



## wwPDB EM Validation Summary Report ⓘ

May 28, 2024 – 04:23 AM EDT

PDB ID : 7RRO  
EMDB ID : EMD-24664  
Title : Structure of the 48-nm repeat doublet microtubule from bovine tracheal cilia  
Authors : Gui, M.; Anderson, J.R.; Botsch, J.J.; Meleppattu, S.; Singh, S.K.; Zhang, Q.;  
Brown, A.  
Deposited on : 2021-08-10  
Resolution : 3.40 Å(reported)

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

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

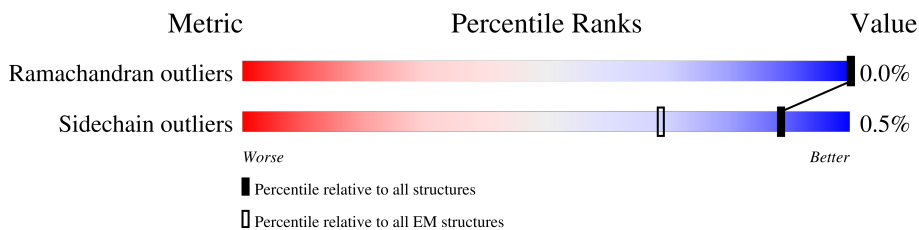
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	0	232	8% (red), 17% (green), 83% (grey)
1	7	232	29% (red), 50% (green), 48% (grey), . (yellow)
2	1	877	16% (red), 17% (green), 83% (grey)
2	2	877	24% (red), 33% (green), 67% (grey)
3	3	514	25% (red), 59% (green), 40% (grey)
3	4	514	16% (red), 42% (green), 58% (grey)
4	5	377	81% (red), 97% (green), .. (grey)
4	6	377	64% (red), 97% (green), .. (grey)
5	8	196	61% (red), 94% (green), ... (grey)

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Mol	Chain	Length	Quality of chain
5	9	196	15% 18% 82%
6	A	494	19% 33% 66%
6	B	494	40% 71% 28%
7	A0	418	5% 52% 47%
7	A1	418	8% 94% 5%
7	A2	418	11% 93% 6%
7	A3	418	12% 79% 20%
7	A4	418	8% 92%
8	AA	452	9% 96%
8	AC	452	6% 96%
8	AE	452	5% 96%
8	AG	452	5% 96%
8	AI	452	6% 96%
8	AK	452	96%
8	AM	452	7% 96%
8	BA	452	15% 95% 5%
8	BC	452	7% 97%
8	BE	452	11% 96%
8	BG	452	7% 96%
8	BI	452	11% 95% 5%
8	BK	452	6% 96%
8	BM	452	11% 94% 5%
8	CA	452	31% 95%
8	CC	452	8% 95%
8	CE	452	18% 97%

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Mol	Chain	Length	Quality of chain
8	CG	452	12% 96%
8	CI	452	17% 96%
8	CK	452	11% 97%
8	CM	452	21% 96%
8	DA	452	57% 87% 11%
8	DC	452	24% 94% 5%
8	DE	452	29% 94% 5%
8	DG	452	19% 94% 5%
8	DI	452	32% 94% 5%
8	DK	452	27% 95% 5%
8	DM	452	36% 93% 5%
8	EC	452	32% 96%
8	EE	452	40% 96%
8	EG	452	34% 96%
8	EI	452	37% 94%
8	EK	452	40% 94%
8	EM	452	46% 94% 5%
8	FC	452	35% 94% 5%
8	FE	452	38% 93% 6%
8	FG	452	37% 92% 6%
8	FI	452	39% 94% 6%
8	FK	452	47% 92% 6%
8	FM	452	47% 94% 5%
8	GC	452	8% 97%
8	GE	452	37% 95% 5%

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Mol	Chain	Length	Quality of chain
8	GG	452	15% 97% ..
8	GI	452	10% 95% 5%
8	GK	452	34% 93% 5%
8	GM	452	13% 95% ..
8	HC	452	13% 94% 6%
8	HE	452	40% 94% 5%
8	HG	452	24% 94% 5%
8	HI	452	15% 95% 5%
8	HK	452	40% 95% 5%
8	HM	452	22% 94% 5%
8	HO	452	10% 85% 15%
8	IC	452	34% 95% 5%
8	IE	452	21% 95% .
8	IG	452	40% 97% ..
8	II	452	29% 95% ..
8	IK	452	39% 96% ..
8	IM	452	32% 95% 5%
8	IO	452	58% 94% 6%
8	JC	452	27% 95% .
8	JE	452	26% 95% 5%
8	JG	452	29% 94% 5%
8	JI	452	33% 94% 5%
8	JK	452	31% 96% ..
8	JM	452	30% 94% 5%
8	KC	452	. 95% ..

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Mol	Chain	Length	Quality of chain
8	KE	452	94% . 5%
8	KG	452	95% 5%
8	KI	452	93% . 5%
8	KK	452	94% . 5%
8	KM	452	95% .
8	KO	452	90% 10%
8	LC	452	5% 96% ..
8	LE	452	7% 96% ..
8	LG	452	5% 97% .
8	LI	452	97% ..
8	LK	452	97% .
8	LM	452	95% . 5%
8	MC	452	14% 96% ..
8	ME	452	17% 94% 5%
8	MG	452	13% 94% . 5%
8	MI	452	15% 95% . 5%
8	MK	452	18% 95% ..
8	MM	452	15% 94% . 5%
8	NA	452	64% 94% . 5%
8	NC	452	60% 94% 5%
8	NE	452	62% 93% . 5%
8	NG	452	58% 95% ..
8	NI	452	67% 95% ..
8	NK	452	59% 94% . 5%
8	OA	452	55% 94% . 5%

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Mol	Chain	Length	Quality of chain
8	OC	452	39% 94% 5%
8	OE	452	53% 95% .
8	OG	452	39% 95% . .
8	OI	452	56% 94% . .
8	OK	452	39% 94% . 5%
8	PA	452	69% 94% . 5%
8	PC	452	49% 95% . .
8	PE	452	67% 94% . 5%
8	PG	452	47% 94% . 5%
8	PI	452	69% 94% . 6%
8	PK	452	47% 94% . 5%
8	PM	452	75% 94% . 5%
8	QA	452	77% 93% . 5%
8	QC	452	54% 94% . 5%
8	QE	452	71% 94% . 5%
8	QG	452	50% 94% . 5%
8	QI	452	72% 94% . 5%
8	QK	452	49% 94% . 5%
8	QM	452	73% 94% . 5%
8	RA	452	79% 94% . 5%
8	RC	452	49% 94% . .
8	RE	452	69% 94% . 5%
8	RG	452	49% 94% . 5%
8	RI	452	69% 95% 5%
8	RK	452	47% 93% . 5%

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Mol	Chain	Length	Quality of chain
8	RM	452	61% 94% • 5%
8	SA	452	81% 94% • 5%
8	SC	452	54% 94% • 5%
8	SE	452	67% 94% • 5%
8	SG	452	58% 94% • 5%
8	SI	452	63% 94% • 6%
8	SK	452	48% 95% •
8	SM	452	56% 94% • 5%
8	TC	452	65% 93% • 5%
8	TE	452	76% 94% • •
8	TG	452	65% 94% • 5%
8	TI	452	77% 94% • 5%
8	TK	452	60% 95% • •
8	TM	452	64% 94% • 5%
8	UC	452	57% 95% • •
8	UE	452	61% 95% •
8	UG	452	47% 95% • •
8	UI	452	55% 95% • •
8	UK	452	51% 96% •
8	UM	452	45% 95% • 5%
8	VC	452	45% 97% • •
8	VE	452	47% 95% • •
8	VG	452	46% 96% • •
8	VI	452	42% 95% • •
8	VK	452	49% 97% •

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Mol	Chain	Length	Quality of chain
8	VM	452	31% 94% 5%
8	WC	452	37% 96% ..
8	WE	452	31% 94% 5%
8	WG	452	41% 96% ..
8	WI	452	27% 94% 5%
8	WK	452	42% 96% .
8	WM	452	22% 94% 5%
9	AB	445	. 97% ..
9	AD	445	. 96% ..
9	AF	445	. 96% ..
9	AH	445	5% 97% ..
9	AJ	445	. 94% ..
9	AL	445	. 96% ..
9	BB	445	8% 95% ..
9	BD	445	7% 95% ..
9	BF	445	6% 95% ..
9	BH	445	7% 94% ..
9	BJ	445	9% 96% .
9	BL	445	6% 94% ..
9	CB	445	13% 94% ..
9	CD	445	11% 95% ..
9	CF	445	16% 96% ..
9	CH	445	13% 94% ..
9	CJ	445	17% 94% ..
9	CL	445	12% 94% ..

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Mol	Chain	Length	Quality of chain
9	DB	445	35% 95%
9	DD	445	18% 95%
9	DF	445	28% 95%
9	DH	445	16% 93%
9	DJ	445	29% 95%
9	DL	445	21% 94%
9	DN	445	65% 86% 13%
9	EB	445	47% 94%
9	ED	445	27% 94%
9	EF	445	41% 95%
9	EH	445	28% 94%
9	EJ	445	44% 94%
9	EL	445	33% 94%
9	EN	445	75% 95%
9	FB	445	51% 96%
9	FD	445	31% 95%
9	FF	445	42% 95%
9	FH	445	27% 94%
9	FJ	445	48% 95%
9	FL	445	33% 93%
9	FN	445	67% 96%
9	GB	445	8% 96%
9	GD	445	18% 96%
9	GF	445	24% 95%
9	GH	445	11% 94%

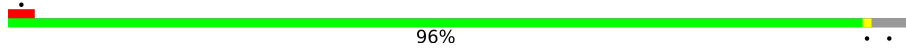
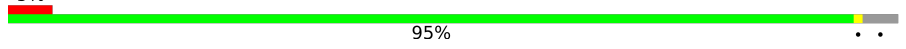
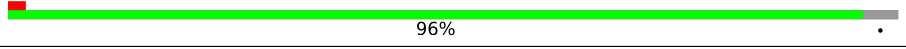
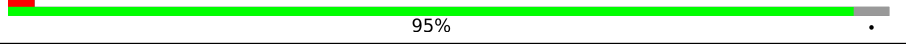
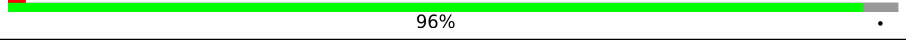
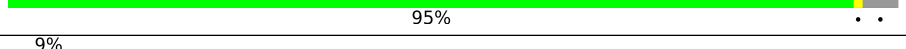
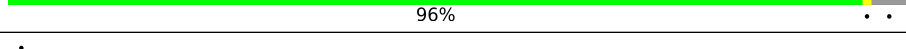
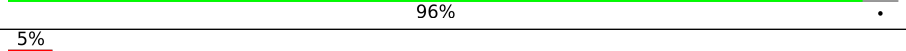
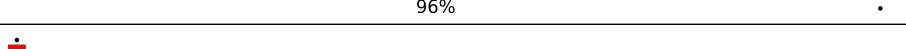
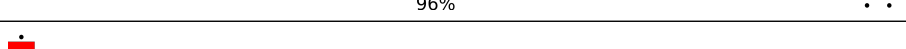
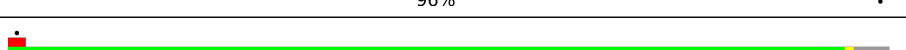
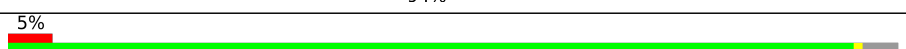
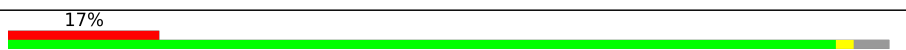
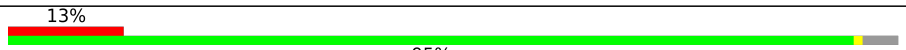
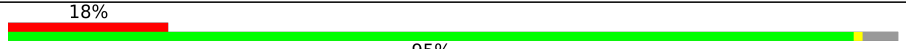
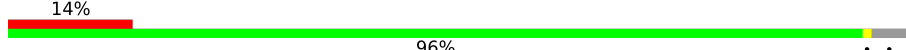
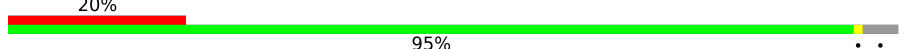
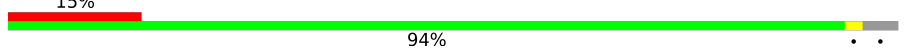
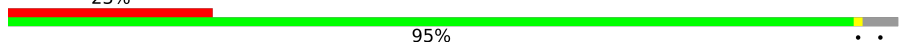
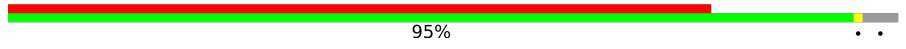
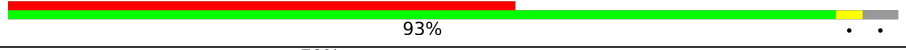
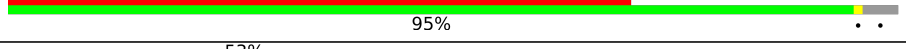
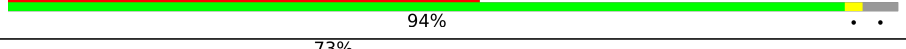
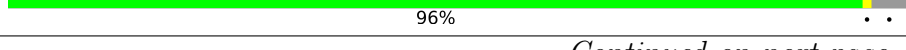

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Mol	Chain	Length	Quality of chain
9	GJ	445	17% 96%
9	GL	445	22% 95%
9	GN	445	96%
9	HB	445	12% 95%
9	HD	445	25% 95%
9	HF	445	49% 96%
9	HH	445	14% 95%
9	HJ	445	24% 95%
9	HL	445	43% 94%
9	HN	445	14% 95%
9	IB	445	43% 82% 17%
9	ID	445	21% 95%
9	IF	445	35% 95%
9	IH	445	29% 95%
9	IJ	445	38% 95%
9	IL	445	32% 94%
9	IN	445	41% 96%
9	JB	445	32% 95%
9	JD	445	20% 95%
9	JF	445	37% 95%
9	JH	445	27% 95%
9	JJ	445	35% 94%
9	JL	445	23% 94%
9	JN	445	50% 96%
9	KB	445	9% 90% 9%

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Mol	Chain	Length	Quality of chain
9	KD	445	 96%
9	KF	445	 95%
9	KH	445	 96%
9	KJ	445	 95%
9	KL	445	 96%
9	KN	445	 95%
9	LB	445	 96%
9	LD	445	 96%
9	LF	445	 96%
9	LH	445	 96%
9	LJ	445	 96%
9	LL	445	 94%
9	LN	445	 95%
9	MB	445	 93%
9	MD	445	 95%
9	MF	445	 95%
9	MH	445	 96%
9	MJ	445	 95%
9	ML	445	 94%
9	MN	445	 95%
9	N0	445	 95%
9	NB	445	 93%
9	ND	445	 95%
9	NF	445	 94%
9	NH	445	 96%

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Mol	Chain	Length	Quality of chain
9	NJ	445	57% 96% ..
9	NL	445	69% 94% ..
9	O0	445	69% 92% 7%
9	OB	445	42% 95% .
9	OD	445	56% 95% .5%
9	OF	445	41% 96% .
9	OH	445	60% 96% .
9	OJ	445	43% 95% ..
9	OL	445	56% 95% 5%
9	PB	445	51% 95% ..
9	PD	445	63% 96% .
9	PF	445	47% 95% ..
9	PH	445	64% 96% .
9	PJ	445	55% 95% ..
9	PL	445	60% 93% ..
9	QB	445	58% 96% .
9	QD	445	68% 95% ..
9	QF	445	50% 95% ..
9	QH	445	62% 95% ..
9	QJ	445	52% 96% ..
9	QL	445	61% 95% ..
9	RB	445	60% 96% .
9	RD	445	65% 96% .
9	RF	445	57% 94% ..
9	RH	445	59% 95% ..

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Mol	Chain	Length	Quality of chain
9	RJ	445	60% 95%
9	RL	445	50% 94%
9	SB	445	61% 94%
9	SD	445	55% 95%
9	SF	445	61% 95%
9	SH	445	56% 96%
9	SJ	445	62% 95%
9	SL	445	48% 95%
9	TB	445	74% 95%
9	TD	445	66% 95%
9	TF	445	77% 95%
9	TH	445	65% 95%
9	TJ	445	74% 95%
9	TL	445	57% 94%
9	UB	445	68% 95%
9	UD	445	51% 96%
9	UF	445	62% 96%
9	UH	445	43% 96%
9	UJ	445	67% 94%
9	UL	445	41% 95%
9	UN	445	71% 95%
9	VB	445	61% 95%
9	VD	445	38% 95%
9	VF	445	60% 95%
9	VH	445	40% 96%

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Mol	Chain	Length	Quality of chain
9	VJ	445	57% 96%
9	VL	445	29% 95%
9	VN	445	45% 96%
9	WB	445	49% 95%
9	WD	445	23% 94%
9	WF	445	42% 95%
9	WH	445	25% 96%
9	WJ	445	46% 95%
9	WL	445	22% 95%
9	WN	445	28% 95%
10	B0	430	44% 56%
10	B1	430	8% 96%
10	B2	430	11% 96%
10	B3	430	13% 88% 11%
10	B4	430	11% 89%
10	B5	430	9% 12% 88%
10	B6	430	60% 83% 17%
10	B7	430	75% 95%
10	B8	430	81% 91% 6%
10	B9	430	40% 43% 57%
11	C	101	50% 87% 10%
12	C0	490	6% 94%
12	C1	490	13% 67% 32%
12	C2	490	17% 80% 20%
12	C3	490	22% 80% 20%

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Mol	Chain	Length	Quality of chain
12	C4	490	13% 43% 56%
12	C5	490	16% 23% 77%
12	C6	490	59% 78% 21%
12	C7	490	63% 83% 16%
12	C8	490	67% 82% 17%
12	C9	490	20% 22% 77%
12	F0	490	17% 28% 72%
12	F1	490	48% 85% 14%
12	F2	490	51% 85% 14%
12	F3	490	53% 76% 23%
12	F4	490	15% 20% 80%
13	D	484	20% 30% 70%
14	D0	447	9% 65% 35%
14	D1	447	9% 95% 5%
14	D2	447	15% 95% 5%
14	D3	447	10% 70% 29%
14	D5	447	98%
14	D6	447	54% 70% 29%
14	D7	447	74% 91% 7%
14	D8	447	76% 91% 8%
14	D9	447	56% 61% 38%
15	E	321	18% 79% 21%
15	F	321	21% 79% 21%
16	E0	208	23% 31% 67%
16	E1	208	47% 58% 39%

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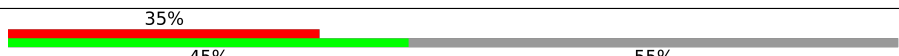
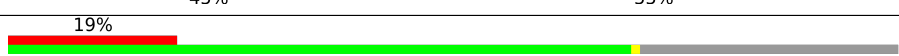
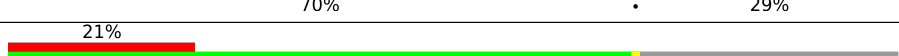
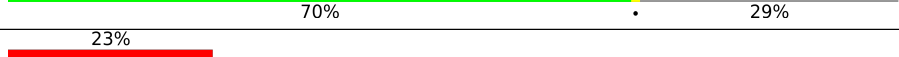





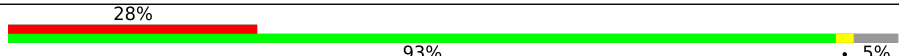
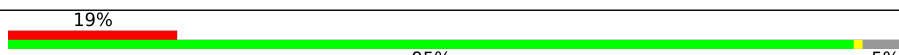
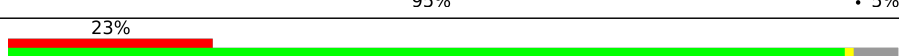
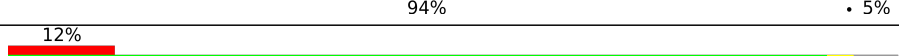
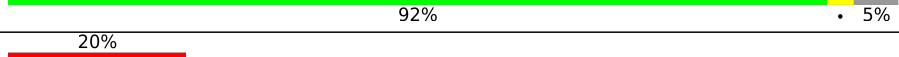
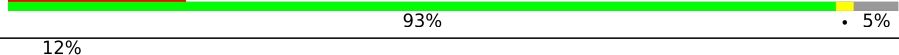
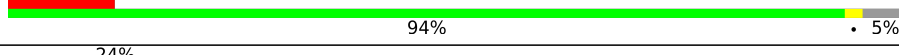
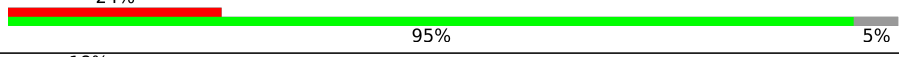




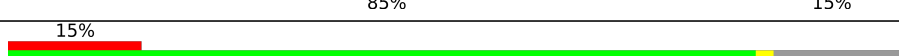



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Mol	Chain	Length	Quality of chain
16	E2	208	57% 66% 31%
16	E3	208	59% 68% 31%
17	G	120	22% 78% 20%
18	H	274	12% 31% 69%
18	I	274	29% 55% 45%
18	J	274	20% 55% 45%
18	K	274	34% 55% 45%
18	L	274	18% 55% 45%
18	M	274	27% 55% 45%
18	N	274	25% 57% 43%
19	H1	687	13% 27% 72%
19	H2	687	19% 35% 64%
19	H3	687	7% 15% 85%
20	H4	621	15% 30% 69%
20	H5	621	20% 39% 60%
20	H6	621	6% 20% 80%
21	H7	1044	10% 55% 44%
21	H8	1044	10% 55% 45%
21	H9	1044	7% 34% 66%
22	I1	683	9% 28% 72%
22	I2	683	12% 28% 72%
23	I3	212	29% 87% 12%
23	I4	212	28% 88% 12%
24	O	377	8% 92%
24	P	377	16% 97%

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Mol	Chain	Length	Quality of chain
24	Q	377	
24	R	377	
24	S	377	
25	T	640	
25	U	640	
25	V	640	
26	W	733	
26	X	733	
26	Y	733	
26	Z	733	
27	XA	193	
27	XB	193	
27	XC	193	
27	XD	193	
27	XE	193	
27	XF	193	
27	XG	193	
28	YB	257	
28	YC	257	
28	YD	257	
28	YE	257	
28	YF	257	
28	YG	257	
29	a	549	
29	b	549	

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Mol	Chain	Length	Quality of chain
29	c	549	48% 50% 50%
29	d	549	37% 38% 61%
30	e	623	43% 97% ..
30	f	623	45% 96% ..
30	g	623	29% 96% ..
31	h	259	34% 57% 43%
31	i	259	47% 89% 9%
31	j	259	47% 90% 9%
31	k	259	36% 90% 9%
32	l	196	16% 58% 42%
32	m	196	14% 58% 41%
32	n	196	13% 60% 40%
33	o	547	59% 69% 31%
33	p	547	15% 18% 82%
34	q	170	13% 45% 54%
34	r	170	14% 45% 54%
34	s	170	9% 46% 54%
35	t	1497	12% 12% 88%
36	y	136	8% 46% 54%
36	z	136	18% 84% 15%

## 2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 1276281 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 Protein C9orf135 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	40	330	205	63	61	1	0	0
1	7	121	806	494	146	164	2	0	0

- Molecule 2 is a protein called EF-hand domain family member B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	152	921	570	172	178	1	0	0
2	2	292	1526	915	312	299		0	0

- Molecule 3 is a protein called Methyl-CpG binding domain protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	306	2295	1393	444	448	10	0	0
3	4	217	1855	1127	350	364	14	0	0

- Molecule 4 is a protein called Nucleoside diphosphate kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	372	2533	1589	451	481	12	0	0
4	6	372	2947	1880	499	546	22	0	0

- Molecule 5 is a protein called Uncharacterized protein C1orf158 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	191	Total	C	N	O	S	0	0
			1607	1037	288	281	1		
5	9	35	Total	C	N	O		0	0
			287	181	51	55			

- Molecule 6 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	170	Total	C	N	O	S	0	0
			1427	869	270	281	7		
6	B	354	Total	C	N	O	S	0	0
			3044	1882	553	592	17		

- Molecule 7 is a protein called Tektin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A0	221	Total	C	N	O	S	0	0
			1797	1120	329	341	7		
7	A1	396	Total	C	N	O	S	0	0
			3258	2026	592	631	9		
7	A2	393	Total	C	N	O	S	0	0
			3238	2016	589	624	9		
7	A3	334	Total	C	N	O	S	0	0
			2759	1716	498	537	8		
7	A4	34	Total	C	N	O		0	0
			290	179	61	50			

- Molecule 8 is a protein called Tubulin alpha-1D chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AA	438	Total	C	N	O	S	0	0
			3422	2165	582	653	22		
8	AC	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
8	AE	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
8	AG	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
8	AI	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
8	AK	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AM	439	3430	2170	583	654	23	0	0
8	BA	430	3372	2136	573	641	22	0	0
8	BC	440	3437	2175	584	655	23	0	0
8	BE	433	3396	2151	576	646	23	0	0
8	BG	440	3437	2175	584	655	23	0	0
8	BI	430	3374	2138	573	640	23	0	0
8	BK	439	3430	2170	583	654	23	0	0
8	BM	430	3372	2137	573	639	23	0	0
8	CA	438	3422	2165	582	653	22	0	0
8	CC	438	3424	2167	582	652	23	0	0
8	CE	438	3424	2167	582	652	23	0	0
8	CG	439	3430	2170	583	654	23	0	0
8	CI	439	3430	2170	583	654	23	0	0
8	CK	439	3430	2170	583	654	23	0	0
8	CM	439	3430	2170	583	654	23	0	0
8	DA	401	3140	1992	535	594	19	0	0
8	DC	429	3366	2134	572	637	23	0	0
8	DE	430	3372	2137	573	639	23	0	0
8	DG	431	3379	2142	574	640	23	0	0
8	DI	429	3364	2133	572	636	23	0	0
8	DK	430	3372	2137	573	639	23	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	DM	430	3372	2137	573	639	23	0	0
8	EC	439	3430	2170	583	654	23	0	0
8	EE	441	3446	2180	585	658	23	0	0
8	EG	437	3416	2163	581	649	23	0	0
8	EI	436	3408	2158	580	648	22	0	0
8	EK	440	3437	2175	584	655	23	0	0
8	EM	428	3358	2130	571	634	23	0	0
8	FC	431	3379	2142	574	640	23	0	0
8	FE	425	3339	2118	568	631	22	0	0
8	FG	426	3346	2123	569	632	22	0	0
8	FI	427	3347	2121	570	633	23	0	0
8	FK	424	3326	2109	566	629	22	0	0
8	FM	429	3365	2132	572	638	23	0	0
8	GC	440	3437	2175	584	655	23	0	0
8	GE	430	3371	2138	573	637	23	0	0
8	GG	440	3437	2175	584	655	23	0	0
8	GI	429	3365	2135	572	635	23	0	0
8	GK	429	3364	2133	572	636	23	0	0
8	GM	439	3430	2170	583	654	23	0	0
8	HC	427	3350	2126	570	631	23	0	0
8	HE	430	3374	2138	573	640	23	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	HG	430	3371	2138	573	637	23	0	0
8	HI	430	3371	2138	573	637	23	0	0
8	HK	431	3379	2142	574	640	23	0	0
8	HM	429	3365	2132	572	638	23	0	0
8	HO	386	3037	1926	518	572	21	0	0
8	IC	429	3365	2135	572	635	23	0	0
8	IE	432	3388	2147	575	643	23	0	0
8	IG	440	3437	2175	584	655	23	0	0
8	II	432	3387	2146	575	643	23	0	0
8	IK	440	3437	2175	584	655	23	0	0
8	IM	431	3378	2140	574	641	23	0	0
8	IO	427	3350	2125	570	633	22	0	0
8	JC	432	3384	2143	575	643	23	0	0
8	JE	430	3372	2137	573	639	23	0	0
8	JG	428	3358	2130	571	634	23	0	0
8	JI	429	3366	2134	572	637	23	0	0
8	JK	440	3437	2175	584	655	23	0	0
8	JM	430	3372	2137	573	639	23	0	0
8	KC	432	3384	2143	575	643	23	0	0
8	KE	431	3380	2141	574	642	23	0	0
8	KG	430	3370	2136	573	638	23	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	KI	428	3358	2130	571	634	23	0	0
8	KK	430	3372	2137	573	639	23	0	0
8	KM	432	3376	2138	575	641	22	0	0
8	KO	408	3217	2040	546	608	23	0	0
8	LC	440	3437	2175	584	655	23	0	0
8	LE	440	3437	2175	584	655	23	0	0
8	LG	440	3437	2175	584	655	23	0	0
8	LI	440	3437	2175	584	655	23	0	0
8	LK	440	3437	2175	584	655	23	0	0
8	LM	431	3378	2140	574	641	23	0	0
8	MC	439	3430	2170	583	654	23	0	0
8	ME	429	3366	2134	572	637	23	0	0
8	MG	430	3372	2137	573	639	23	0	0
8	MI	431	3379	2142	574	640	23	0	0
8	MK	440	3437	2175	584	655	23	0	0
8	MM	431	3376	2138	574	642	22	0	0
8	NA	430	3372	2136	573	641	22	0	0
8	NC	429	3365	2135	572	635	23	0	0
8	NE	430	3374	2140	573	638	23	0	0
8	NG	432	3387	2146	575	643	23	0	0
8	NI	432	3387	2146	575	643	23	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	NK	430	Total 3374	C 2138	N 573	O 640	S 23	0	0
8	OA	428	Total 3358	C 2129	N 571	O 636	S 22	0	0
8	OC	429	Total 3366	C 2134	N 572	O 637	S 23	0	0
8	OE	433	Total 3396	C 2151	N 576	O 646	S 23	0	0
8	OG	433	Total 3391	C 2148	N 576	O 644	S 23	0	0
8	OI	432	Total 3387	C 2146	N 575	O 643	S 23	0	0
8	OK	431	Total 3380	C 2141	N 574	O 642	S 23	0	0
8	PA	430	Total 3372	C 2136	N 573	O 641	S 22	0	0
8	PC	432	Total 3386	C 2144	N 575	O 644	S 23	0	0
8	PE	431	Total 3380	C 2143	N 574	O 640	S 23	0	0
8	PG	430	Total 3371	C 2138	N 573	O 637	S 23	0	0
8	PI	427	Total 3349	C 2123	N 570	O 634	S 22	0	0
8	PK	430	Total 3371	C 2138	N 573	O 637	S 23	0	0
8	PM	430	Total 3372	C 2137	N 573	O 639	S 23	0	0
8	QA	431	Total 3376	C 2138	N 574	O 642	S 22	0	0
8	QC	430	Total 3372	C 2137	N 573	O 639	S 23	0	0
8	QE	430	Total 3372	C 2137	N 573	O 639	S 23	0	0
8	QG	431	Total 3380	C 2141	N 574	O 642	S 23	0	0
8	QI	429	Total 3366	C 2134	N 572	O 637	S 23	0	0
8	QK	431	Total 3380	C 2141	N 574	O 642	S 23	0	0
8	QM	431	Total 3378	C 2140	N 574	O 641	S 23	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	RA	429	Total 3364	C 2132	N 572	O 638	S 22	0	0
8	RC	432	Total 3387	C 2146	N 575	O 643	S 23	0	0
8	RE	428	Total 3358	C 2130	N 571	O 634	S 23	0	0
8	RG	430	Total 3372	C 2137	N 573	O 639	S 23	0	0
8	RI	431	Total 3379	C 2142	N 574	O 640	S 23	0	0
8	RK	431	Total 3379	C 2142	N 574	O 640	S 23	0	0
8	RM	428	Total 3356	C 2128	N 571	O 635	S 22	0	0
8	SA	430	Total 3372	C 2136	N 573	O 641	S 22	0	0
8	SC	430	Total 3372	C 2137	N 573	O 639	S 23	0	0
8	SE	431	Total 3381	C 2142	N 574	O 642	S 23	0	0
8	SG	431	Total 3379	C 2142	N 574	O 640	S 23	0	0
8	SI	427	Total 3358	C 2129	N 569	O 637	S 23	0	0
8	SK	432	Total 3387	C 2146	N 575	O 643	S 23	0	0
8	SM	431	Total 3378	C 2140	N 574	O 641	S 23	0	0
8	TC	430	Total 3371	C 2138	N 573	O 637	S 23	0	0
8	TE	432	Total 3388	C 2147	N 575	O 643	S 23	0	0
8	TG	430	Total 3371	C 2138	N 573	O 637	S 23	0	0
8	TI	430	Total 3371	C 2138	N 573	O 637	S 23	0	0
8	TK	432	Total 3387	C 2146	N 575	O 643	S 23	0	0
8	TM	430	Total 3372	C 2137	N 573	O 639	S 23	0	0
8	UC	433	Total 3393	C 2149	N 576	O 645	S 23	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	UE	432	Total	C	N	O	S	0	0
			3388	2147	575	643	23		
8	UG	433	Total	C	N	O	S	0	0
			3393	2149	576	645	23		
8	UI	433	Total	C	N	O	S	0	0
			3393	2149	576	645	23		
8	UK	433	Total	C	N	O	S	0	0
			3391	2148	576	644	23		
8	UM	431	Total	C	N	O	S	0	0
			3378	2140	574	641	23		
8	VC	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
8	VE	433	Total	C	N	O	S	0	0
			3396	2151	576	646	23		
8	VG	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
8	VI	433	Total	C	N	O	S	0	0
			3393	2149	576	645	23		
8	VK	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
8	VM	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
8	WC	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
8	WE	431	Total	C	N	O	S	0	0
			3380	2141	574	642	23		
8	WG	439	Total	C	N	O	S	0	0
			3430	2170	583	654	23		
8	WI	431	Total	C	N	O	S	0	0
			3380	2141	574	642	23		
8	WK	438	Total	C	N	O	S	0	0
			3424	2167	582	652	23		
8	WM	431	Total	C	N	O	S	0	0
			3378	2140	574	641	23		

- Molecule 9 is a protein called Tubulin beta-4B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AB	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
9	AD	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	AF	436	Total 3424	C 2150	N 584	O 664	S 26	0	0
9	AH	436	Total 3424	C 2150	N 584	O 664	S 26	0	0
9	AJ	436	Total 3424	C 2150	N 584	O 664	S 26	0	0
9	AL	435	Total 3416	C 2145	N 583	O 663	S 25	0	0
9	BB	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	BD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	BF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	BH	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	BJ	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	BL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
9	CB	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	CD	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	CF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	CH	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	CJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	CL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
9	DB	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	DD	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	DF	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	DH	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	DJ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	DL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
9	DN	387	Total 3035	C 1911	N 519	O 582	S 23	0	0
9	EB	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	ED	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	EF	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	EH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	EJ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	EL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
9	EN	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	FB	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	FD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	FF	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	FH	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	FJ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	FL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
9	FN	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	GB	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	GD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	GF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	GH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	GJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	GL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
9	GN	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	HB	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	HD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	HF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	HH	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	HJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	HL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
9	HN	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	IB	370	Total 2905	C 1824	N 501	O 557	S 23	0	0
9	ID	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	IF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	IH	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	IJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	IL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	IN	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	JB	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	JD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	JF	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	JH	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	JJ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	JL	426	3348	2105	574	643	26	0	0
9	JN	426	3348	2105	574	643	26	0	0
9	KB	403	3165	1989	539	613	24	0	0
9	KD	428	3361	2112	576	647	26	0	0
9	KF	427	3356	2109	575	646	26	0	0
9	KH	429	3368	2116	577	649	26	0	0
9	KJ	426	3348	2105	574	643	26	0	0
9	KL	429	3368	2116	577	649	26	0	0
9	KN	428	3361	2112	576	647	26	0	0
9	LB	428	3361	2112	576	647	26	0	0
9	LD	427	3356	2109	575	646	26	0	0
9	LF	428	3361	2112	576	647	26	0	0
9	LH	428	3361	2112	576	647	26	0	0
9	LJ	428	3361	2112	576	647	26	0	0
9	LL	426	3348	2105	574	643	26	0	0
9	LN	428	3361	2112	576	647	26	0	0
9	MB	426	3348	2105	574	643	26	0	0
9	MD	426	3348	2105	574	643	26	0	0
9	MF	428	3361	2112	576	647	26	0	0
9	MH	428	3361	2112	576	647	26	0	0
9	MJ	426	3348	2105	574	643	26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	ML	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	MN	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
9	NO	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	NB	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	ND	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	NF	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	NH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	NJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	NL	425	Total 3339	C 2100	N 572	O 641	S 26	0	0
9	OO	412	Total 3224	C 2024	N 553	O 623	S 24	0	0
9	OB	425	Total 3339	C 2100	N 572	O 641	S 26	0	0
9	OD	424	Total 3327	C 2091	N 571	O 639	S 26	0	0
9	OF	425	Total 3339	C 2100	N 572	O 641	S 26	0	0
9	OH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	OJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	OL	424	Total 3327	C 2091	N 571	O 639	S 26	0	0
9	PB	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	PD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
9	PF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	PH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
9	PJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	PL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
9	QB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	QD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	QF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	QH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	QJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	QL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	RB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	RD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	RF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	RH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	RJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	RL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	SB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	SD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	SF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	SH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	SJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	SL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	TB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	TD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	TF	428	3361	2112	576	647	26	0	0
9	TH	428	3361	2112	576	647	26	0	0
9	TJ	428	3361	2112	576	647	26	0	0
9	TL	426	3348	2105	574	643	26	0	0
9	UB	428	3361	2112	576	647	26	0	0
9	UD	427	3356	2109	575	646	26	0	0
9	UF	428	3361	2112	576	647	26	0	0
9	UH	428	3361	2112	576	647	26	0	0
9	UJ	428	3361	2112	576	647	26	0	0
9	UL	426	3348	2105	574	643	26	0	0
9	UN	428	3361	2112	576	647	26	0	0
9	VB	428	3361	2112	576	647	26	0	0
9	VD	427	3356	2109	575	646	26	0	0
9	VF	427	3356	2109	575	646	26	0	0
9	VH	428	3361	2112	576	647	26	0	0
9	VJ	428	3361	2112	576	647	26	0	0
9	VL	426	3348	2105	574	643	26	0	0
9	VN	428	3361	2112	576	647	26	0	0
9	WB	428	3361	2112	576	647	26	0	0
9	WD	427	3356	2109	575	646	26	0	0
9	WF	426	3348	2105	574	643	26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	WH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	WJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	WL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	WN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

- Molecule 10 is a protein called Tektin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B0	189	Total	C	N	O	S	0	0
			1538	941	290	301	6		
10	B1	416	Total	C	N	O	S	0	0
			3391	2090	627	660	14		
10	B2	416	Total	C	N	O	S	0	0
			3391	2090	627	660	14		
10	B3	383	Total	C	N	O	S	0	0
			3113	1920	568	610	15		
10	B4	49	Total	C	N	O	S	0	0
			406	248	79	77	2		
10	B5	51	Total	C	N	O	S	0	0
			419	257	81	79	2		
10	B6	358	Total	C	N	O	S	0	0
			2911	1793	534	570	14		
10	B7	414	Total	C	N	O	S	0	0
			3372	2080	621	657	14		
10	B8	403	Total	C	N	O	S	0	0
			3284	2025	607	638	14		
10	B9	187	Total	C	N	O	S	0	0
			1523	933	287	297	6		

- Molecule 11 is a protein called Uncharacterized protein C1orf189 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	91	Total	C	N	O	S	0	0
			785	495	151	133	6		

- Molecule 12 is a protein called Tektin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C0	30	Total	C	N	O		0	0
			261	157	50	54			
12	C1	334	Total	C	N	O	S	0	0
			2710	1667	493	537	13		
12	C2	394	Total	C	N	O	S	0	0
			3208	1974	588	631	15		
12	C3	394	Total	C	N	O	S	0	0
			3208	1974	588	631	15		
12	C4	215	Total	C	N	O	S	0	0
			1745	1083	314	335	13		
12	C5	113	Total	C	N	O	S	0	0
			908	559	165	181	3		
12	C6	385	Total	C	N	O	S	0	0
			3131	1925	573	618	15		
12	C7	413	Total	C	N	O	S	0	0
			3359	2066	615	661	17		
12	C8	407	Total	C	N	O	S	0	0
			3310	2039	602	653	16		
12	C9	112	Total	C	N	O	S	0	0
			926	559	177	187	3		
12	F0	139	Total	C	N	O	S	0	0
			1156	714	214	226	2		
12	F1	421	Total	C	N	O	S	0	0
			3433	2121	624	672	16		
12	F2	421	Total	C	N	O	S	0	0
			3433	2121	624	672	16		
12	F3	378	Total	C	N	O	S	0	0
			3064	1884	561	604	15		
12	F4	99	Total	C	N	O	S	0	0
			809	500	147	159	3		

- Molecule 13 is a protein called Sperm associated antigen 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	147	Total	C	N	O	S	0	0
			944	587	174	182	1		

- Molecule 14 is a protein called Tektin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D0	291	Total	C	N	O	S	0	0
			2377	1468	435	462	12		
14	D1	425	Total	C	N	O	S	0	0
			3483	2143	653	672	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	D2	425	Total	C	N	O	S	0	0
			3483	2143	653	672	15		
14	D3	316	Total	C	N	O	S	0	0
			2593	1603	483	495	12		
14	D5	9	Total	C	N	O	S	0	0
			77	46	18	12	1		
14	D6	319	Total	C	N	O	S	0	0
			2619	1617	489	501	12		
14	D7	414	Total	C	N	O	S	0	0
			3390	2085	634	656	15		
14	D8	413	Total	C	N	O	S	0	0
			3381	2080	632	654	15		
14	D9	277	Total	C	N	O	S	0	0
			2259	1395	410	443	11		

- Molecule 15 is a protein called Cilia and flagella associated protein 161.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	255	Total	C	N	O	S	0	0
			2055	1302	369	373	11		
15	F	255	Total	C	N	O	S	0	0
			2055	1302	369	373	11		

- Molecule 16 is a protein called TEKTIPI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E0	68	Total	C	N	O	S	0	0
			581	371	113	96	1		
16	E1	127	Total	C	N	O	S	0	0
			1062	675	200	185	2		
16	E2	144	Total	C	N	O	S	0	0
			1202	766	220	214	2		
16	E3	144	Total	C	N	O	S	0	0
			1202	766	220	214	2		

- Molecule 17 is a protein called Pierce2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	96	Total	C	N	O	S	0	0
			775	496	130	142	7		

- Molecule 18 is a protein called Protein FAM166B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	84	Total	C	N	O	S	0	0
			647	421	111	110	5		
18	I	152	Total	C	N	O	S	0	0
			1188	780	201	201	6		
18	J	152	Total	C	N	O	S	0	0
			1188	780	201	201	6		
18	K	152	Total	C	N	O	S	0	0
			1188	780	201	201	6		
18	L	152	Total	C	N	O	S	0	0
			1188	780	201	201	6		
18	M	152	Total	C	N	O	S	0	0
			1188	780	201	201	6		
18	N	155	Total	C	N	O	S	0	0
			1218	797	209	206	6		

- Molecule 19 is a protein called Coiled-coil domain containing 114.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H1	192	Total	C	N	O	S	0	0
			1571	959	306	300	6		
19	H2	250	Total	C	N	O	S	0	0
			2069	1261	414	386	8		
19	H3	105	Total	C	N	O	S	0	0
			880	530	182	164	4		

- Molecule 20 is a protein called Outer dynein arm-docking complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H4	193	Total	C	N	O	S	0	0
			1625	1009	304	308	4		
20	H5	249	Total	C	N	O	S	0	0
			2097	1303	390	399	5		
20	H6	125	Total	C	N	O	S	0	0
			1060	666	198	195	1		

- Molecule 21 is a protein called Armadillo repeat containing 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	H7	580	Total	C	N	O	0	0
			2867	1707	580	580		
21	H8	579	Total	C	N	O	0	0
			2862	1704	579	579		

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Mol	Chain	Residues	Atoms				AltConf	Trace
21	H9	358	Total	C	N	O	0	0
			1768	1052	358	358		

- Molecule 22 is a protein called TTC25 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I1	192	Total	C	N	O	S	0	0
			1300	812	232	249	7		
22	I2	192	Total	C	N	O	S	0	0
			1300	812	232	249	7		

- Molecule 23 is a protein called EF-hand calcium-binding domain-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	I3	186	Total	C	N	O	0	0
			921	549	186	186		
23	I4	187	Total	C	N	O	0	0
			925	551	187	187		

- Molecule 24 is a protein called RIB43A-like with coiled-coils protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	31	Total	C	N	O	0	0	
			270	170	58	42			
24	P	373	Total	C	N	O	S	0	0
			3104	1890	607	592	15		
24	Q	39	Total	C	N	O	S	0	0
			317	193	58	63	3		
24	R	249	Total	C	N	O	S	0	0
			2041	1239	395	397	10		
24	S	170	Total	C	N	O	S	0	0
			1412	857	277	271	7		

- Molecule 25 is a protein called EF-hand domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	452	Total	C	N	O	S	0	0
			3726	2406	627	678	15		
25	U	452	Total	C	N	O	S	0	0
			3726	2406	627	678	15		
25	V	452	Total	C	N	O	S	0	0
			3726	2406	627	678	15		



- Molecule 26 is a protein called EFHC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	553	Total	C	N	O	S	0	0
			4558	2931	763	841	23		
26	X	636	Total	C	N	O	S	0	0
			5234	3358	881	968	27		
26	Y	636	Total	C	N	O	S	0	0
			5234	3358	881	968	27		
26	Z	449	Total	C	N	O	S	0	0
			3691	2365	618	687	21		

- Molecule 27 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	XA	184	Total	C	N	O	S	0	0
			1532	984	268	273	7		
27	XB	184	Total	C	N	O	S	0	0
			1532	984	268	273	7		
27	XC	184	Total	C	N	O	S	0	0
			1532	984	268	273	7		
27	XD	184	Total	C	N	O	S	0	0
			1532	984	268	273	7		
27	XE	184	Total	C	N	O	S	0	0
			1532	984	268	273	7		
27	XF	184	Total	C	N	O	S	0	0
			1532	984	268	273	7		
27	XG	184	Total	C	N	O	S	0	0
			1532	984	268	273	7		

- Molecule 28 is a protein called PACRG protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	YB	219	Total	C	N	O	S	0	0
			1767	1144	298	316	9		
28	YC	219	Total	C	N	O	S	0	0
			1767	1144	298	316	9		
28	YD	219	Total	C	N	O	S	0	0
			1767	1144	298	316	9		
28	YE	219	Total	C	N	O	S	0	0
			1767	1144	298	316	9		
28	YF	219	Total	C	N	O	S	0	0
			1767	1144	298	316	9		
28	YG	219	Total	C	N	O	S	0	0
			1767	1144	298	316	9		

- Molecule 29 is a protein called Cilia and flagella associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	169	Total	C	N	O	S	0	0
			1426	879	270	269	8		
29	b	332	Total	C	N	O	S	0	0
			2854	1723	570	549	12		
29	c	277	Total	C	N	O	S	0	0
			2361	1445	446	455	15		
29	d	215	Total	C	N	O	S	0	0
			1830	1110	368	346	6		

- Molecule 30 is a protein called Cilia and flagella associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	610	Total	C	N	O	S	0	0
			4722	2990	823	877	32		
30	f	610	Total	C	N	O	S	0	0
			4722	2990	823	877	32		
30	g	610	Total	C	N	O	S	0	0
			4722	2990	823	877	32		

- Molecule 31 is a protein called Enkurin, TRPC channel interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	148	Total	C	N	O	S	0	0
			1220	772	213	231	4		
31	i	235	Total	C	N	O	S	0	0
			1939	1242	336	354	7		
31	j	235	Total	C	N	O	S	0	0
			1939	1242	336	354	7		
31	k	235	Total	C	N	O	S	0	0
			1939	1242	336	354	7		

- Molecule 32 is a protein called Protein Flattop.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	l	114	Total	C	N	O	S	0	0
			894	569	162	161	2		
32	m	116	Total	C	N	O	S	0	0
			910	580	165	163	2		
32	n	118	Total	C	N	O	S	0	0
			928	590	169	167	2		

- Molecule 33 is a protein called Coiled-coil domain containing 173.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	378	Total	C	N	O	S	0	0
			2068	1246	415	405	2		
33	p	100	Total	C	N	O	S	0	0
			835	524	144	164	3		

- Molecule 34 is a protein called Chromosome 3 C1orf194 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	q	79	Total	C	N	O	0	0
			631	395	116	120		
34	r	79	Total	C	N	O	0	0
			631	395	116	120		
34	s	79	Total	C	N	O	0	0
			631	395	116	120		

- Molecule 35 is a protein called EFCAB6.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	t	178	Total	C	N	O	0	0
			882	526	178	178		

- Molecule 36 is a protein called Pierce1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	y	63	Total	C	N	O	S	0	0
			515	329	88	94	4		
36	z	115	Total	C	N	O	S	0	0
			950	602	168	175	5		

- Molecule 37 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
37	CA	1	Total 32	C 10	N 5	O 14	P 3	0
37	CC	1	Total 32	C 10	N 5	O 14	P 3	0
37	CE	1	Total 32	C 10	N 5	O 14	P 3	0
37	CG	1	Total 32	C 10	N 5	O 14	P 3	0
37	CI	1	Total 32	C 10	N 5	O 14	P 3	0
37	CK	1	Total 32	C 10	N 5	O 14	P 3	0
37	CM	1	Total 32	C 10	N 5	O 14	P 3	0
37	DA	1	Total 32	C 10	N 5	O 14	P 3	0
37	DC	1	Total 32	C 10	N 5	O 14	P 3	0
37	DE	1	Total 32	C 10	N 5	O 14	P 3	0
37	DG	1	Total 32	C 10	N 5	O 14	P 3	0
37	DI	1	Total 32	C 10	N 5	O 14	P 3	0
37	DK	1	Total 32	C 10	N 5	O 14	P 3	0
37	DM	1	Total 32	C 10	N 5	O 14	P 3	0
37	EC	1	Total 32	C 10	N 5	O 14	P 3	0
37	EE	1	Total 32	C 10	N 5	O 14	P 3	0
37	EG	1	Total 32	C 10	N 5	O 14	P 3	0
37	EI	1	Total 32	C 10	N 5	O 14	P 3	0
37	EK	1	Total 32	C 10	N 5	O 14	P 3	0
37	EM	1	Total 32	C 10	N 5	O 14	P 3	0
37	FC	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	
37	FE	1	Total 32	C 10	N 5	O 14	P 3	0
37	FG	1	Total 32	C 10	N 5	O 14	P 3	0
37	FI	1	Total 32	C 10	N 5	O 14	P 3	0
37	FK	1	Total 32	C 10	N 5	O 14	P 3	0
37	FM	1	Total 32	C 10	N 5	O 14	P 3	0
37	GC	1	Total 32	C 10	N 5	O 14	P 3	0
37	GE	1	Total 32	C 10	N 5	O 14	P 3	0
37	GG	1	Total 32	C 10	N 5	O 14	P 3	0
37	GI	1	Total 32	C 10	N 5	O 14	P 3	0
37	GK	1	Total 32	C 10	N 5	O 14	P 3	0
37	GM	1	Total 32	C 10	N 5	O 14	P 3	0
37	HC	1	Total 32	C 10	N 5	O 14	P 3	0
37	HE	1	Total 32	C 10	N 5	O 14	P 3	0
37	HG	1	Total 32	C 10	N 5	O 14	P 3	0
37	HI	1	Total 32	C 10	N 5	O 14	P 3	0
37	HK	1	Total 32	C 10	N 5	O 14	P 3	0
37	HM	1	Total 32	C 10	N 5	O 14	P 3	0
37	HO	1	Total 32	C 10	N 5	O 14	P 3	0
37	IC	1	Total 32	C 10	N 5	O 14	P 3	0
37	IE	1	Total 32	C 10	N 5	O 14	P 3	0
37	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	
37	II	1	Total 32	C 10	N 5	O 14	P 3	0
37	IK	1	Total 32	C 10	N 5	O 14	P 3	0
37	IM	1	Total 32	C 10	N 5	O 14	P 3	0
37	IO	1	Total 32	C 10	N 5	O 14	P 3	0
37	JC	1	Total 32	C 10	N 5	O 14	P 3	0
37	JE	1	Total 32	C 10	N 5	O 14	P 3	0
37	JG	1	Total 32	C 10	N 5	O 14	P 3	0
37	JI	1	Total 32	C 10	N 5	O 14	P 3	0
37	JK	1	Total 32	C 10	N 5	O 14	P 3	0
37	JM	1	Total 32	C 10	N 5	O 14	P 3	0
37	KC	1	Total 32	C 10	N 5	O 14	P 3	0
37	KE	1	Total 32	C 10	N 5	O 14	P 3	0
37	KG	1	Total 32	C 10	N 5	O 14	P 3	0
37	KI	1	Total 32	C 10	N 5	O 14	P 3	0
37	KK	1	Total 32	C 10	N 5	O 14	P 3	0
37	KM	1	Total 32	C 10	N 5	O 14	P 3	0
37	KO	1	Total 32	C 10	N 5	O 14	P 3	0
37	LC	1	Total 32	C 10	N 5	O 14	P 3	0
37	LE	1	Total 32	C 10	N 5	O 14	P 3	0
37	LG	1	Total 32	C 10	N 5	O 14	P 3	0
37	LI	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	
37	LK	1	Total 32	C 10	N 5	O 14	P 3	0
37	LM	1	Total 32	C 10	N 5	O 14	P 3	0
37	MC	1	Total 32	C 10	N 5	O 14	P 3	0
37	ME	1	Total 32	C 10	N 5	O 14	P 3	0
37	MG	1	Total 32	C 10	N 5	O 14	P 3	0
37	MI	1	Total 32	C 10	N 5	O 14	P 3	0
37	MK	1	Total 32	C 10	N 5	O 14	P 3	0
37	MM	1	Total 32	C 10	N 5	O 14	P 3	0
37	NA	1	Total 32	C 10	N 5	O 14	P 3	0
37	NC	1	Total 32	C 10	N 5	O 14	P 3	0
37	NE	1	Total 32	C 10	N 5	O 14	P 3	0
37	NG	1	Total 32	C 10	N 5	O 14	P 3	0
37	NI	1	Total 32	C 10	N 5	O 14	P 3	0
37	NK	1	Total 32	C 10	N 5	O 14	P 3	0
37	OA	1	Total 32	C 10	N 5	O 14	P 3	0
37	OC	1	Total 32	C 10	N 5	O 14	P 3	0
37	OE	1	Total 32	C 10	N 5	O 14	P 3	0
37	OG	1	Total 32	C 10	N 5	O 14	P 3	0
37	OI	1	Total 32	C 10	N 5	O 14	P 3	0
37	OK	1	Total 32	C 10	N 5	O 14	P 3	0
37	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	
37	PC	1	Total 32	C 10	N 5	O 14	P 3	0
37	PE	1	Total 32	C 10	N 5	O 14	P 3	0
37	PG	1	Total 32	C 10	N 5	O 14	P 3	0
37	PI	1	Total 32	C 10	N 5	O 14	P 3	0
37	PK	1	Total 32	C 10	N 5	O 14	P 3	0
37	PM	1	Total 32	C 10	N 5	O 14	P 3	0
37	QA	1	Total 32	C 10	N 5	O 14	P 3	0
37	QC	1	Total 32	C 10	N 5	O 14	P 3	0
37	QE	1	Total 32	C 10	N 5	O 14	P 3	0
37	QG	1	Total 32	C 10	N 5	O 14	P 3	0
37	QI	1	Total 32	C 10	N 5	O 14	P 3	0
37	QK	1	Total 32	C 10	N 5	O 14	P 3	0
37	QM	1	Total 32	C 10	N 5	O 14	P 3	0
37	RA	1	Total 32	C 10	N 5	O 14	P 3	0
37	RC	1	Total 32	C 10	N 5	O 14	P 3	0
37	RE	1	Total 32	C 10	N 5	O 14	P 3	0
37	RG	1	Total 32	C 10	N 5	O 14	P 3	0
37	RI	1	Total 32	C 10	N 5	O 14	P 3	0
37	RK	1	Total 32	C 10	N 5	O 14	P 3	0
37	RM	1	Total 32	C 10	N 5	O 14	P 3	0
37	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	
37	SC	1	Total 32	C 10	N 5	O 14	P 3	0
37	SE	1	Total 32	C 10	N 5	O 14	P 3	0
37	SG	1	Total 32	C 10	N 5	O 14	P 3	0
37	SI	1	Total 32	C 10	N 5	O 14	P 3	0
37	SK	1	Total 32	C 10	N 5	O 14	P 3	0
37	SM	1	Total 32	C 10	N 5	O 14	P 3	0
37	TC	1	Total 32	C 10	N 5	O 14	P 3	0
37	TE	1	Total 32	C 10	N 5	O 14	P 3	0
37	TG	1	Total 32	C 10	N 5	O 14	P 3	0
37	TI	1	Total 32	C 10	N 5	O 14	P 3	0
37	TK	1	Total 32	C 10	N 5	O 14	P 3	0
37	TM	1	Total 32	C 10	N 5	O 14	P 3	0
37	UC	1	Total 32	C 10	N 5	O 14	P 3	0
37	UE	1	Total 32	C 10	N 5	O 14	P 3	0
37	UG	1	Total 32	C 10	N 5	O 14	P 3	0
37	UI	1	Total 32	C 10	N 5	O 14	P 3	0
37	UK	1	Total 32	C 10	N 5	O 14	P 3	0
37	UM	1	Total 32	C 10	N 5	O 14	P 3	0
37	VC	1	Total 32	C 10	N 5	O 14	P 3	0
37	VE	1	Total 32	C 10	N 5	O 14	P 3	0
37	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	
37	VI	1	32	10	5	14	3	0
37	VK	1	32	10	5	14	3	0
37	VM	1	32	10	5	14	3	0
37	WC	1	32	10	5	14	3	0
37	WE	1	32	10	5	14	3	0
37	WG	1	32	10	5	14	3	0
37	WI	1	32	10	5	14	3	0
37	WK	1	32	10	5	14	3	0
37	WM	1	32	10	5	14	3	0

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
38	AA	1	1	1	0
38	AC	1	1	1	0
38	AE	1	1	1	0
38	AG	1	1	1	0
38	AI	1	1	1	0
38	AK	1	1	1	0
38	AM	1	1	1	0
38	BA	1	1	1	0
38	BC	1	1	1	0
38	BE	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
38	BG	1	1	1	0
38	BI	1	1	1	0
38	BK	1	1	1	0
38	BM	1	1	1	0
38	CA	1	1	1	0
38	CC	1	1	1	0
38	CE	1	1	1	0
38	CG	1	1	1	0
38	CI	1	1	1	0
38	CK	1	1	1	0
38	CM	1	1	1	0
38	DA	1	1	1	0
38	DC	1	1	1	0
38	DE	1	1	1	0
38	DG	1	1	1	0
38	DI	1	1	1	0
38	DK	1	1	1	0
38	DM	1	1	1	0
38	EC	1	1	1	0
38	EE	1	1	1	0
38	EG	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
38	EI	1	1	1	0
38	EK	1	1	1	0
38	EM	1	1	1	0
38	FC	1	1	1	0
38	FE	1	1	1	0
38	FG	1	1	1	0
38	FI	1	1	1	0
38	FK	1	1	1	0
38	FM	1	1	1	0
38	GC	1	1	1	0
38	GE	1	1	1	0
38	GG	1	1	1	0
38	GI	1	1	1	0
38	GK	1	1	1	0
38	GM	1	1	1	0
38	HC	1	1	1	0
38	HE	1	1	1	0
38	HG	1	1	1	0
38	HI	1	1	1	0
38	HK	1	1	1	0
38	HM	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
38	HO	1	1	1	0
38	IC	1	1	1	0
38	IE	1	1	1	0
38	IG	1	1	1	0
38	II	1	1	1	0
38	IK	1	1	1	0
38	IM	1	1	1	0
38	IO	1	1	1	0
38	JC	1	1	1	0
38	JE	1	1	1	0
38	JG	1	1	1	0
38	JI	1	1	1	0
38	JK	1	1	1	0
38	JM	1	1	1	0
38	KC	1	1	1	0
38	KE	1	1	1	0
38	KG	1	1	1	0
38	KI	1	1	1	0
38	KK	1	1	1	0
38	KM	1	1	1	0
38	KO	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
38	LC	1	1	1	0
38	LE	1	1	1	0
38	LG	1	1	1	0
38	LI	1	1	1	0
38	LK	1	1	1	0
38	LM	1	1	1	0
38	MC	1	1	1	0
38	ME	1	1	1	0
38	MG	1	1	1	0
38	MI	1	1	1	0
38	MK	1	1	1	0
38	MM	1	1	1	0
38	NA	1	1	1	0
38	NC	1	1	1	0
38	NE	1	1	1	0
38	NG	1	1	1	0
38	NI	1	1	1	0
38	NK	1	1	1	0
38	OA	1	1	1	0
38	OC	1	1	1	0
38	OE	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
38	OG	1	1	1	0
38	OI	1	1	1	0
38	OK	1	1	1	0
38	PA	1	1	1	0
38	PC	1	1	1	0
38	PE	1	1	1	0
38	PG	1	1	1	0
38	PI	1	1	1	0
38	PK	1	1	1	0
38	PM	1	1	1	0
38	QA	1	1	1	0
38	QC	1	1	1	0
38	QE	1	1	1	0
38	QG	1	1	1	0
38	QI	1	1	1	0
38	QK	1	1	1	0
38	QM	1	1	1	0
38	RA	1	1	1	0
38	RC	1	1	1	0
38	RE	1	1	1	0
38	RG	1	1	1	0

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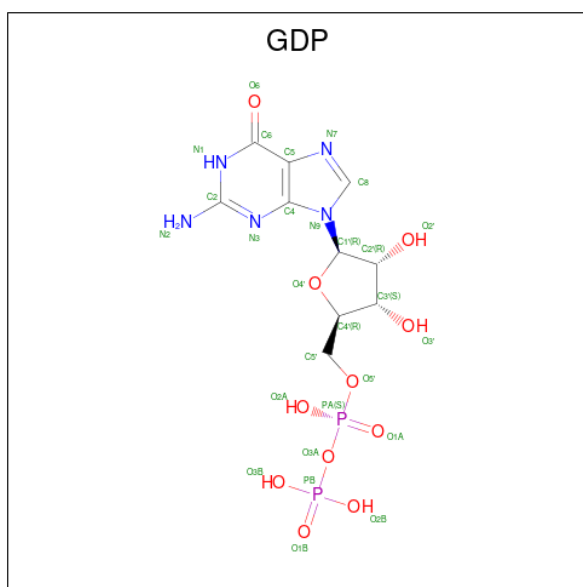
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
38	RI	1	1	1	0
38	RK	1	1	1	0
38	RM	1	1	1	0
38	SA	1	1	1	0
38	SC	1	1	1	0
38	SE	1	1	1	0
38	SG	1	1	1	0
38	SI	1	1	1	0
38	SK	1	1	1	0
38	SM	1	1	1	0
38	TC	1	1	1	0
38	TE	1	1	1	0
38	TG	1	1	1	0
38	TI	1	1	1	0
38	TK	1	1	1	0
38	TM	1	1	1	0
38	UC	1	1	1	0
38	UE	1	1	1	0
38	UG	1	1	1	0
38	UI	1	1	1	0
38	UK	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
38	UM	1	Total 1	Mg 1	0
38	VC	1	Total 1	Mg 1	0
38	VE	1	Total 1	Mg 1	0
38	VG	1	Total 1	Mg 1	0
38	VI	1	Total 1	Mg 1	0
38	VK	1	Total 1	Mg 1	0
38	VM	1	Total 1	Mg 1	0
38	WC	1	Total 1	Mg 1	0
38	WE	1	Total 1	Mg 1	0
38	WG	1	Total 1	Mg 1	0
38	WI	1	Total 1	Mg 1	0
38	WK	1	Total 1	Mg 1	0
38	WM	1	Total 1	Mg 1	0

- Molecule 39 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	AB	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	AD	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	AF	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	AH	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	AJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	AL	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	BB	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	BD	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	BF	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	BH	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	BJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	BL	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	CB	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	CF	1	28	10	5	11	2	0
39	CH	1	28	10	5	11	2	0
39	CJ	1	28	10	5	11	2	0
39	CL	1	28	10	5	11	2	0
39	DB	1	28	10	5	11	2	0
39	DD	1	28	10	5	11	2	0
39	DF	1	28	10	5	11	2	0
39	DH	1	28	10	5	11	2	0
39	DJ	1	28	10	5	11	2	0
39	DL	1	28	10	5	11	2	0
39	DN	1	28	10	5	11	2	0
39	EB	1	28	10	5	11	2	0
39	ED	1	28	10	5	11	2	0
39	EF	1	28	10	5	11	2	0
39	EH	1	28	10	5	11	2	0
39	EJ	1	28	10	5	11	2	0
39	EL	1	28	10	5	11	2	0
39	EN	1	28	10	5	11	2	0
39	FB	1	28	10	5	11	2	0
39	FD	1	28	10	5	11	2	0
39	FF	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	FH	1	28	10	5	11	2	0
39	FJ	1	28	10	5	11	2	0
39	FL	1	28	10	5	11	2	0
39	FN	1	28	10	5	11	2	0
39	GB	1	28	10	5	11	2	0
39	GD	1	28	10	5	11	2	0
39	GF	1	28	10	5	11	2	0
39	GH	1	28	10	5	11	2	0
39	GJ	1	28	10	5	11	2	0
39	GL	1	28	10	5	11	2	0
39	GN	1	28	10	5	11	2	0
39	HB	1	28	10	5	11	2	0
39	HD	1	28	10	5	11	2	0
39	HF	1	28	10	5	11	2	0
39	HH	1	28	10	5	11	2	0
39	HJ	1	28	10	5	11	2	0
39	HL	1	28	10	5	11	2	0
39	HN	1	28	10	5	11	2	0
39	IB	1	28	10	5	11	2	0
39	ID	1	28	10	5	11	2	0
39	IF	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	IH	1	28	10	5	11	2	0
39	IJ	1	28	10	5	11	2	0
39	IL	1	28	10	5	11	2	0
39	IN	1	28	10	5	11	2	0
39	JB	1	28	10	5	11	2	0
39	JD	1	28	10	5	11	2	0
39	JF	1	28	10	5	11	2	0
39	JH	1	28	10	5	11	2	0
39	JJ	1	28	10	5	11	2	0
39	JL	1	28	10	5	11	2	0
39	JN	1	28	10	5	11	2	0
39	KB	1	28	10	5	11	2	0
39	KD	1	28	10	5	11	2	0
39	KF	1	28	10	5	11	2	0
39	KH	1	28	10	5	11	2	0
39	KJ	1	28	10	5	11	2	0
39	KL	1	28	10	5	11	2	0
39	KN	1	28	10	5	11	2	0
39	LB	1	28	10	5	11	2	0
39	LD	1	28	10	5	11	2	0
39	LF	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	LH	1	28	10	5	11	2	0
39	LJ	1	28	10	5	11	2	0
39	LL	1	28	10	5	11	2	0
39	LN	1	28	10	5	11	2	0
39	MB	1	28	10	5	11	2	0
39	MD	1	28	10	5	11	2	0
39	MF	1	28	10	5	11	2	0
39	MH	1	28	10	5	11	2	0
39	MJ	1	28	10	5	11	2	0
39	ML	1	28	10	5	11	2	0
39	MN	1	28	10	5	11	2	0
39	N0	1	28	10	5	11	2	0
39	NB	1	28	10	5	11	2	0
39	ND	1	28	10	5	11	2	0
39	NF	1	28	10	5	11	2	0
39	NH	1	28	10	5	11	2	0
39	NJ	1	28	10	5	11	2	0
39	NL	1	28	10	5	11	2	0
39	O0	1	28	10	5	11	2	0
39	OB	1	28	10	5	11	2	0
39	OD	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	OF	1	28	10	5	11	2	0
39	OH	1	28	10	5	11	2	0
39	OJ	1	28	10	5	11	2	0
39	OL	1	28	10	5	11	2	0
39	PB	1	28	10	5	11	2	0
39	PD	1	28	10	5	11	2	0
39	PF	1	28	10	5	11	2	0
39	PH	1	28	10	5	11	2	0
39	PJ	1	28	10	5	11	2	0
39	PL	1	28	10	5	11	2	0
39	QB	1	28	10	5	11	2	0
39	QD	1	28	10	5	11	2	0
39	QF	1	28	10	5	11	2	0
39	QH	1	28	10	5	11	2	0
39	QJ	1	28	10	5	11	2	0
39	QL	1	28	10	5	11	2	0
39	RB	1	28	10	5	11	2	0
39	RD	1	28	10	5	11	2	0
39	RF	1	28	10	5	11	2	0
39	RH	1	28	10	5	11	2	0
39	RJ	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	RL	1	Total 28	C 10	N 5	O 11	P 2	0
39	SB	1	Total 28	C 10	N 5	O 11	P 2	0
39	SD	1	Total 28	C 10	N 5	O 11	P 2	0
39	SF	1	Total 28	C 10	N 5	O 11	P 2	0
39	SH	1	Total 28	C 10	N 5	O 11	P 2	0
39	SJ	1	Total 28	C 10	N 5	O 11	P 2	0
39	SL	1	Total 28	C 10	N 5	O 11	P 2	0
39	TB	1	Total 28	C 10	N 5	O 11	P 2	0
39	TD	1	Total 28	C 10	N 5	O 11	P 2	0
39	TF	1	Total 28	C 10	N 5	O 11	P 2	0
39	TH	1	Total 28	C 10	N 5	O 11	P 2	0
39	TJ	1	Total 28	C 10	N 5	O 11	P 2	0
39	TL	1	Total 28	C 10	N 5	O 11	P 2	0
39	UB	1	Total 28	C 10	N 5	O 11	P 2	0
39	UD	1	Total 28	C 10	N 5	O 11	P 2	0
39	UF	1	Total 28	C 10	N 5	O 11	P 2	0
39	UH	1	Total 28	C 10	N 5	O 11	P 2	0
39	UJ	1	Total 28	C 10	N 5	O 11	P 2	0
39	UL	1	Total 28	C 10	N 5	O 11	P 2	0
39	UN	1	Total 28	C 10	N 5	O 11	P 2	0
39	VB	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	
39	VD	1	Total 28	10	5	11	2	0
39	VF	1	Total 28	10	5	11	2	0
39	VH	1	Total 28	10	5	11	2	0
39	VJ	1	Total 28	10	5	11	2	0
39	VL	1	Total 28	10	5	11	2	0
39	VN	1	Total 28	10	5	11	2	0
39	WB	1	Total 28	10	5	11	2	0
39	WD	1	Total 28	10	5	11	2	0
39	WF	1	Total 28	10	5	11	2	0
39	WH	1	Total 28	10	5	11	2	0
39	WJ	1	Total 28	10	5	11	2	0
39	WL	1	Total 28	10	5	11	2	0
39	WN	1	Total 28	10	5	11	2	0

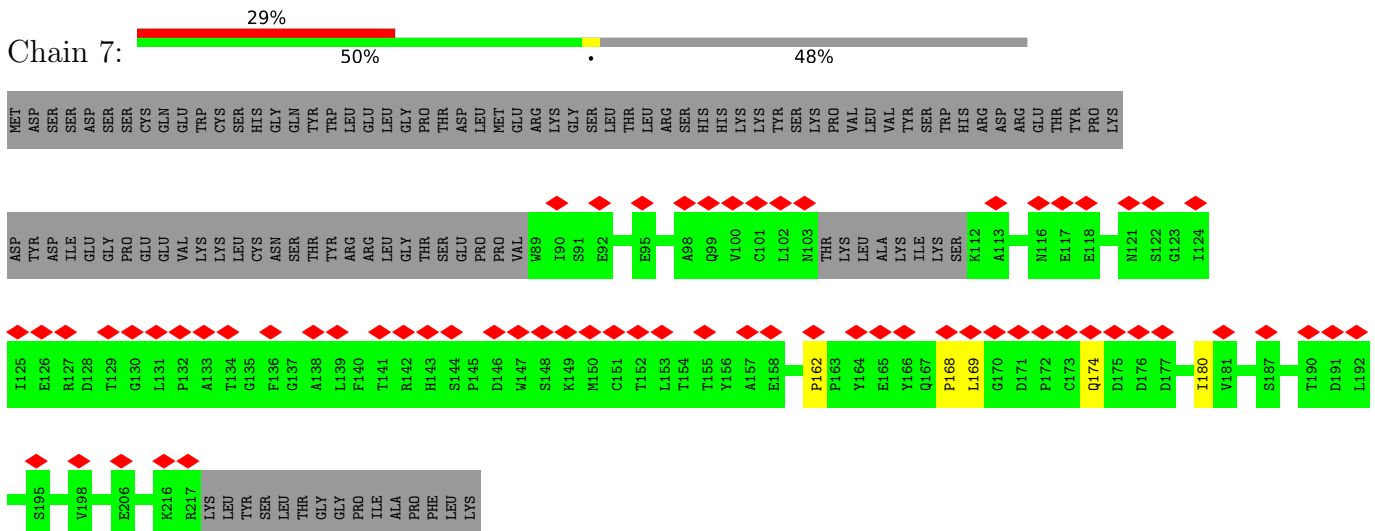
### 3 Residue-property plots [i](#)

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

- Molecule 1: Protein C9orf135 homolog



- Molecule 1: Protein C9orf135 homolog

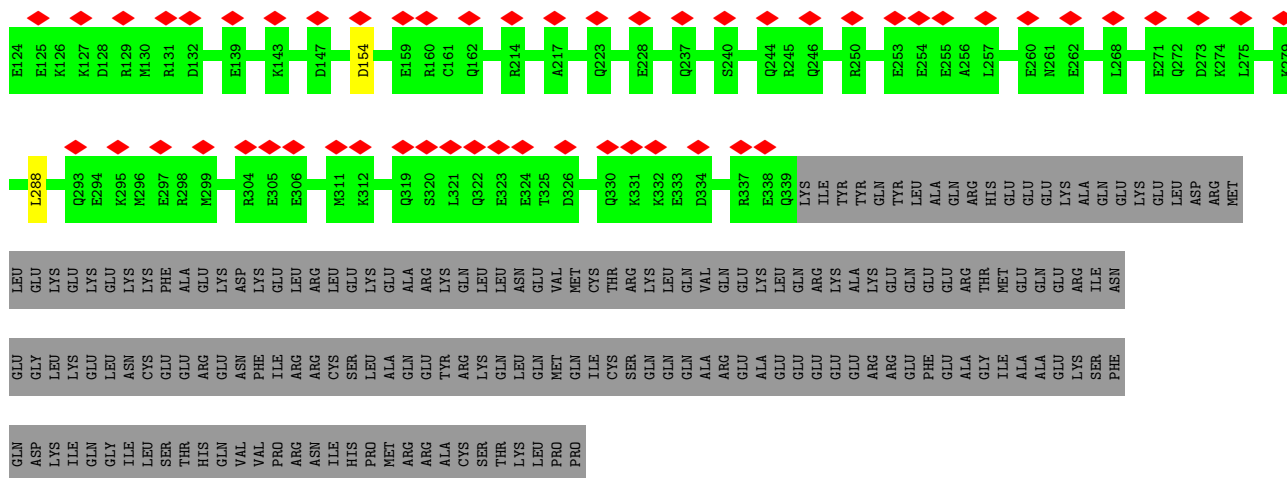


- Molecule 2: EF-hand domain family member B

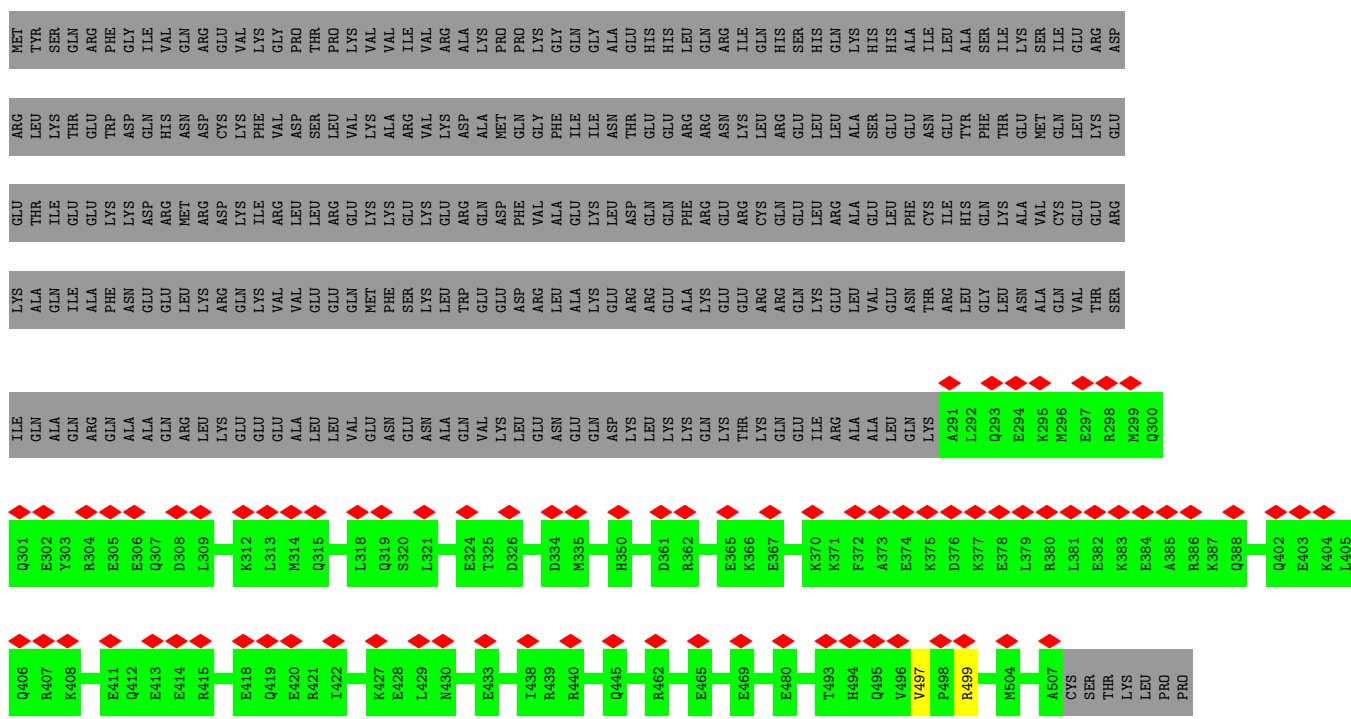




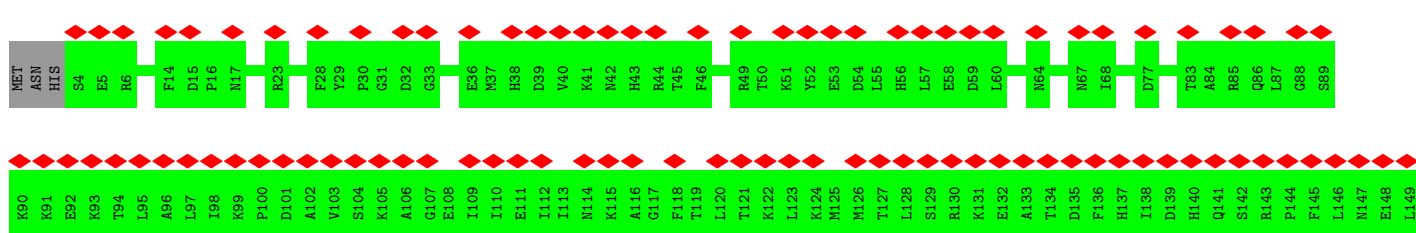
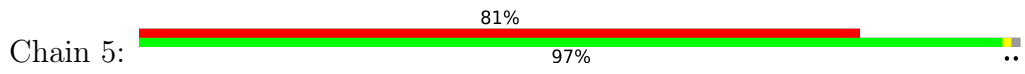


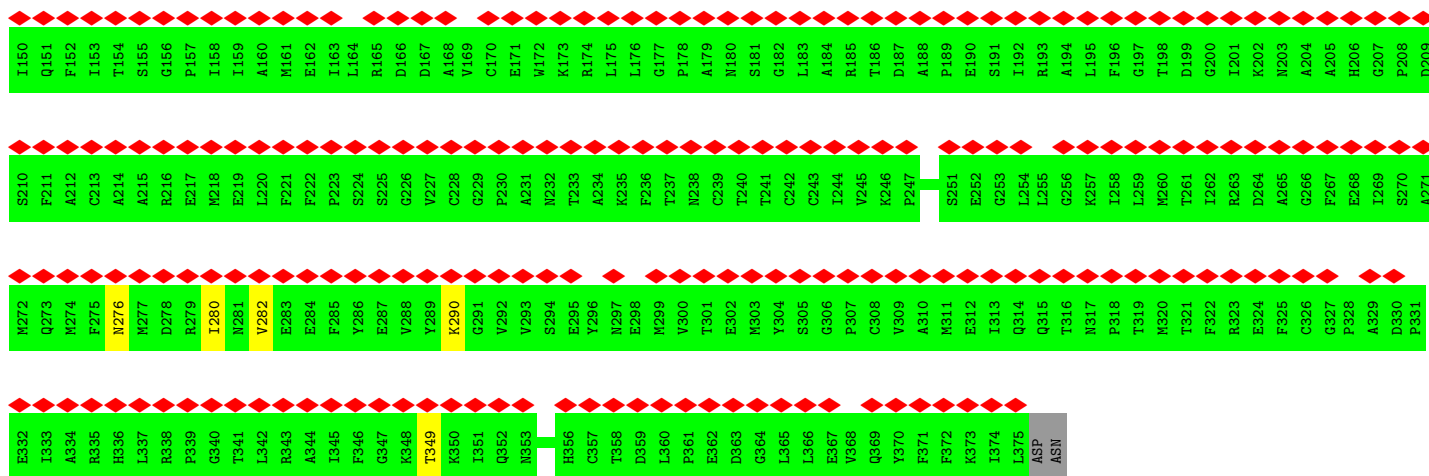


• Molecule 3: Methyl-CpG binding domain protein 1

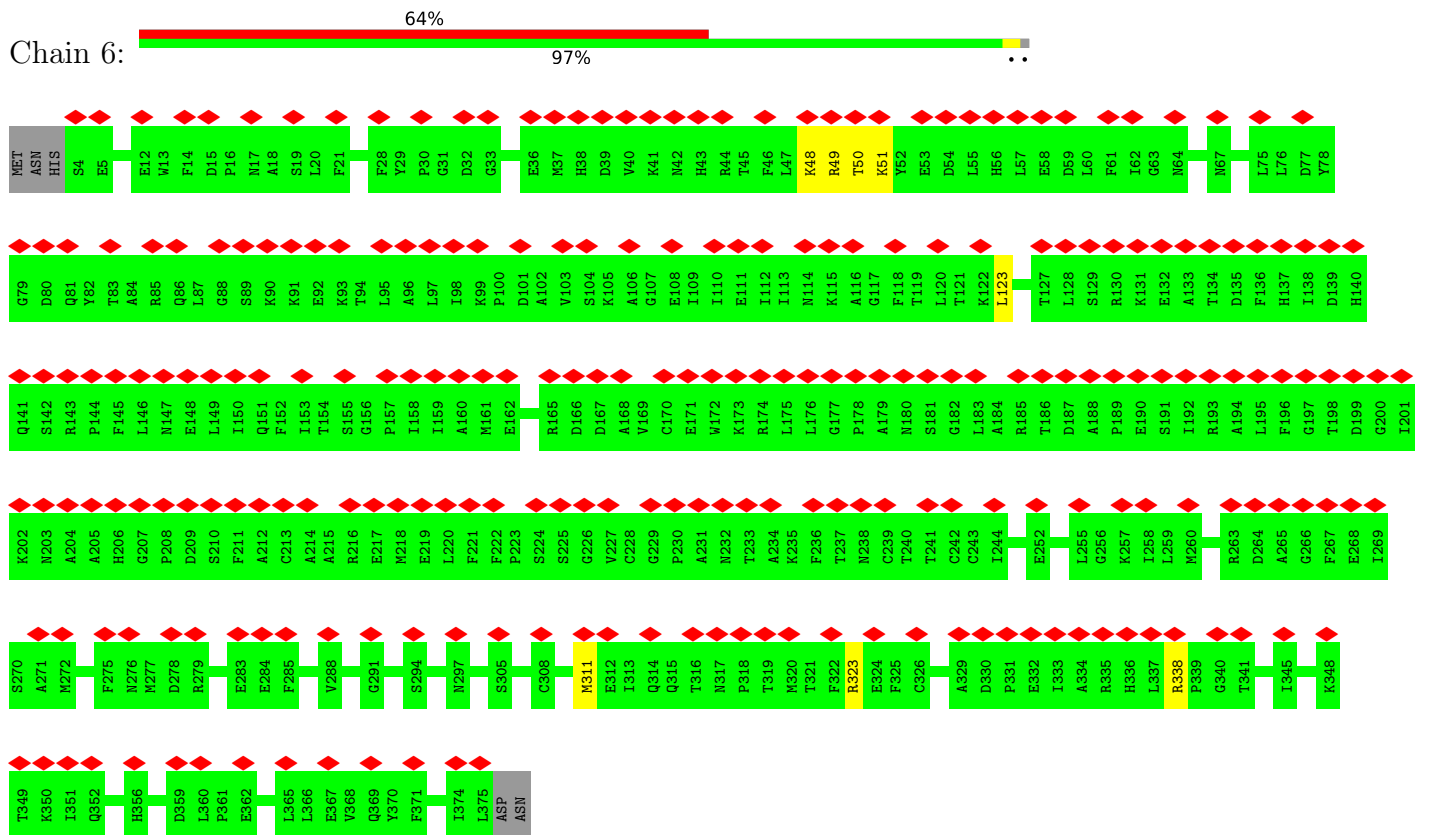


• Molecule 4: Nucleoside diphosphate kinase 7

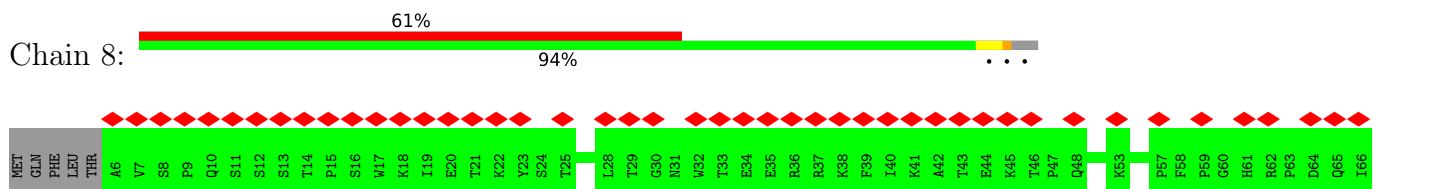


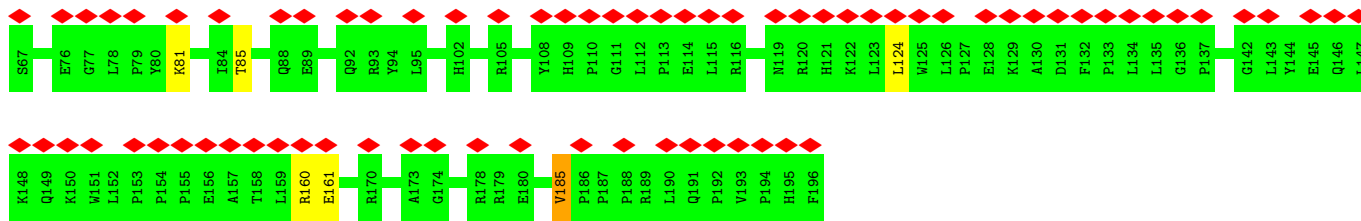


• Molecule 4: Nucleoside diphosphate kinase 7

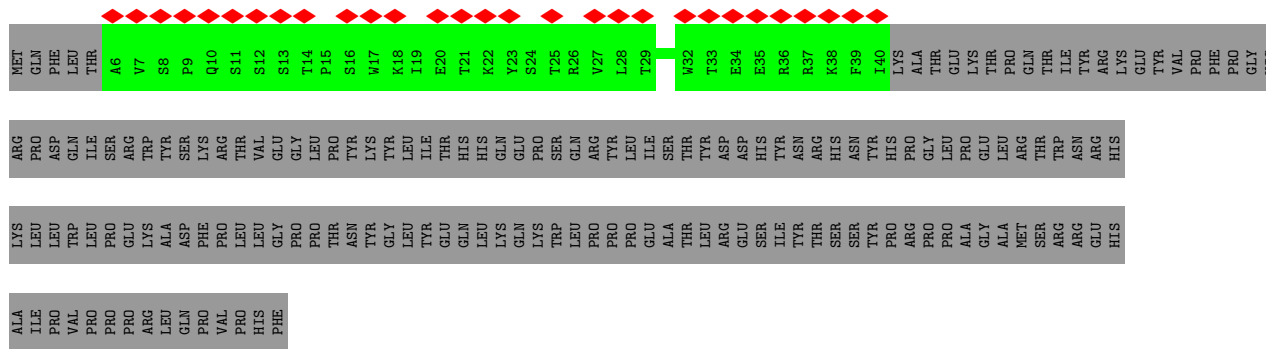


• Molecule 5: Uncharacterized protein C1orf158 homolog

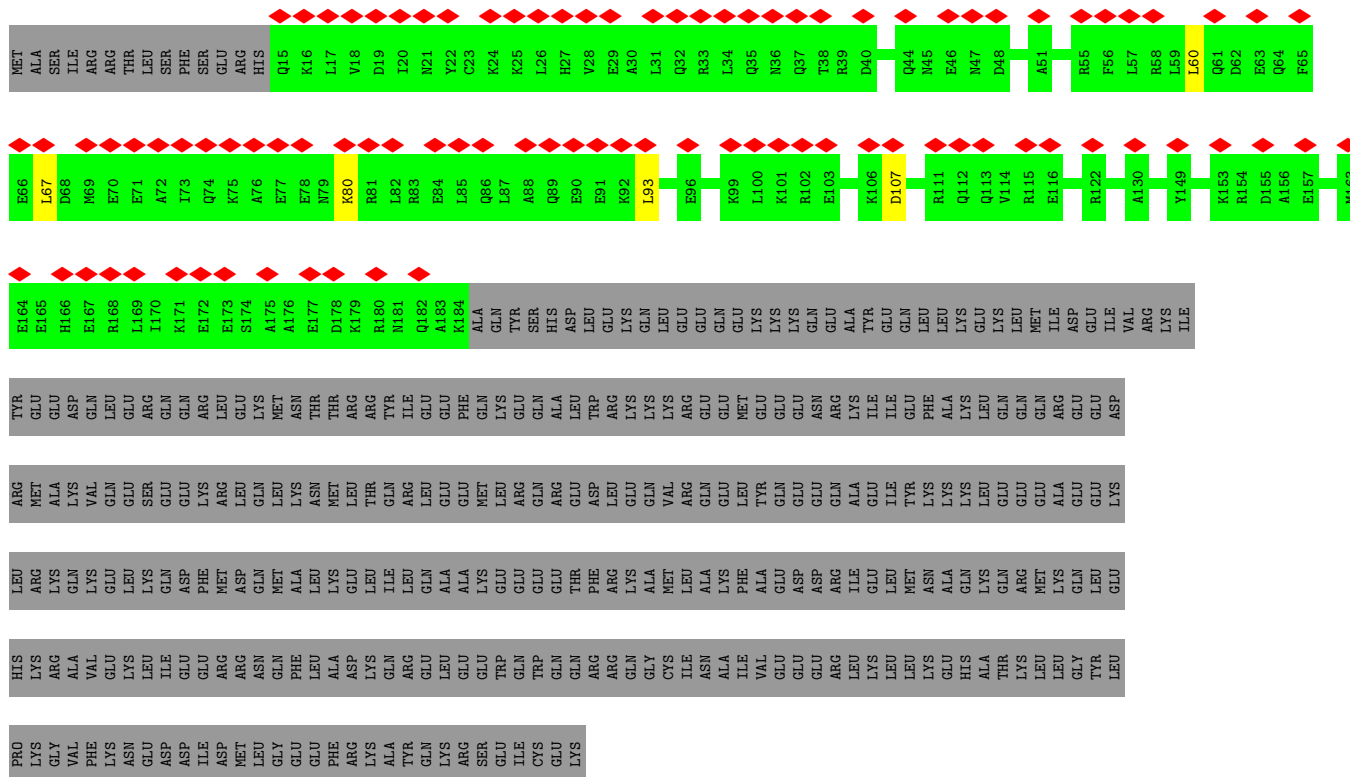




• Molecule 5: Uncharacterized protein C1orf158 homolog

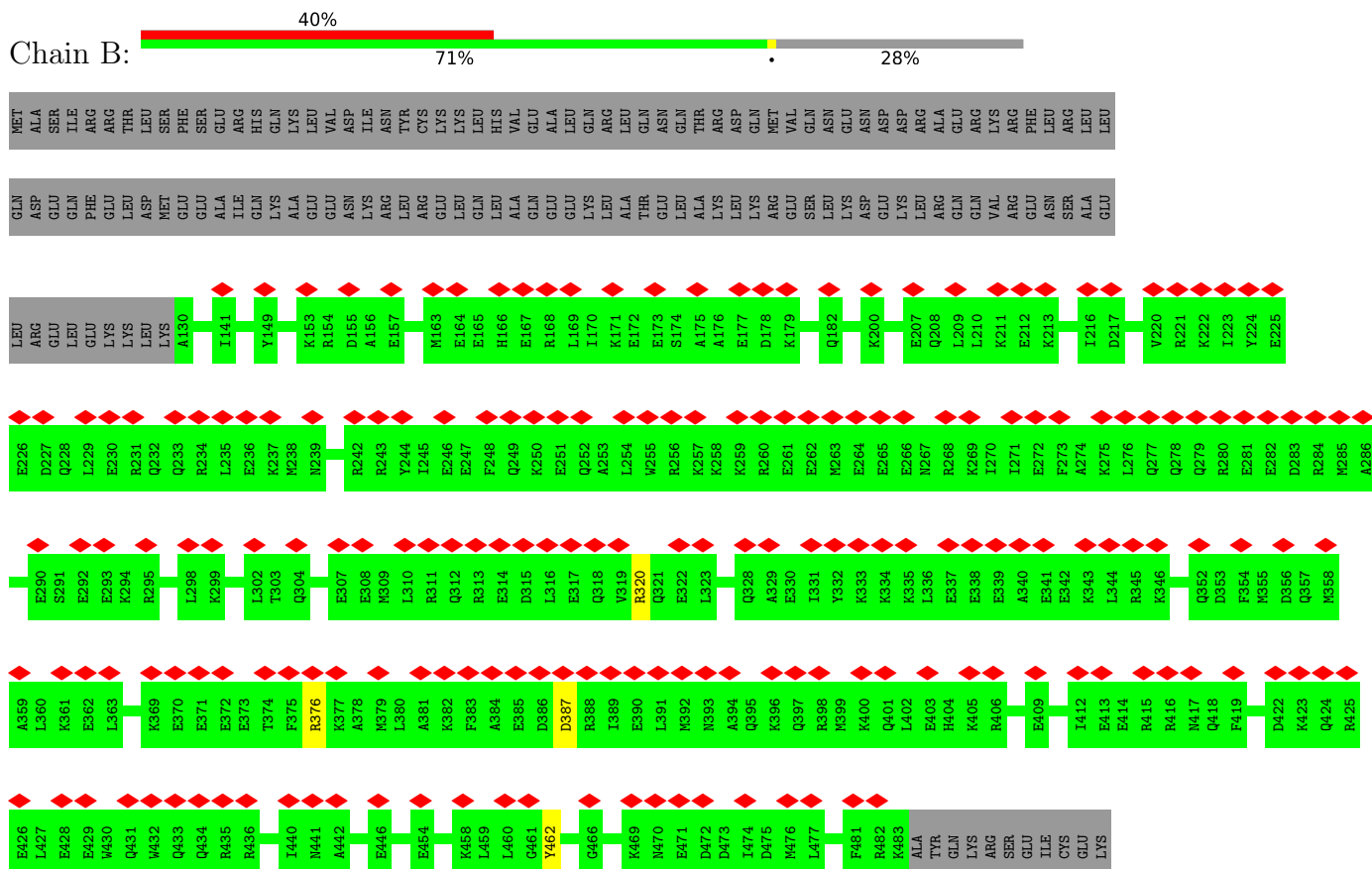


• Molecule 6: Meiosis-specific nuclear structural protein 1

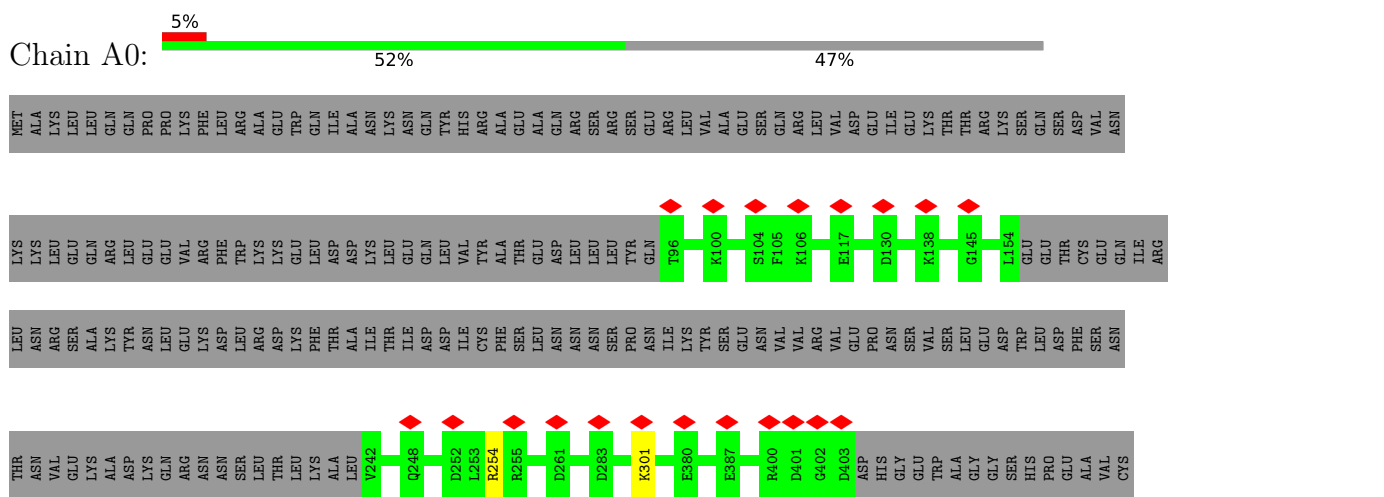


• Molecule 6: Meiosis-specific nuclear structural protein 1

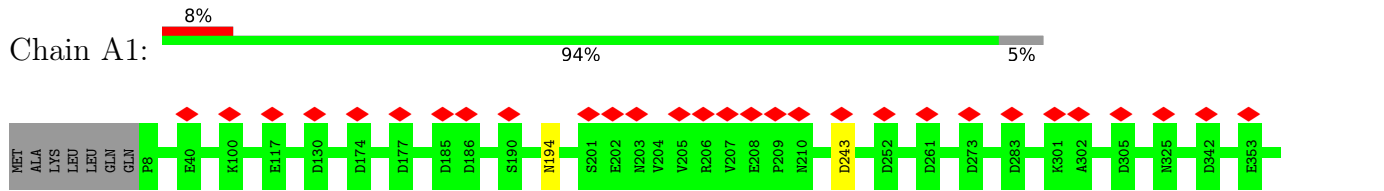


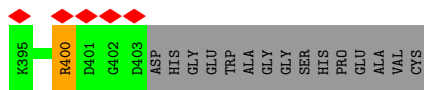


• Molecule 7: Tektin-1

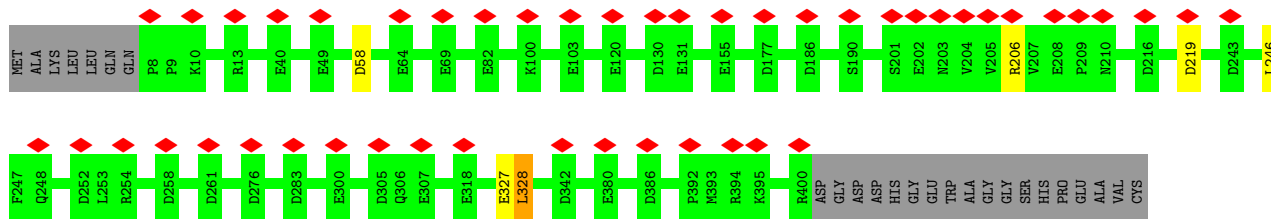


• Molecule 7: Tektin-1

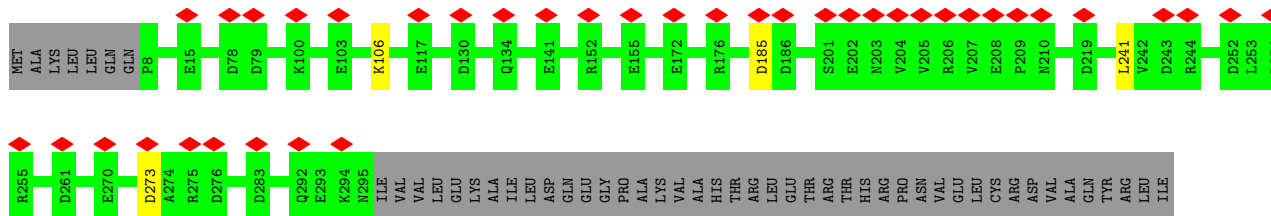
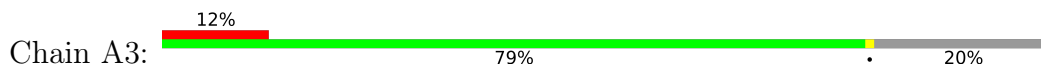




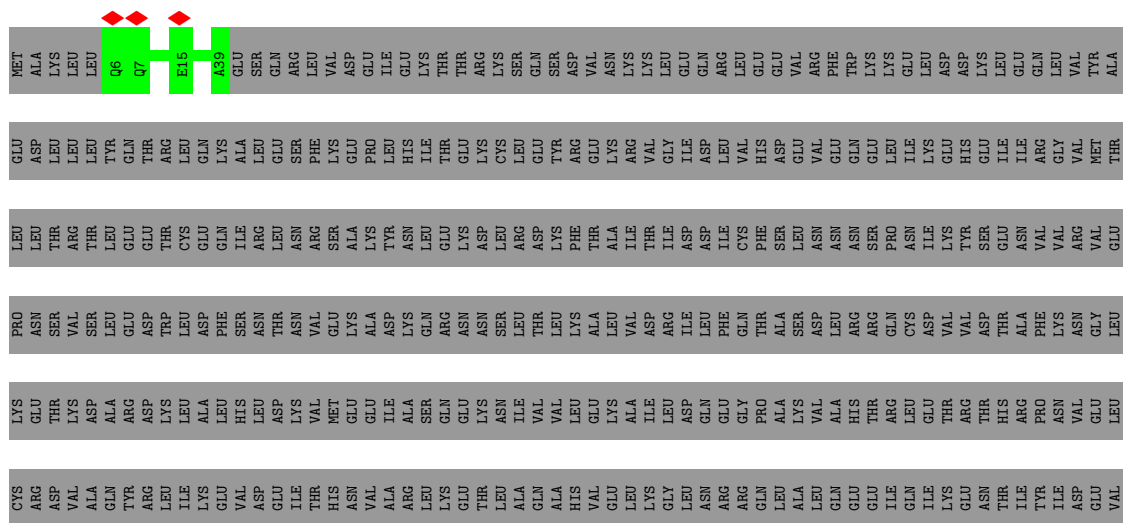
• Molecule 7: Tektin-1



• Molecule 7: Tektin-1

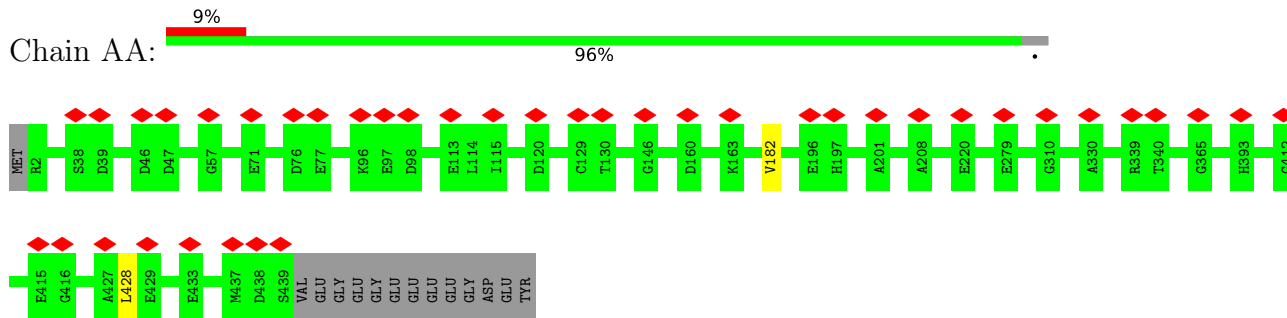


• Molecule 7: Tektin-1

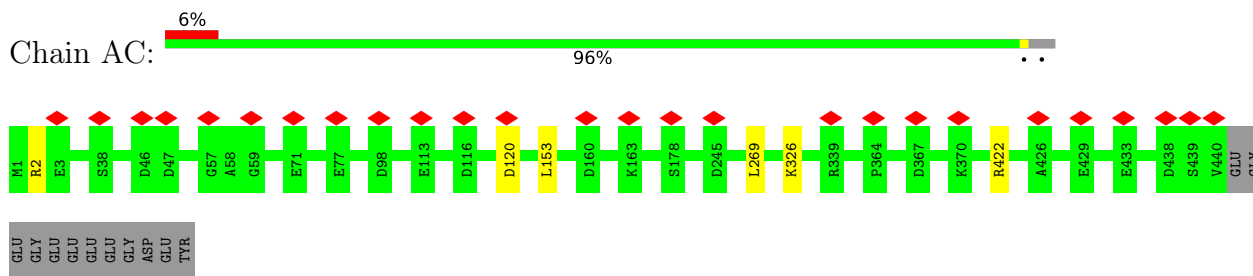


LEU CYS VAL PRO MET ARG LYS SER ILE PRO PRO ARG ASP ASP HIS GLY GLU TRP ALA GLY SER HIS PRO GLU ALA VAL CYS

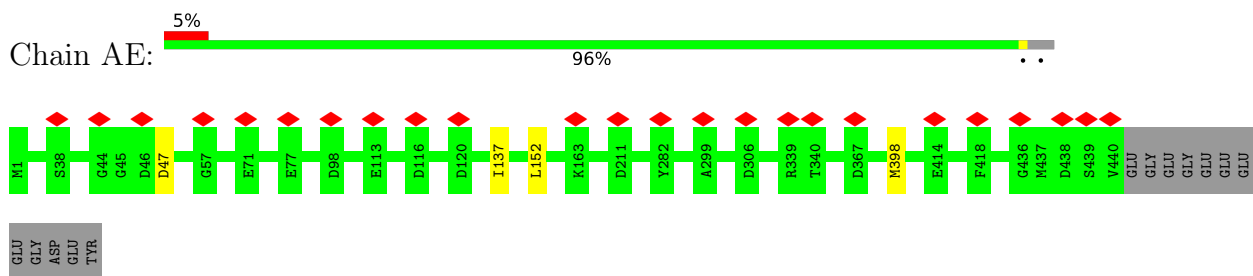
• Molecule 8: Tubulin alpha-1D chain



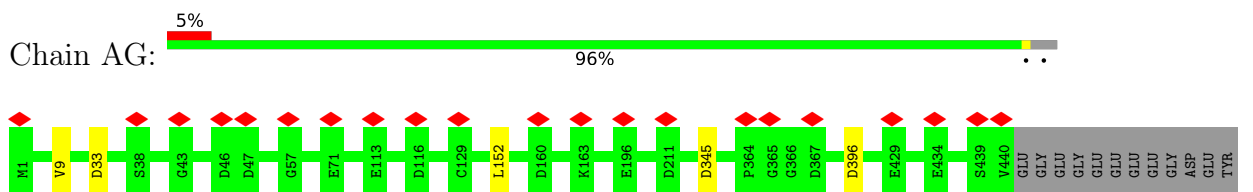
• Molecule 8: Tubulin alpha-1D chain



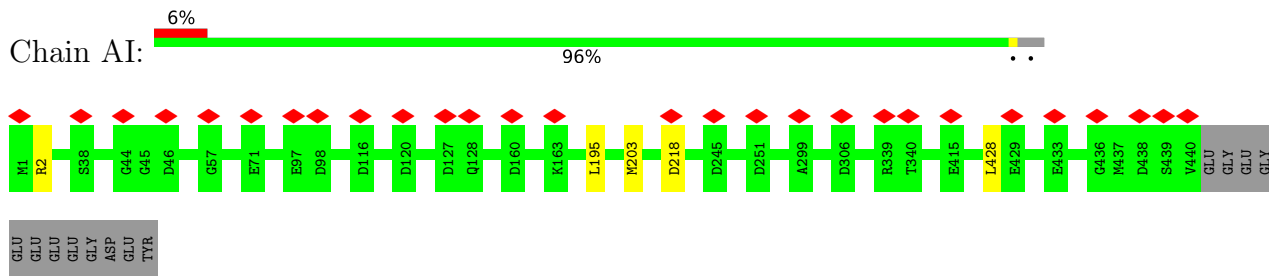
• Molecule 8: Tubulin alpha-1D chain



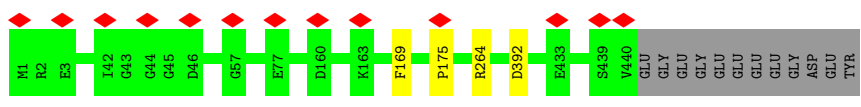
• Molecule 8: Tubulin alpha-1D chain



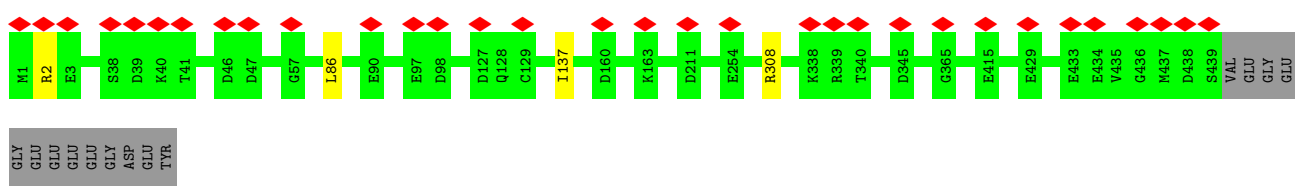
• Molecule 8: Tubulin alpha-1D chain



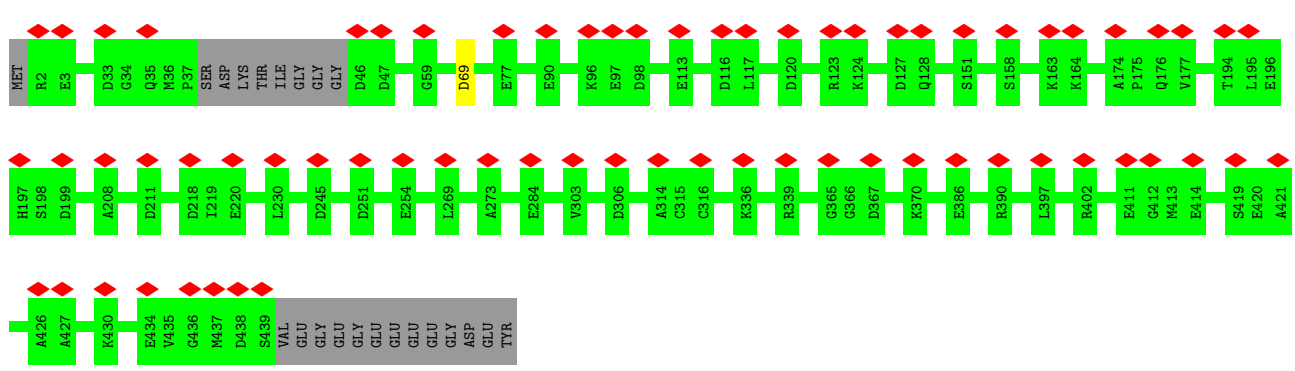
• Molecule 8: Tubulin alpha-1D chain



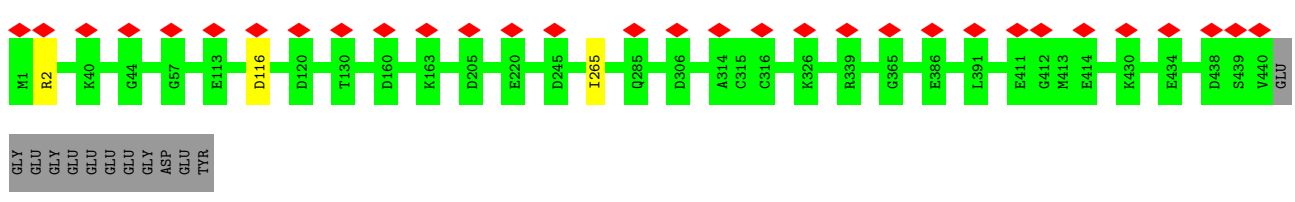
• Molecule 8: Tubulin alpha-1D chain



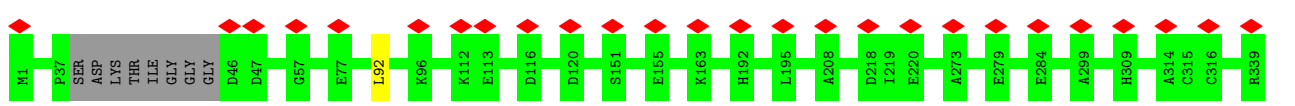
• Molecule 8: Tubulin alpha-1D chain

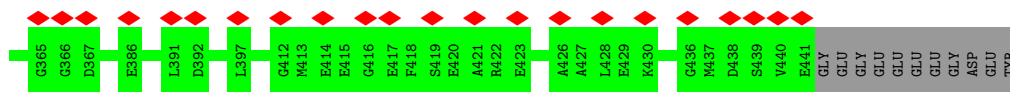


• Molecule 8: Tubulin alpha-1D chain

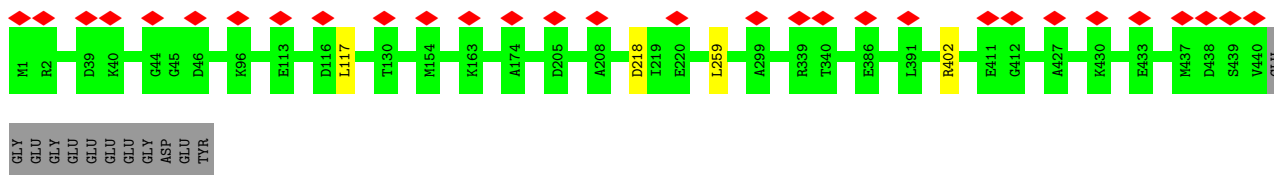


• Molecule 8: Tubulin alpha-1D chain

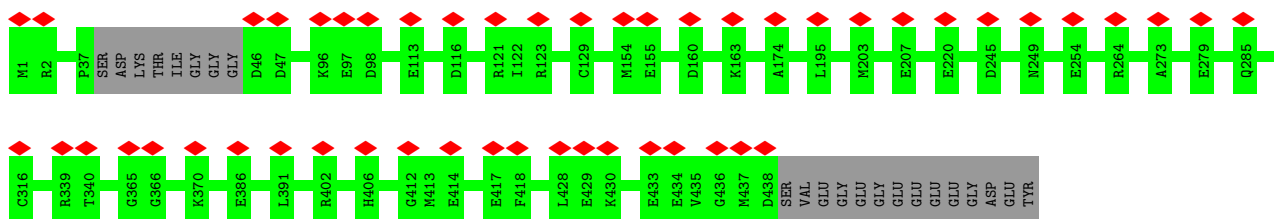
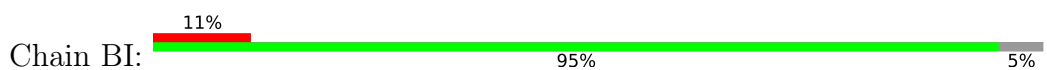




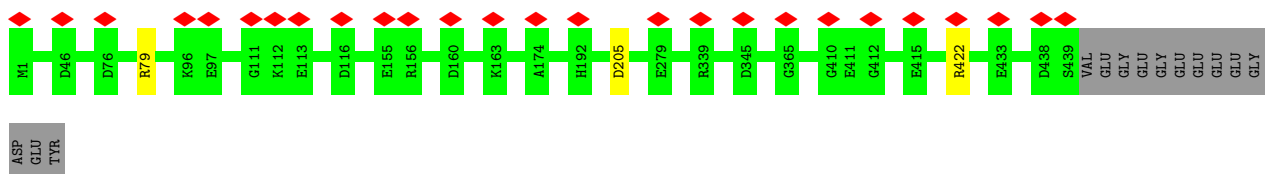
- Molecule 8: Tubulin alpha-1D chain



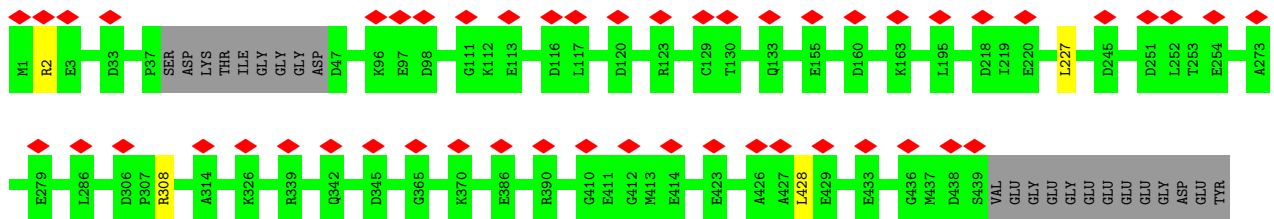
- Molecule 8: Tubulin alpha-1D chain



- Molecule 8: Tubulin alpha-1D chain

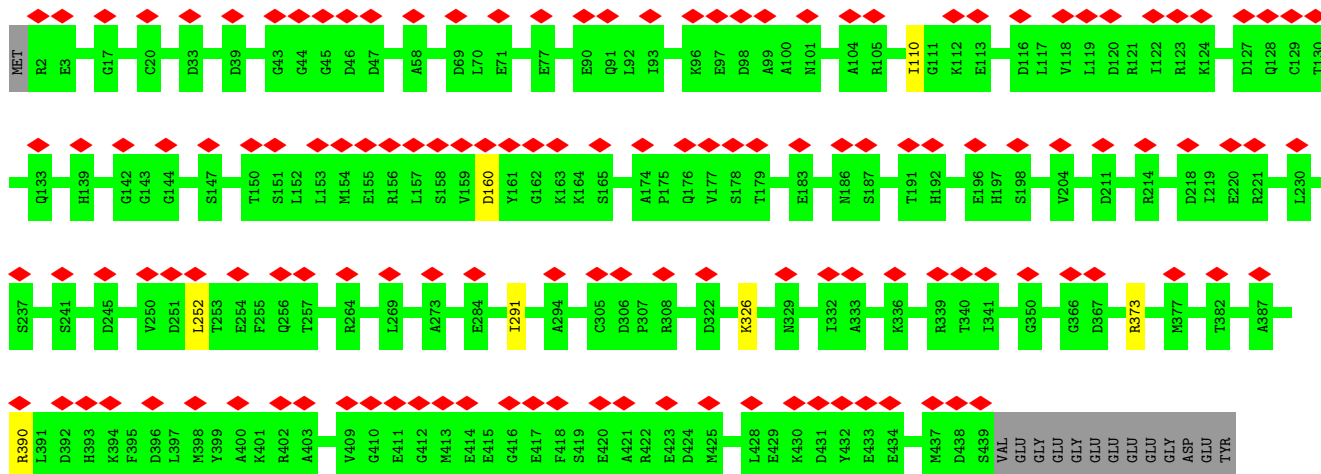


- Molecule 8: Tubulin alpha-1D chain

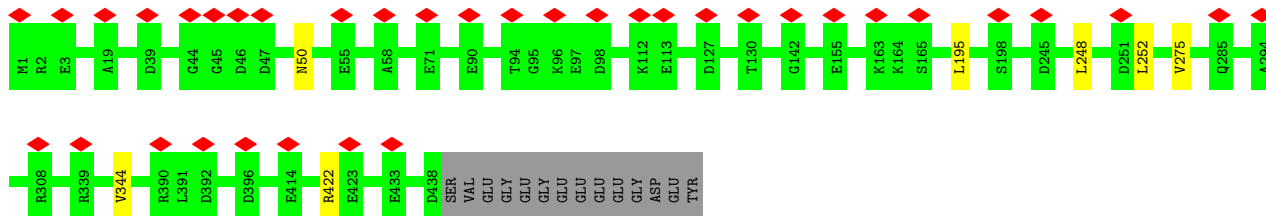


- Molecule 8: Tubulin alpha-1D chain

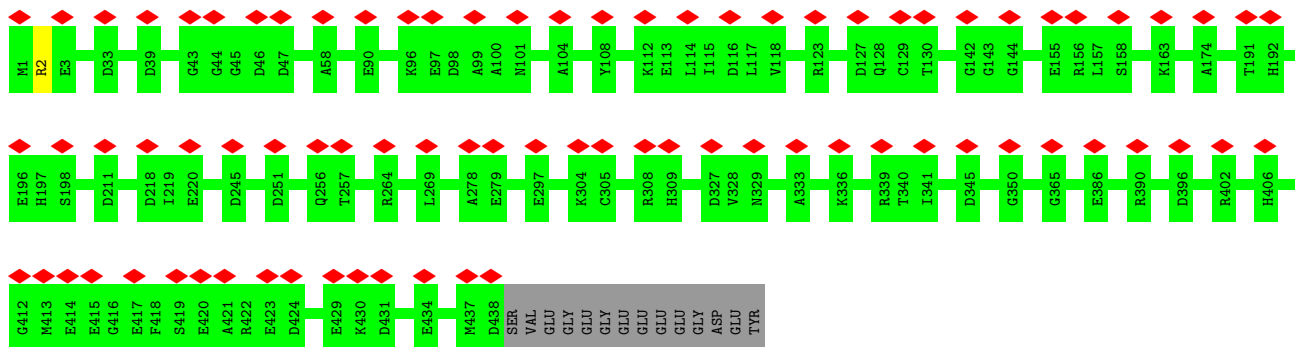




• Molecule 8: Tubulin alpha-1D chain

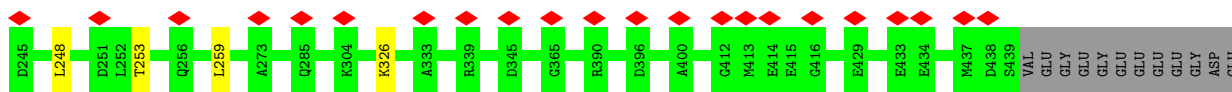


• Molecule 8: Tubulin alpha-1D chain



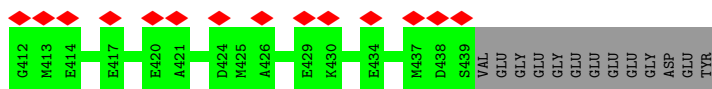
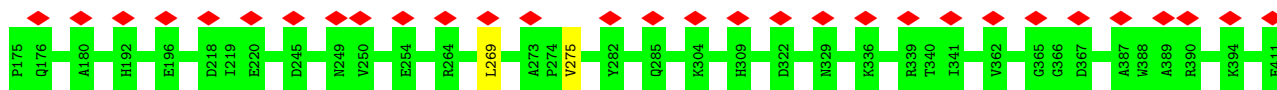
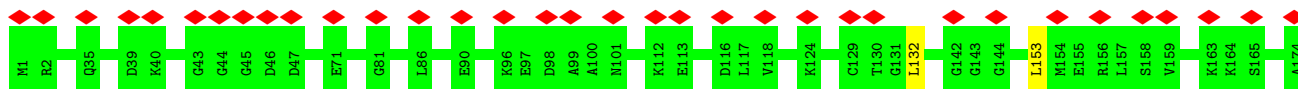
• Molecule 8: Tubulin alpha-1D chain



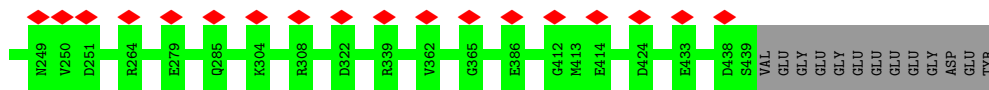
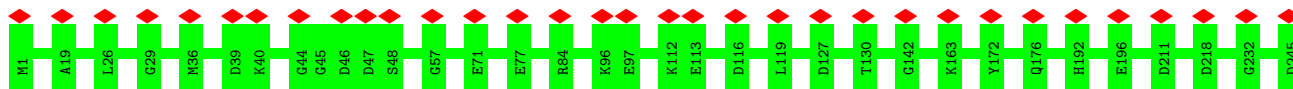


TYR

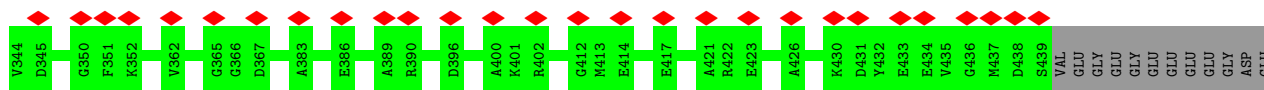
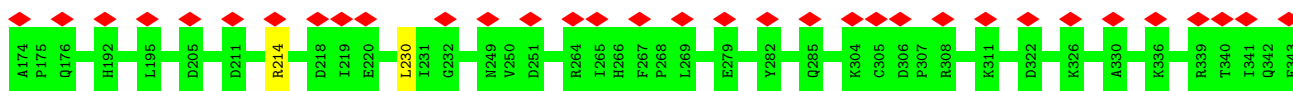
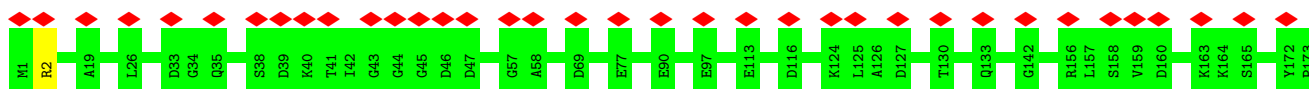
- Molecule 8: Tubulin alpha-1D chain



- Molecule 8: Tubulin alpha-1D chain

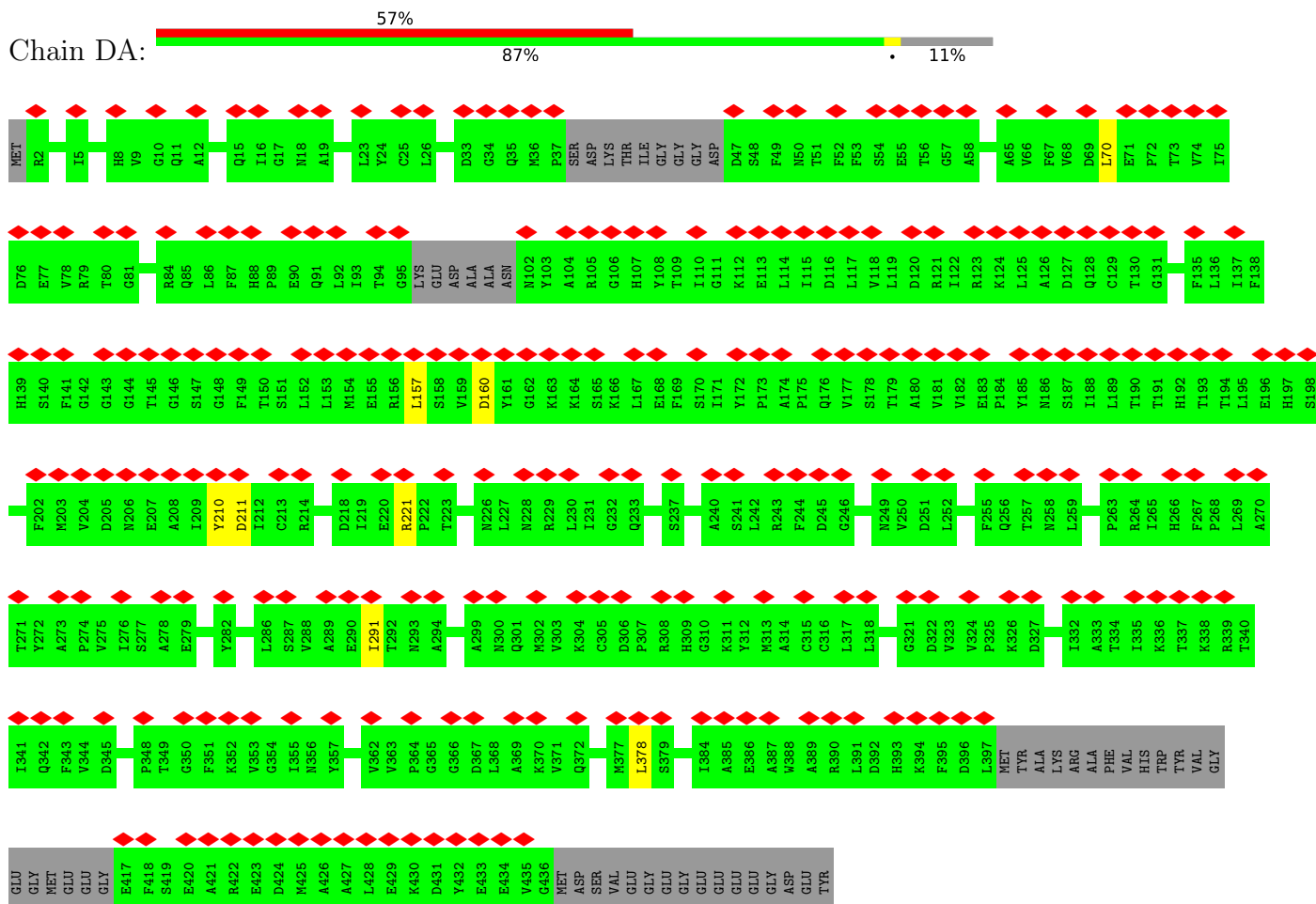


- Molecule 8: Tubulin alpha-1D chain

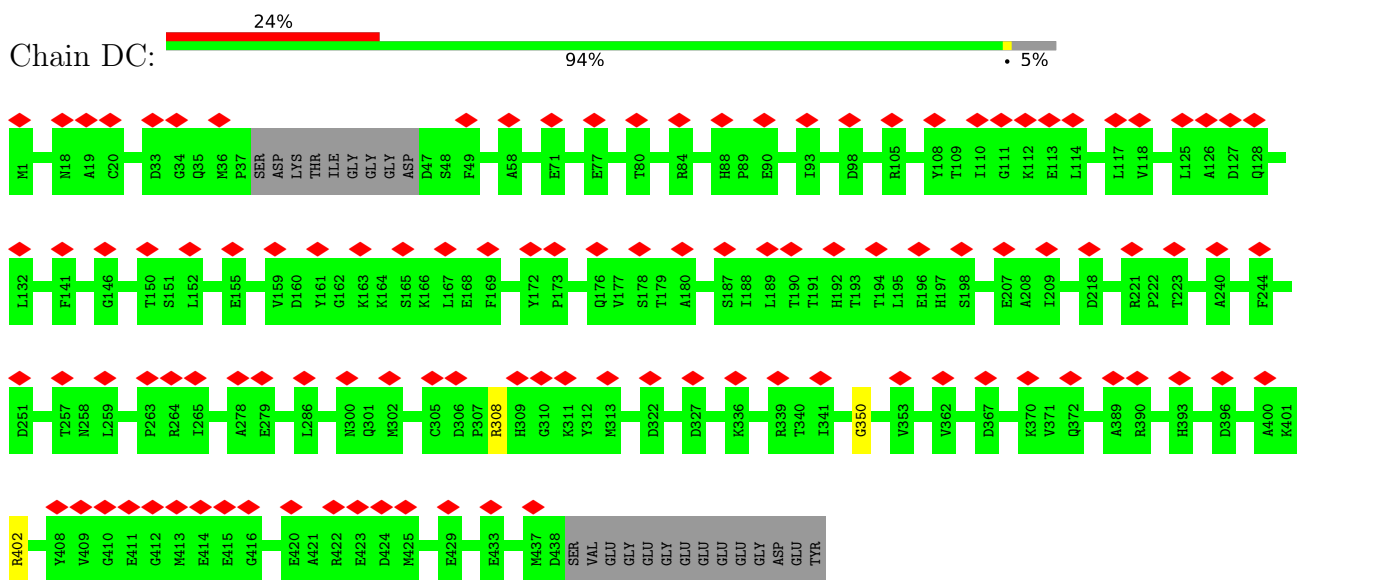


TYR

- Molecule 8: Tubulin alpha-1D chain



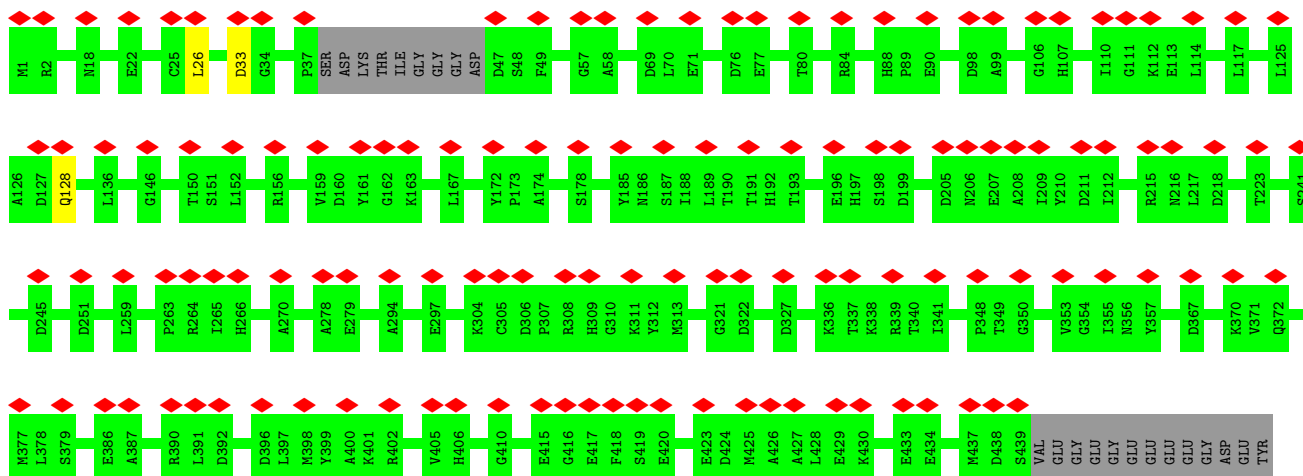
• Molecule 8: Tubulin alpha-1D chain



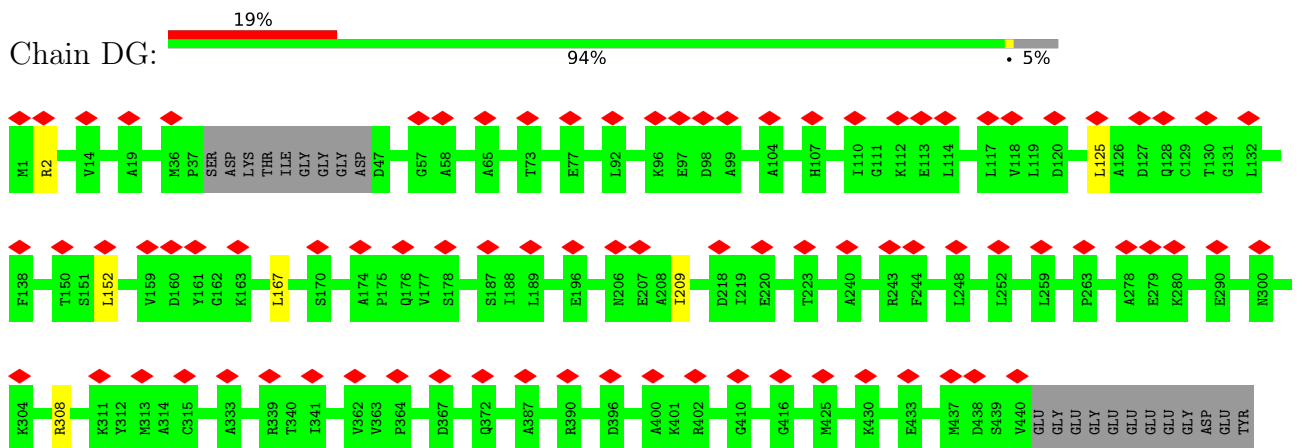
• Molecule 8: Tubulin alpha-1D chain



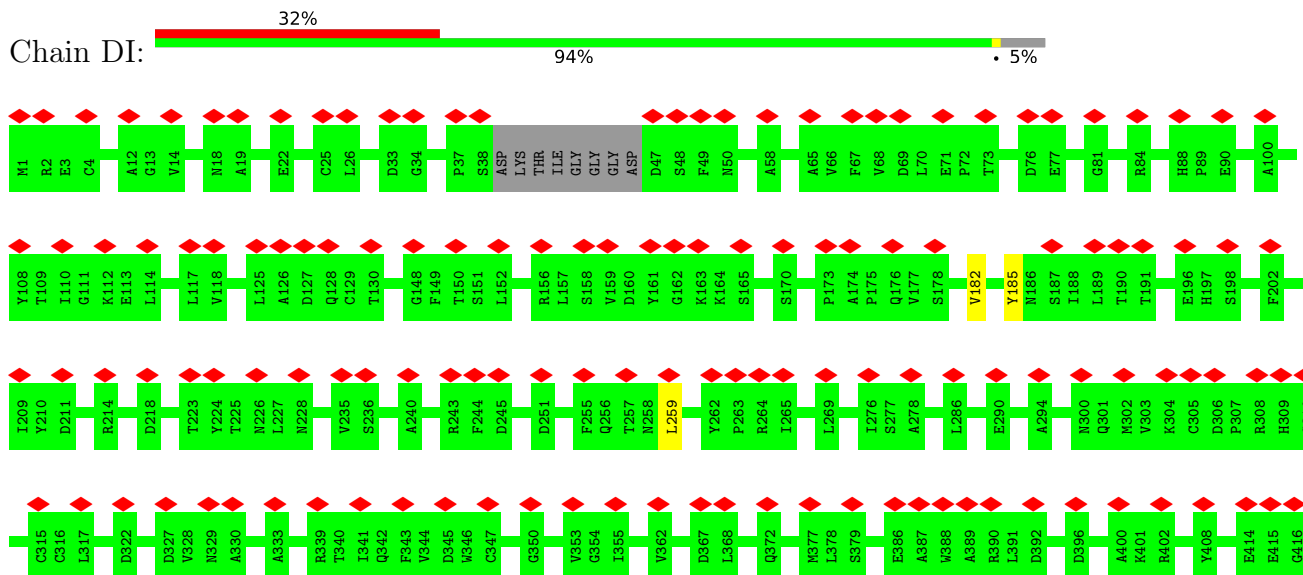


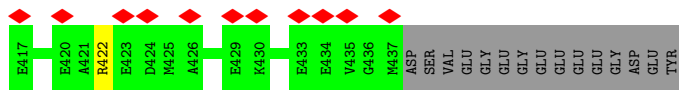


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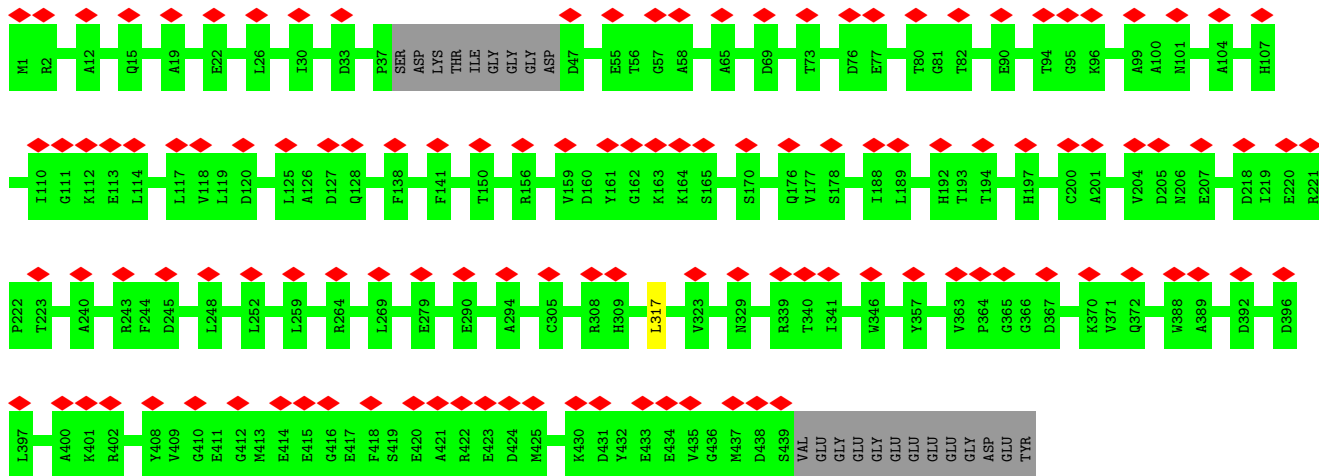


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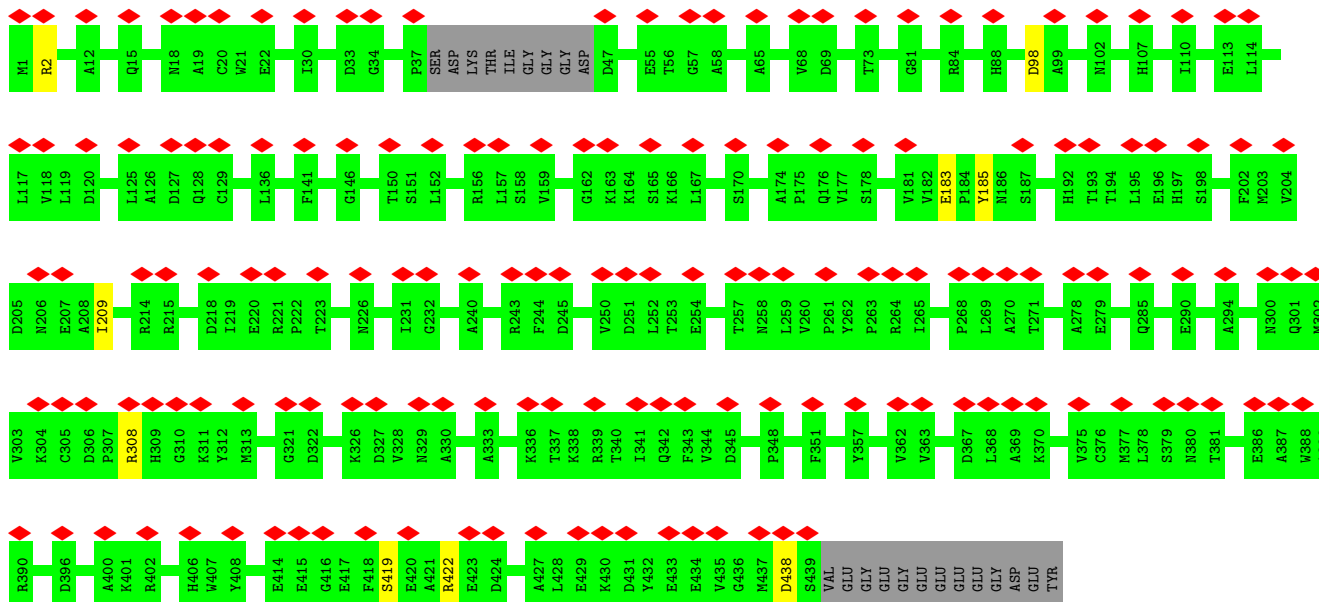




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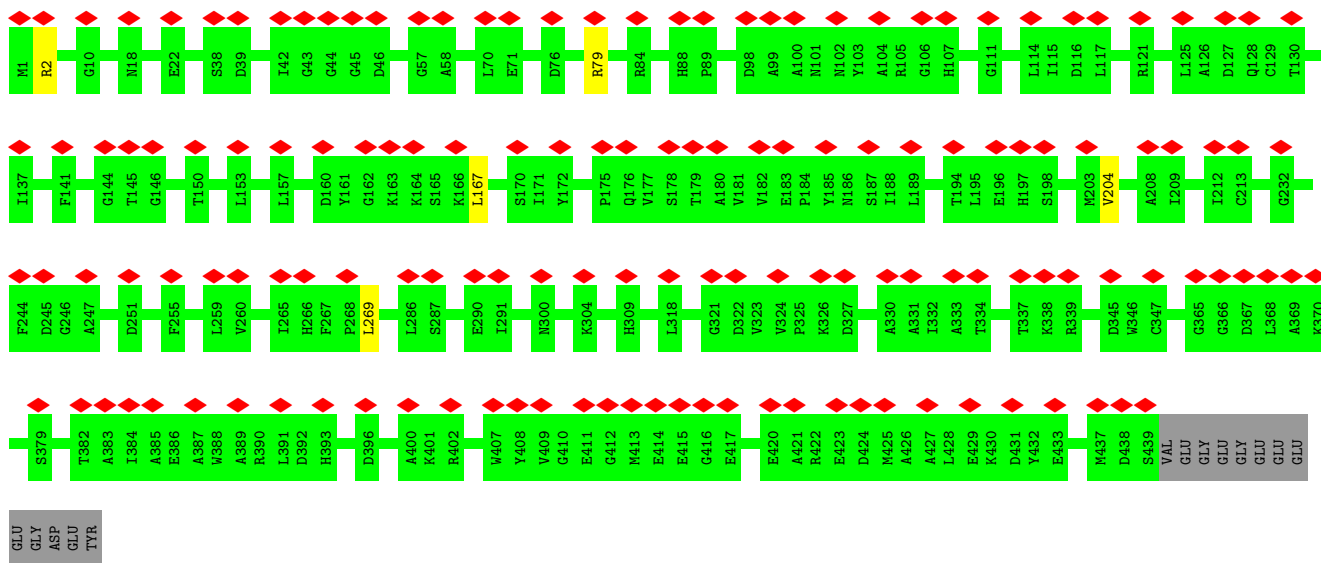


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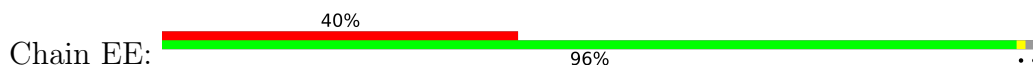


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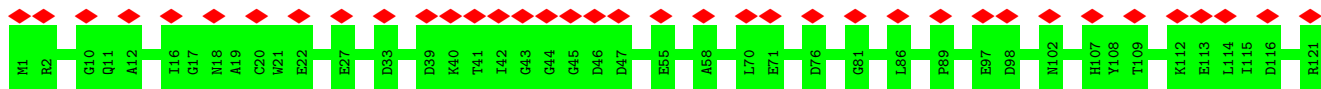


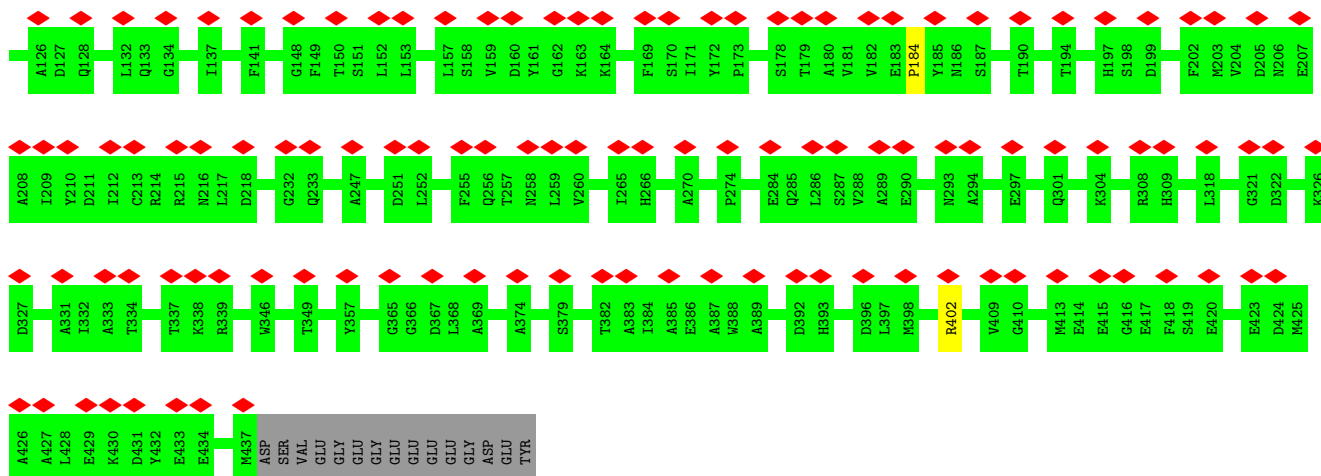


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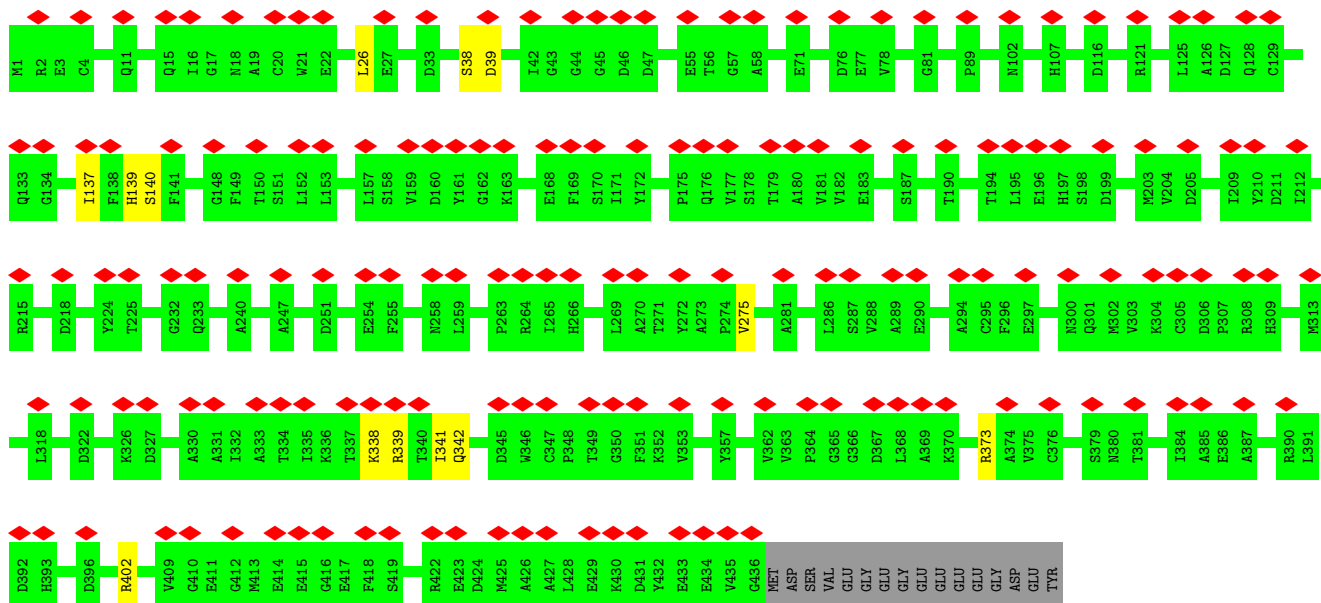


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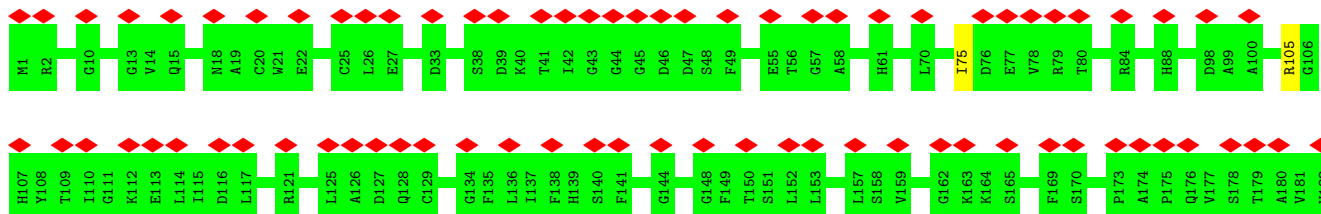
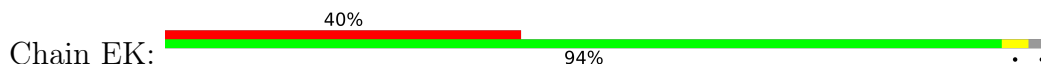


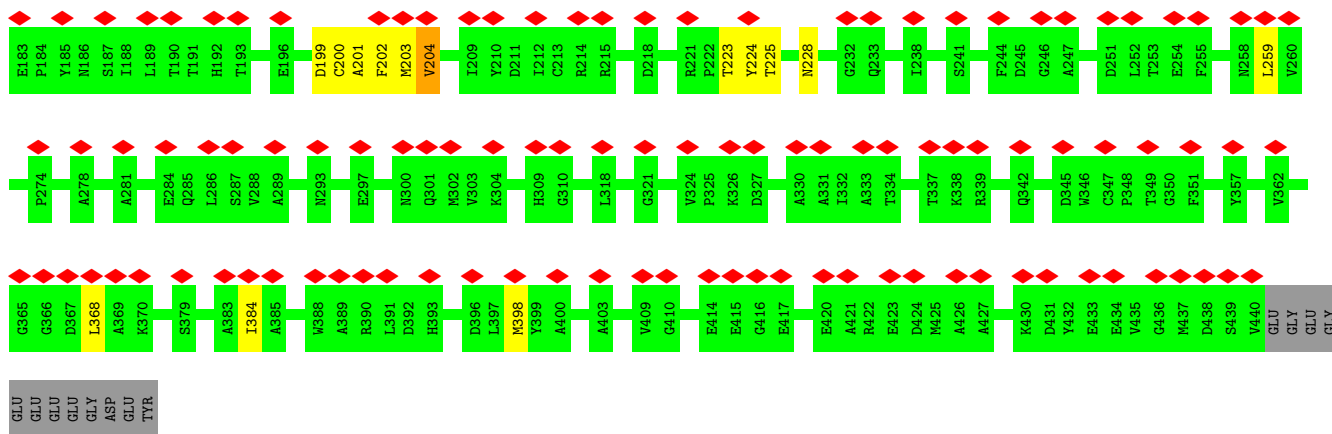


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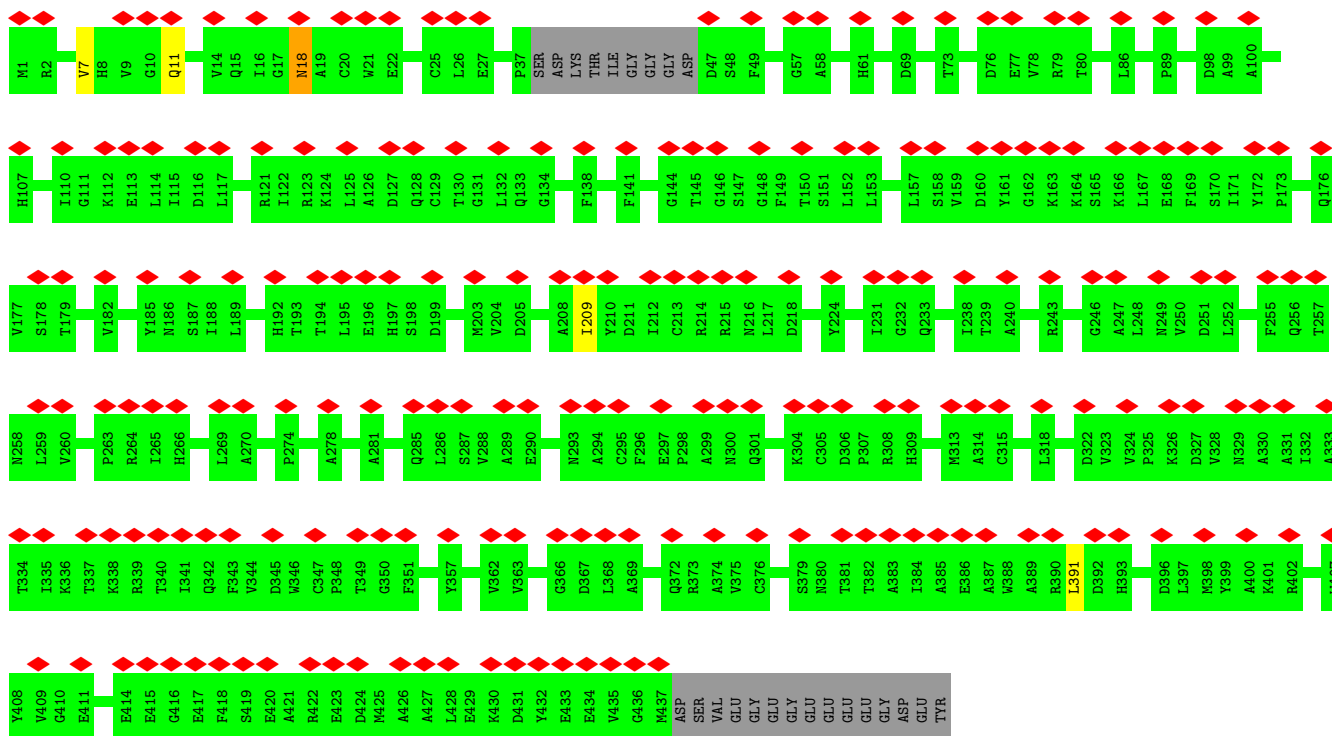


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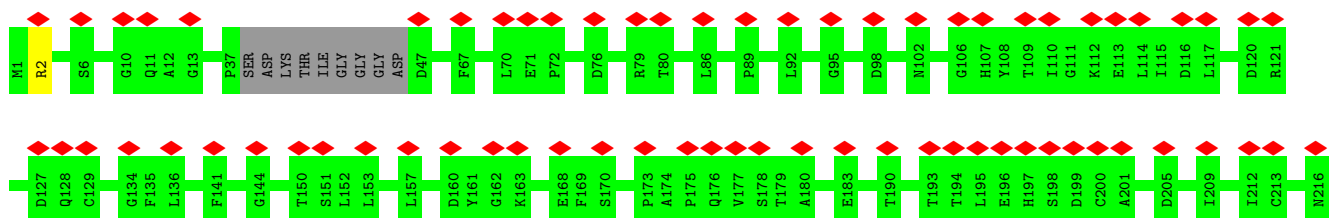


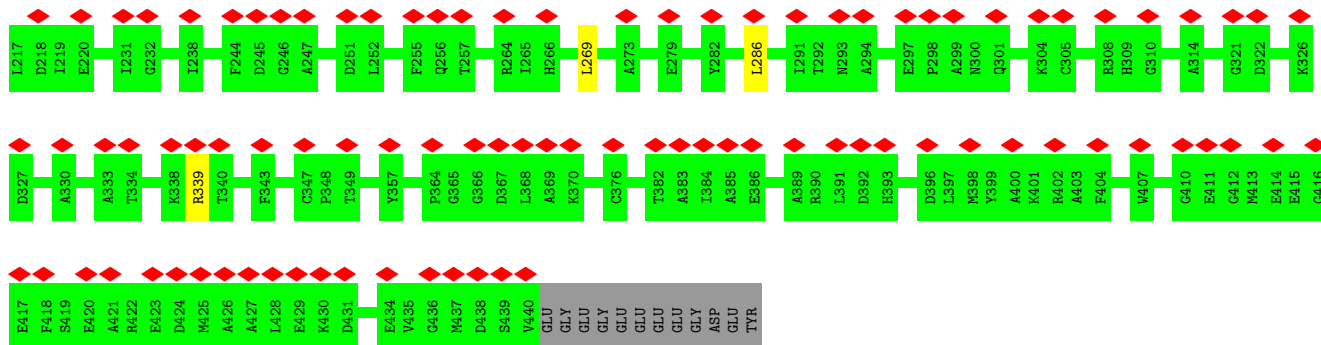


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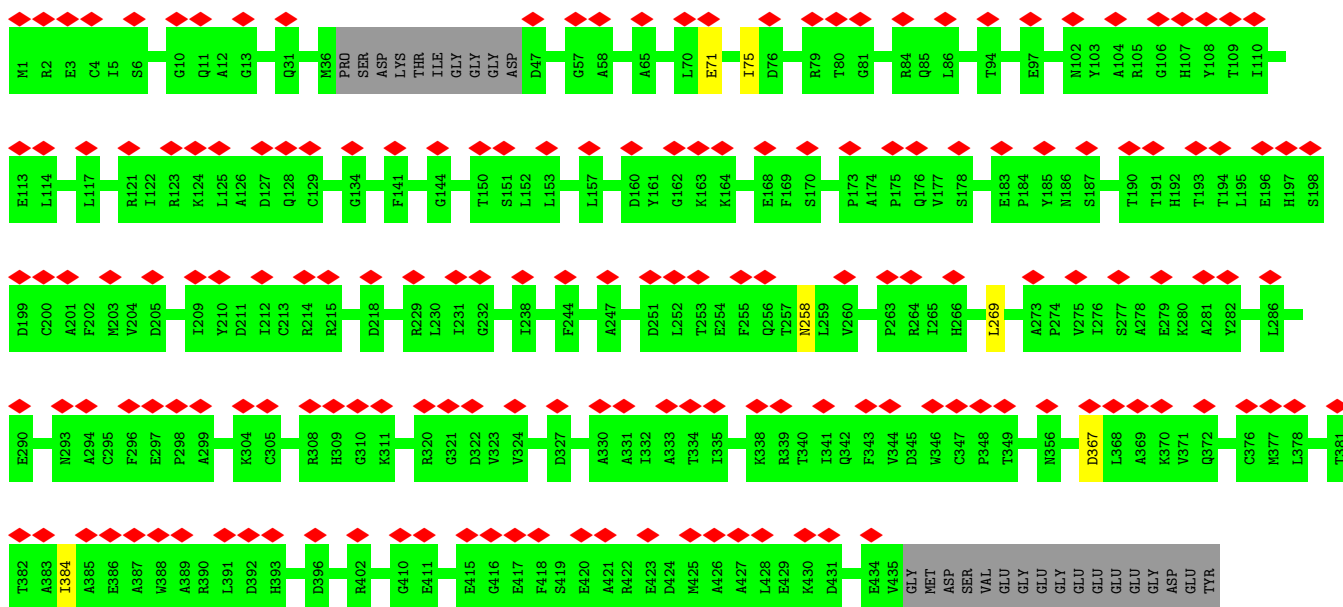
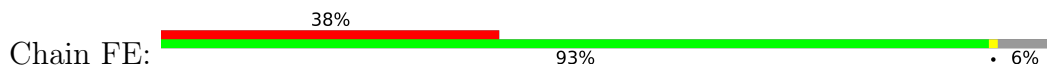


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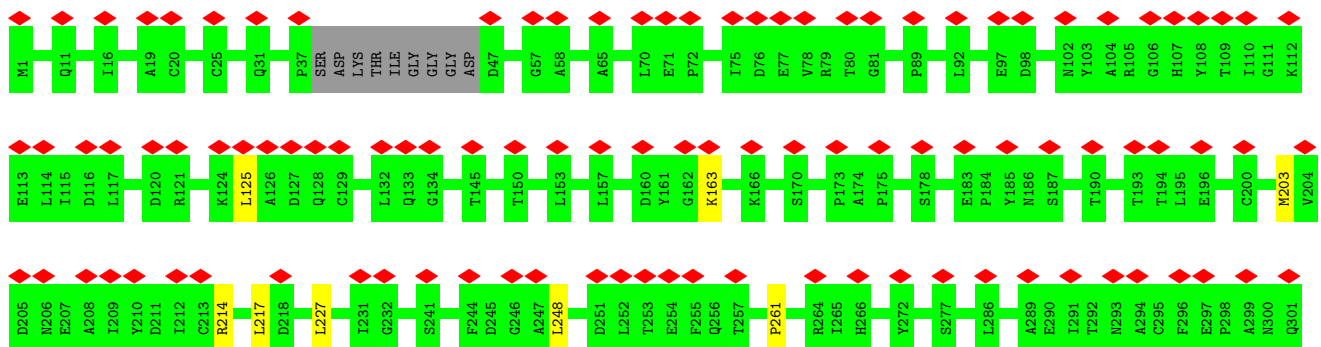


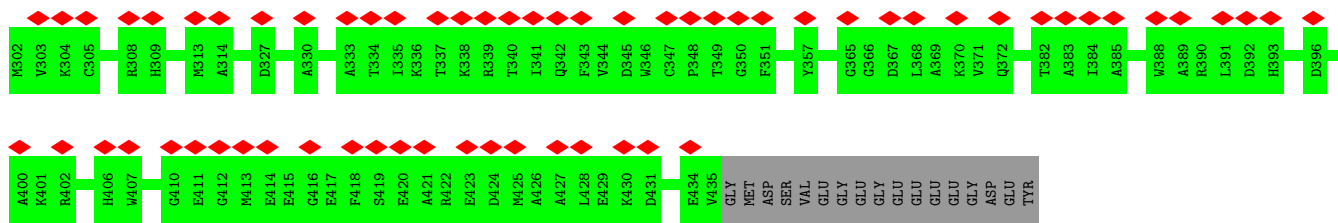


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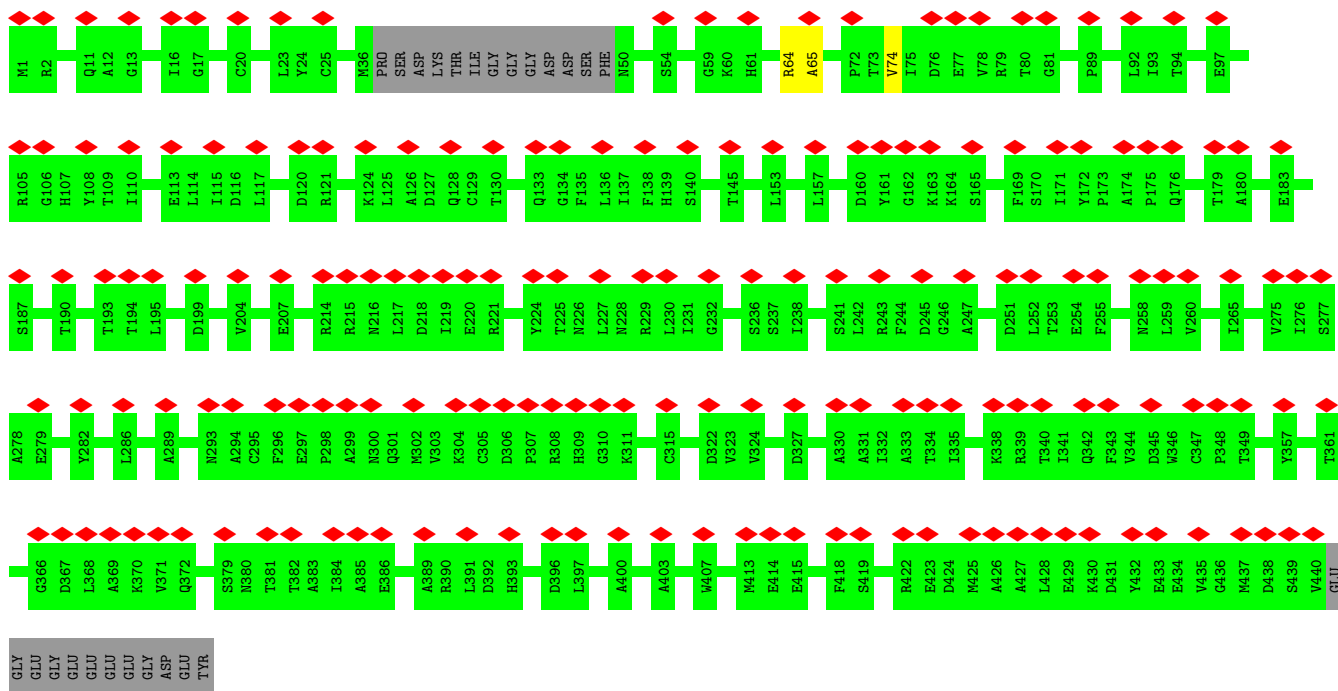
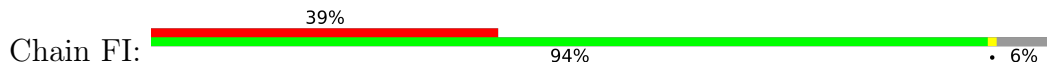


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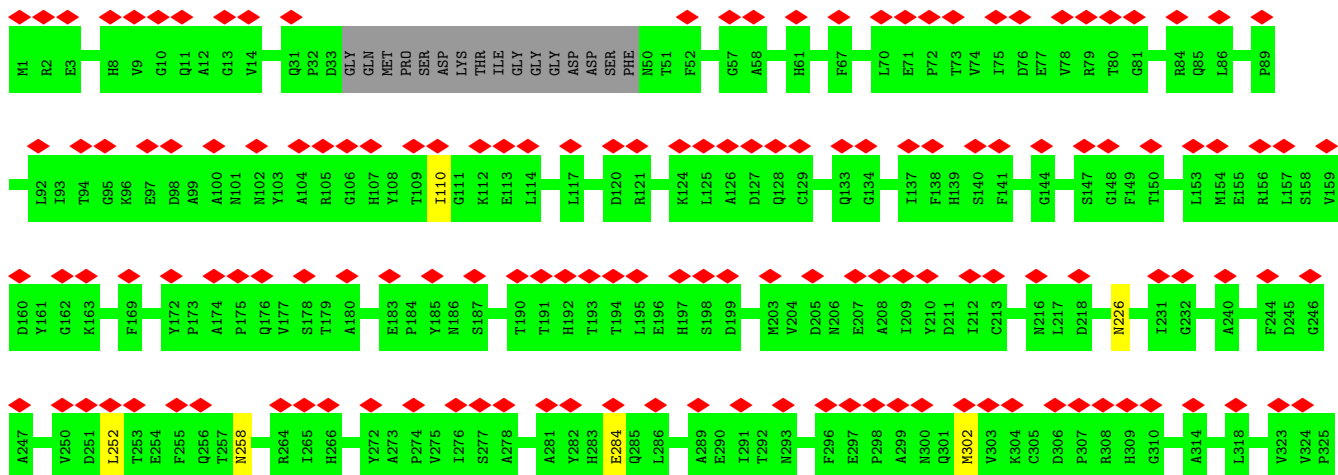


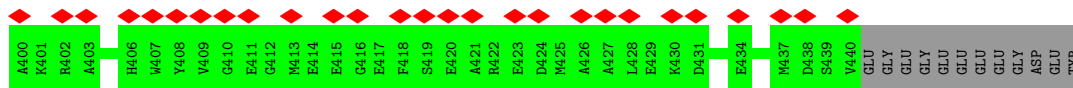
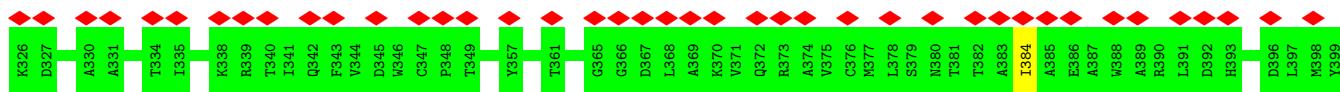


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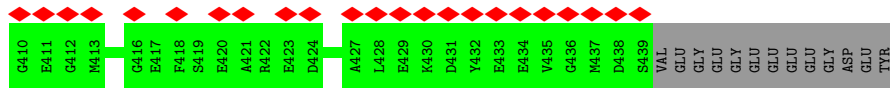
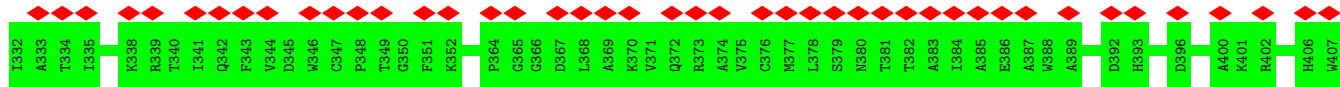
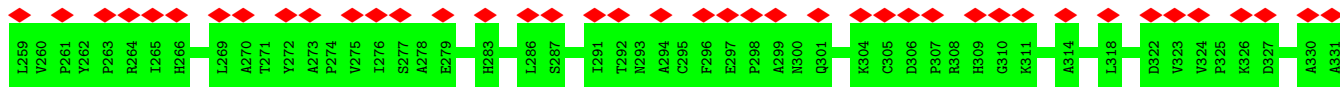
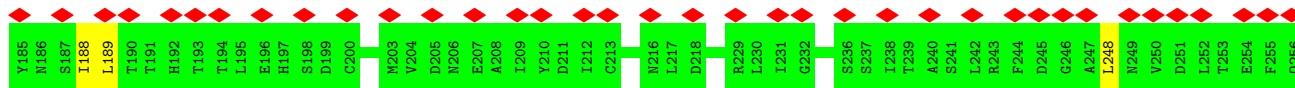
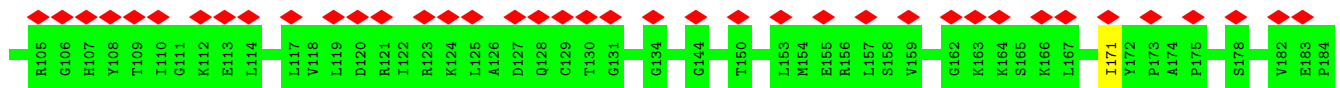
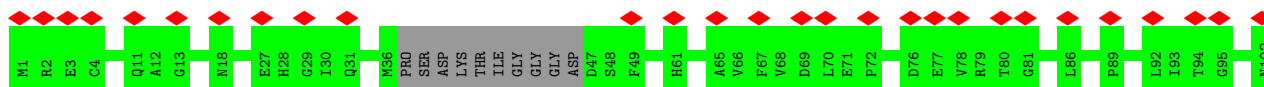


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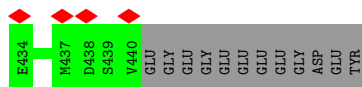
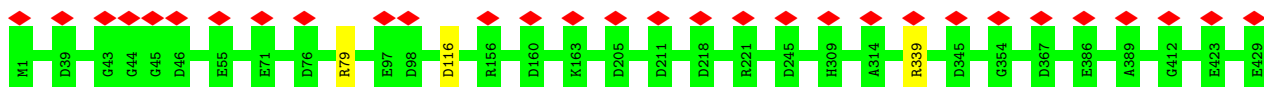




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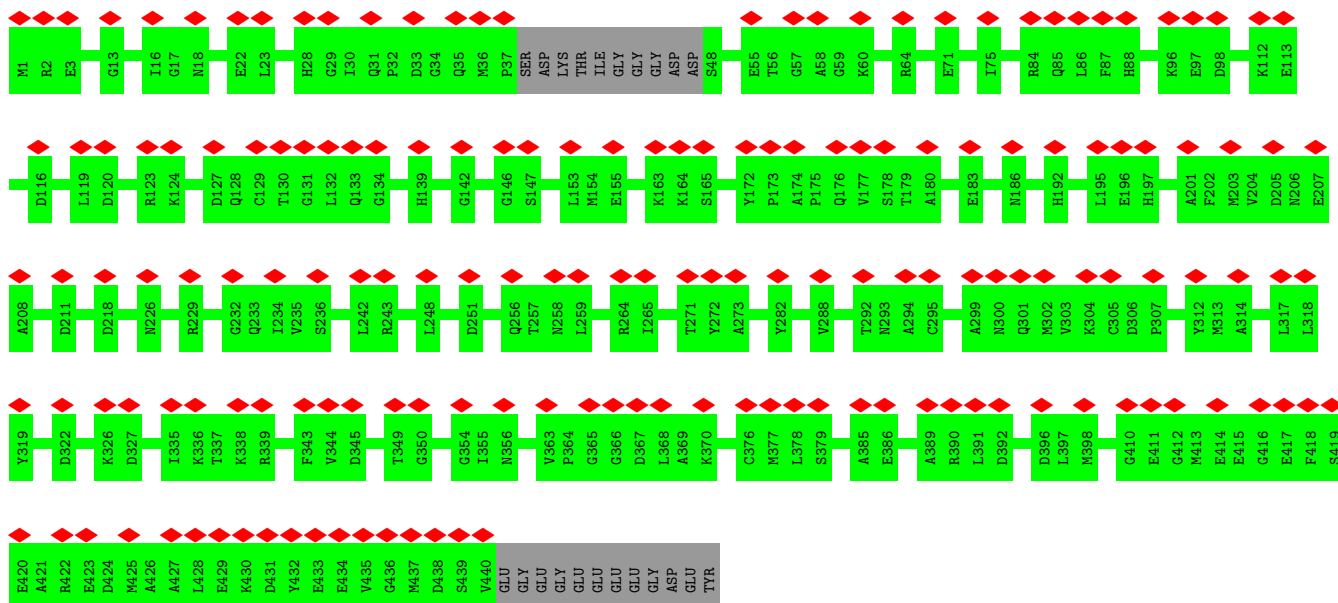
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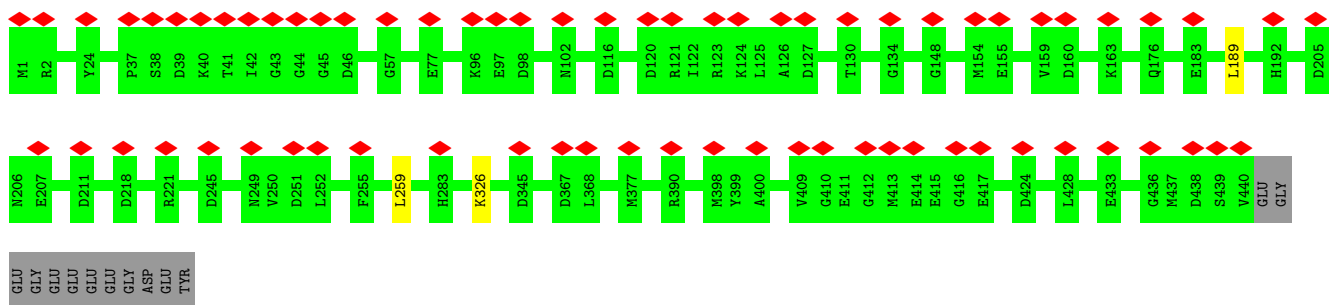
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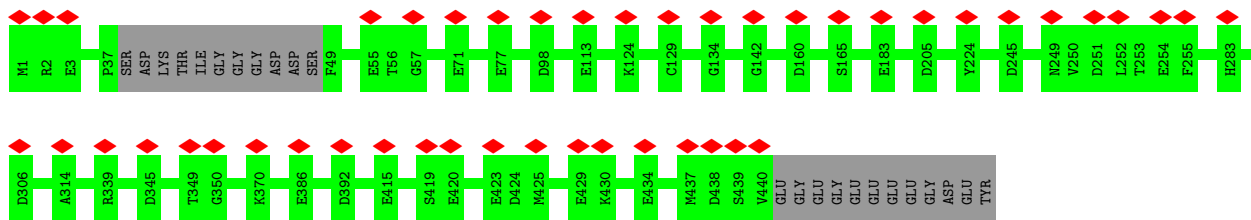




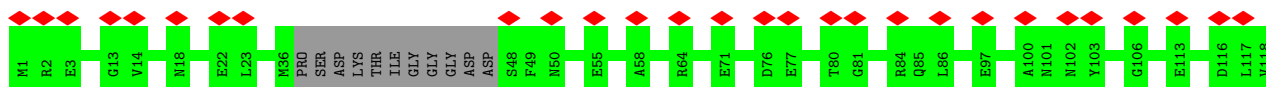
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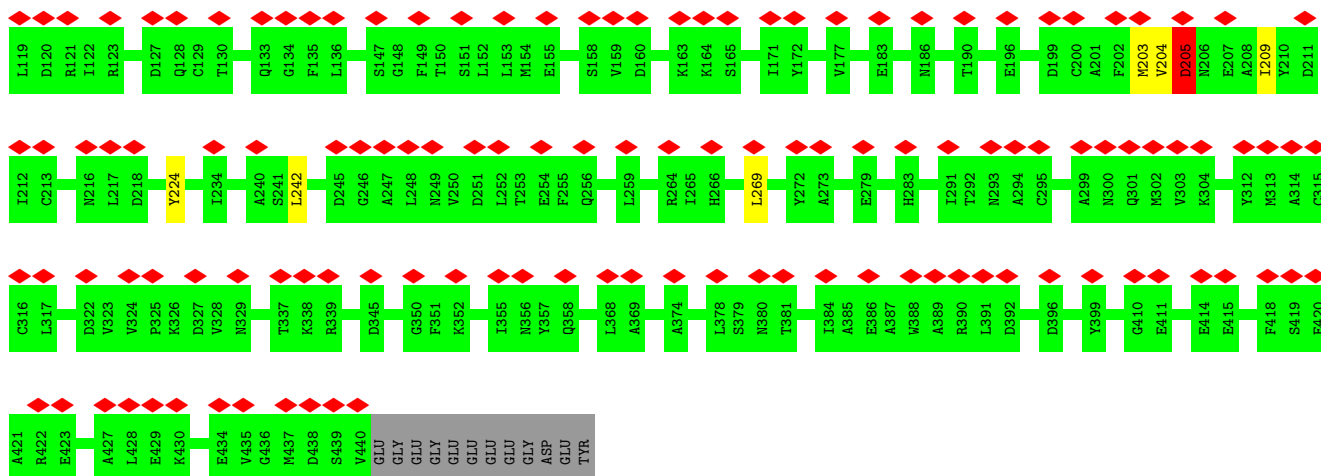


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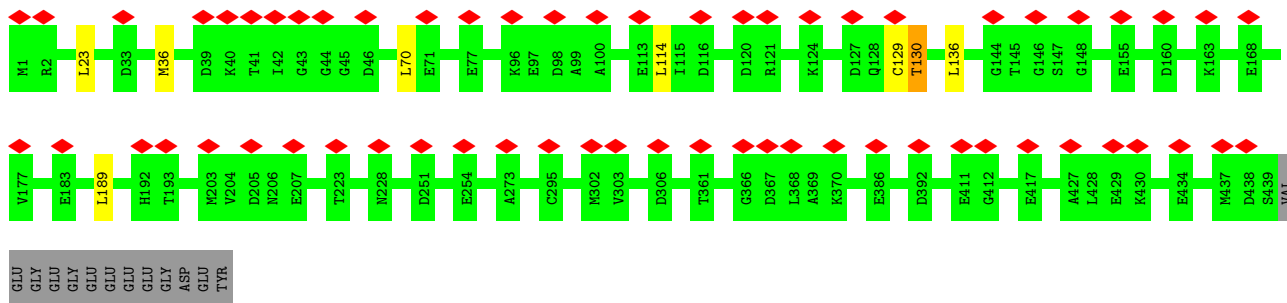


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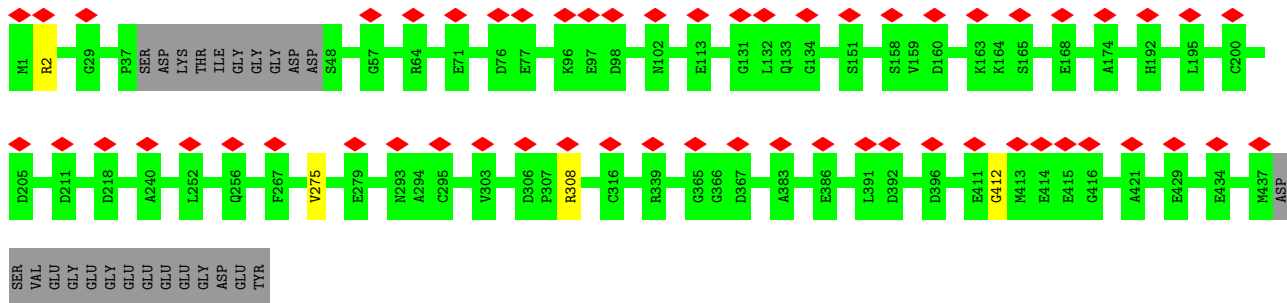




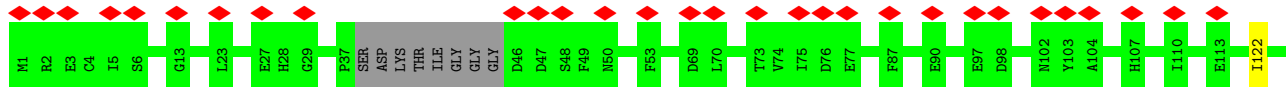
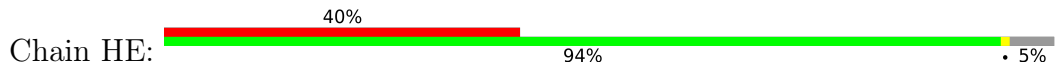
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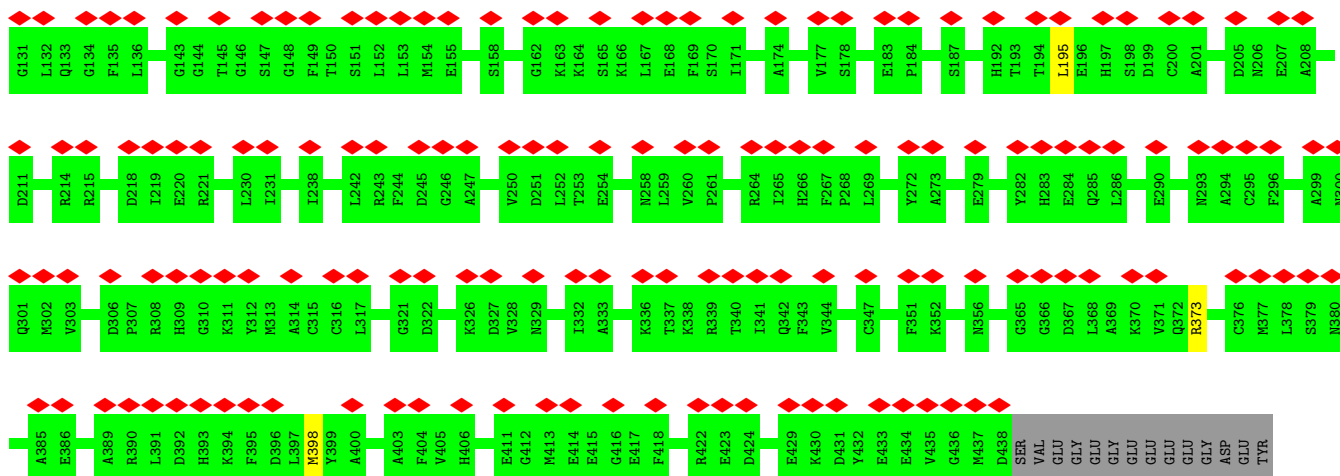


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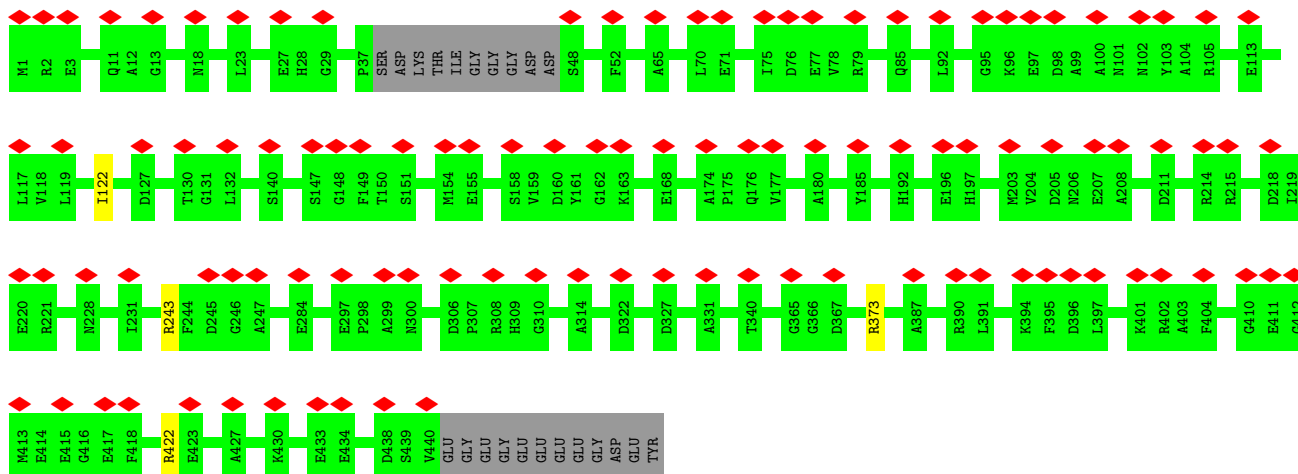
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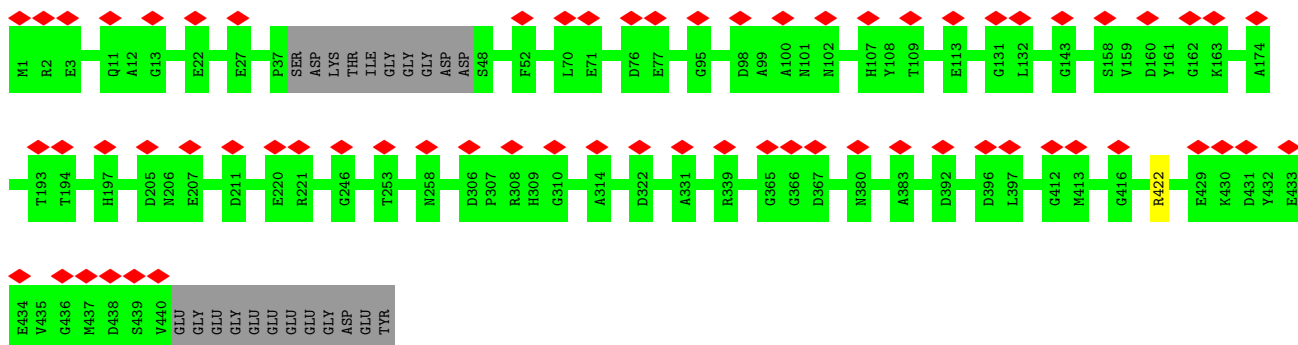
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Chain HG: 24% 94% 5%

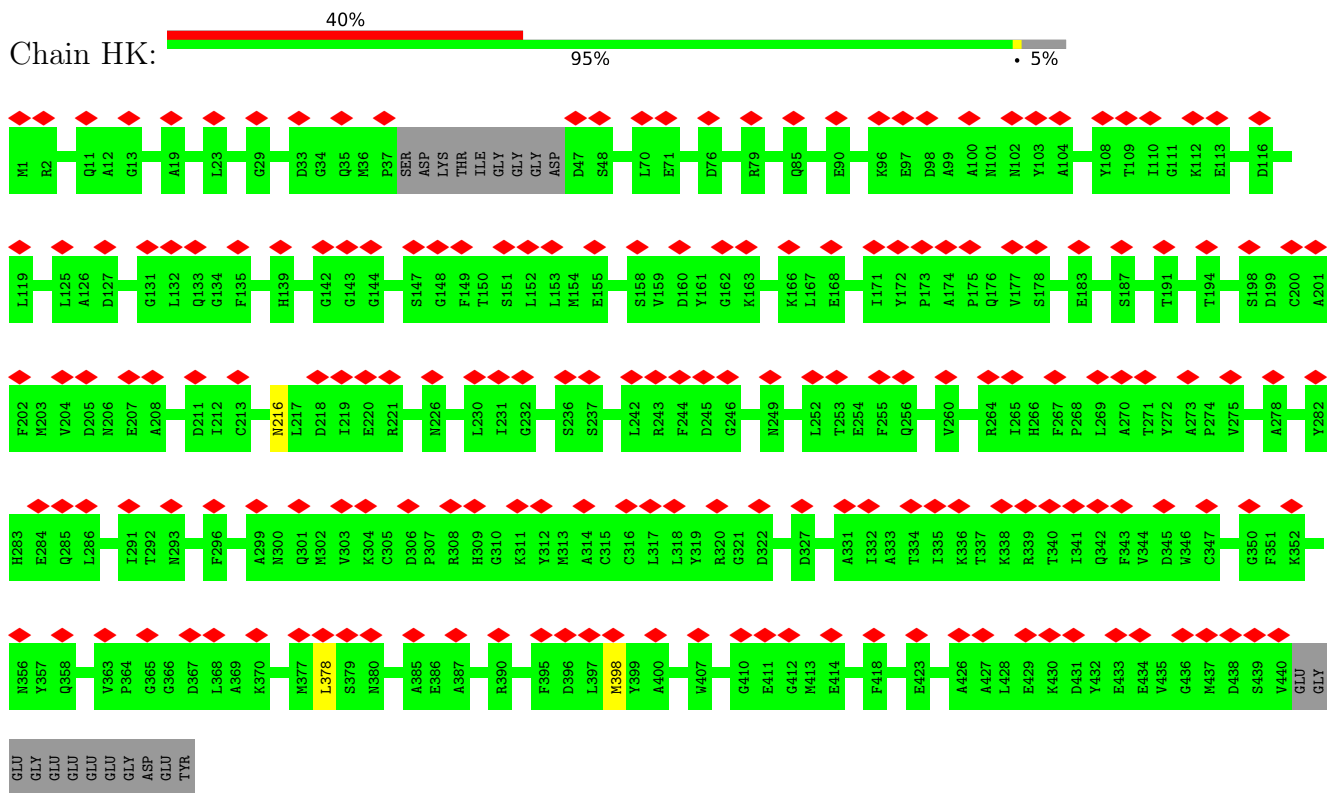


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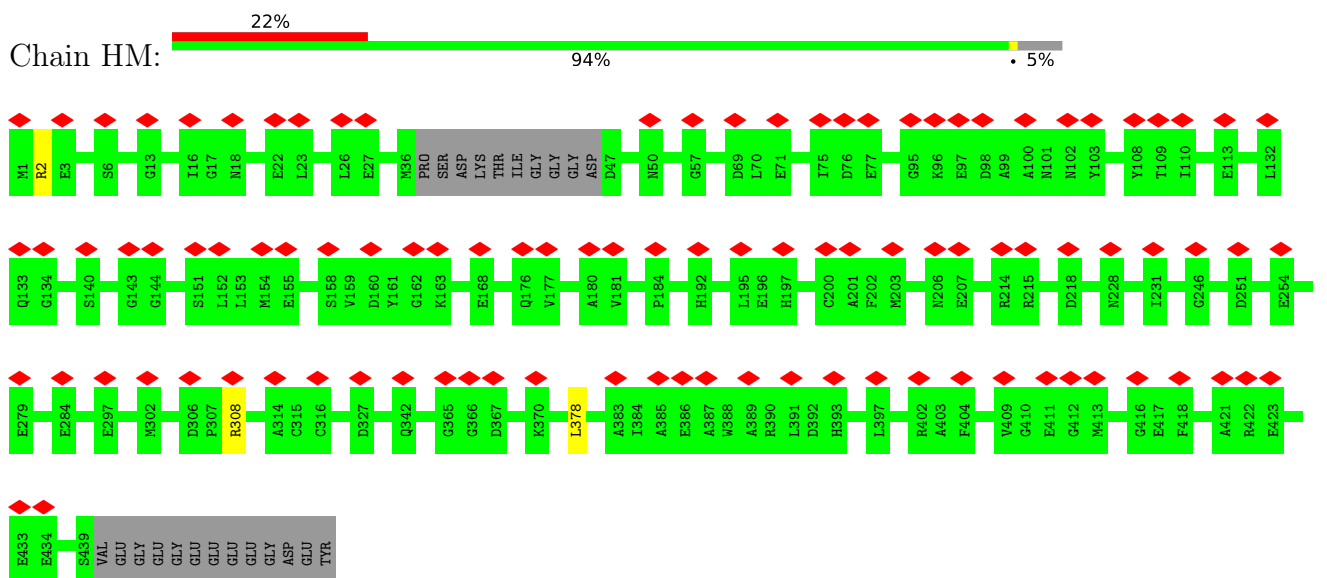
Chain HI: 15% 95% 5%



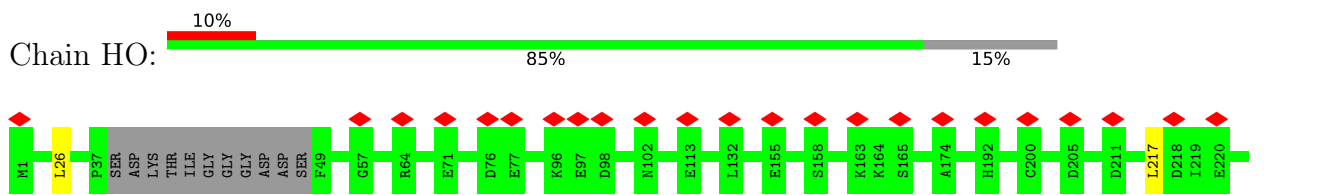
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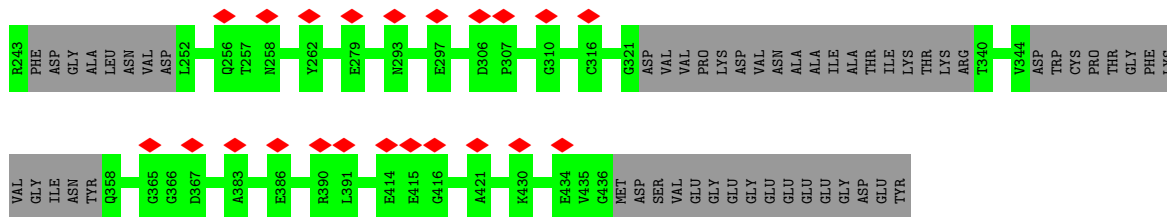


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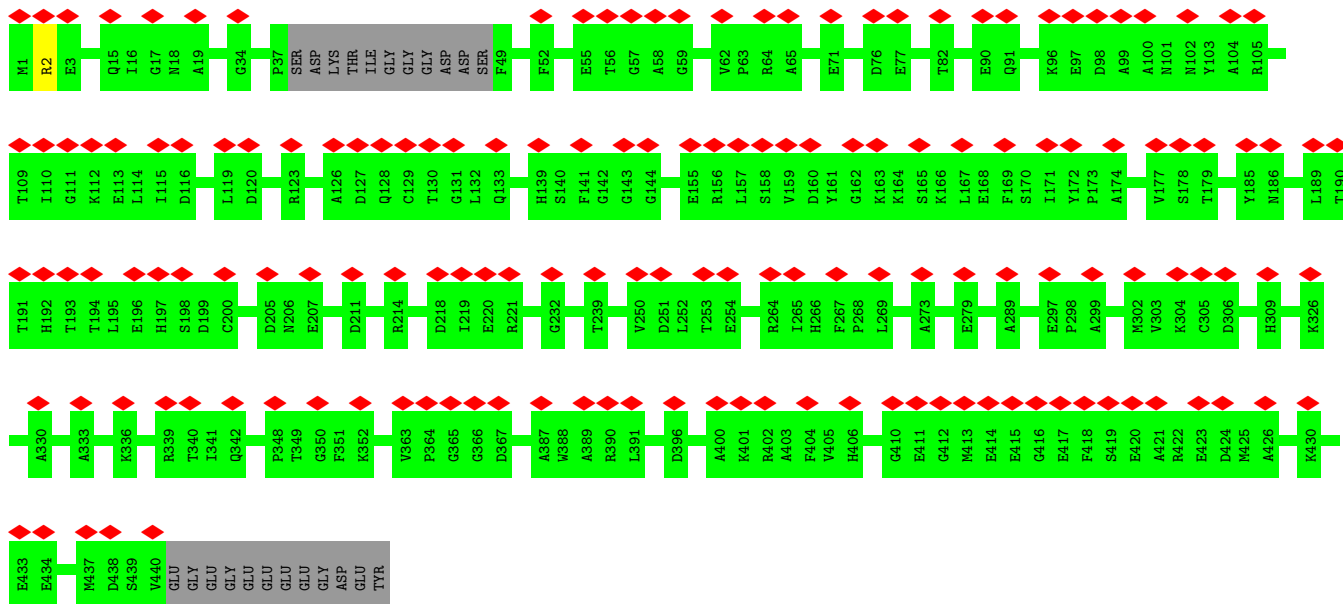


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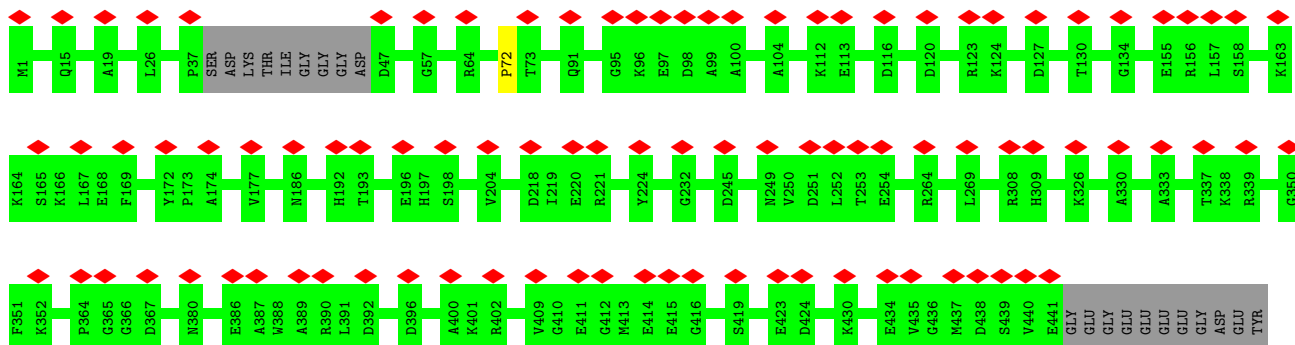




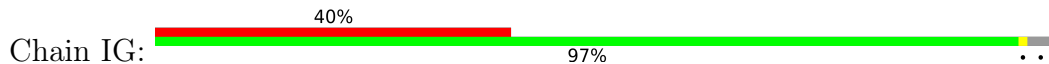
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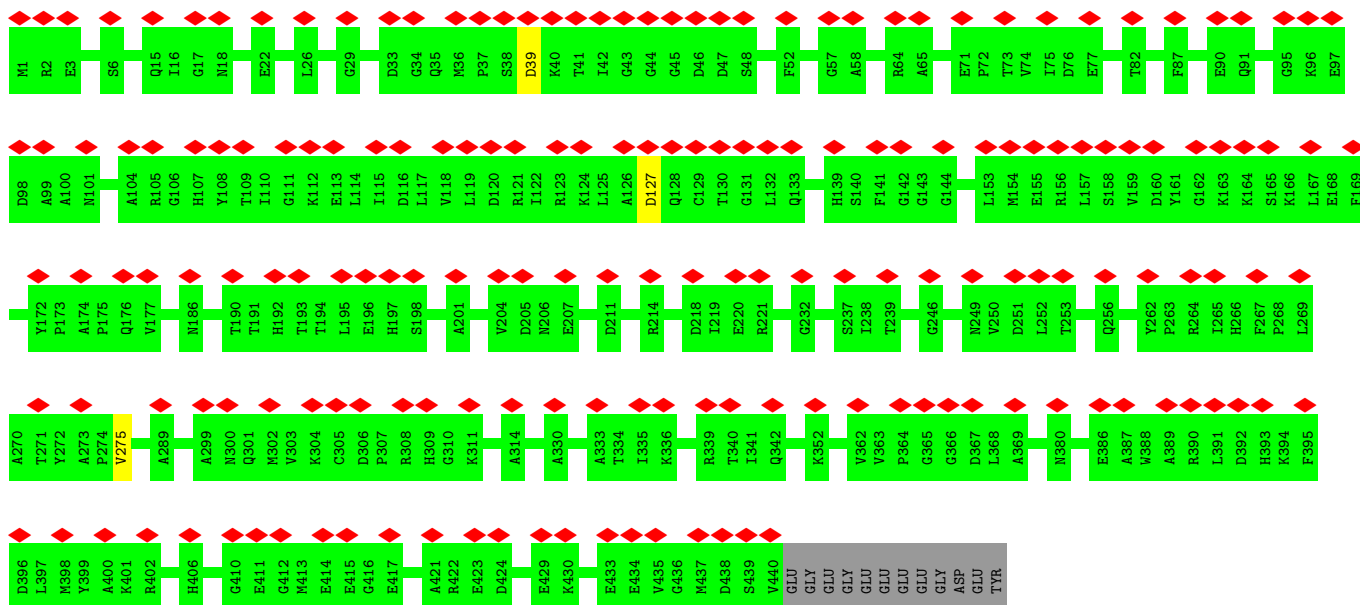


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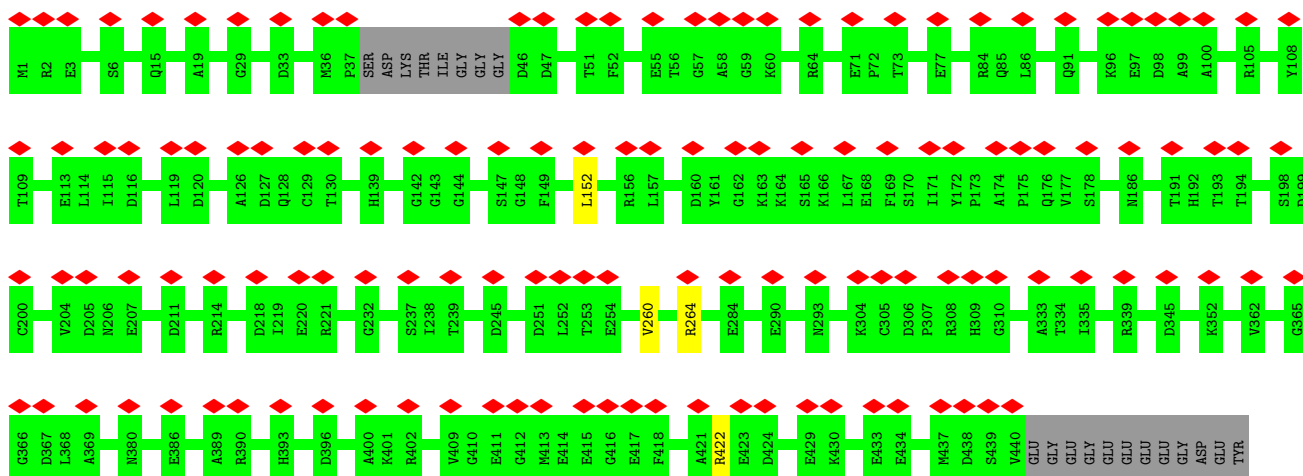
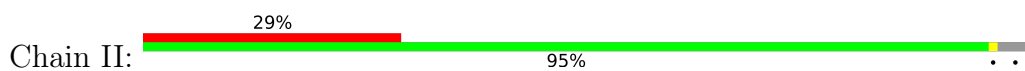


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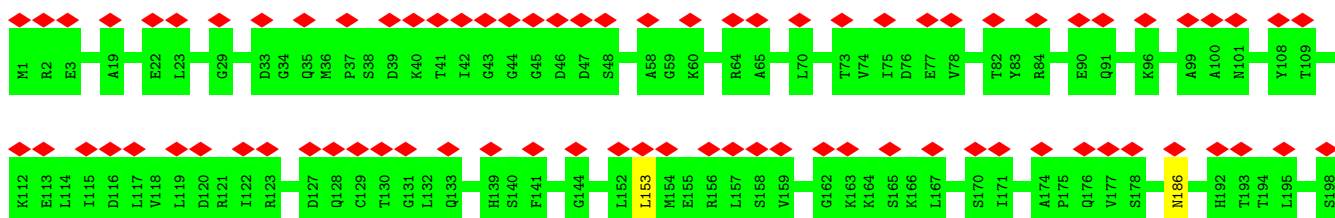
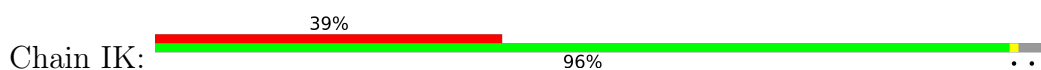


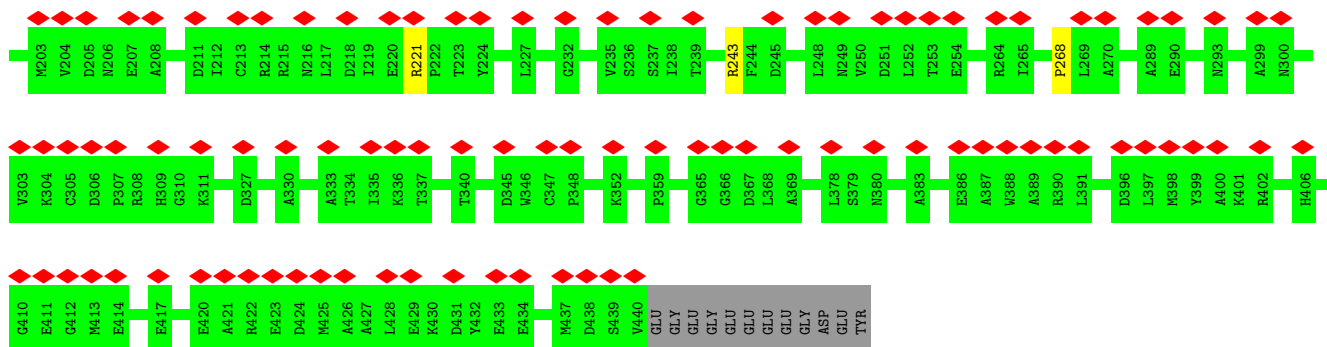


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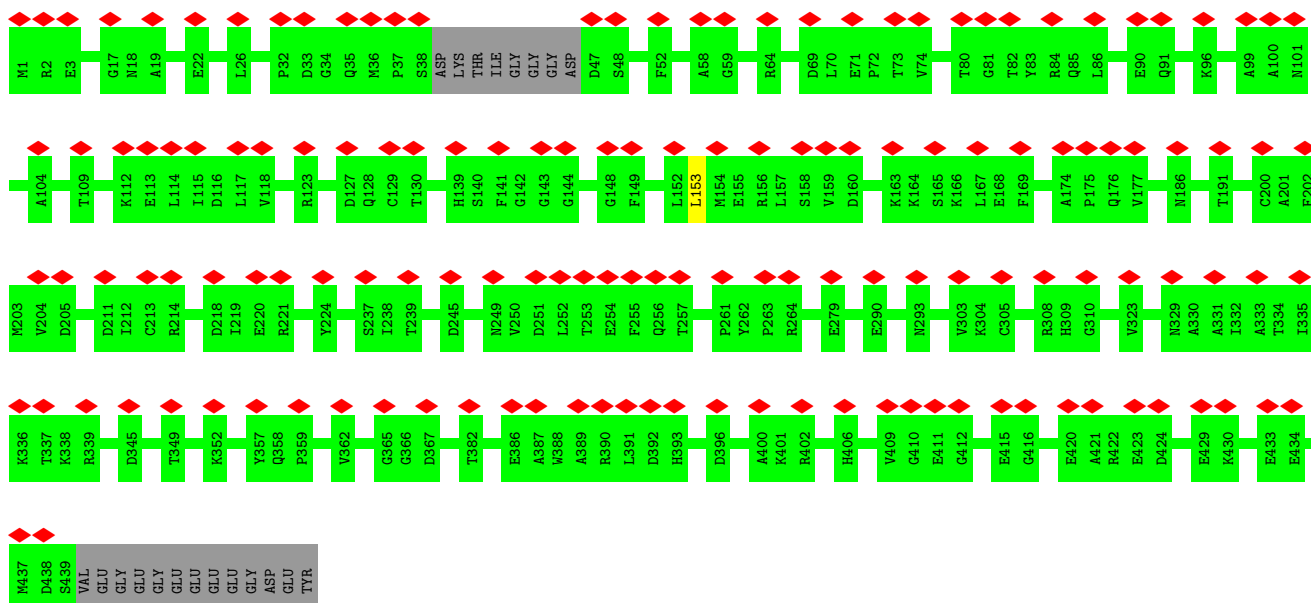


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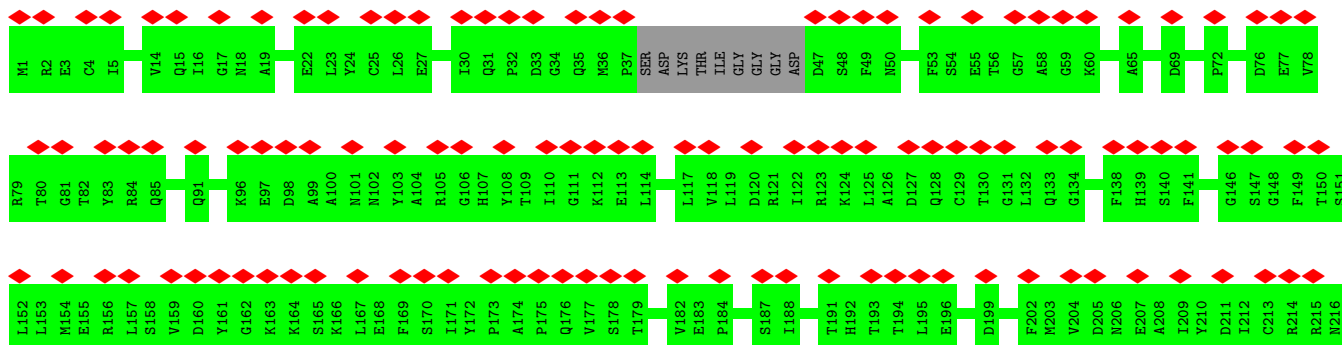


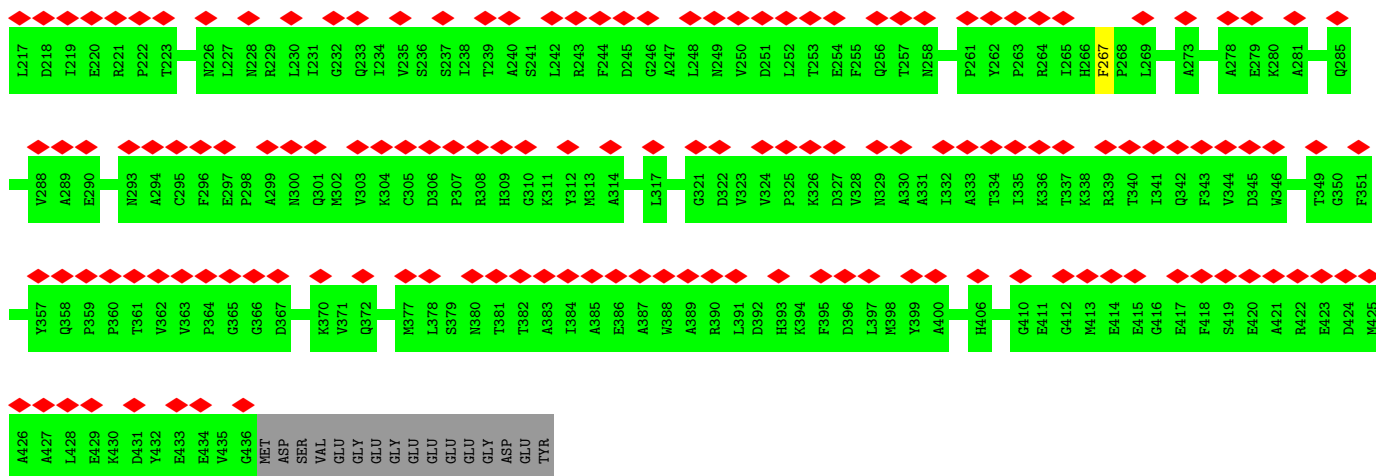


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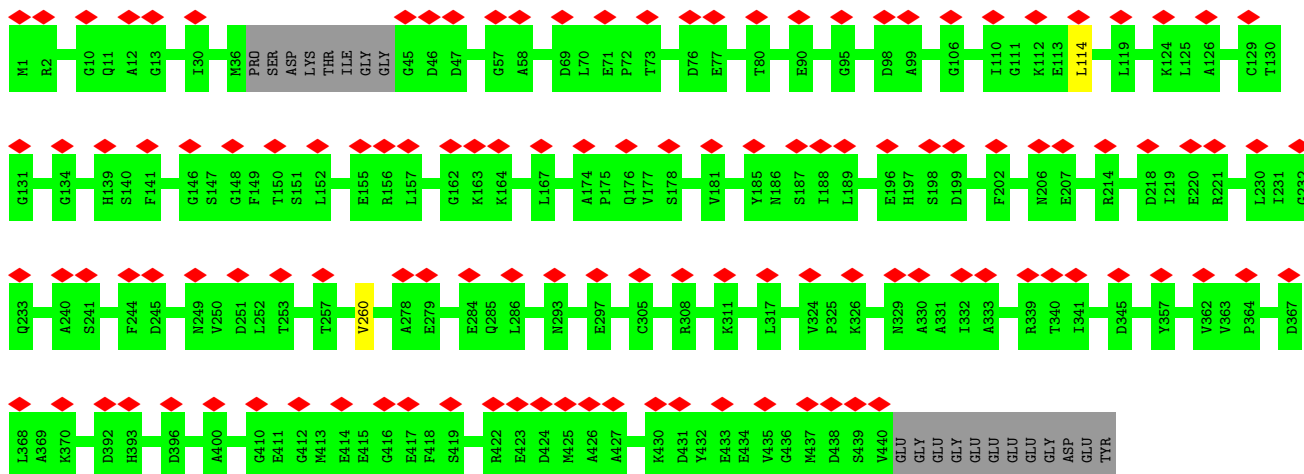


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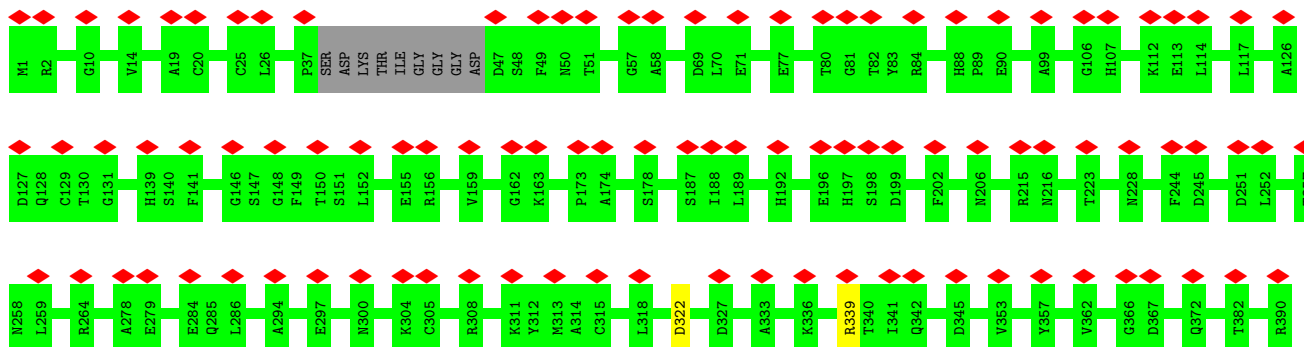




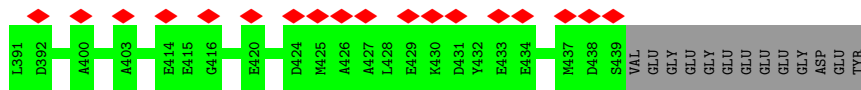
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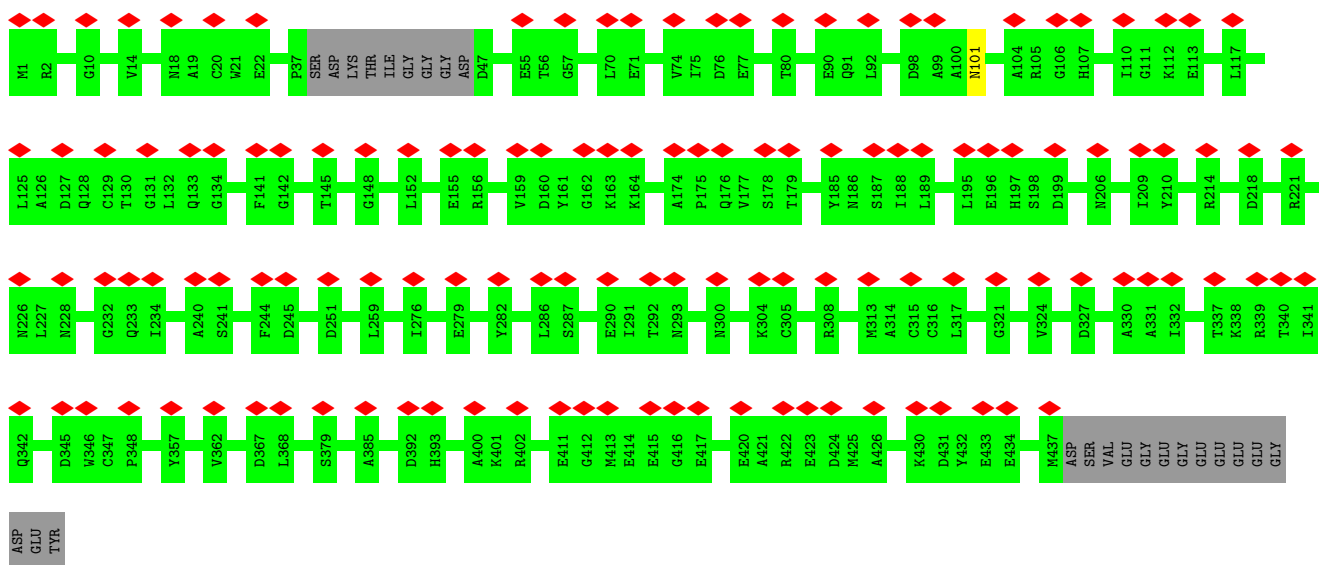
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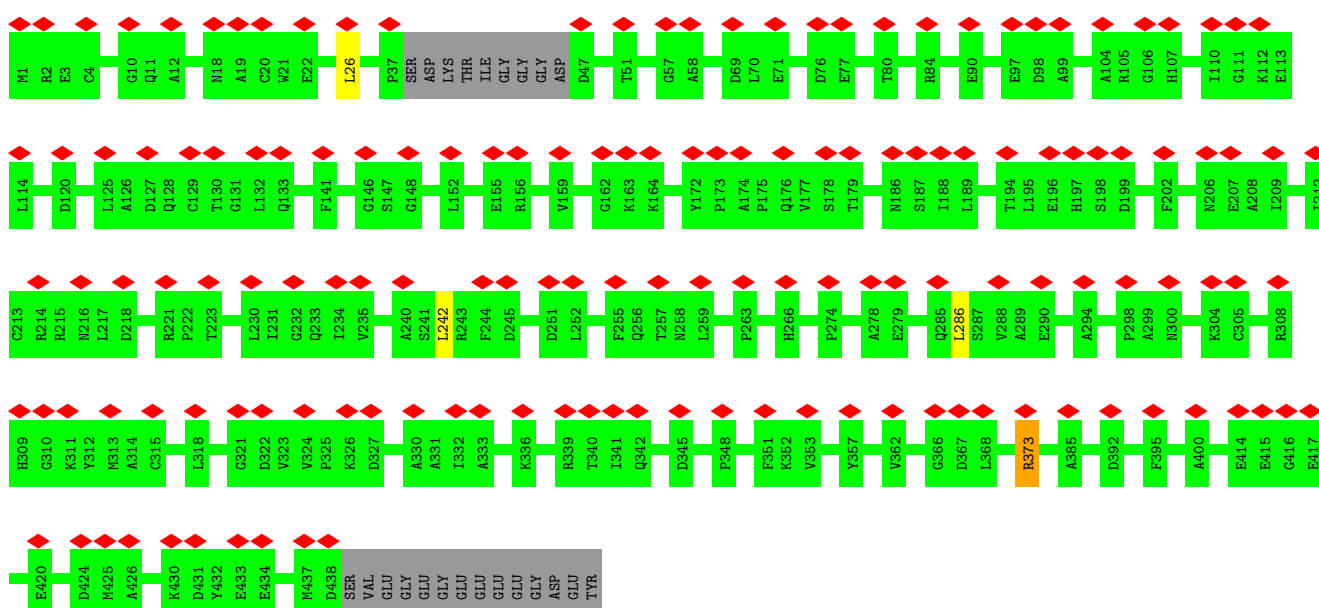
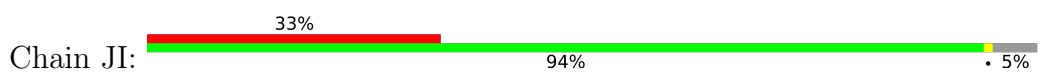




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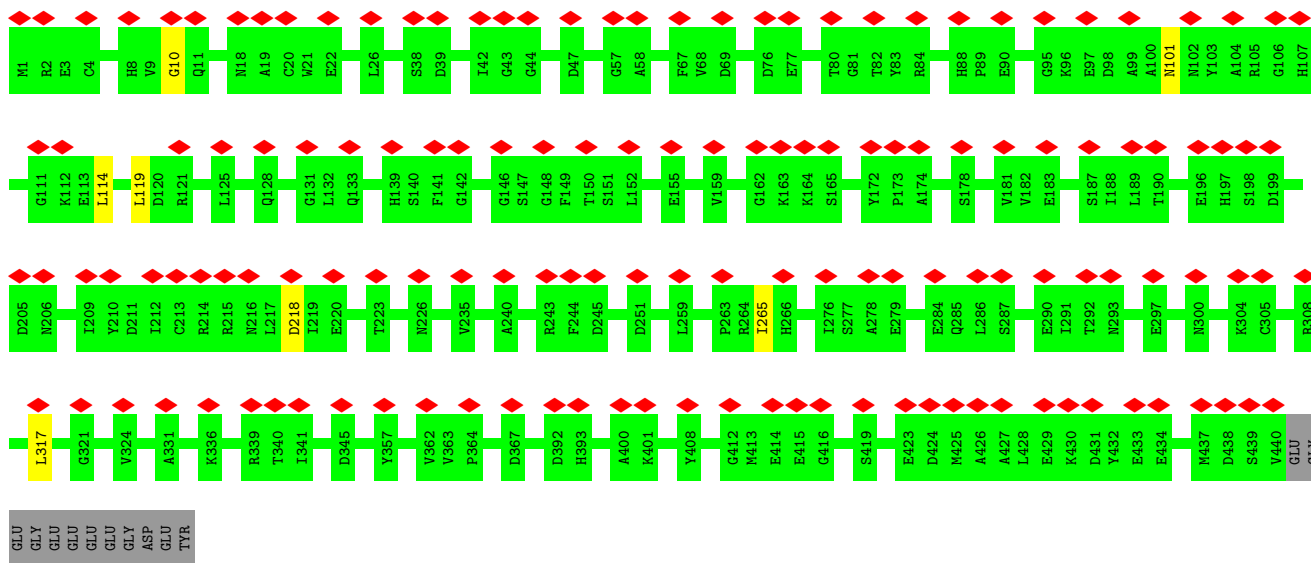


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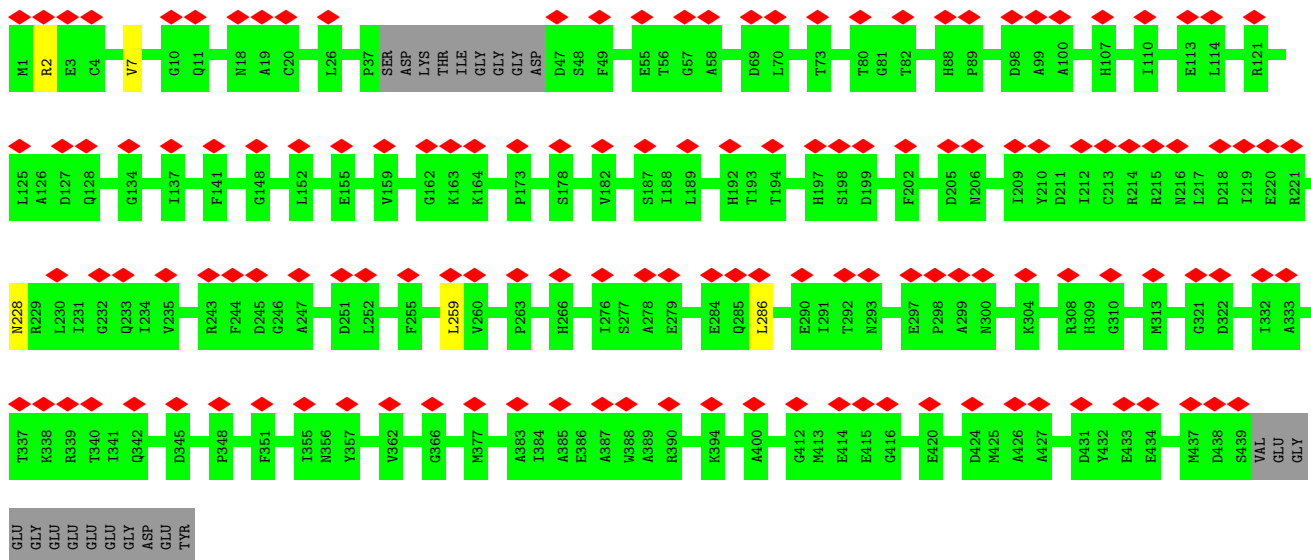


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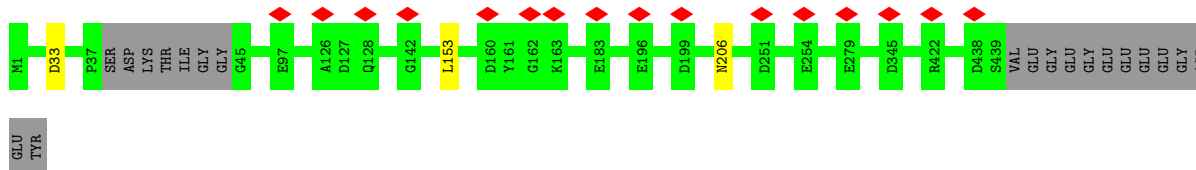




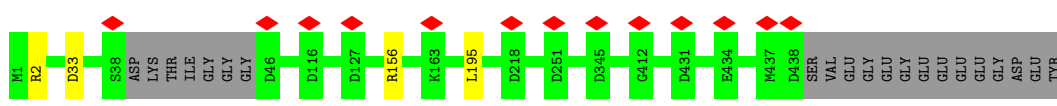
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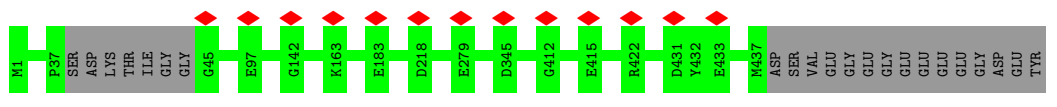
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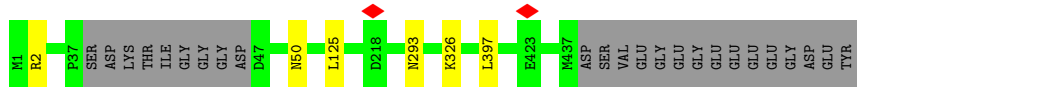
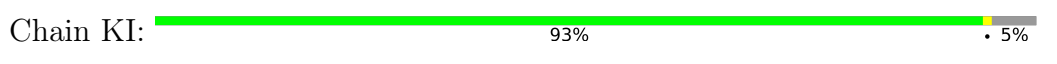
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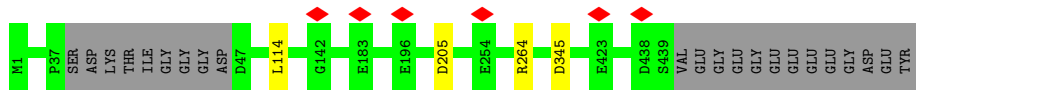
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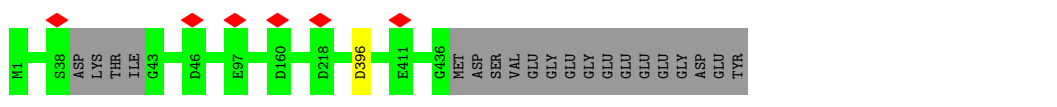
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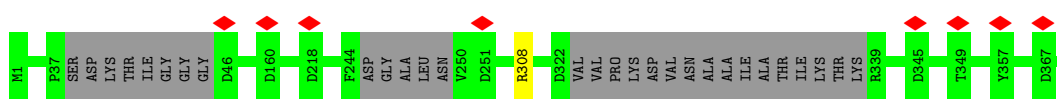
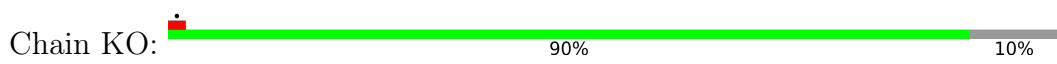
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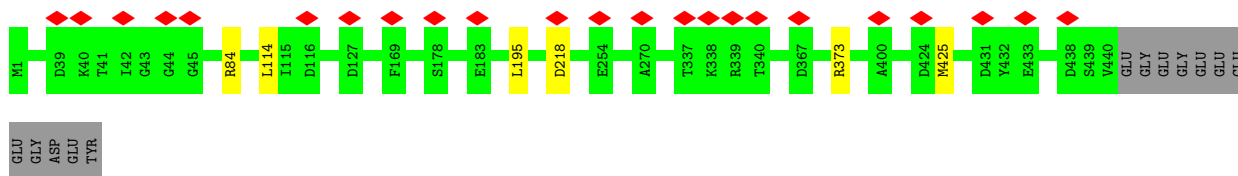


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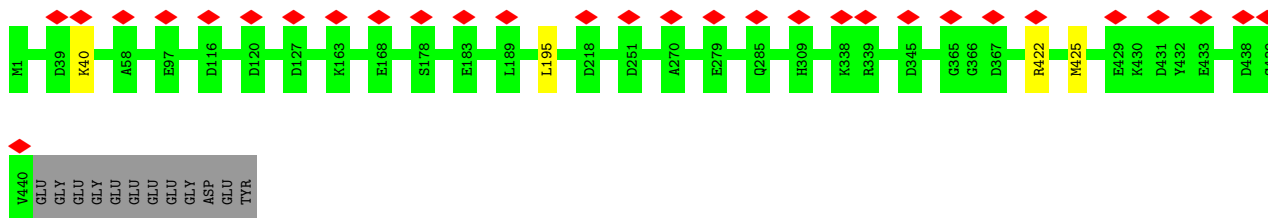


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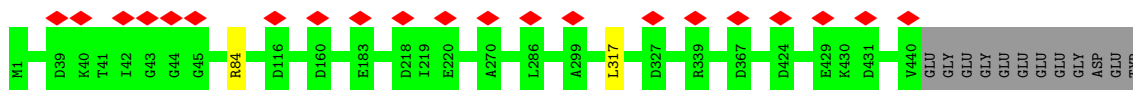




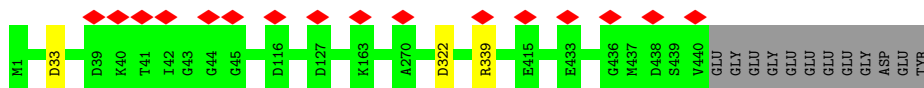
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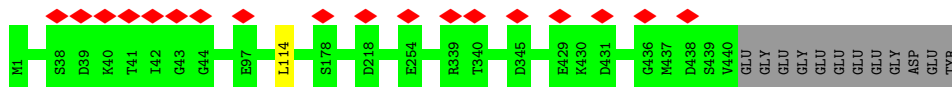
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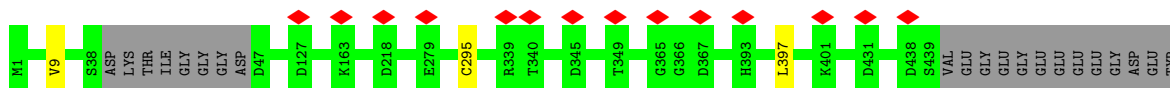
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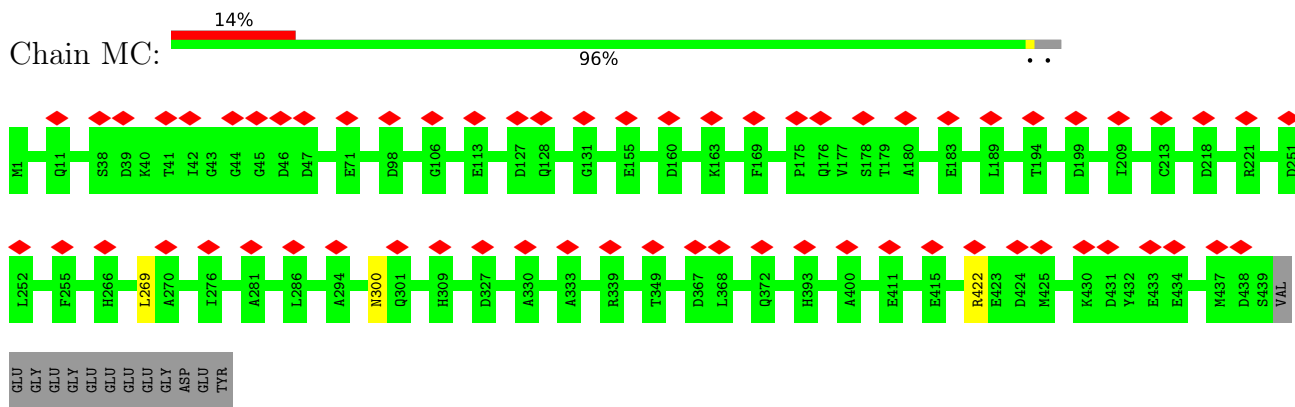
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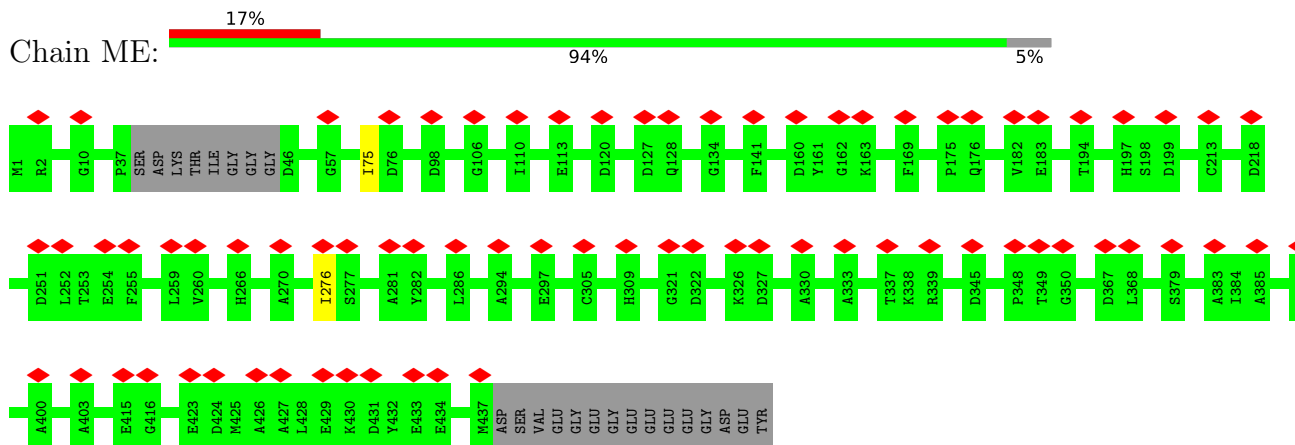
• Molecule 8: Tubulin alpha-1D chain



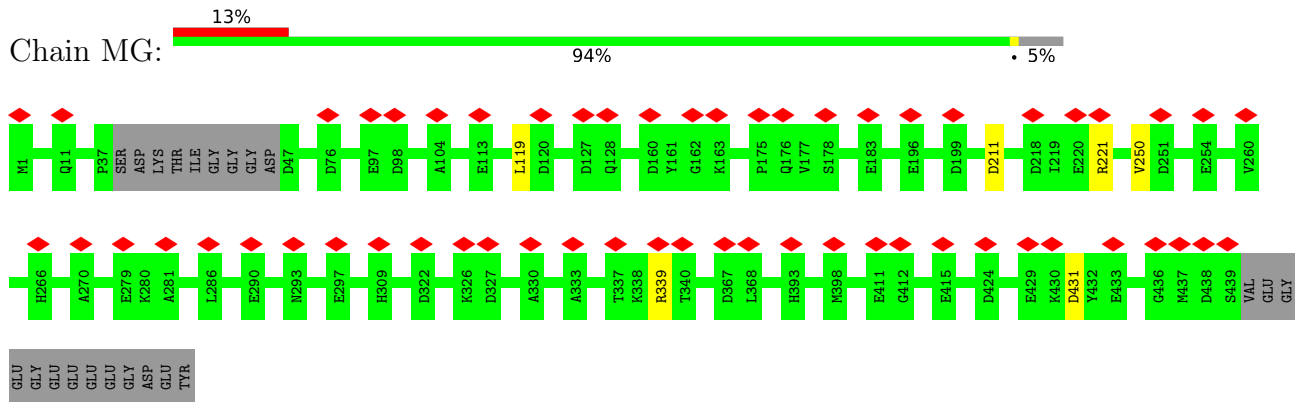
• Molecule 8: Tubulin alpha-1D chain



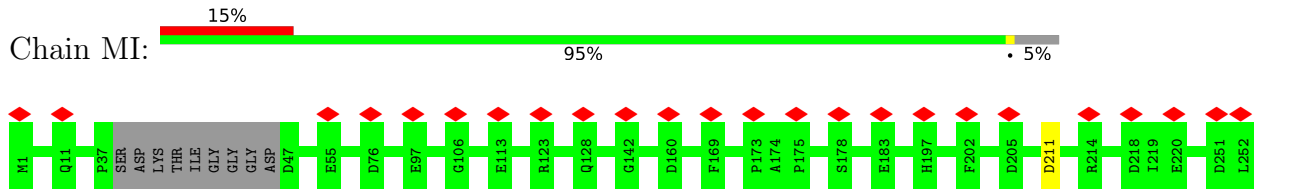
• Molecule 8: Tubulin alpha-1D chain

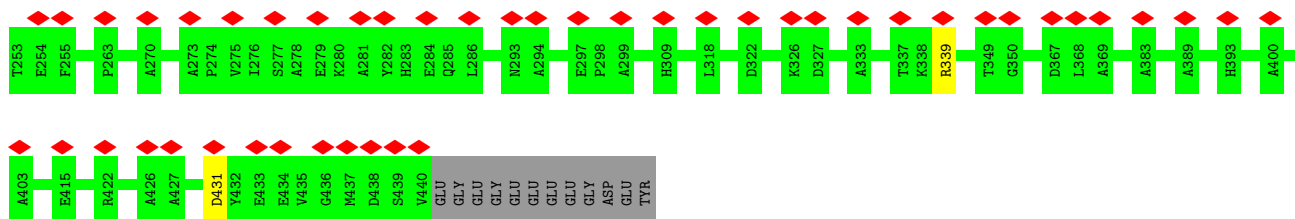


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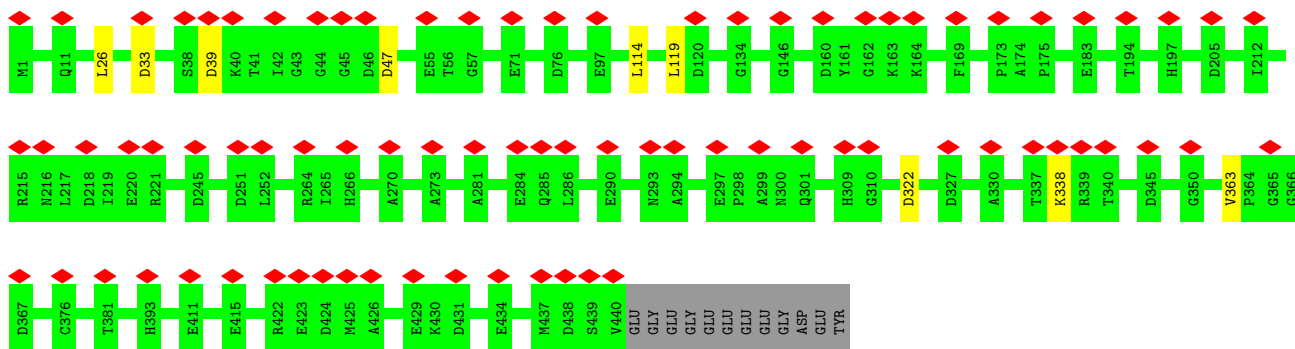


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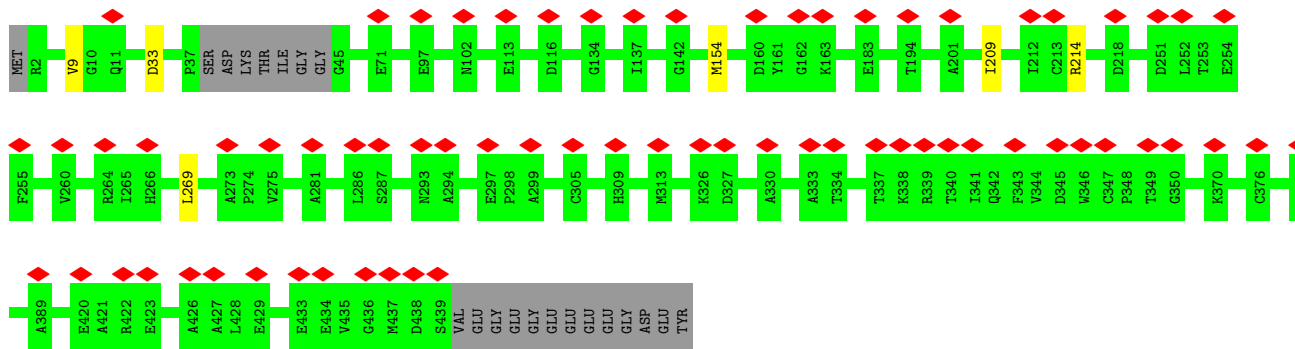




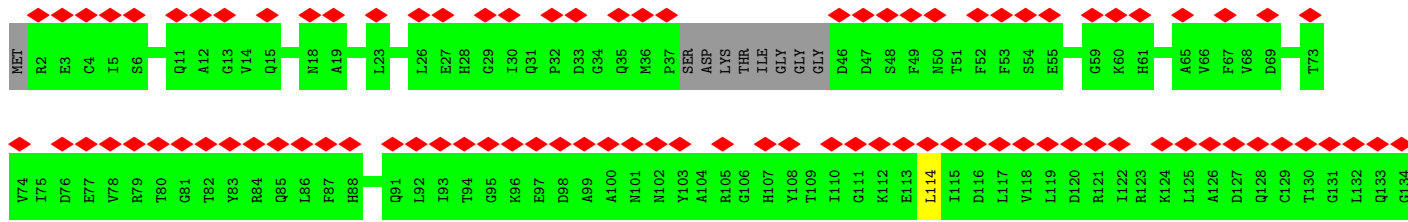
• Molecule 8: Tubulin alpha-1D chain



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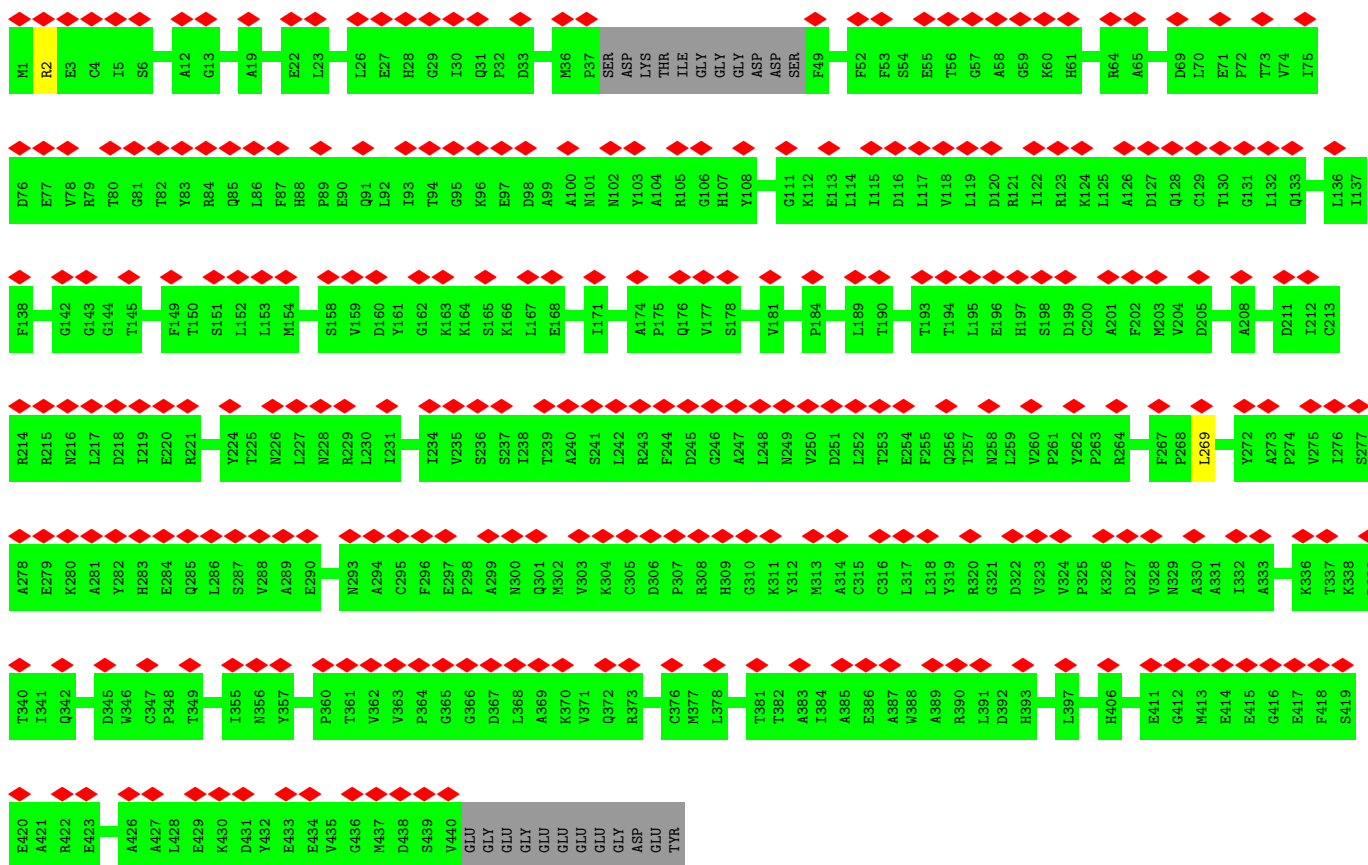


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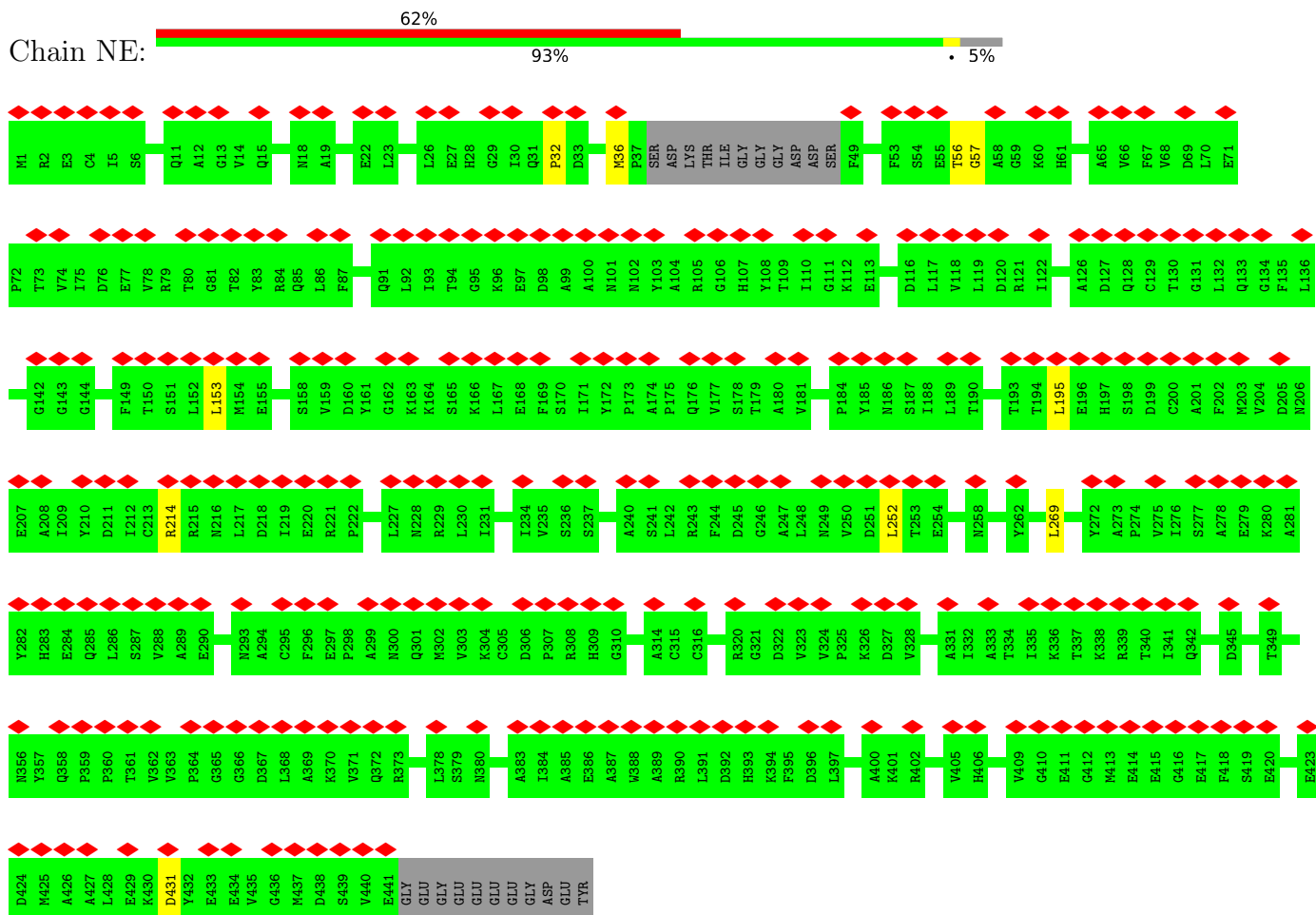




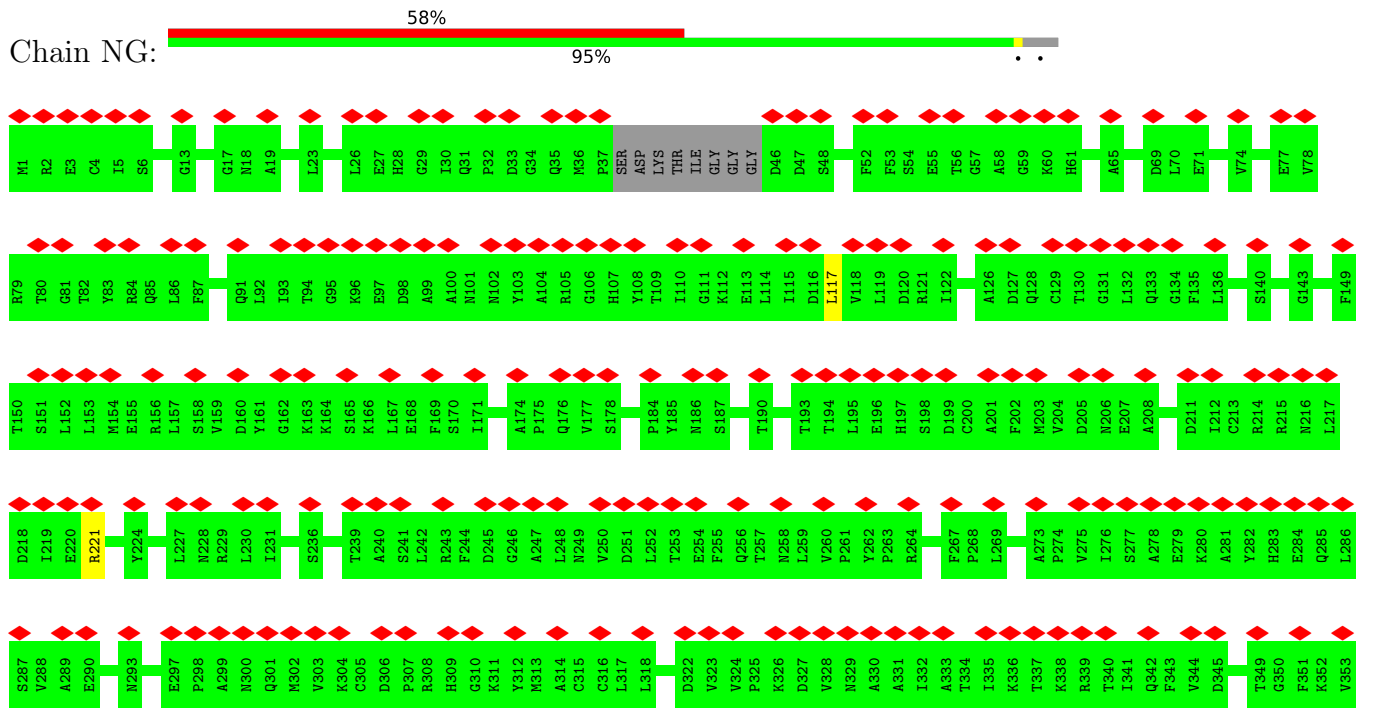
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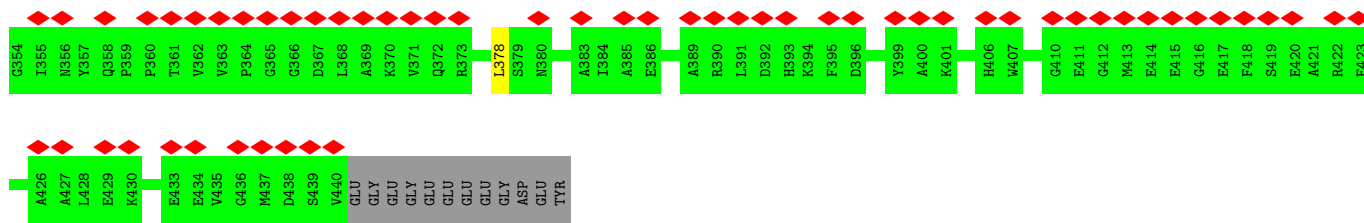
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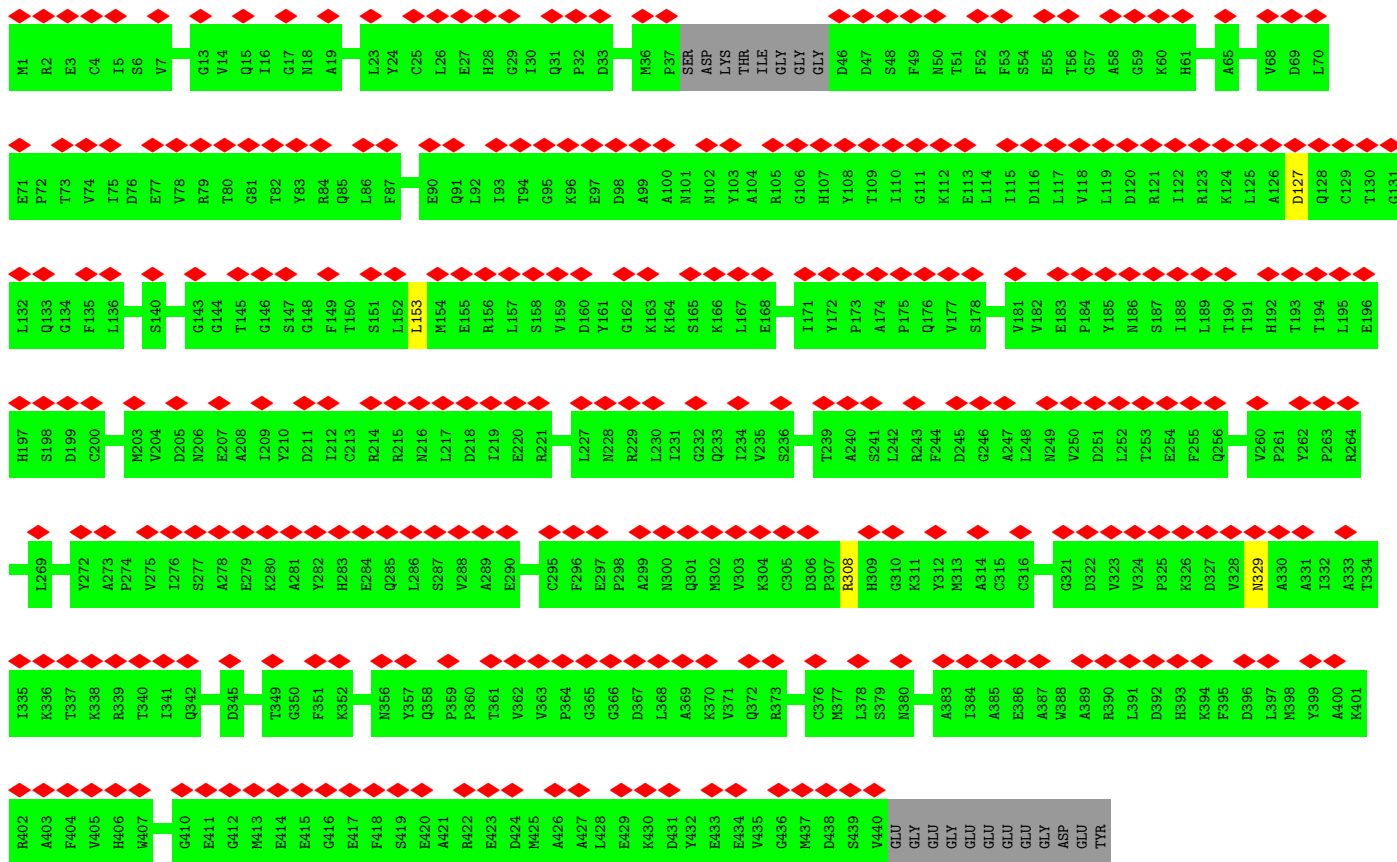
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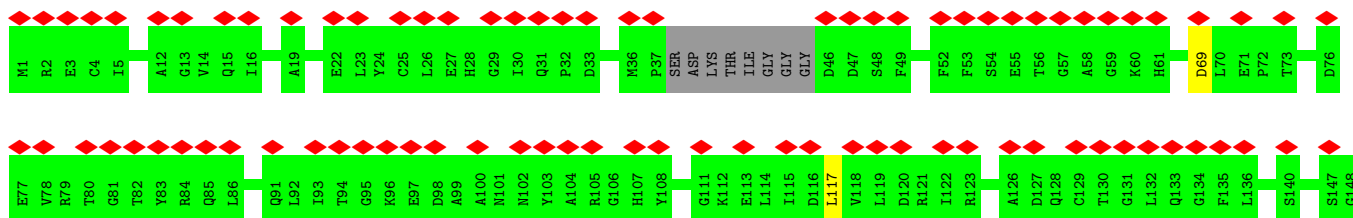


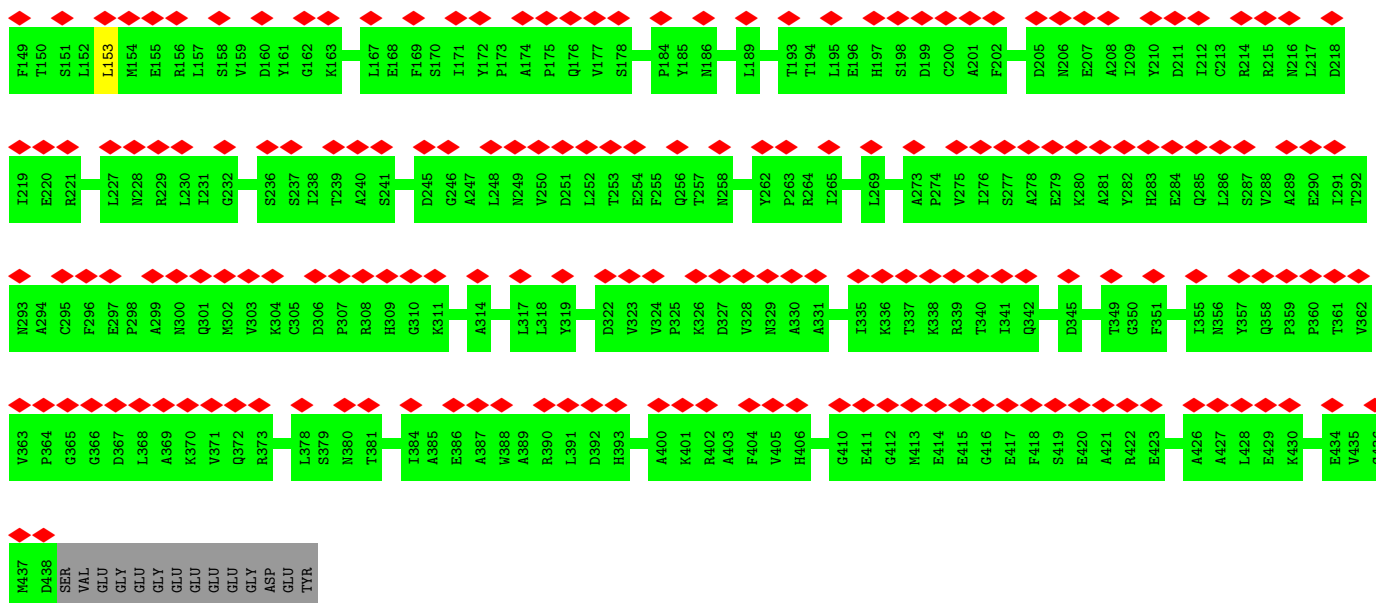


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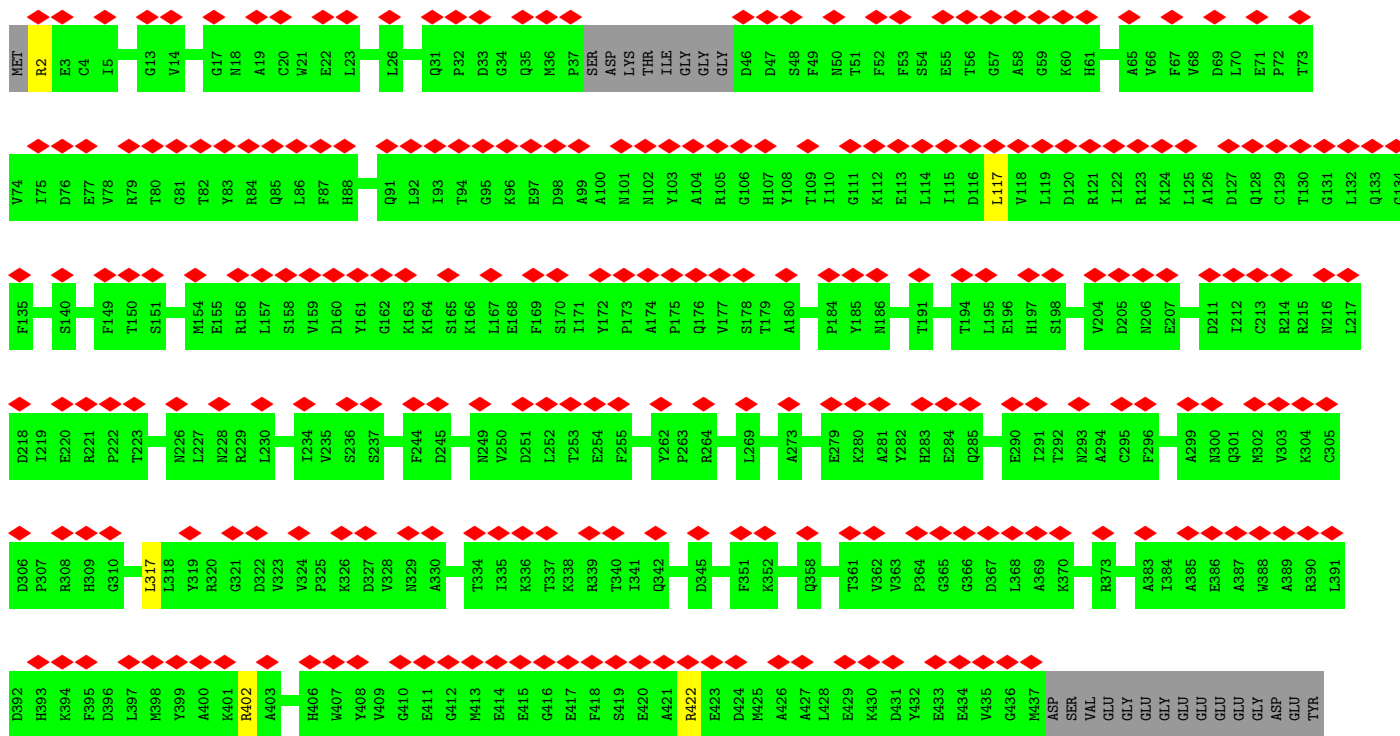


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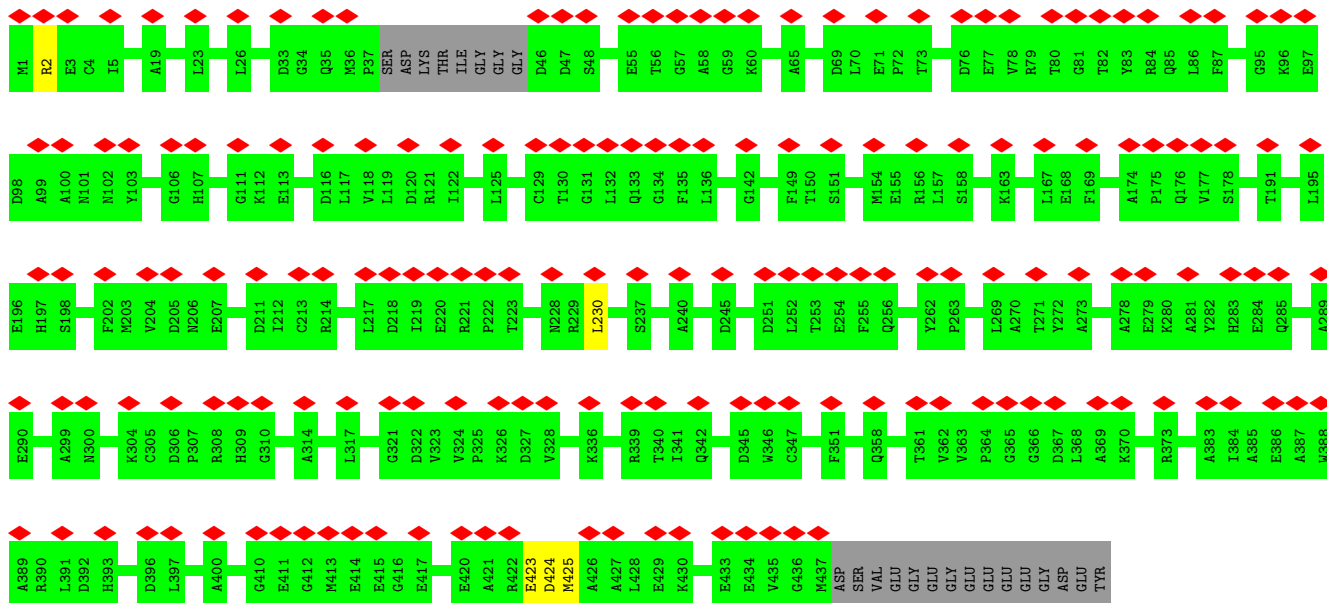


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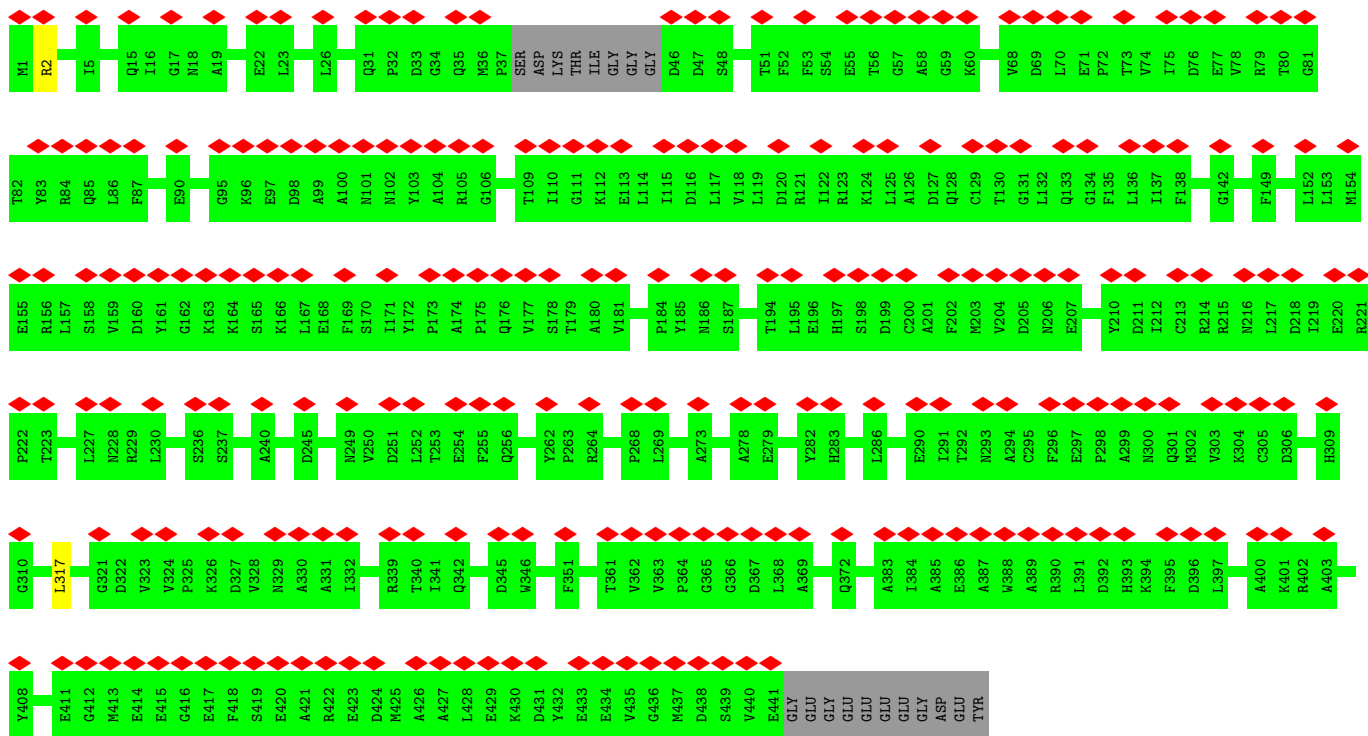


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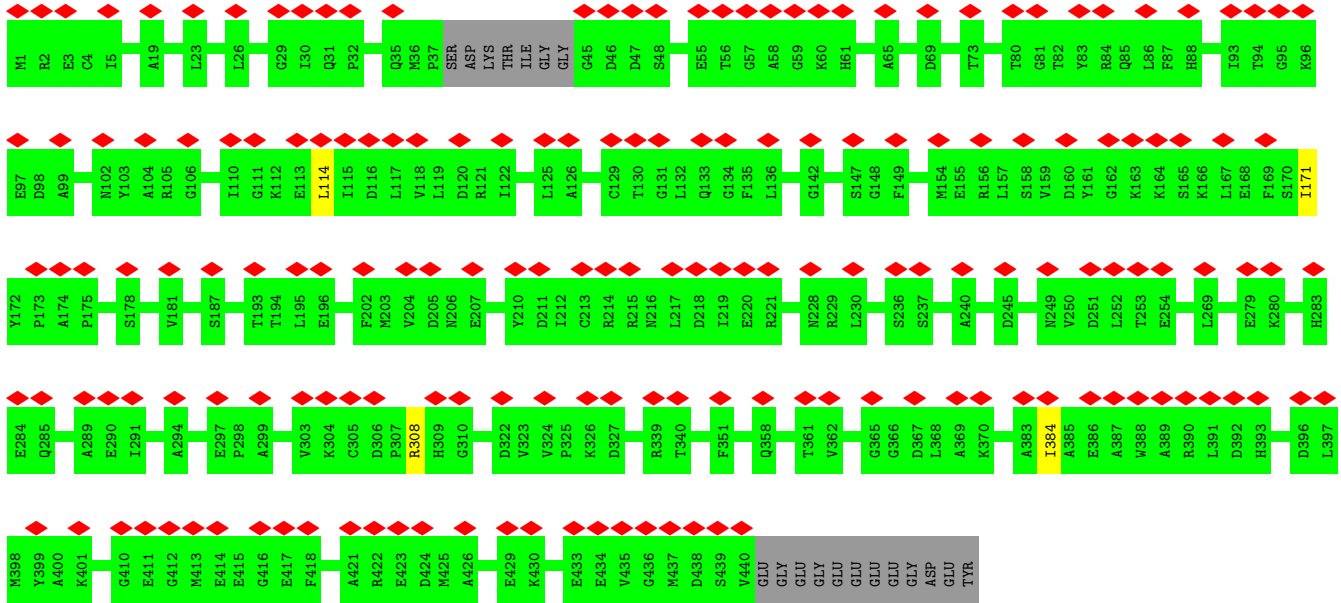


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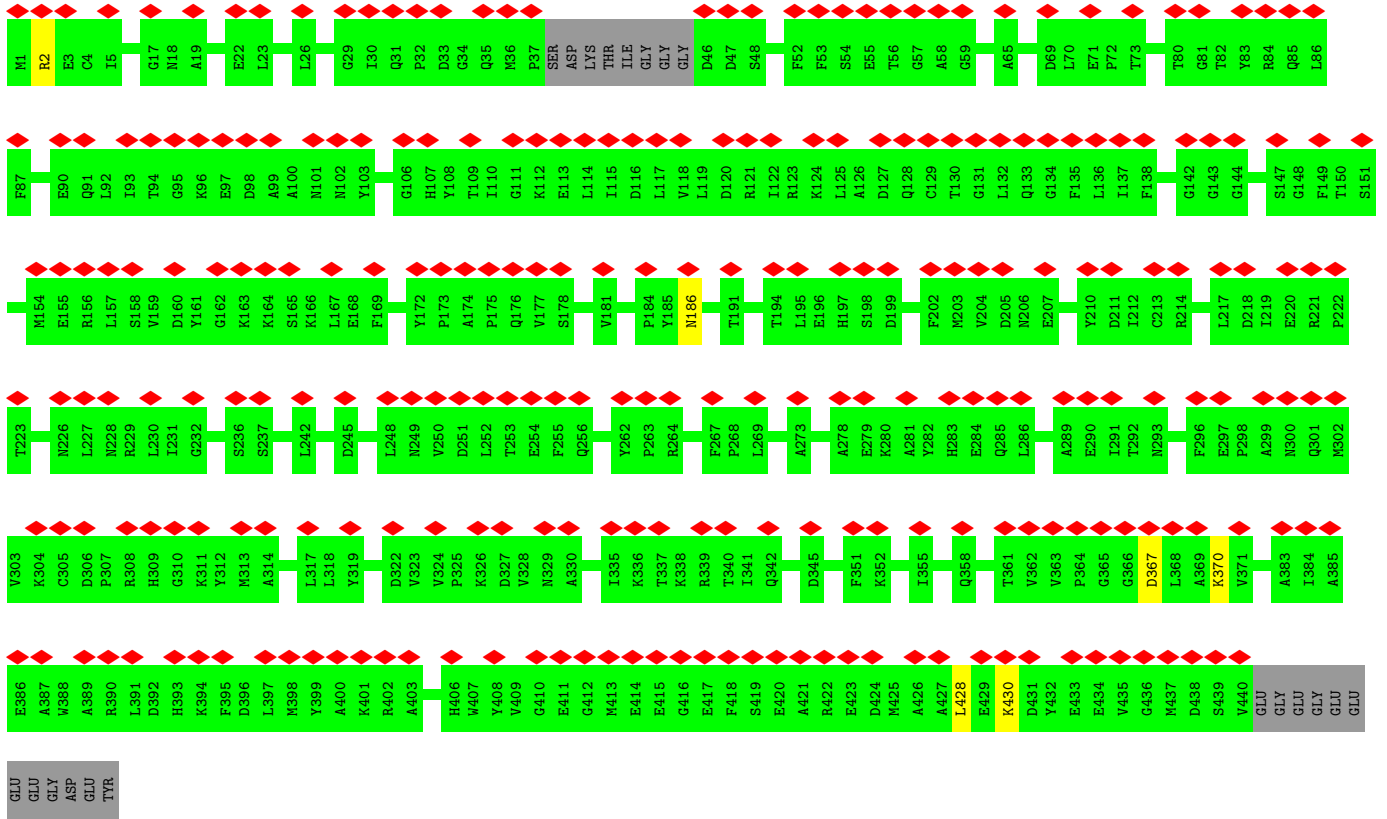


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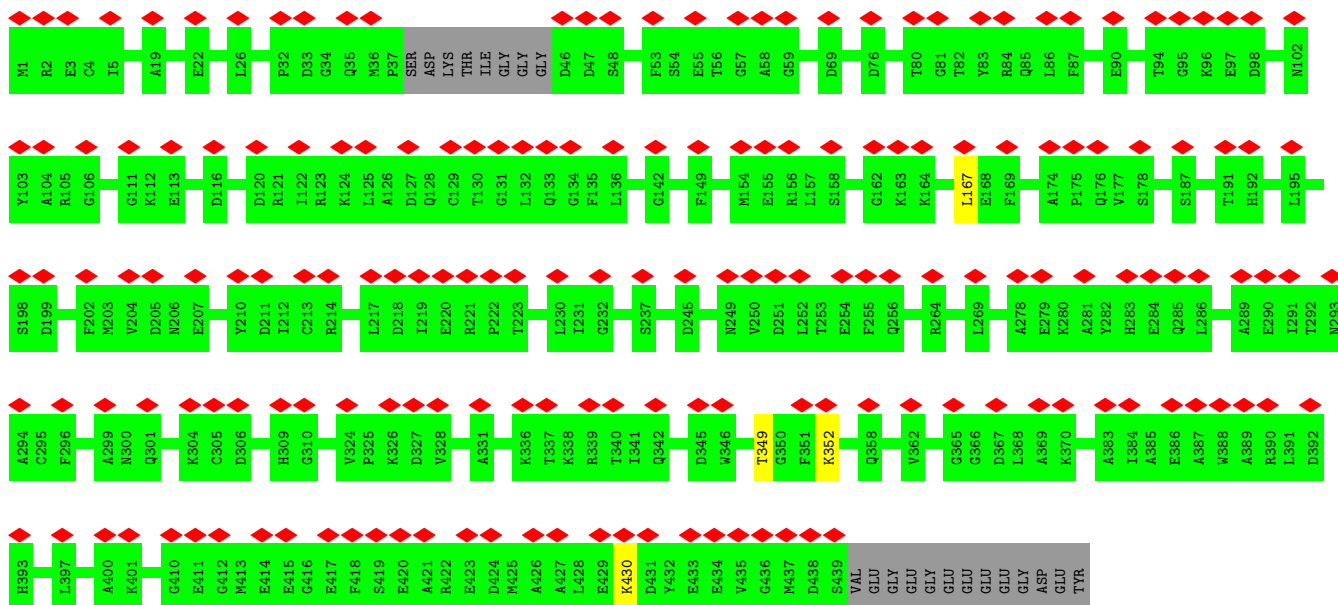


● Molecule 8: Tubulin alpha-1D chain

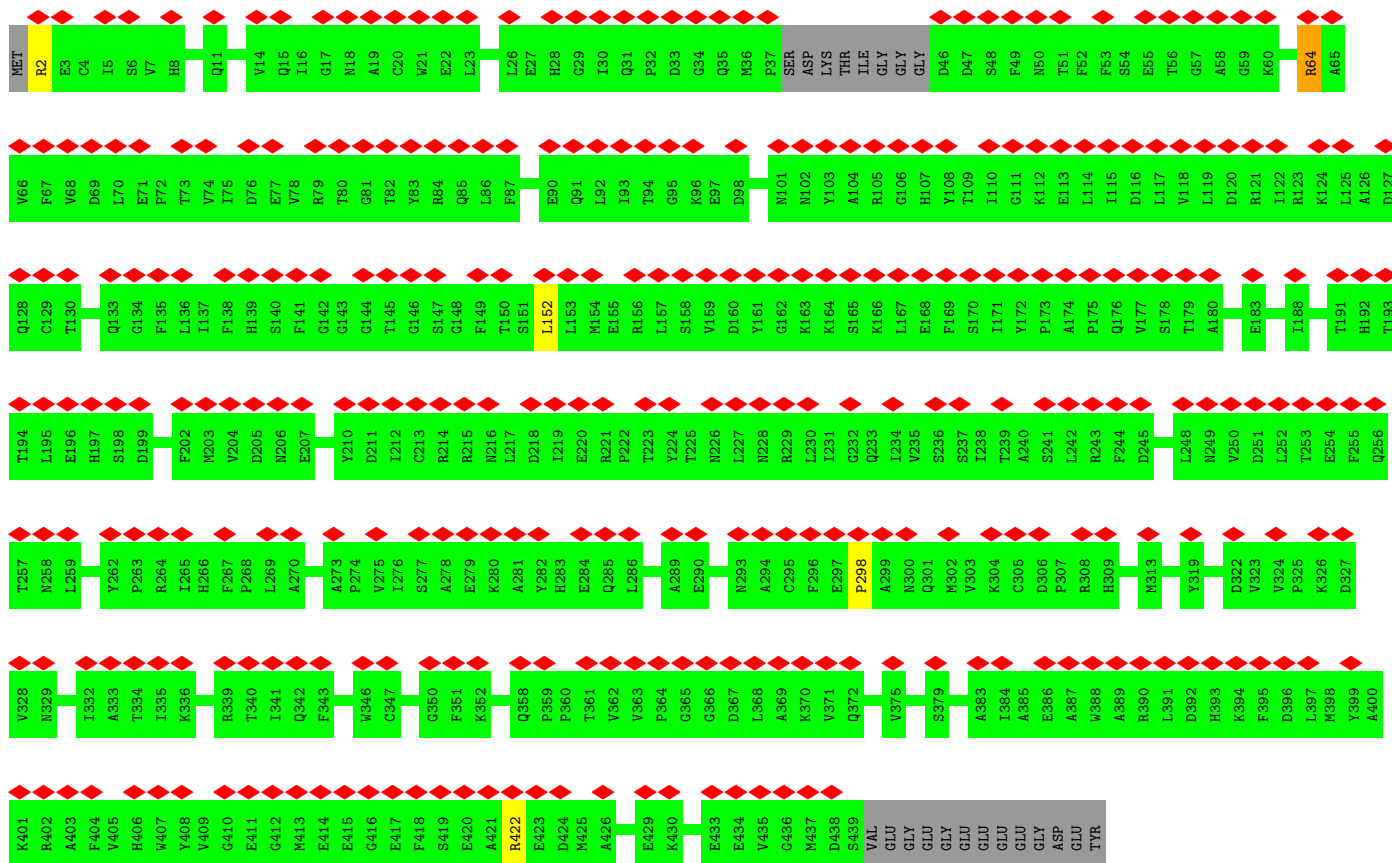


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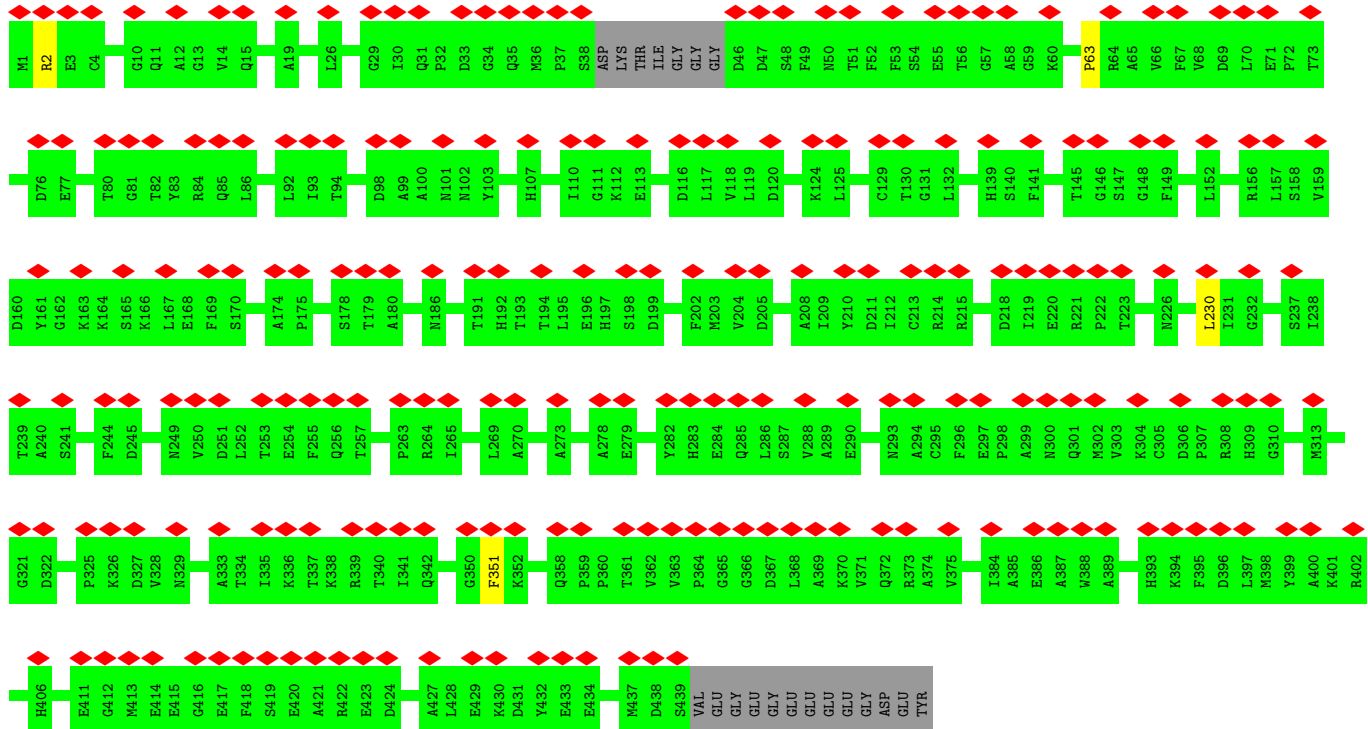




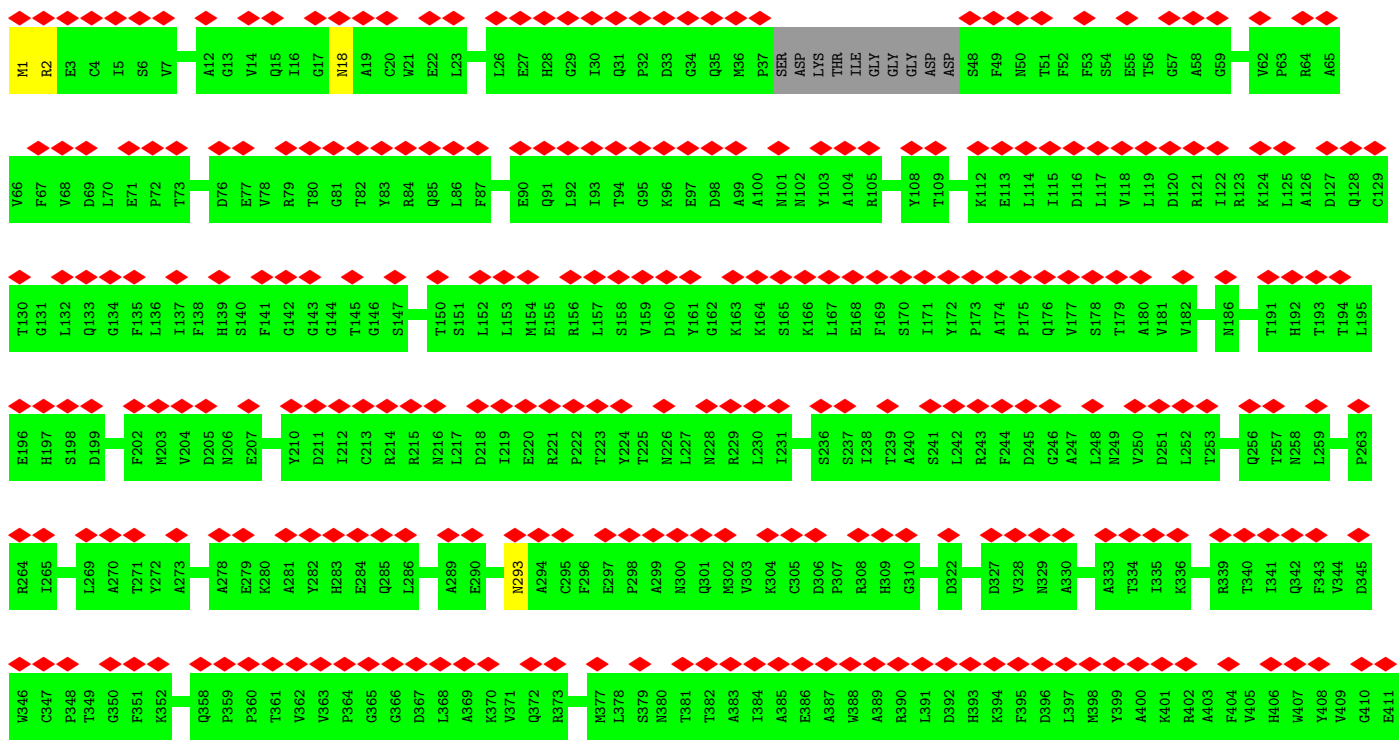
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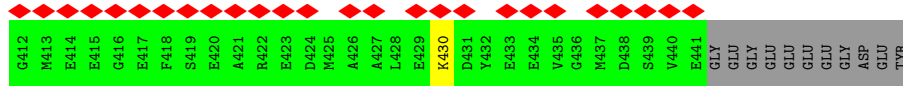


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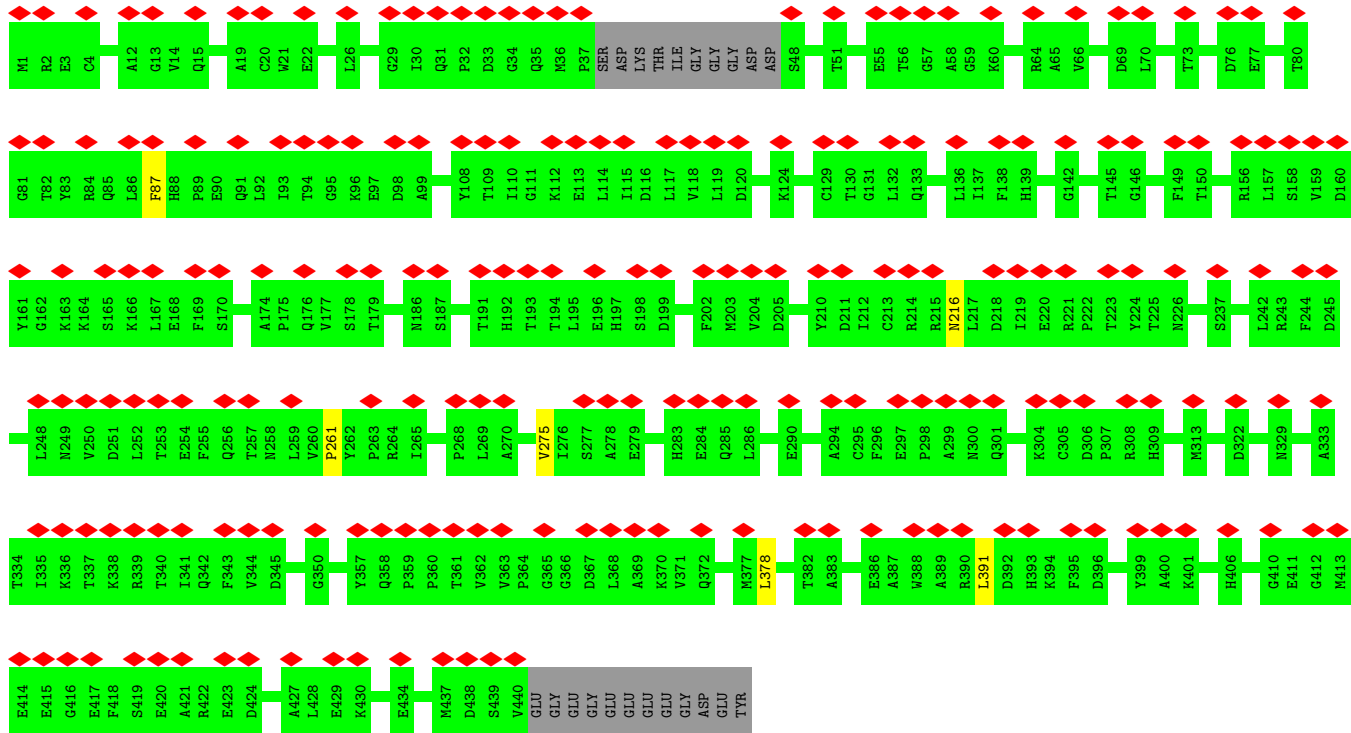


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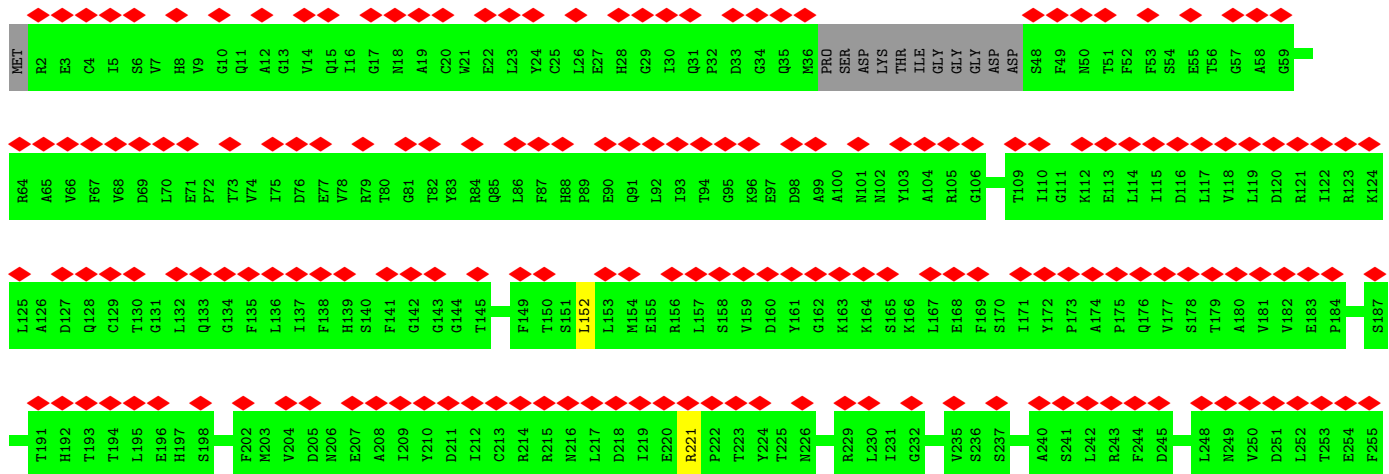
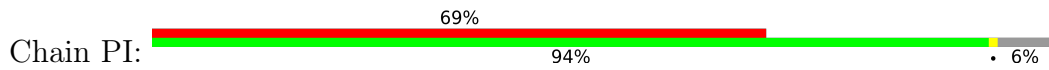


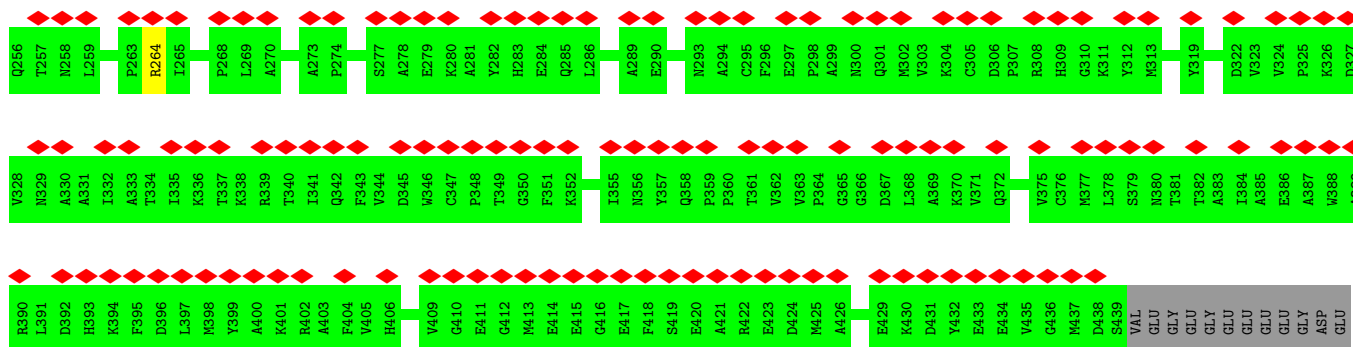


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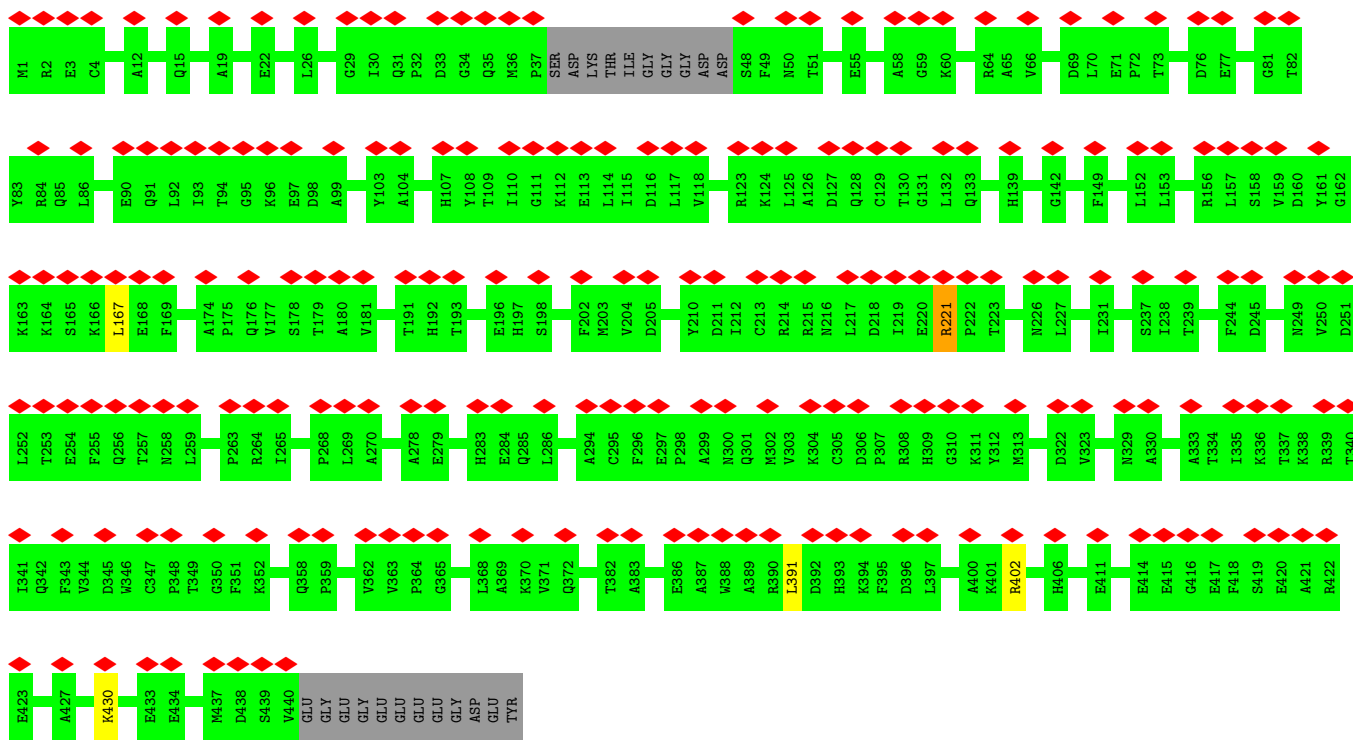
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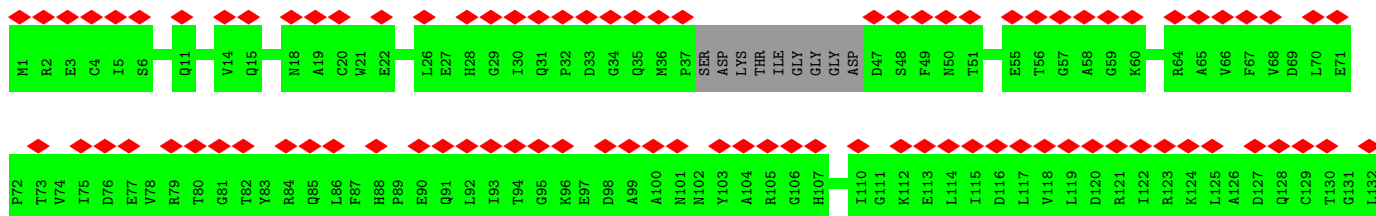
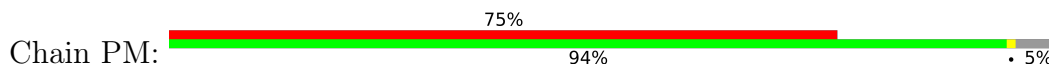


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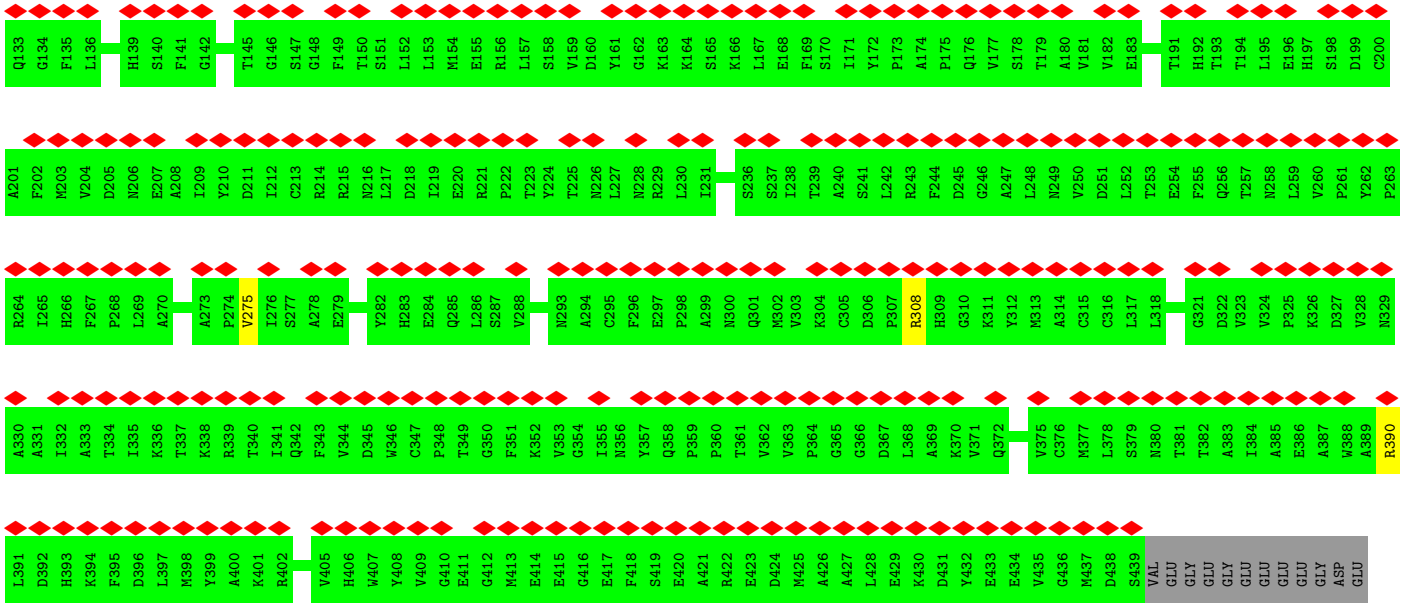
• Molecule 8: Tubulin alpha-1D chain



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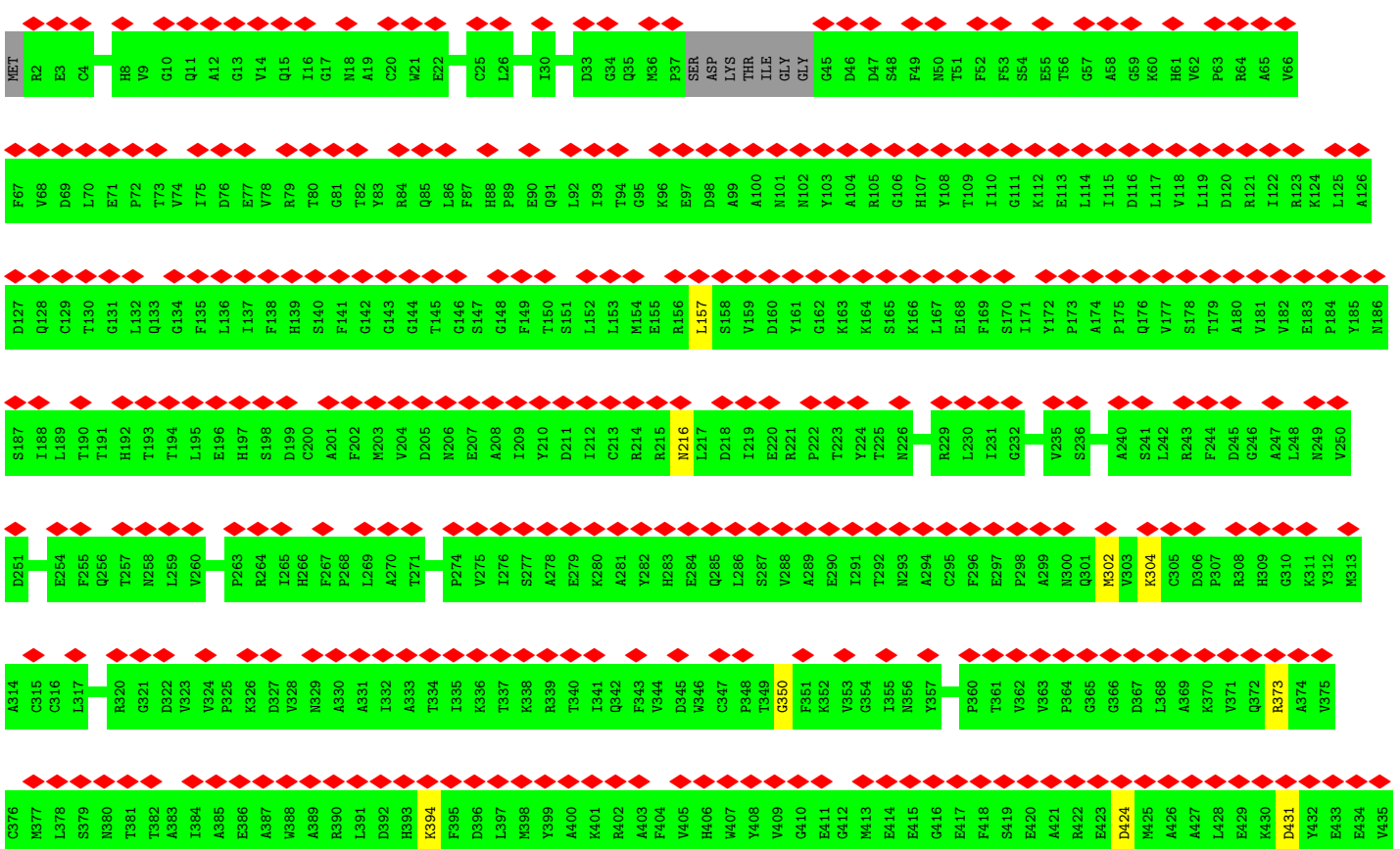
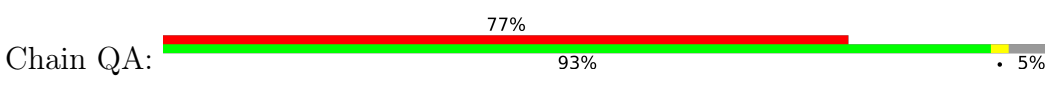


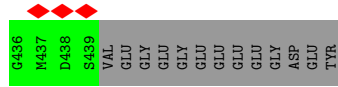




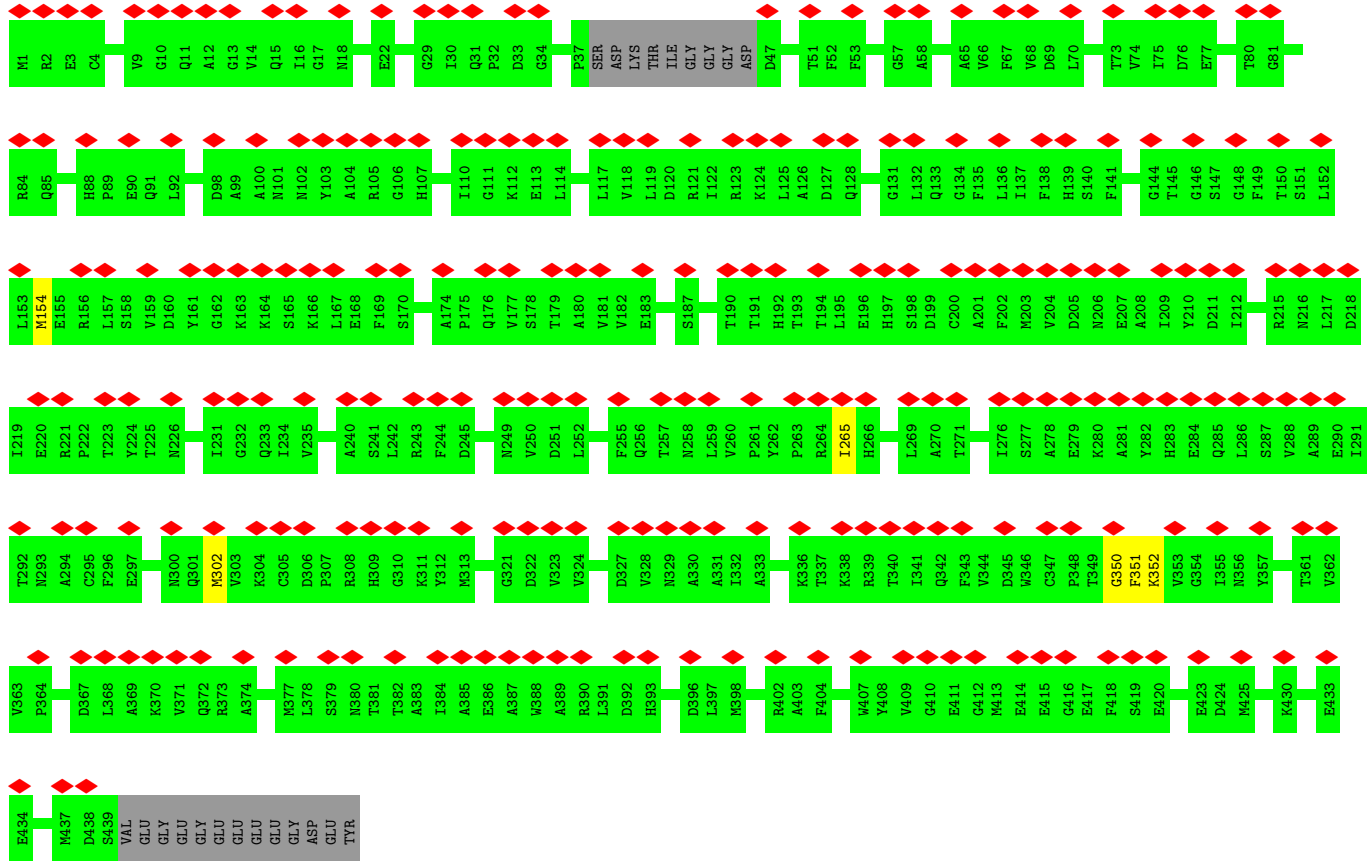
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• Molecule 8: Tubulin alpha-1D chain

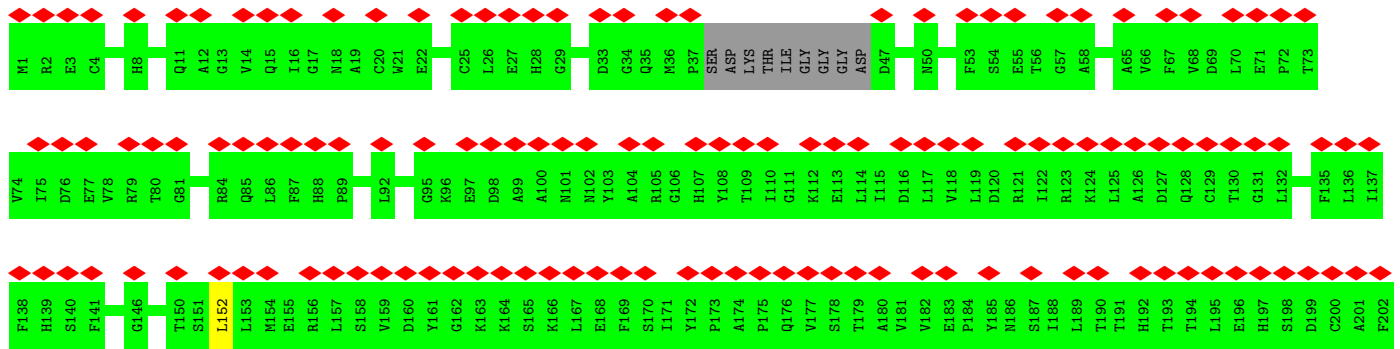
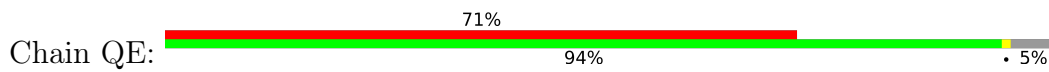


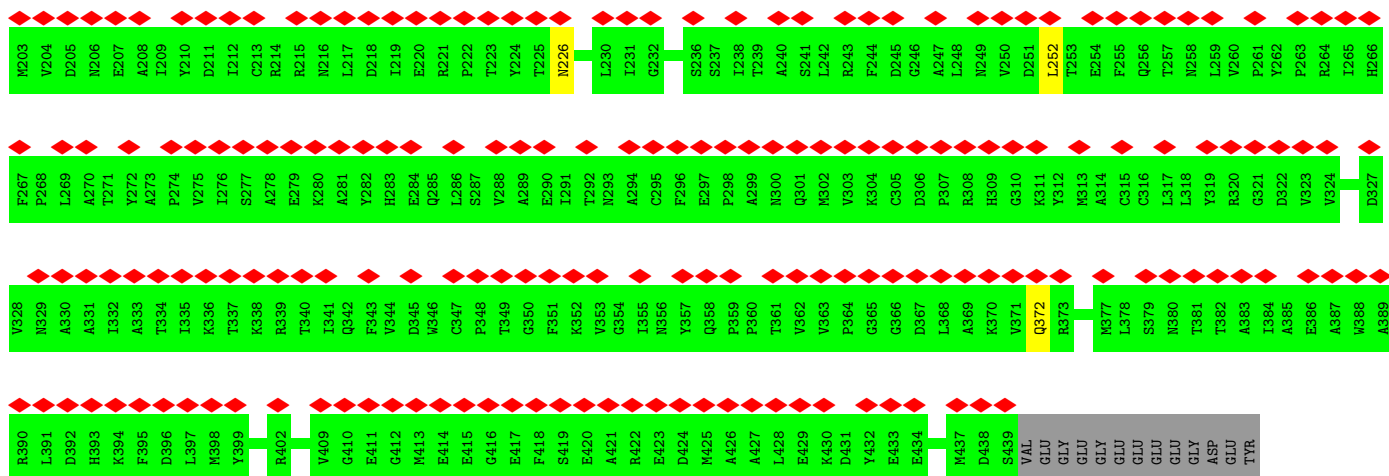


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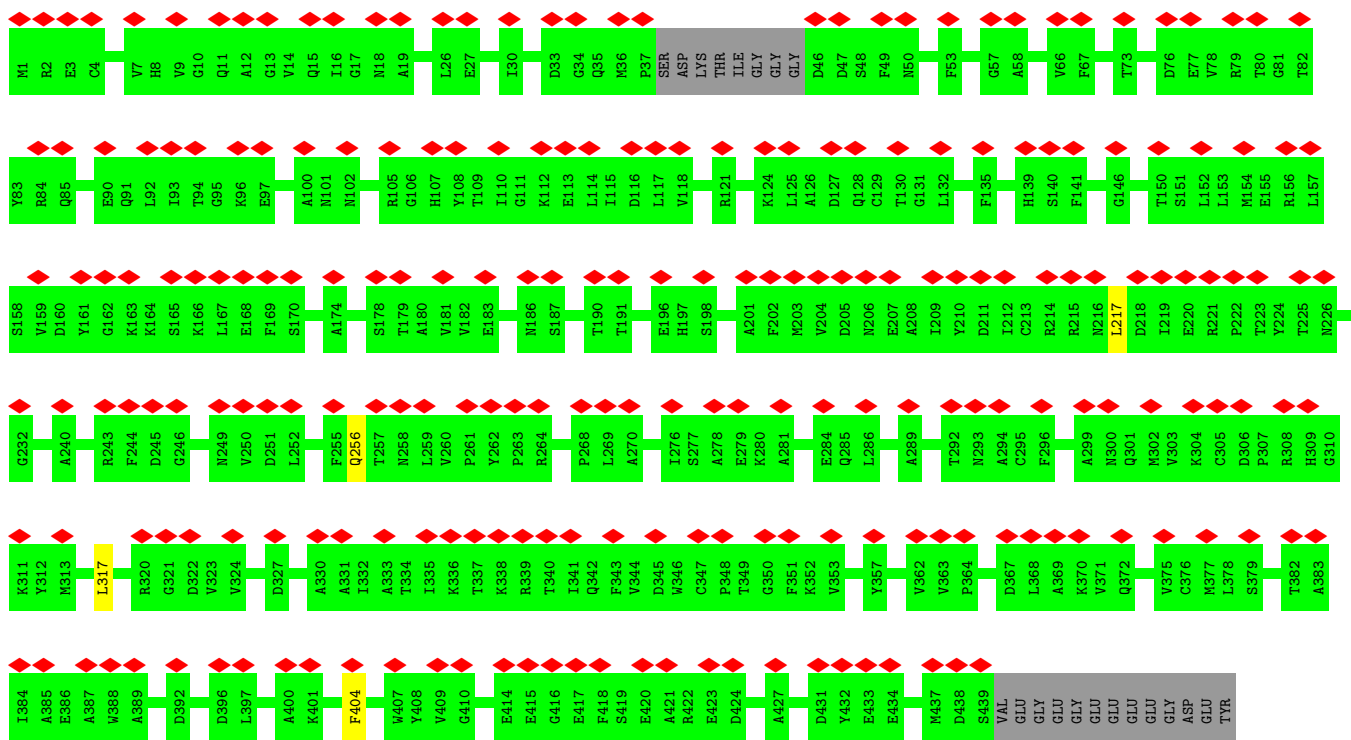


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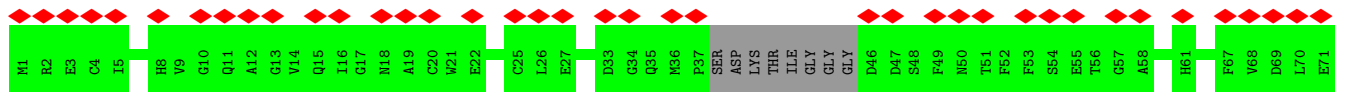
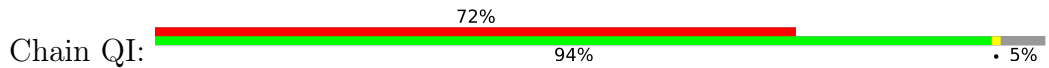


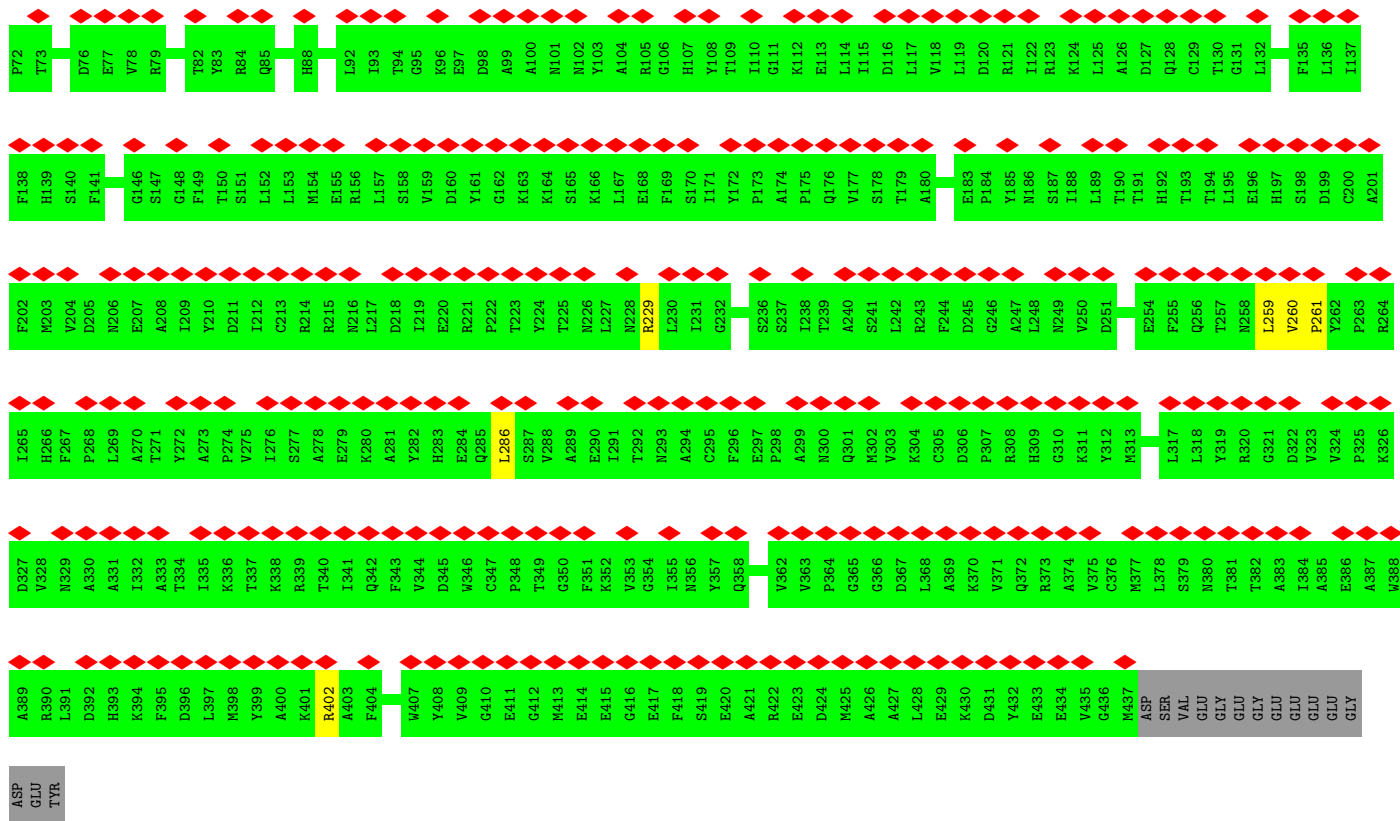


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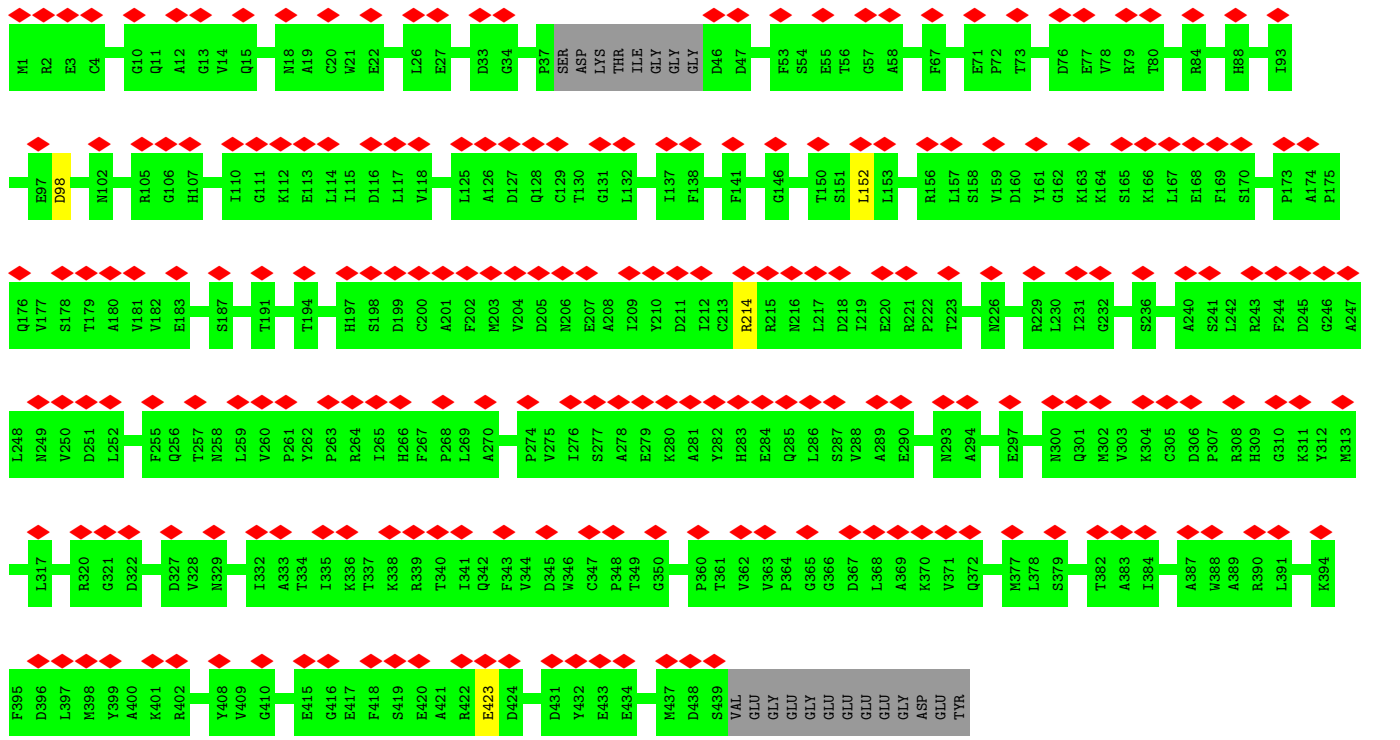


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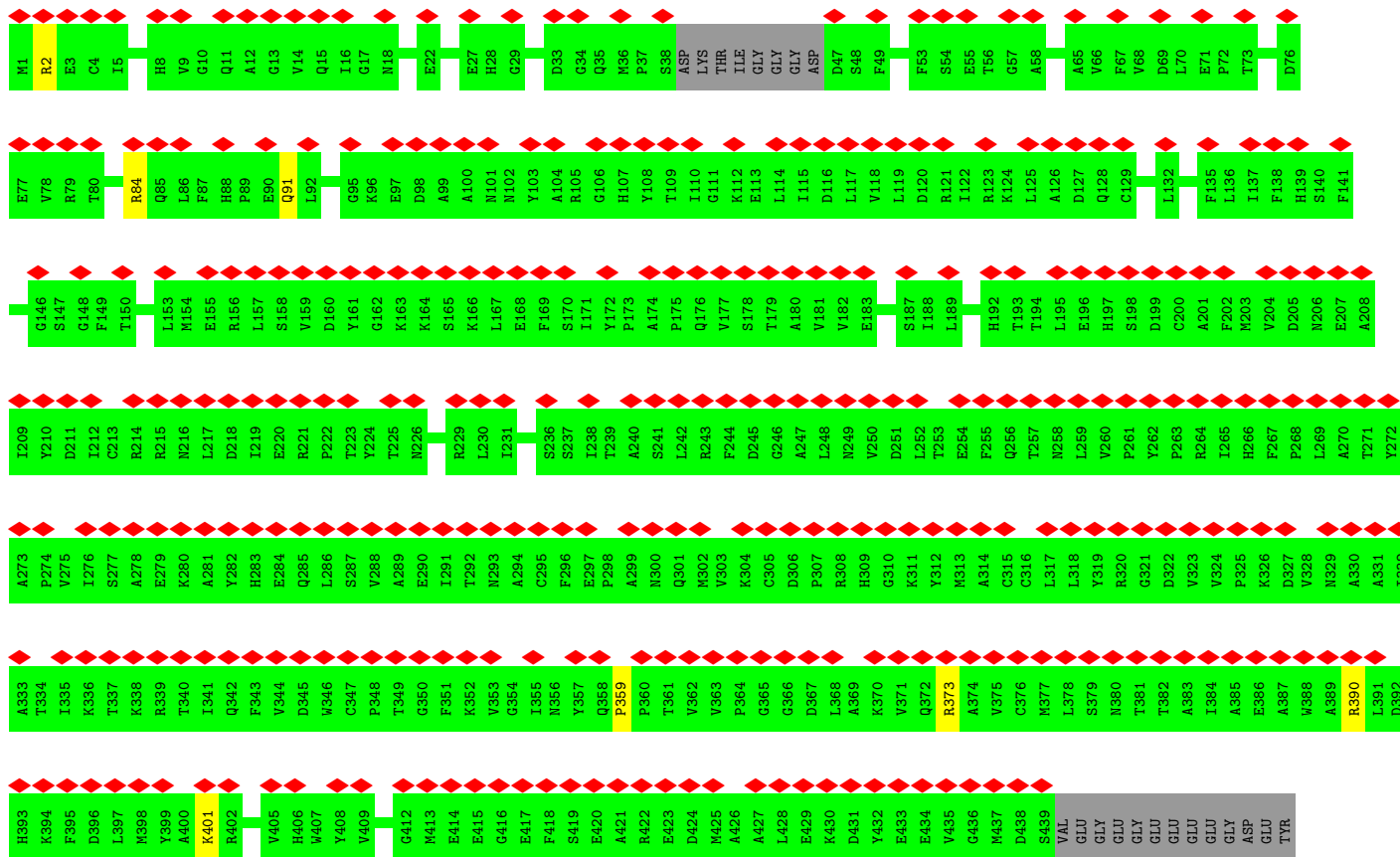
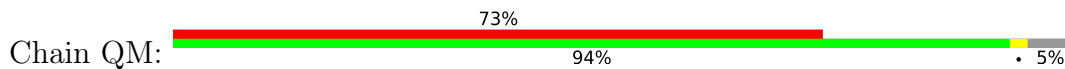




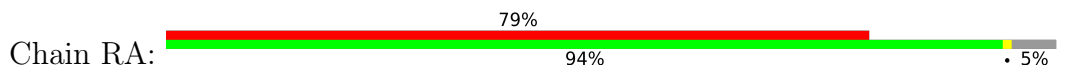
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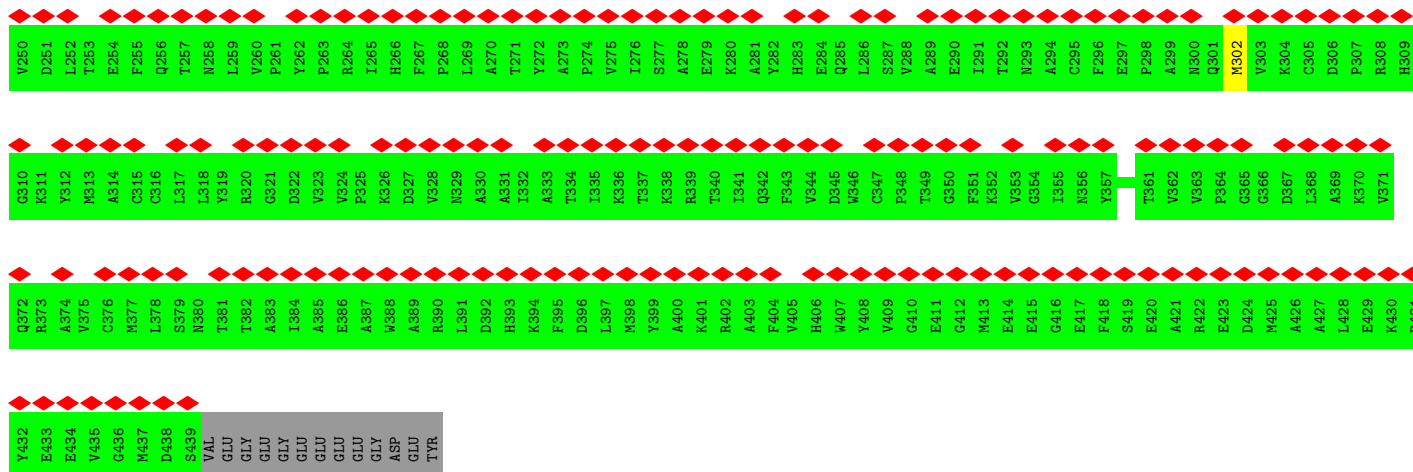


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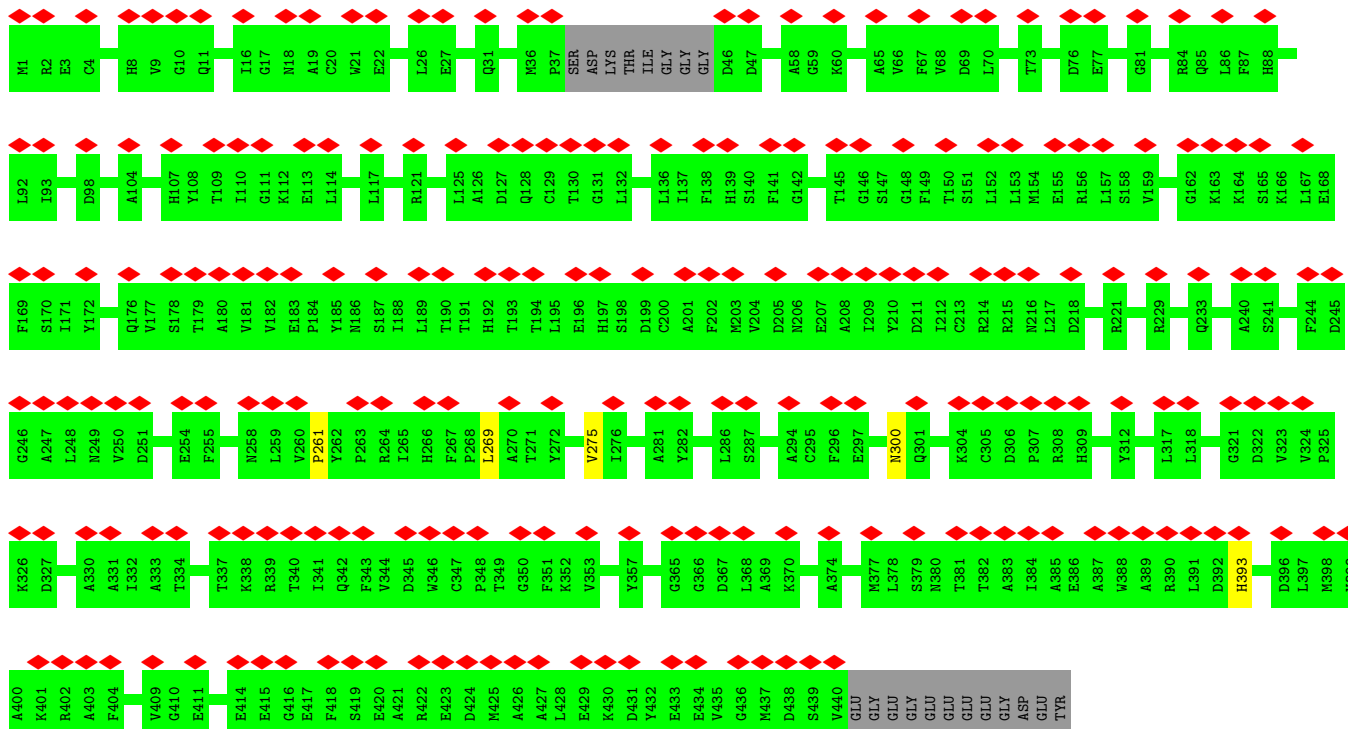


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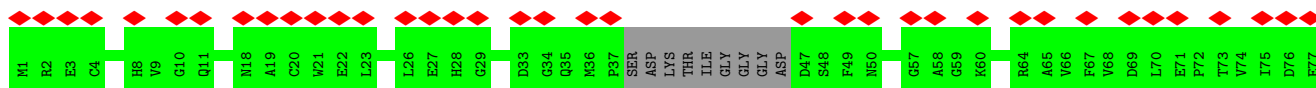


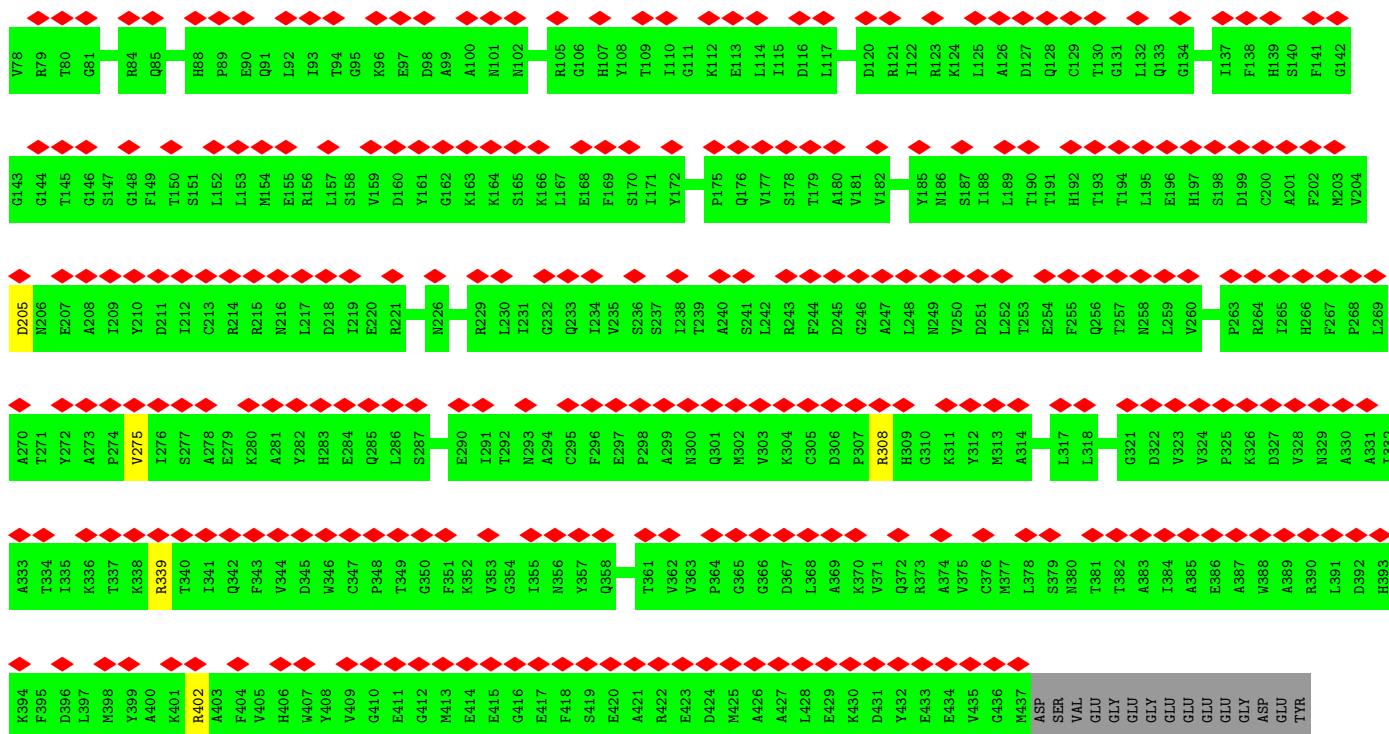


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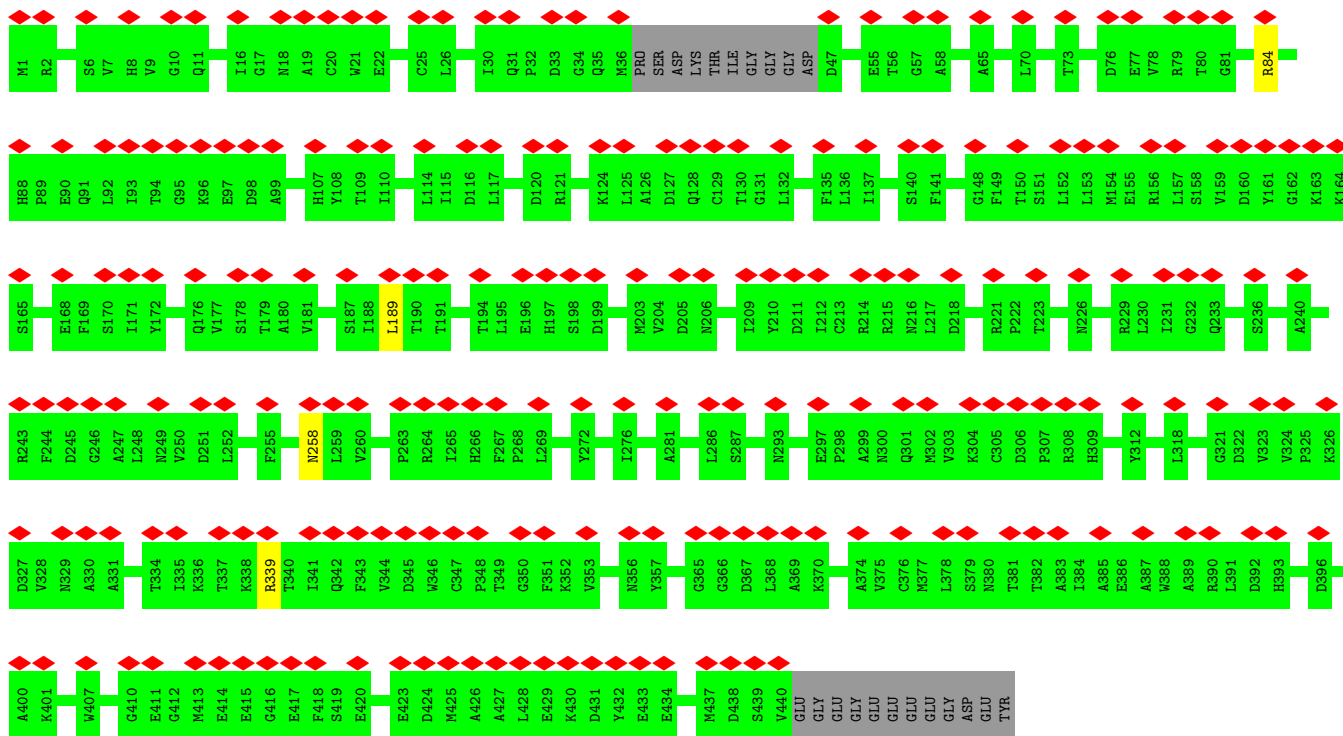


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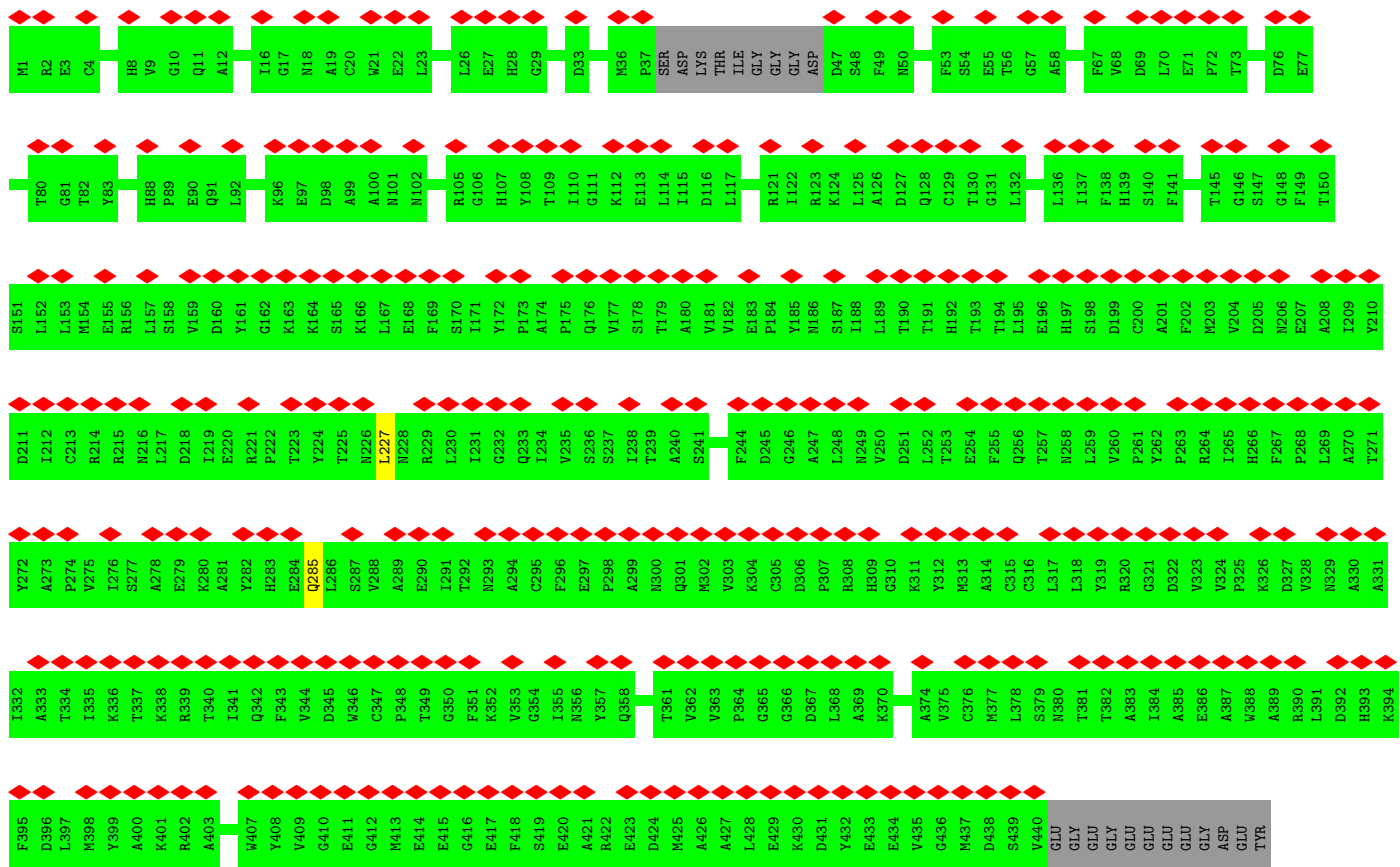




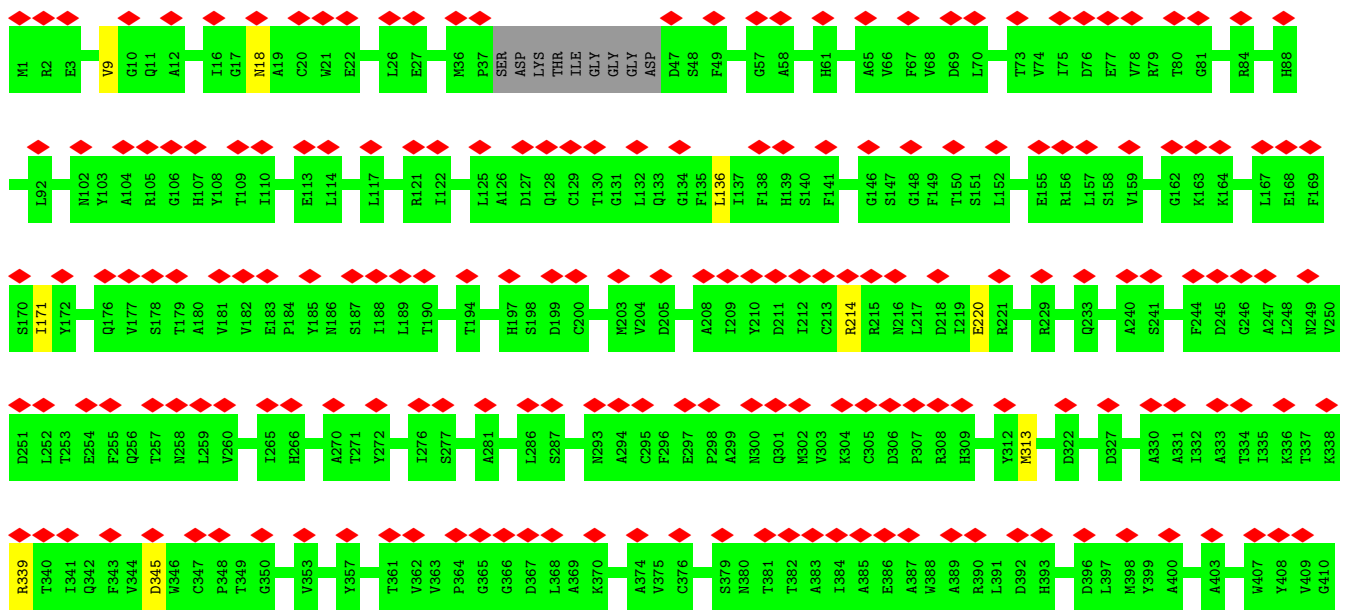
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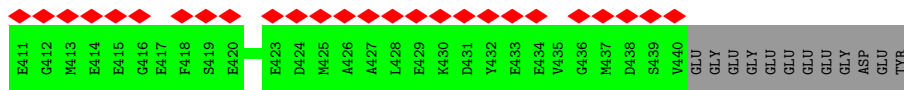
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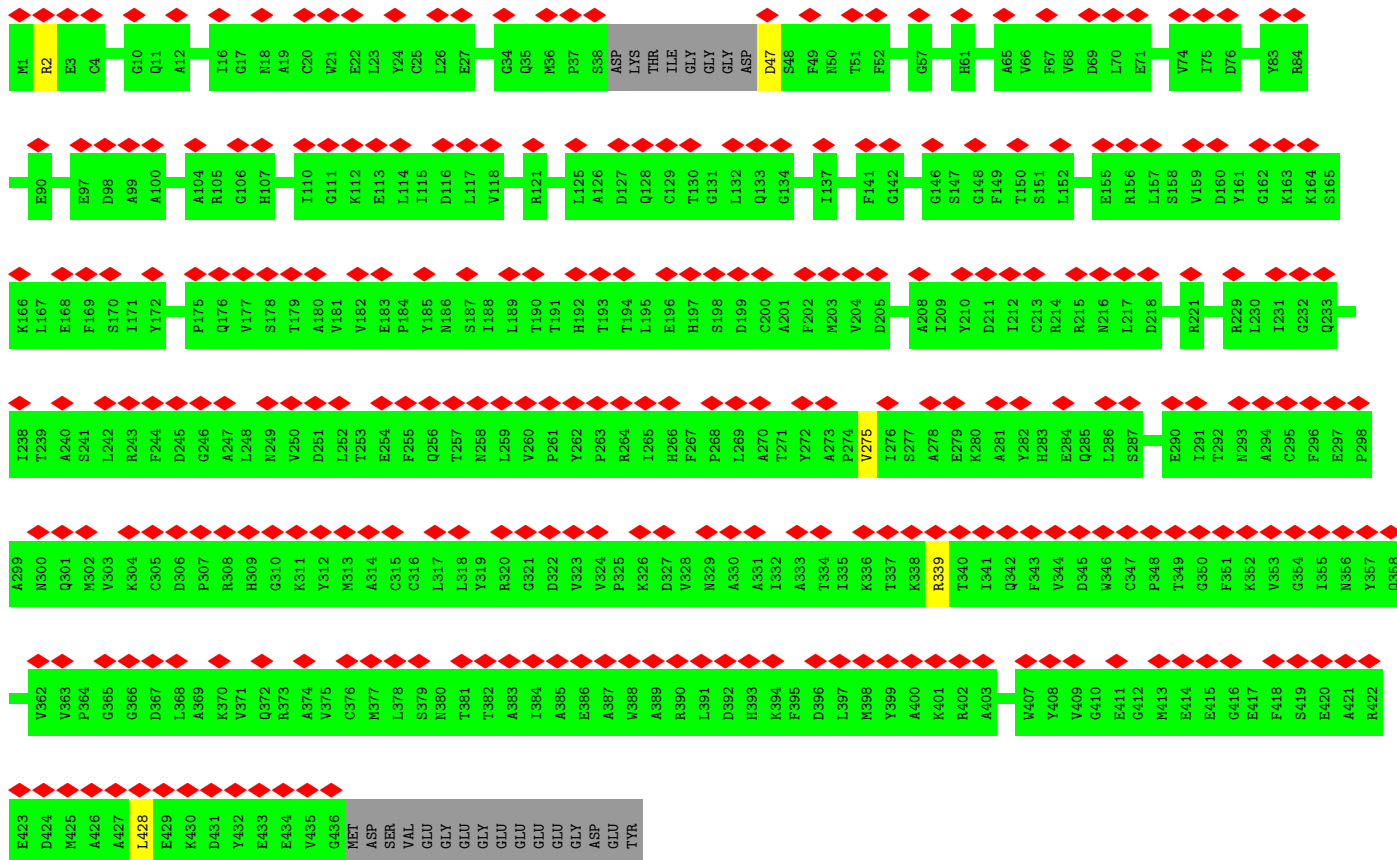
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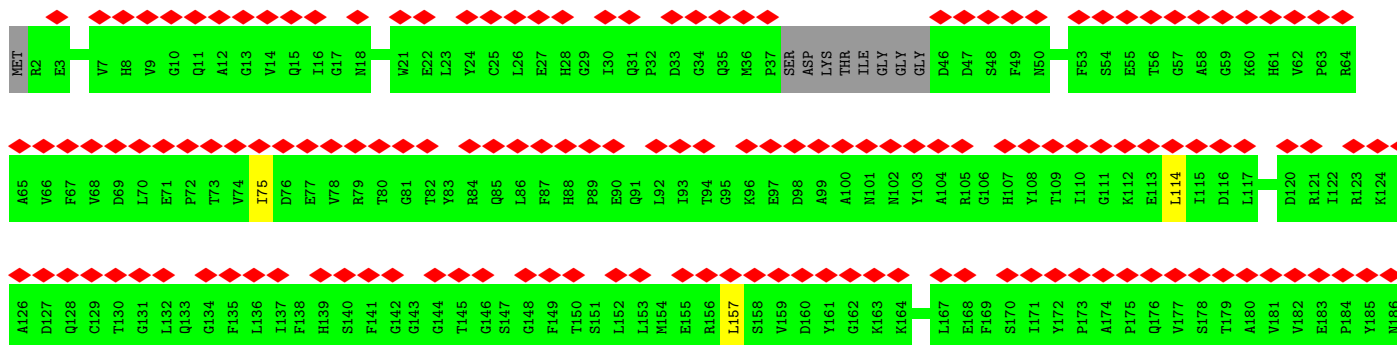
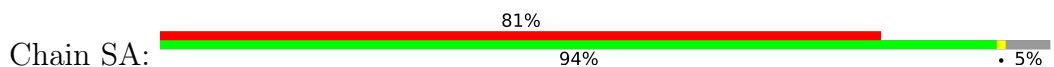


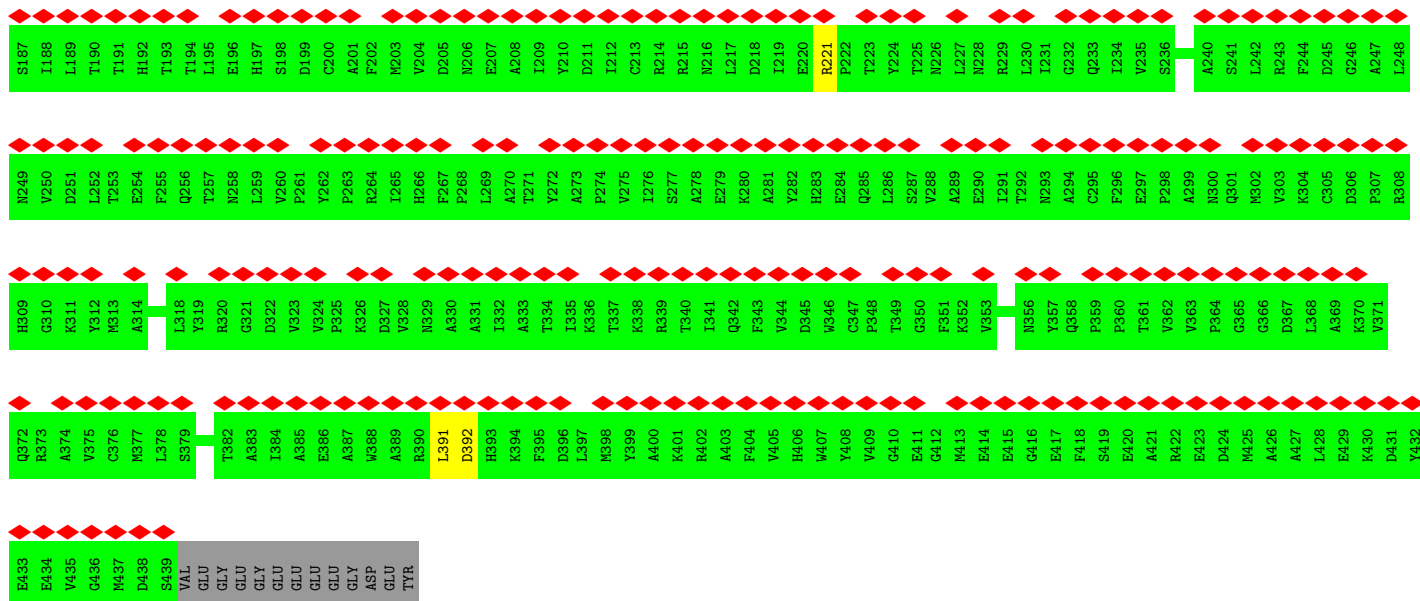


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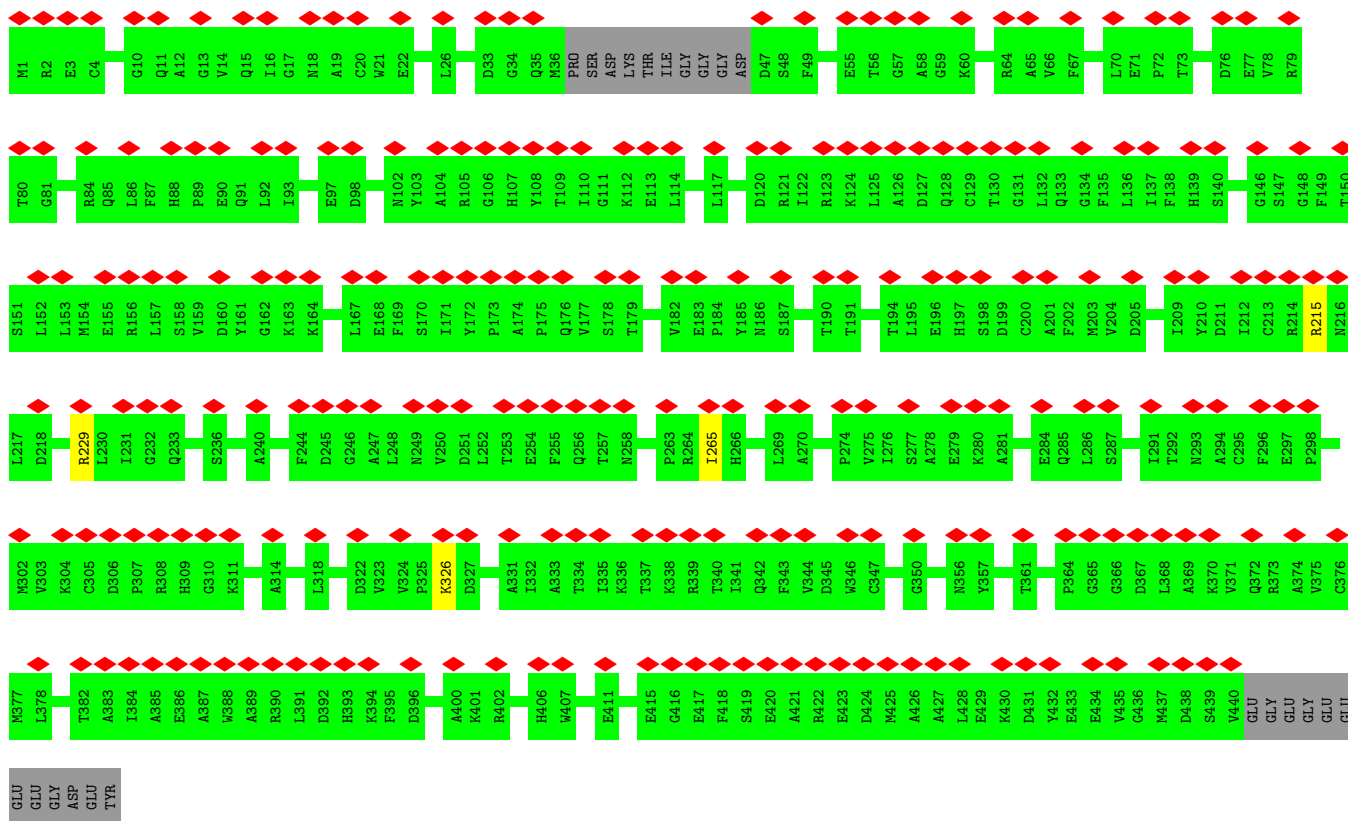


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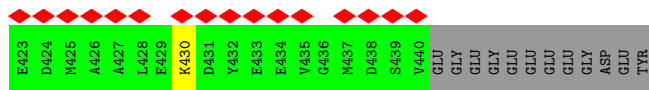
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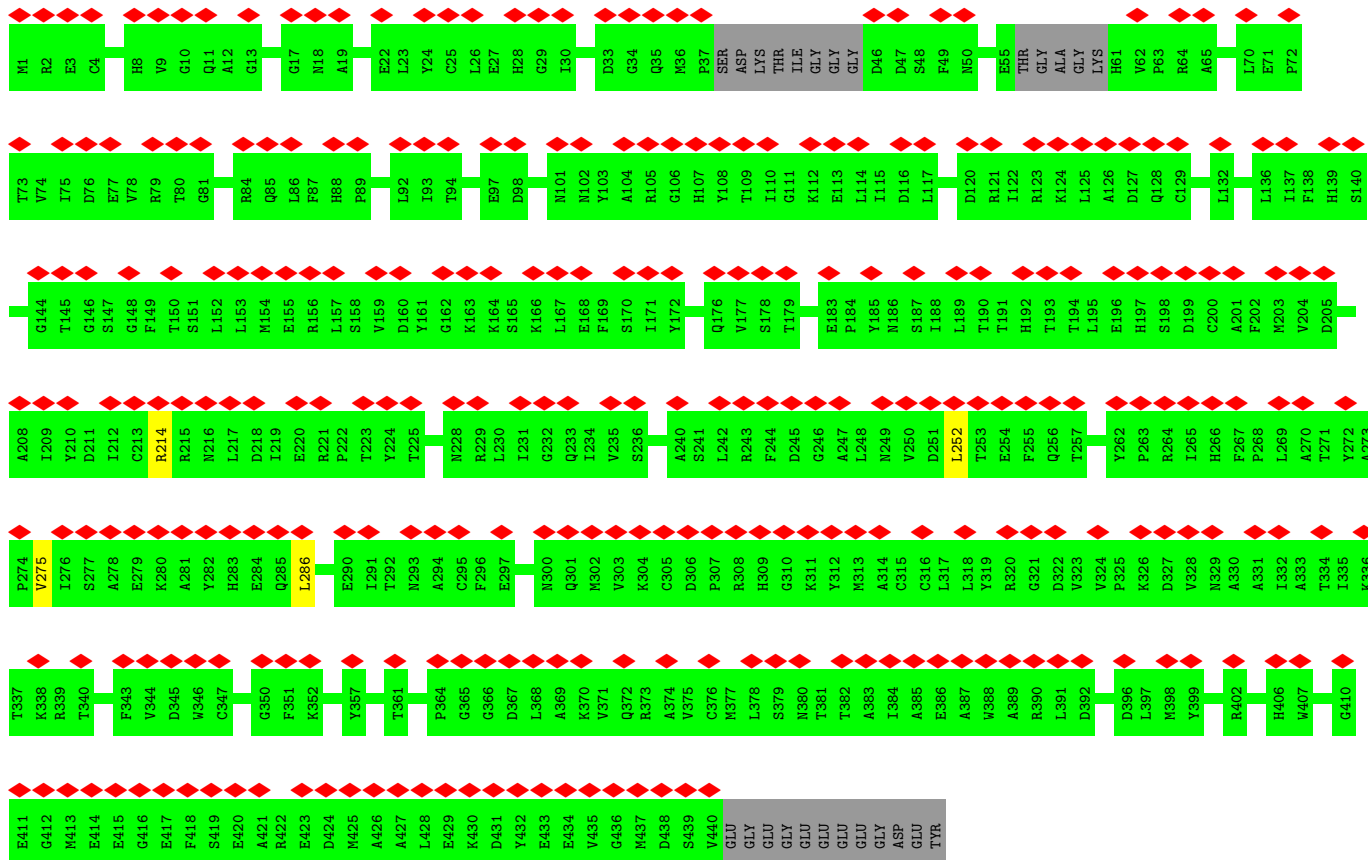
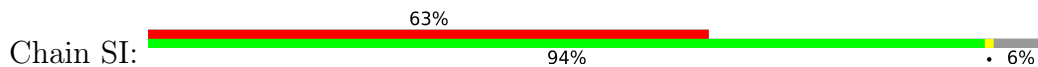
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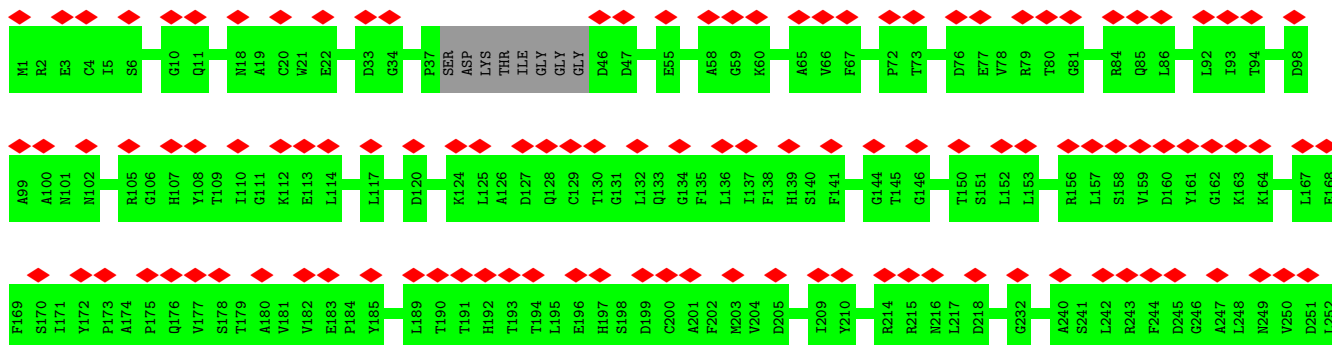


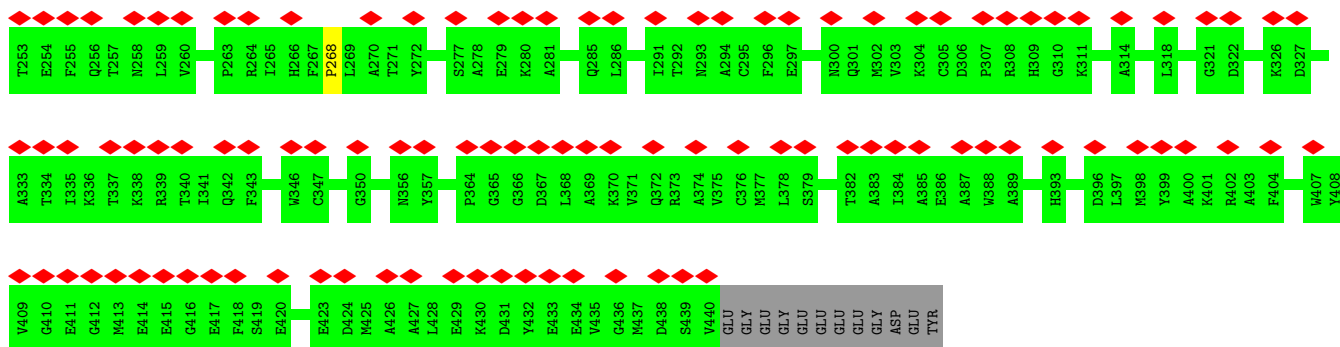


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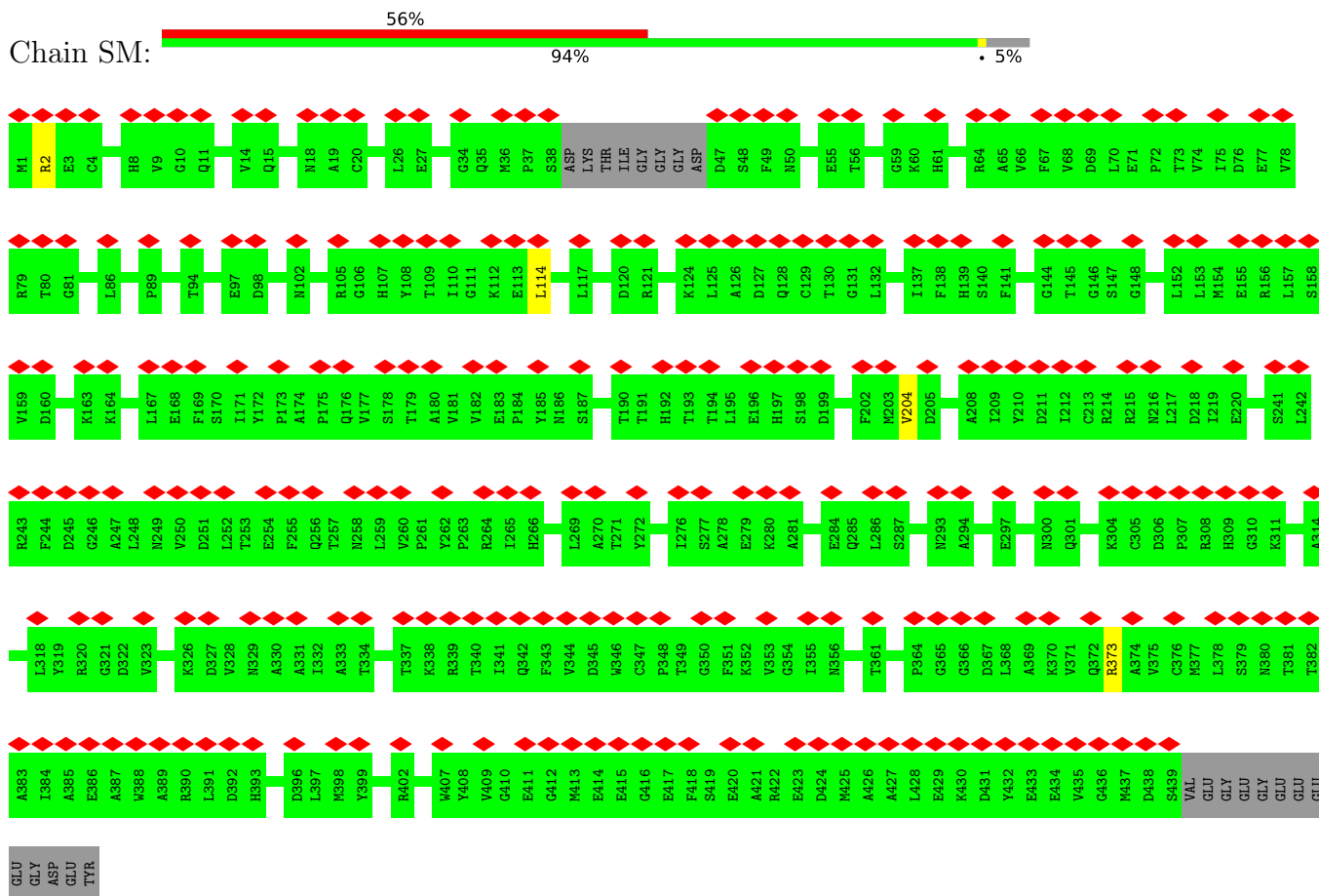


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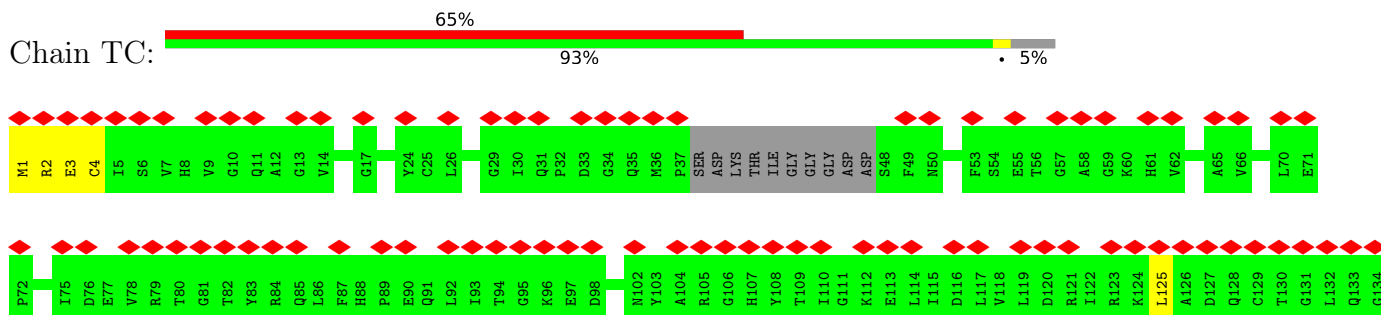


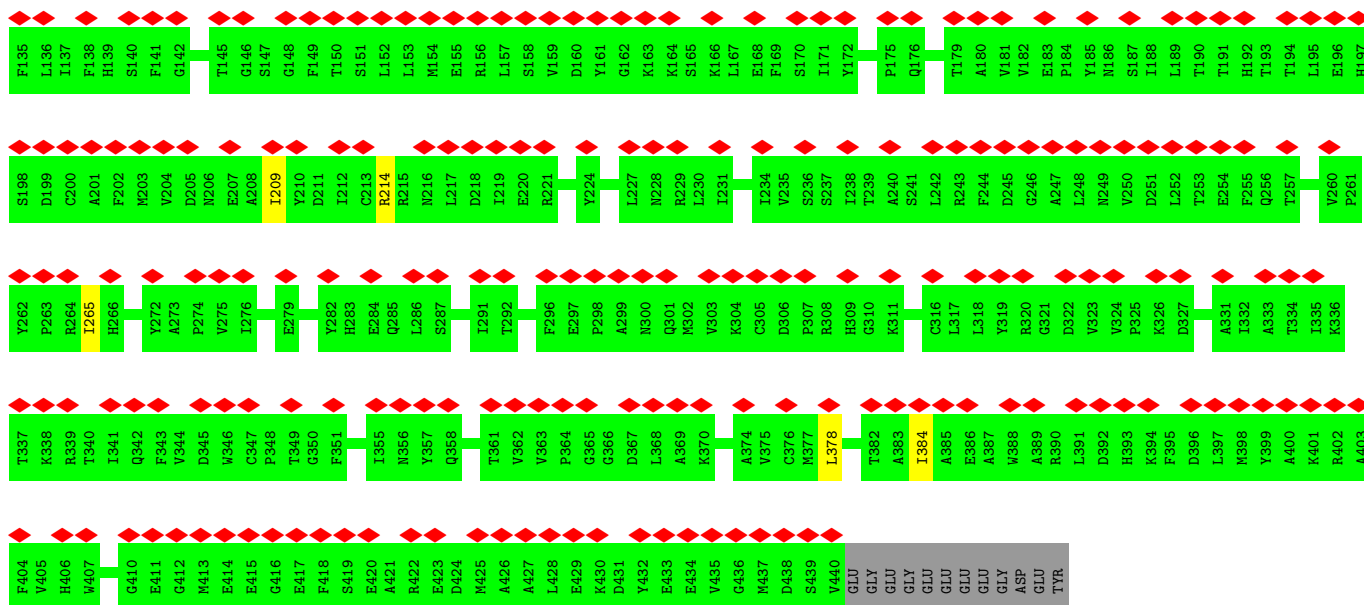


- Molecule 8: Tubulin alpha-1D chain

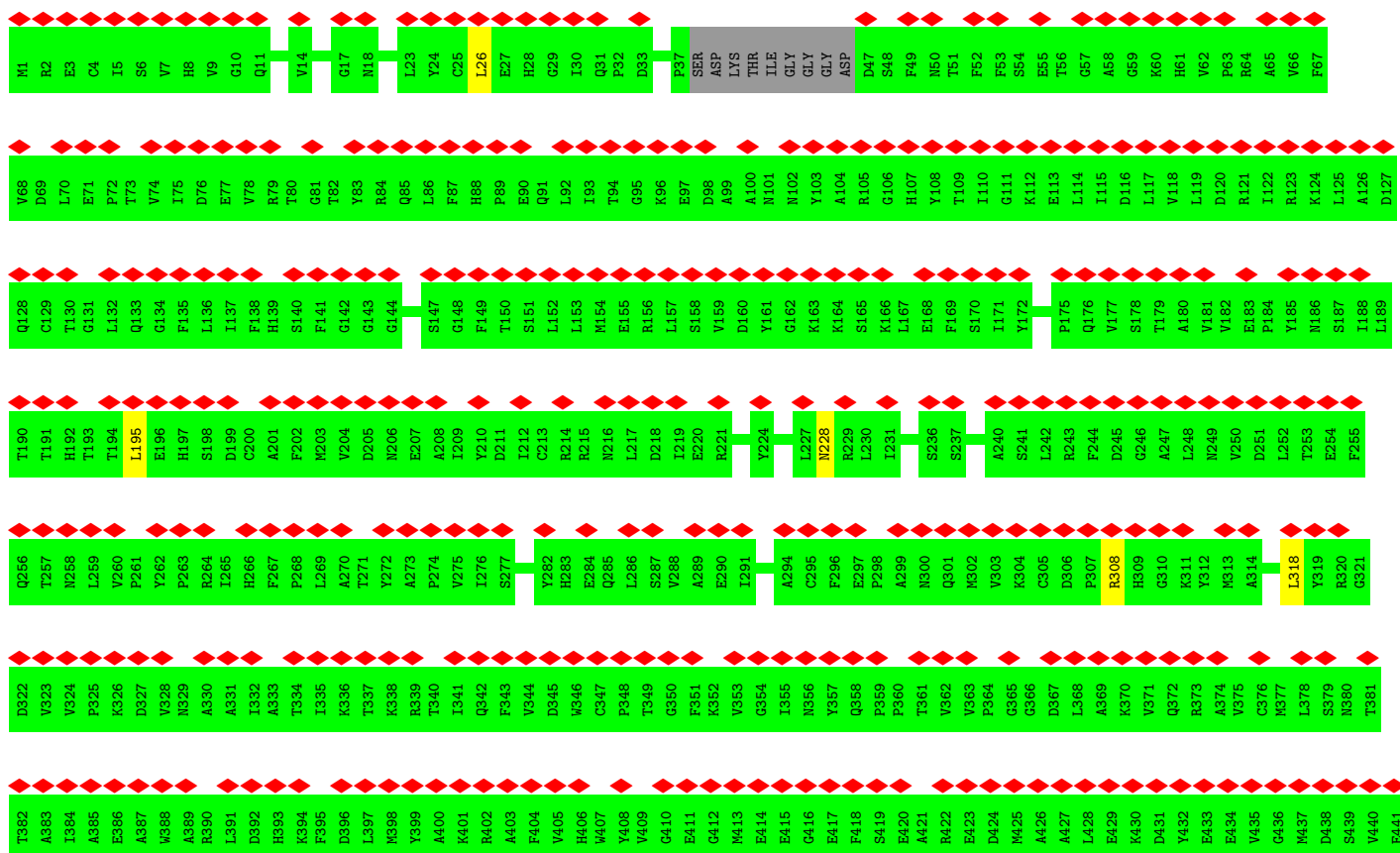
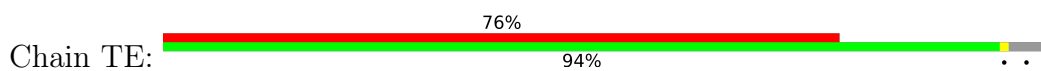


- Molecule 8: Tubulin alpha-1D chain



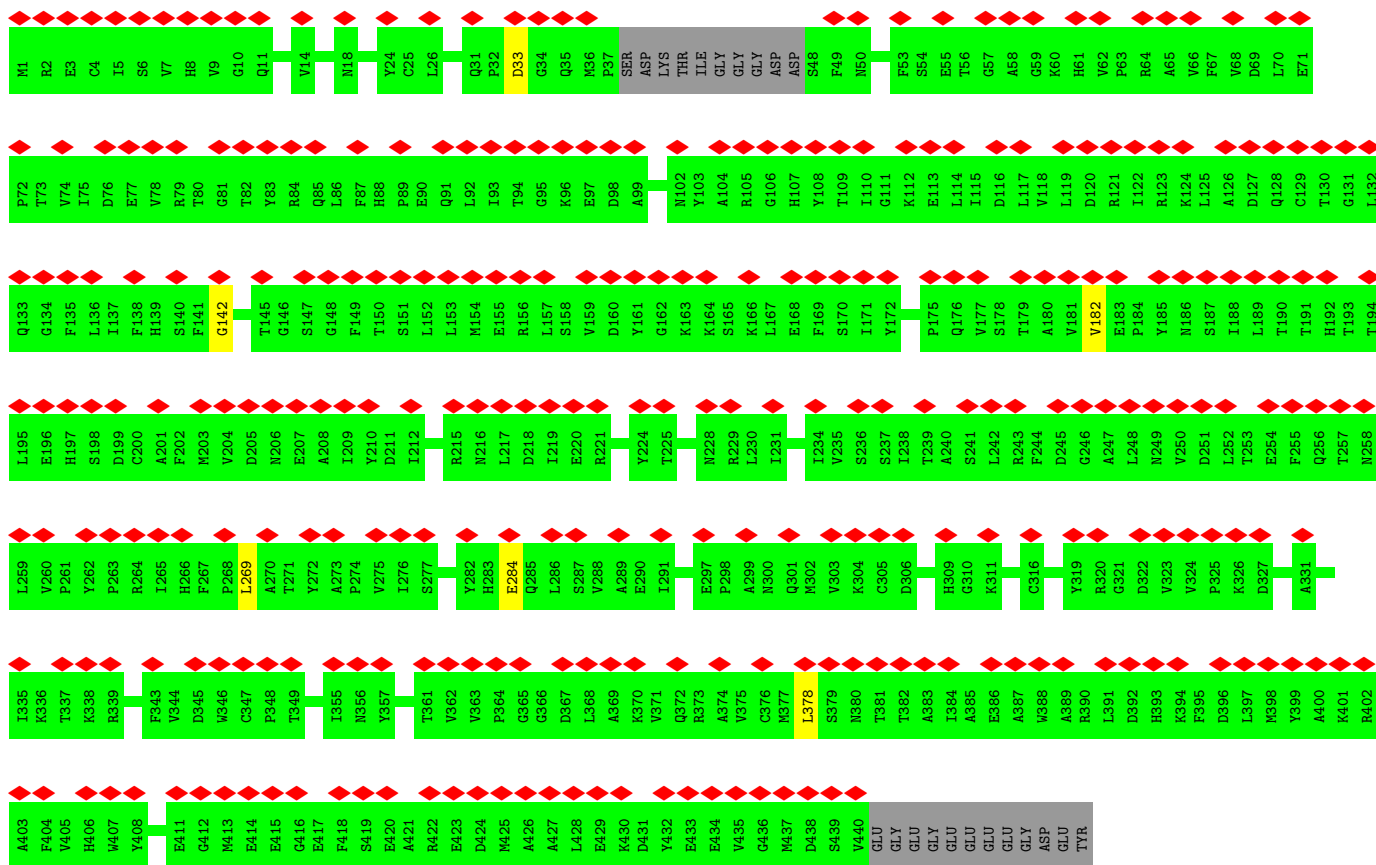


● Molecule 8: Tubulin alpha-1D chain

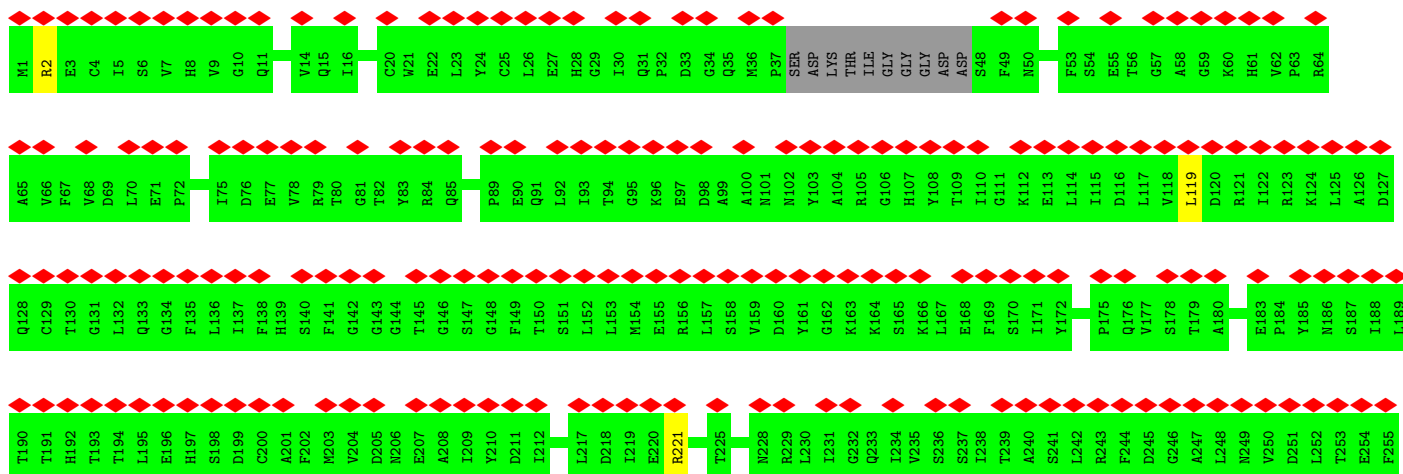
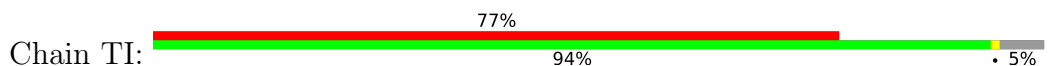


GLY  
GLU  
GLN  
GLU  
GLU  
GLU  
GLU  
GLU  
GLY  
ASP  
ASN  
TYR

• Molecule 8: Tubulin alpha-1D chain

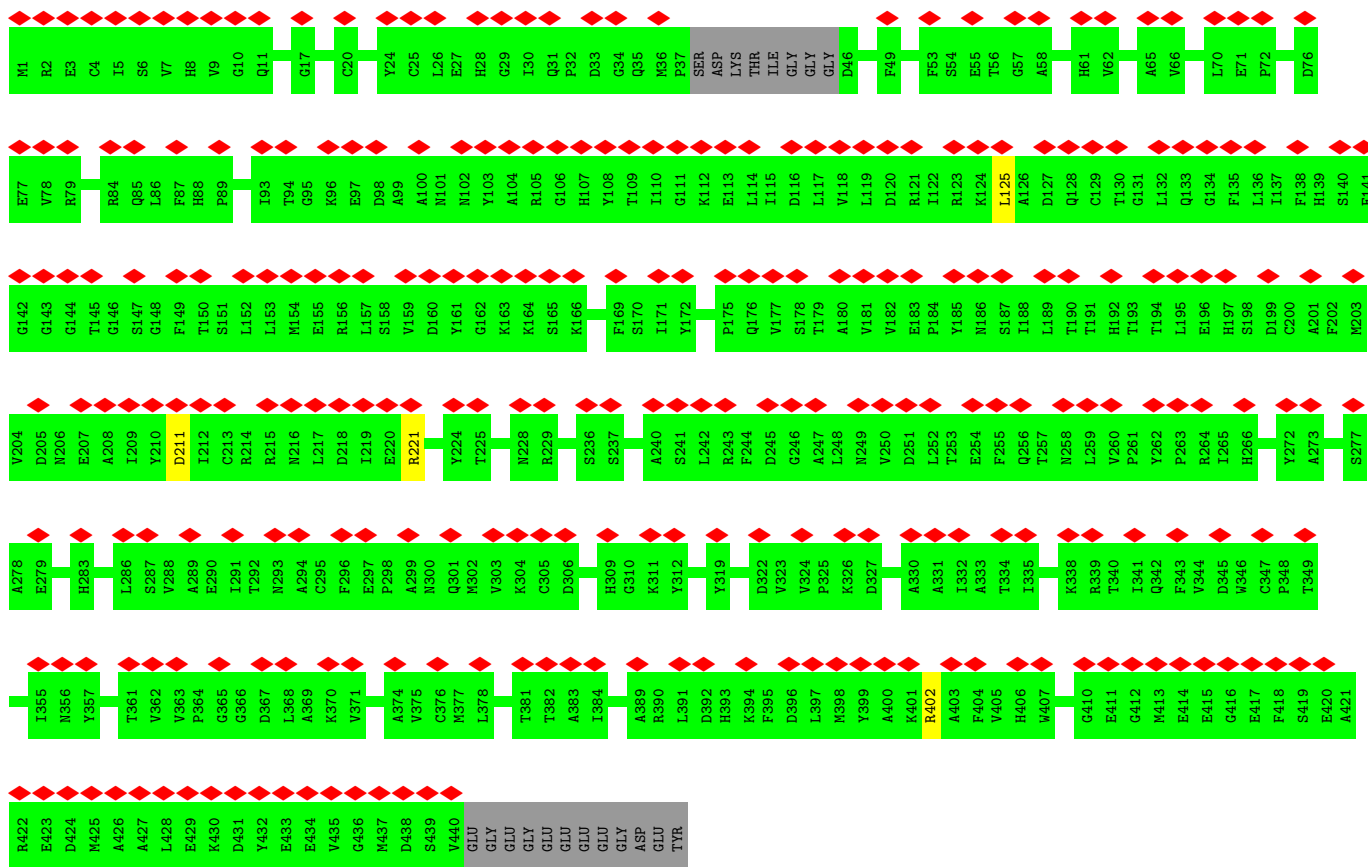


• Molecule 8: Tubulin alpha-1D chain





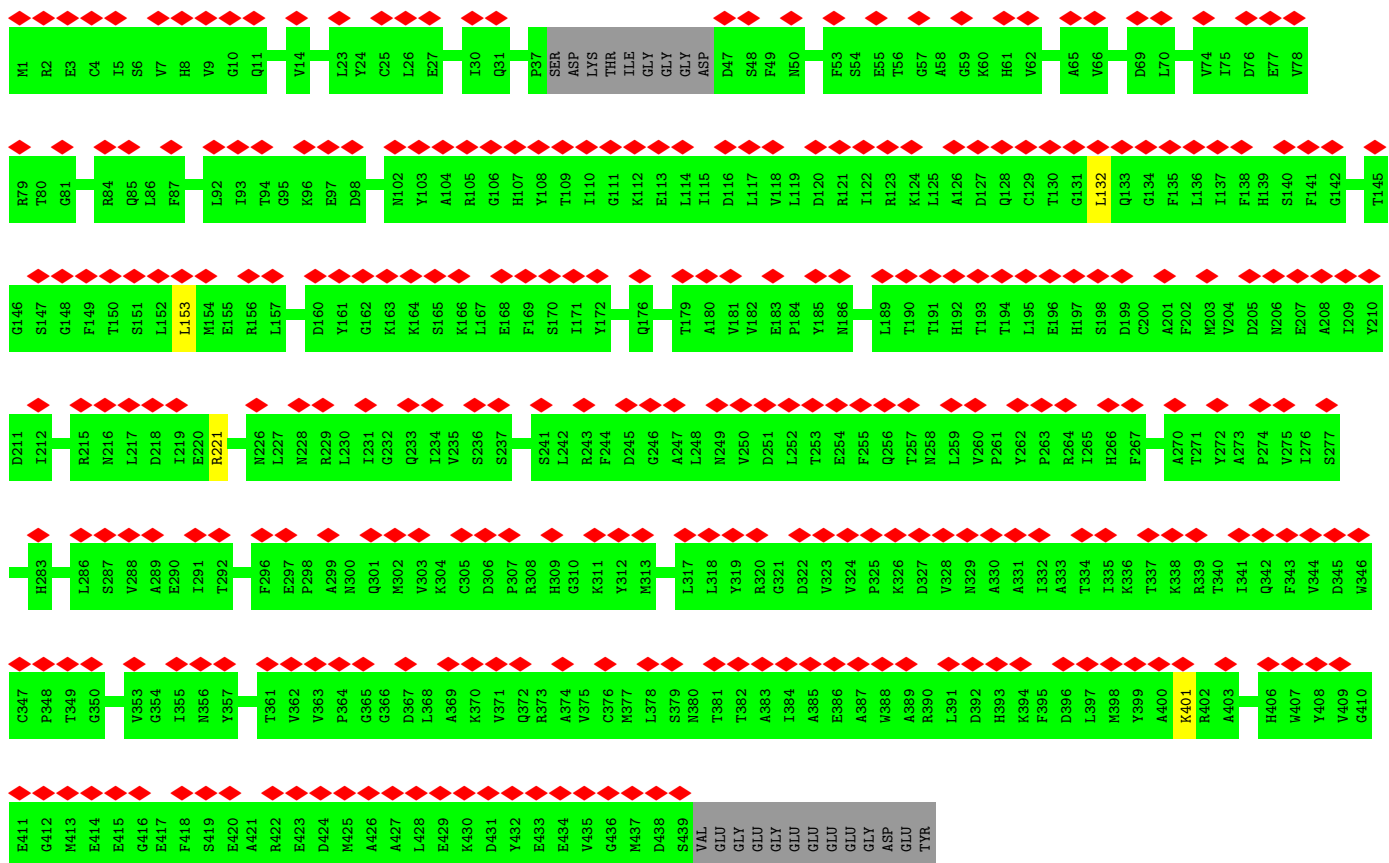
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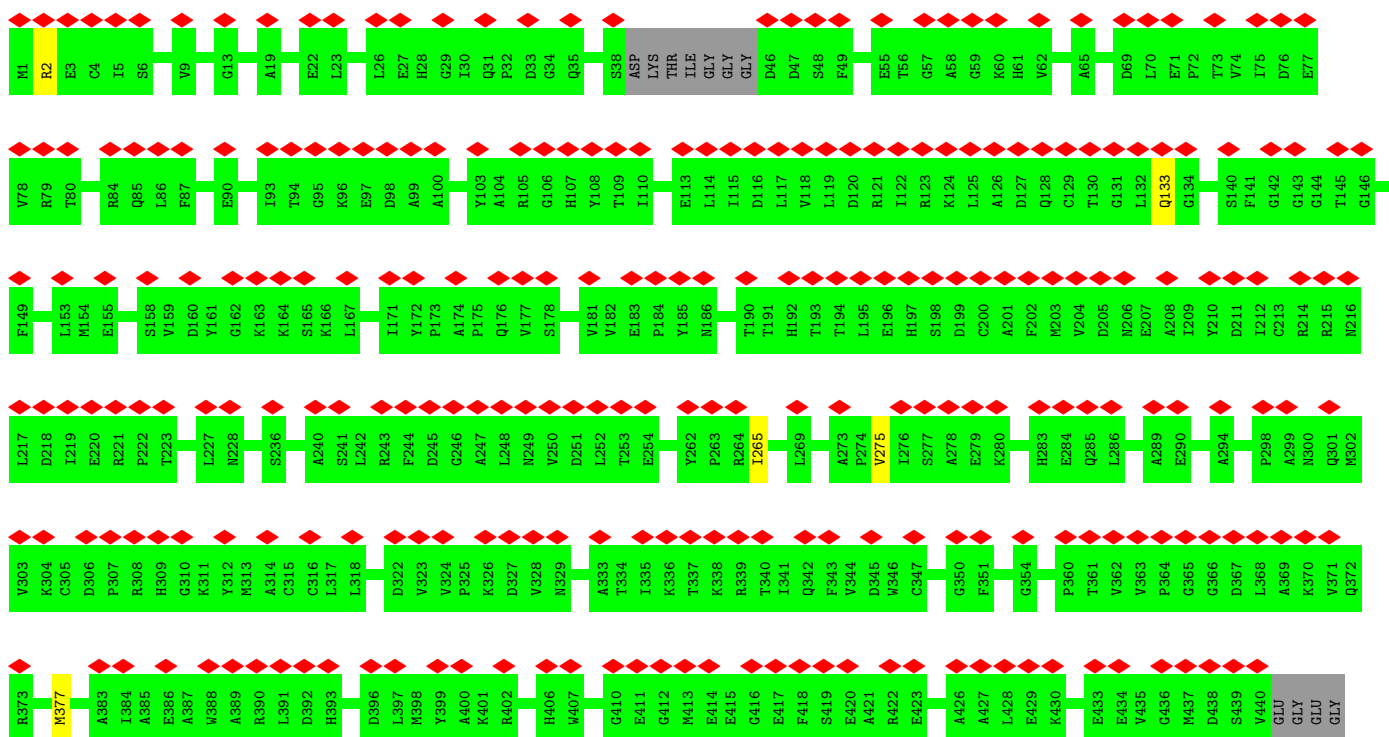
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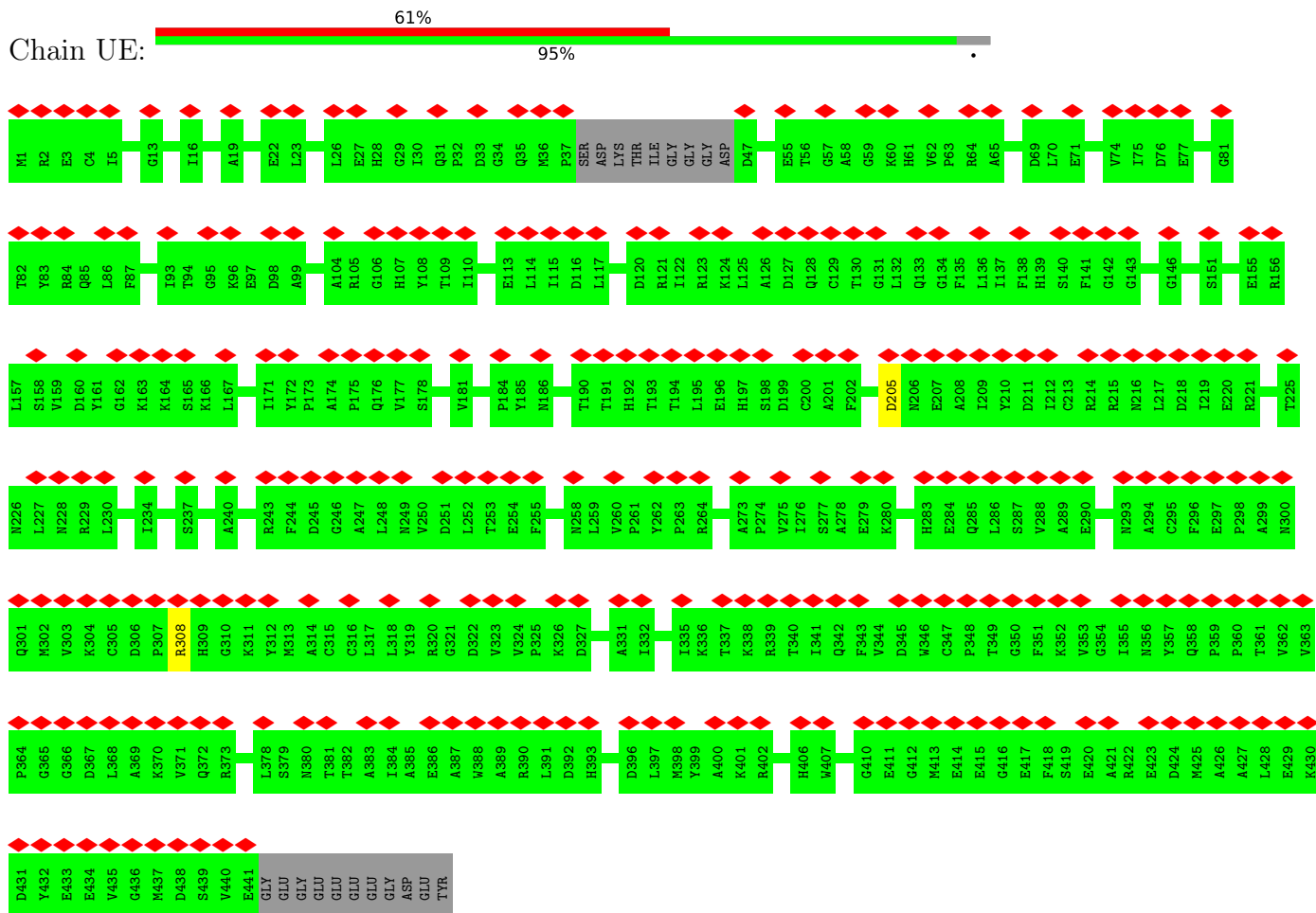


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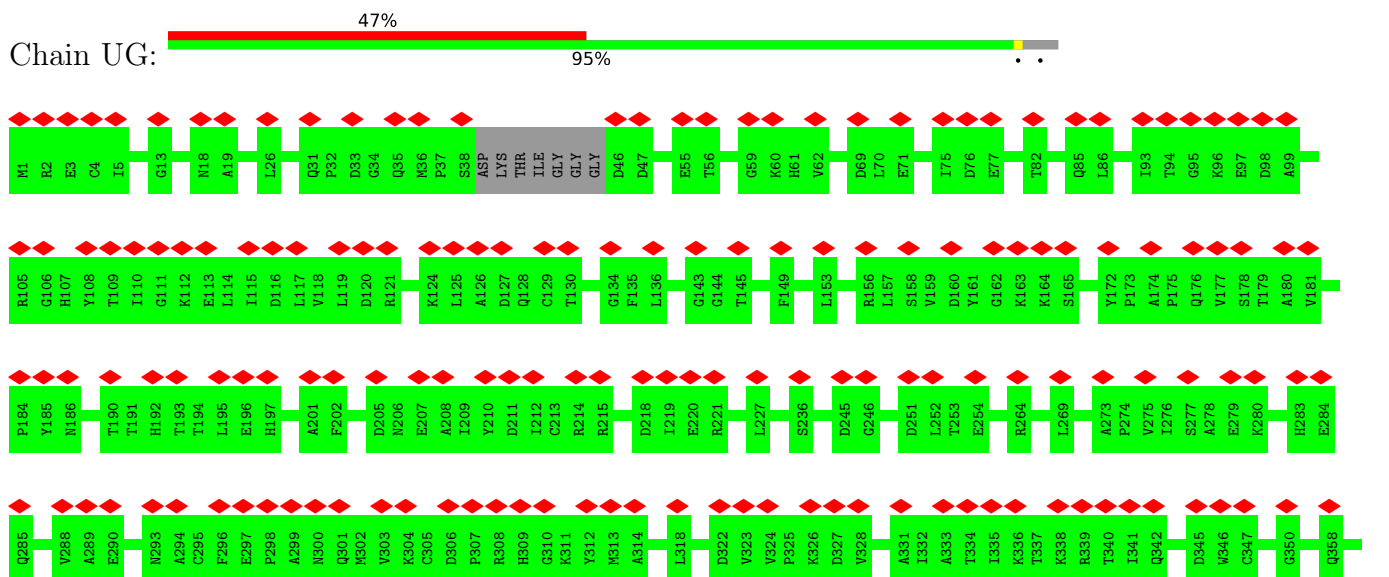


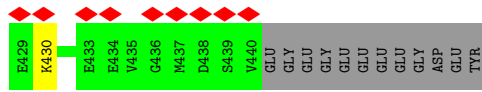
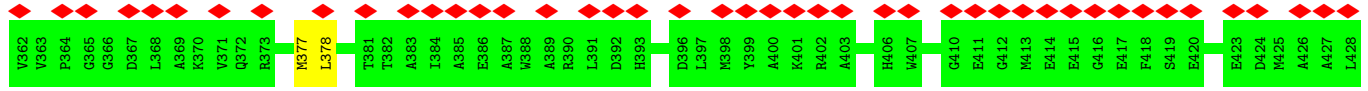
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GLU  
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GLU  
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• Molecule 8: Tubulin alpha-1D chain

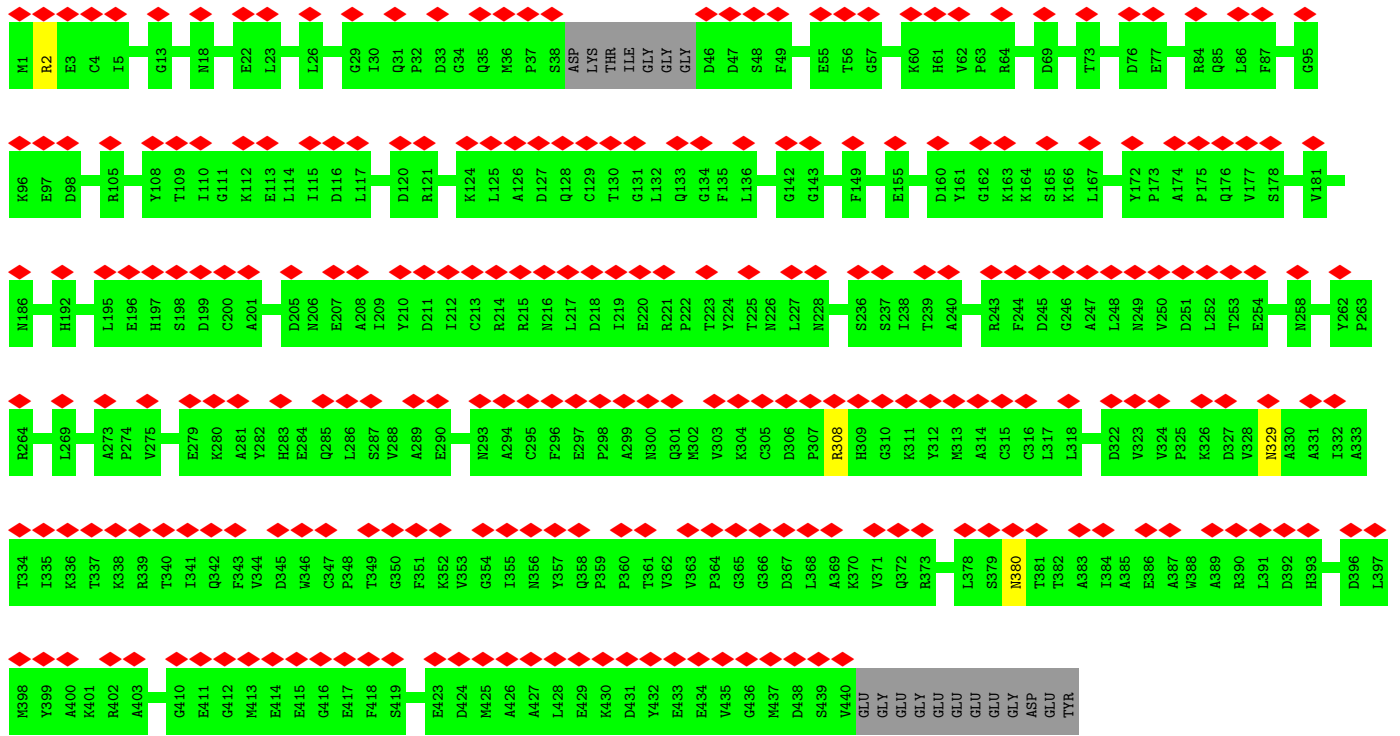


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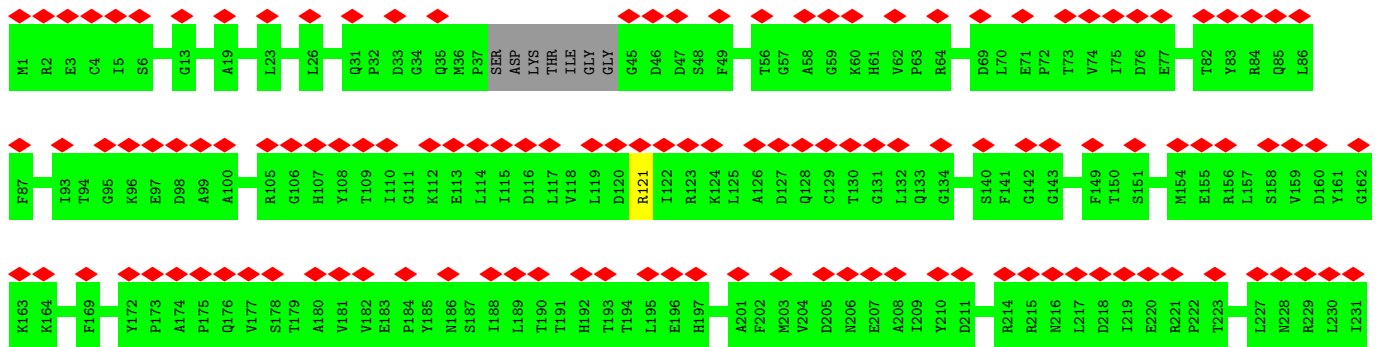


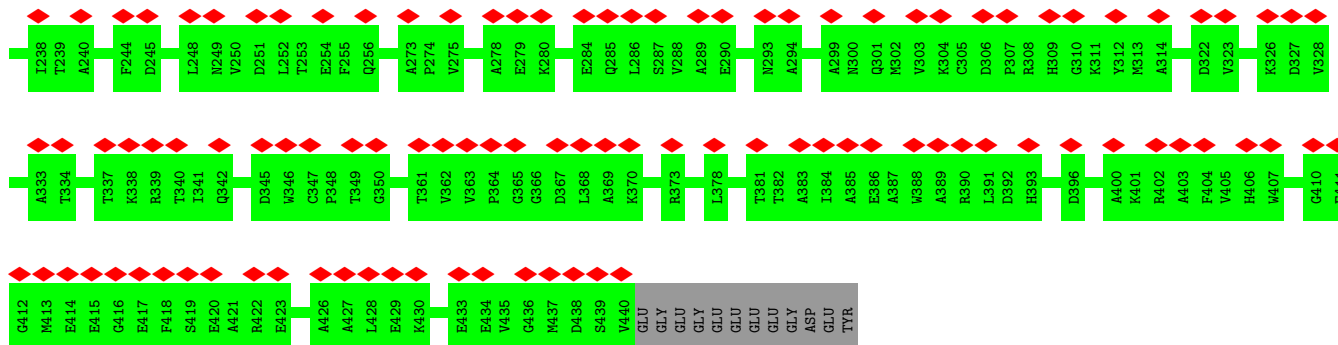


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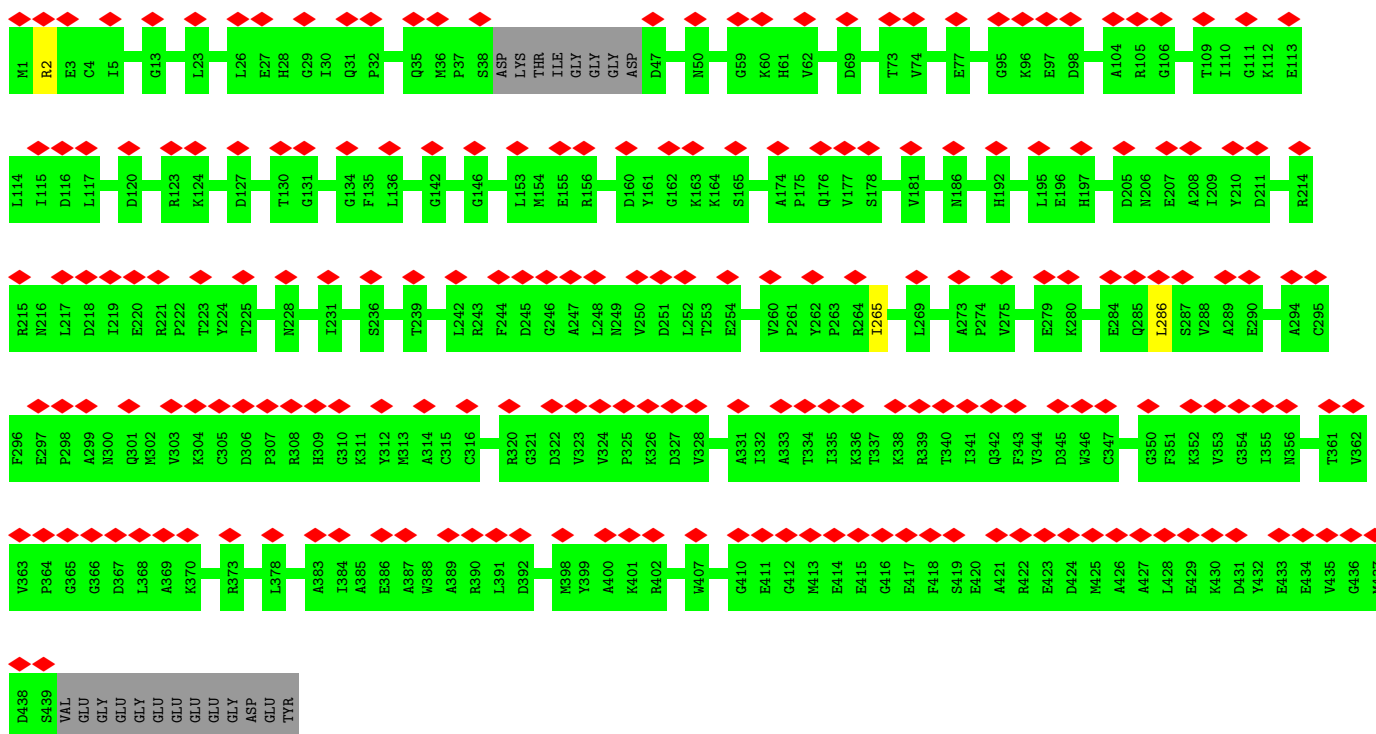


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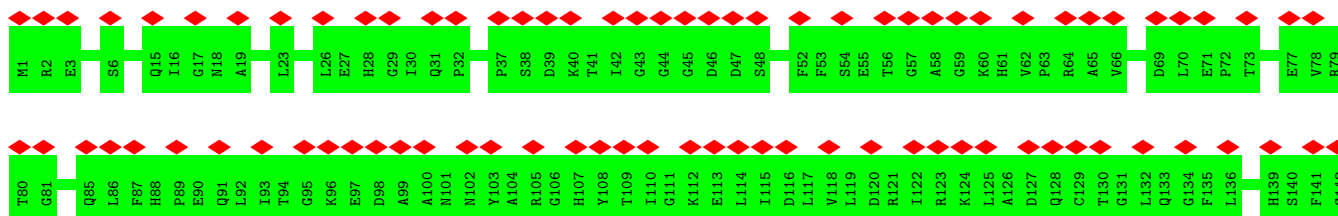


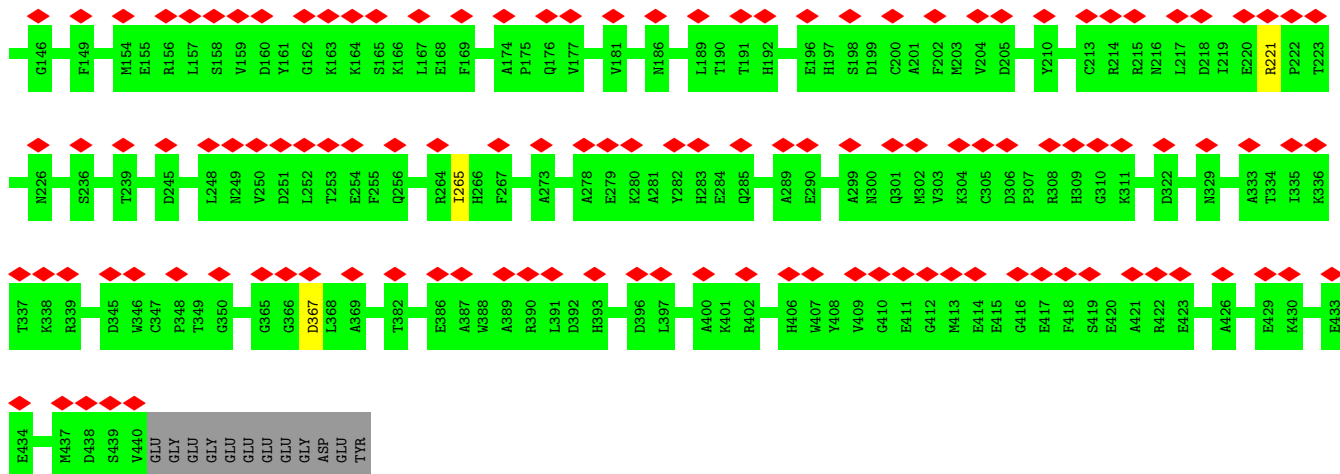


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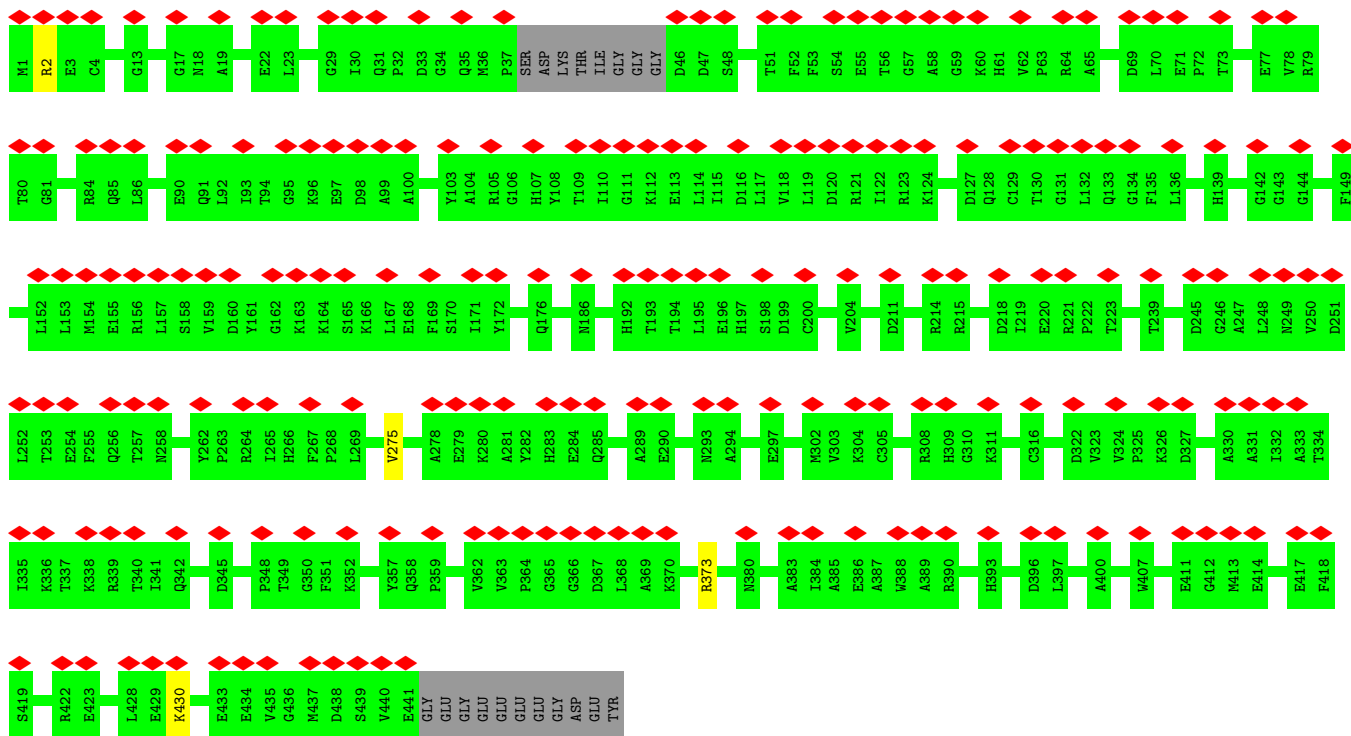


• Molecule 8: Tubulin alpha-1D chain

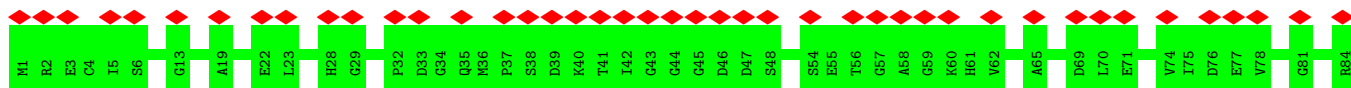


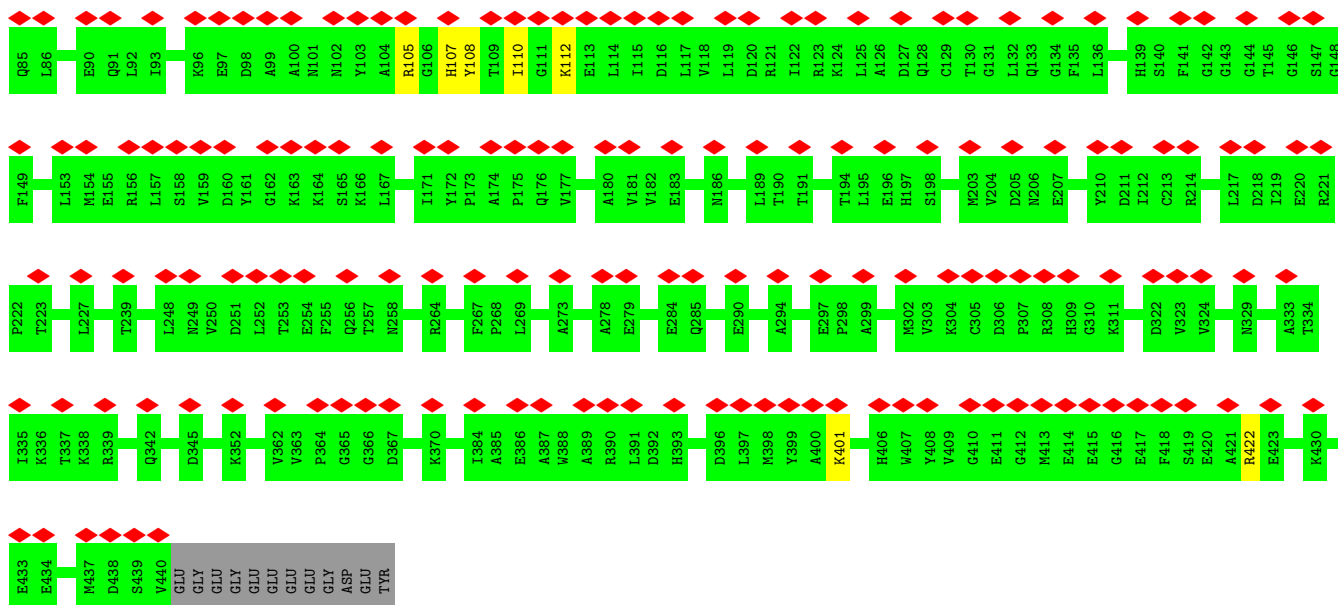


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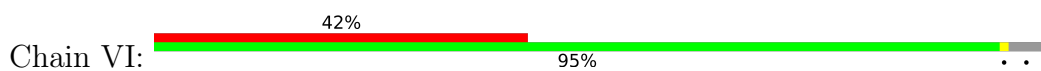


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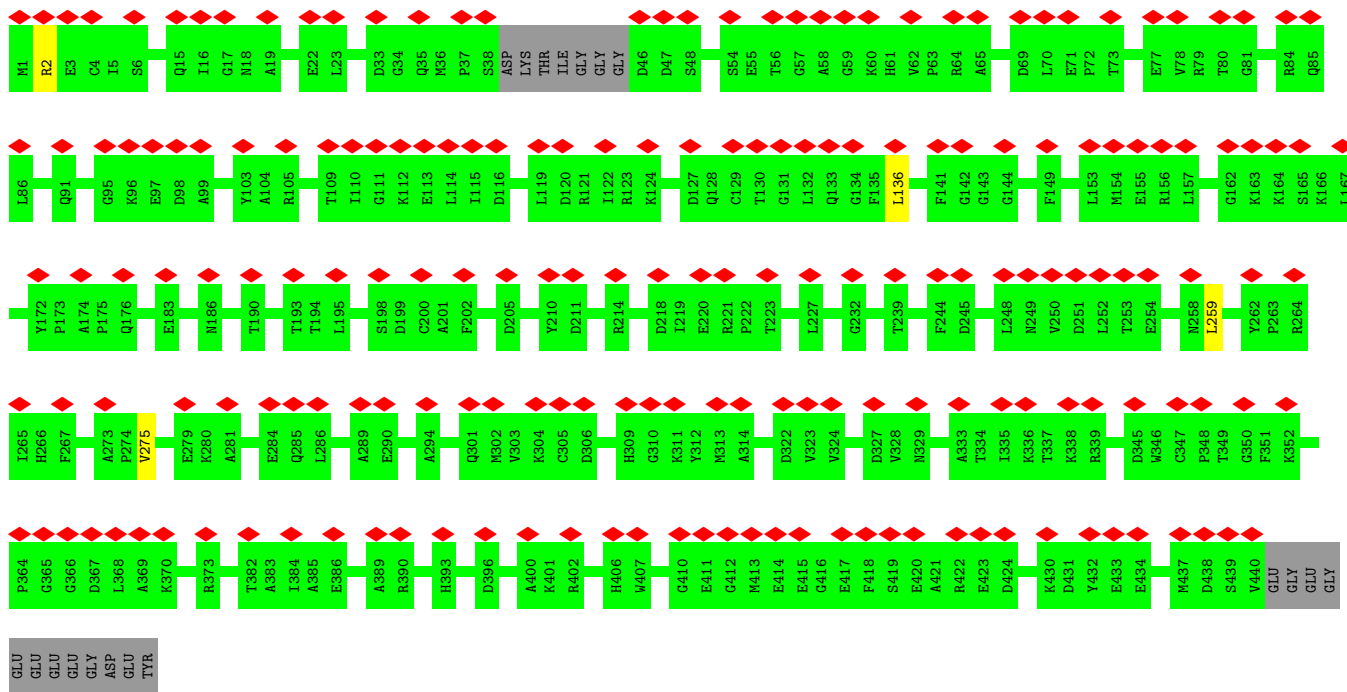




• Molecule 8: Tubulin alpha-1D chain



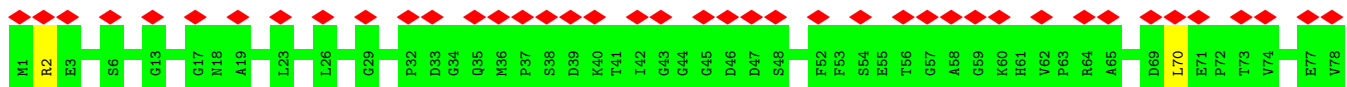
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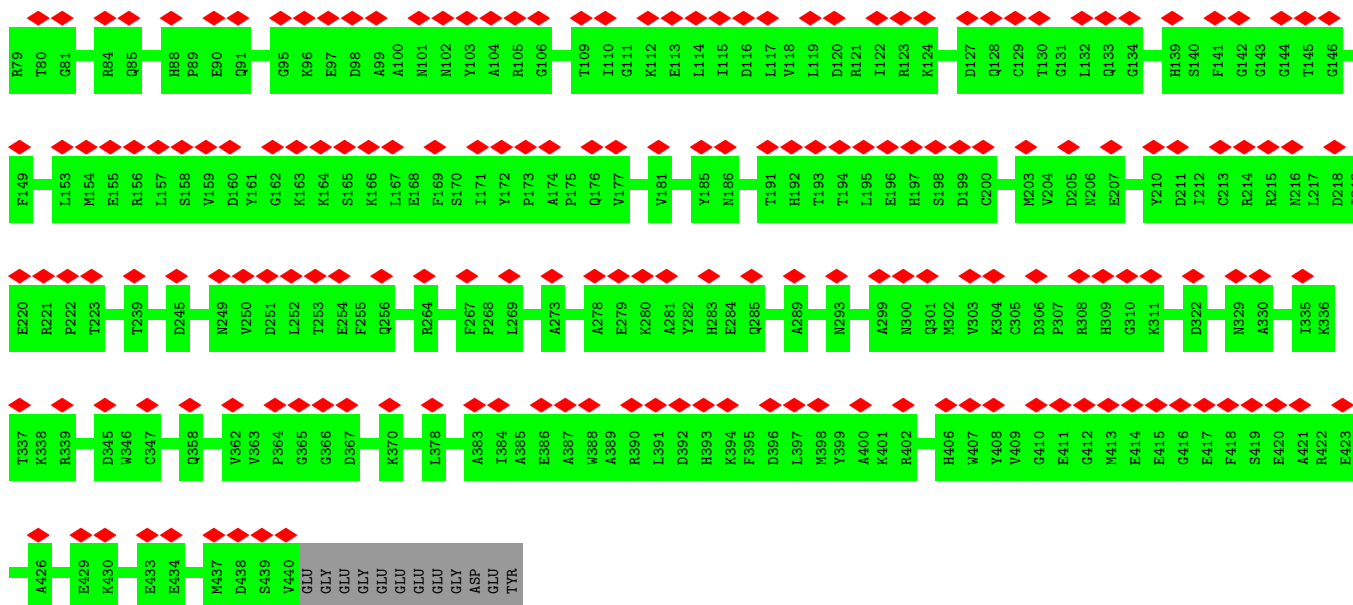


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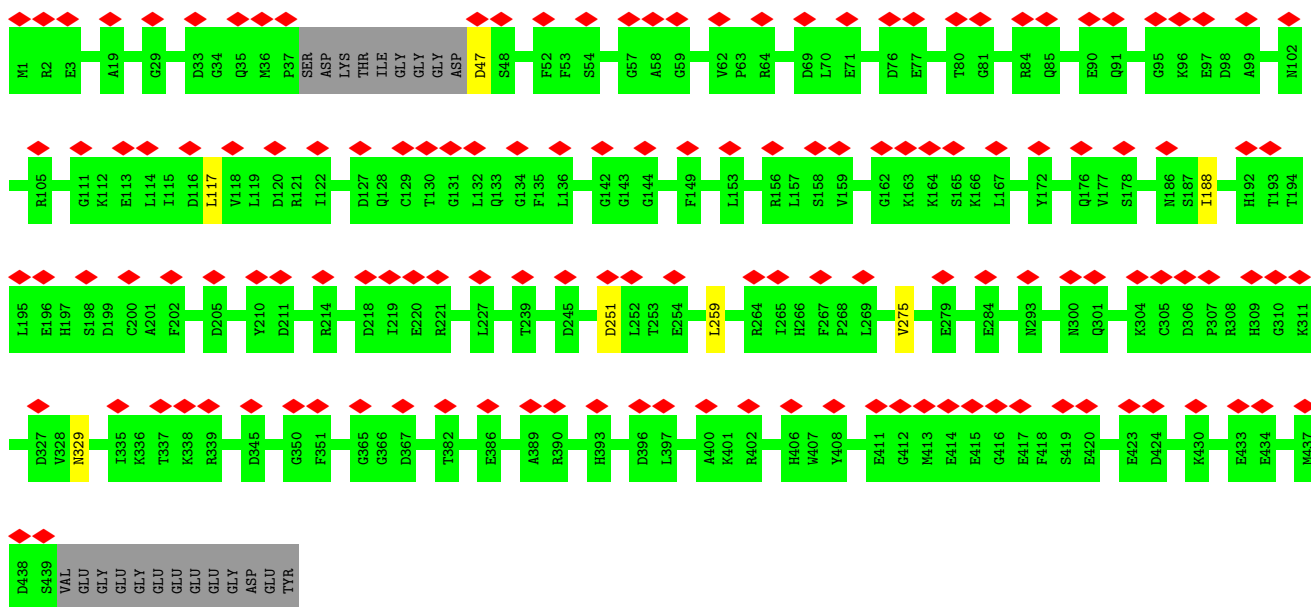


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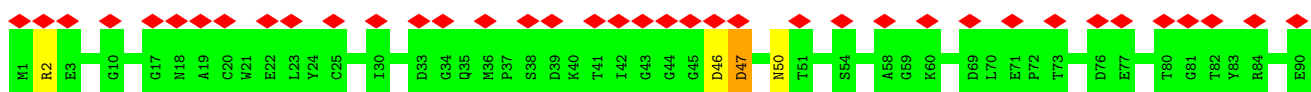
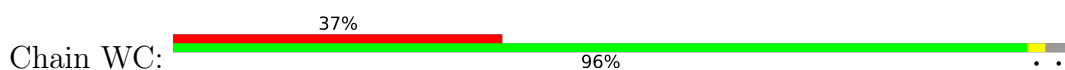


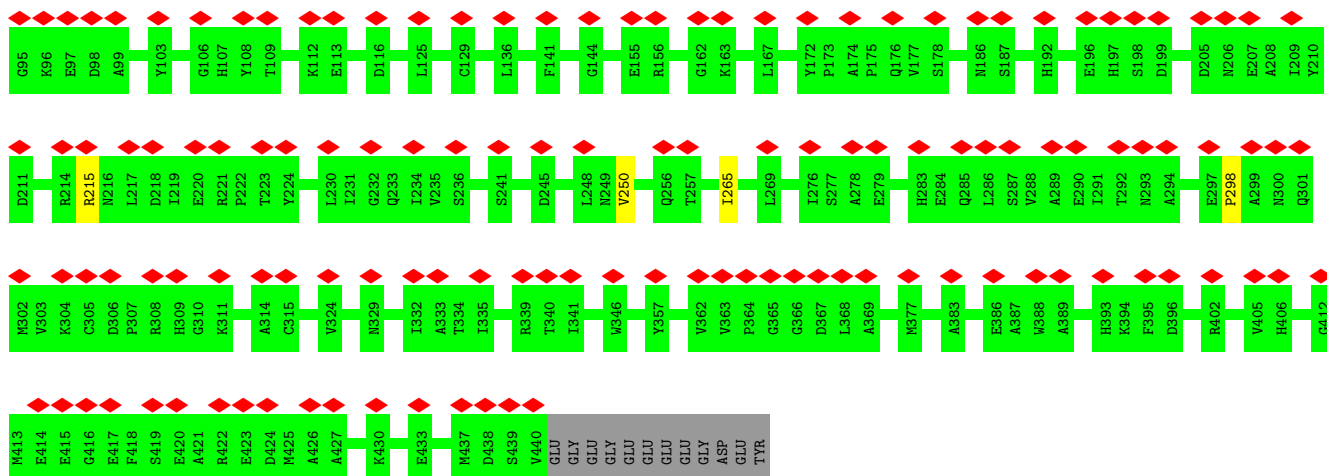


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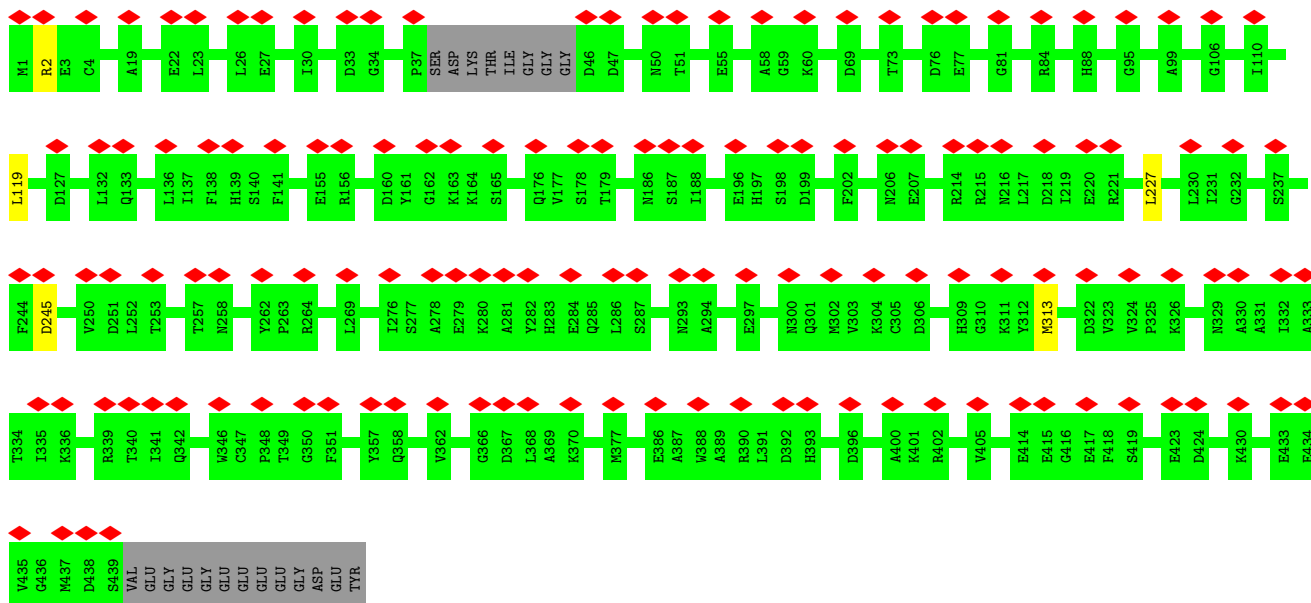


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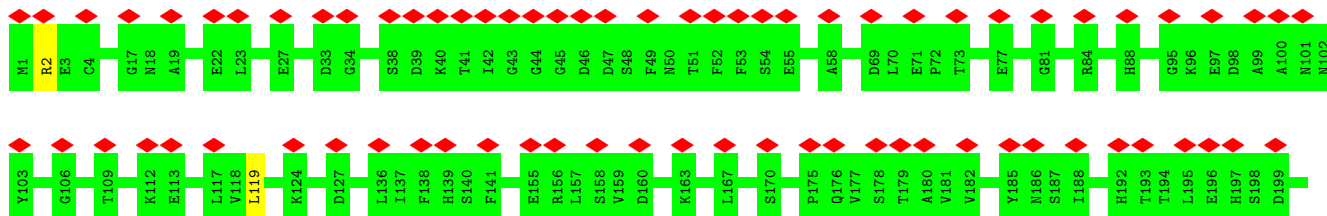
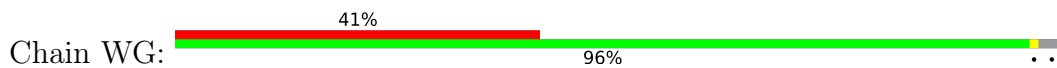




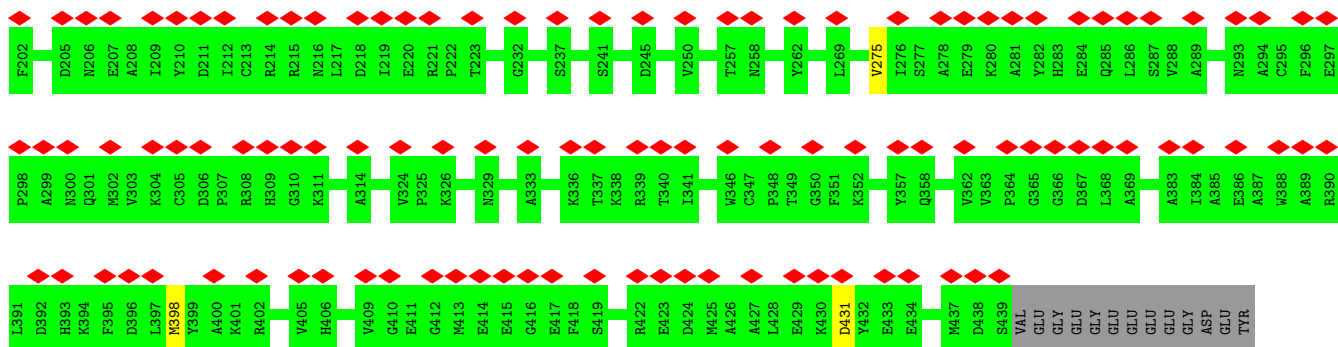
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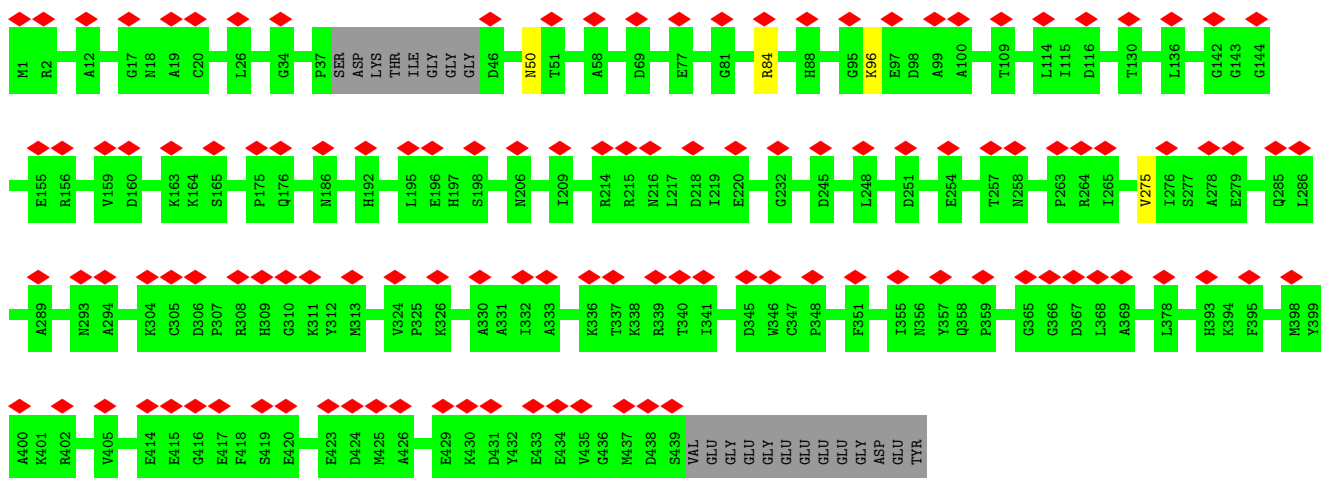
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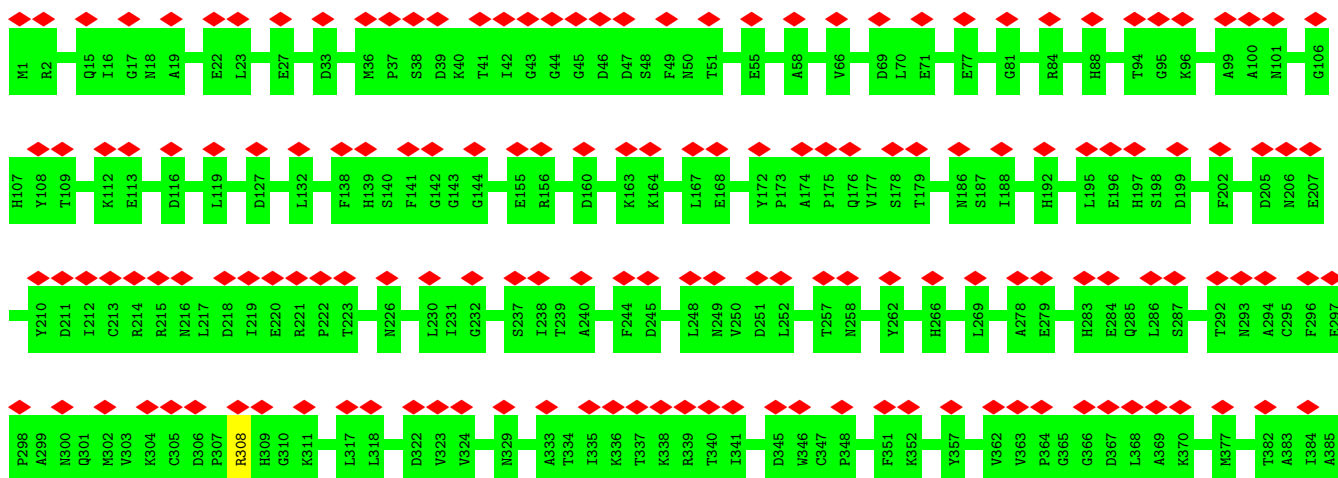


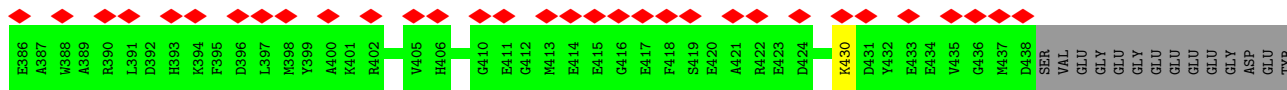


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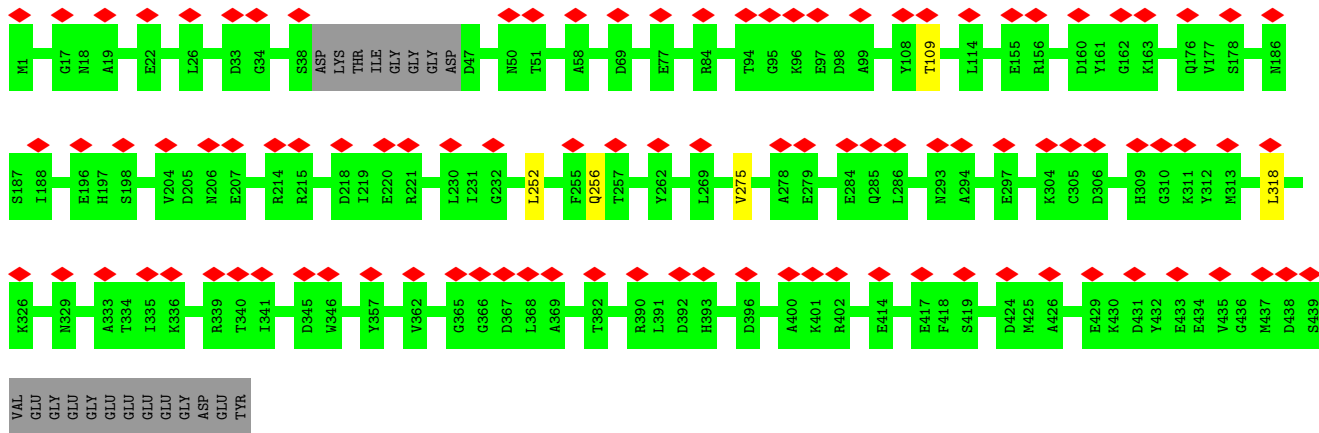


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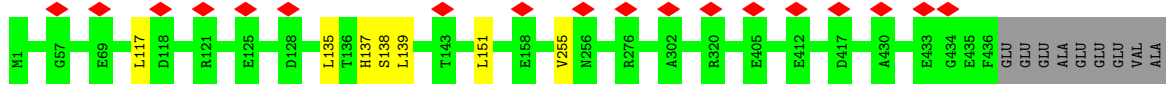
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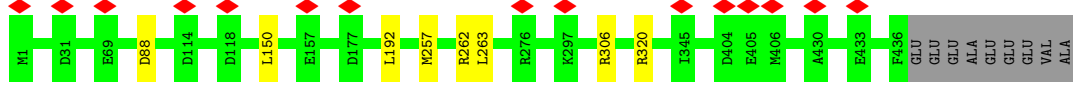
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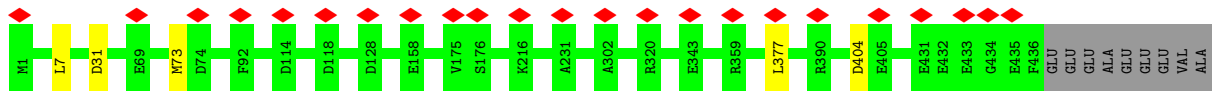
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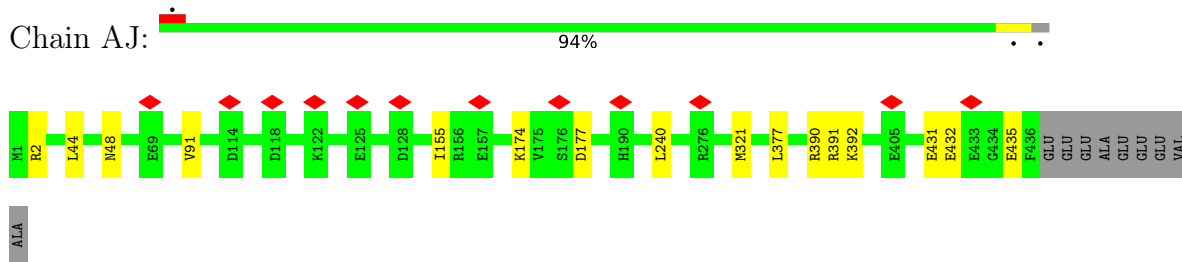
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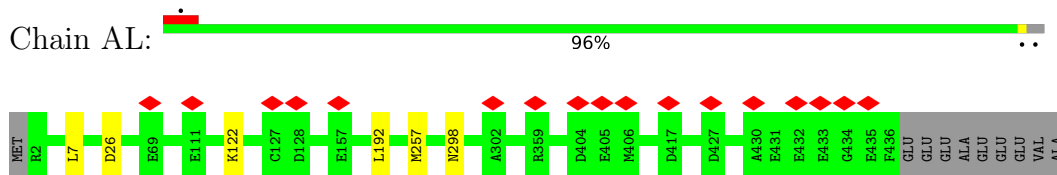
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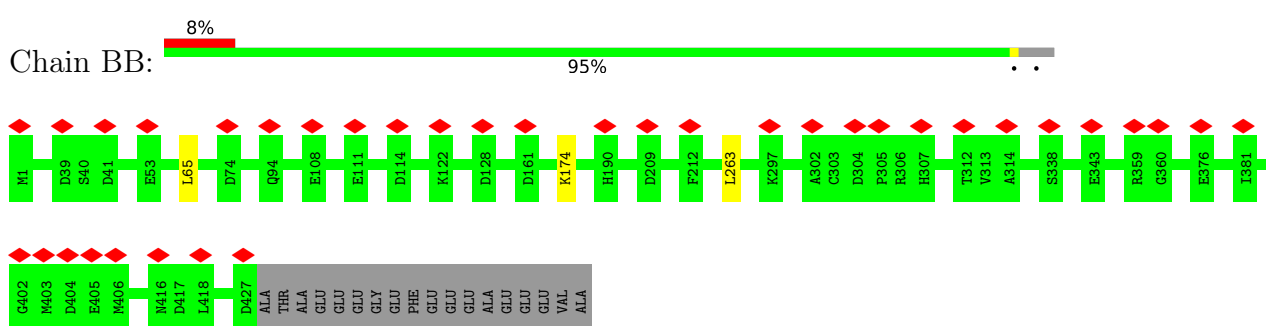
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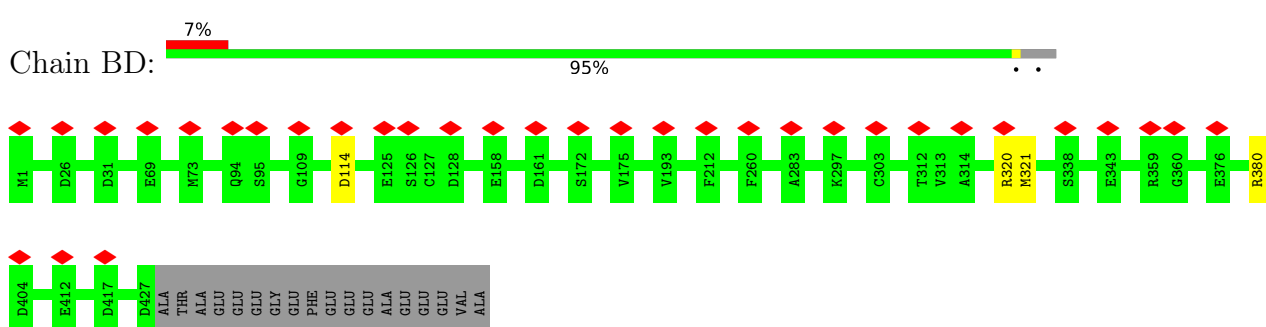
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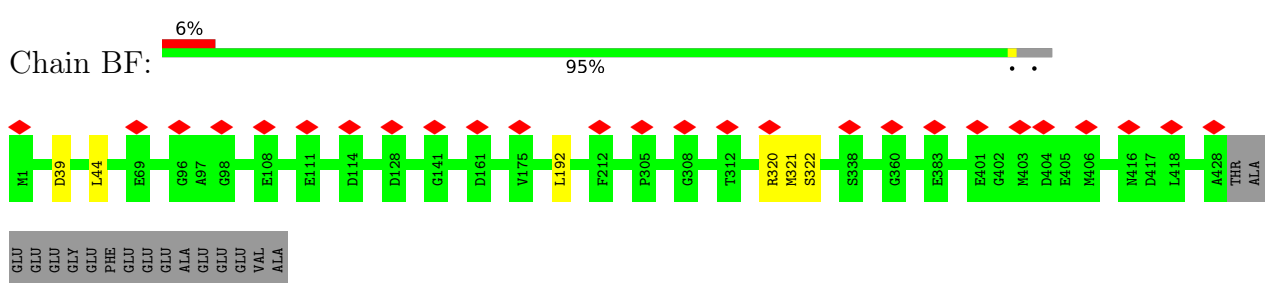
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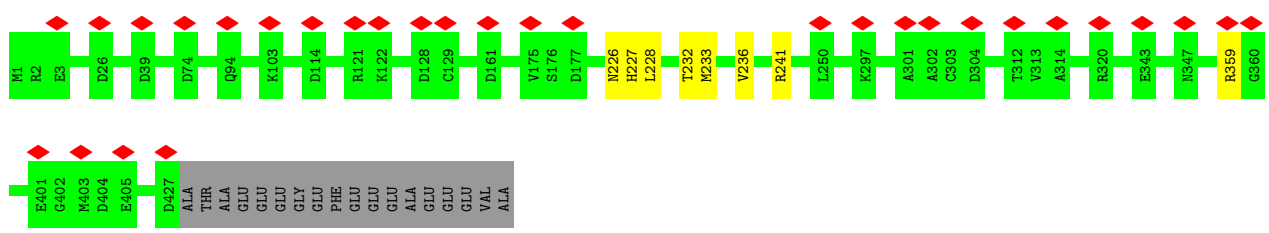
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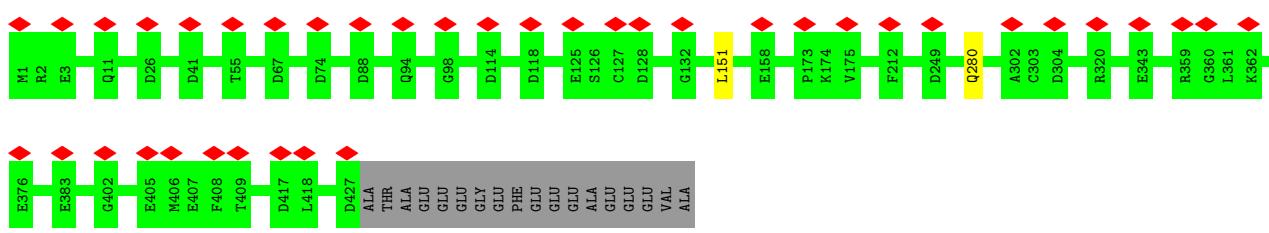
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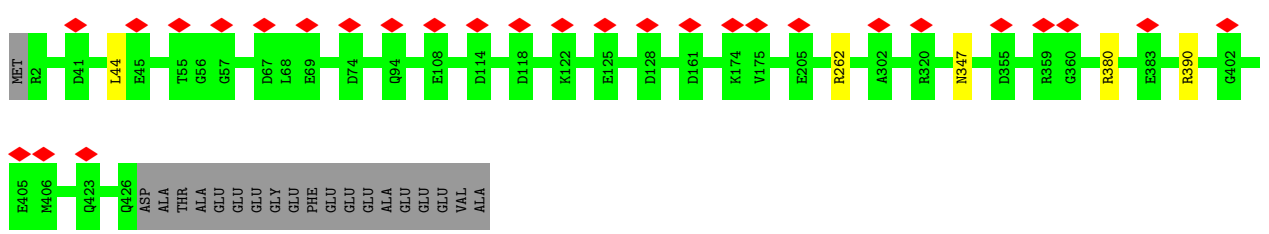
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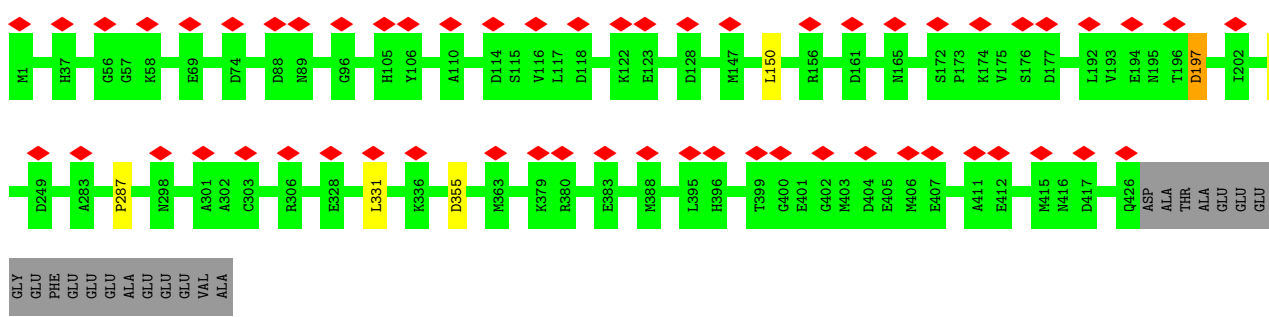
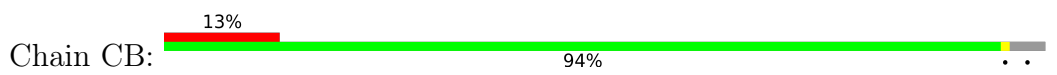
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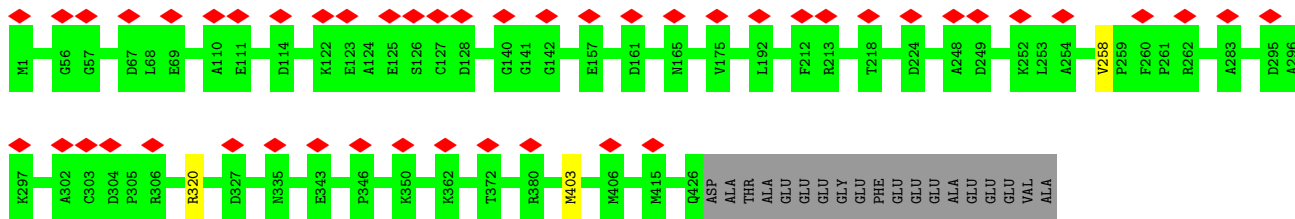


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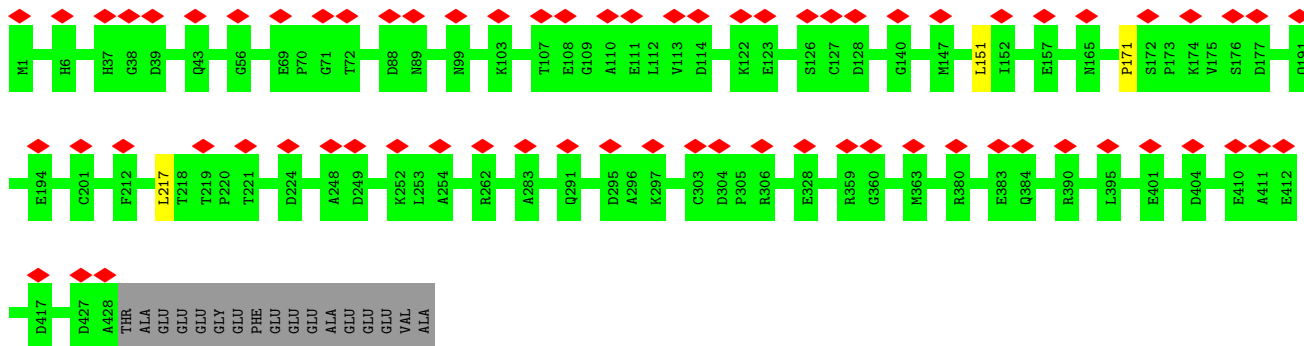


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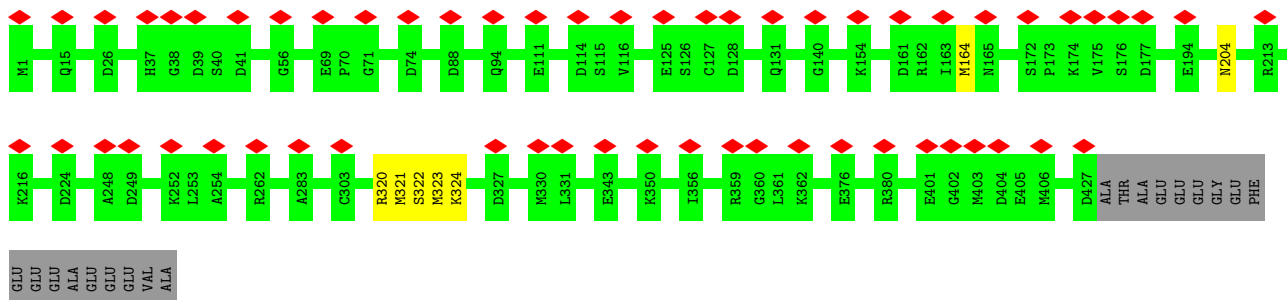




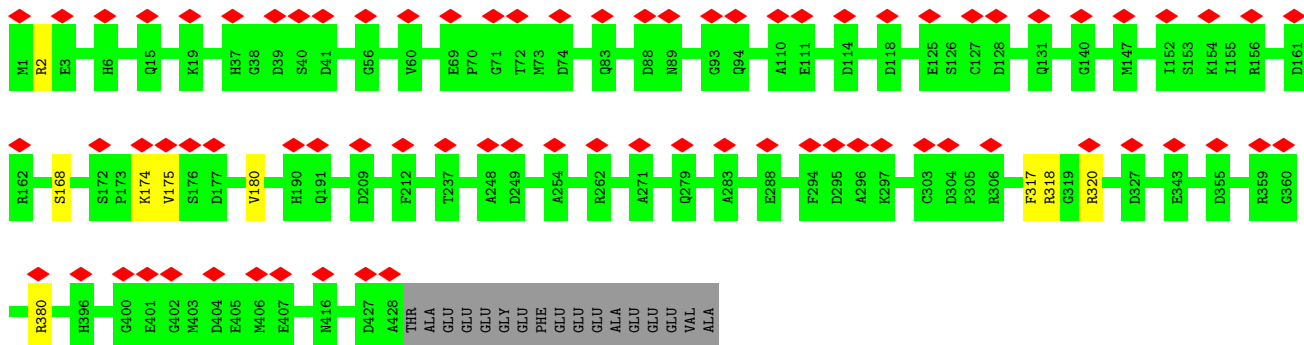
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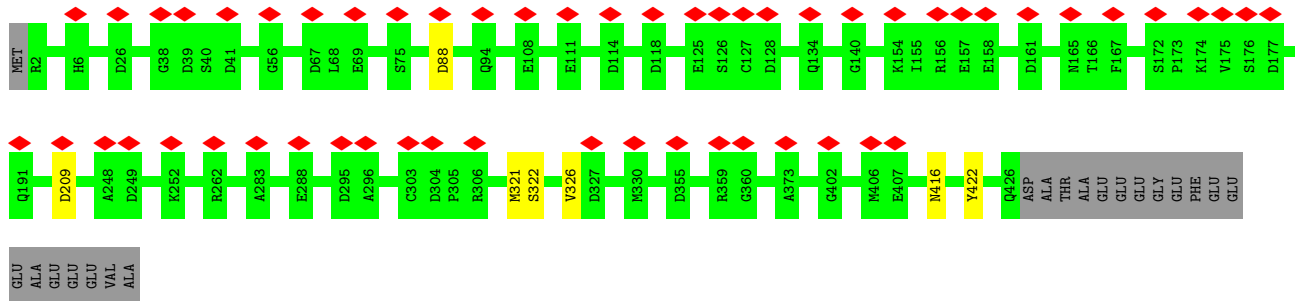
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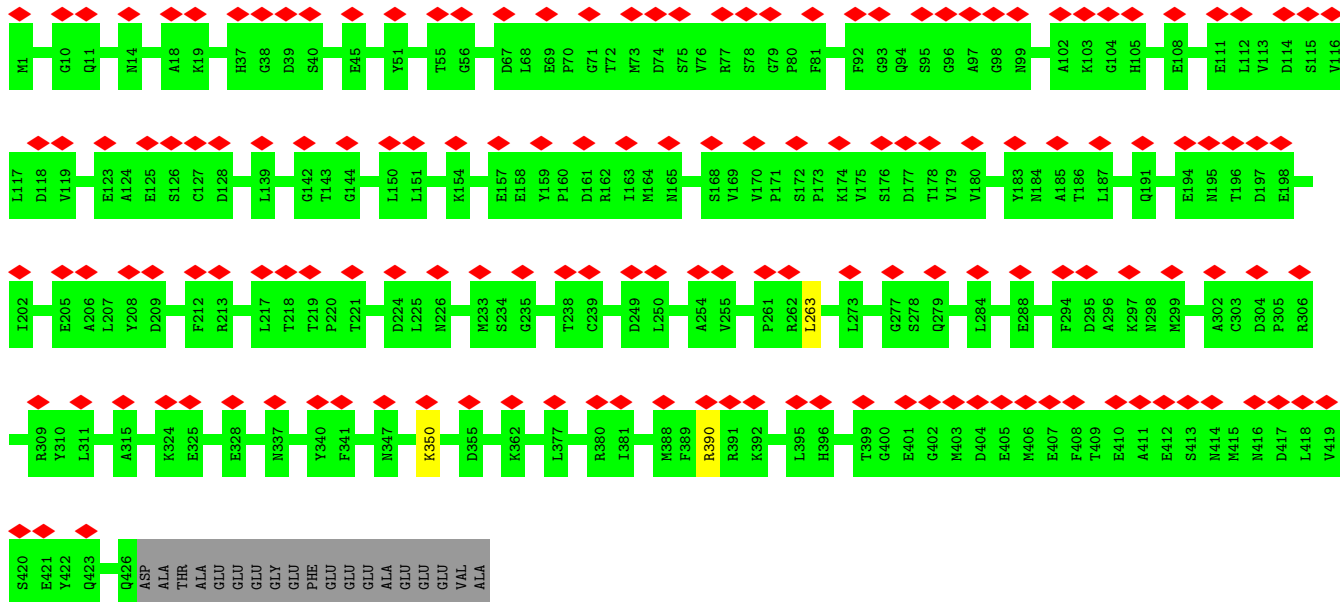
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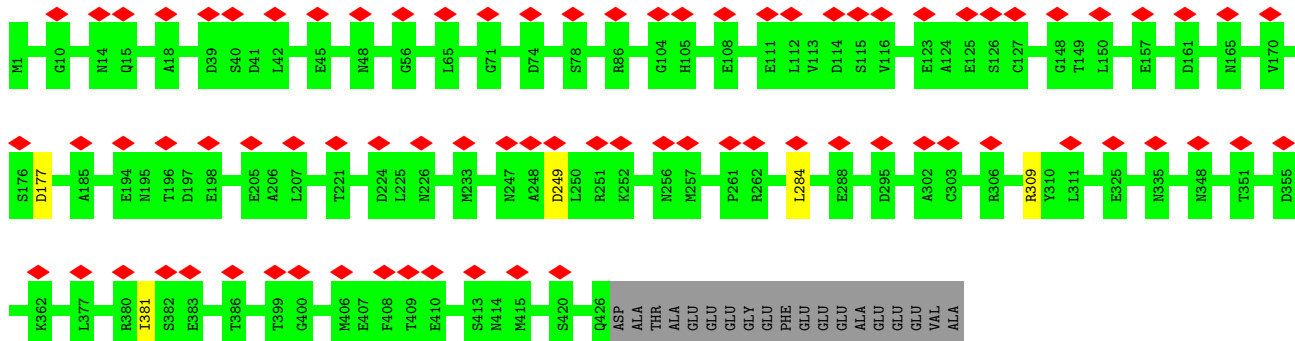
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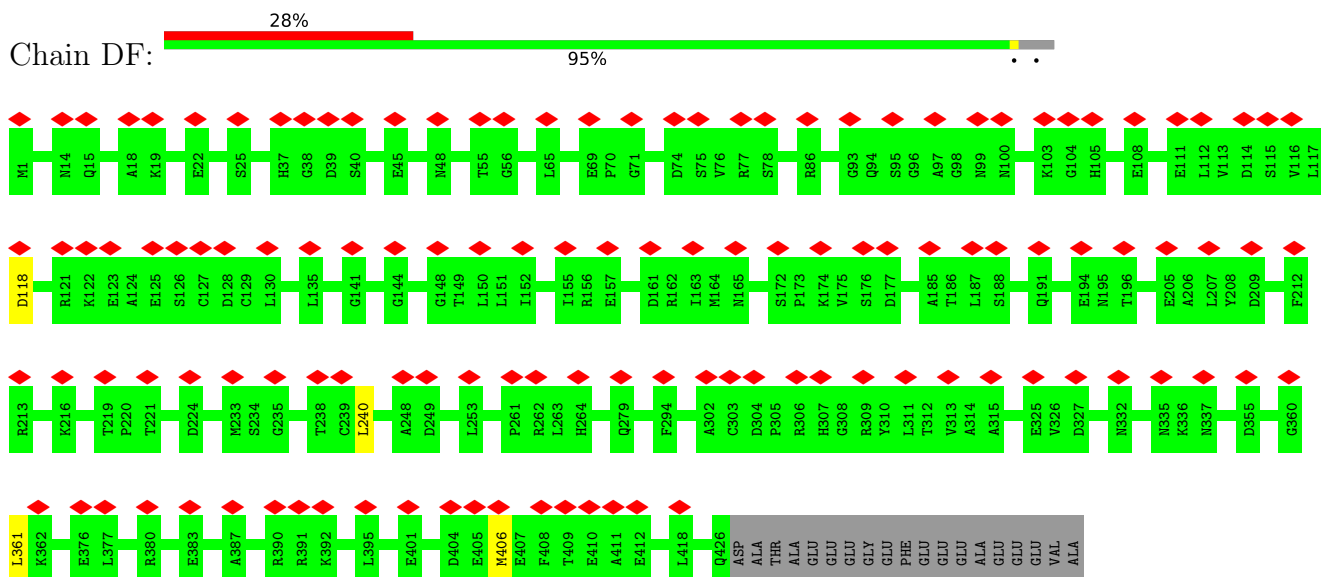
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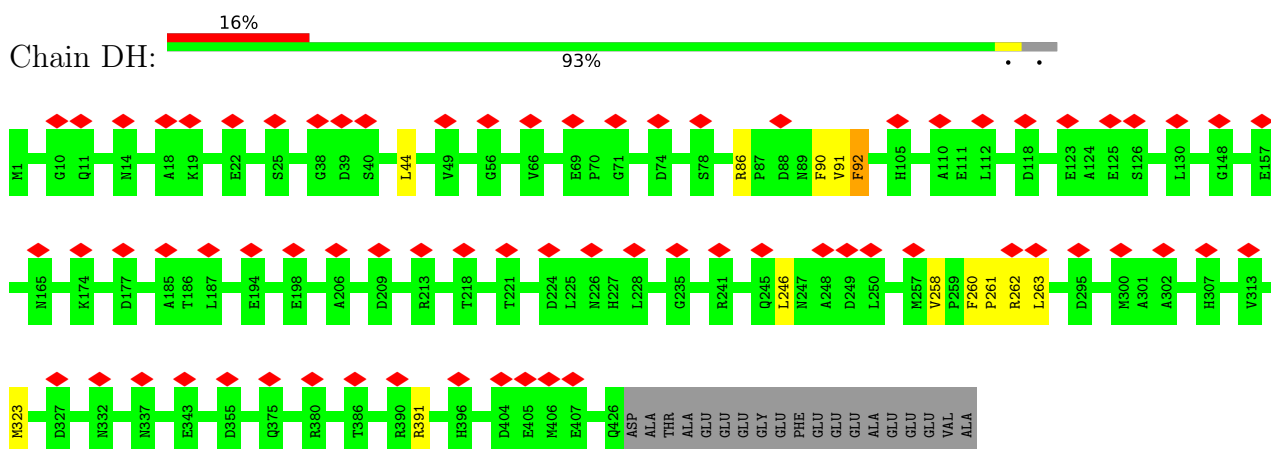
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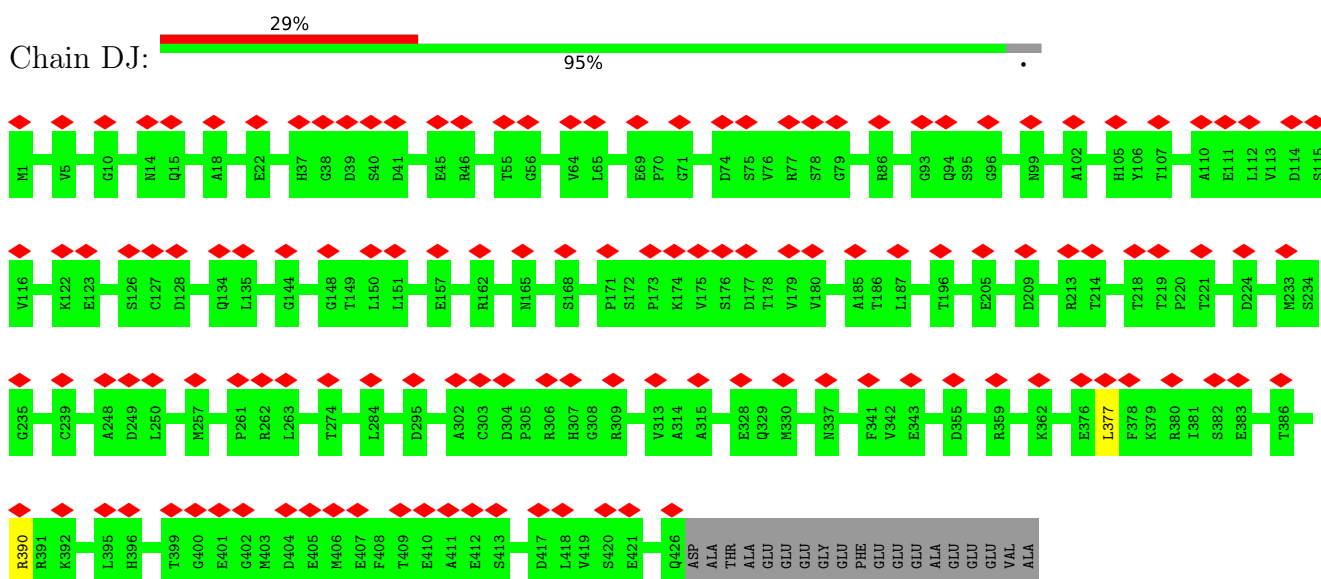
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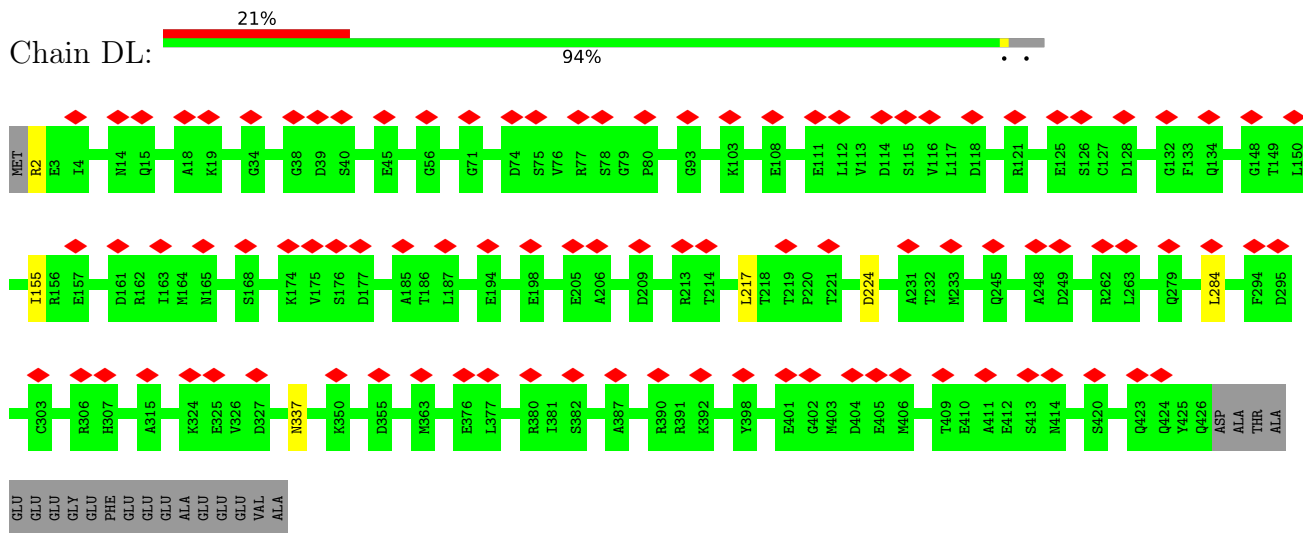
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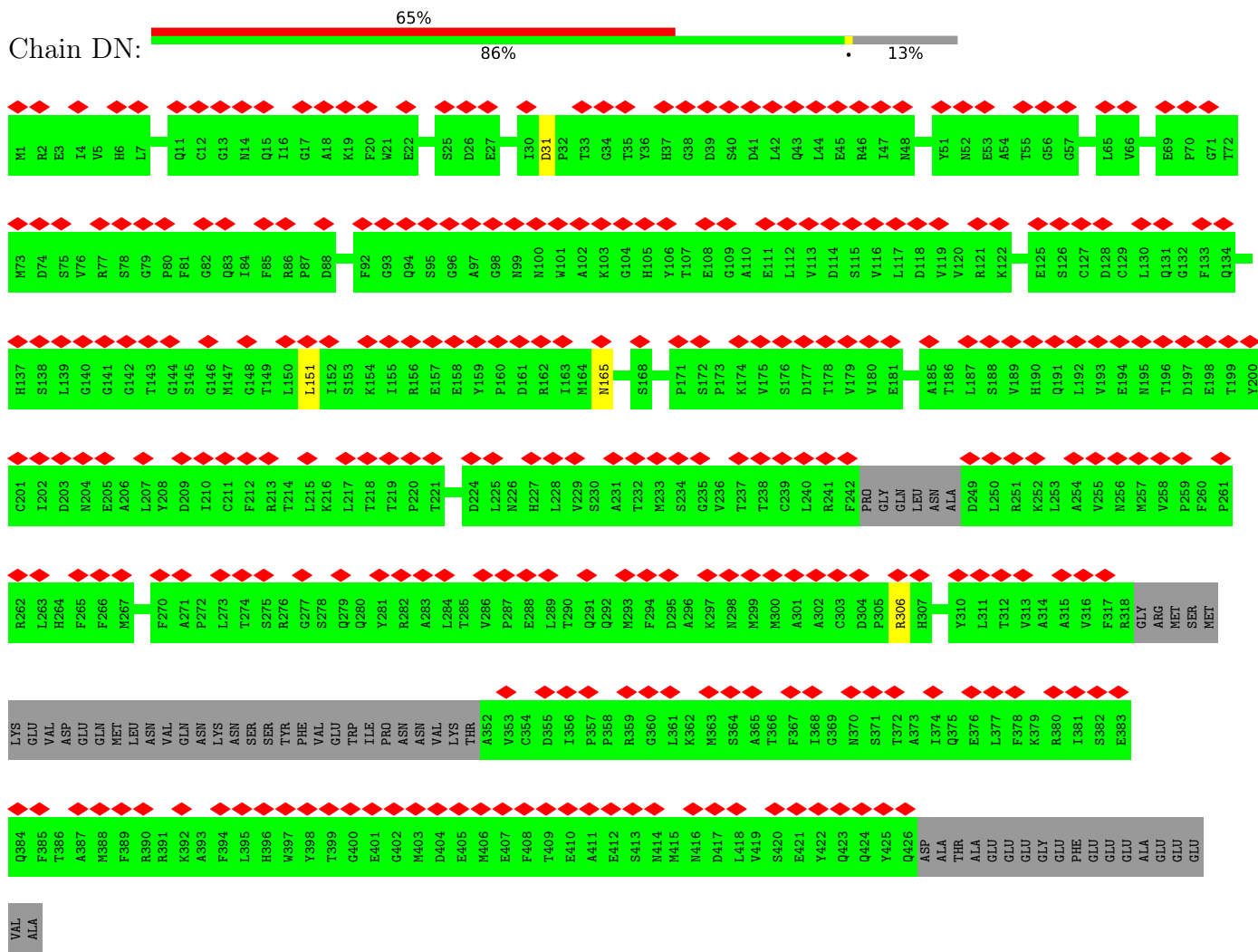
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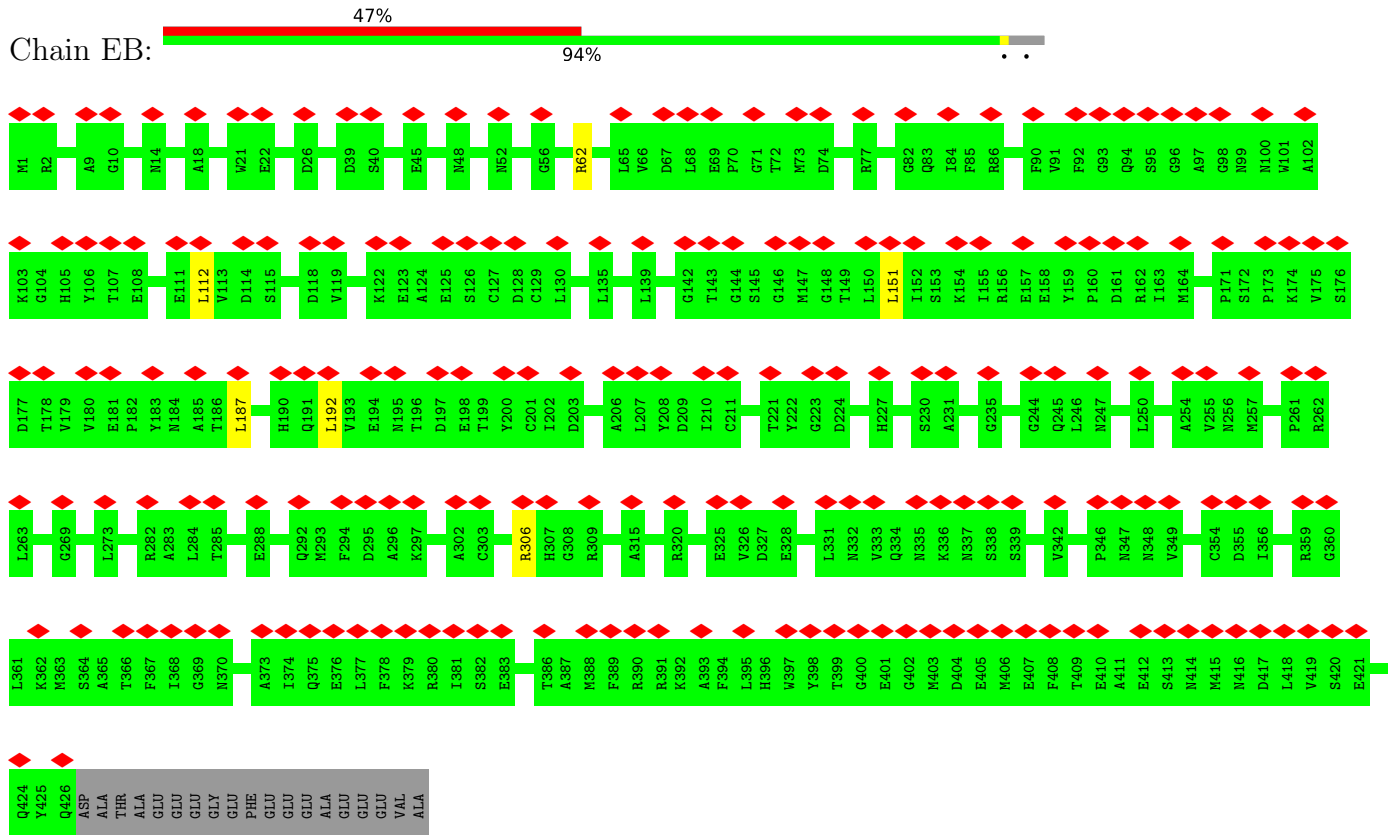


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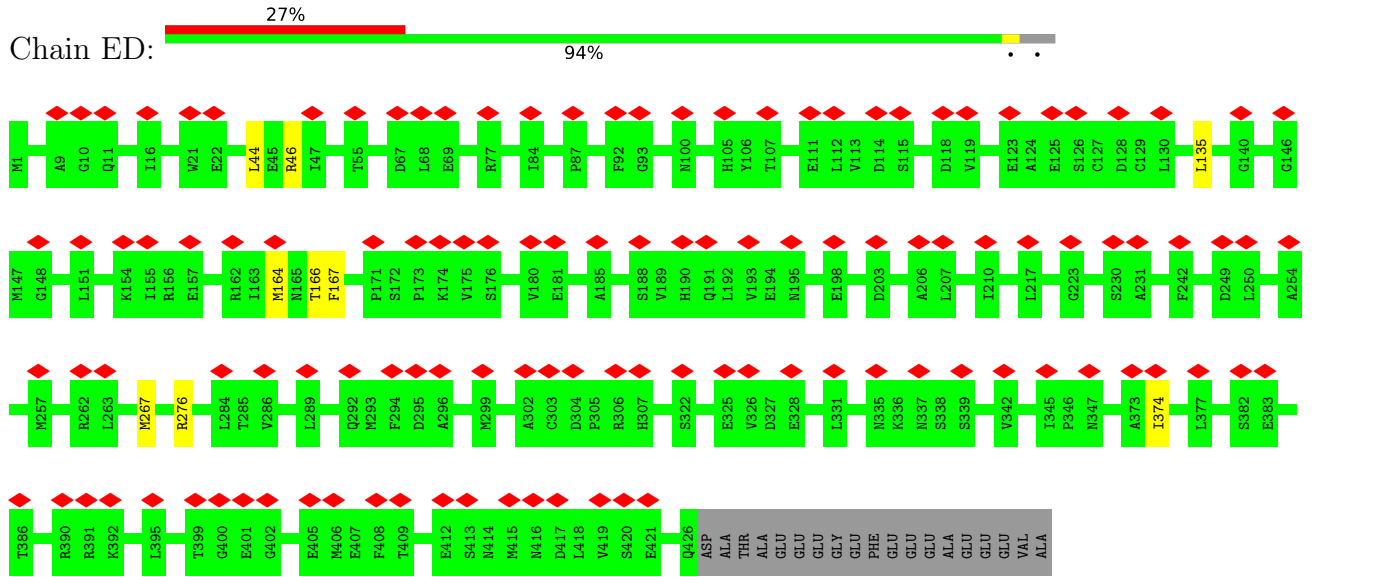


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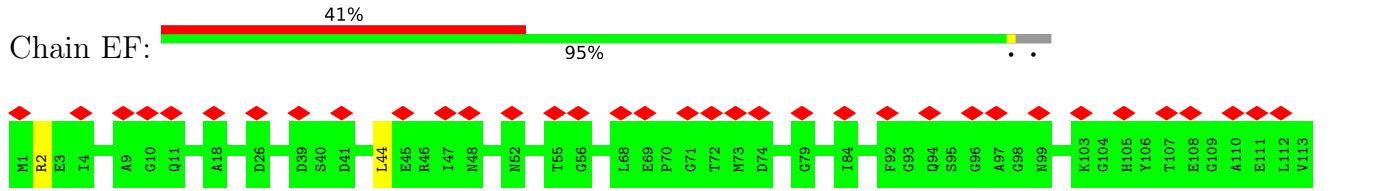


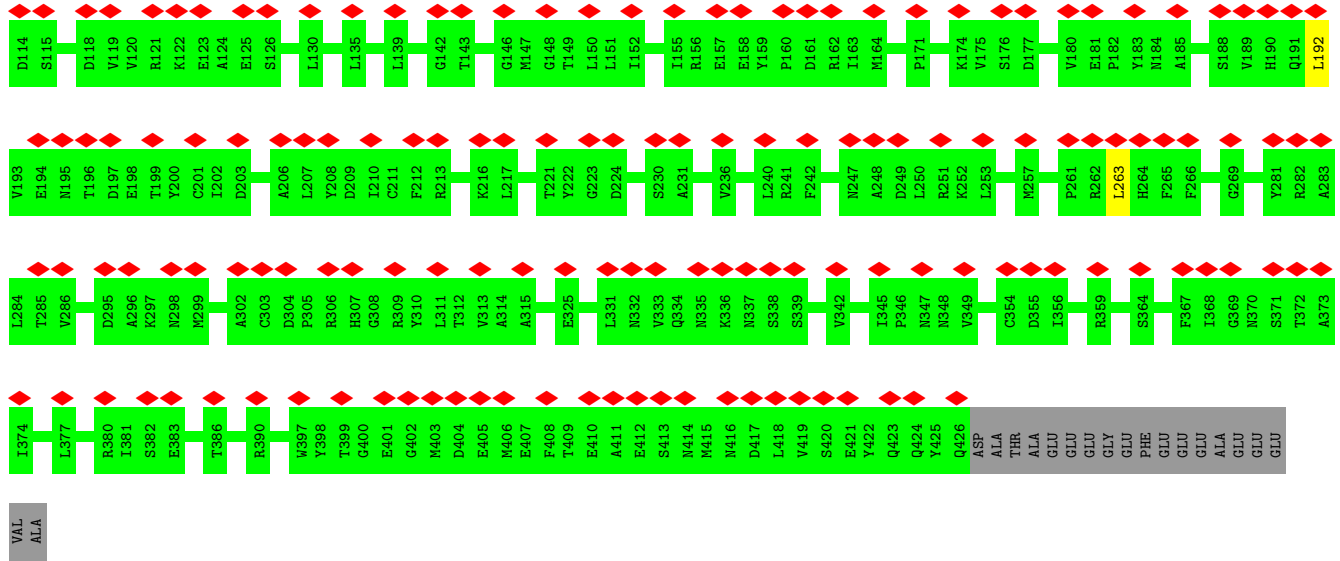


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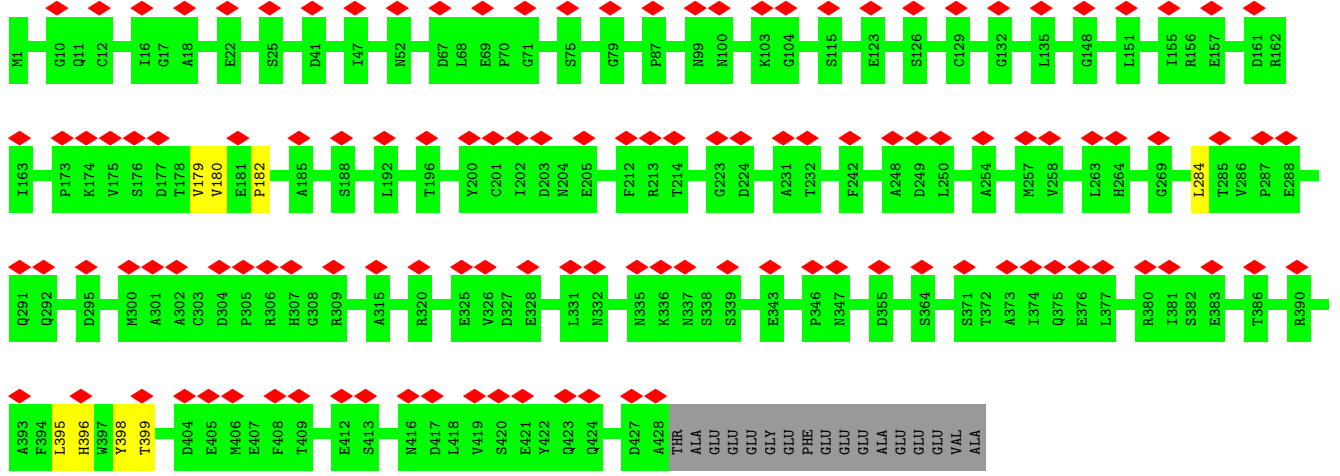


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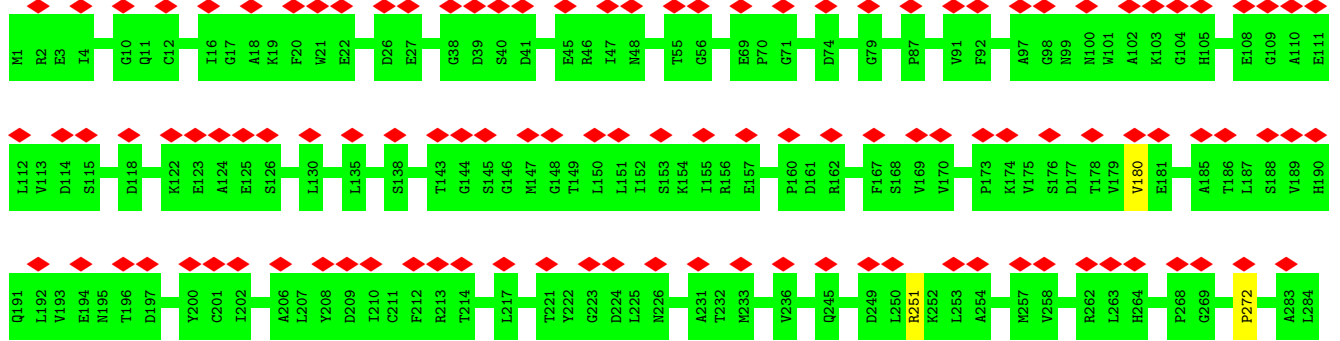
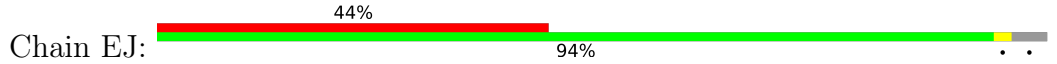


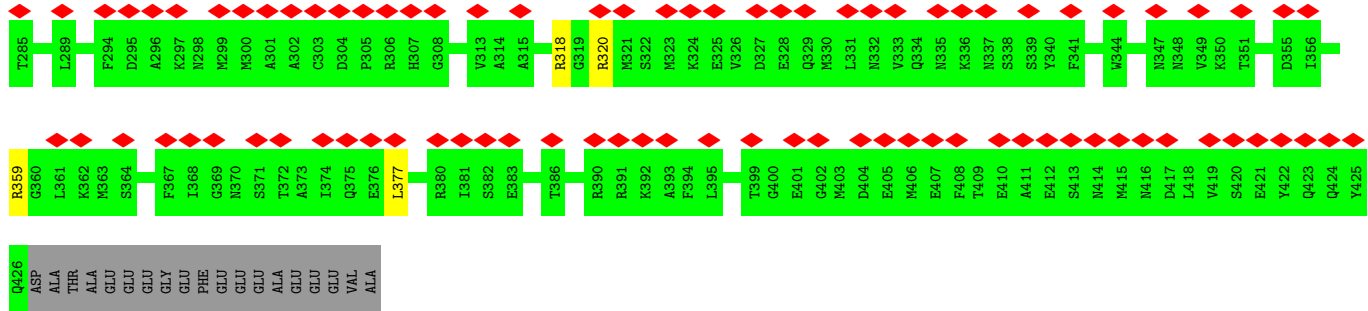


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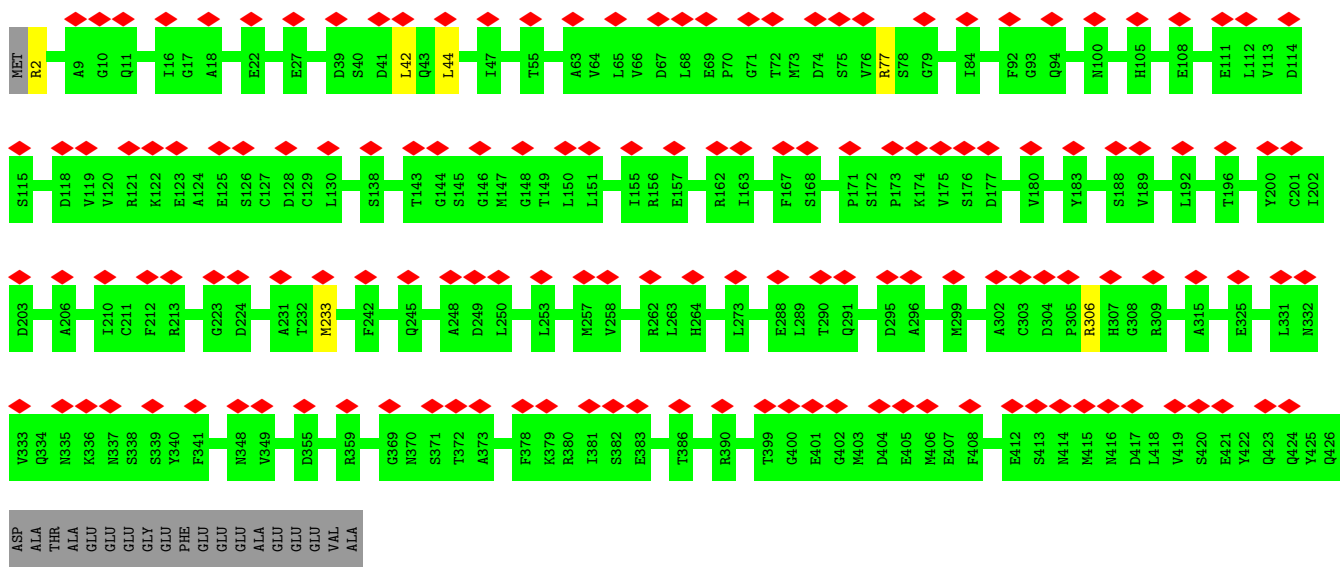


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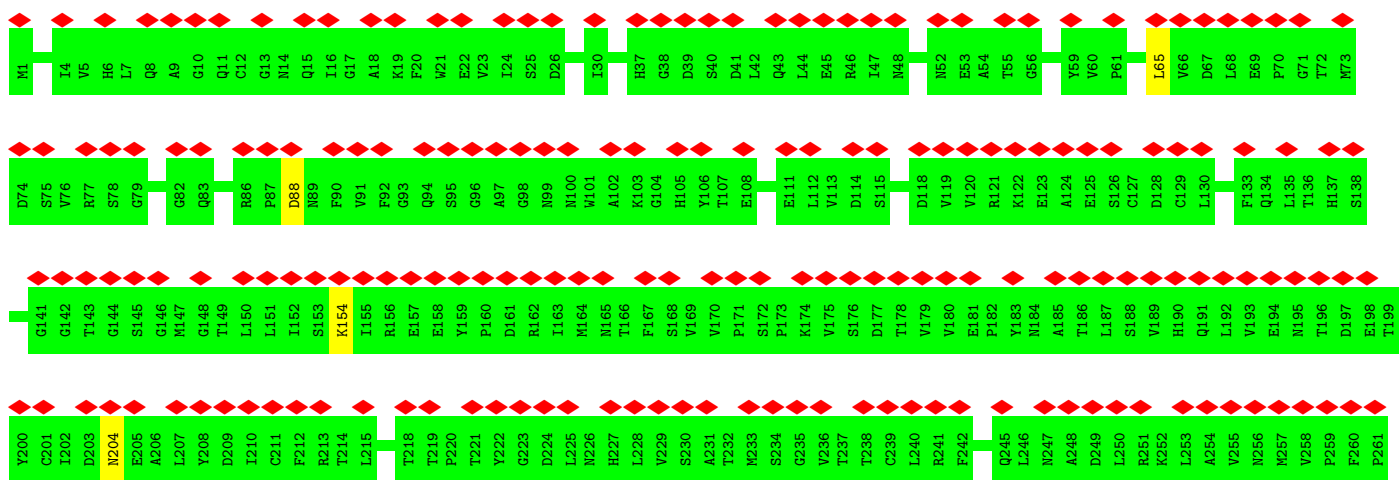
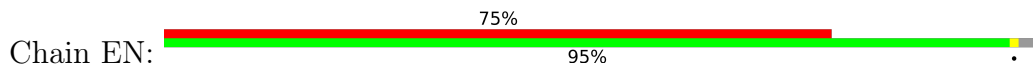


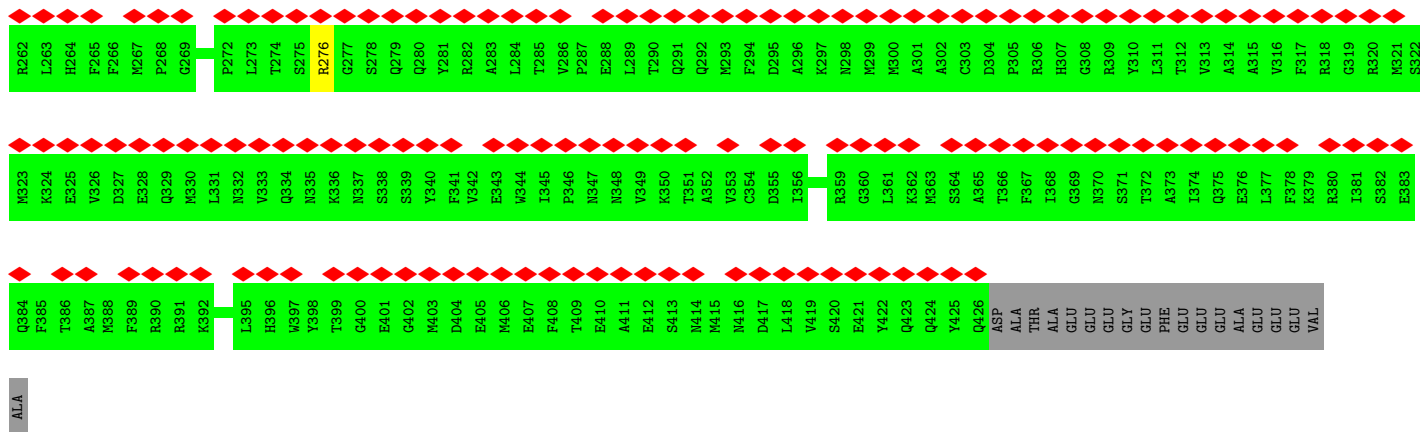


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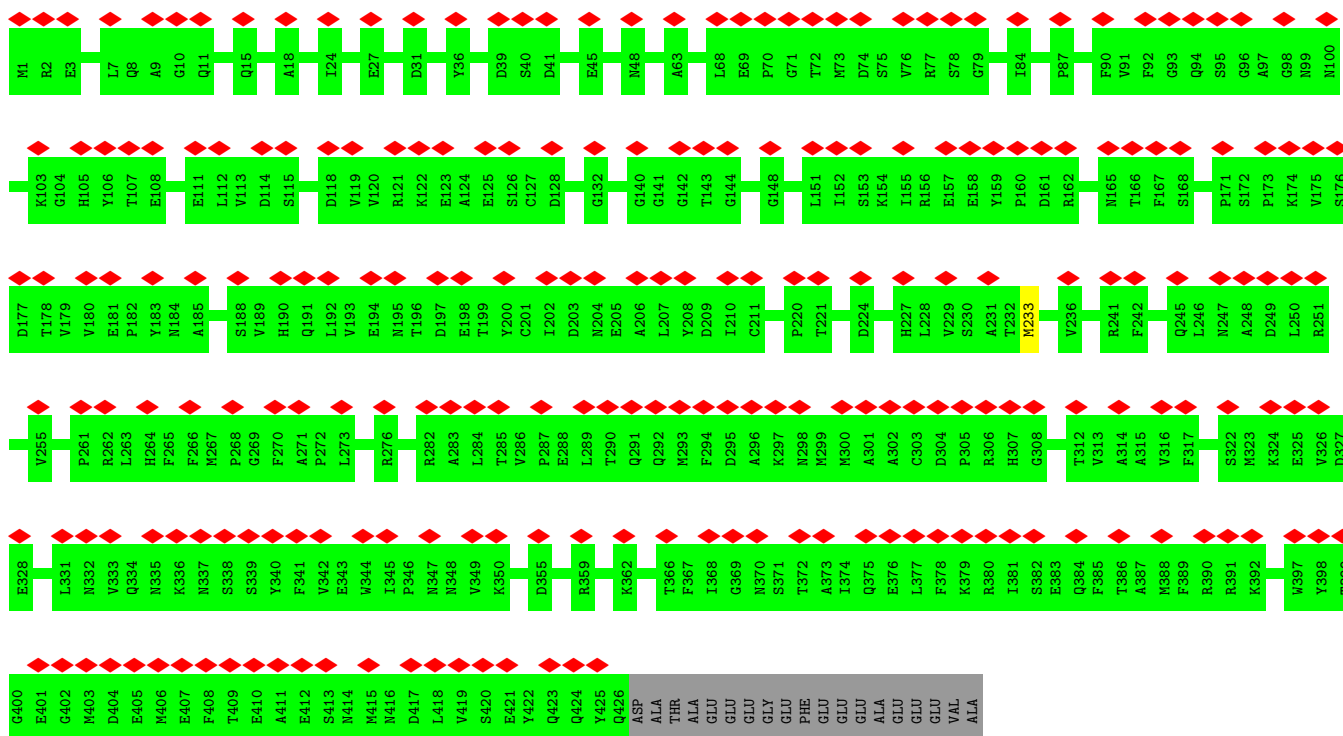


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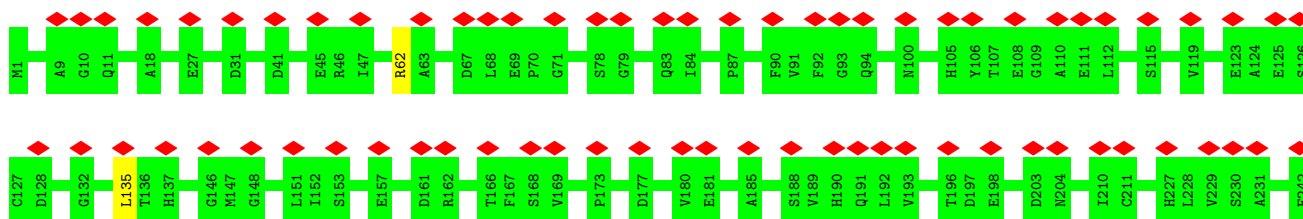


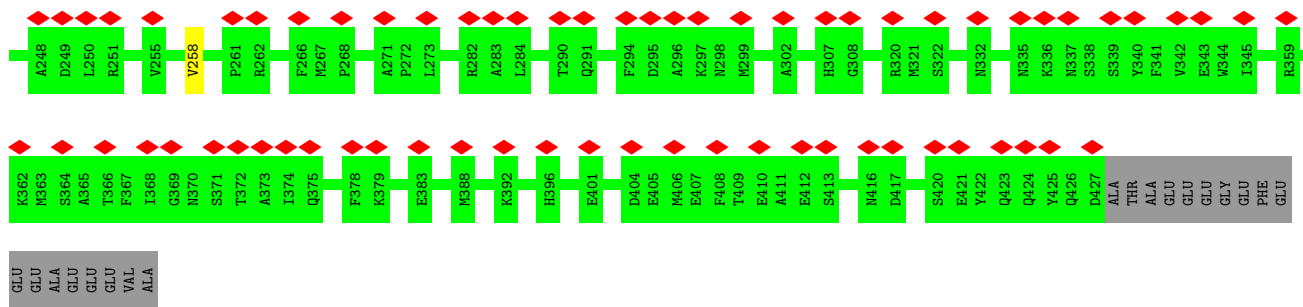


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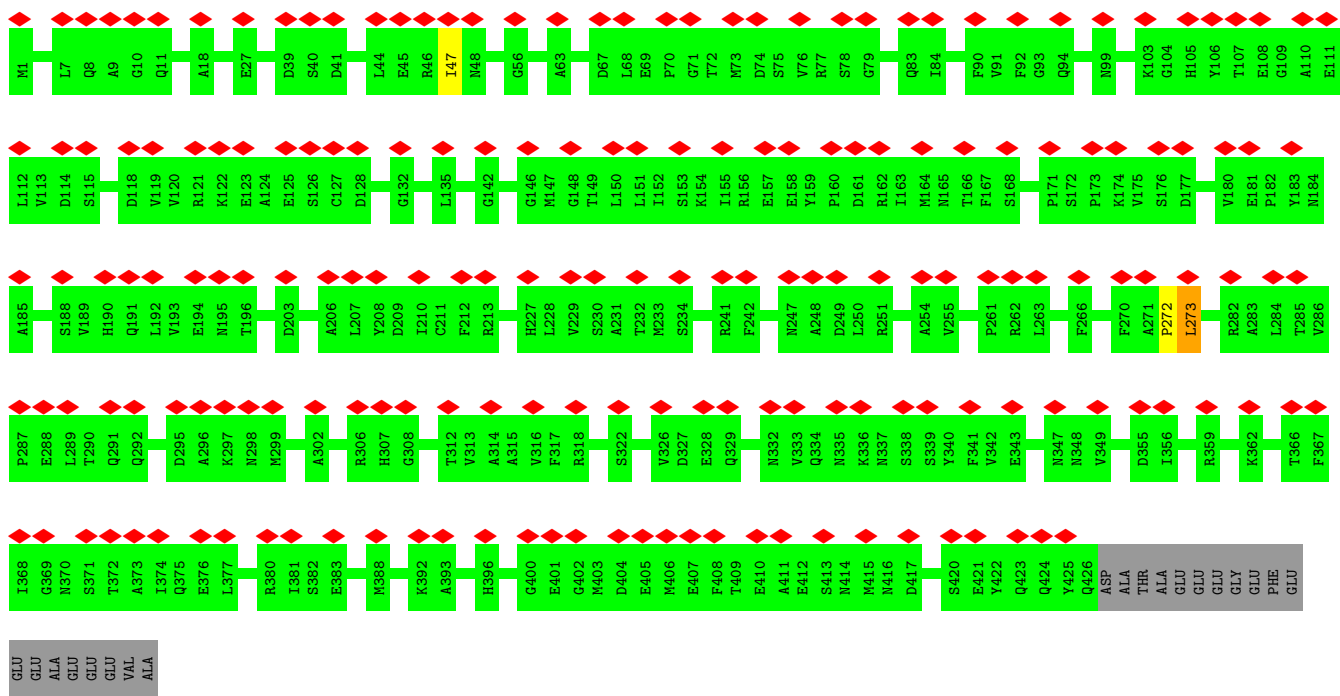
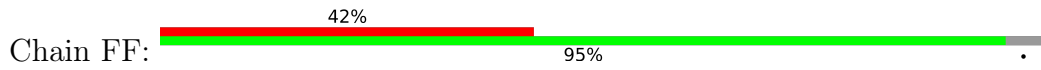


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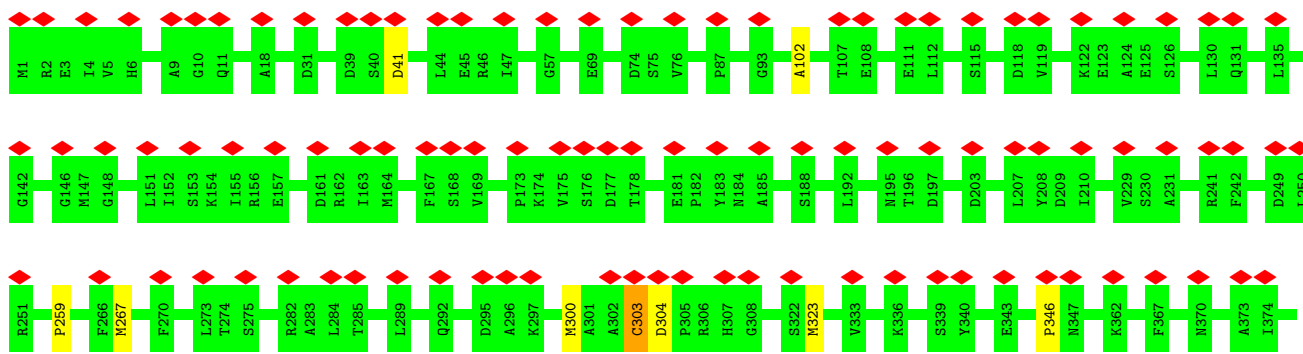


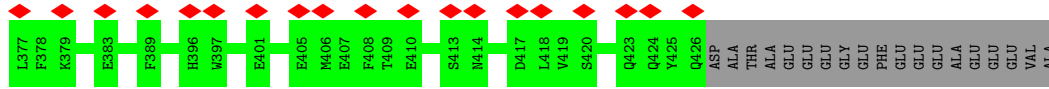


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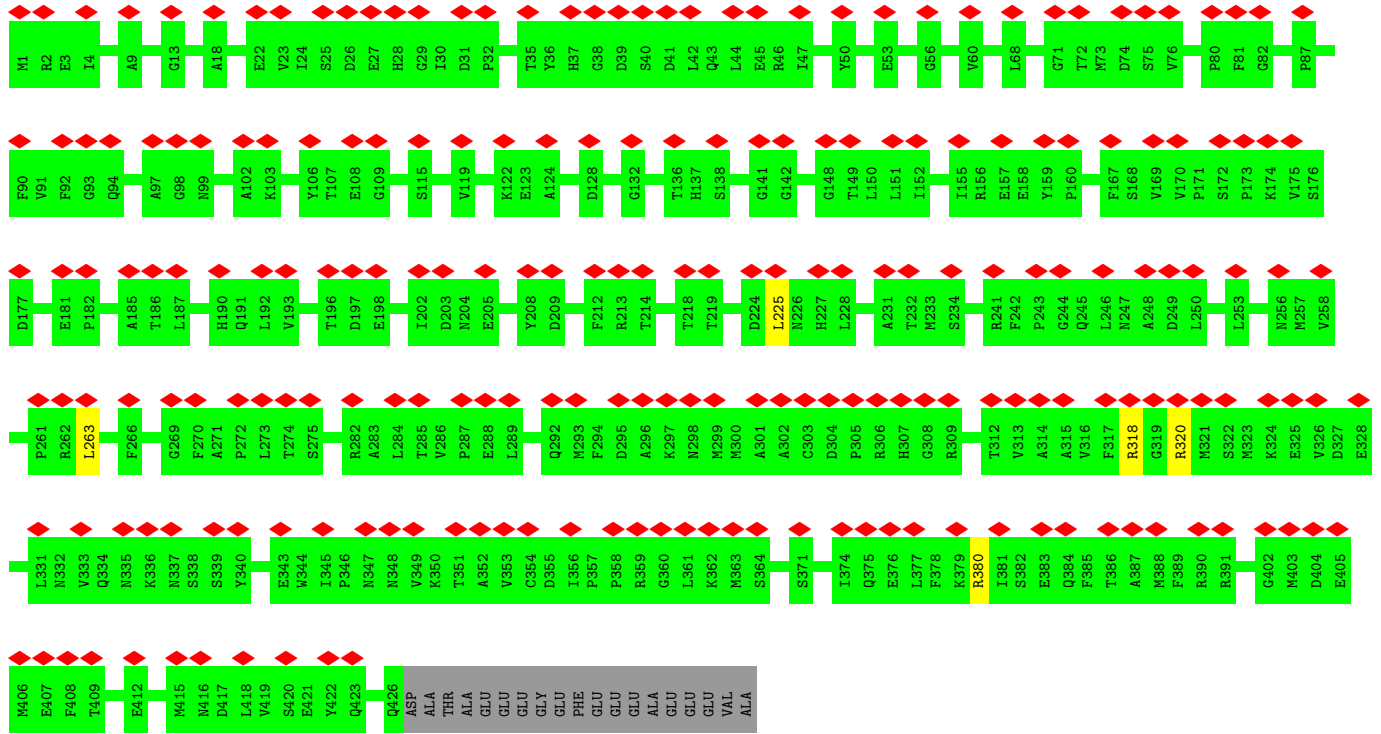


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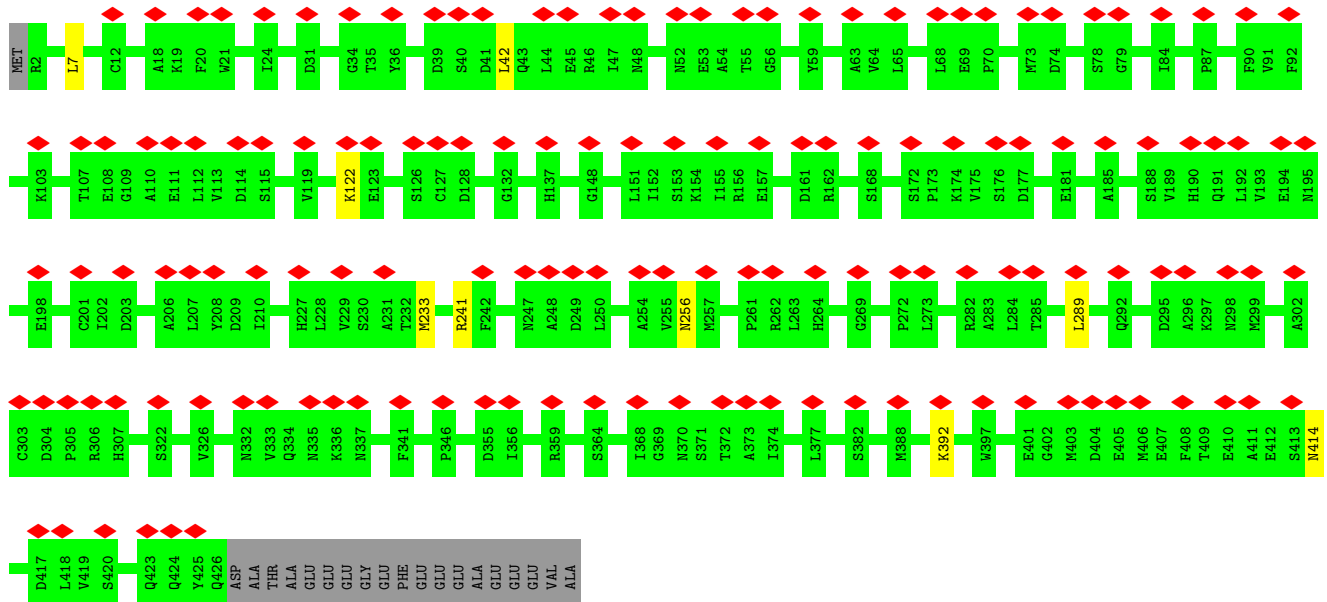




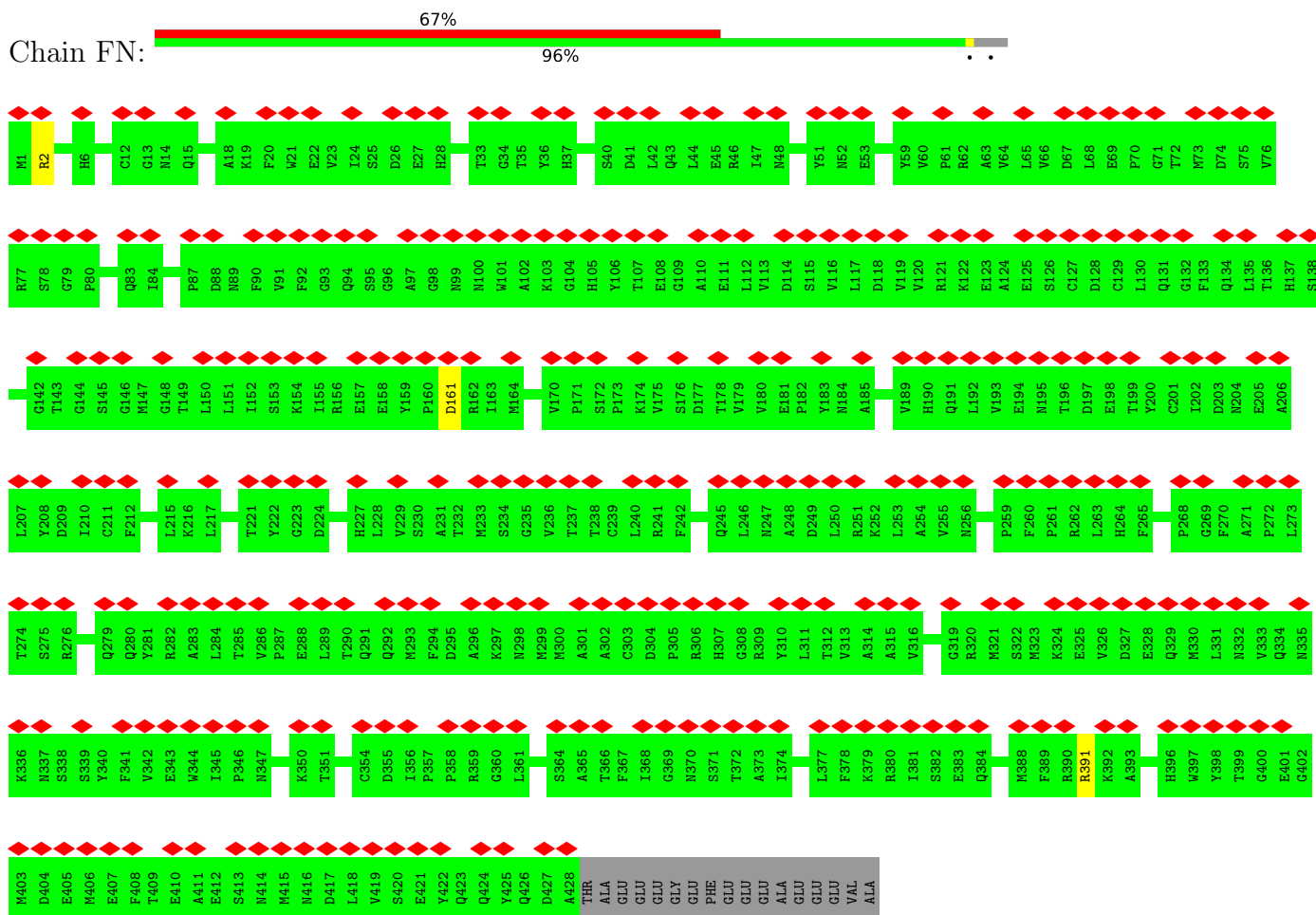
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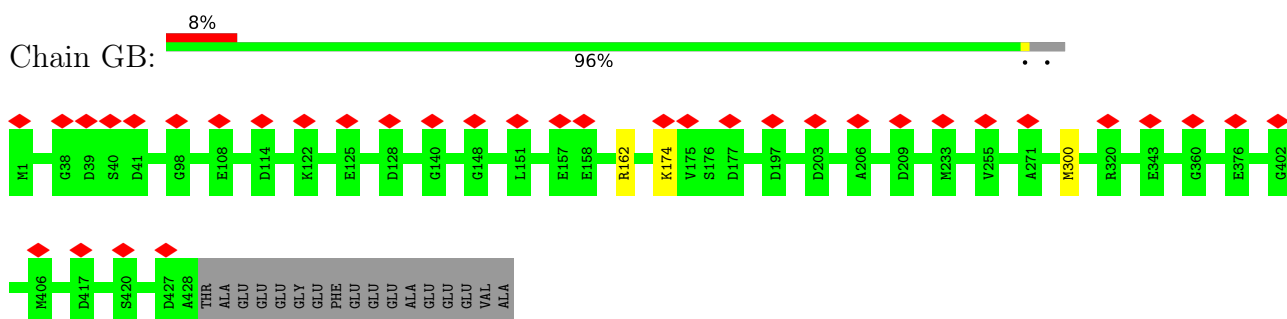
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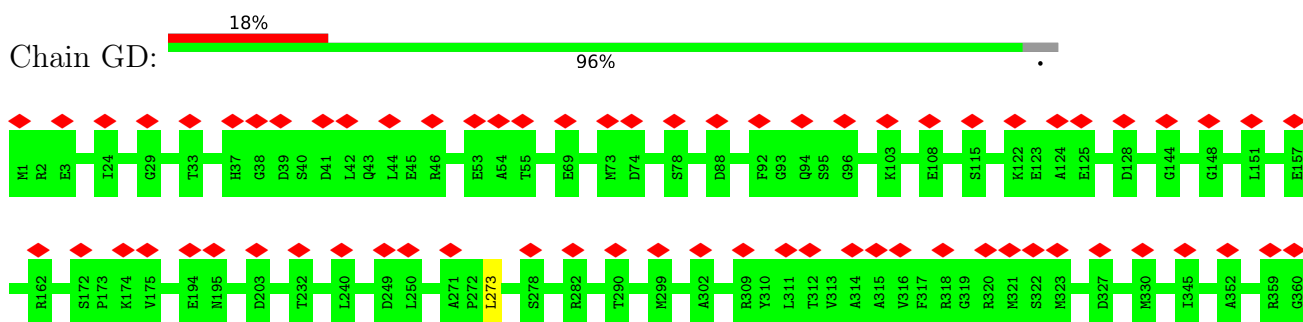
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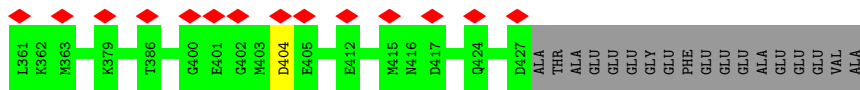


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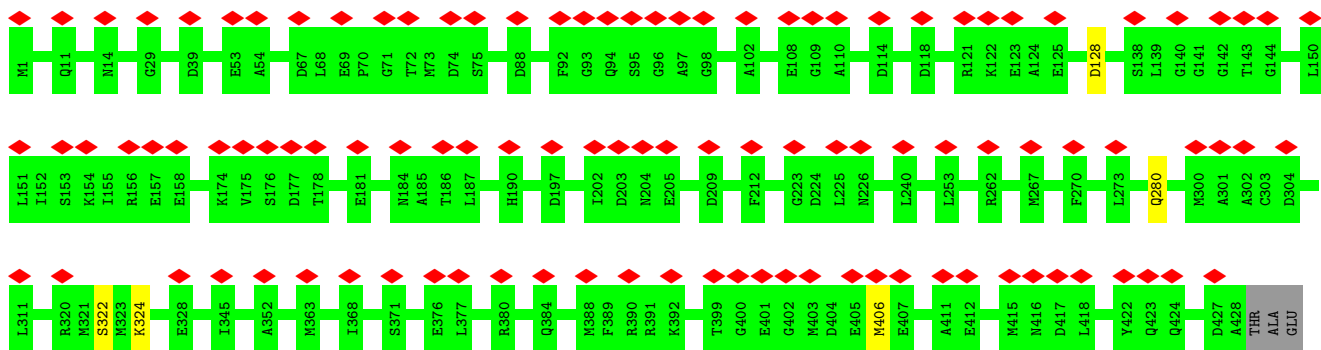


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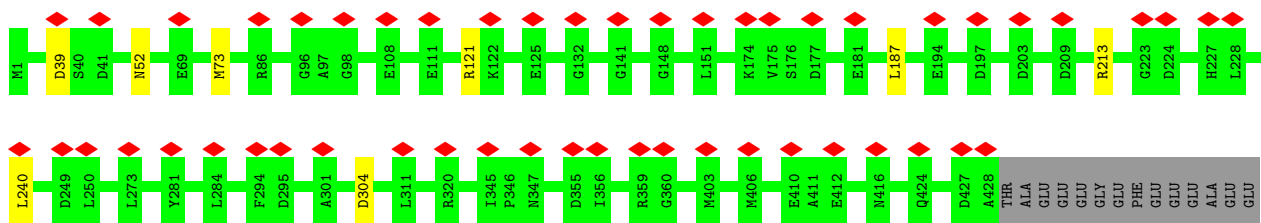


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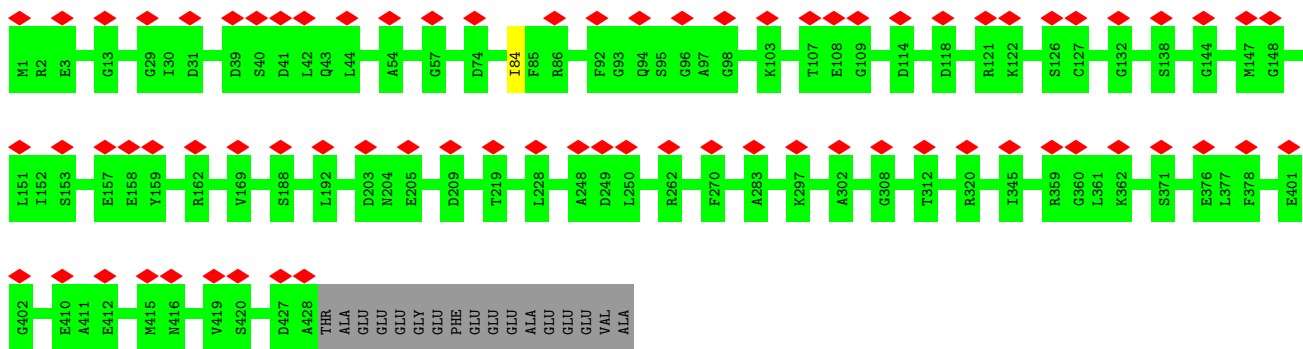
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GLU  
GLY  
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GLU  
GLU  
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GLU  
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VAL  
ALA

• Molecule 9: Tubulin beta-4B chain



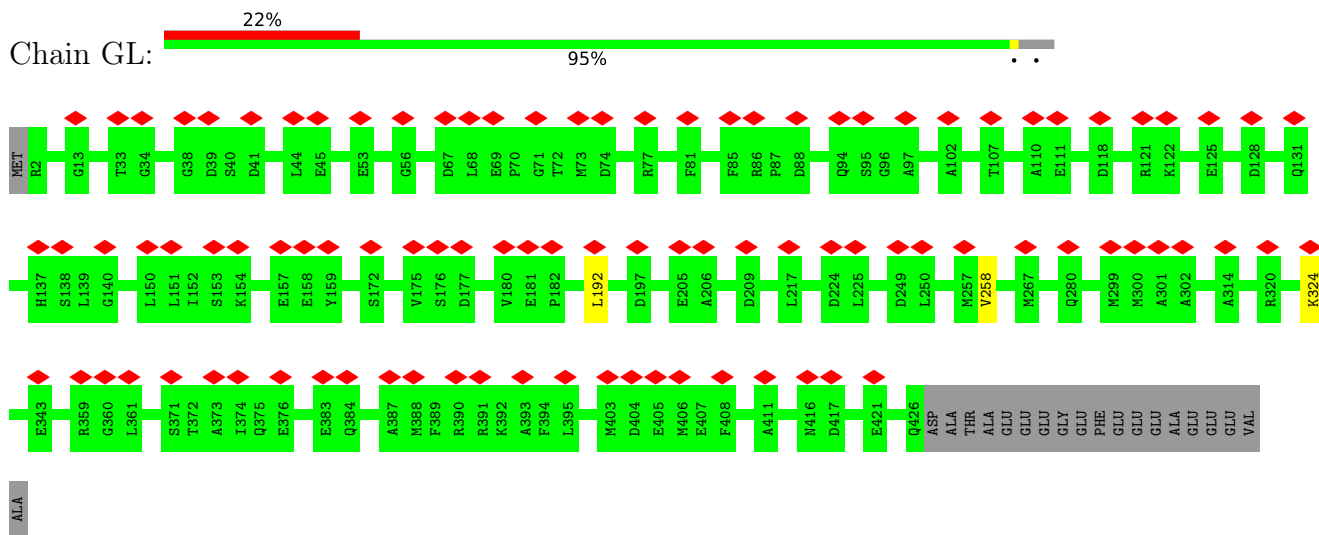
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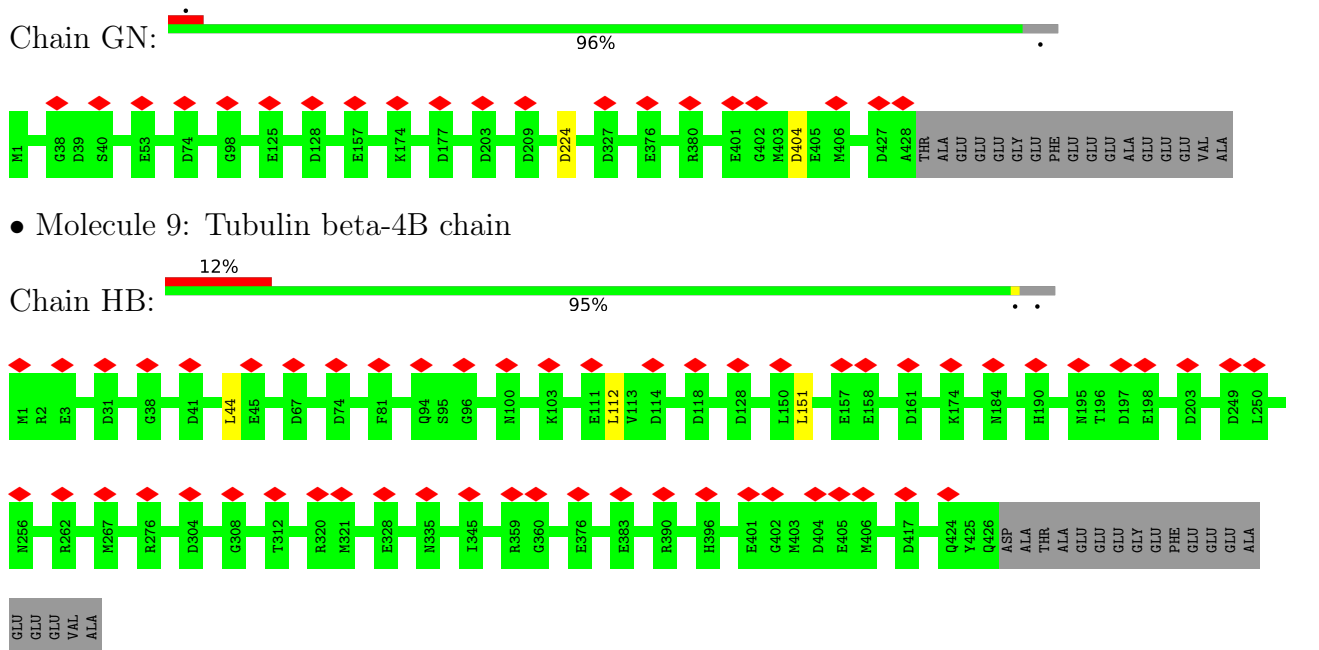


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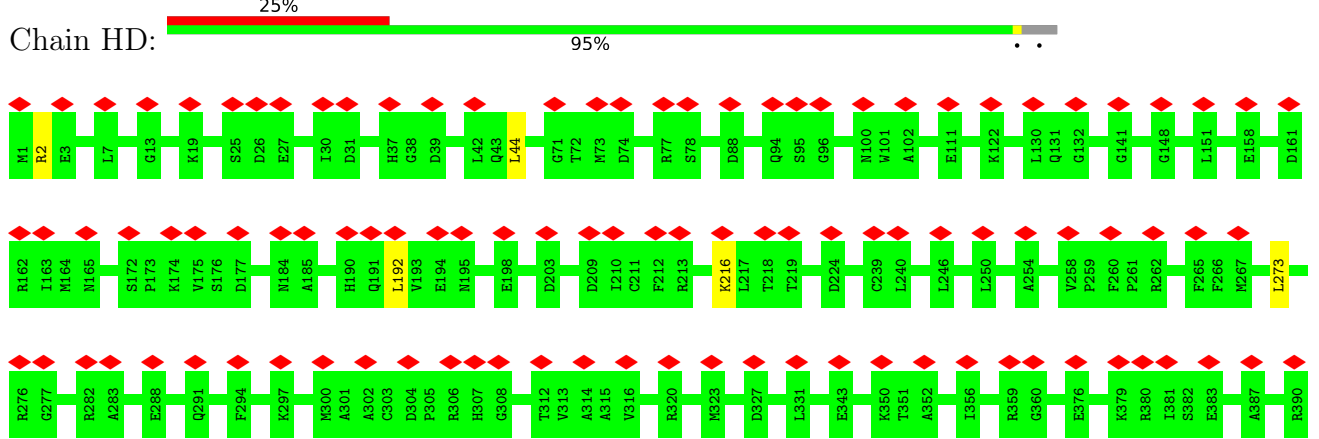


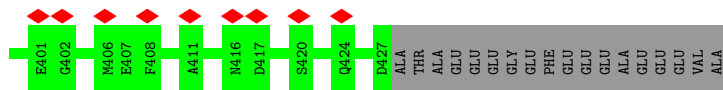


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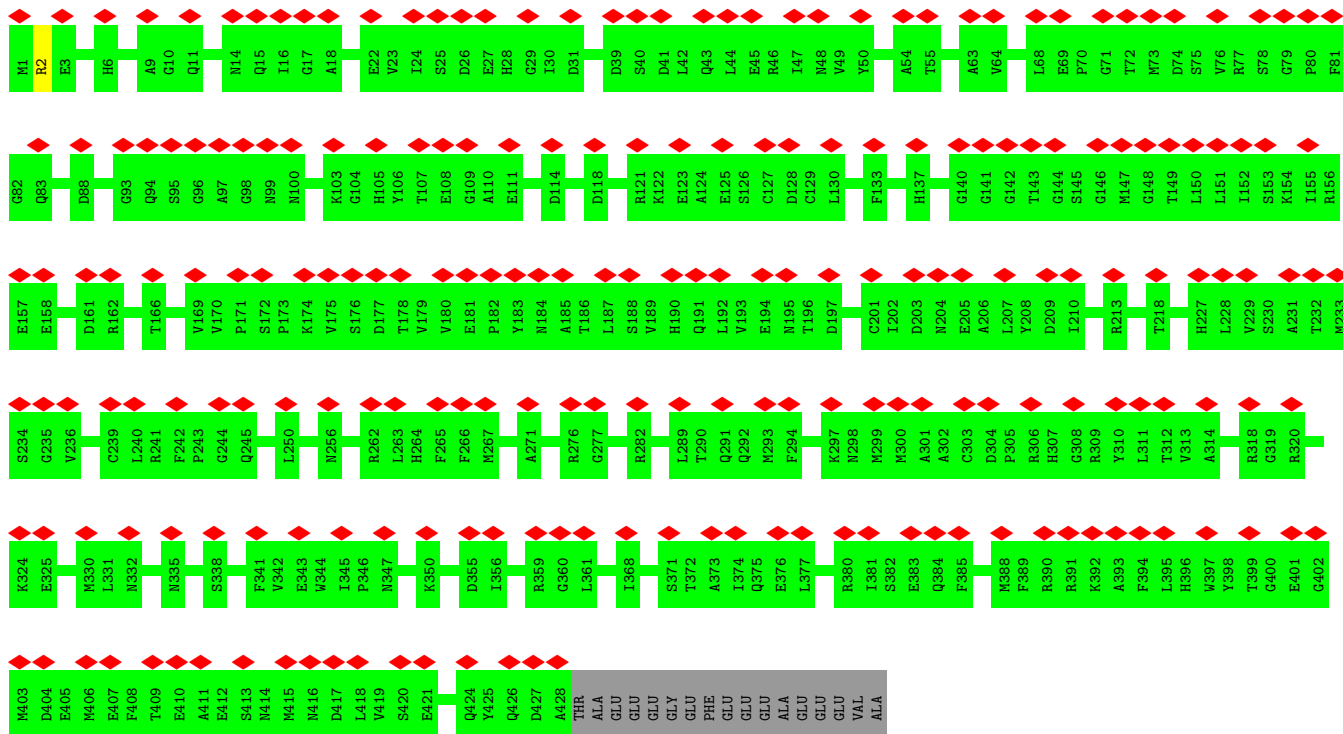


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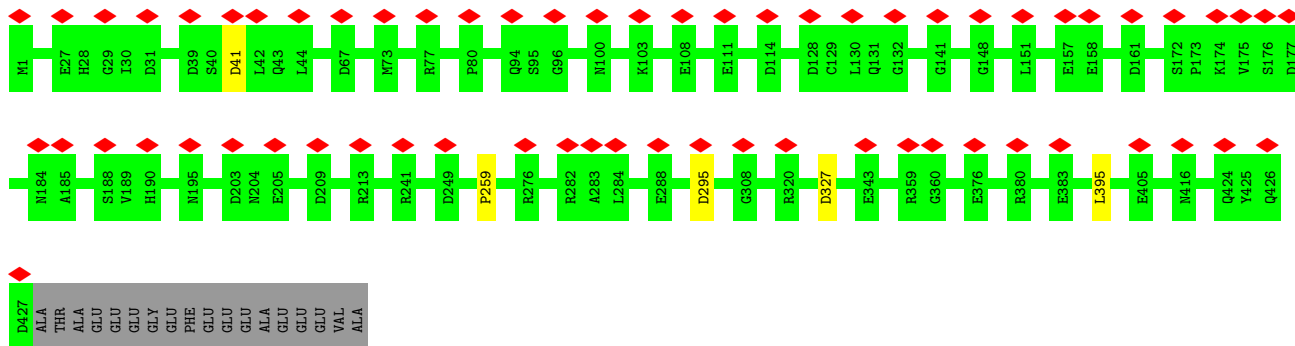




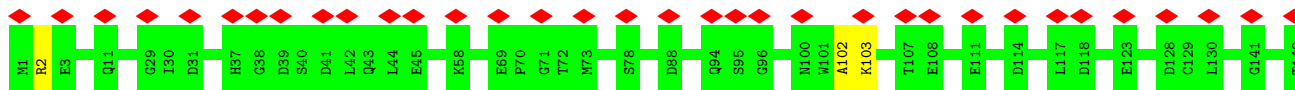
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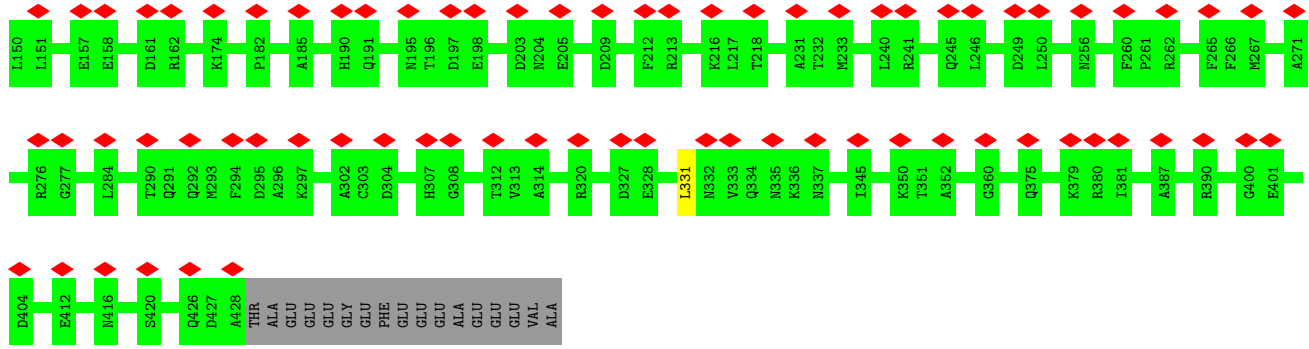


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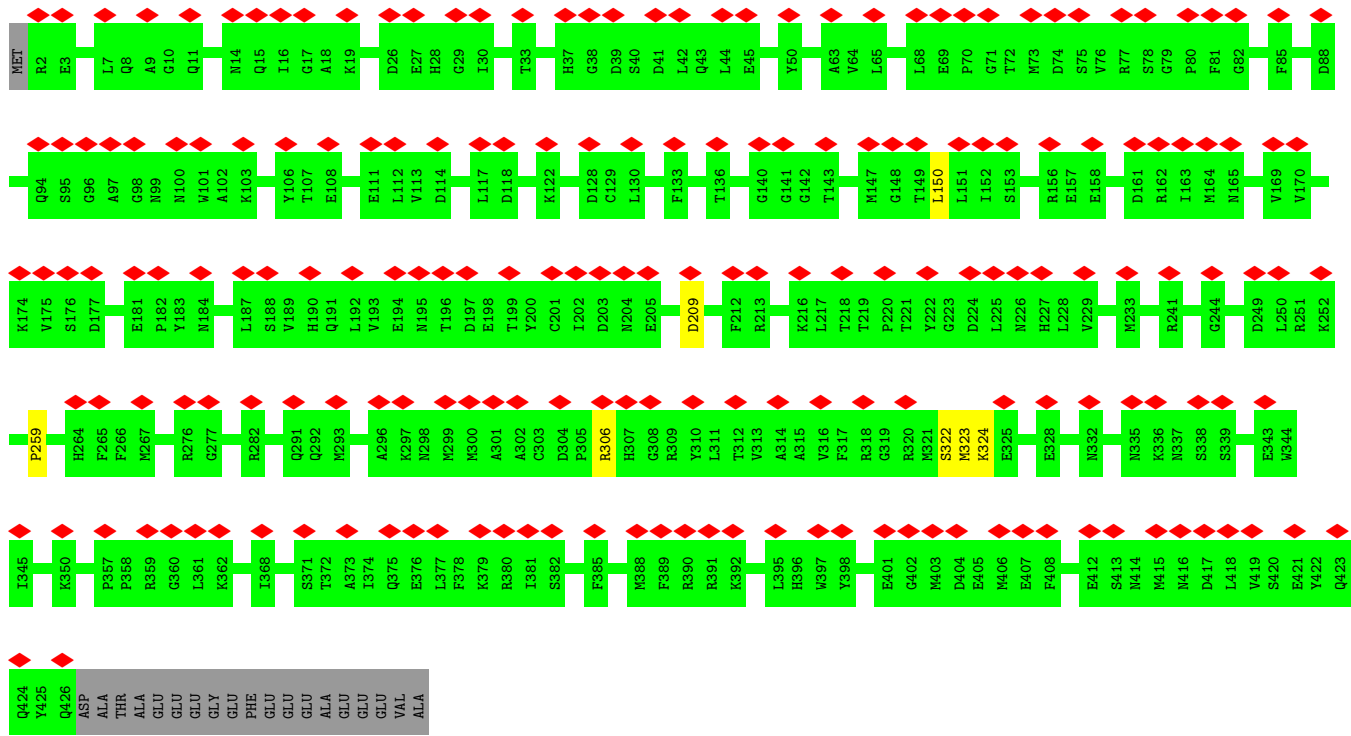


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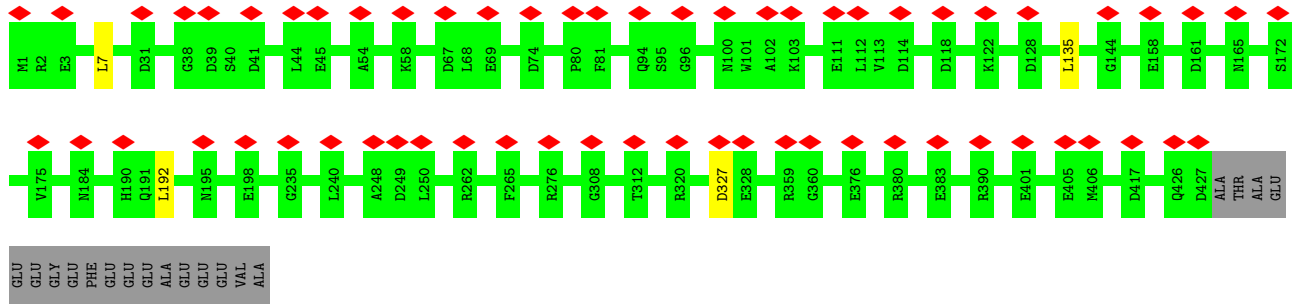




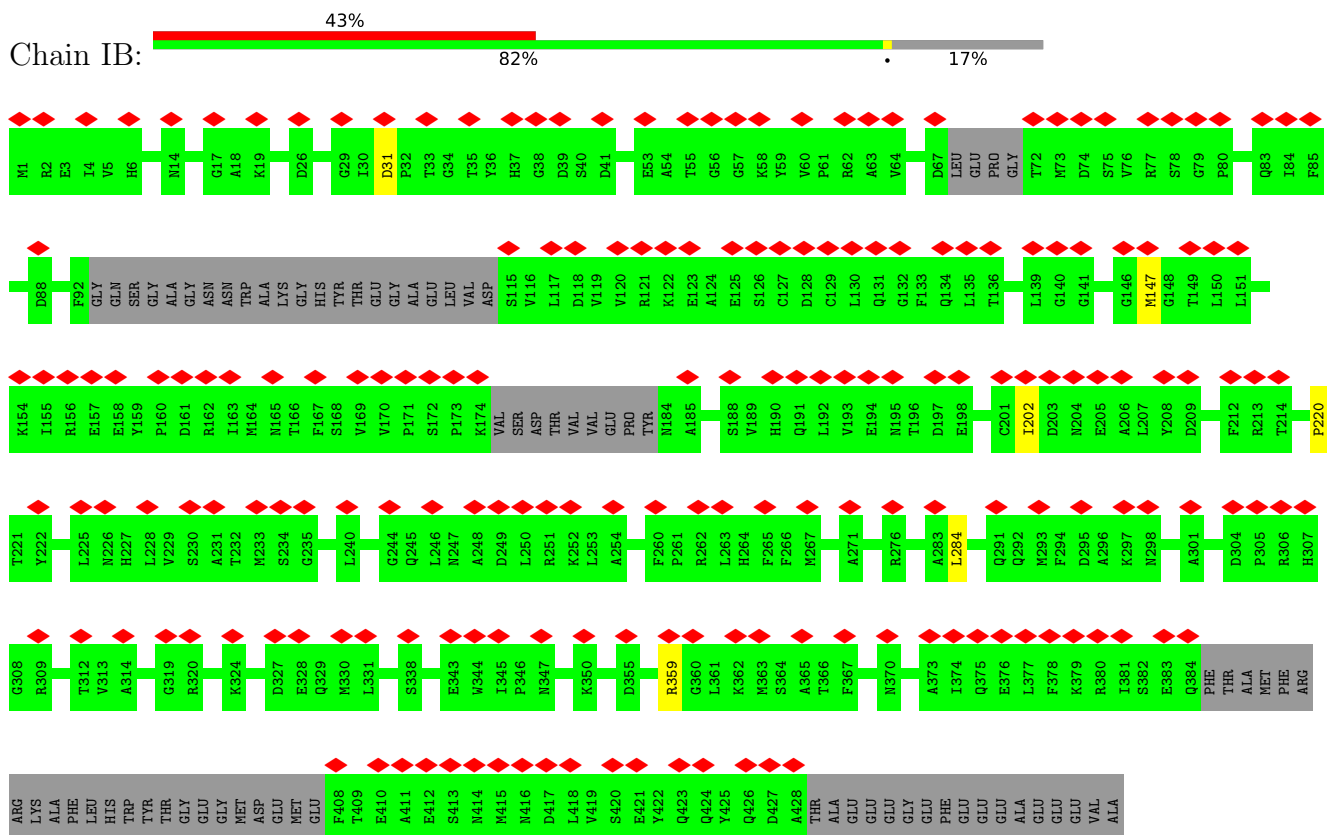
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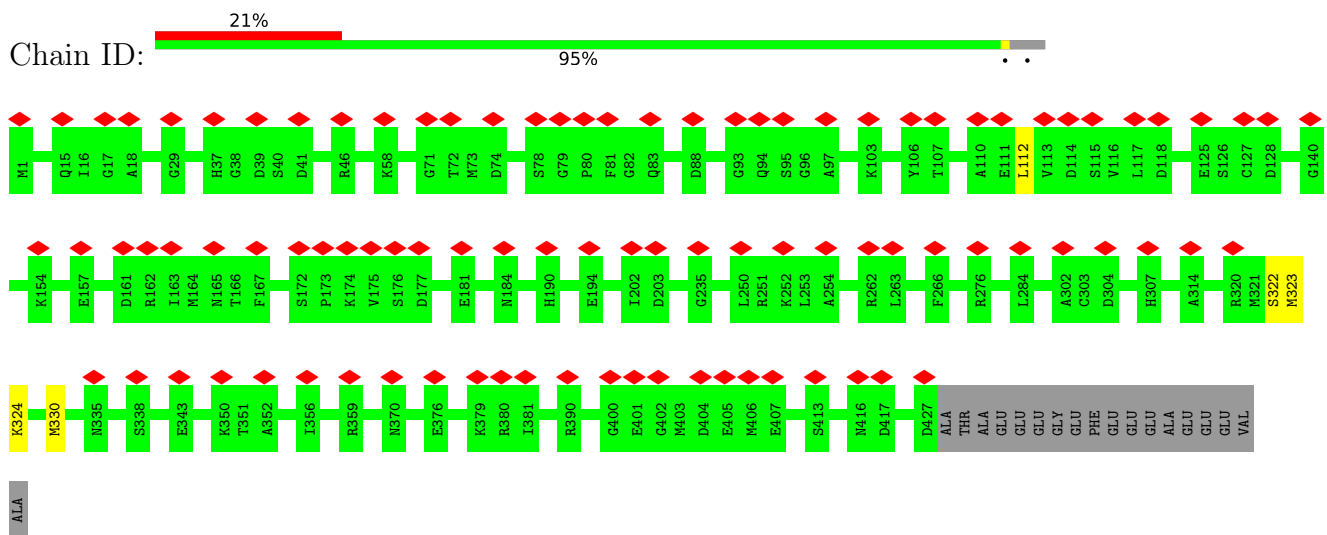
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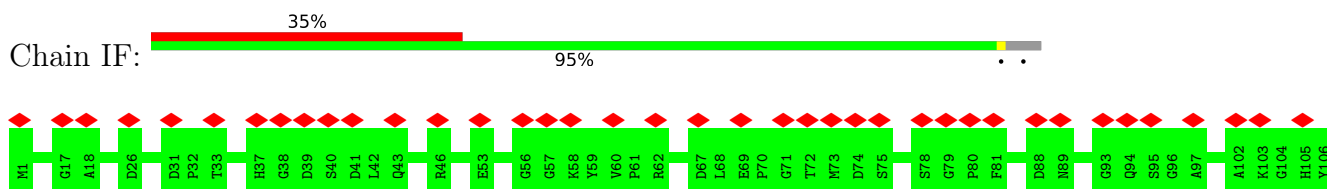
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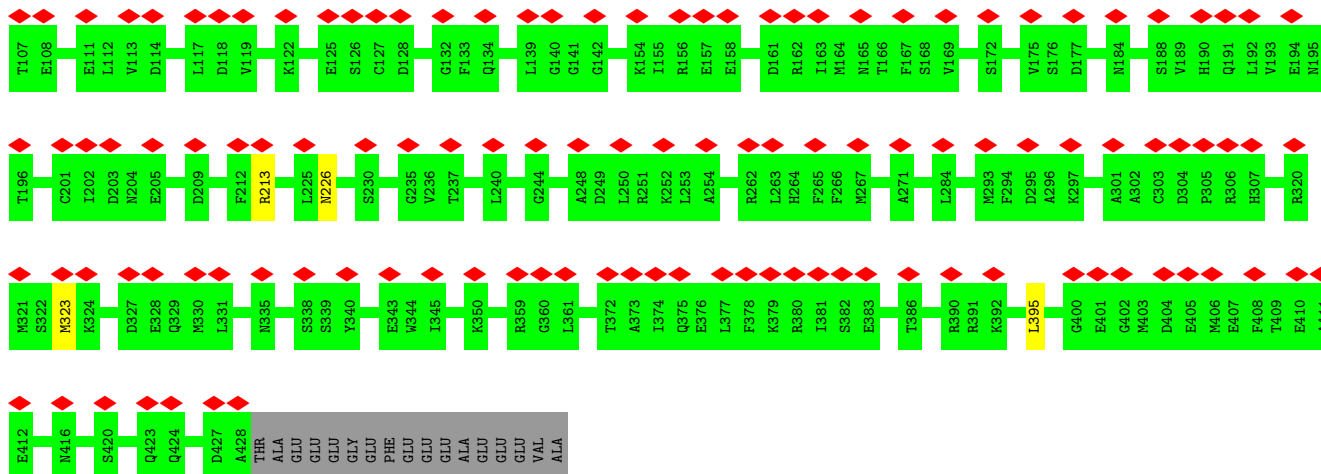


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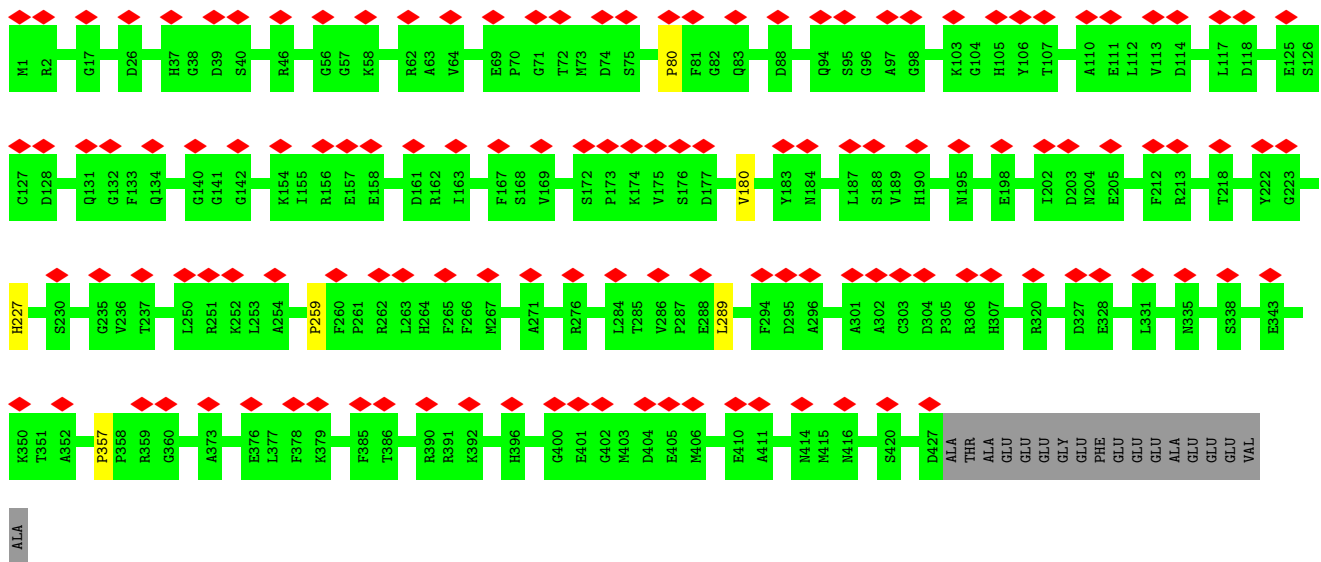


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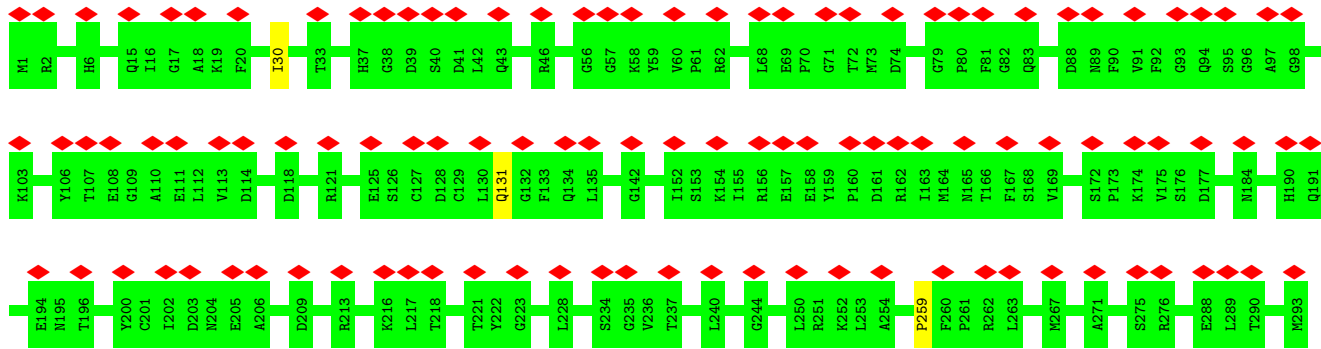


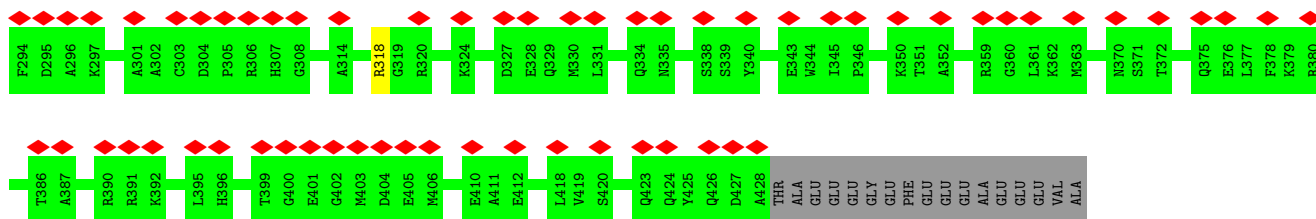


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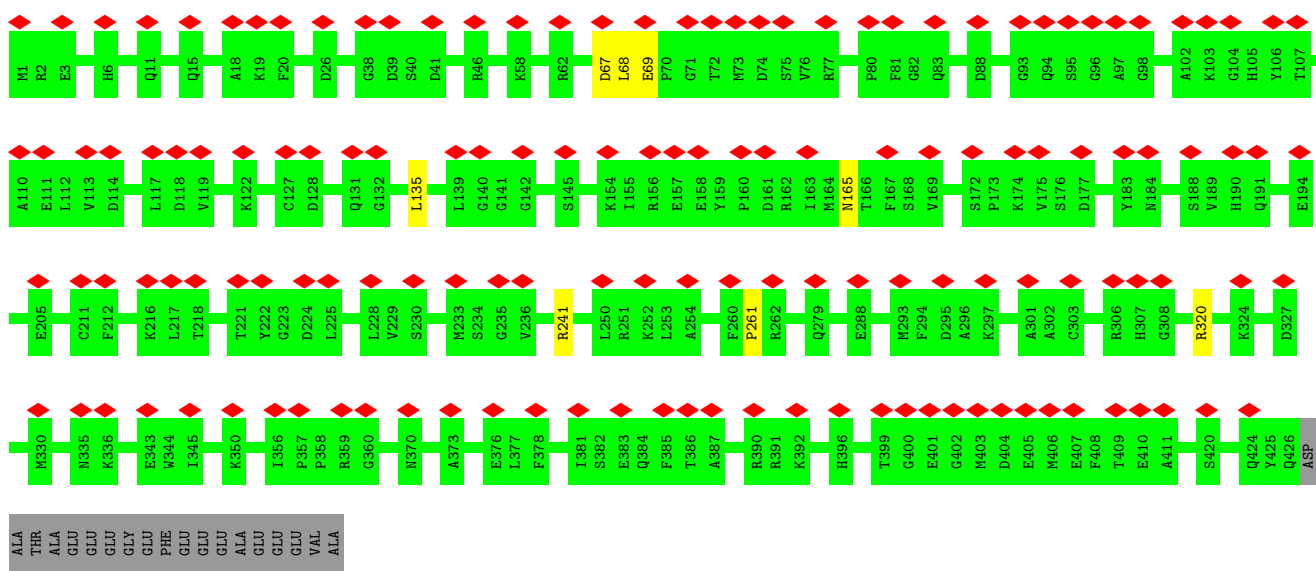
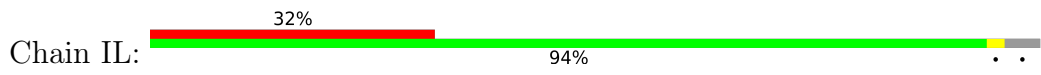


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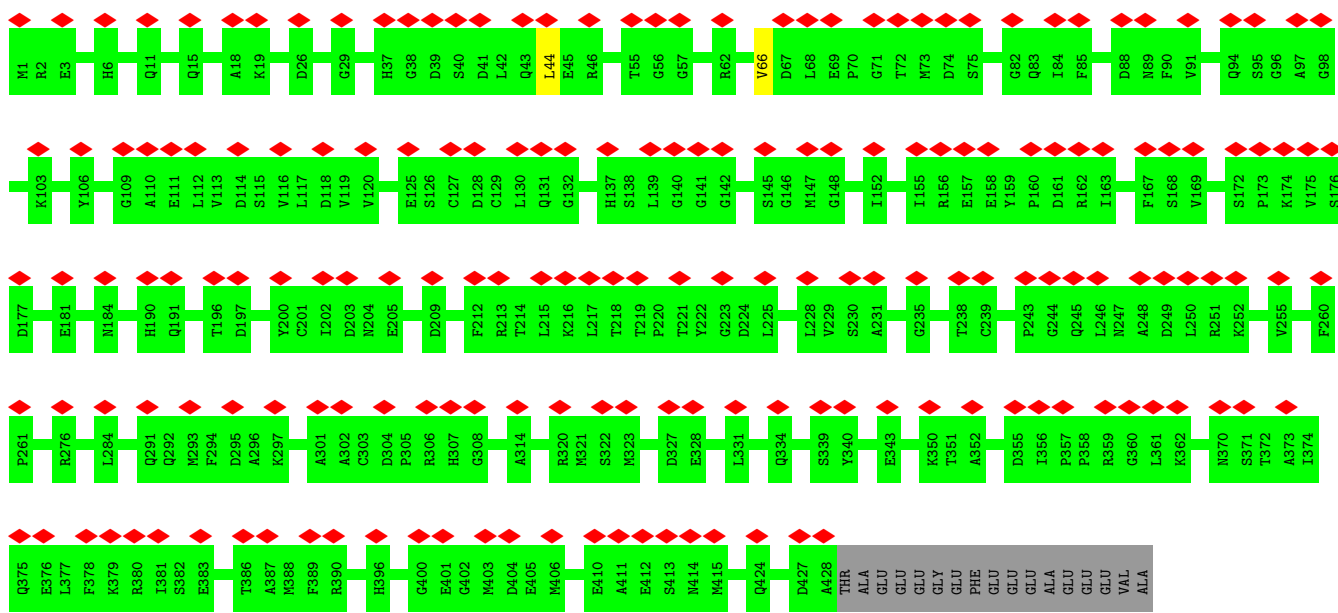
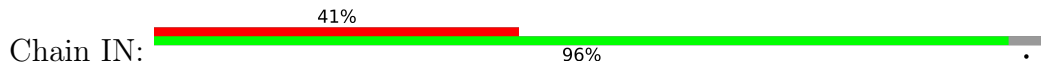




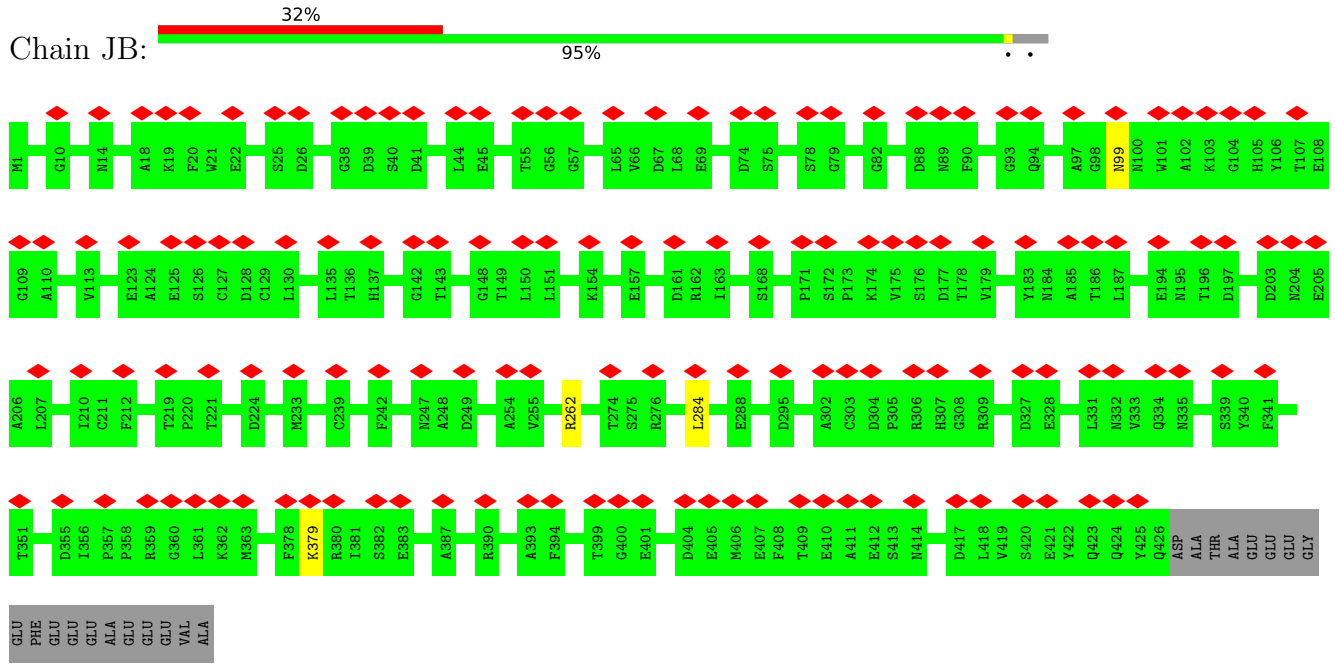
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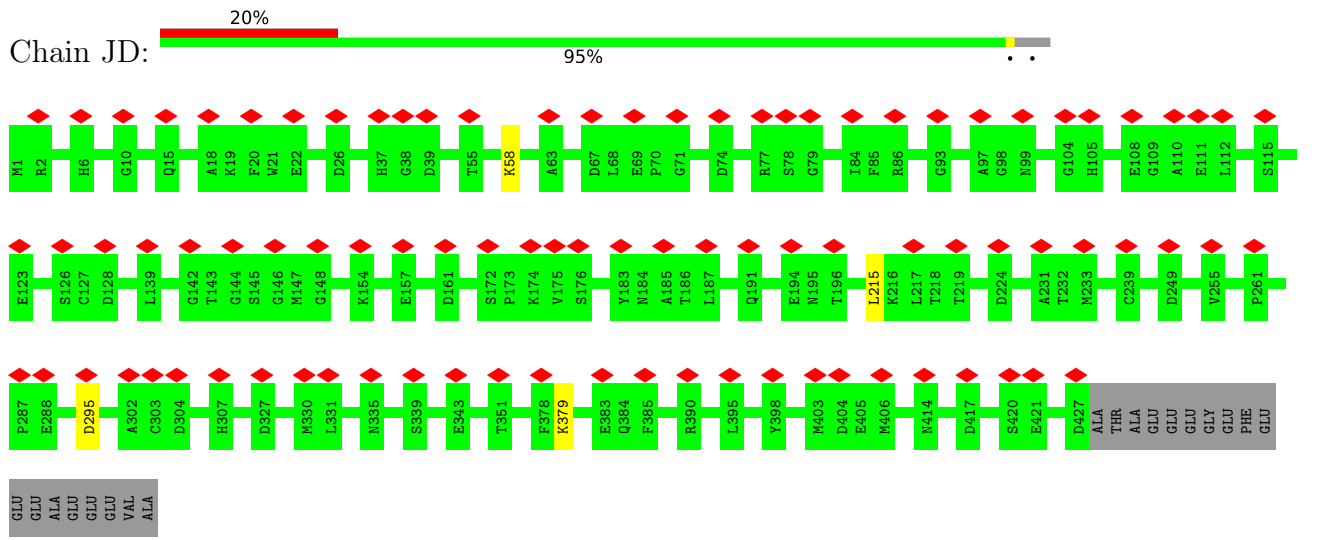
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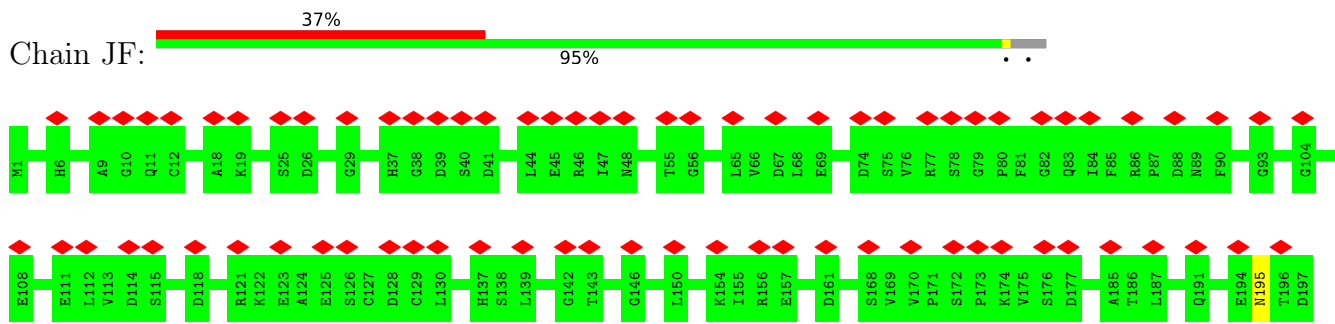
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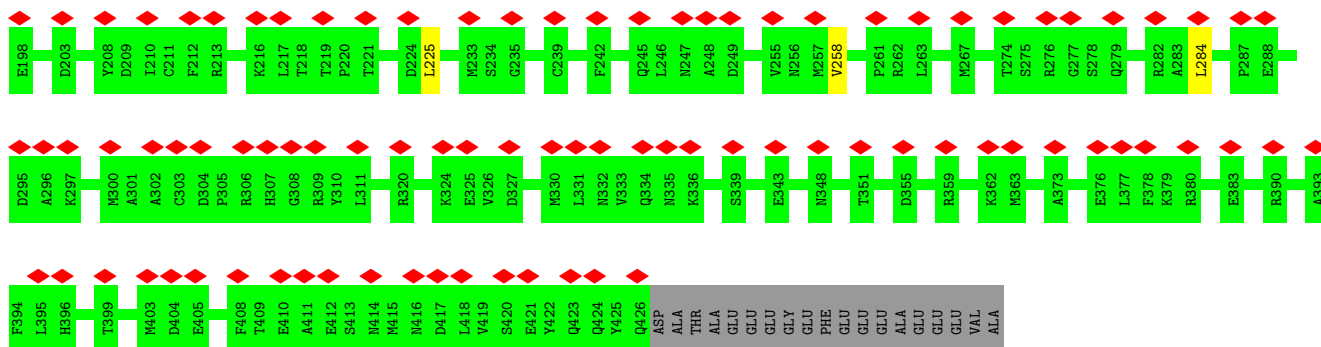


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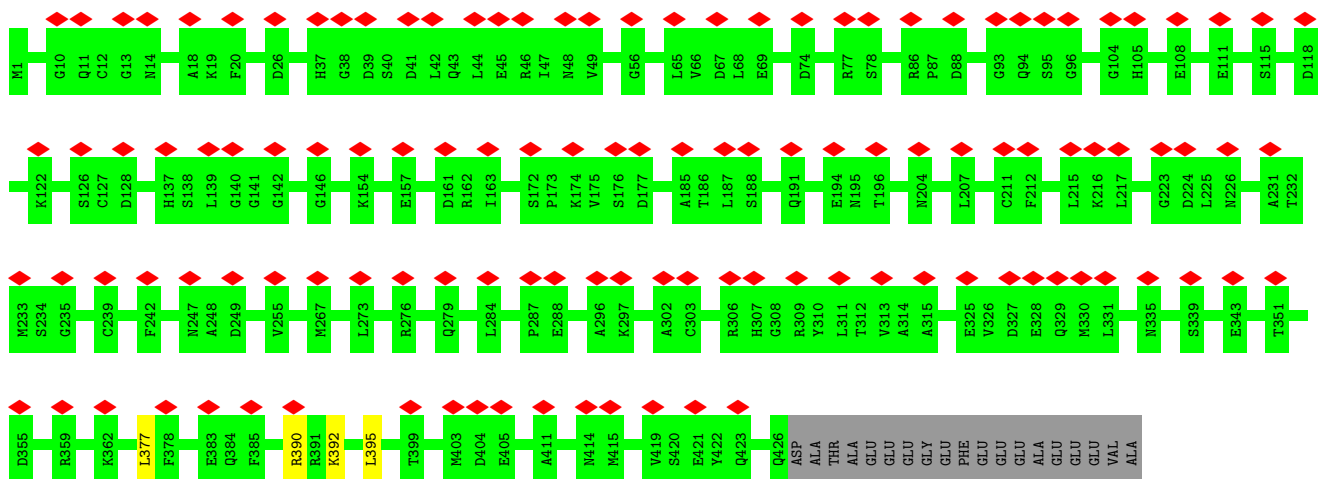


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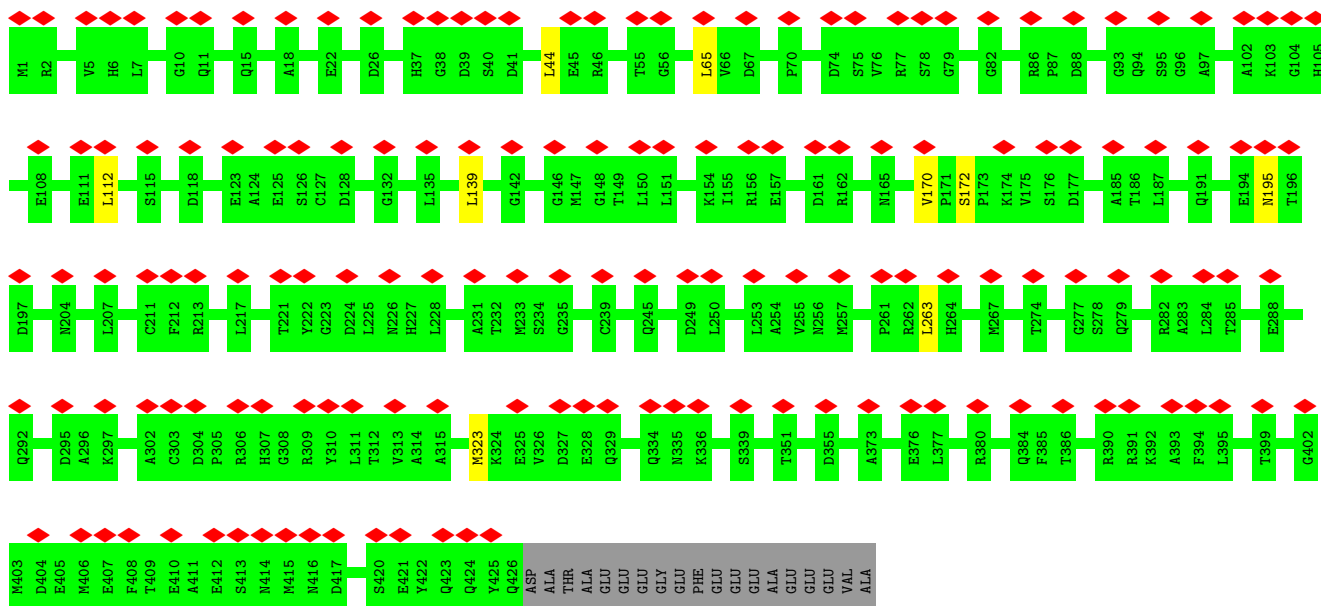




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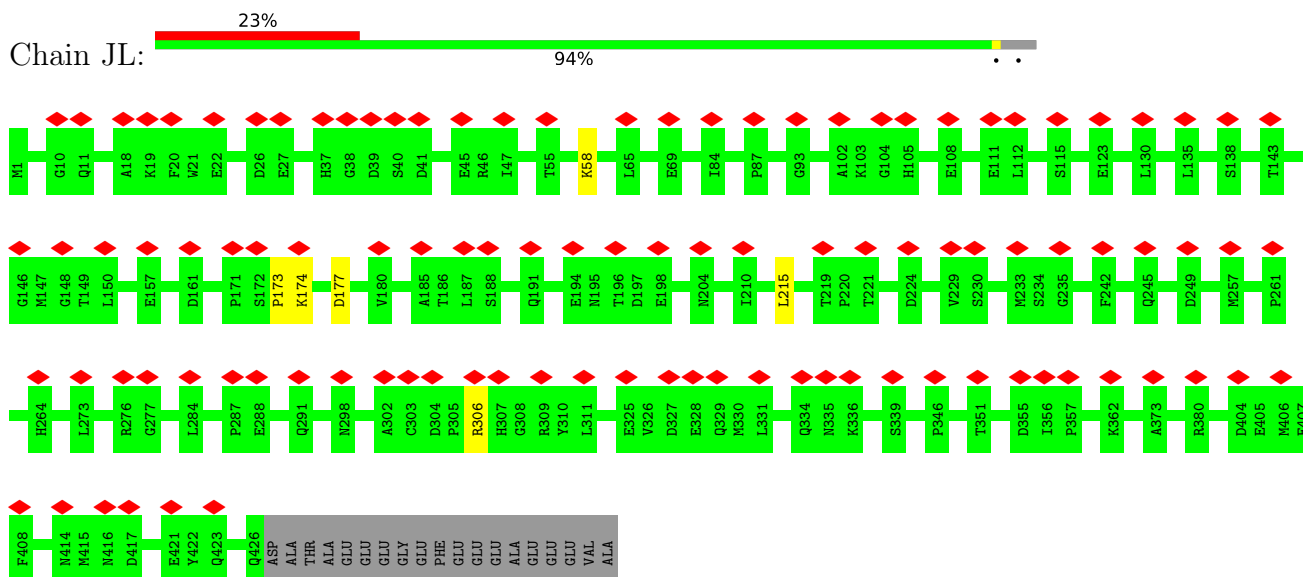


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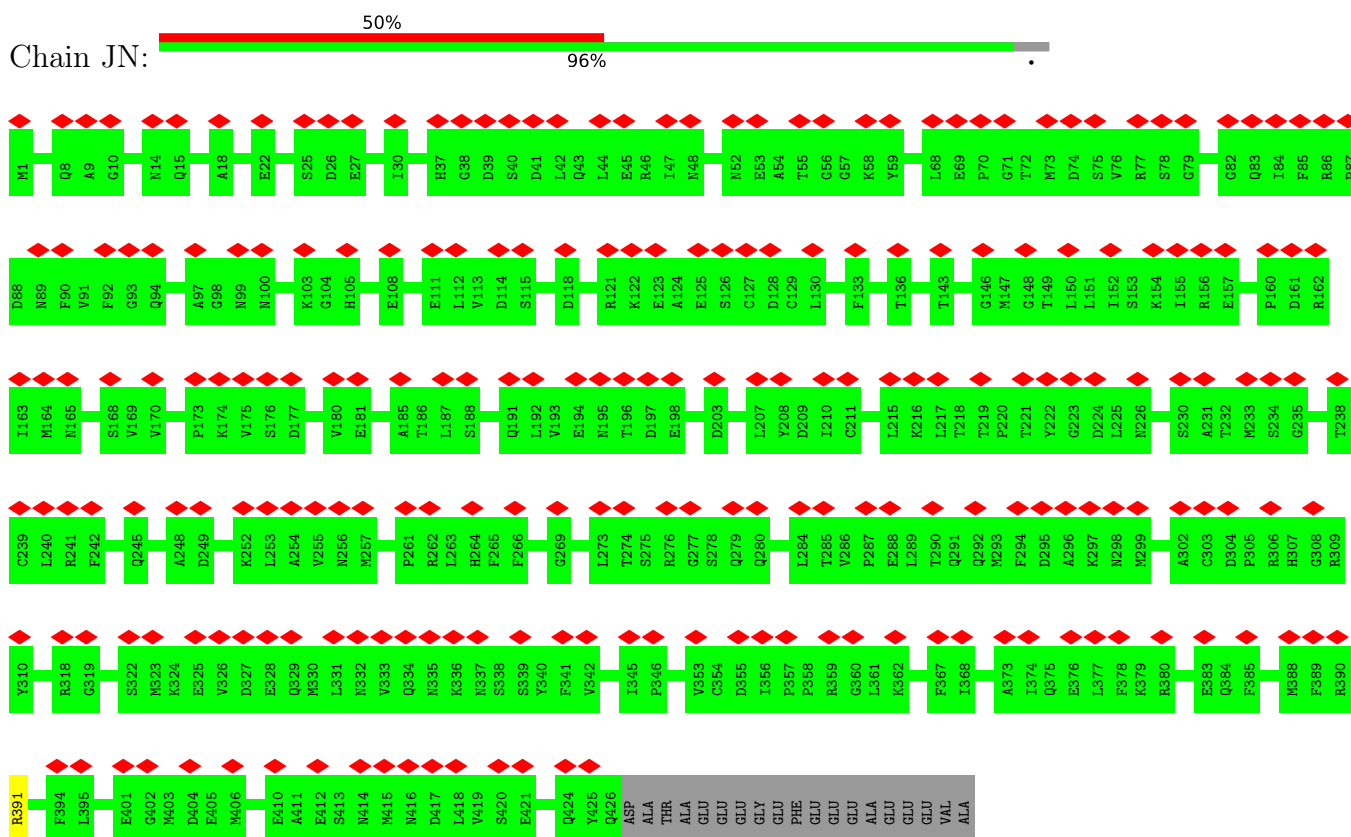




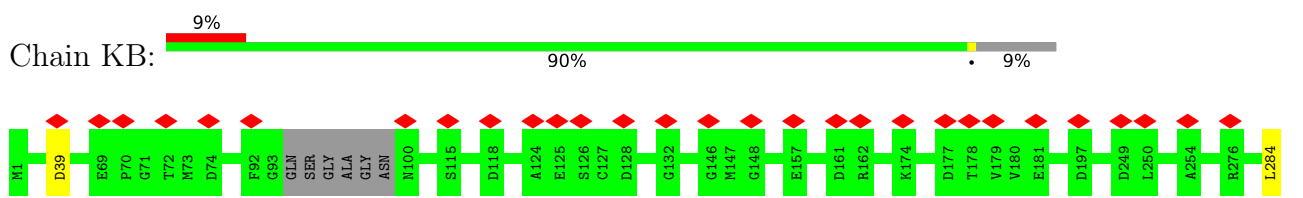
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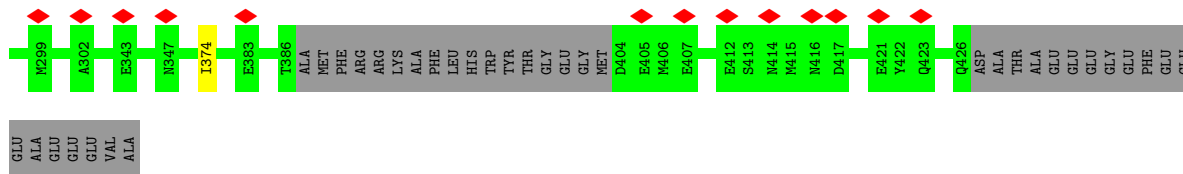


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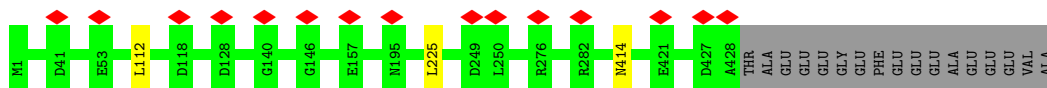


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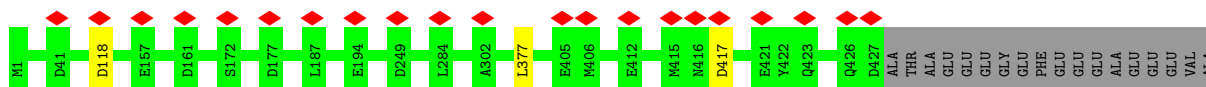




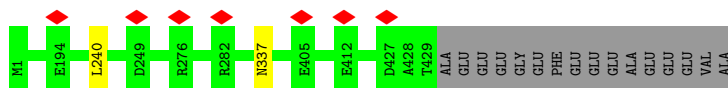
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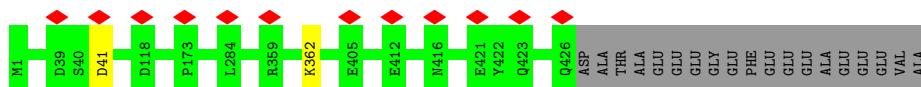
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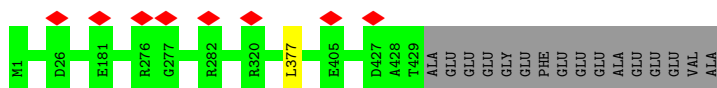
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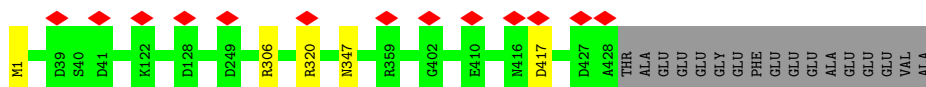
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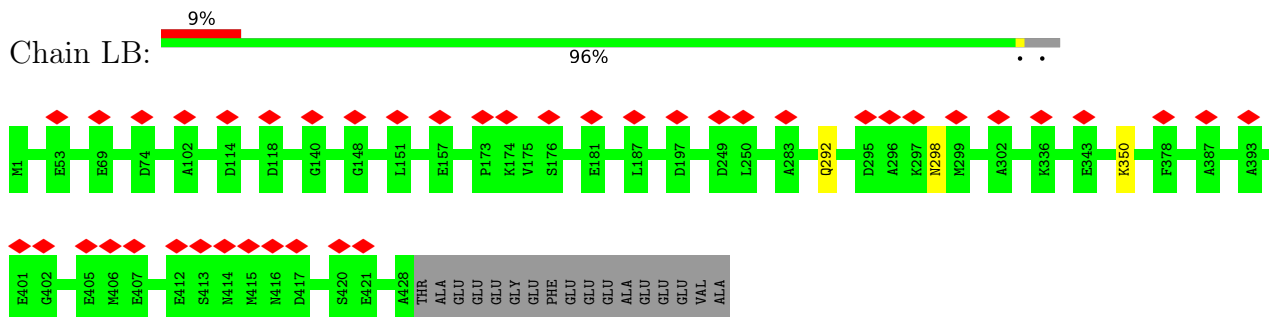
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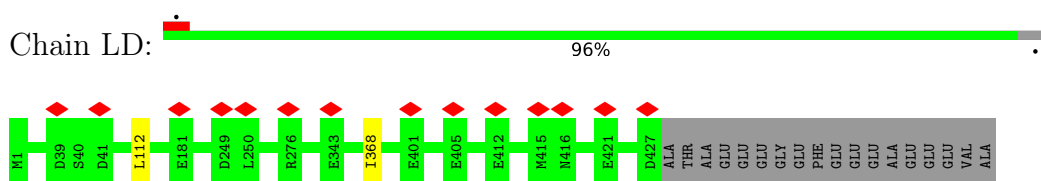
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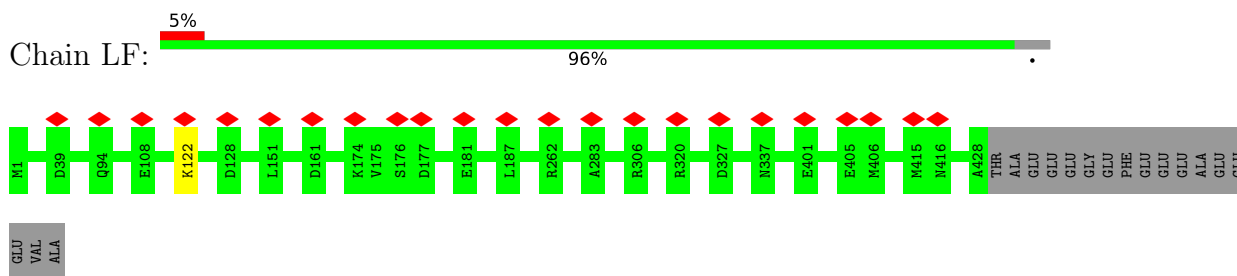
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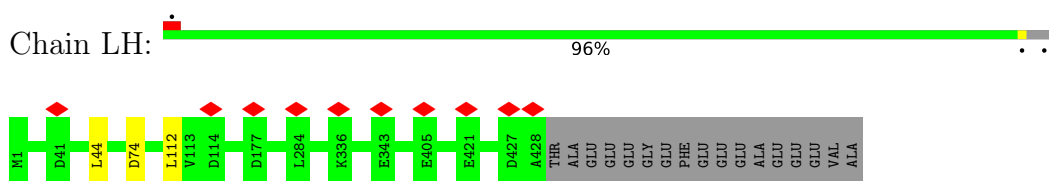
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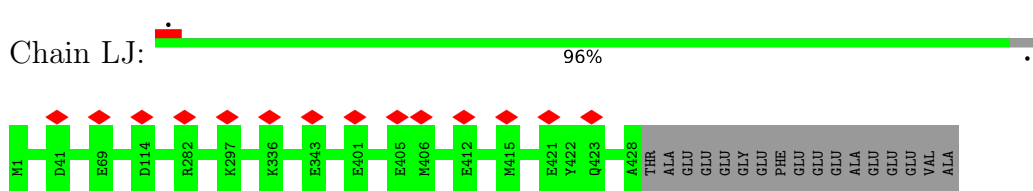
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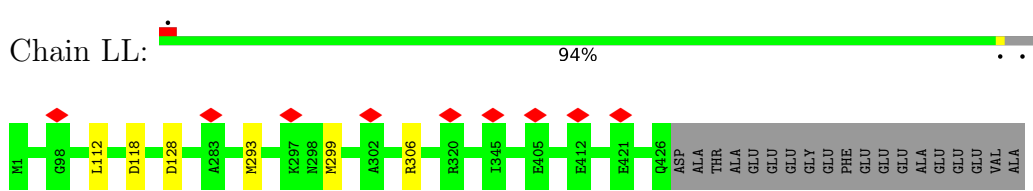
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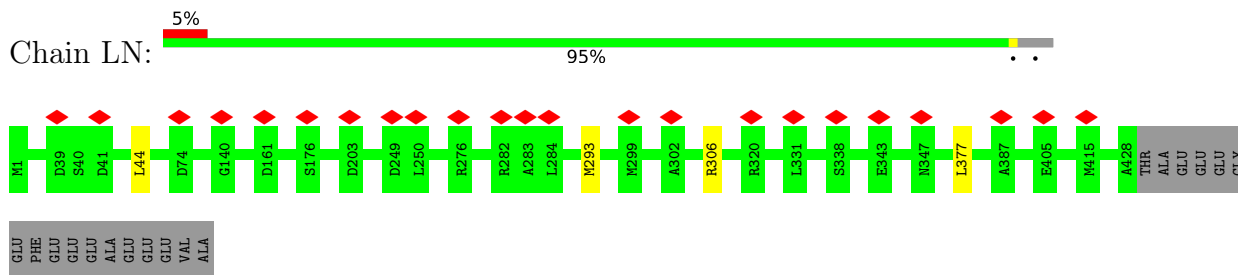
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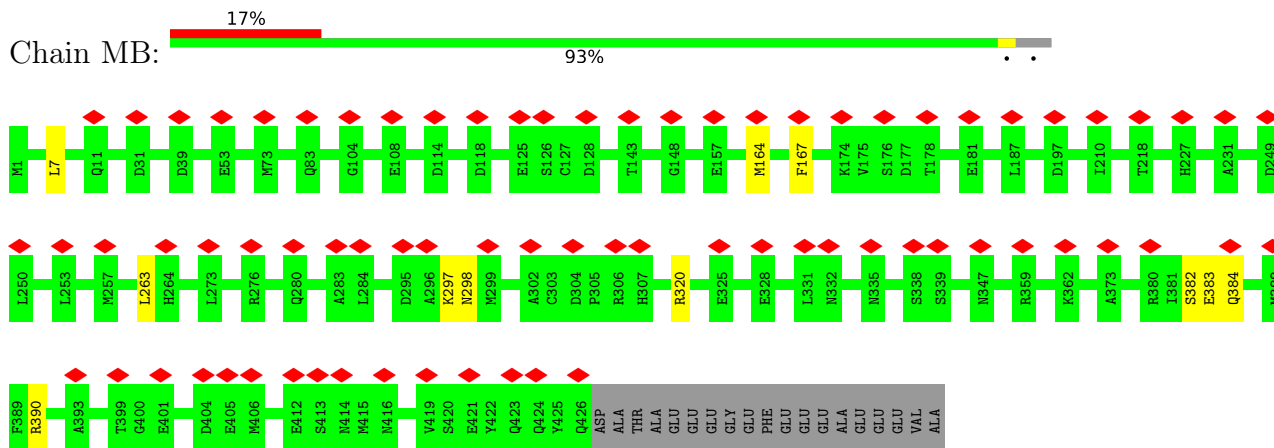
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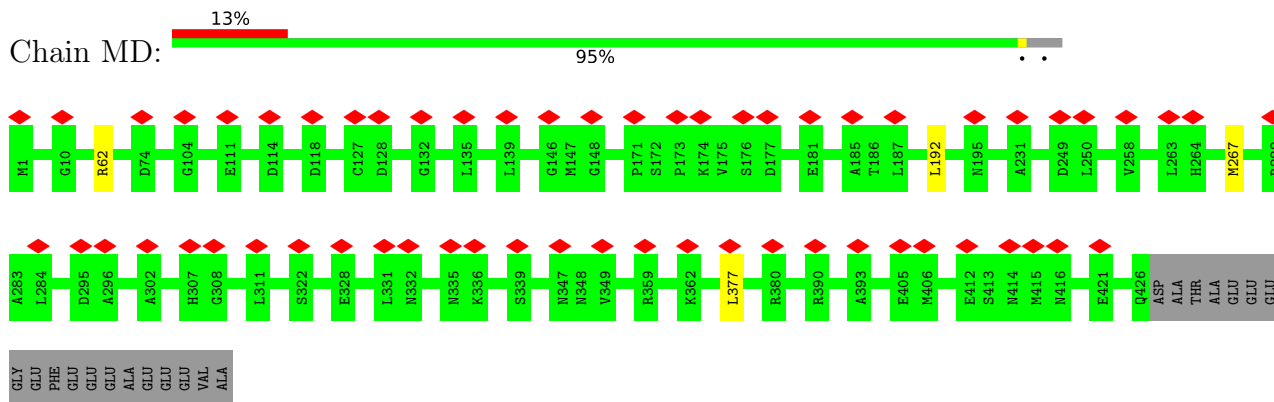
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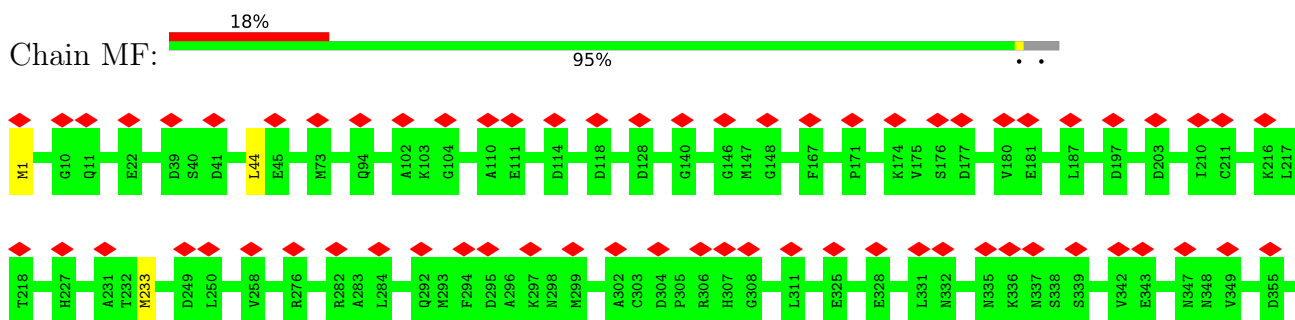
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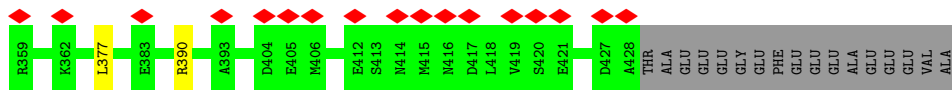


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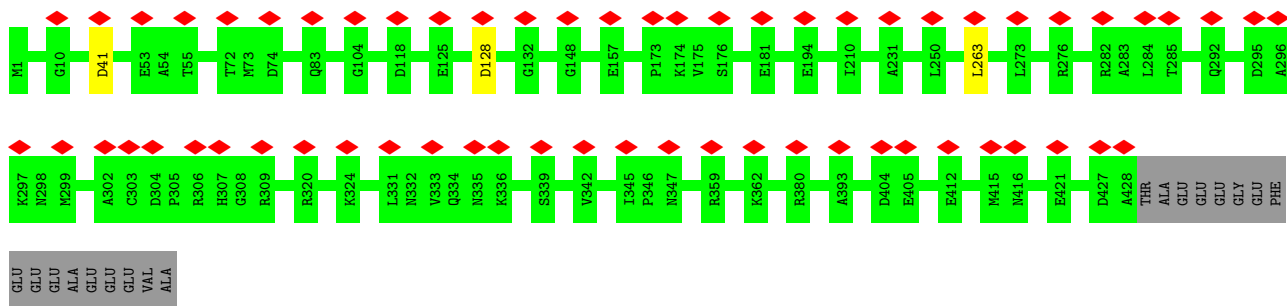


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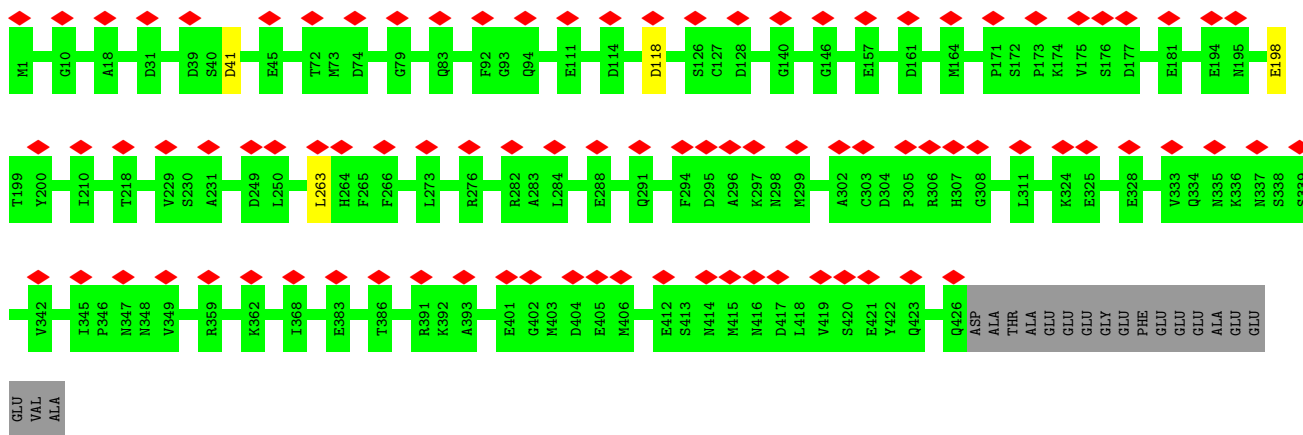




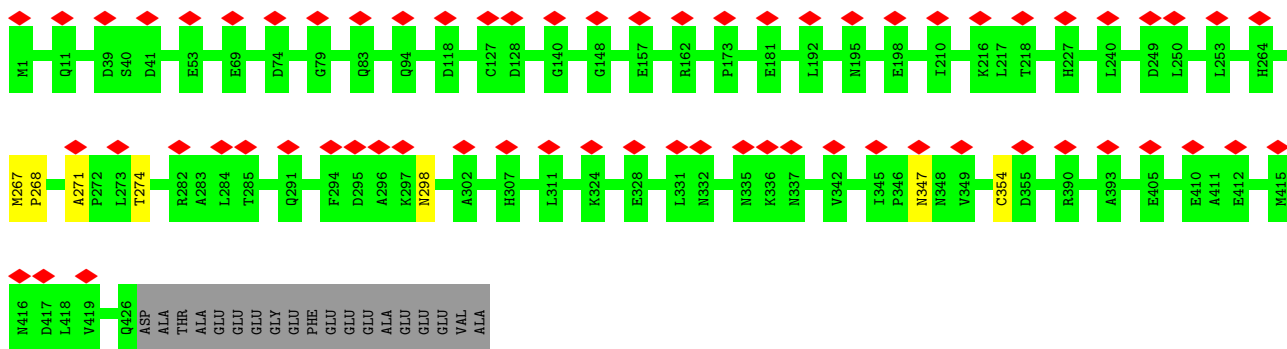
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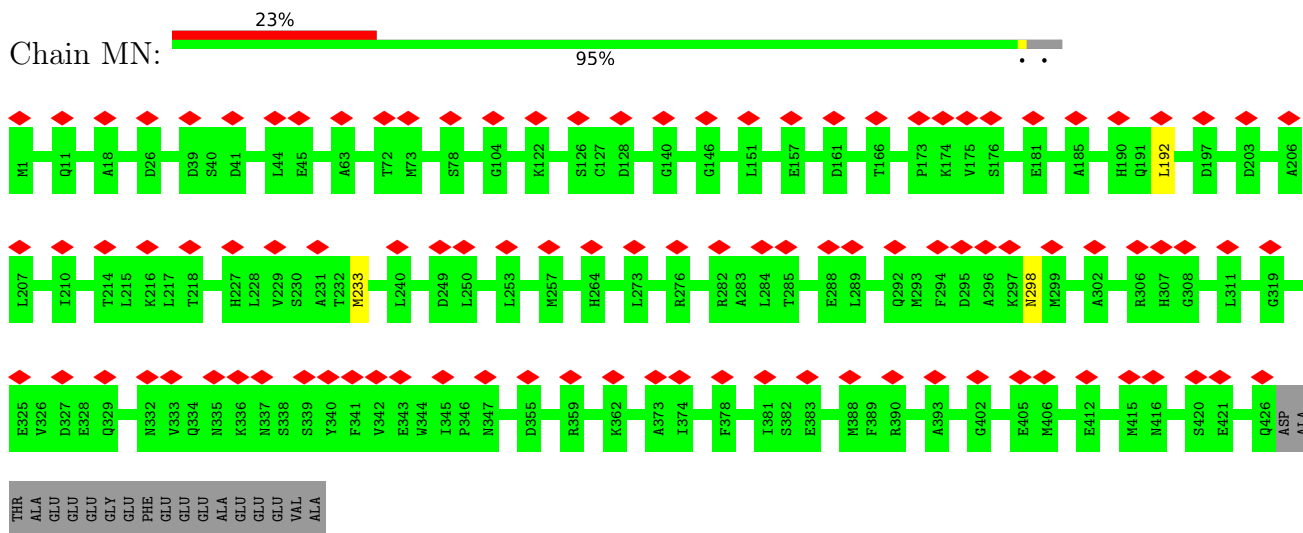
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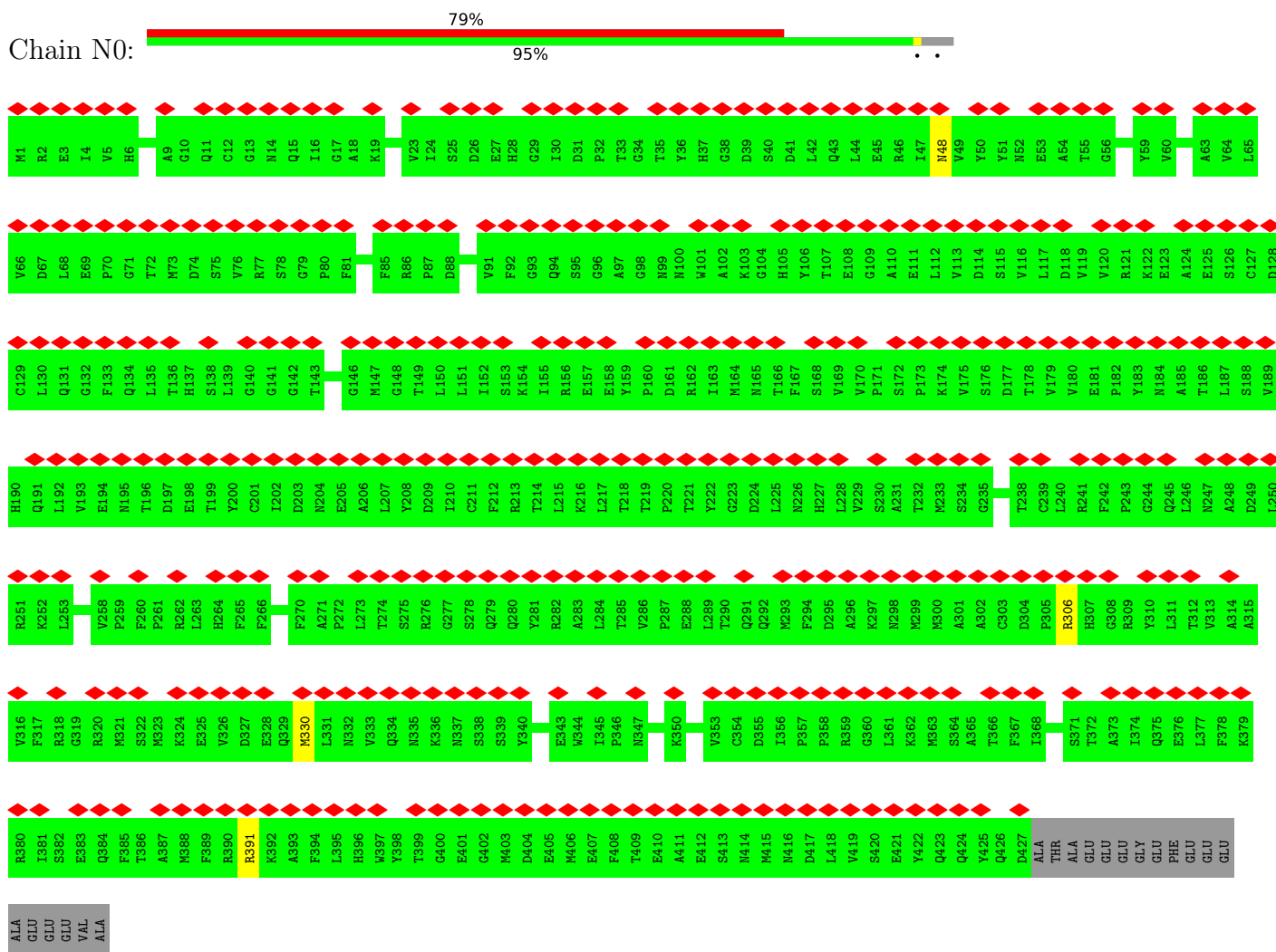
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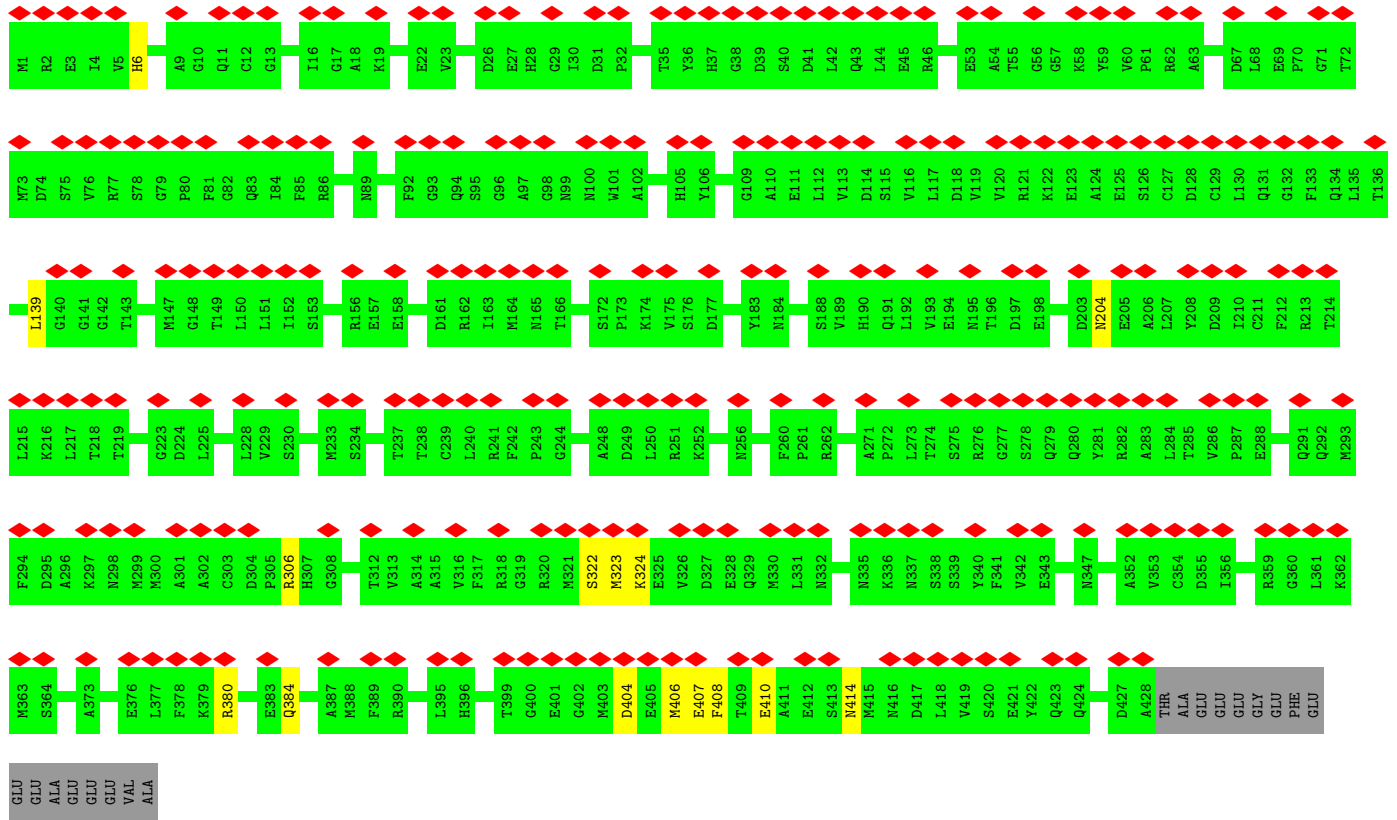


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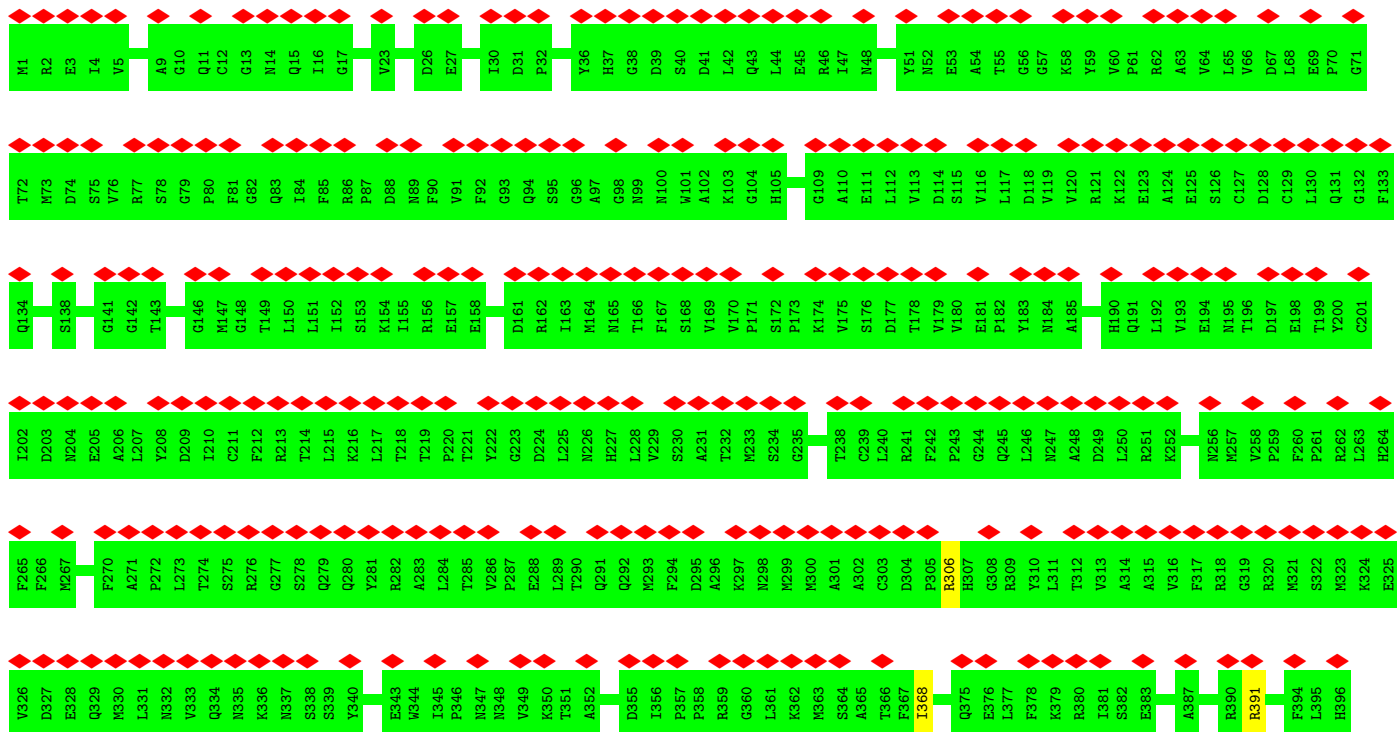


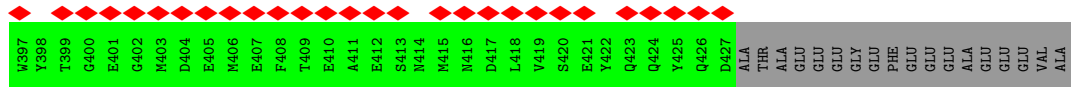
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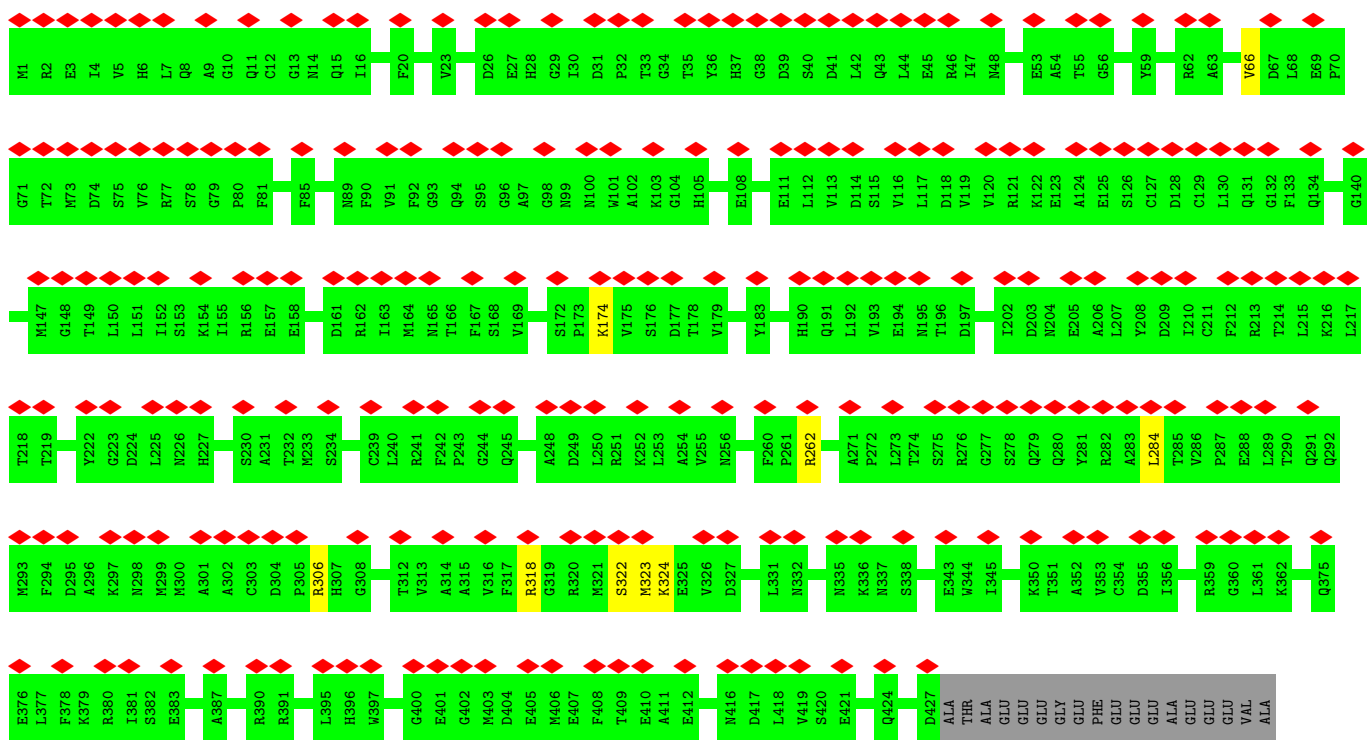


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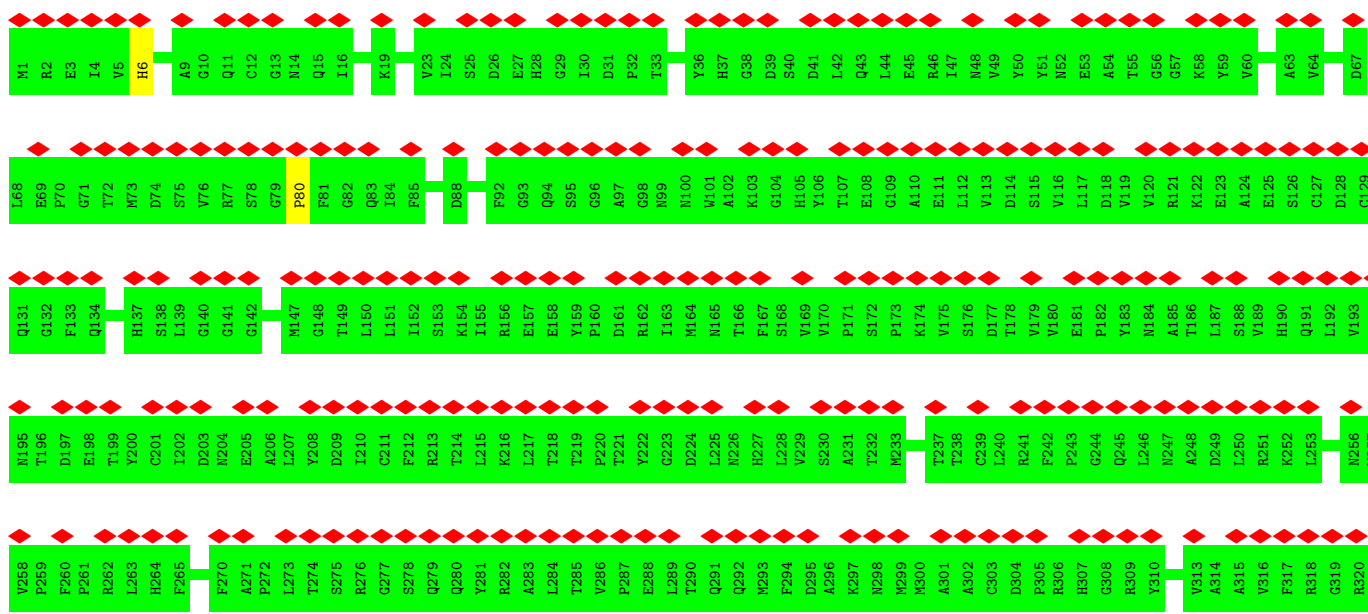
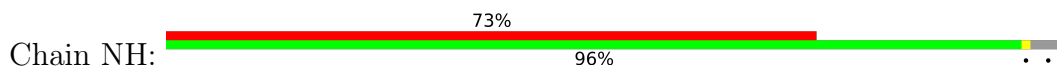




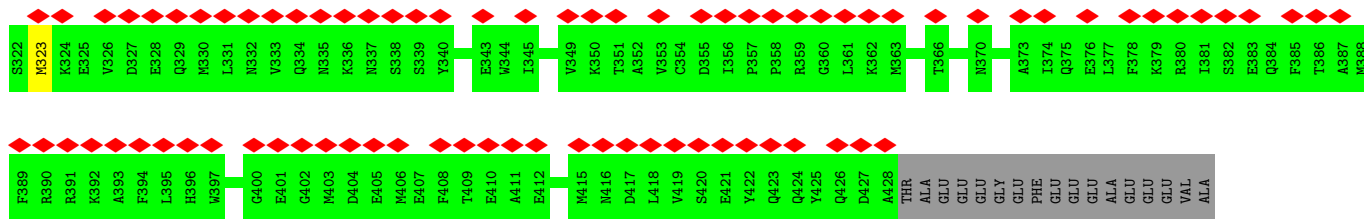
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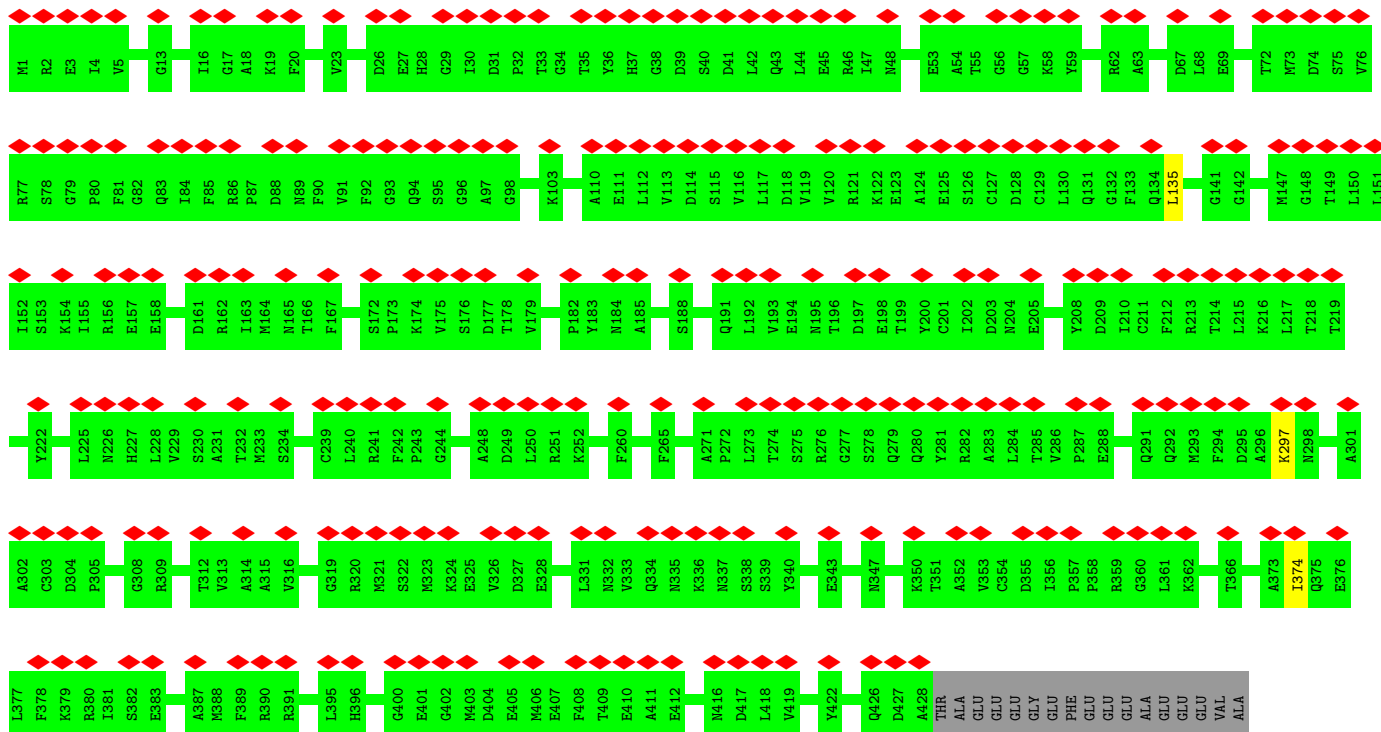
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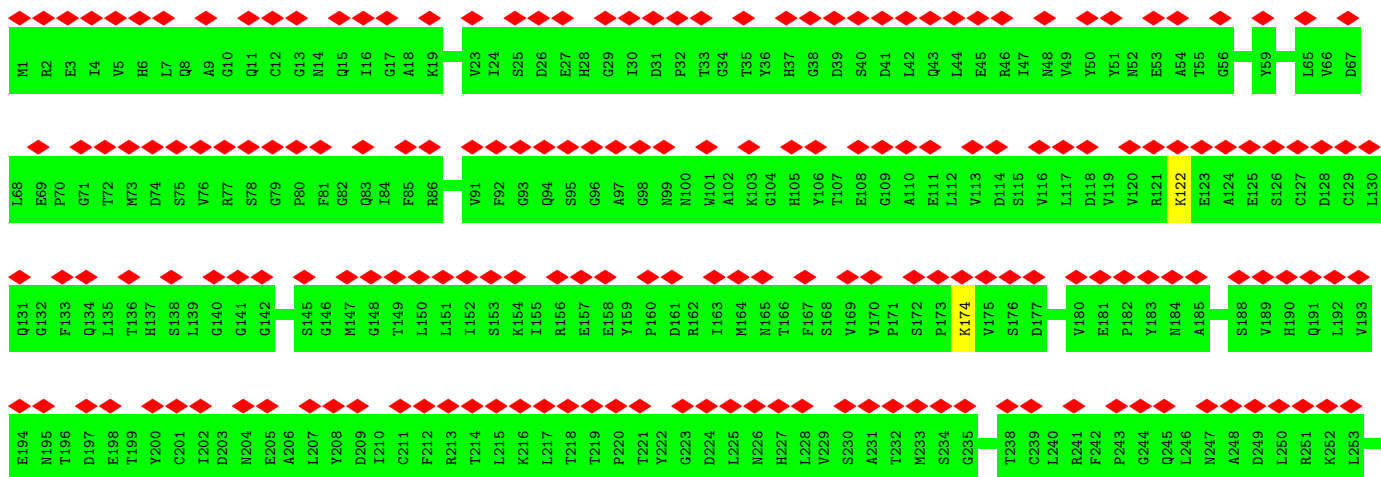
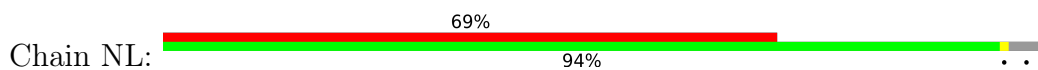


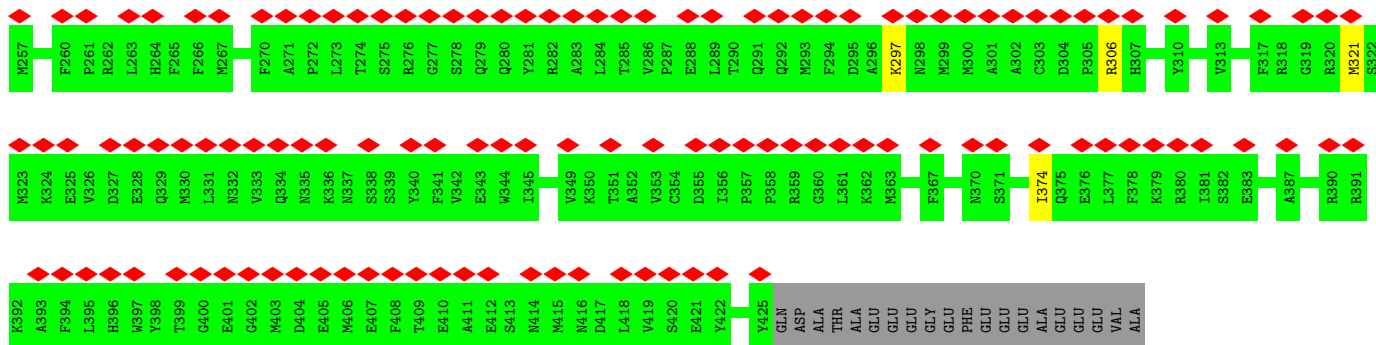


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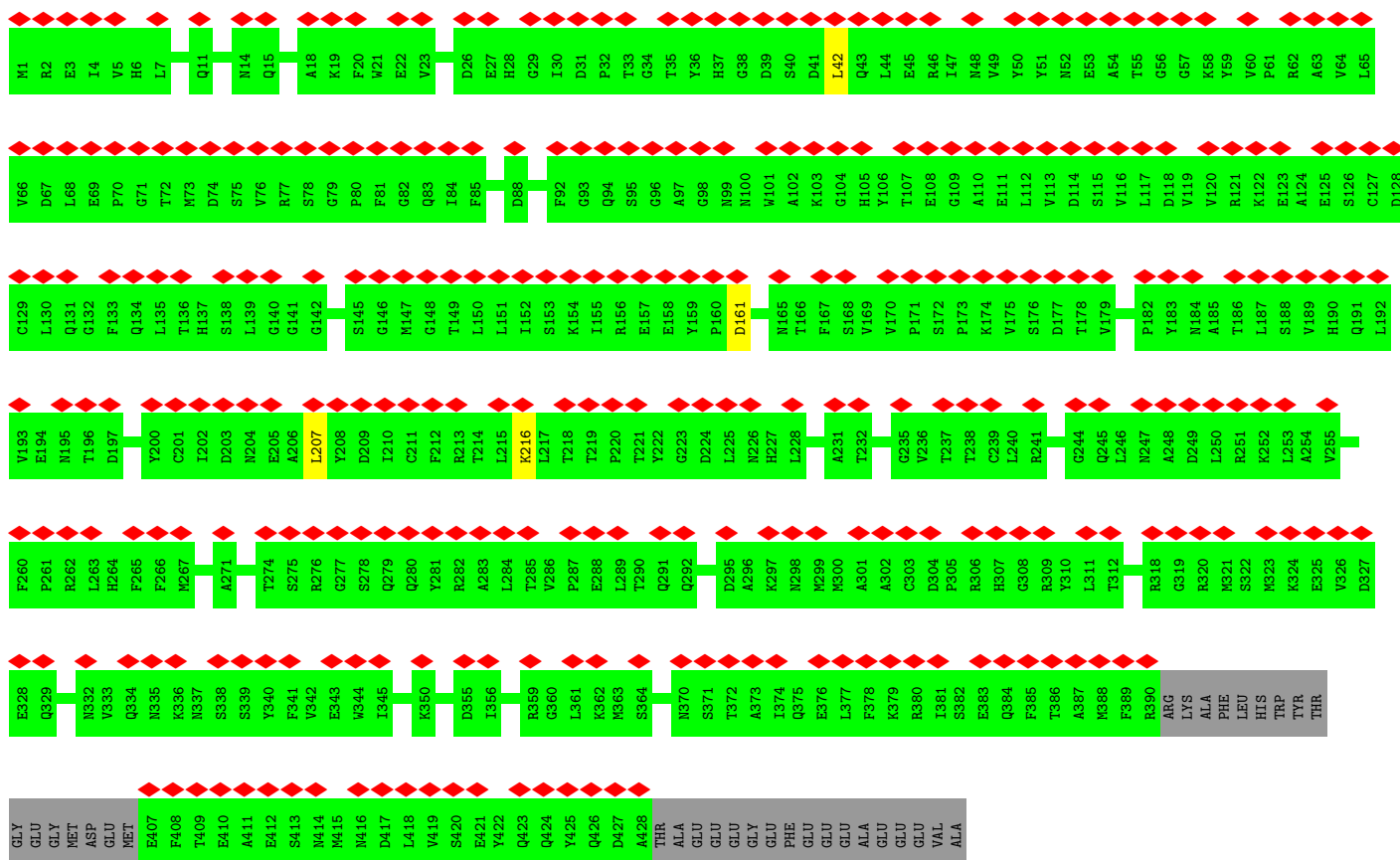


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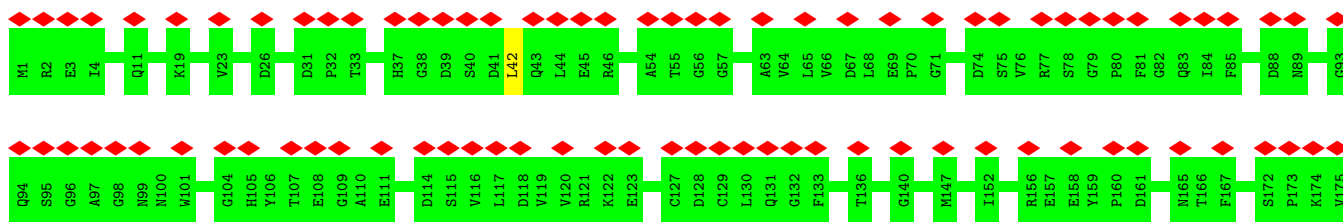
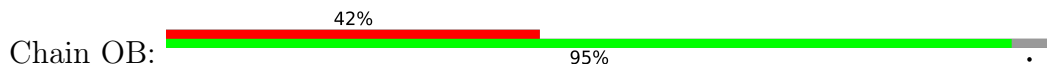


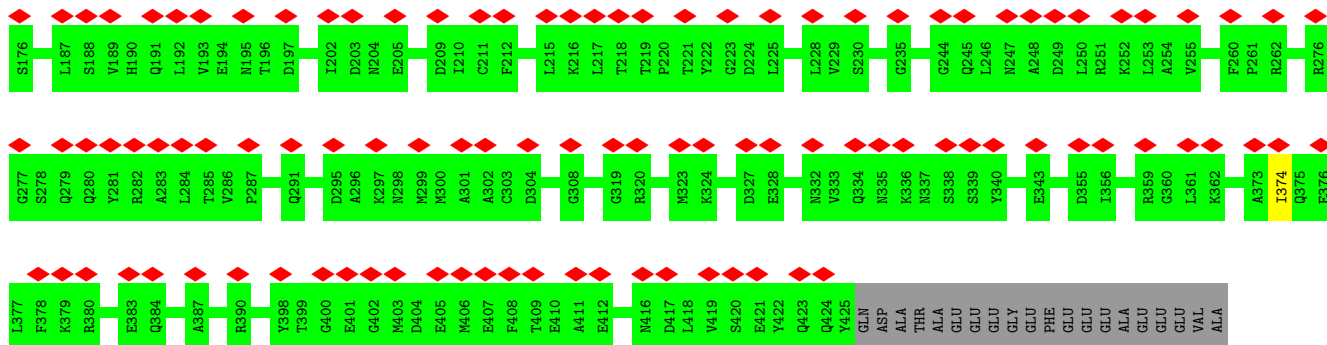


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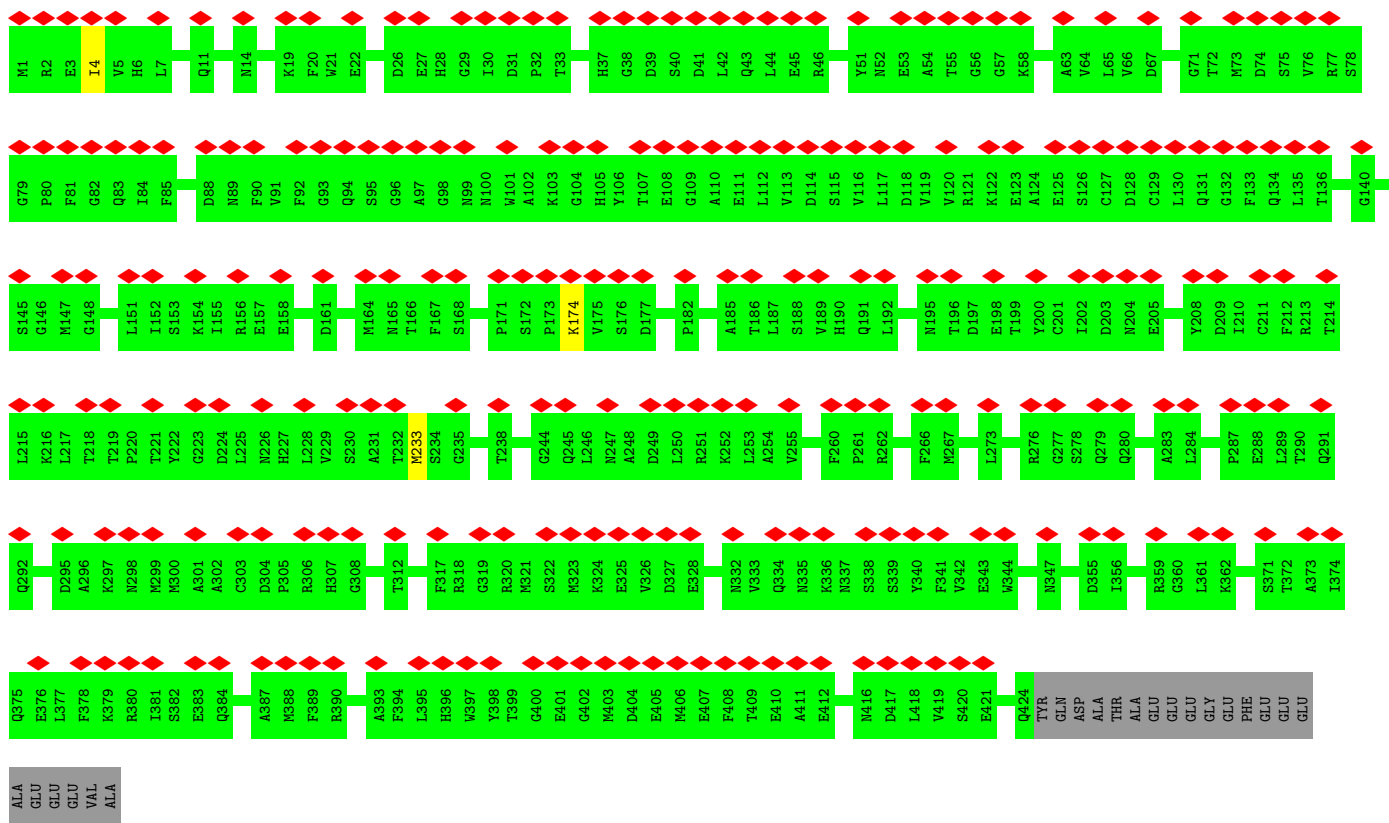


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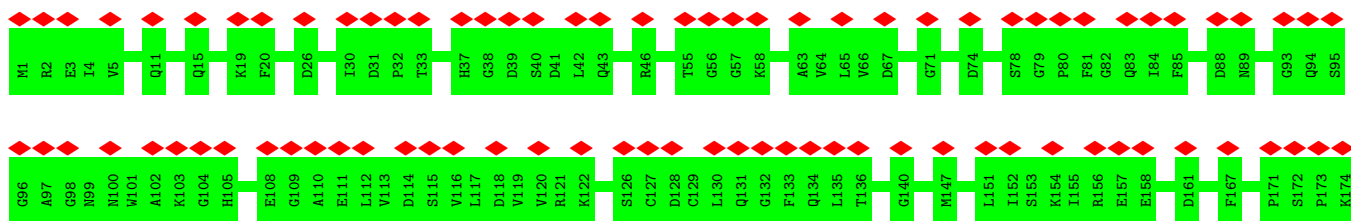
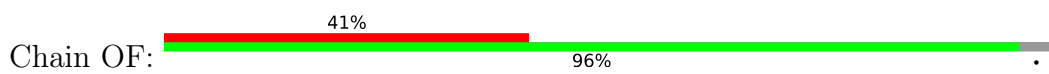


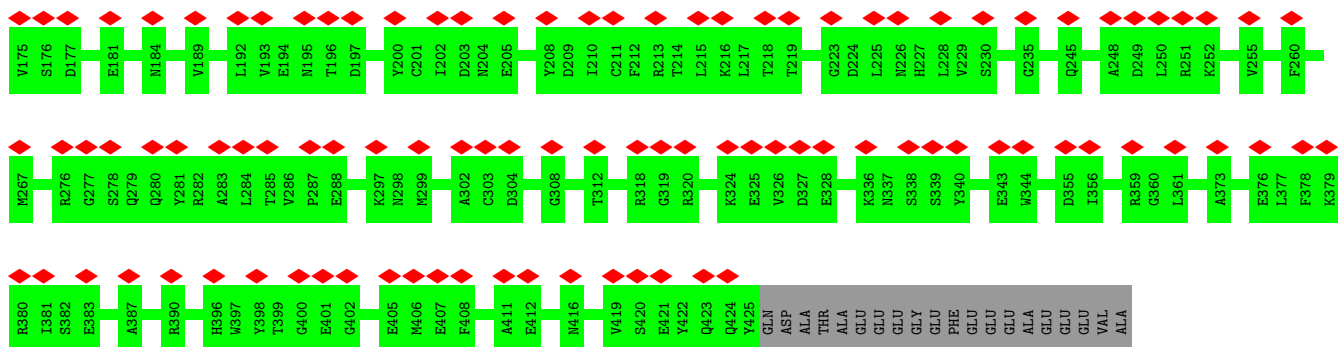


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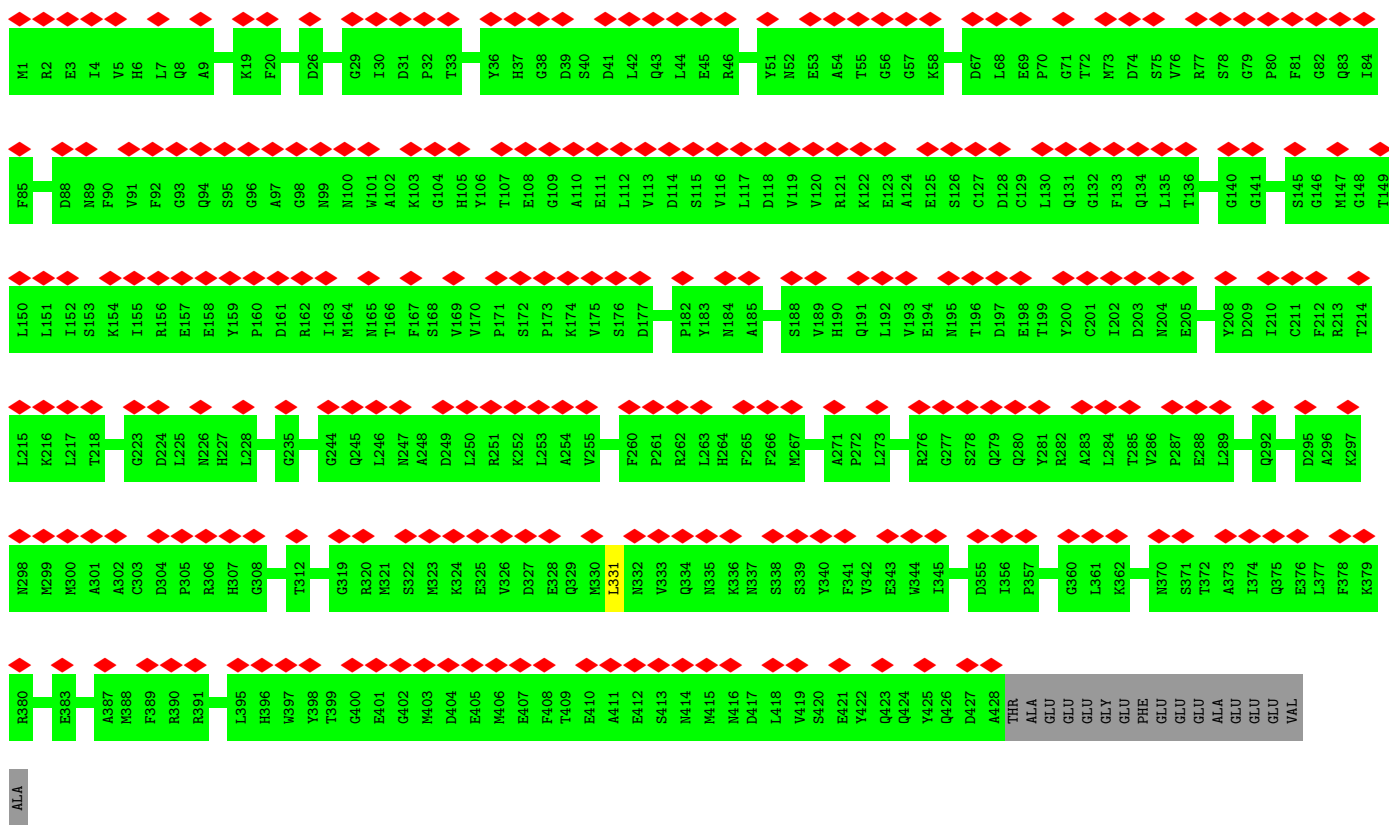


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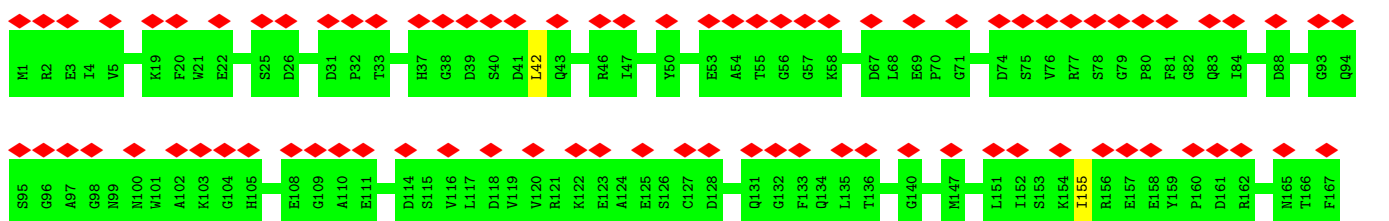
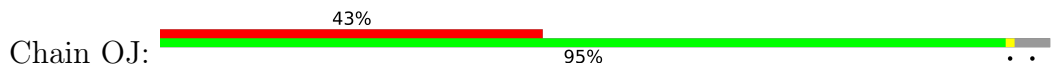


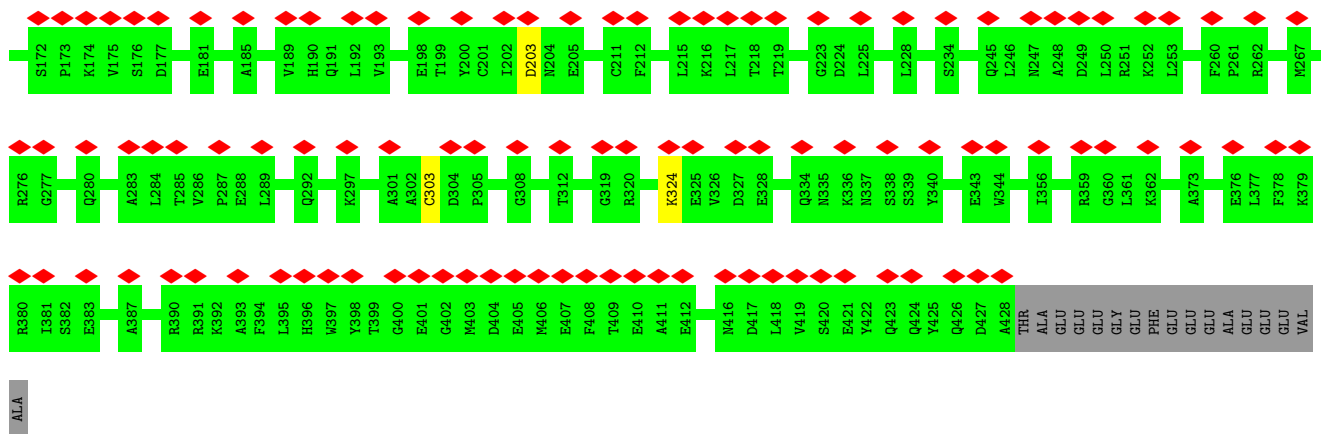


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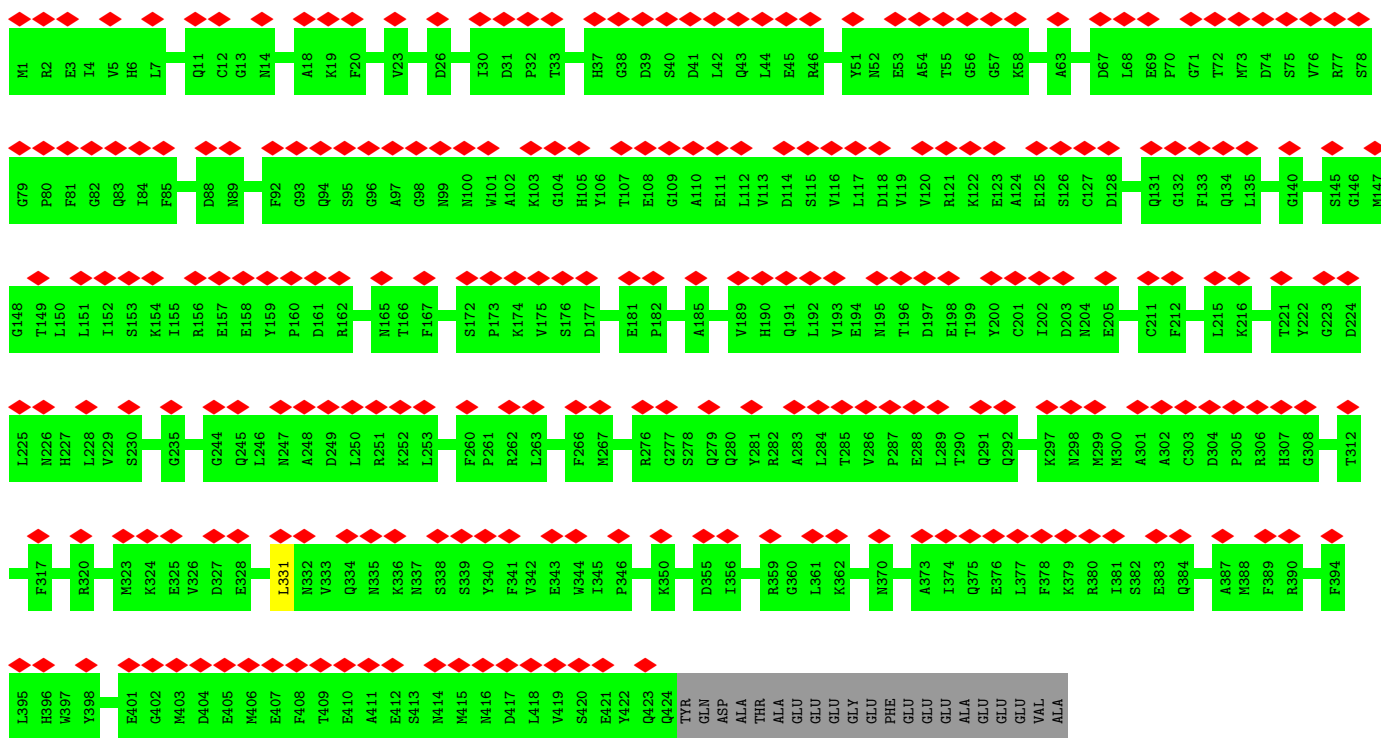


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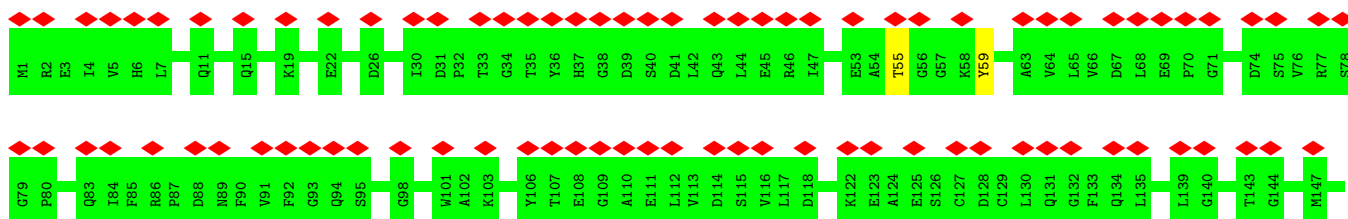


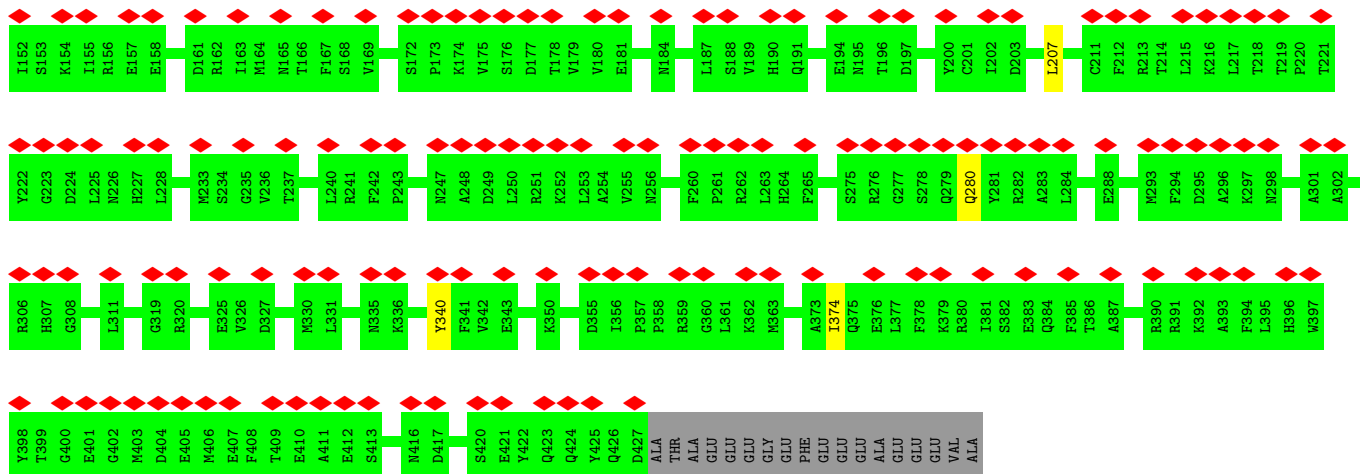


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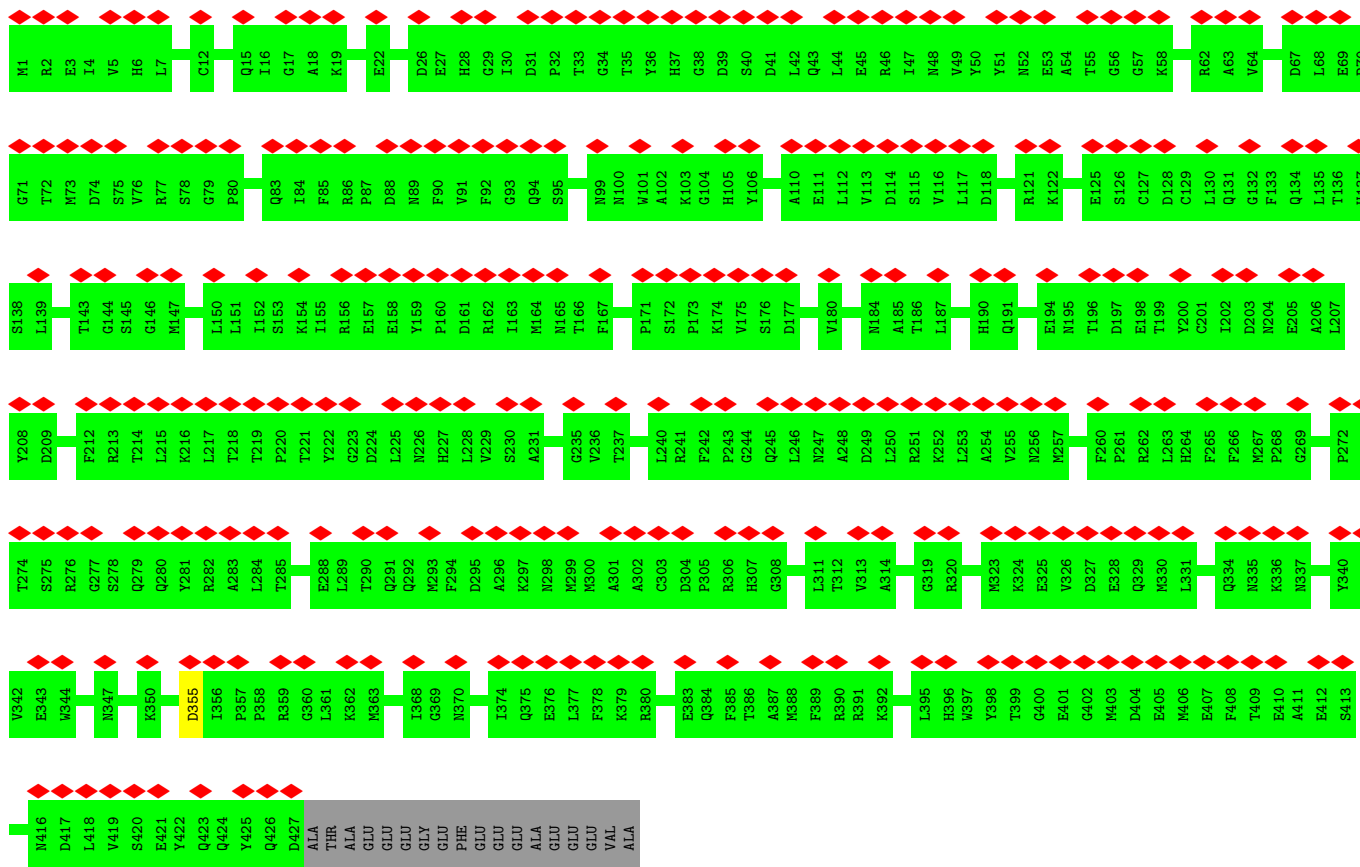


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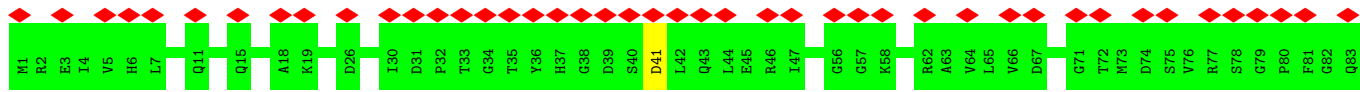


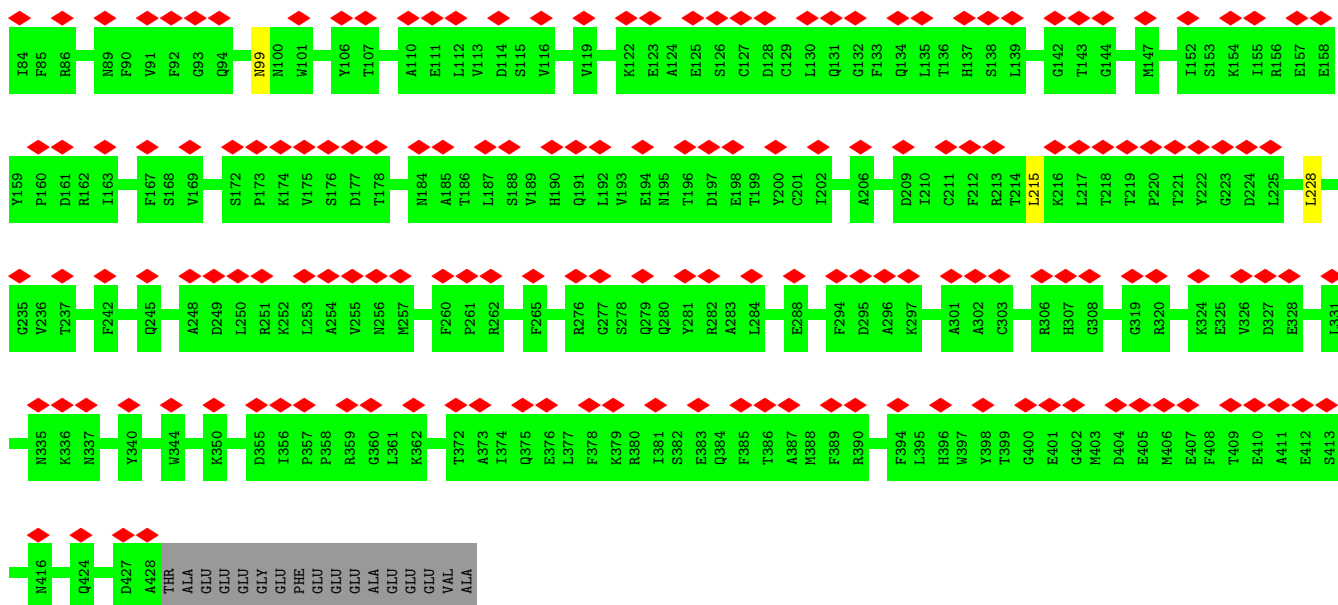


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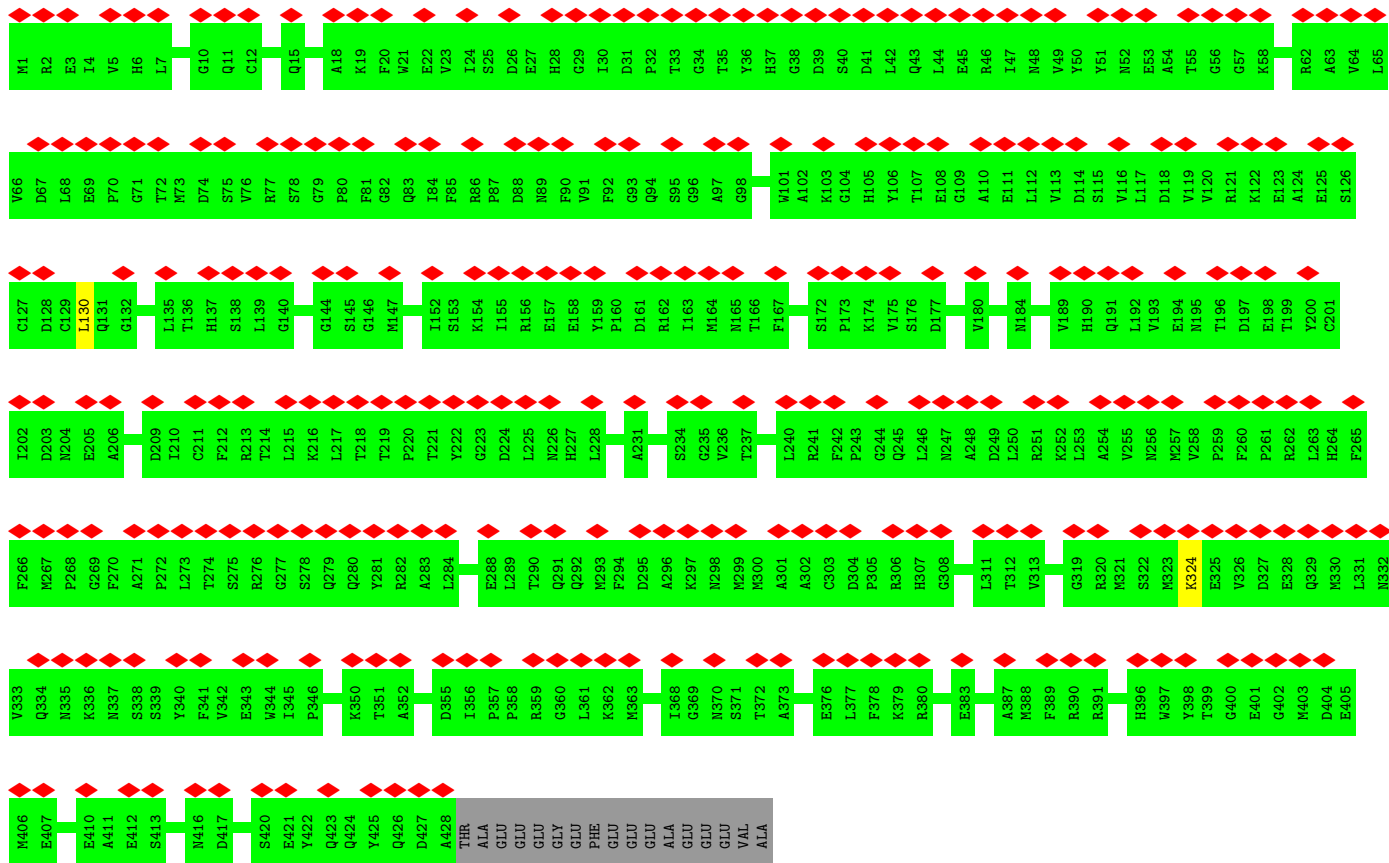


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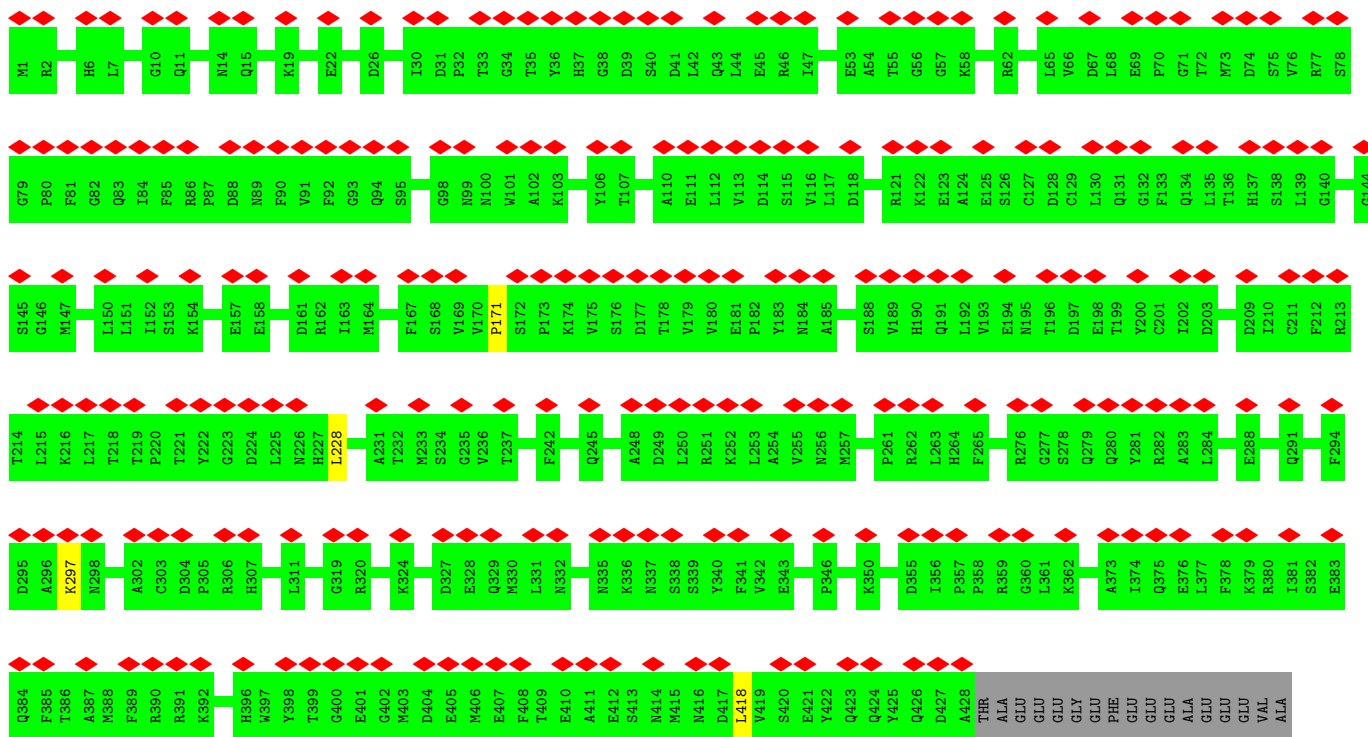


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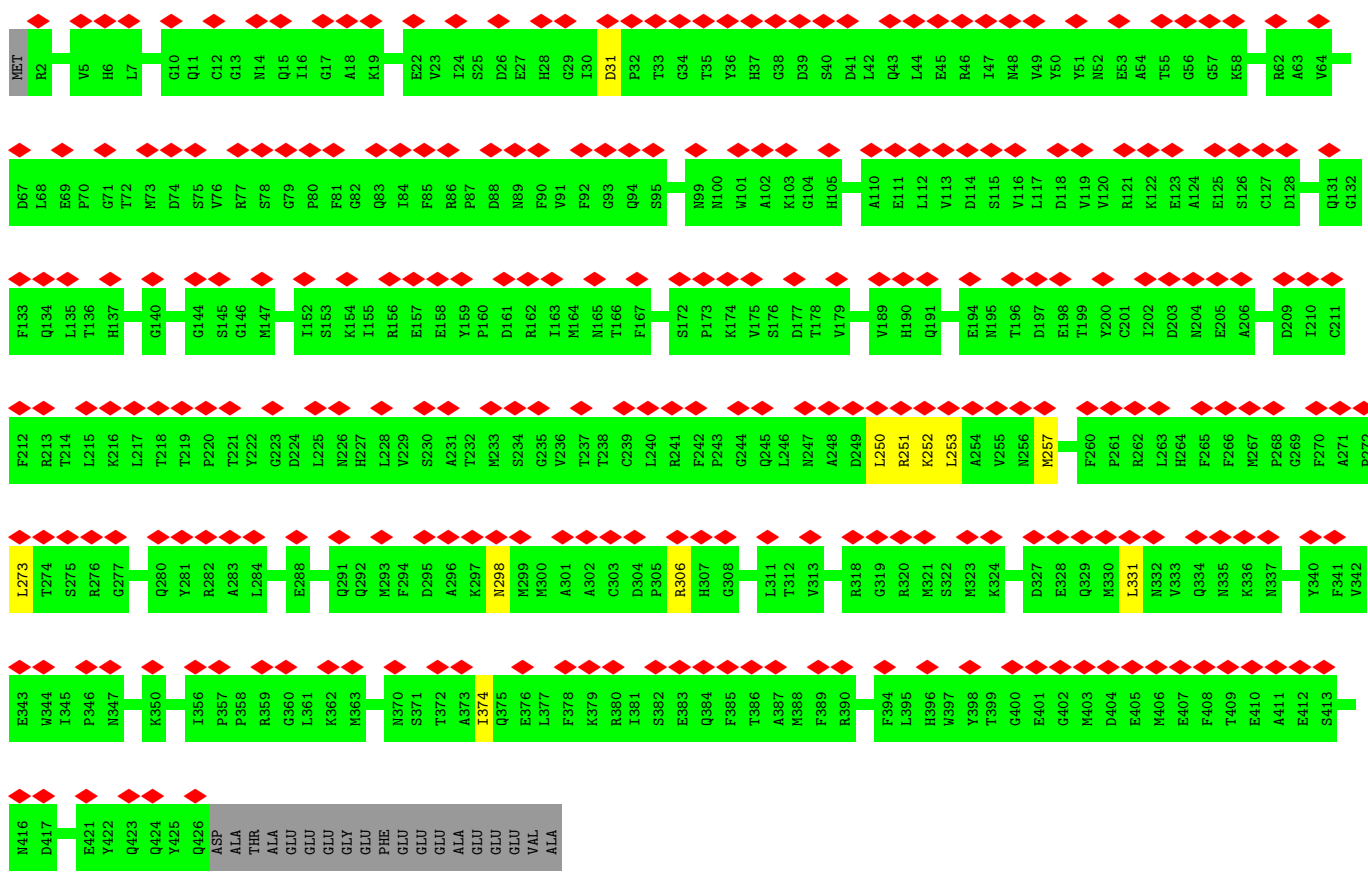


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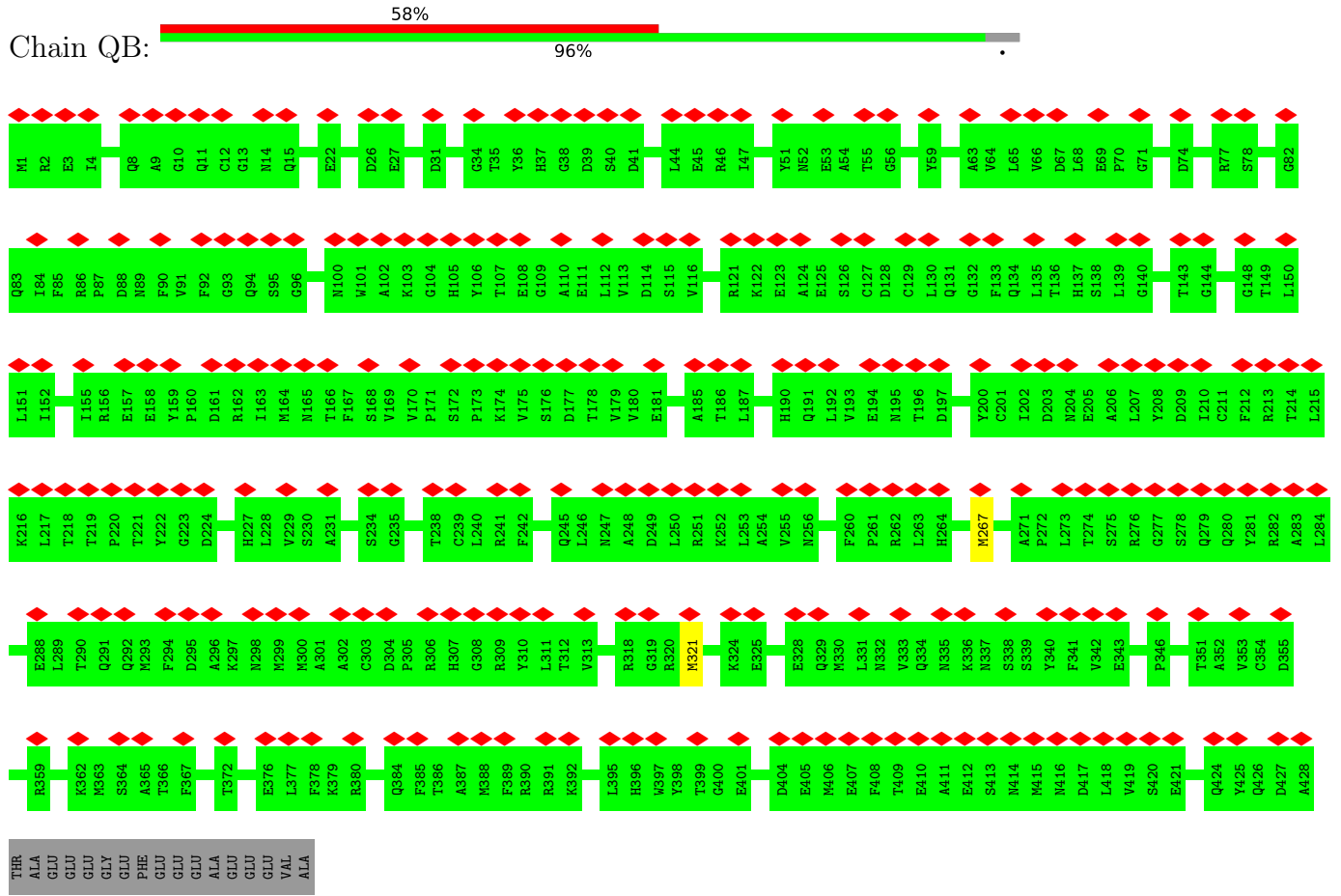


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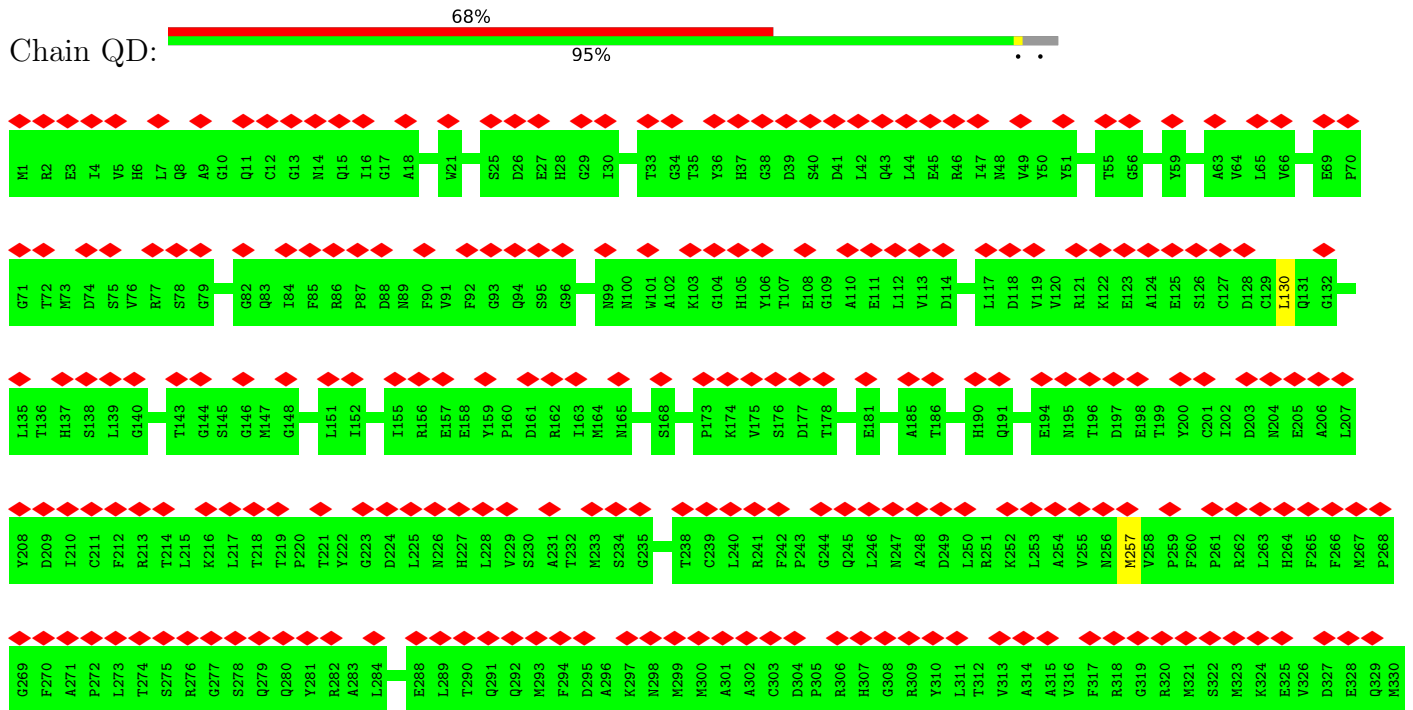


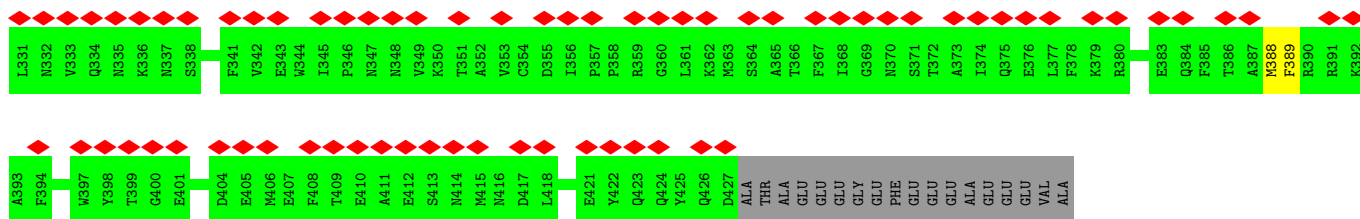


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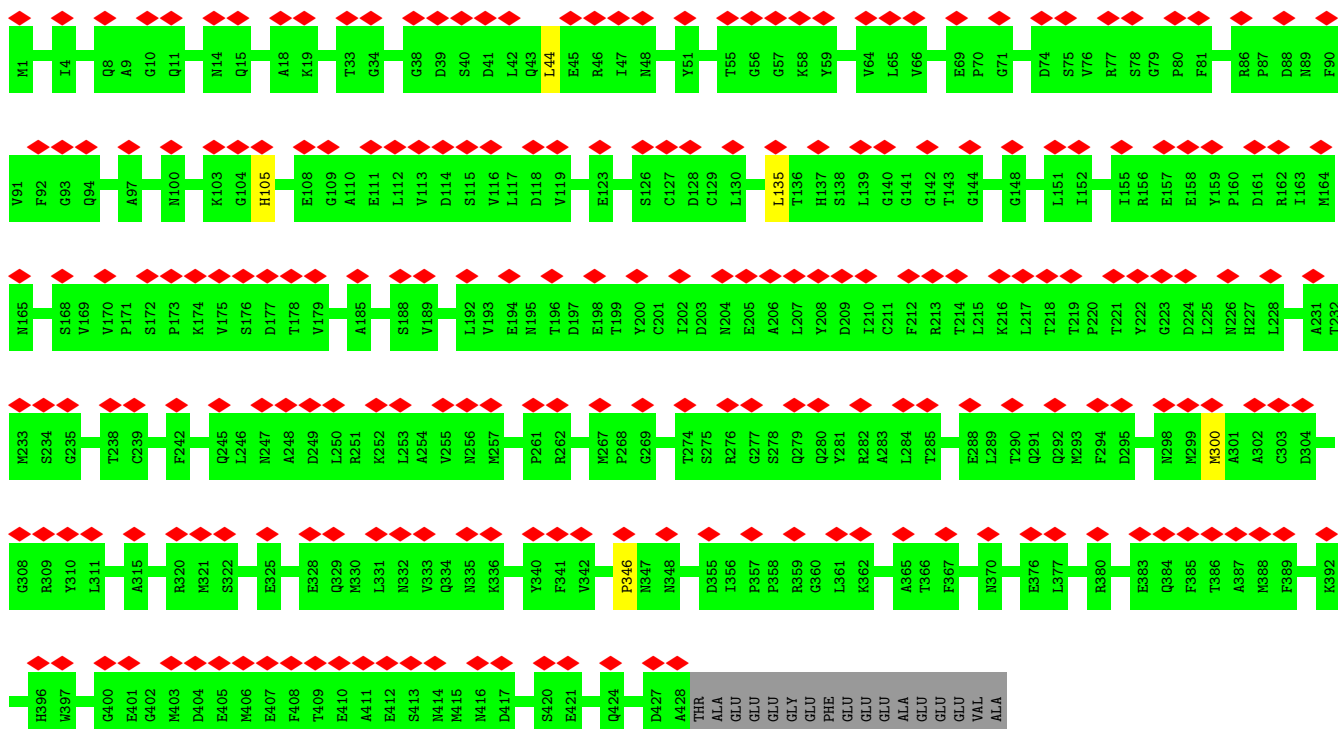


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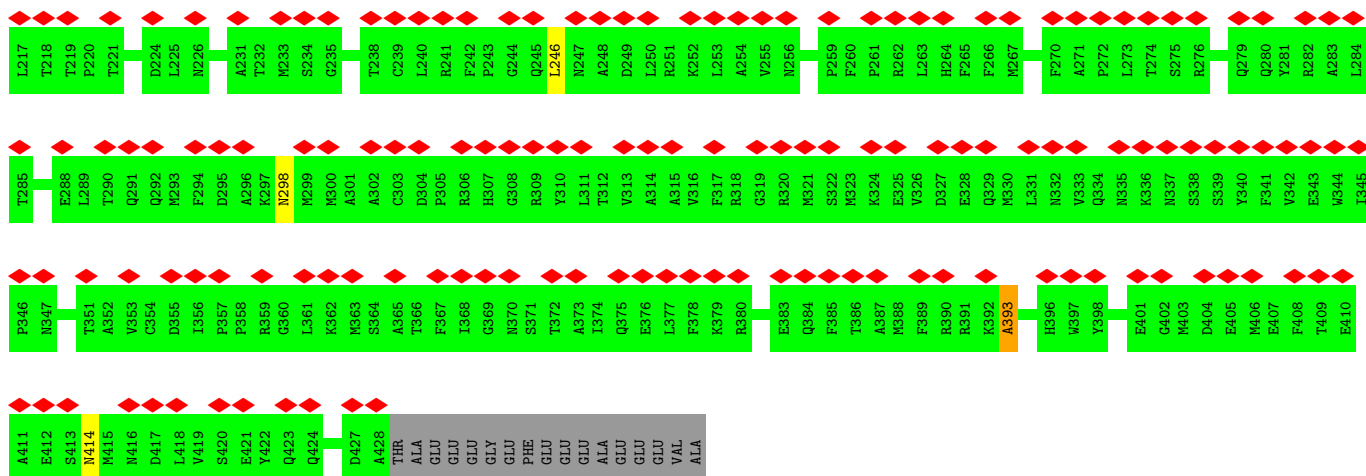


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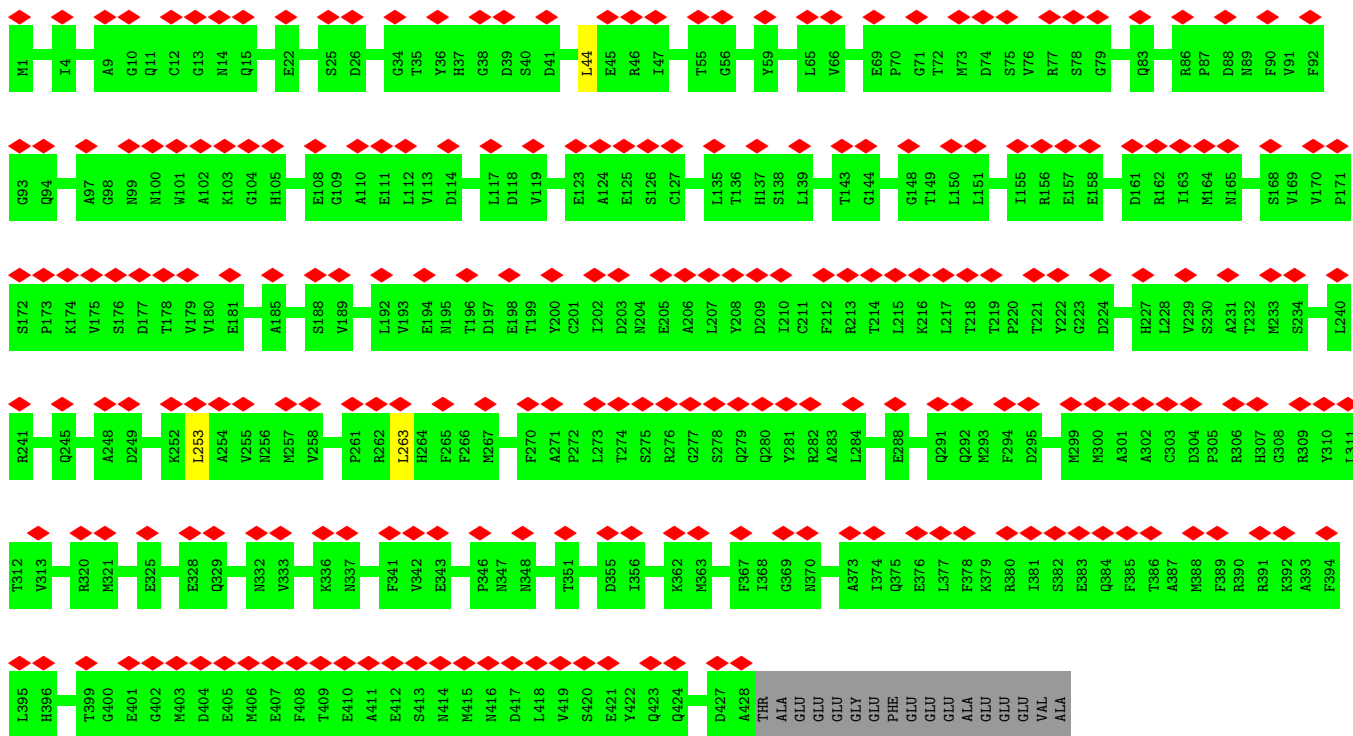


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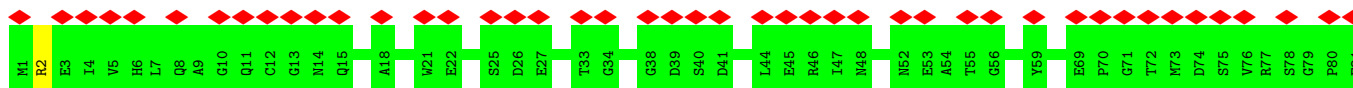




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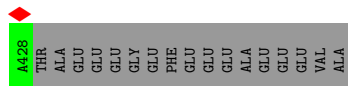


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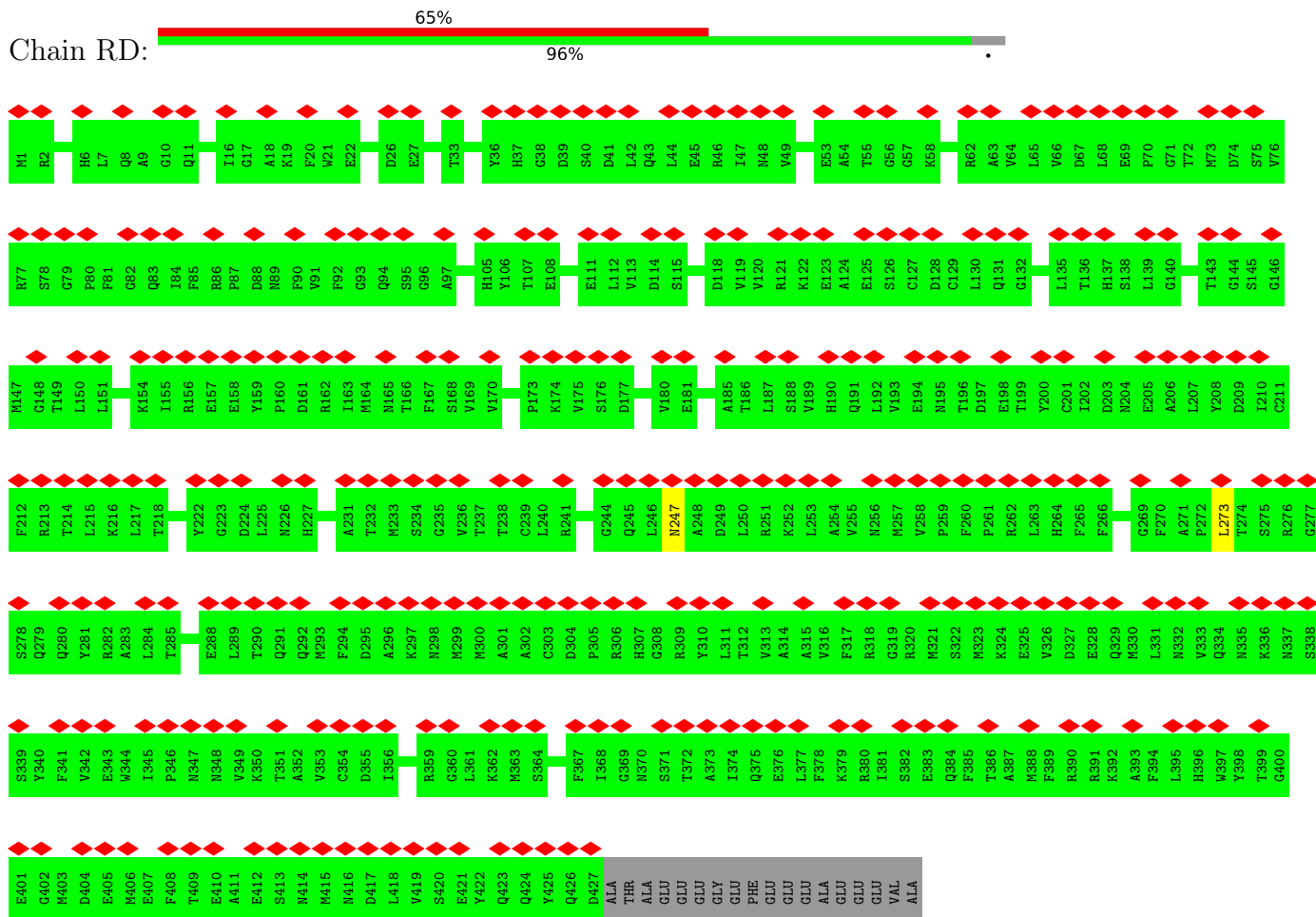




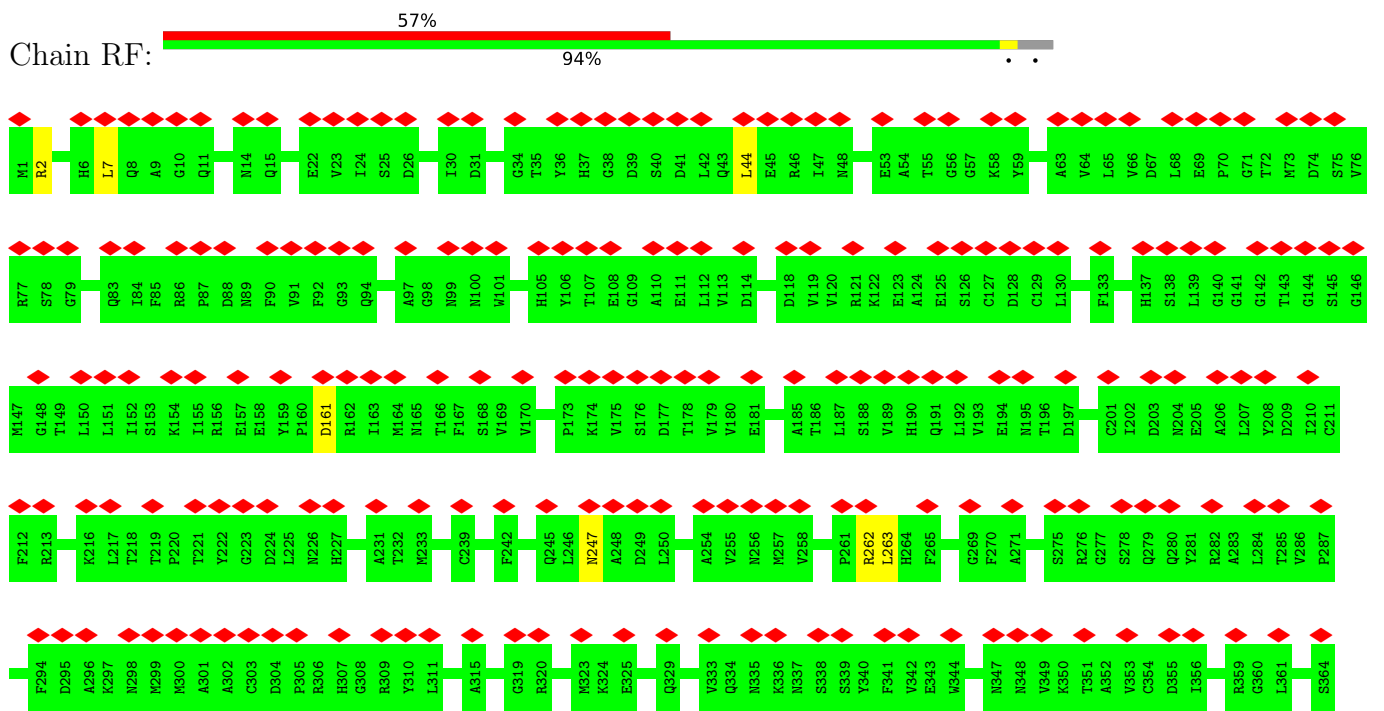
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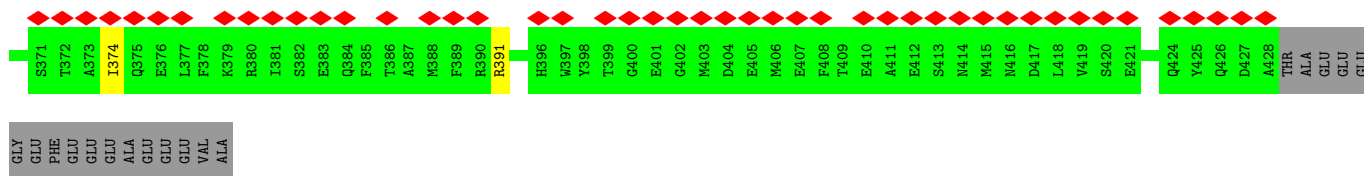


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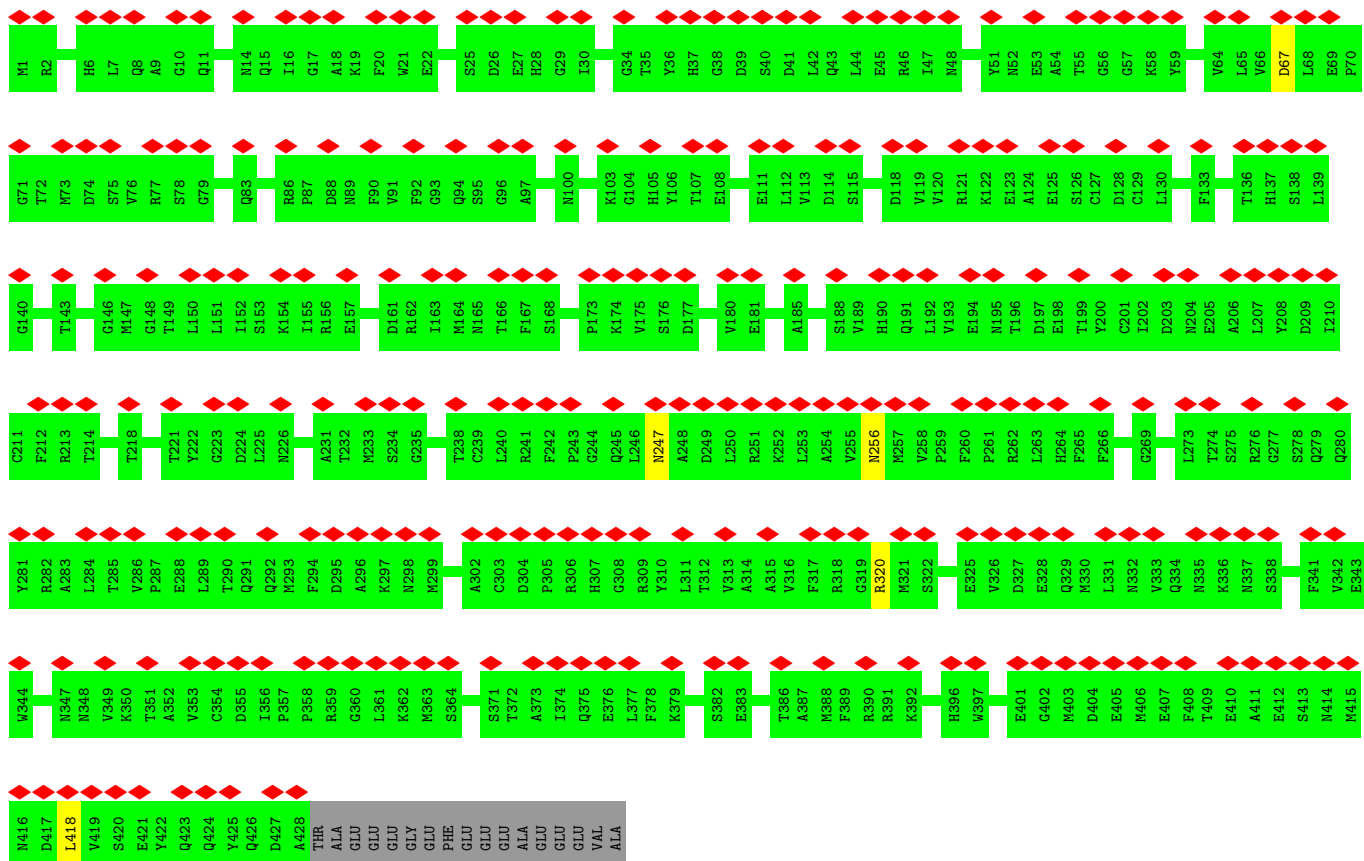


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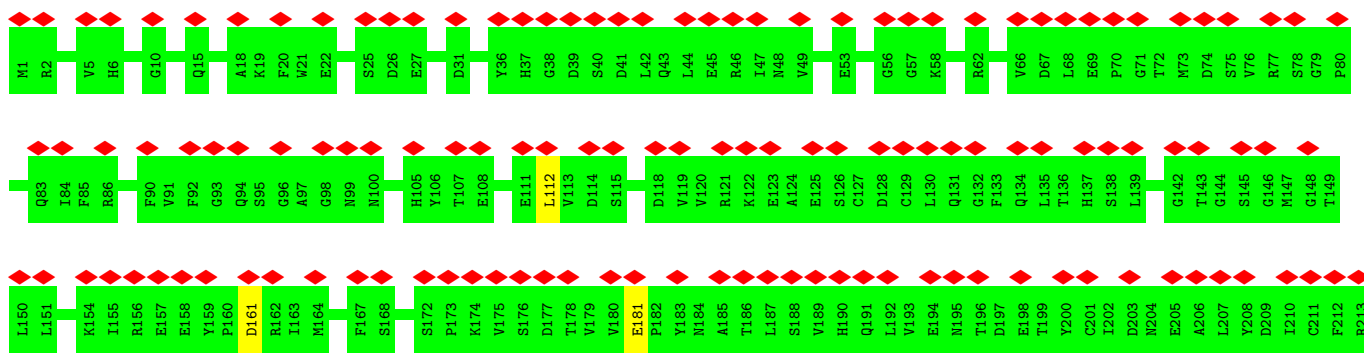


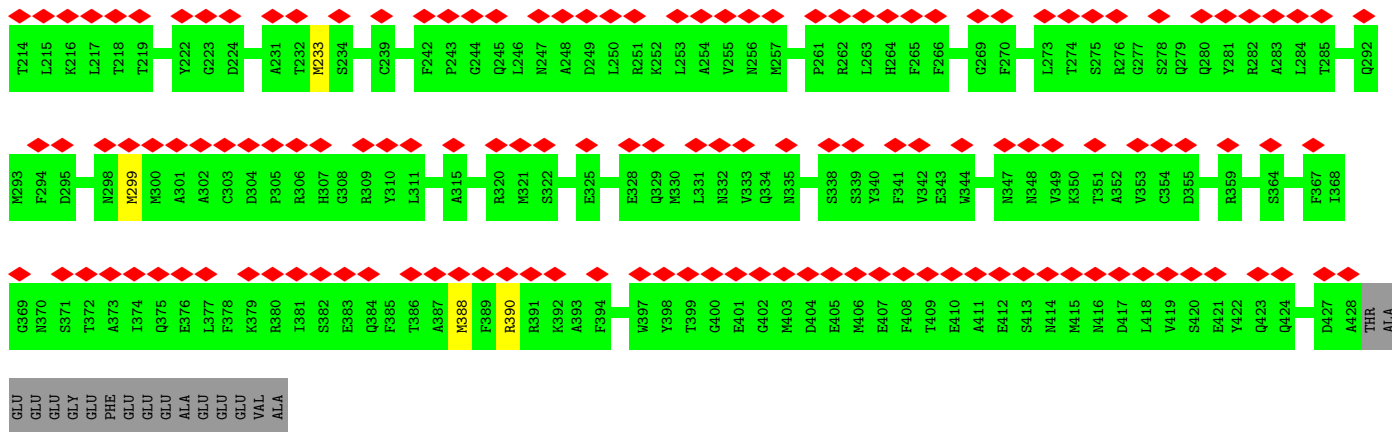


• Molecule 9: Tubulin beta-4B chain

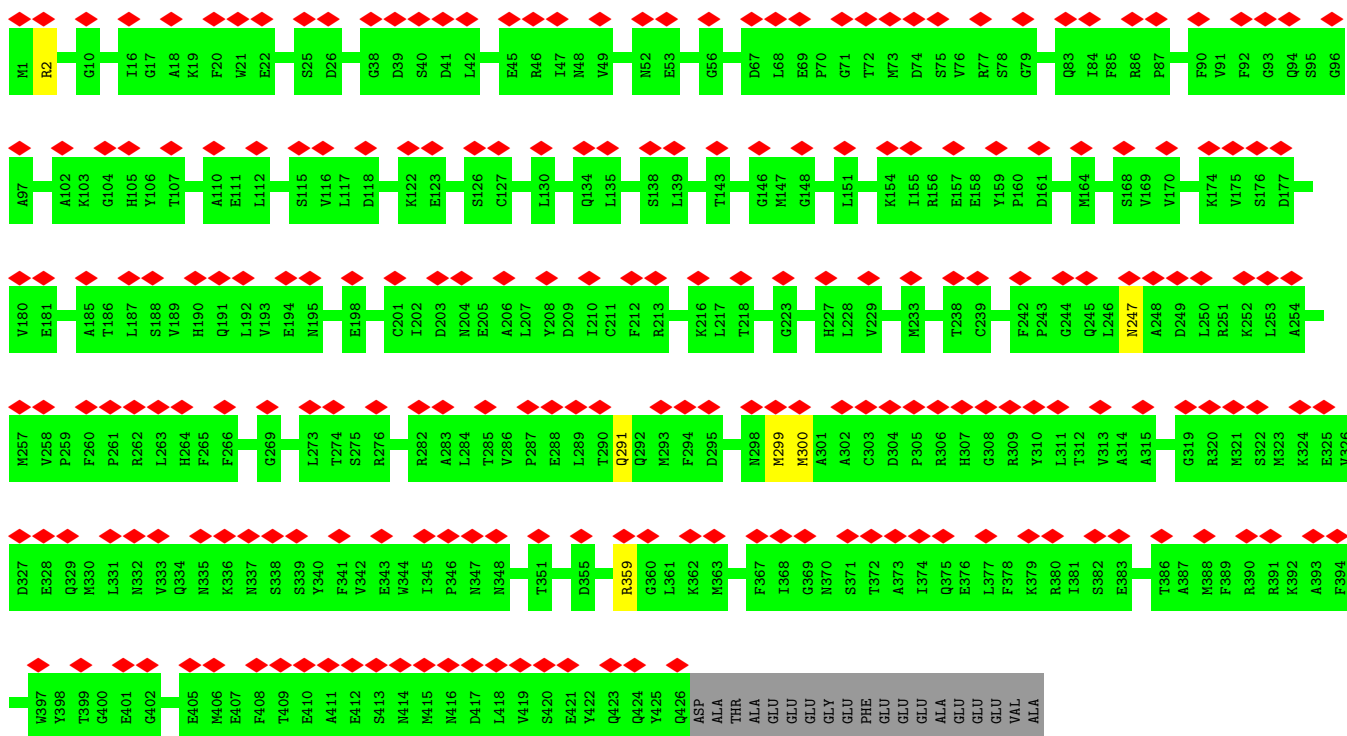


• Molecule 9: Tubulin beta-4B chain

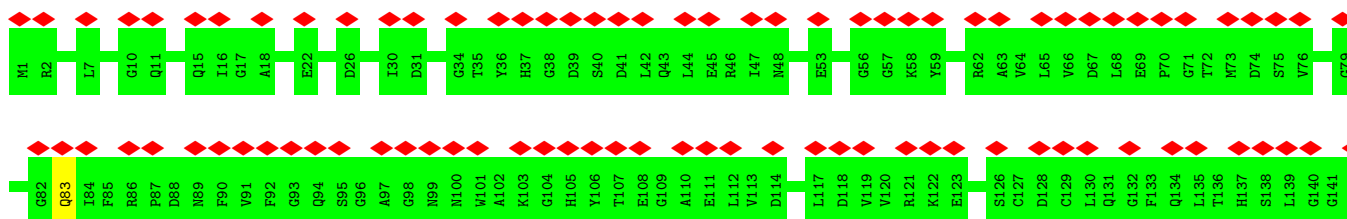


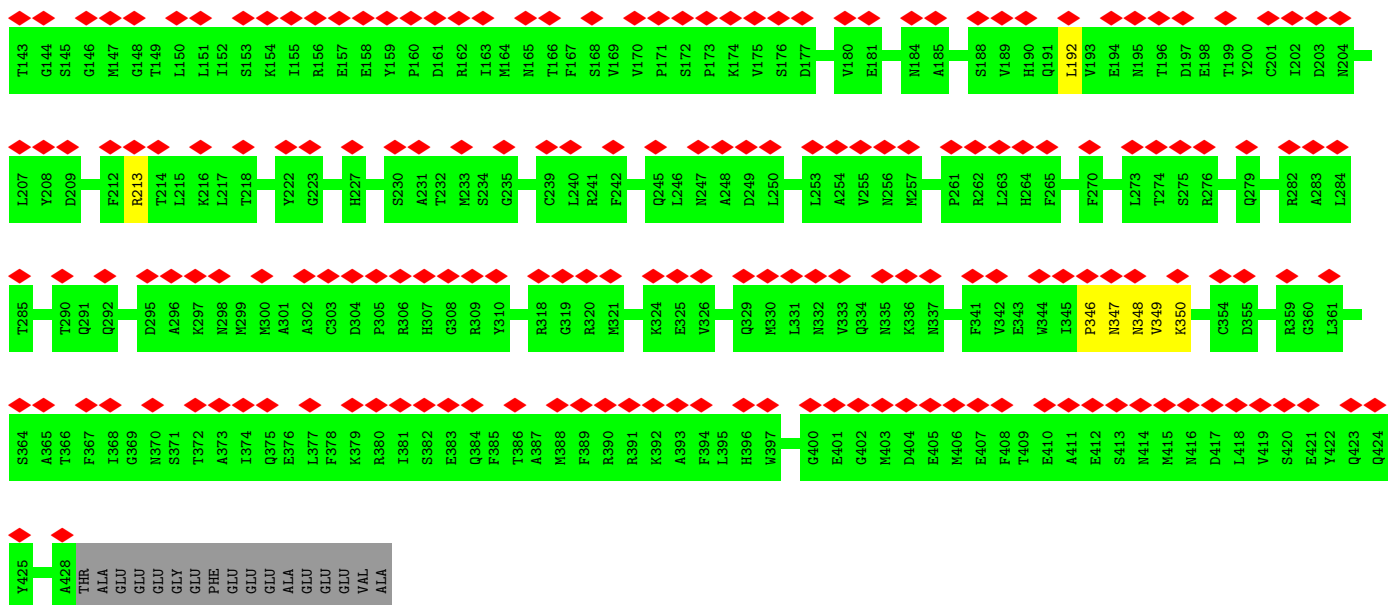


• Molecule 9: Tubulin beta-4B chain

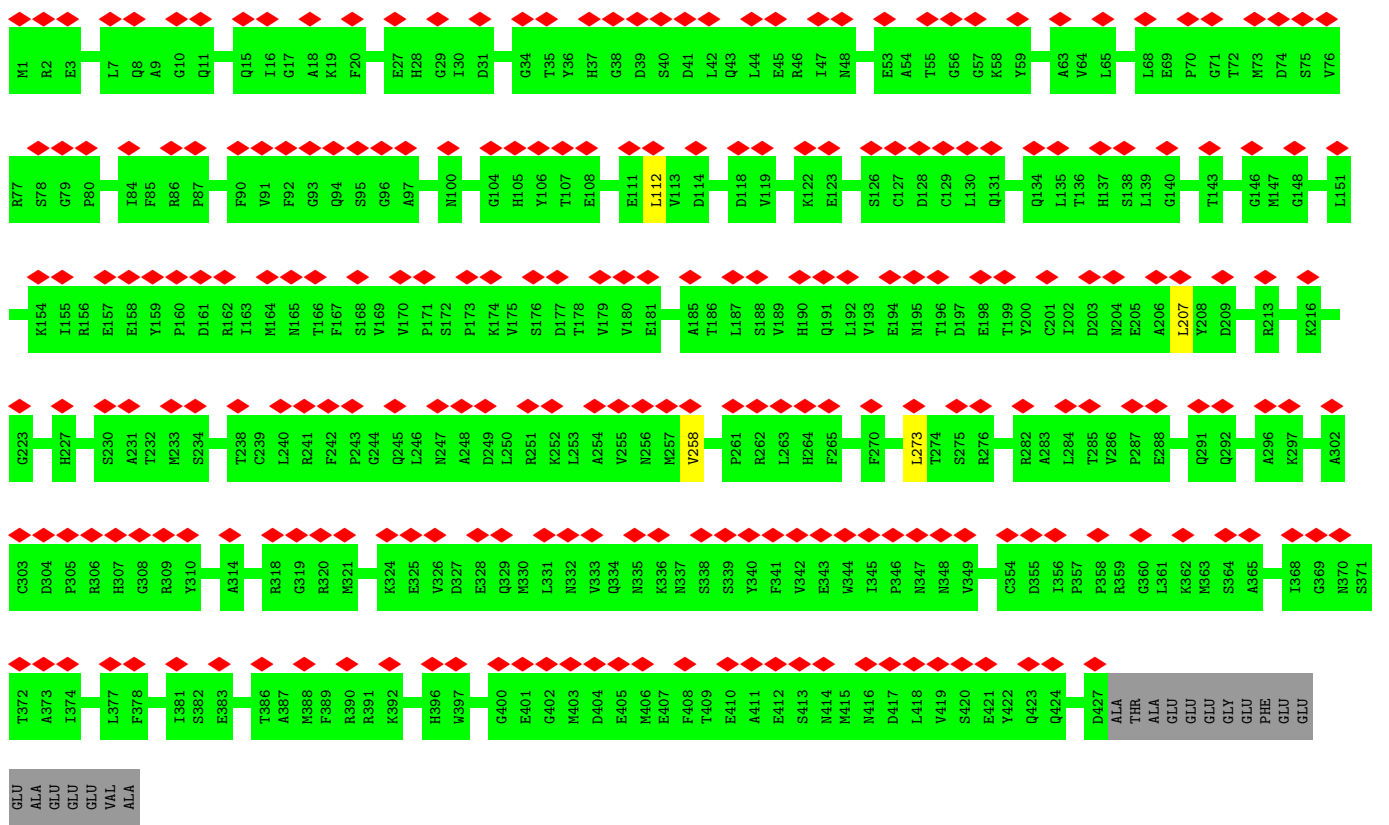


• Molecule 9: Tubulin beta-4B chain





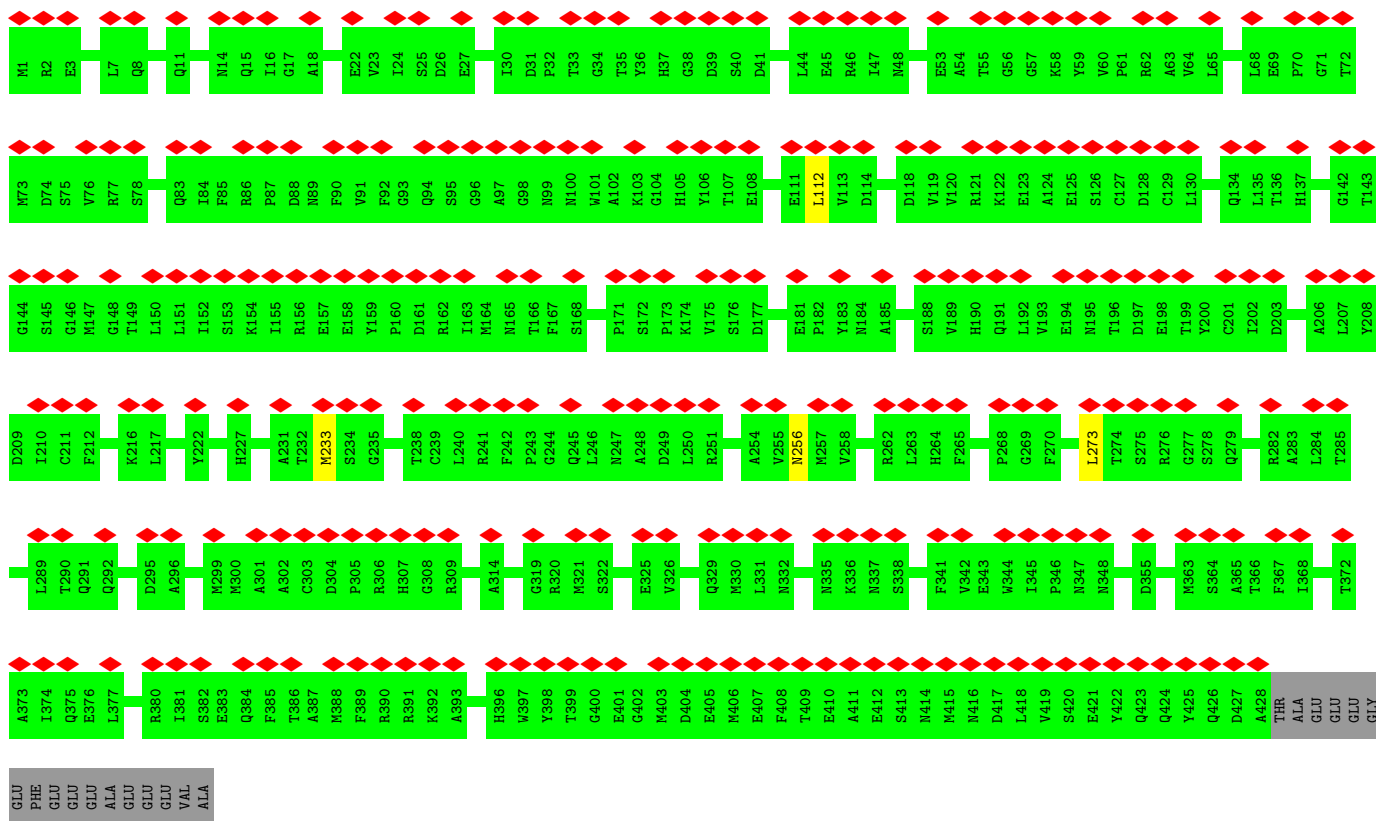
• Molecule 9: Tubulin beta-4B chain



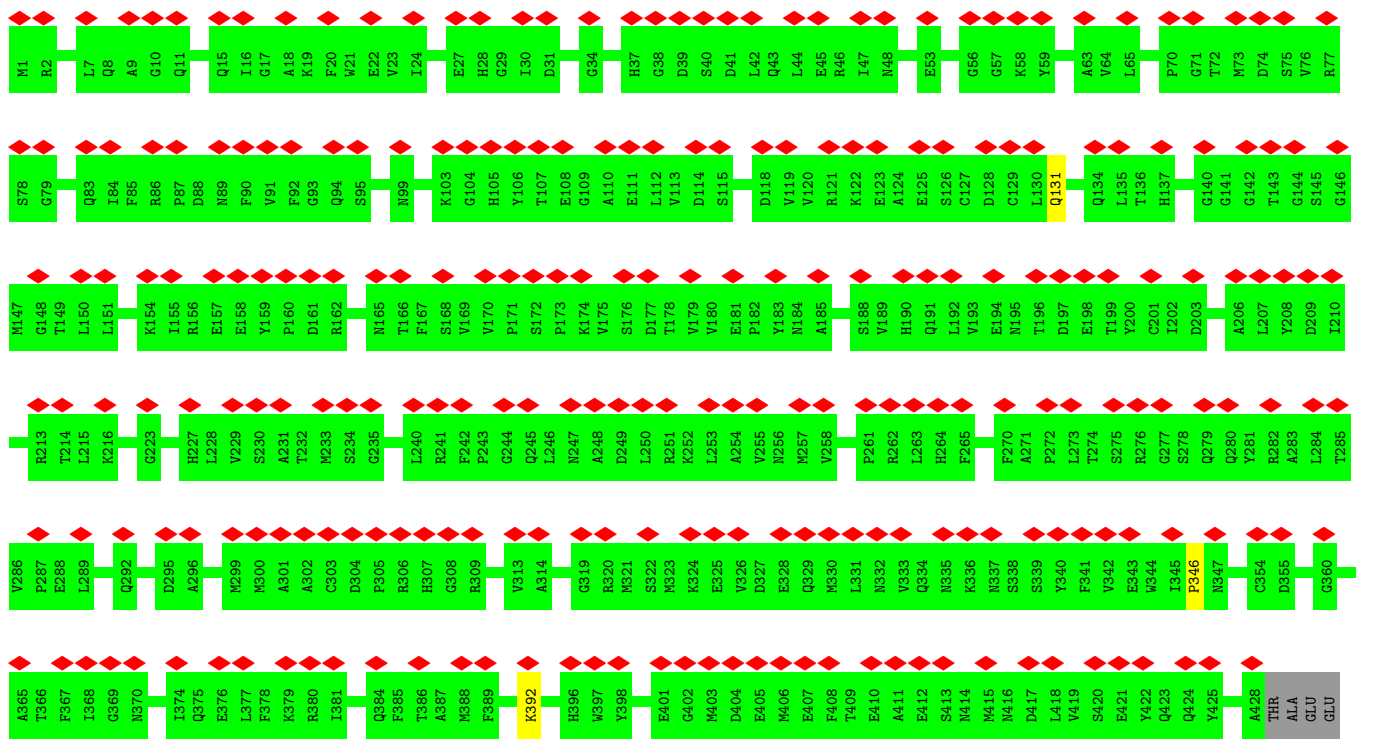
• Molecule 9: Tubulin beta-4B chain





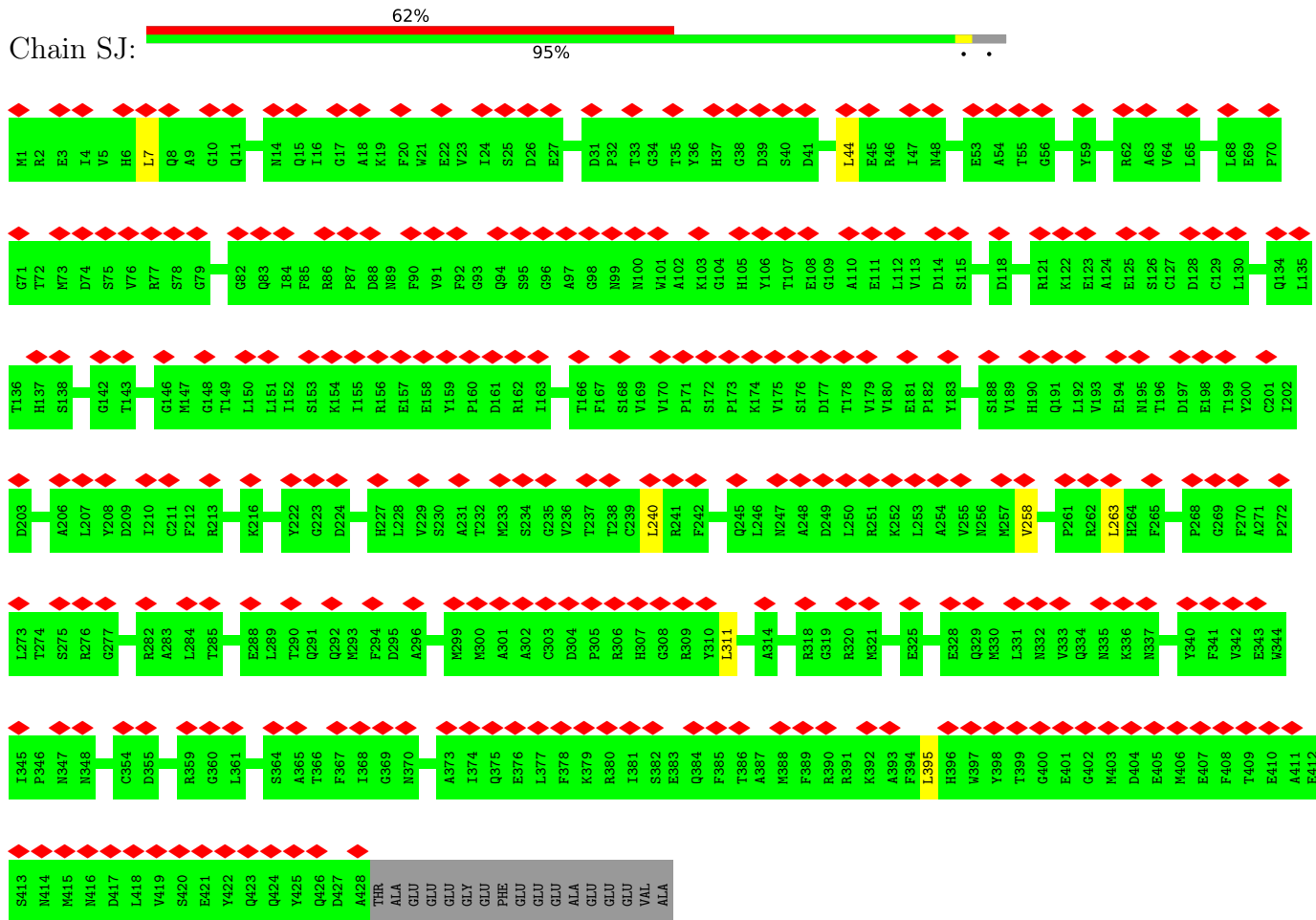


● Molecule 9: Tubulin beta-4B chain

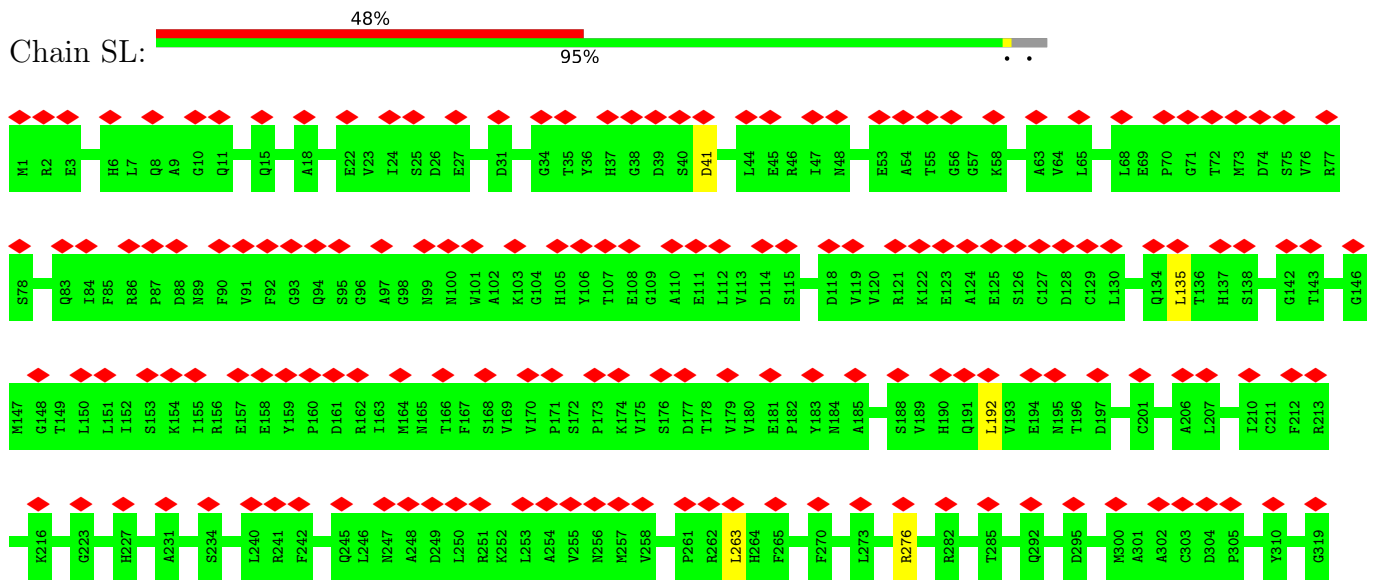


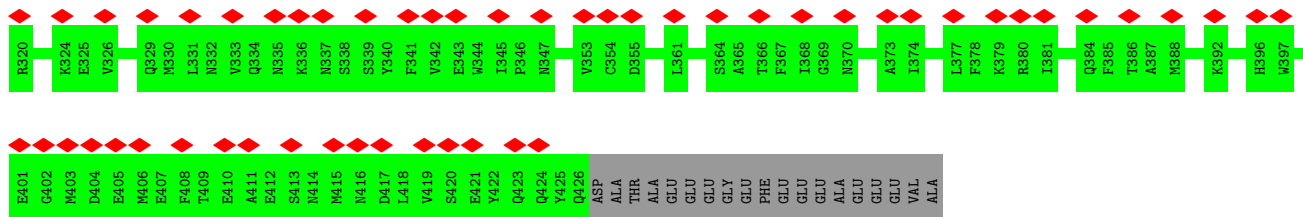
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GLU  
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VAL  
ALA

• Molecule 9: Tubulin beta-4B chain

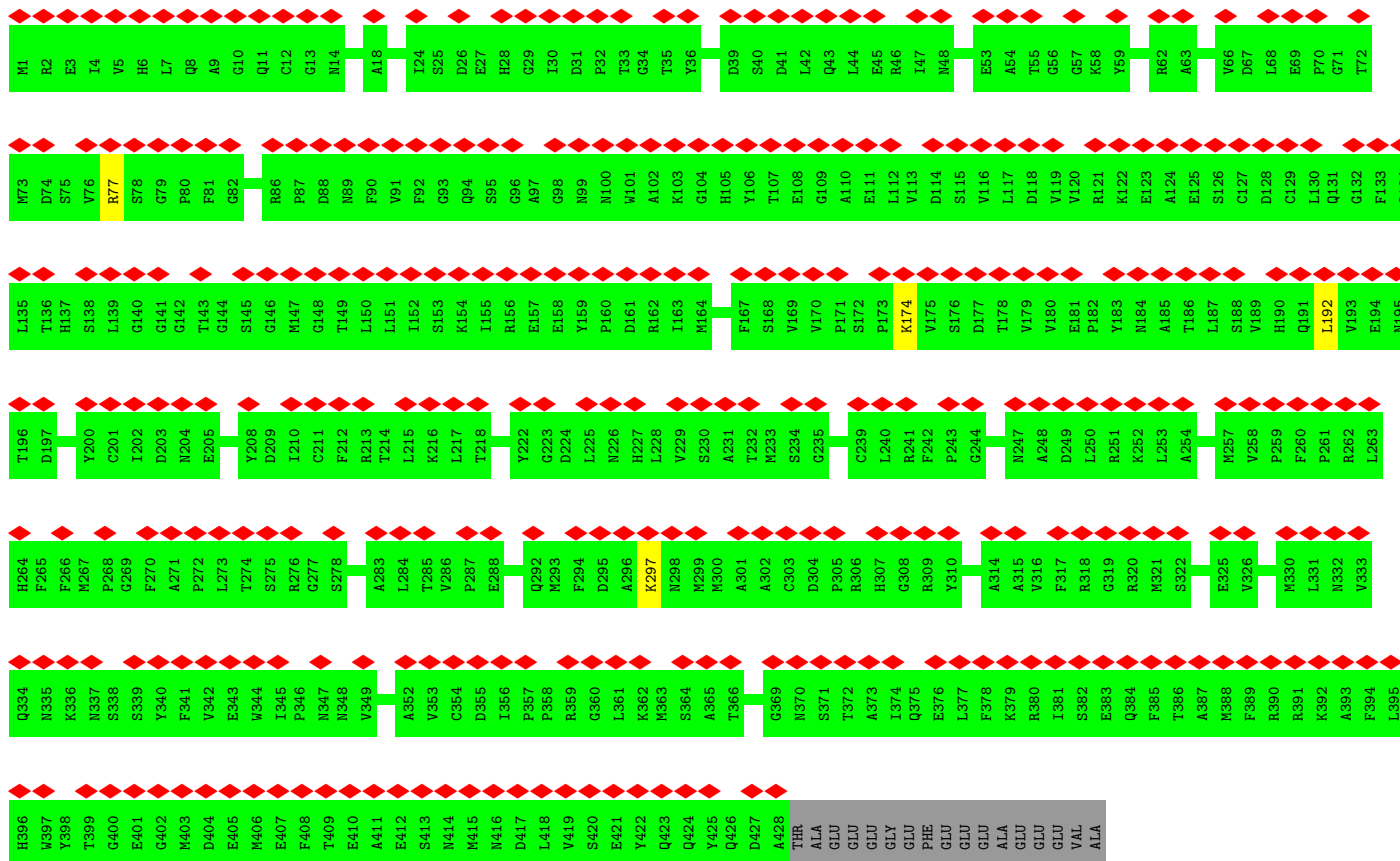
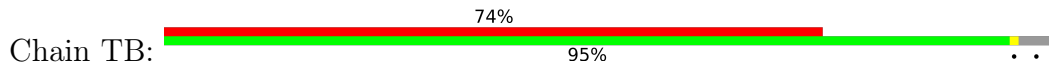


• Molecule 9: Tubulin beta-4B chain

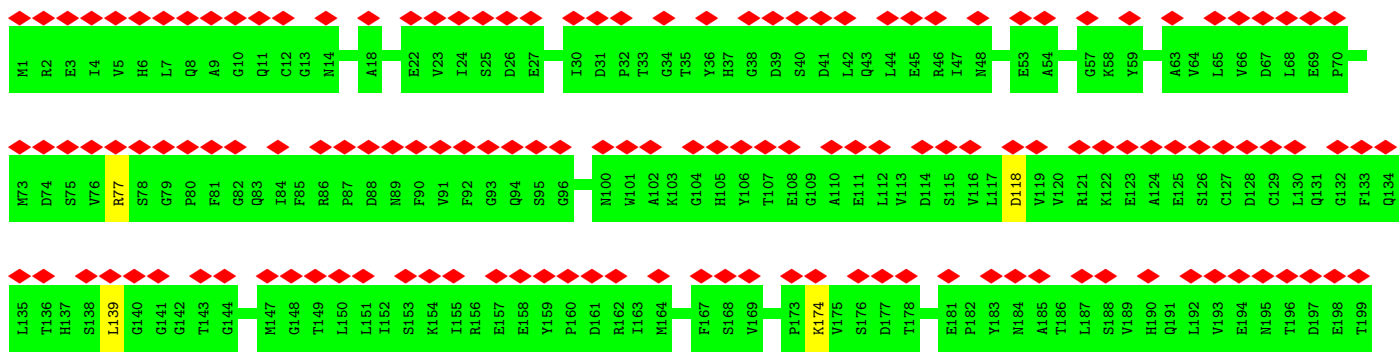


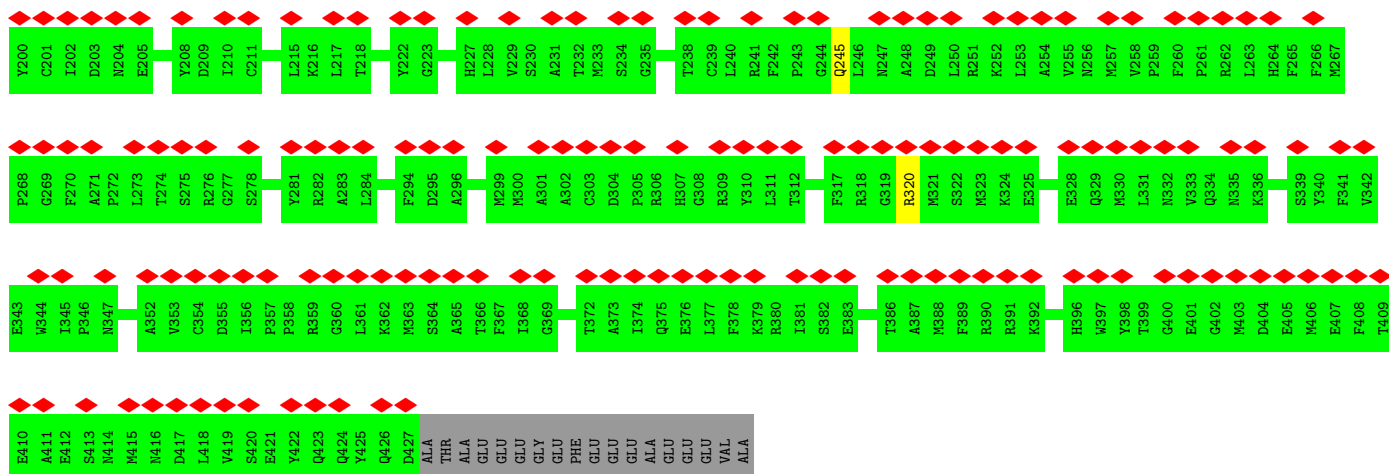


• Molecule 9: Tubulin beta-4B chain

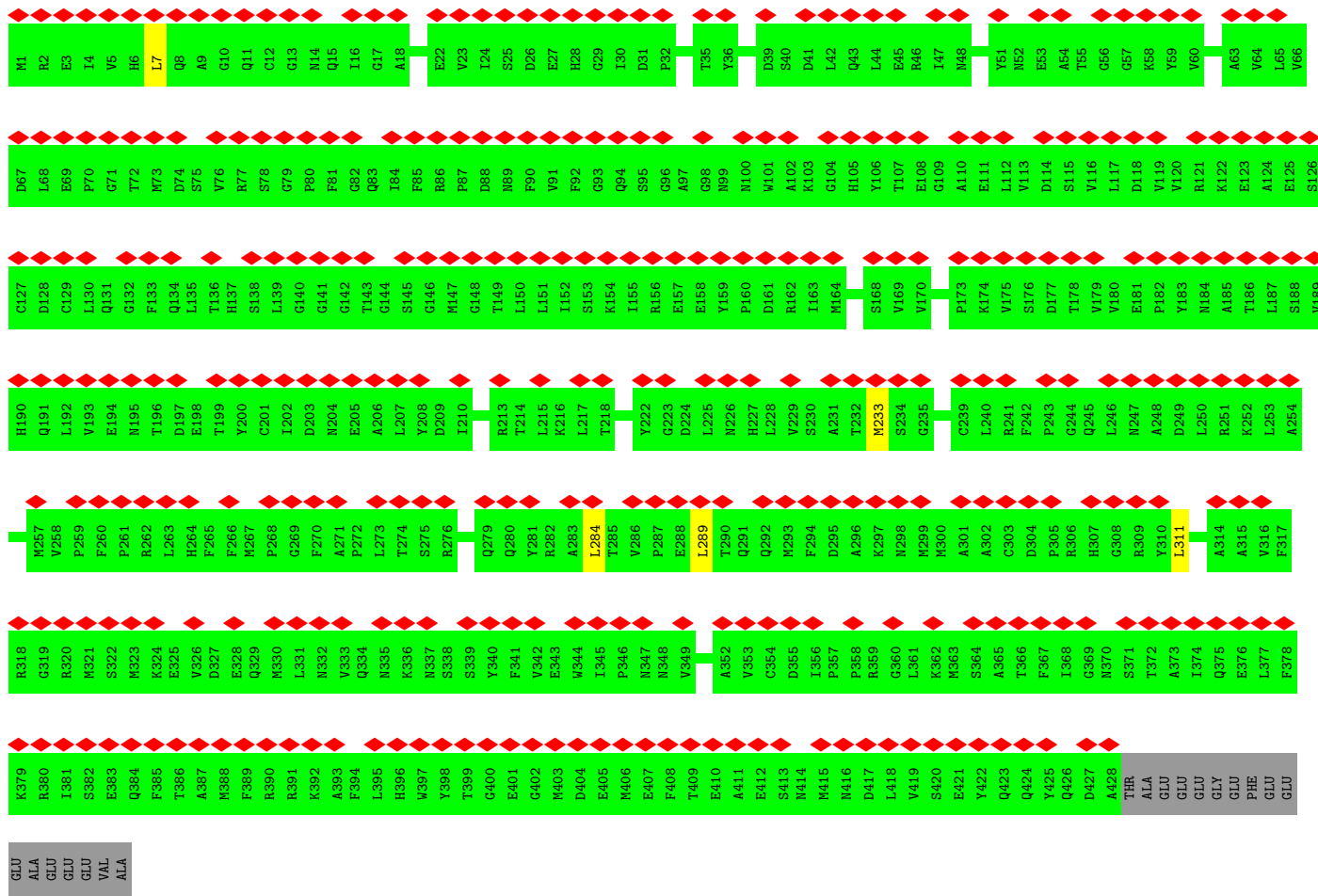
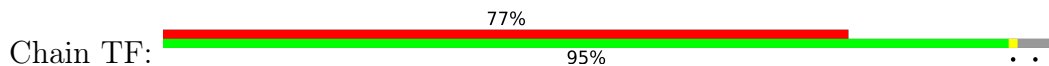


• Molecule 9: Tubulin beta-4B chain



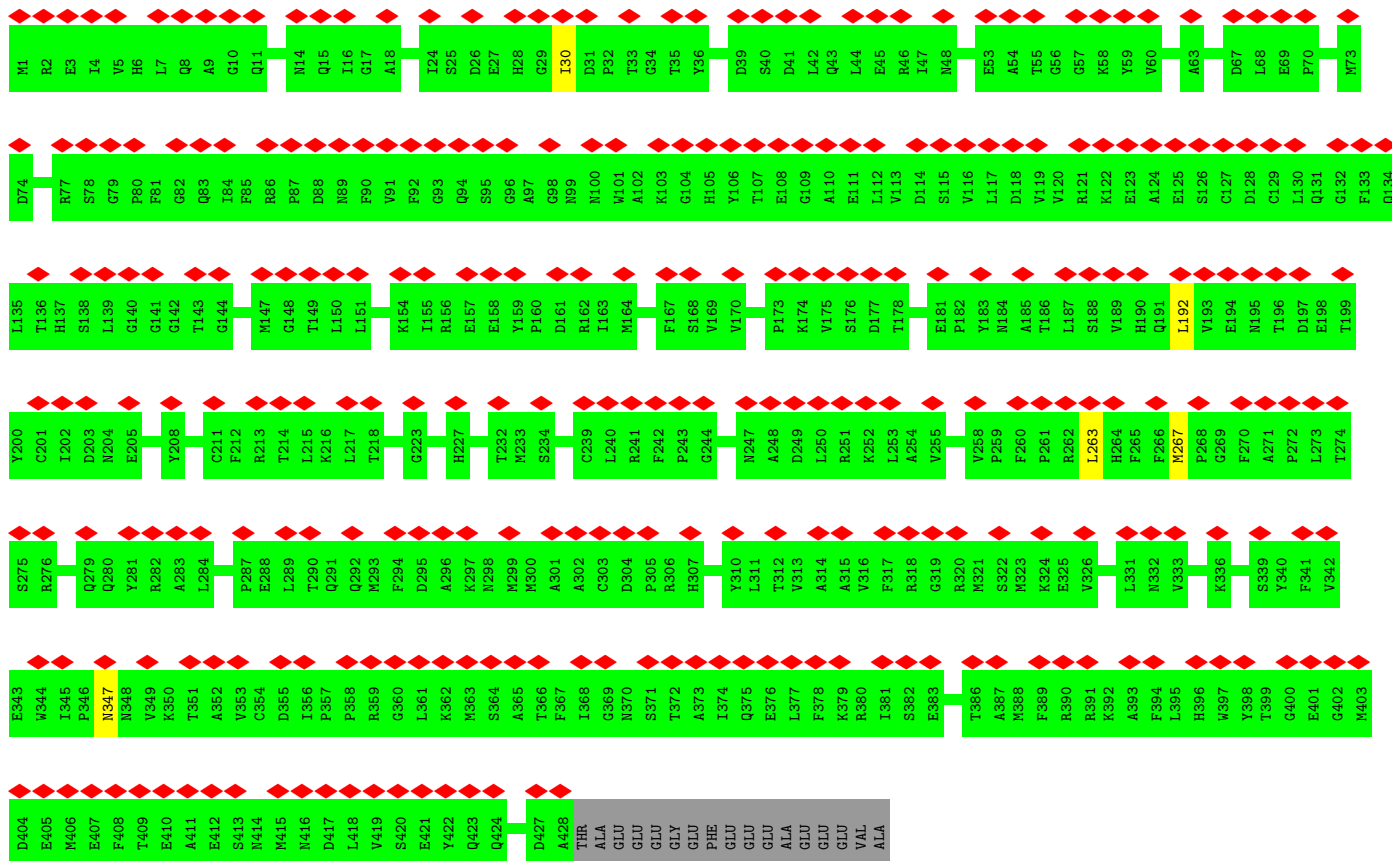


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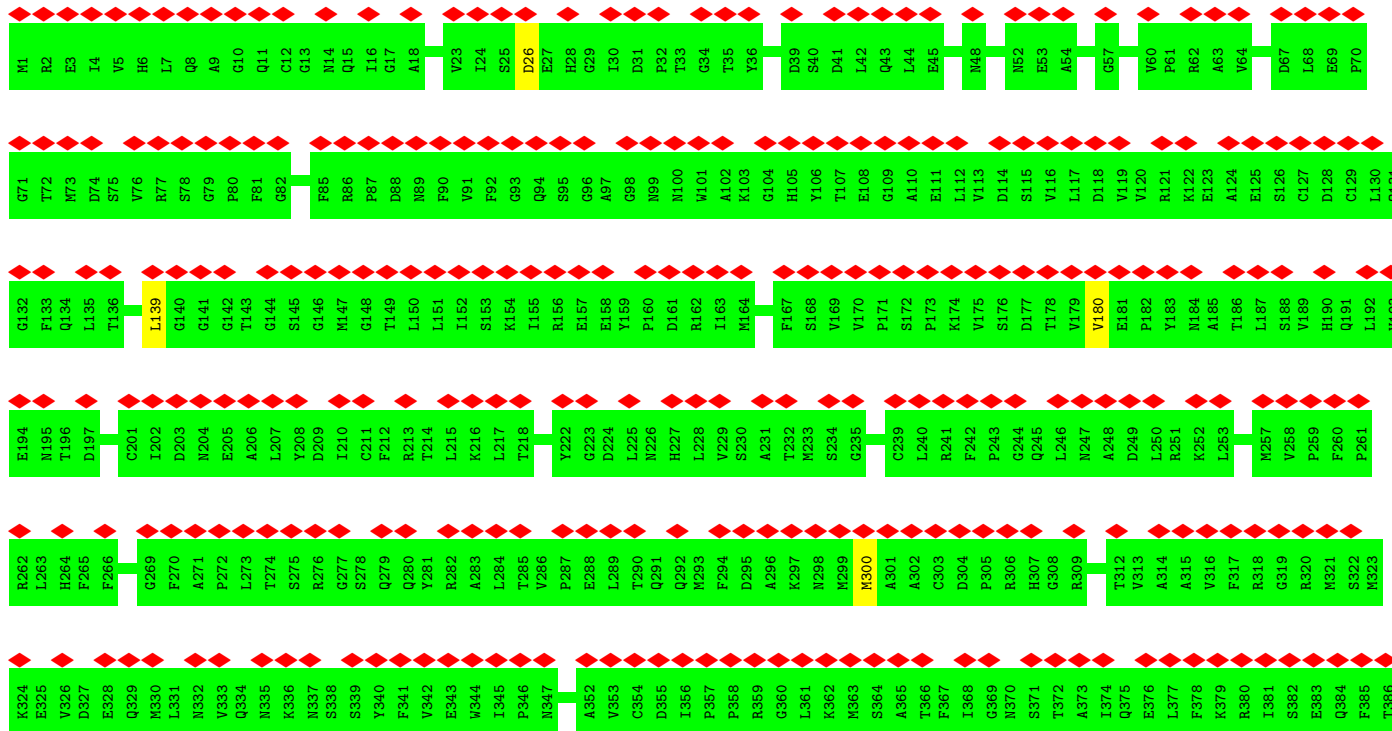
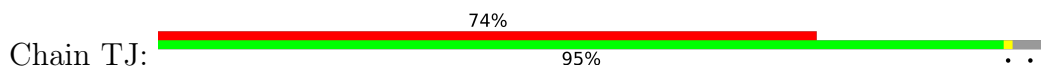


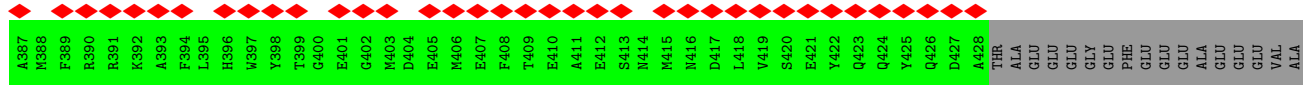
• Molecule 9: Tubulin beta-4B chain



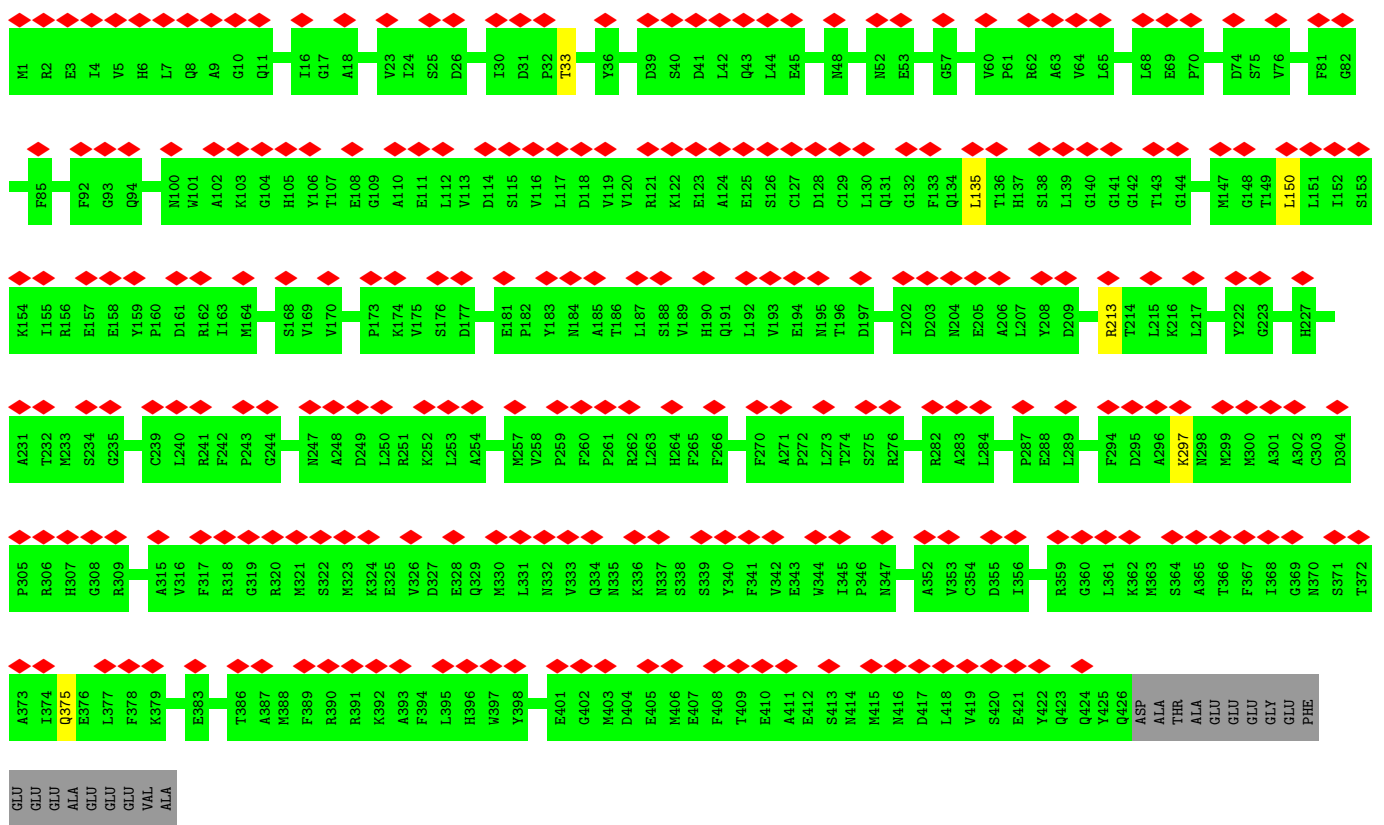


● Molecule 9: Tubulin beta-4B chain

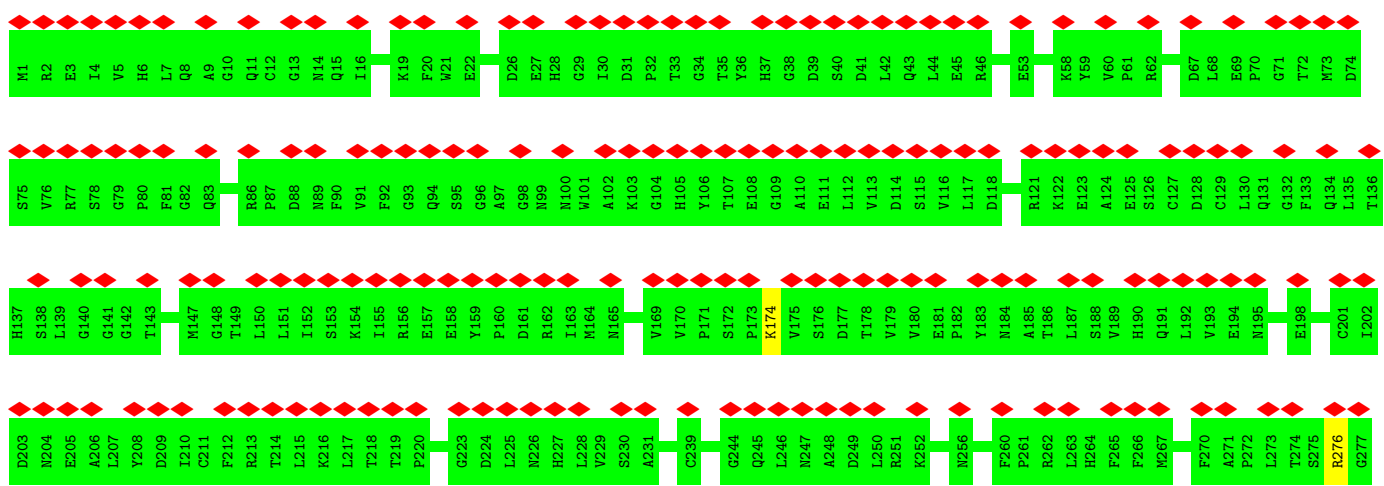


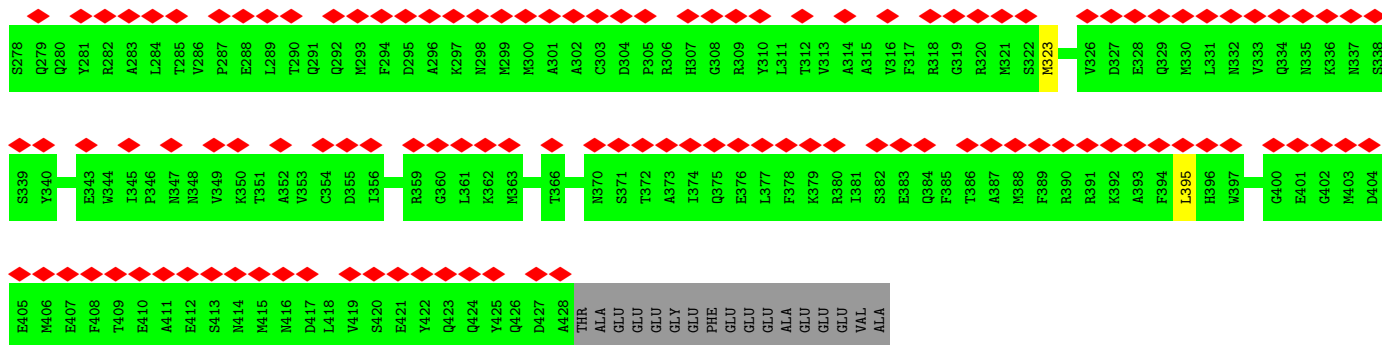


• Molecule 9: Tubulin beta-4B chain

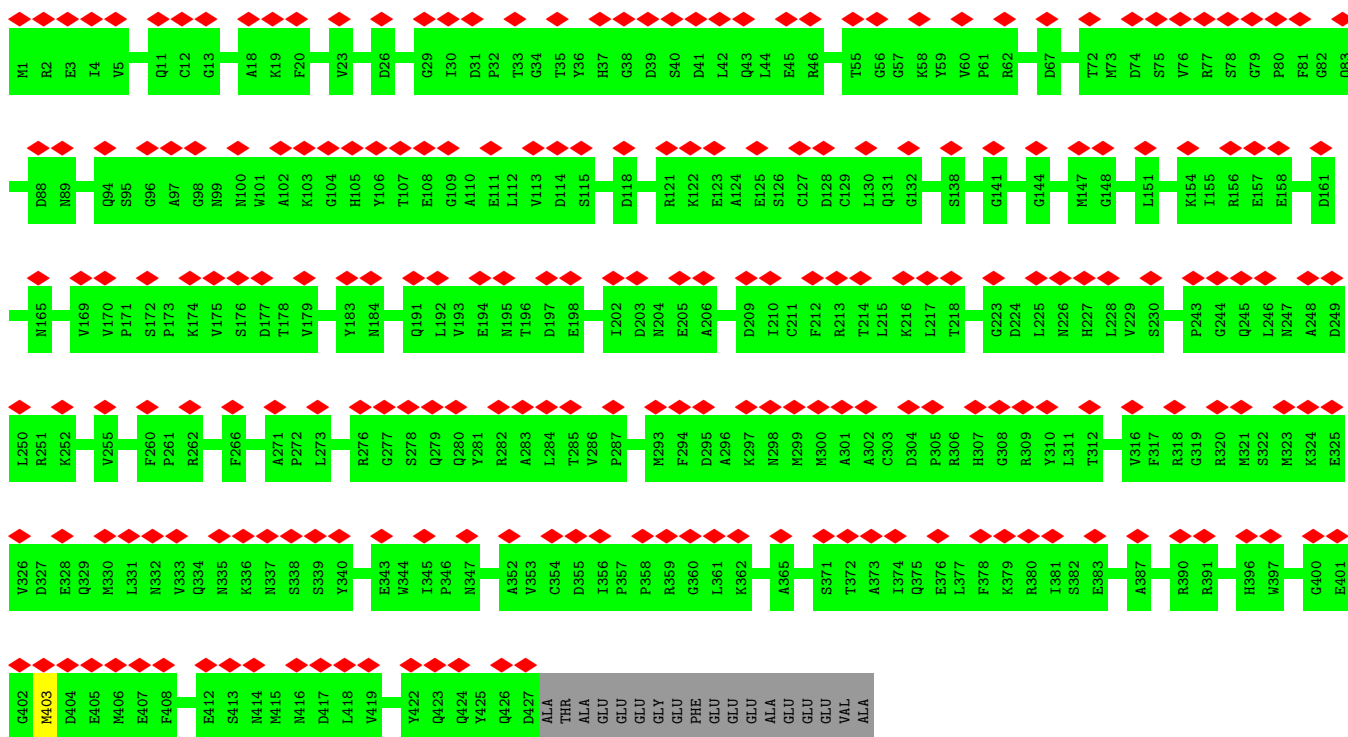


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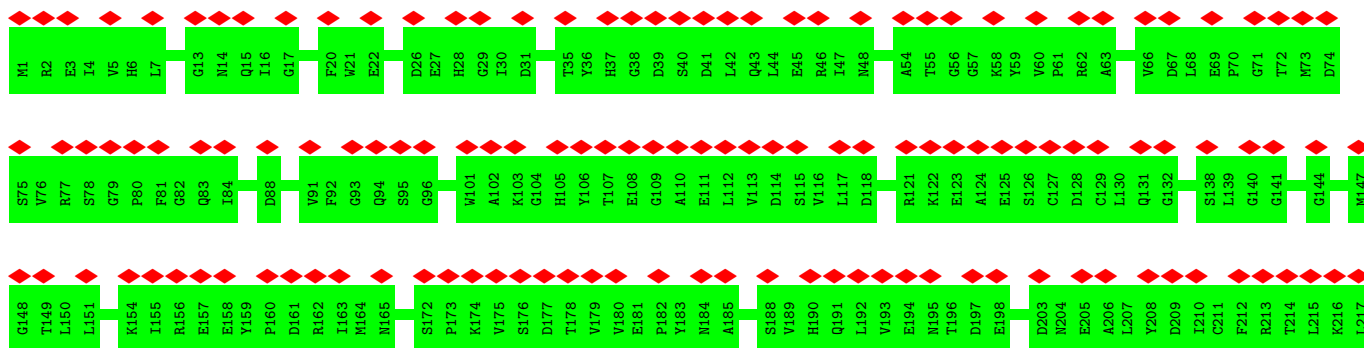


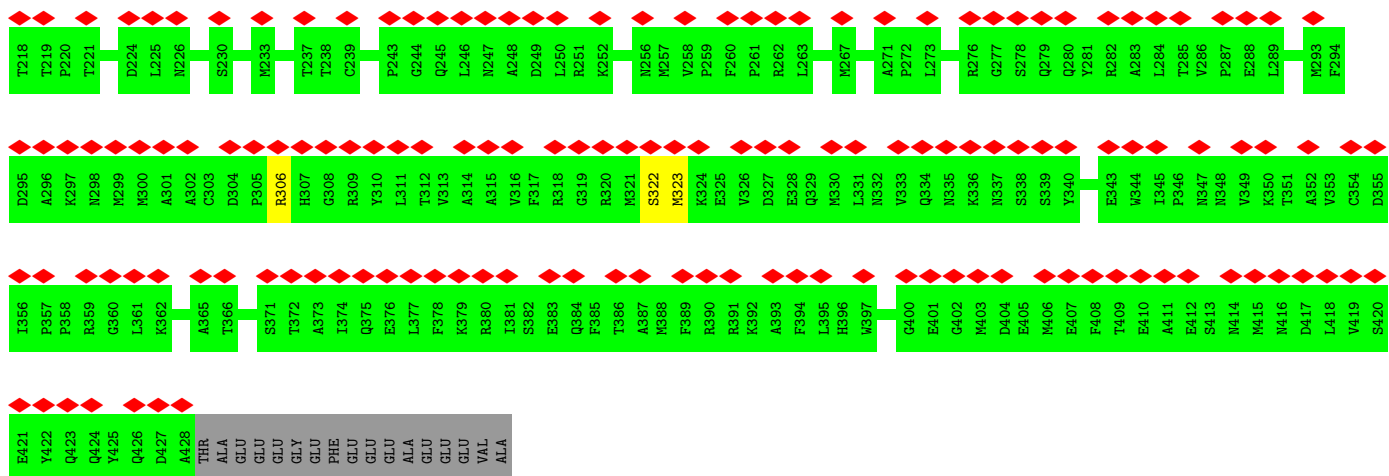


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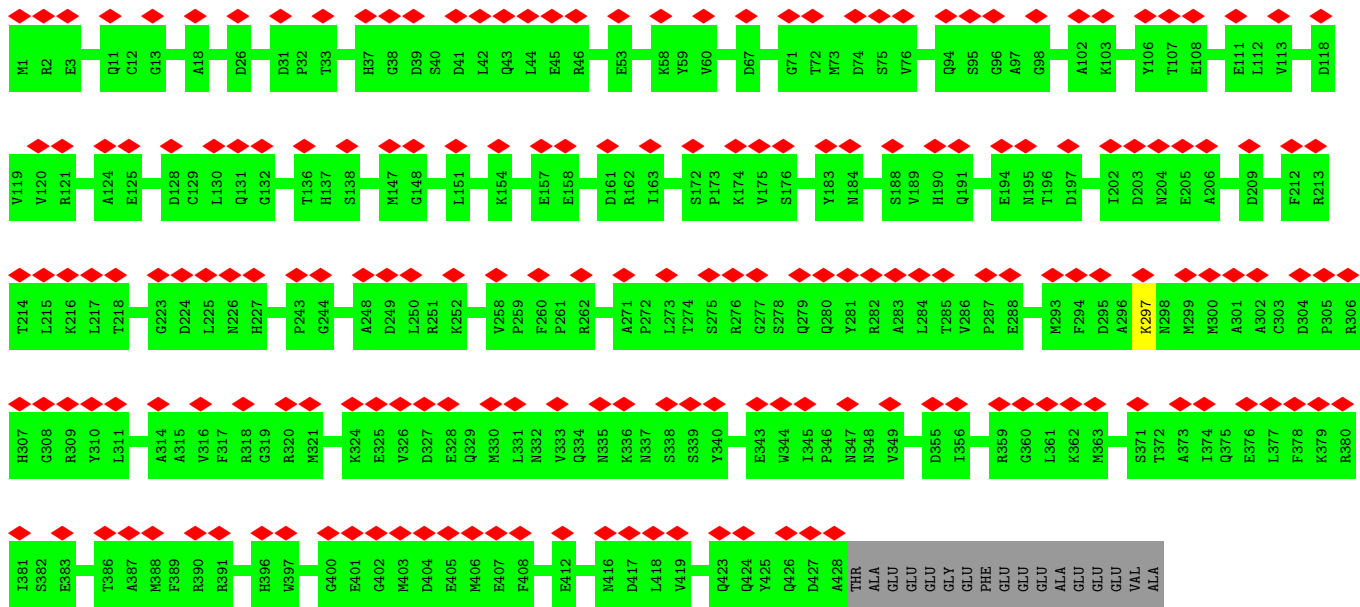
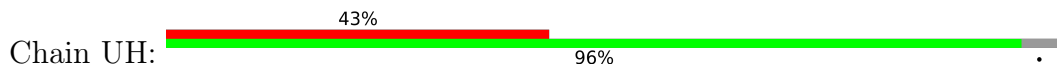


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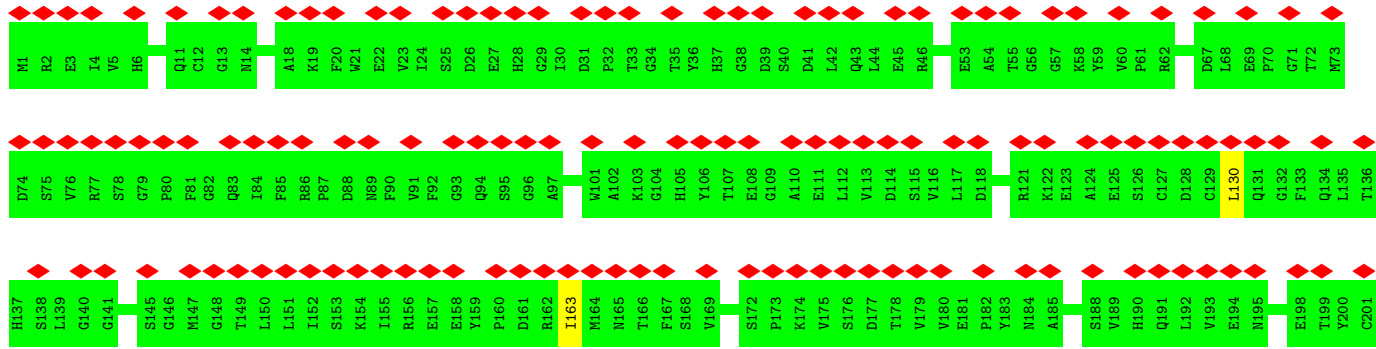
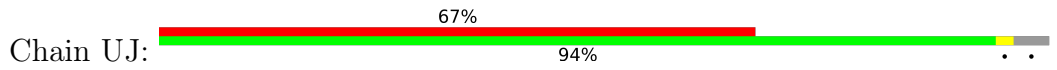




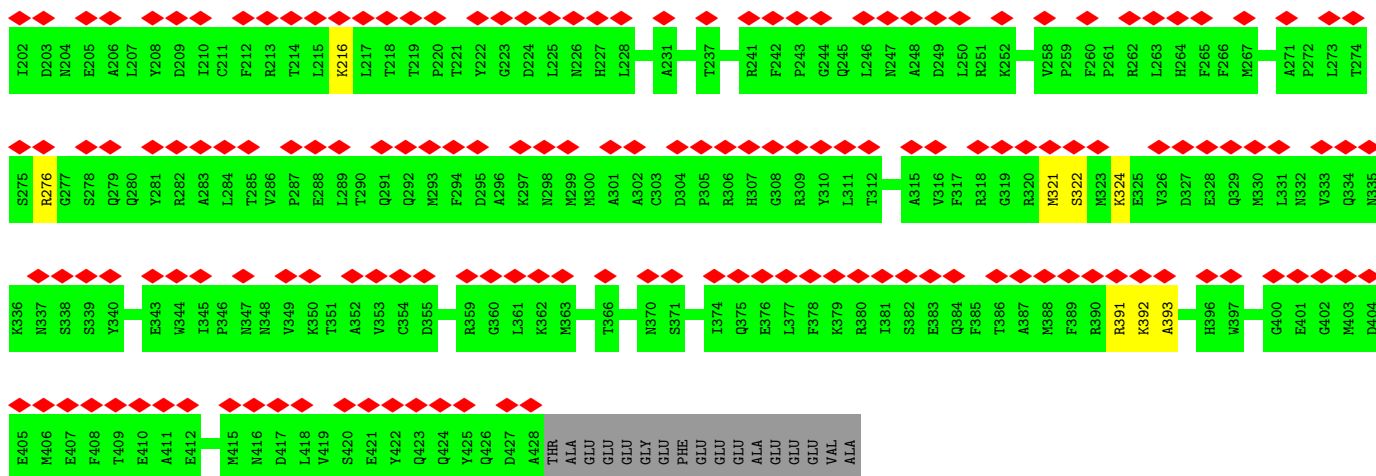
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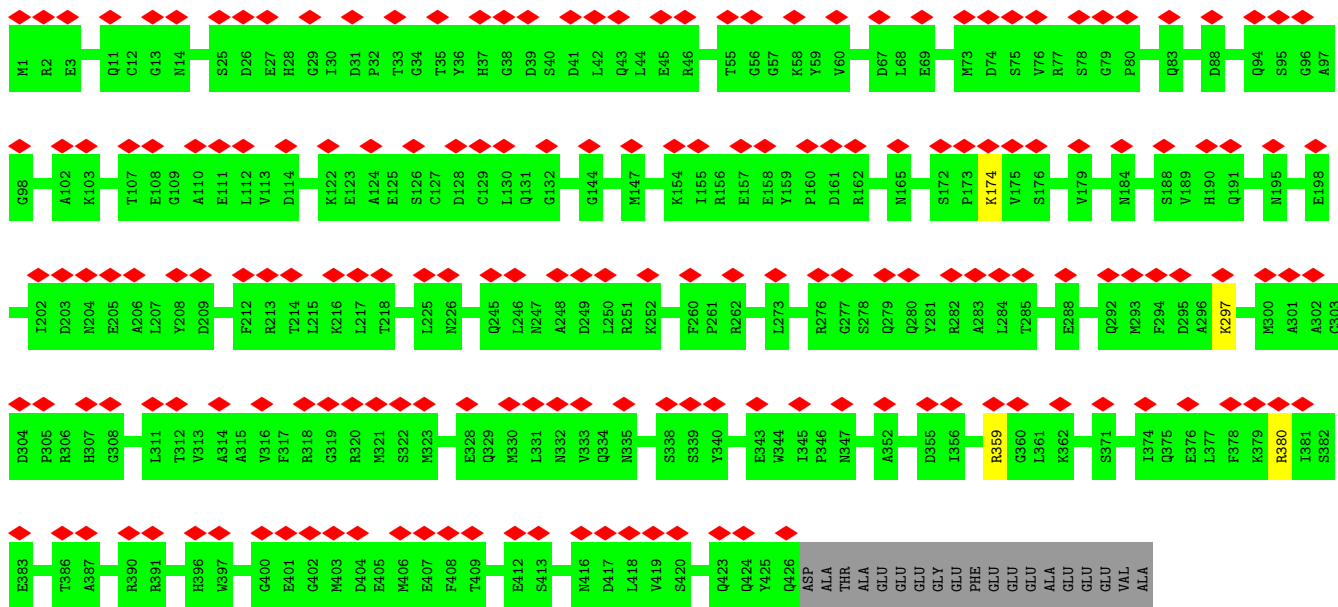
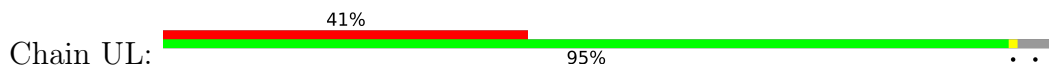
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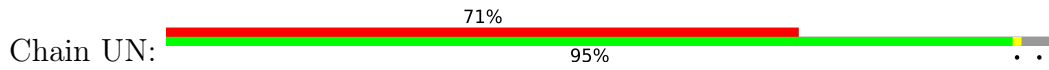


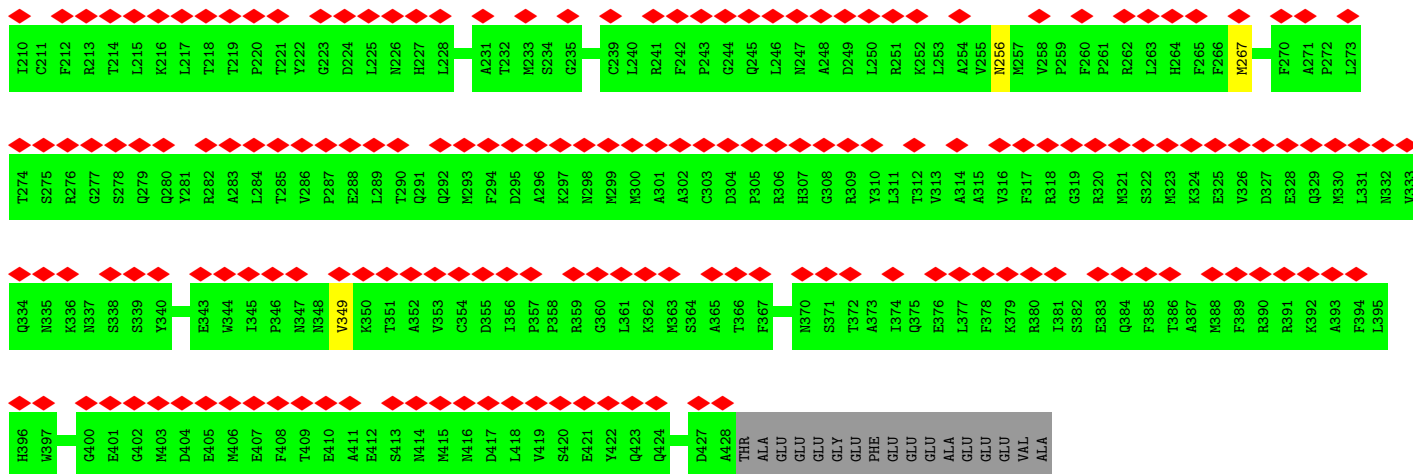


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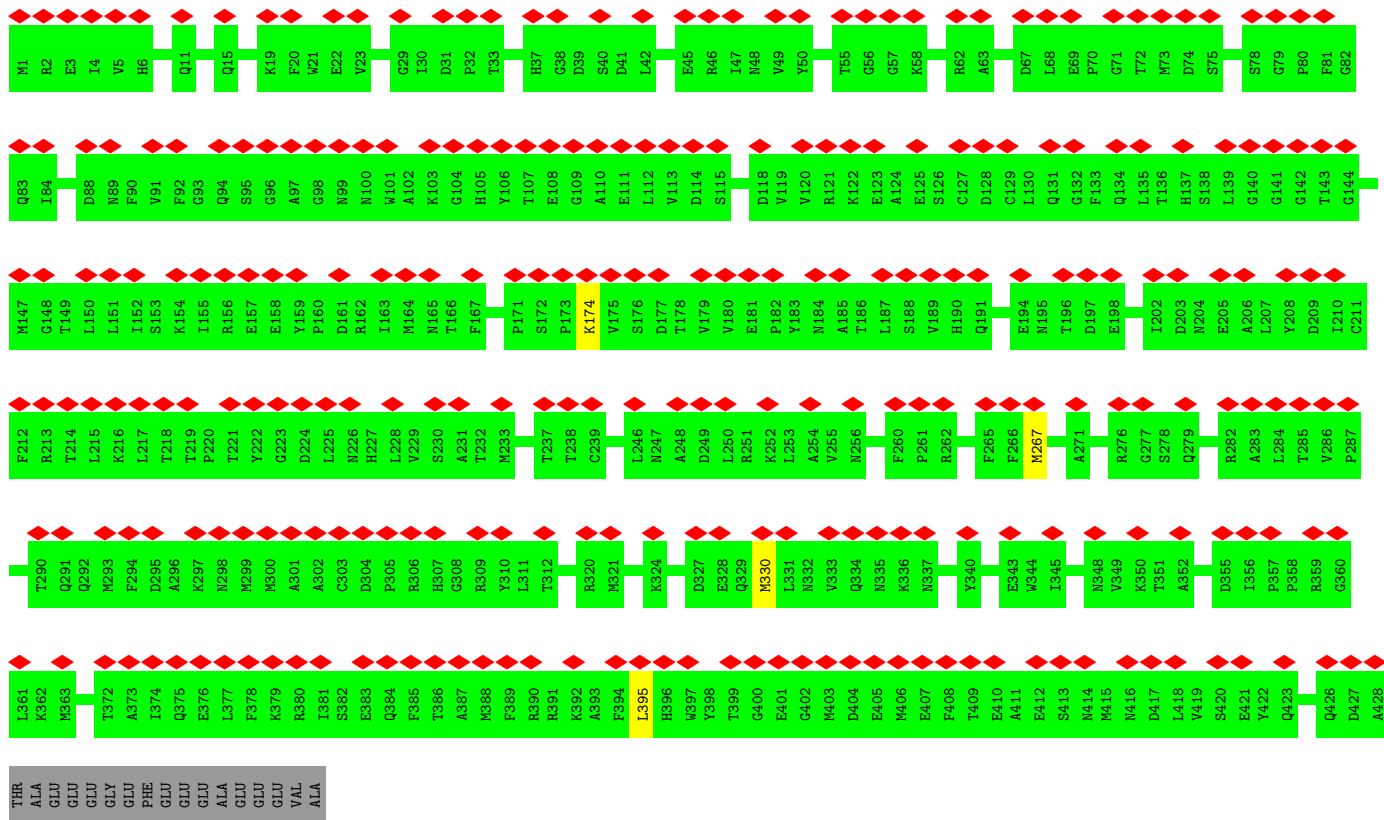


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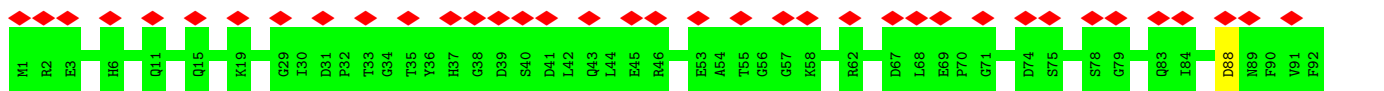
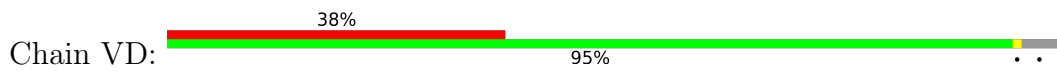


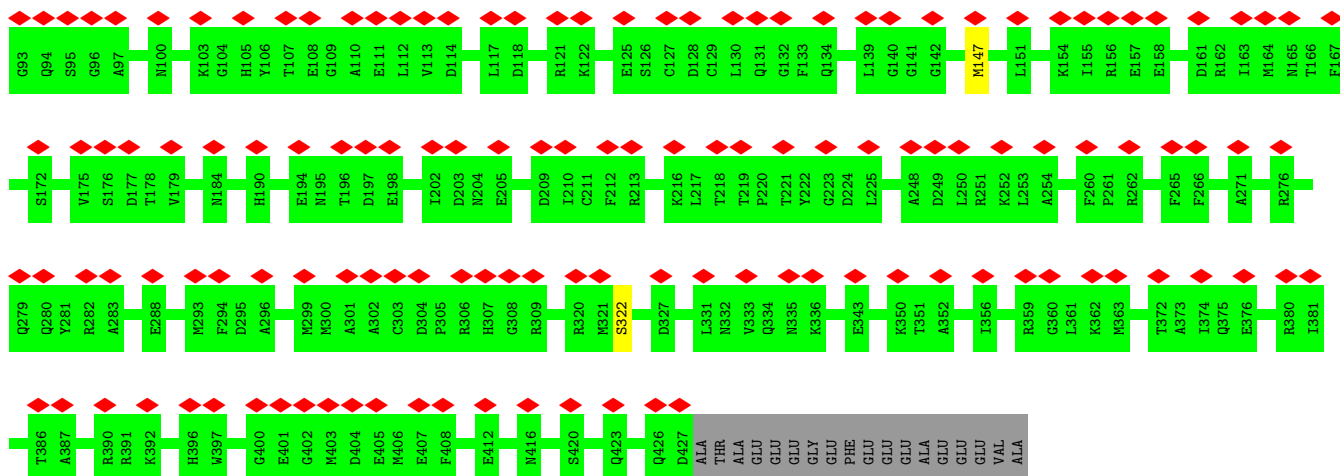


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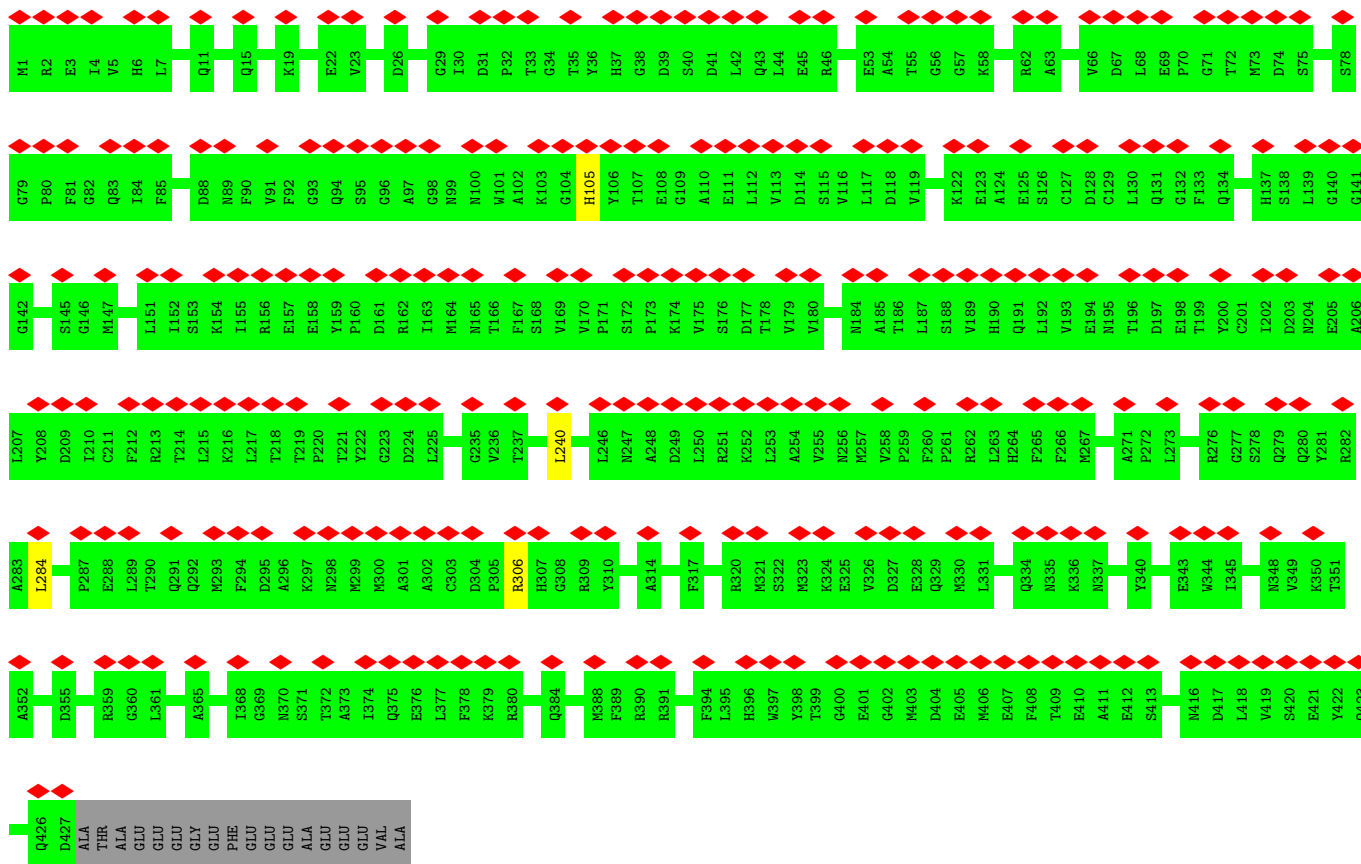


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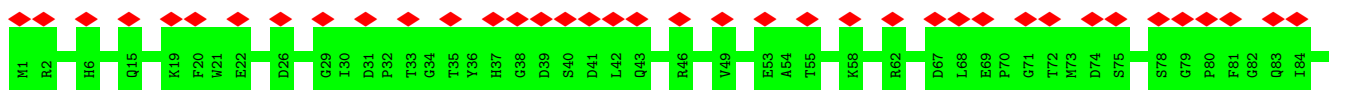
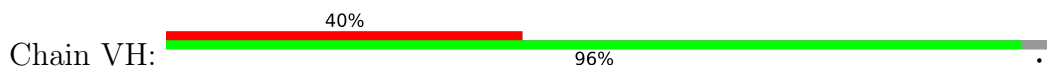


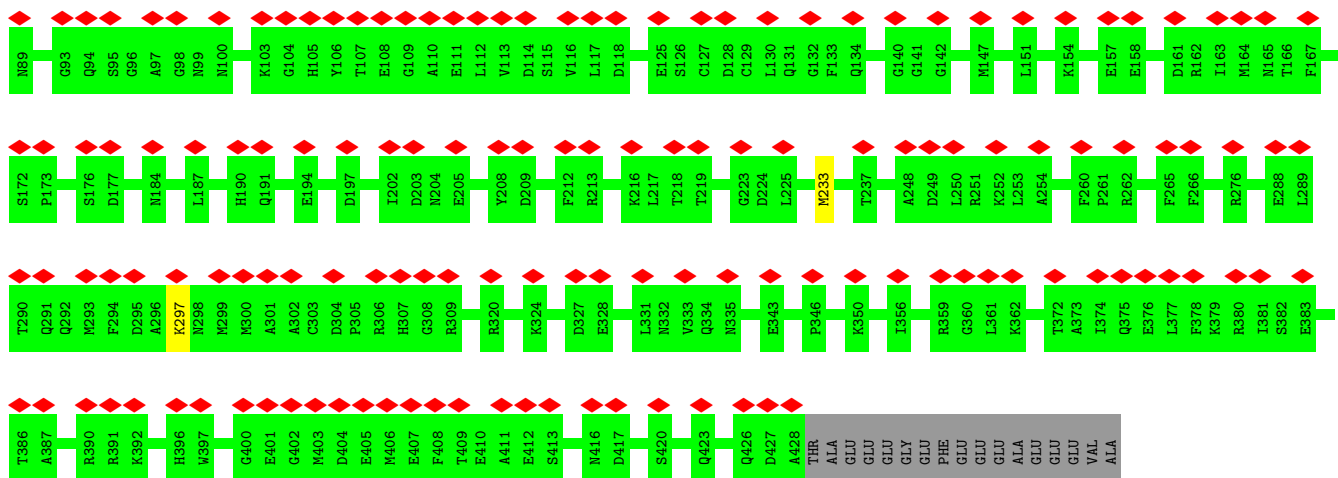


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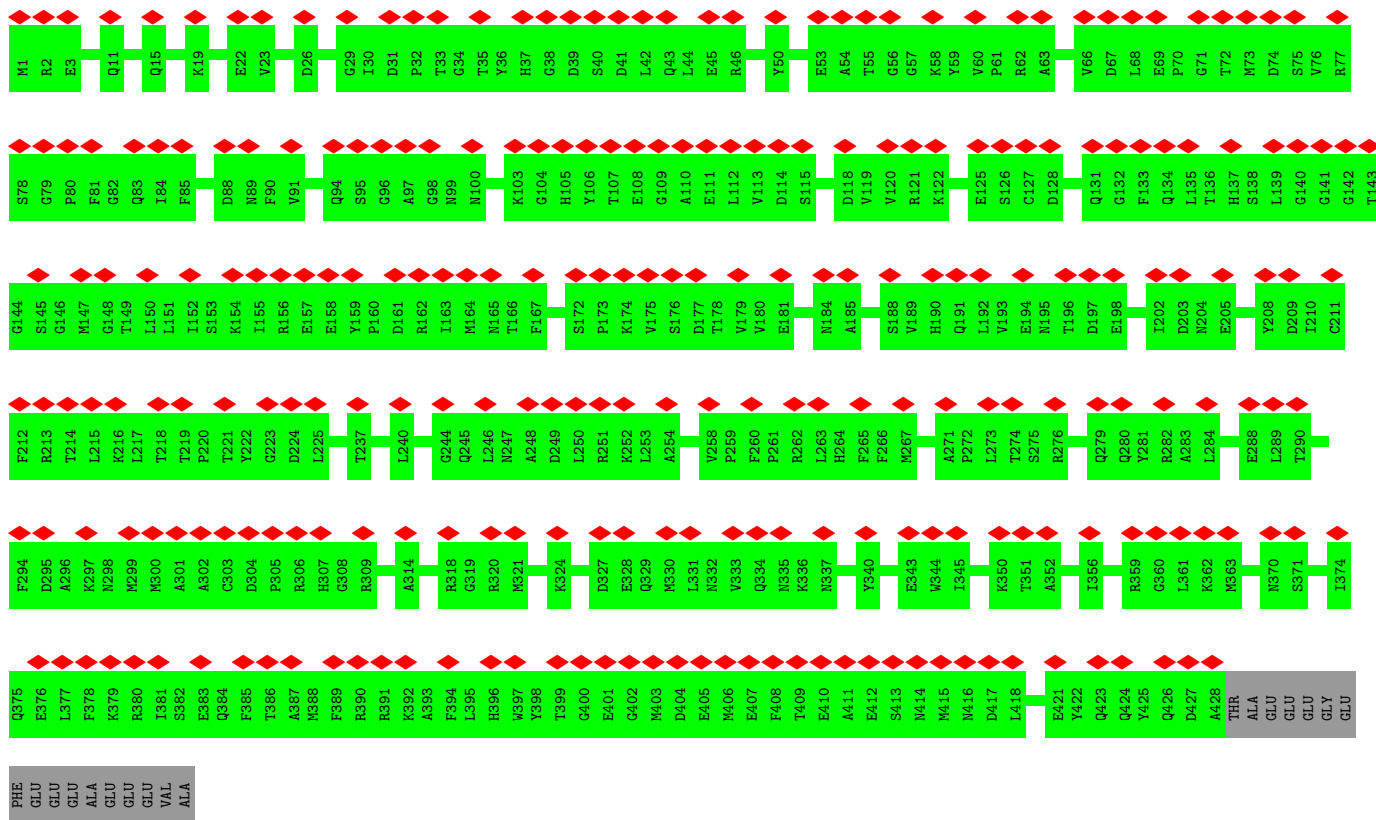


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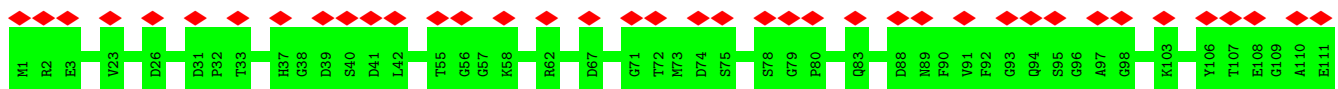


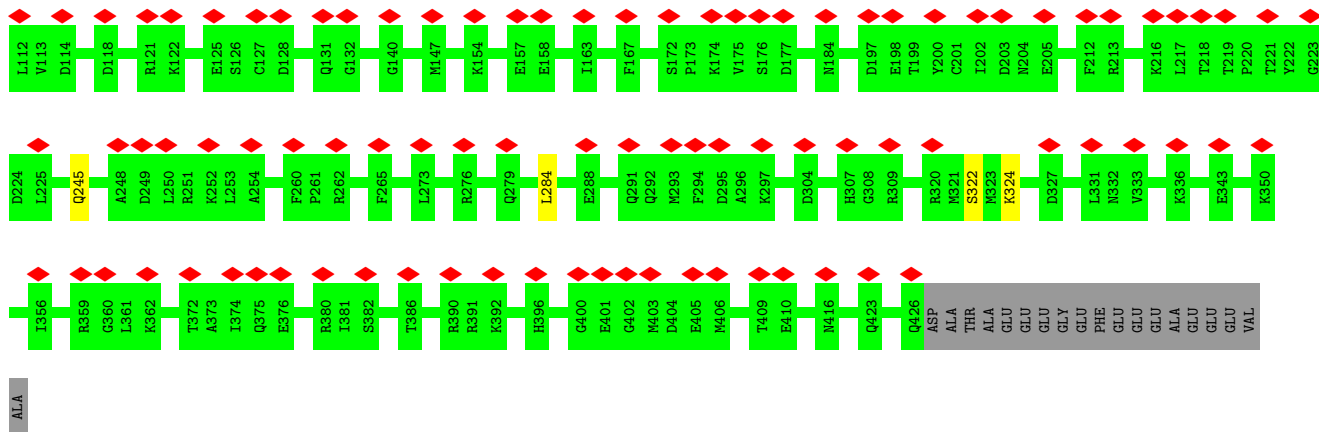


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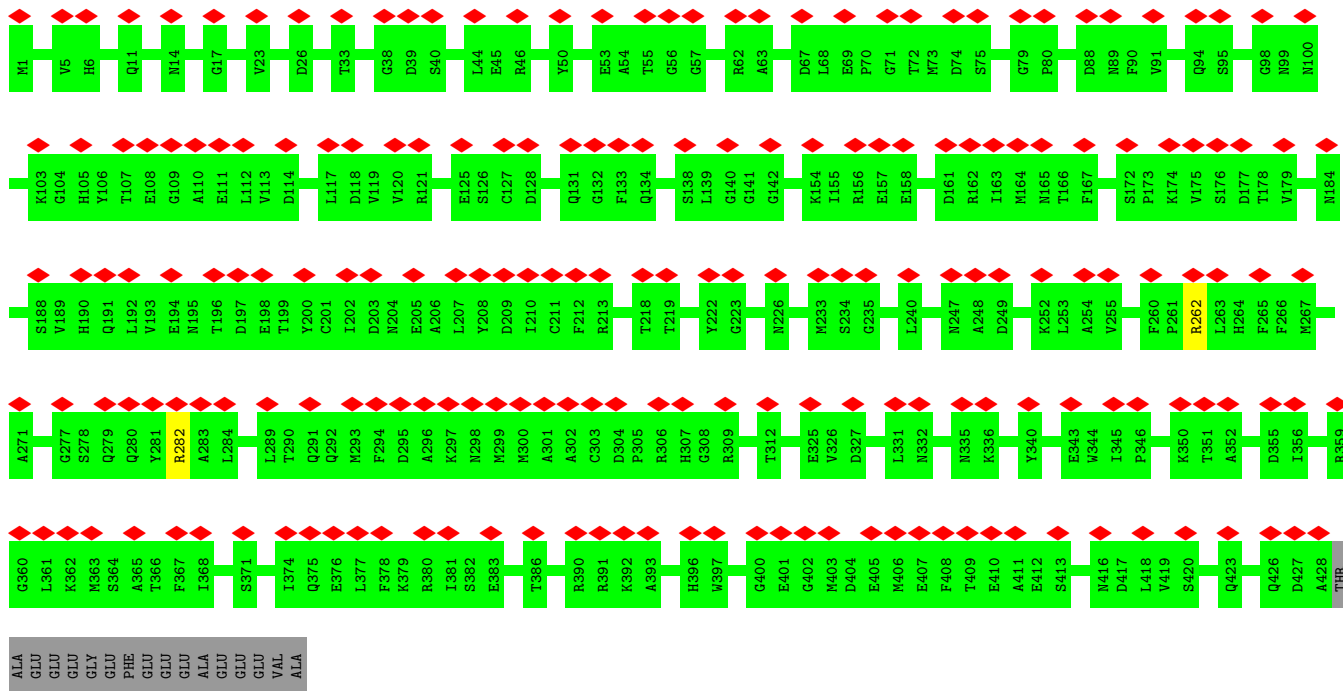


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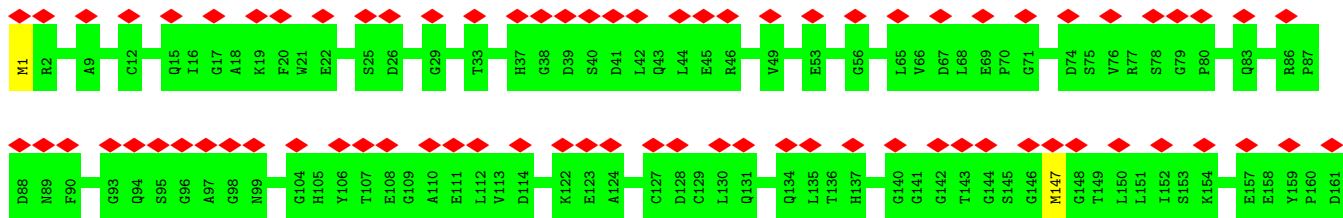


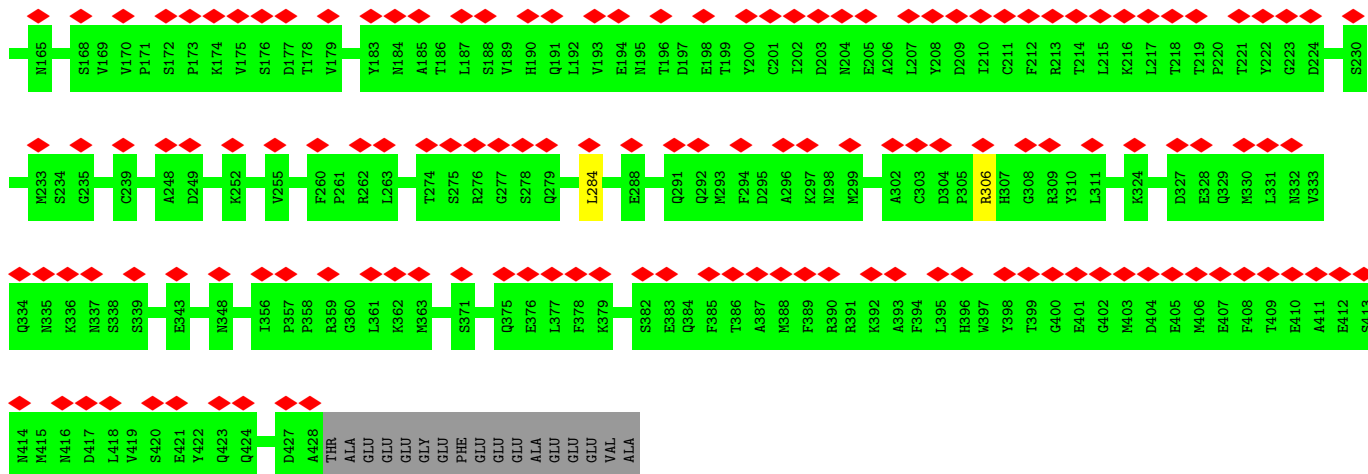


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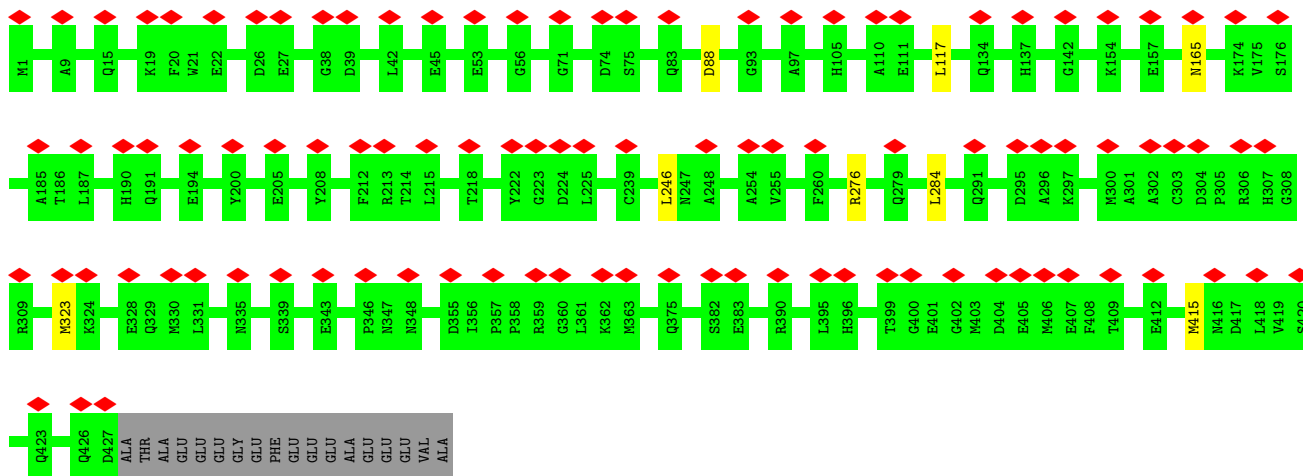


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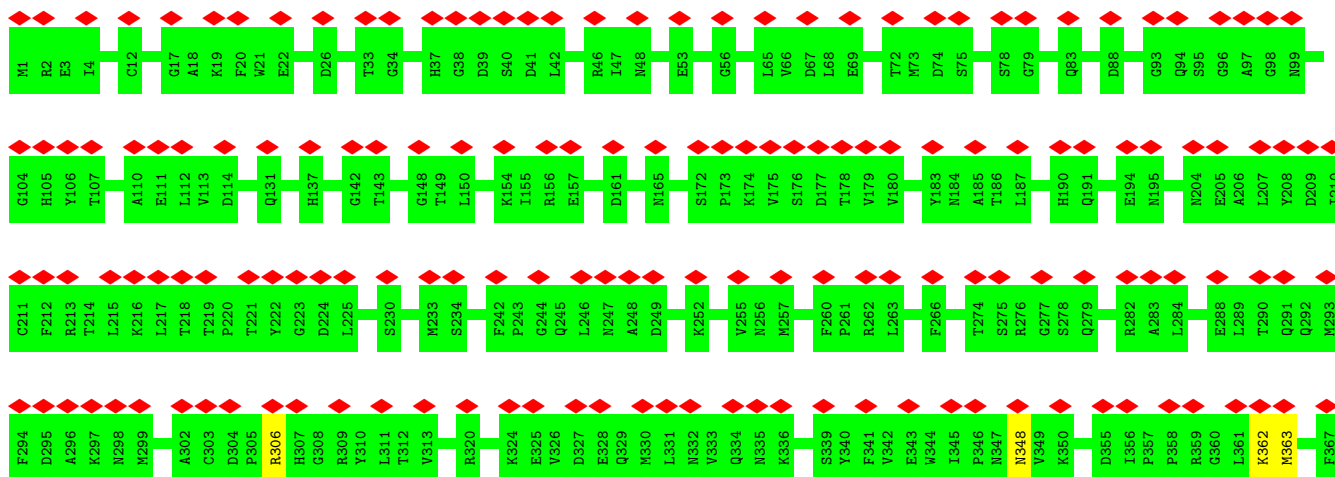
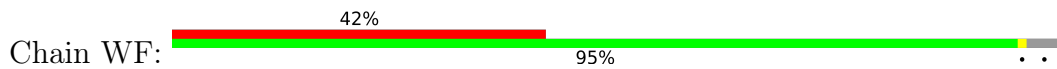


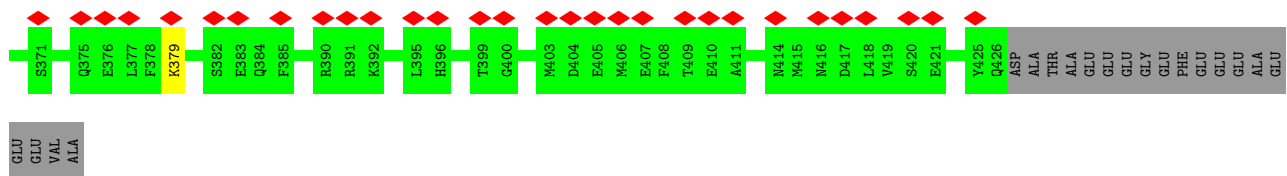


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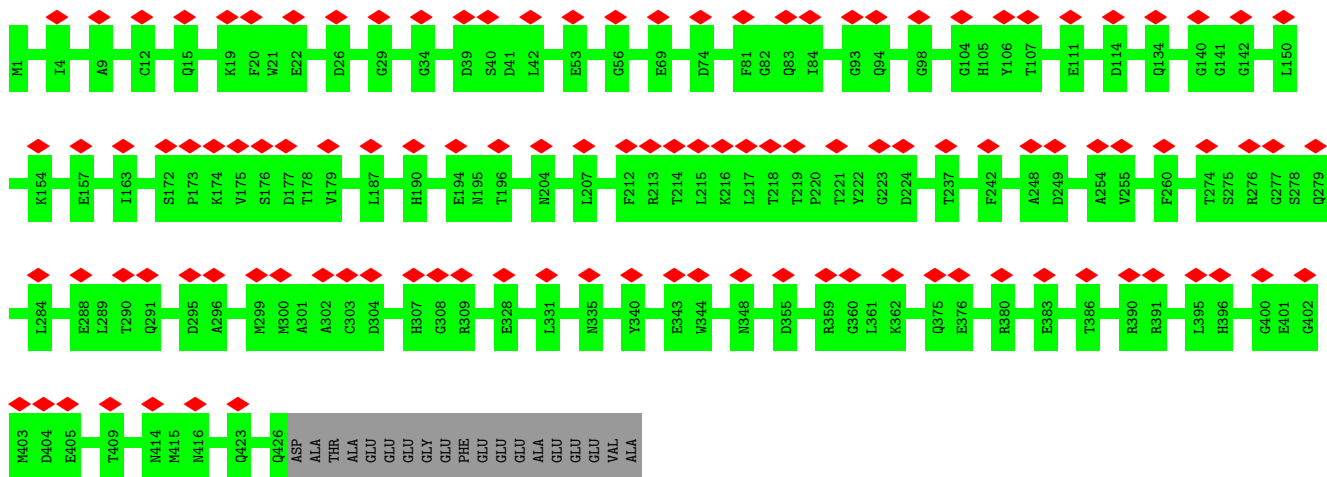


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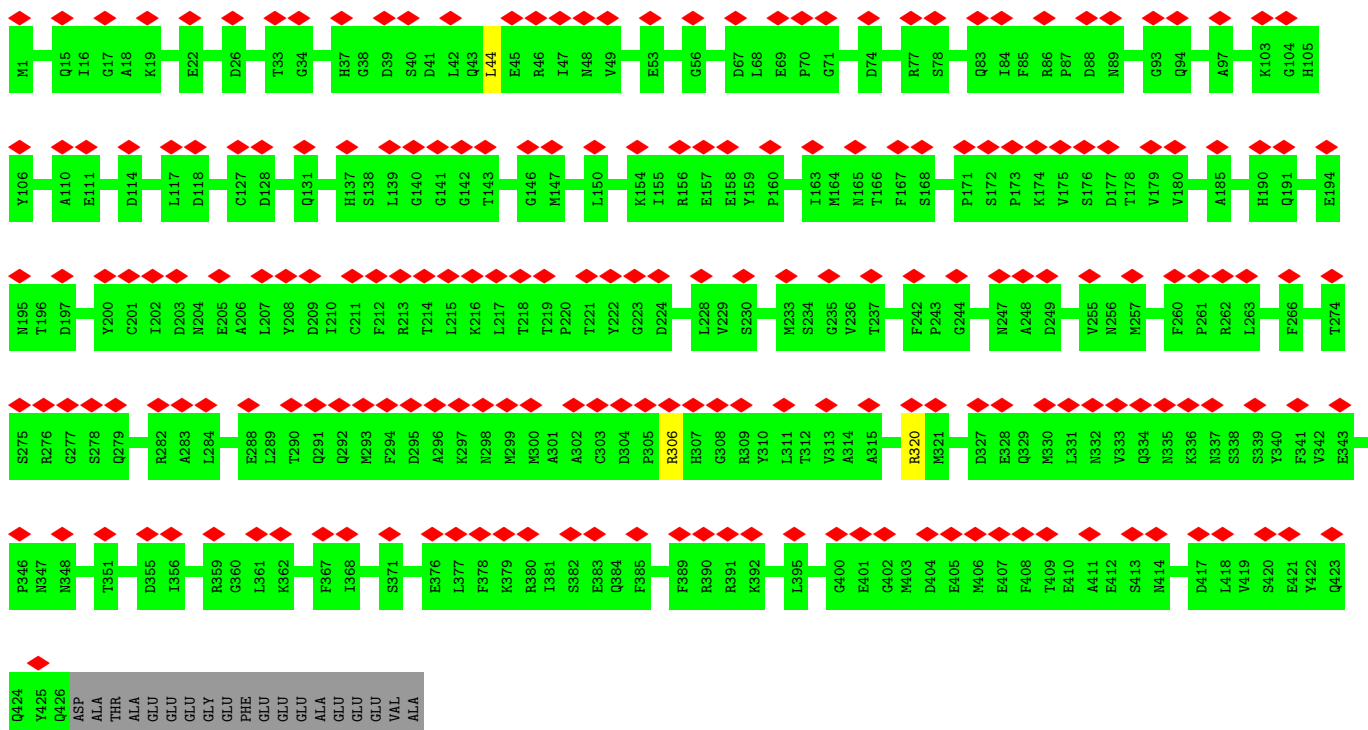




• Molecule 9: Tubulin beta-4B chain



• Molecule 9: Tubulin beta-4B chain

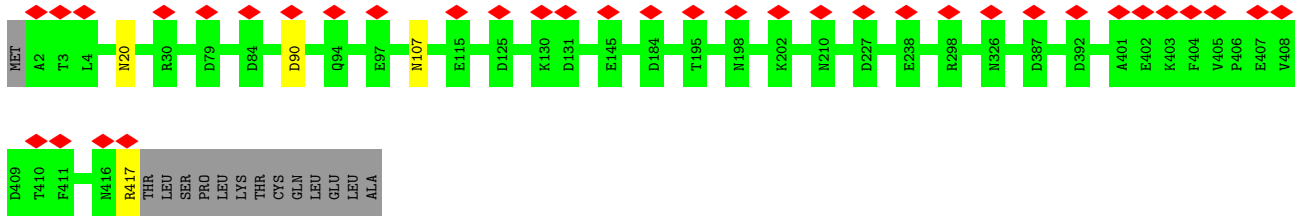




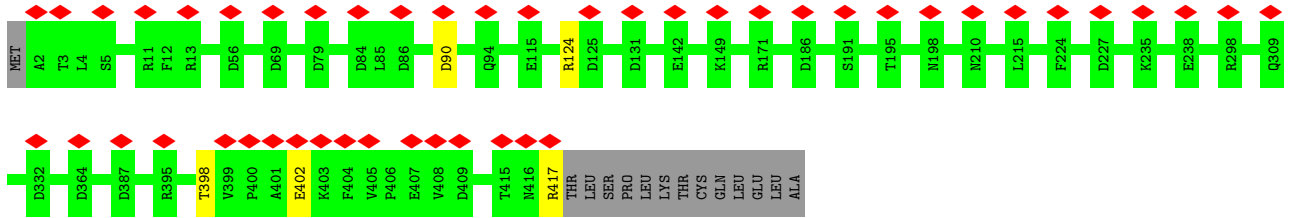




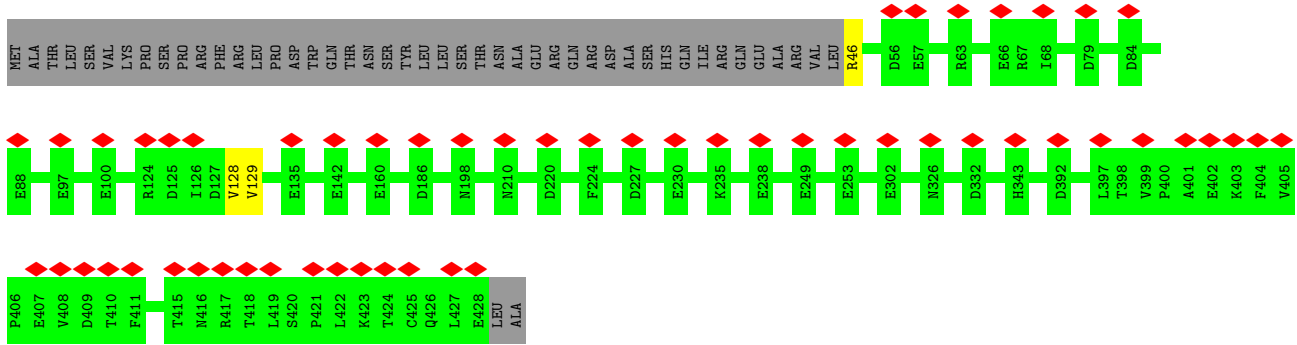
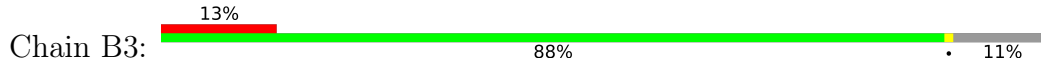
Molecule 10: Tektin-2



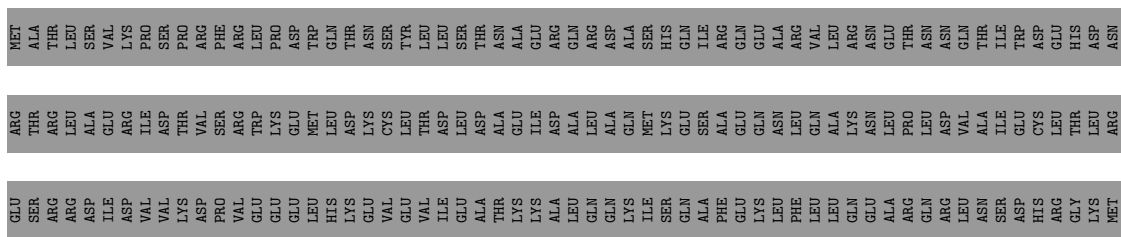
Molecule 10: Tektin-2



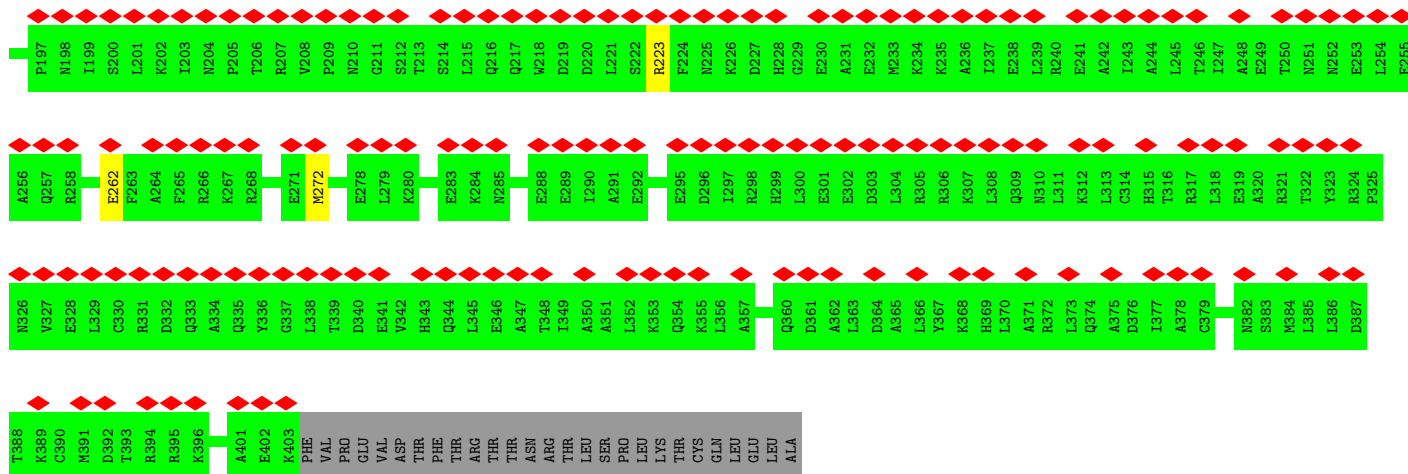
Molecule 10: Tektin-2



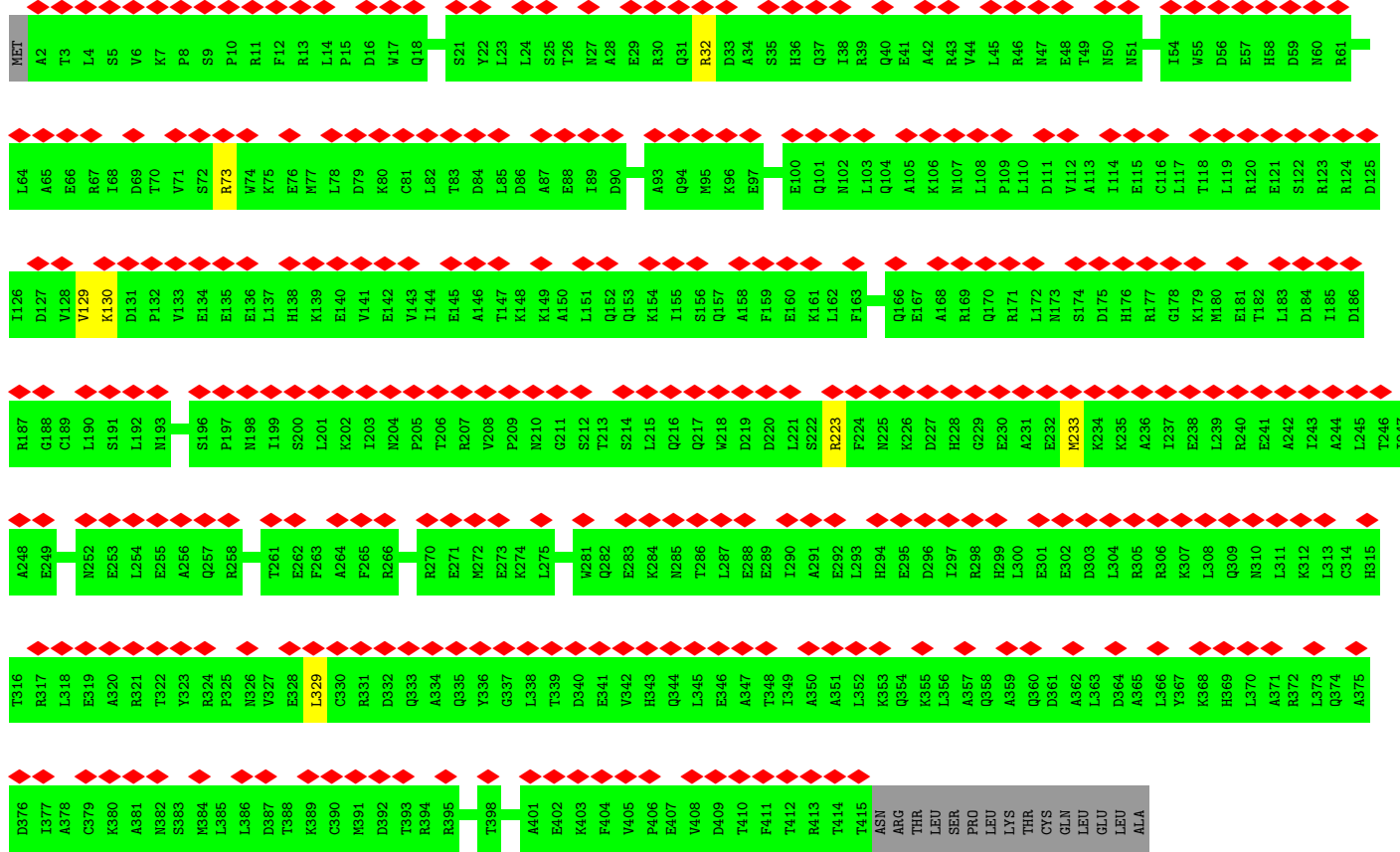
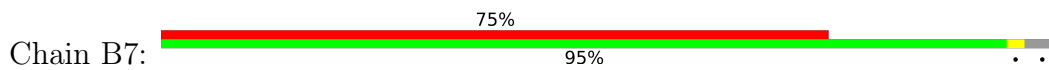
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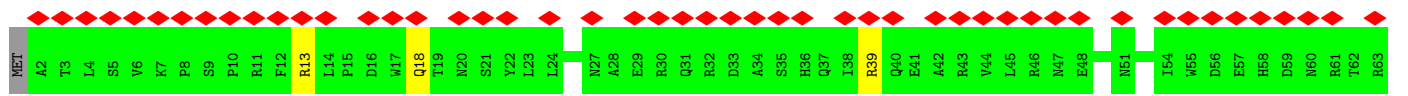
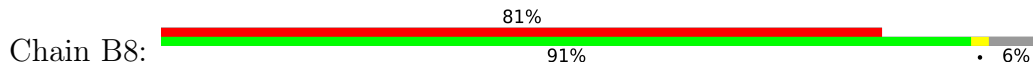


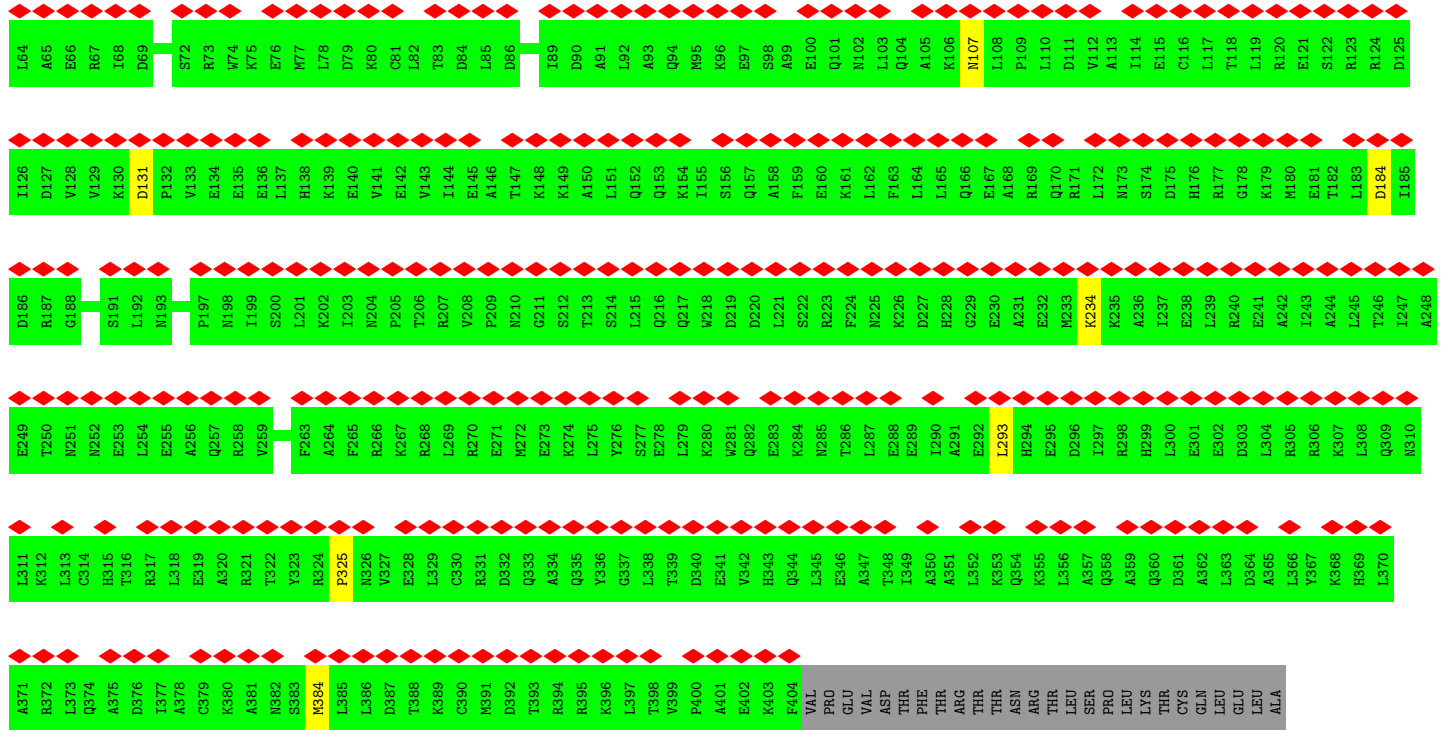


• Molecule 10: Tektin-2

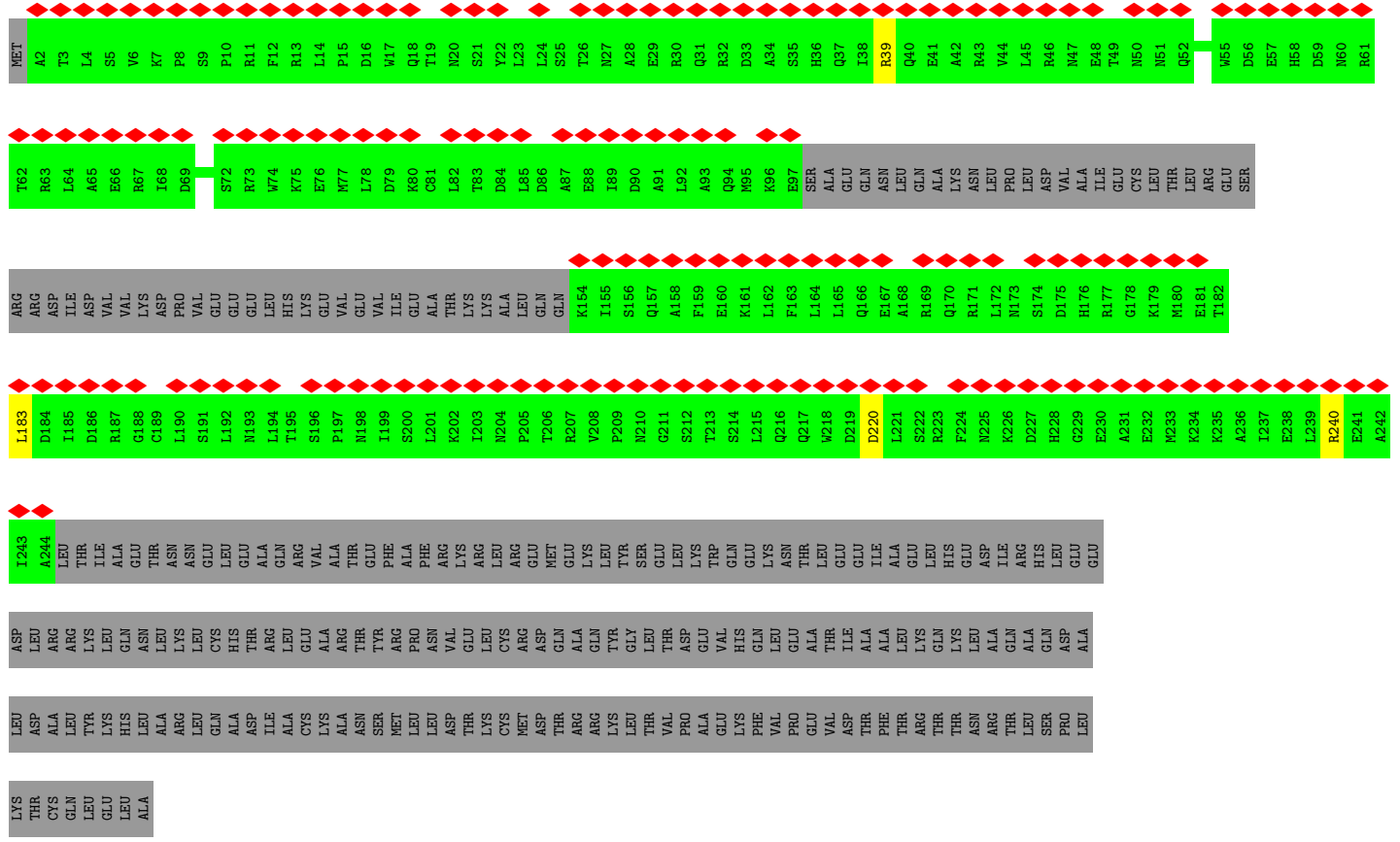


• Molecule 10: Tektin-2

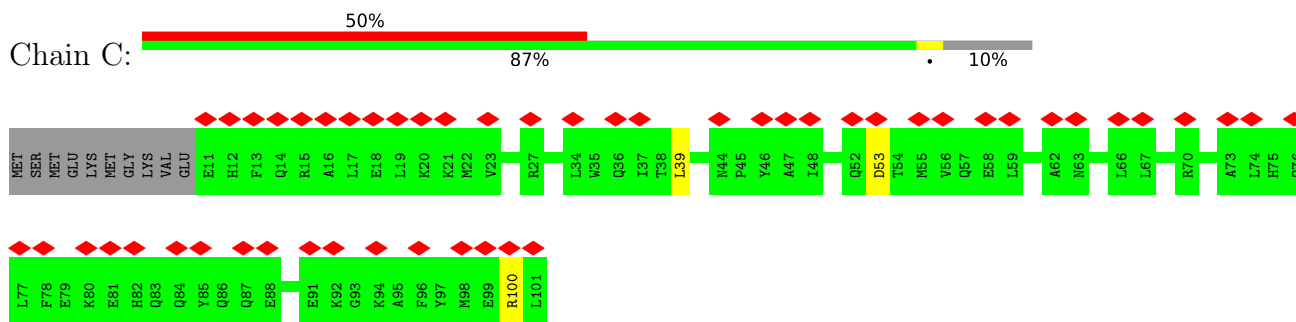




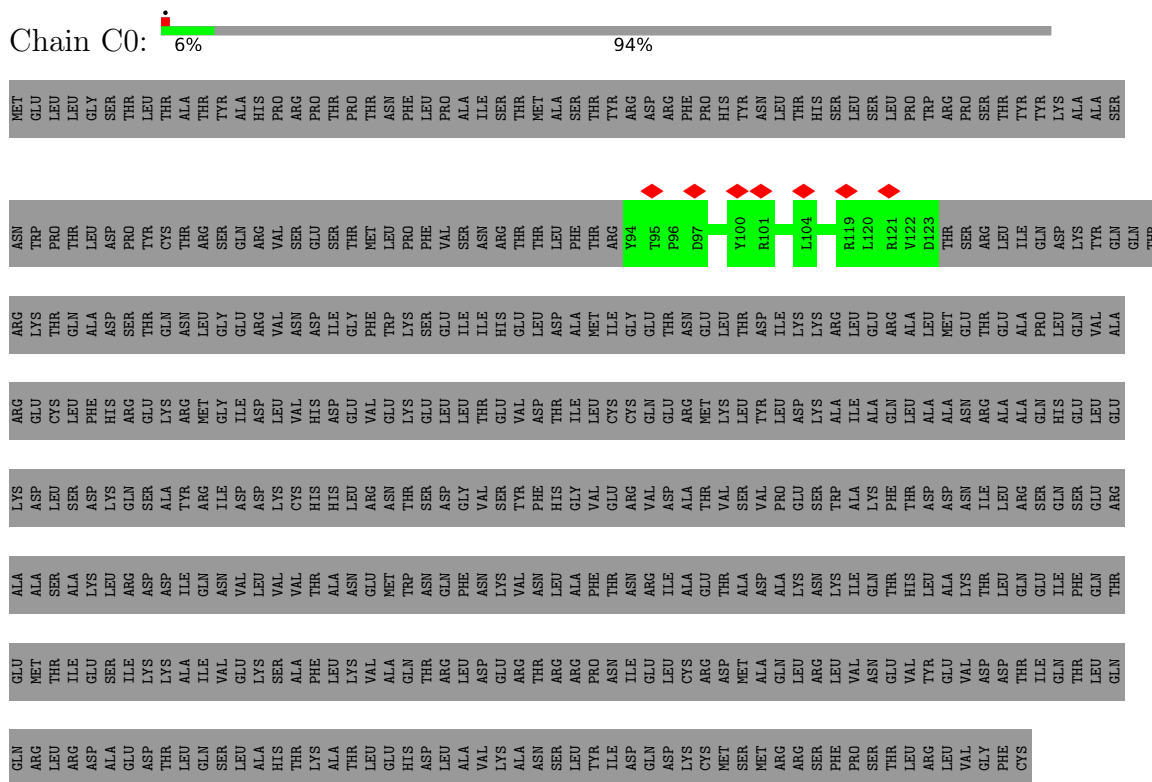
● Molecule 10: Tektin-2



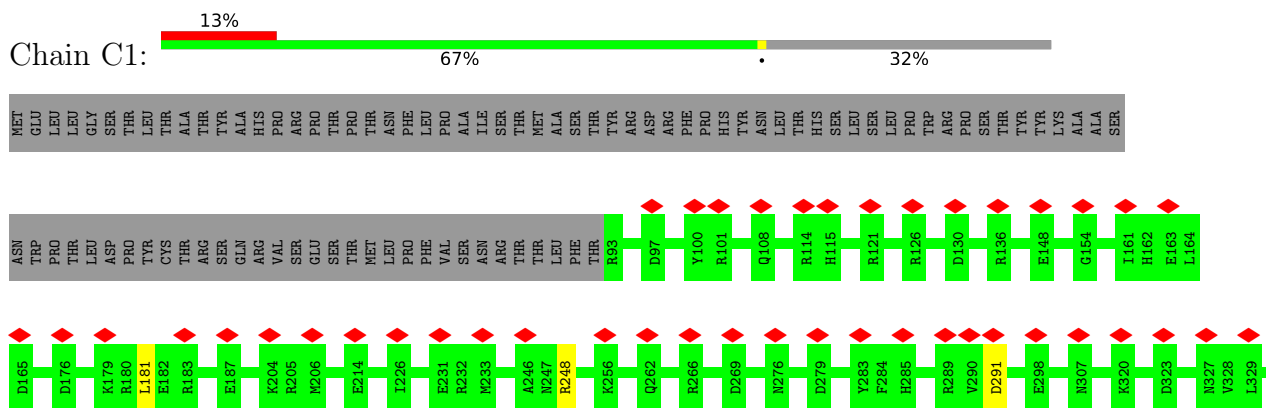
- Molecule 11: Uncharacterized protein C1orf189 homolog

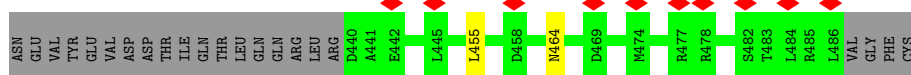
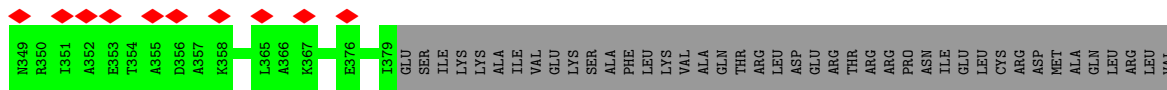


- Molecule 12: Tektin-3

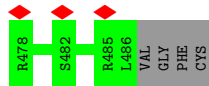
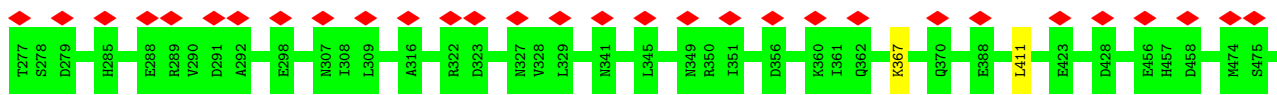
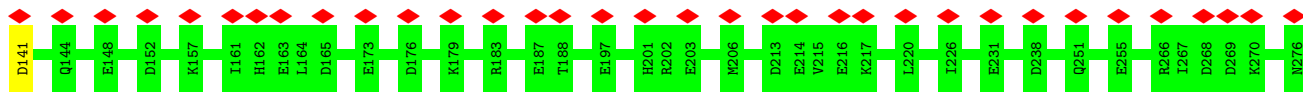
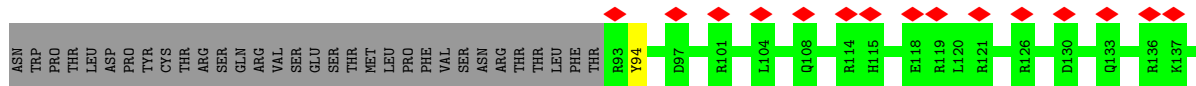
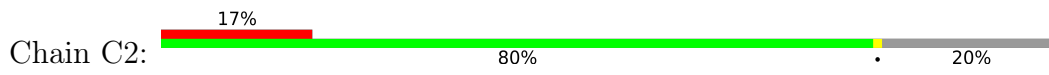


- Molecule 12: Tektin-3

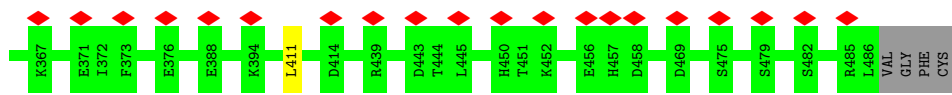
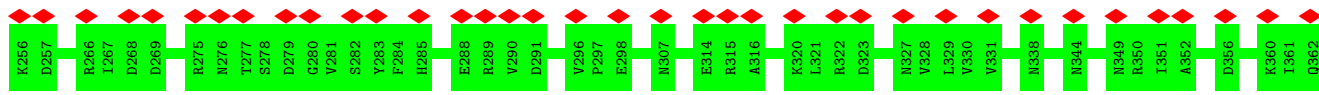
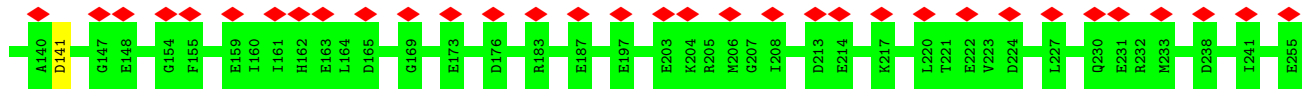
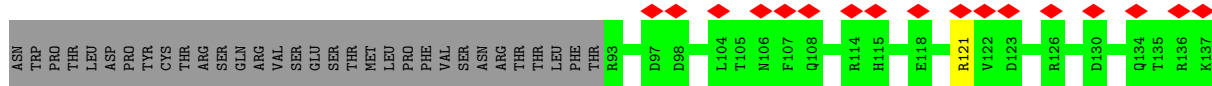
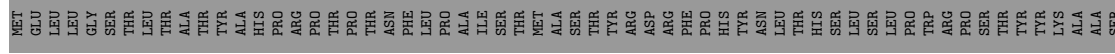
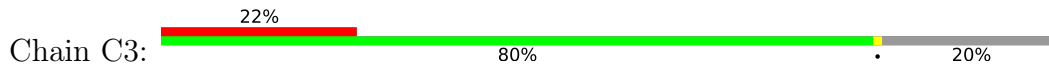




• Molecule 12: Tektin-3



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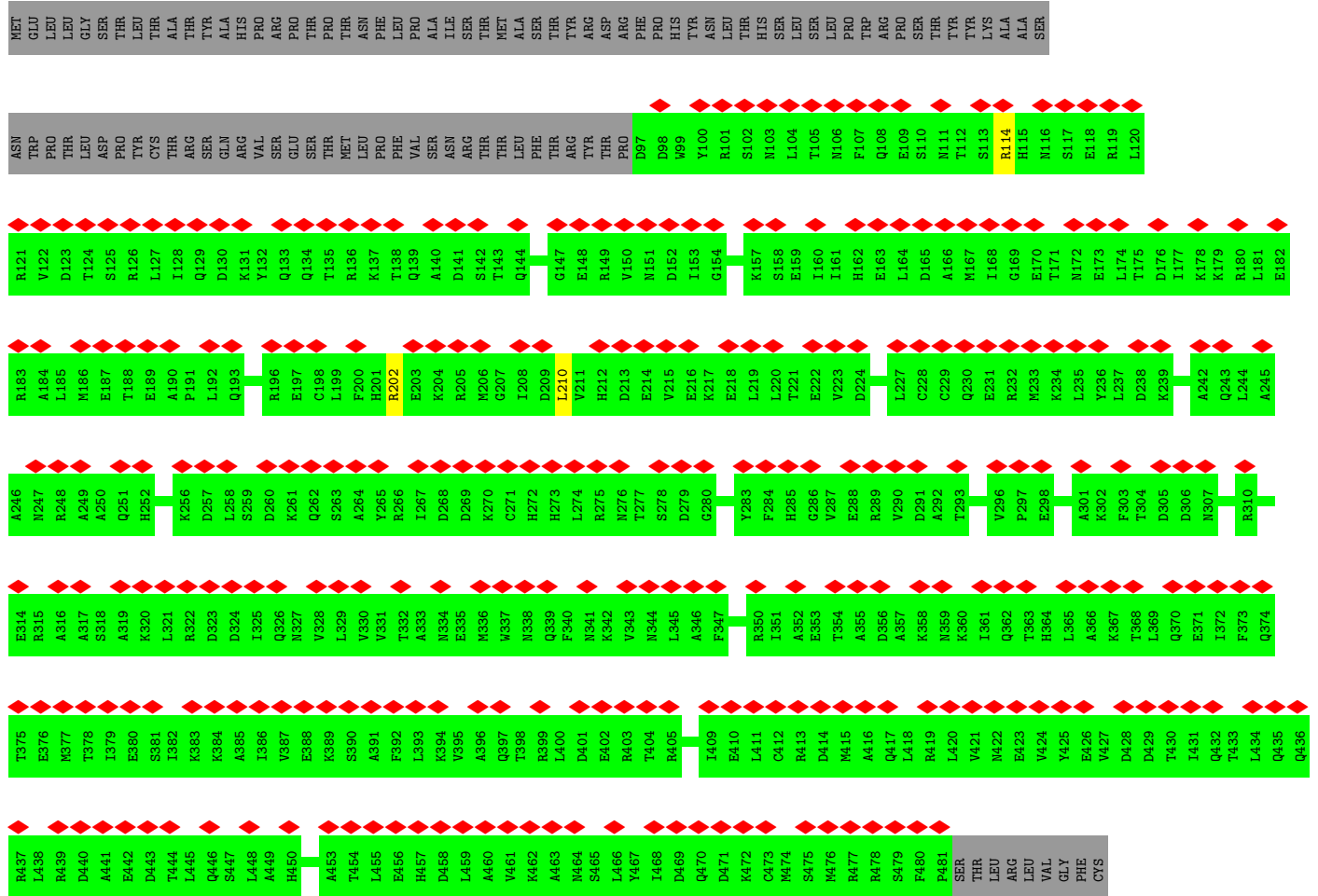
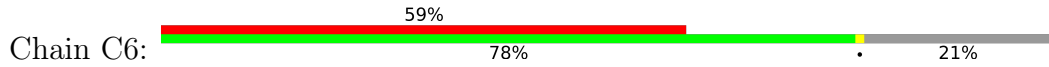


• Molecule 12: Tektin-3

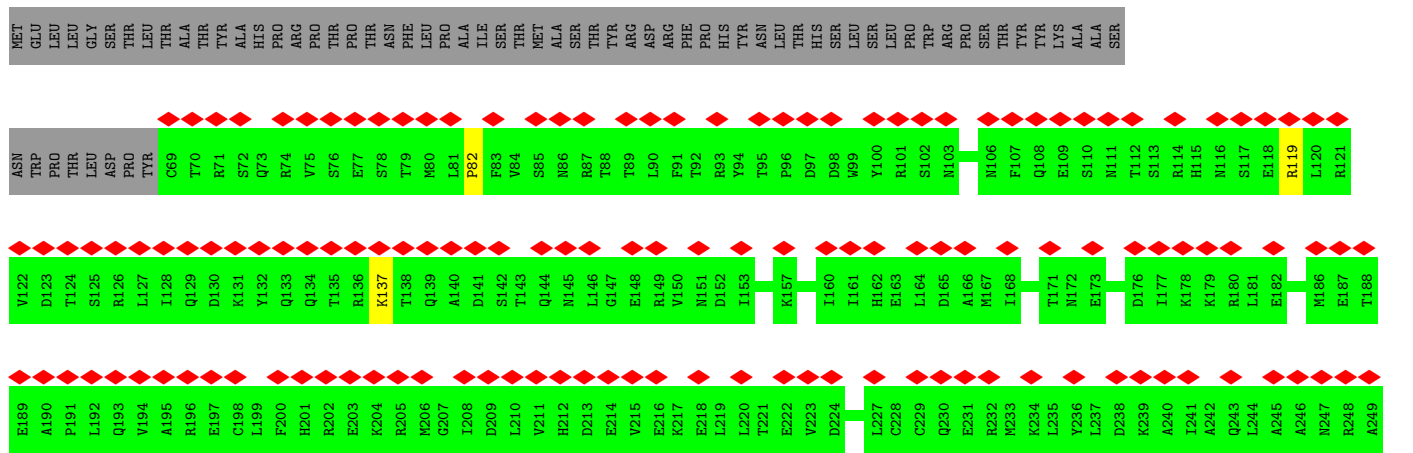
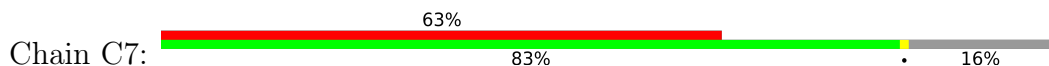


GLY  
PHE  
CYS

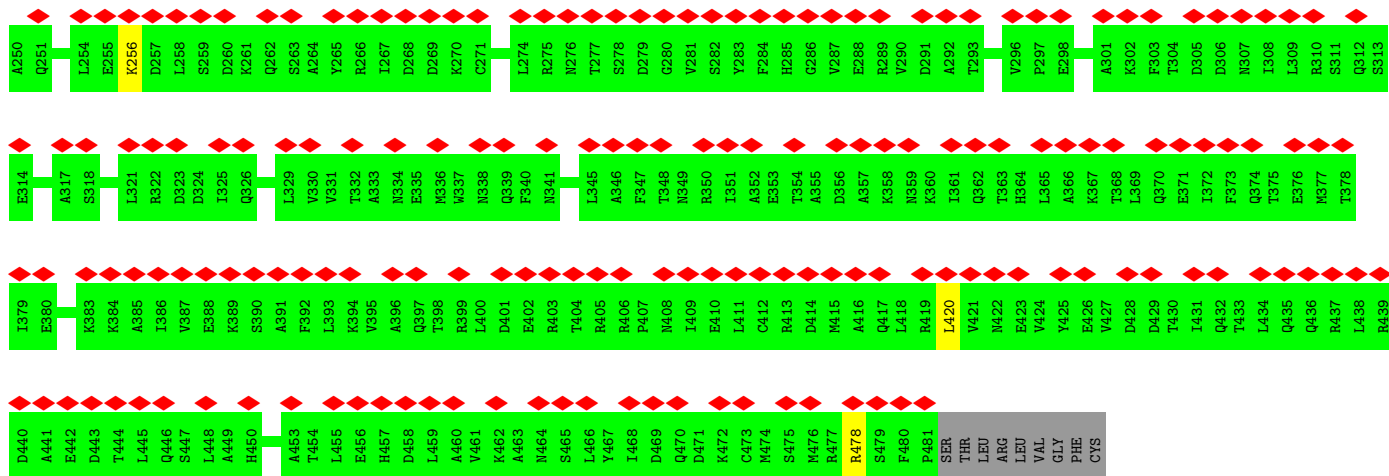
• Molecule 12: Tektin-3



• Molecule 12: Tektin-3

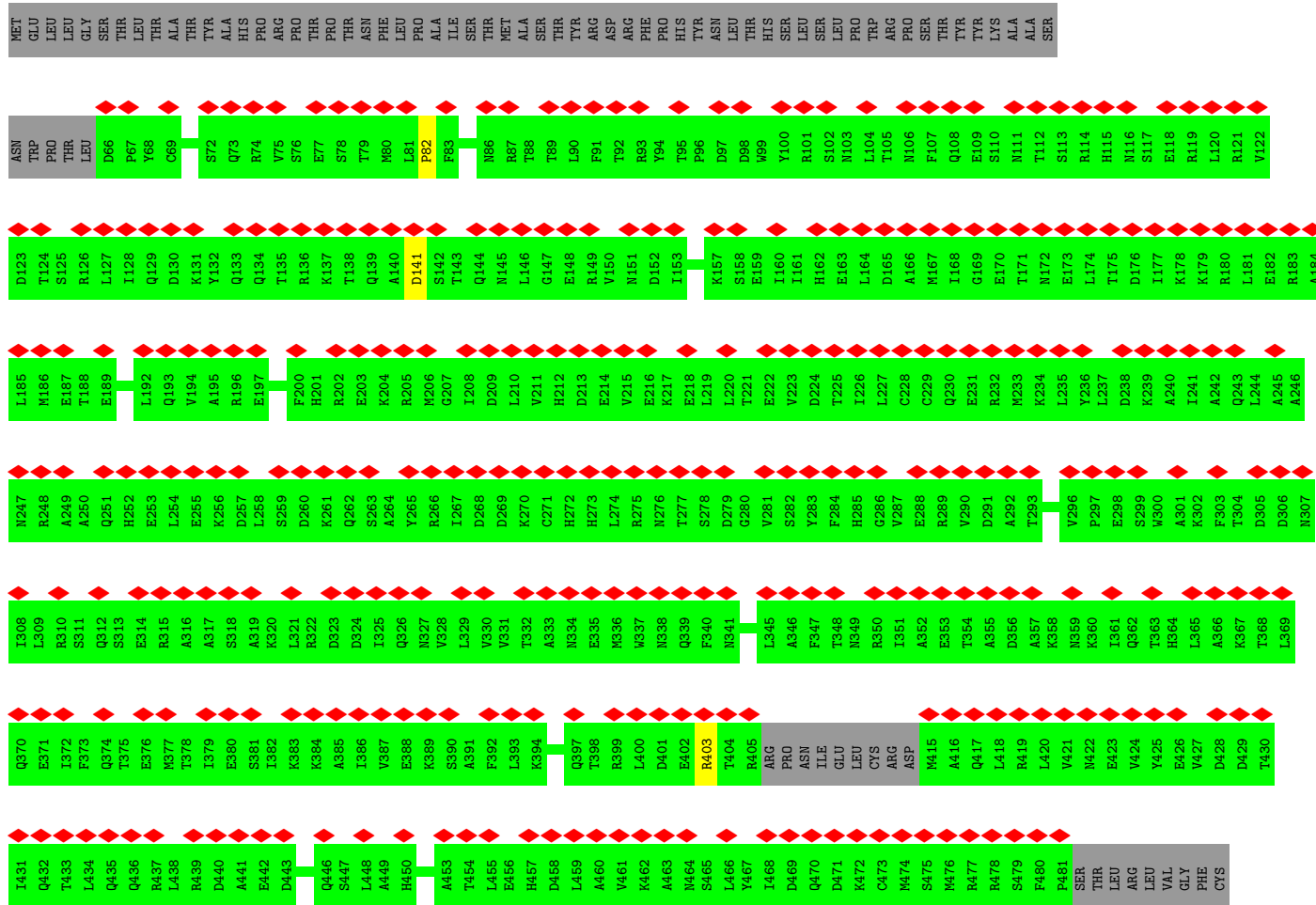






• Molecule 12: Tektin-3

Chain C8:



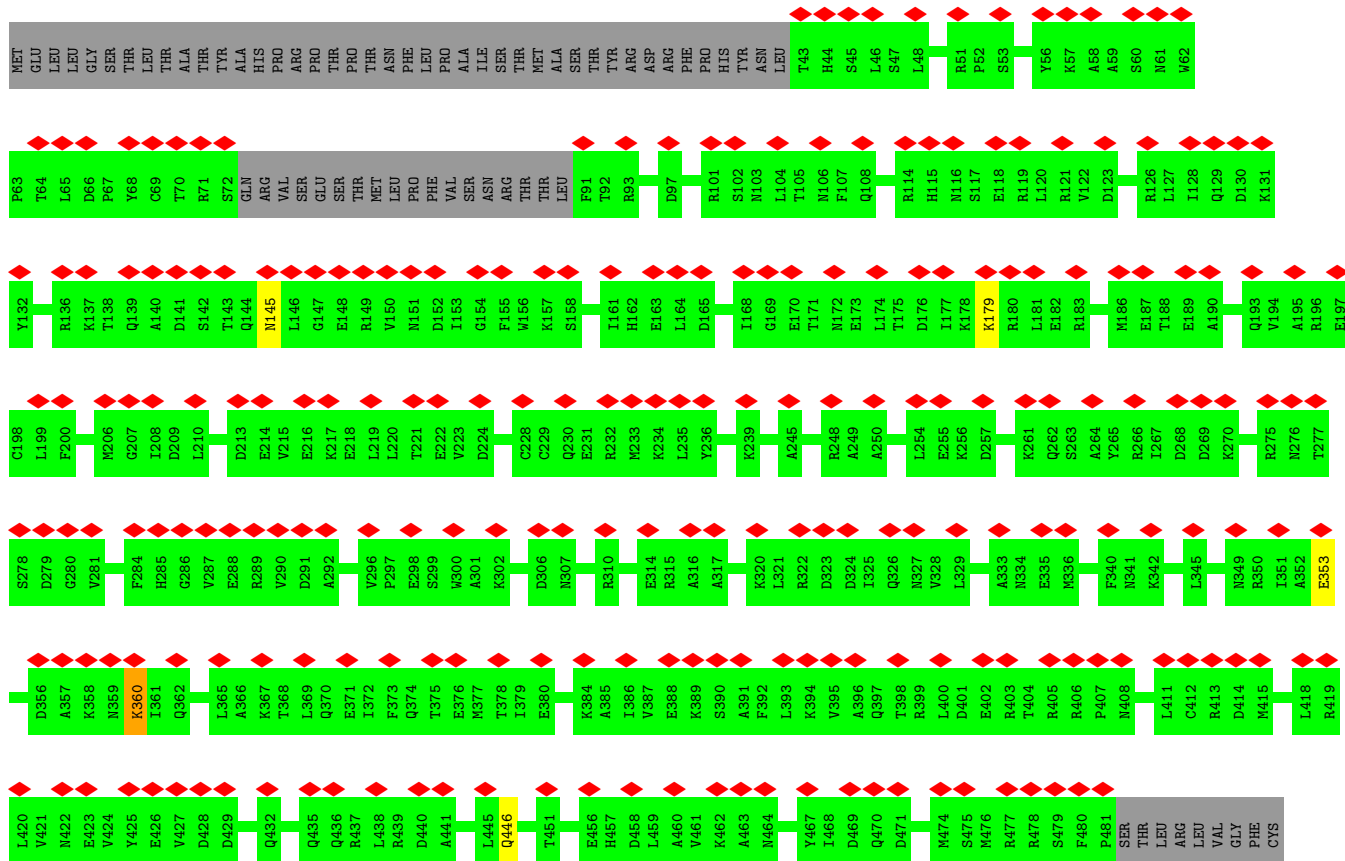
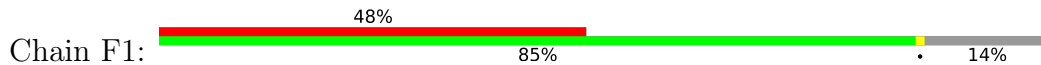
• Molecule 12: Tektin-3

Chain C9:

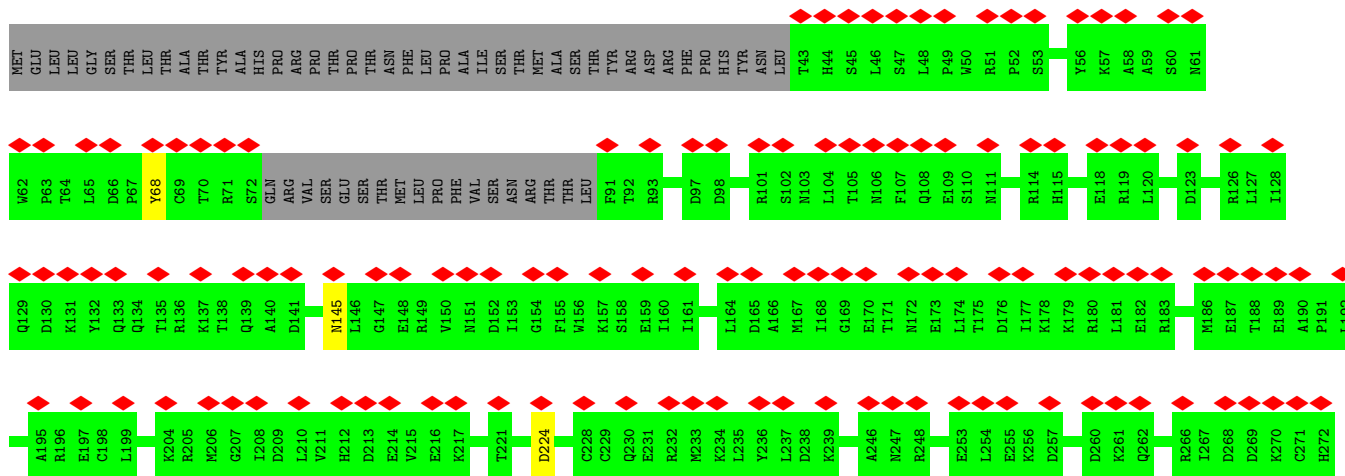
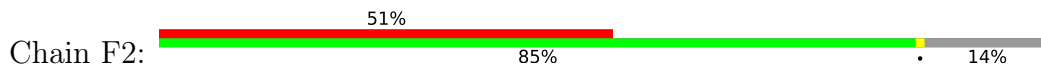


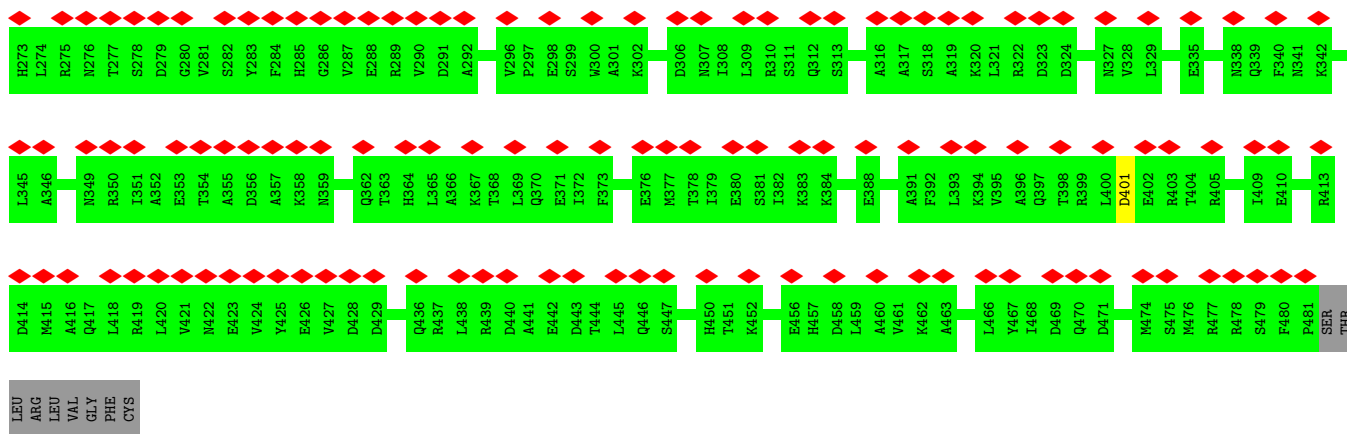
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Molecule 12: Tektin-3

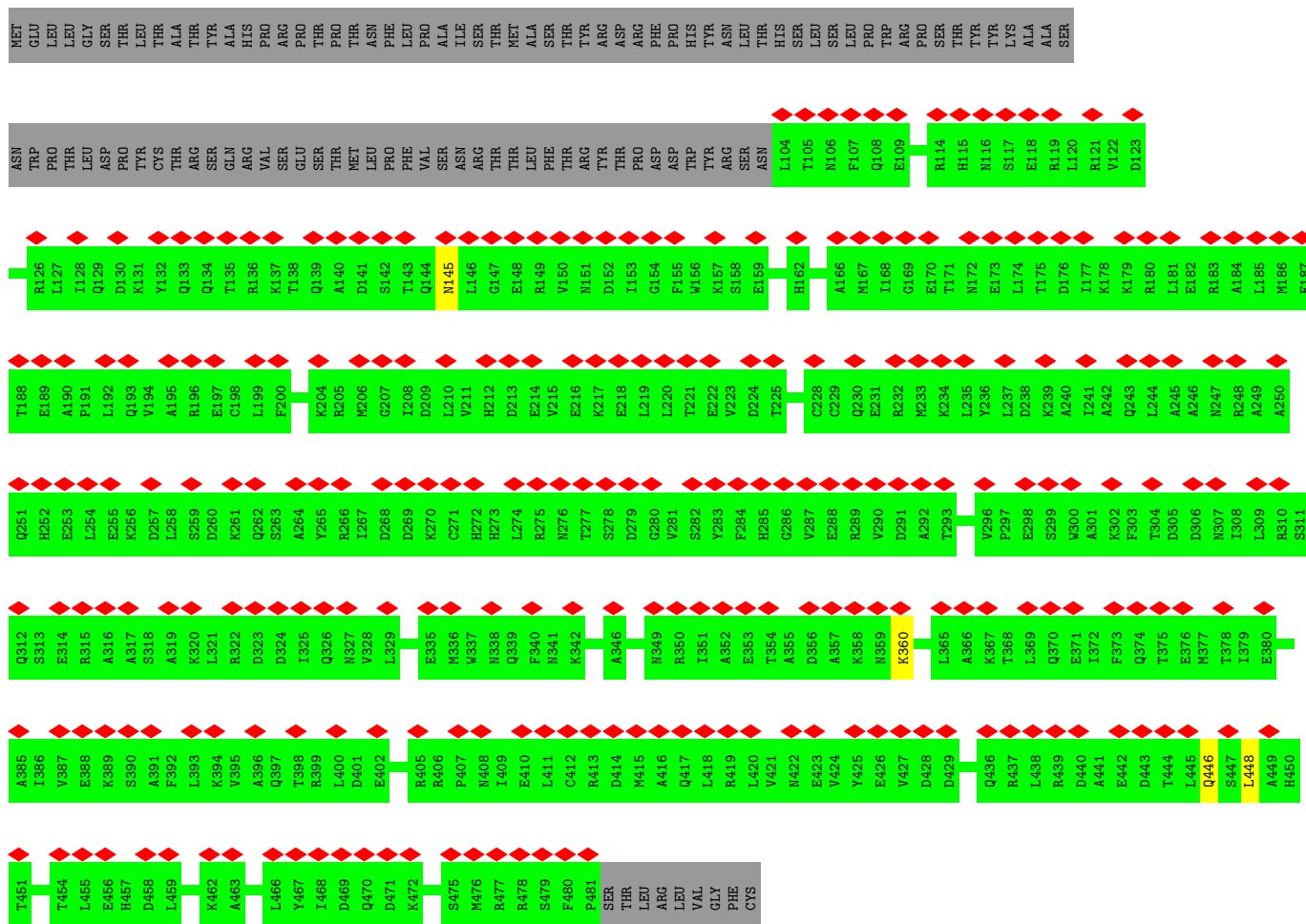
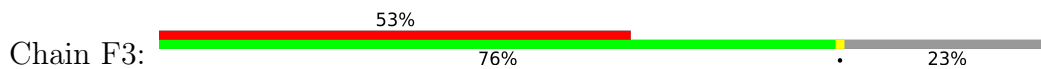


Molecule 12: Tektin-3

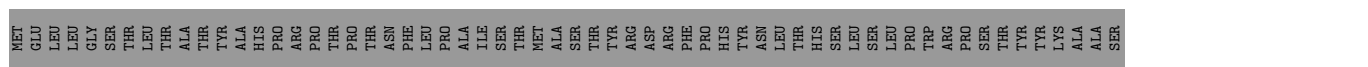


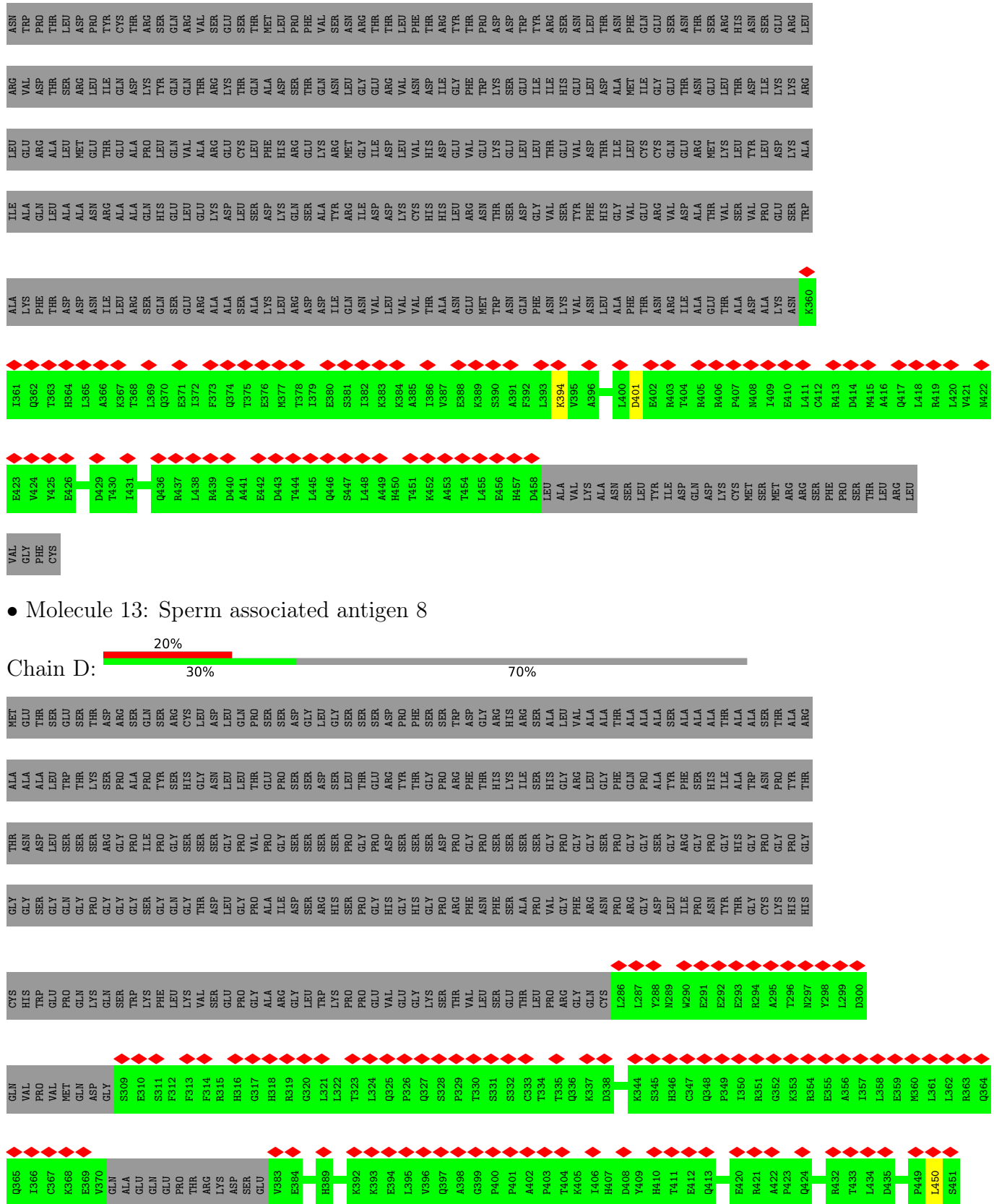


• Molecule 12: Tektin-3



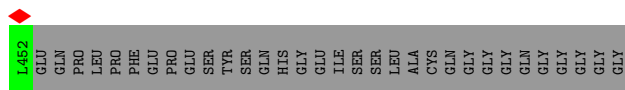
• Molecule 12: Tektin-3



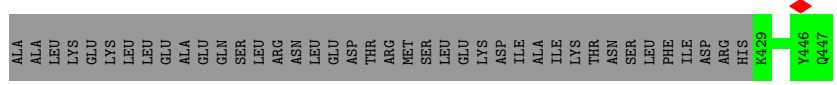
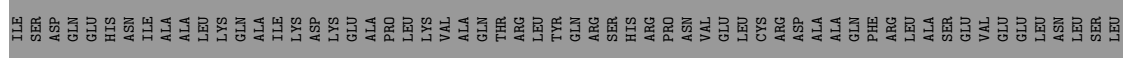
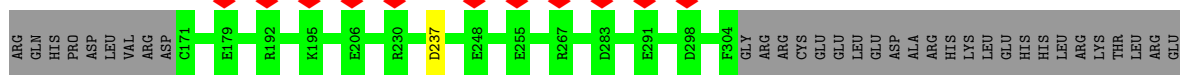
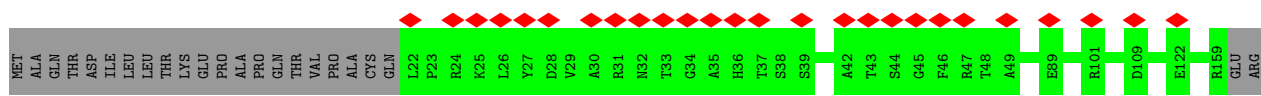


• Molecule 13: Sperm associated antigen 8

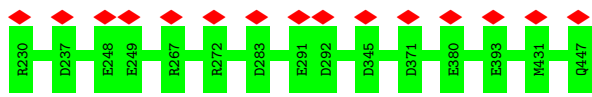
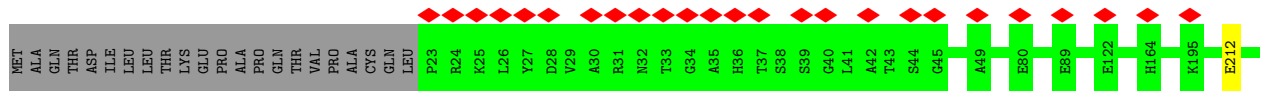




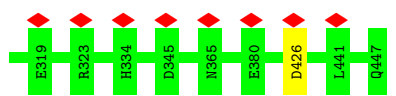
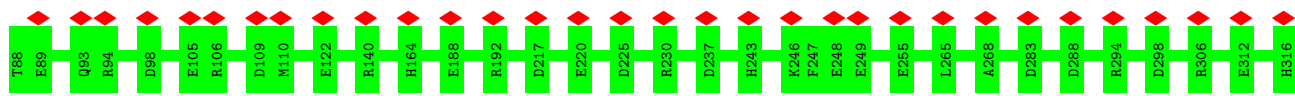
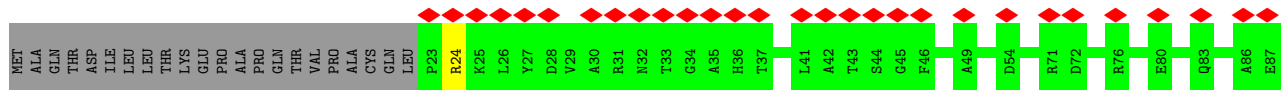
• Molecule 14: Tektin-4



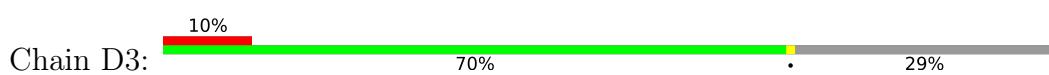
• Molecule 14: Tektin-4

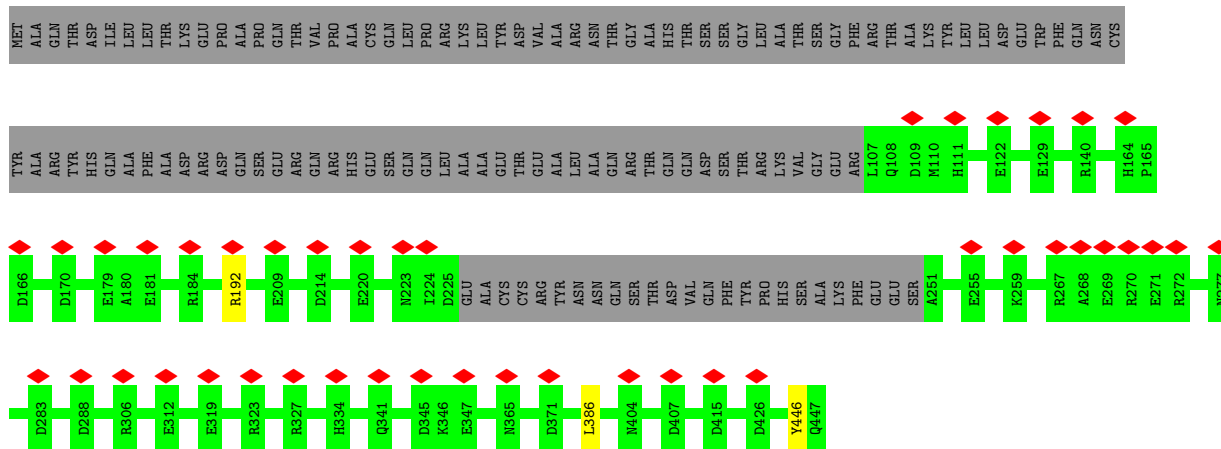


• Molecule 14: Tektin-4

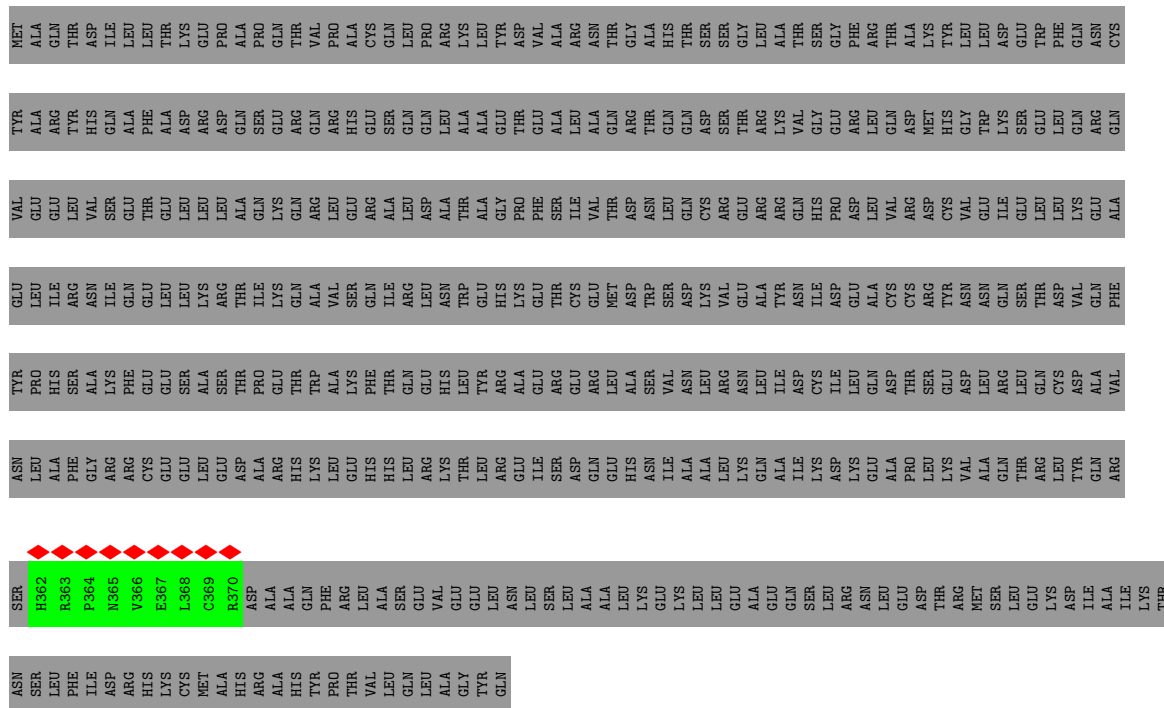


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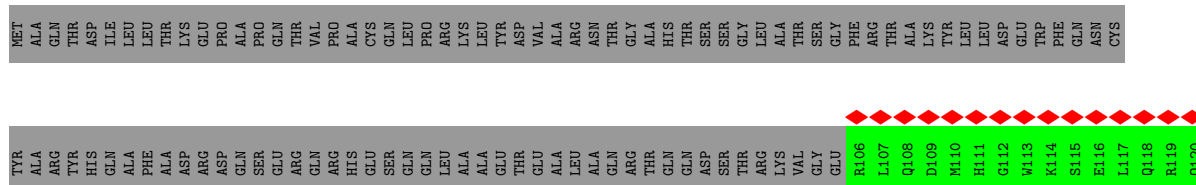
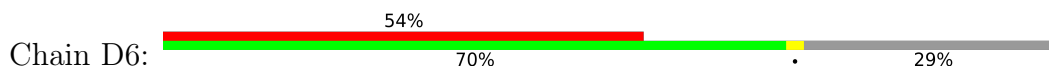


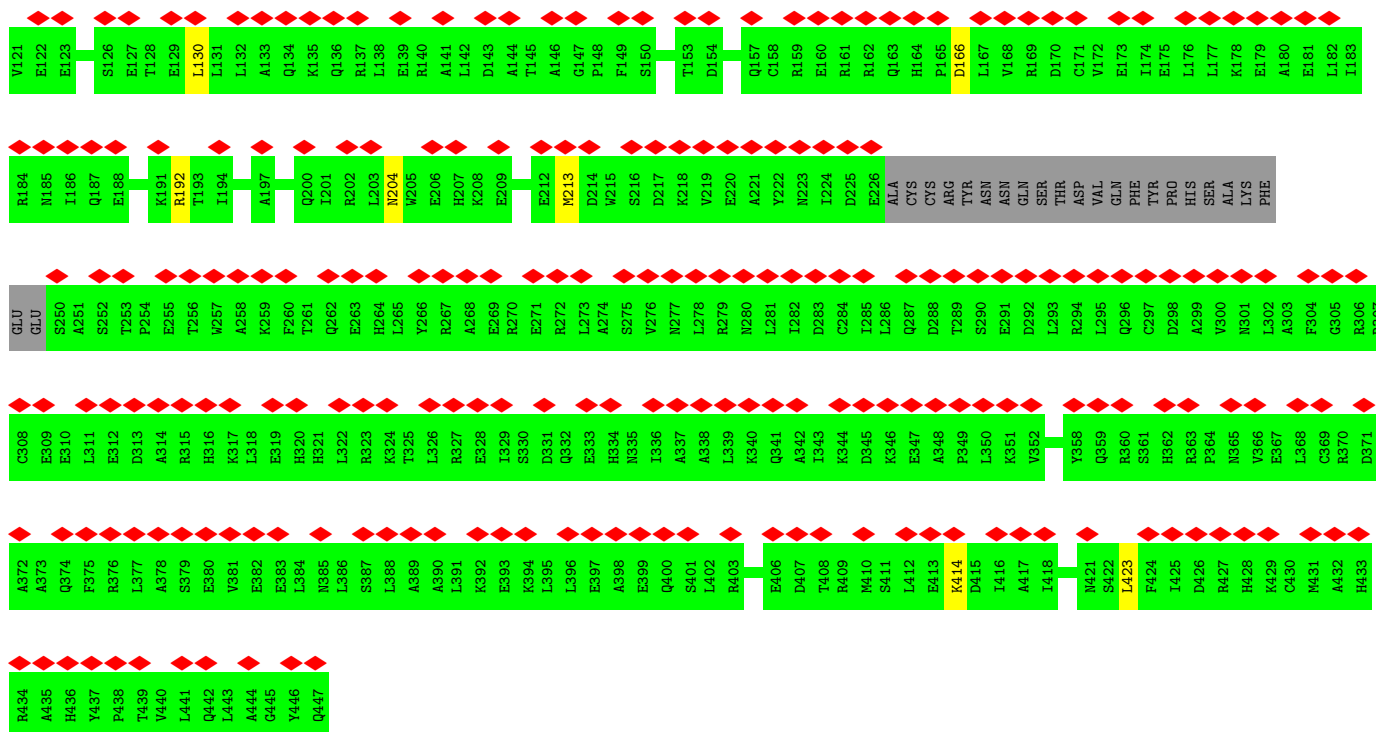


• Molecule 14: Tektin-4

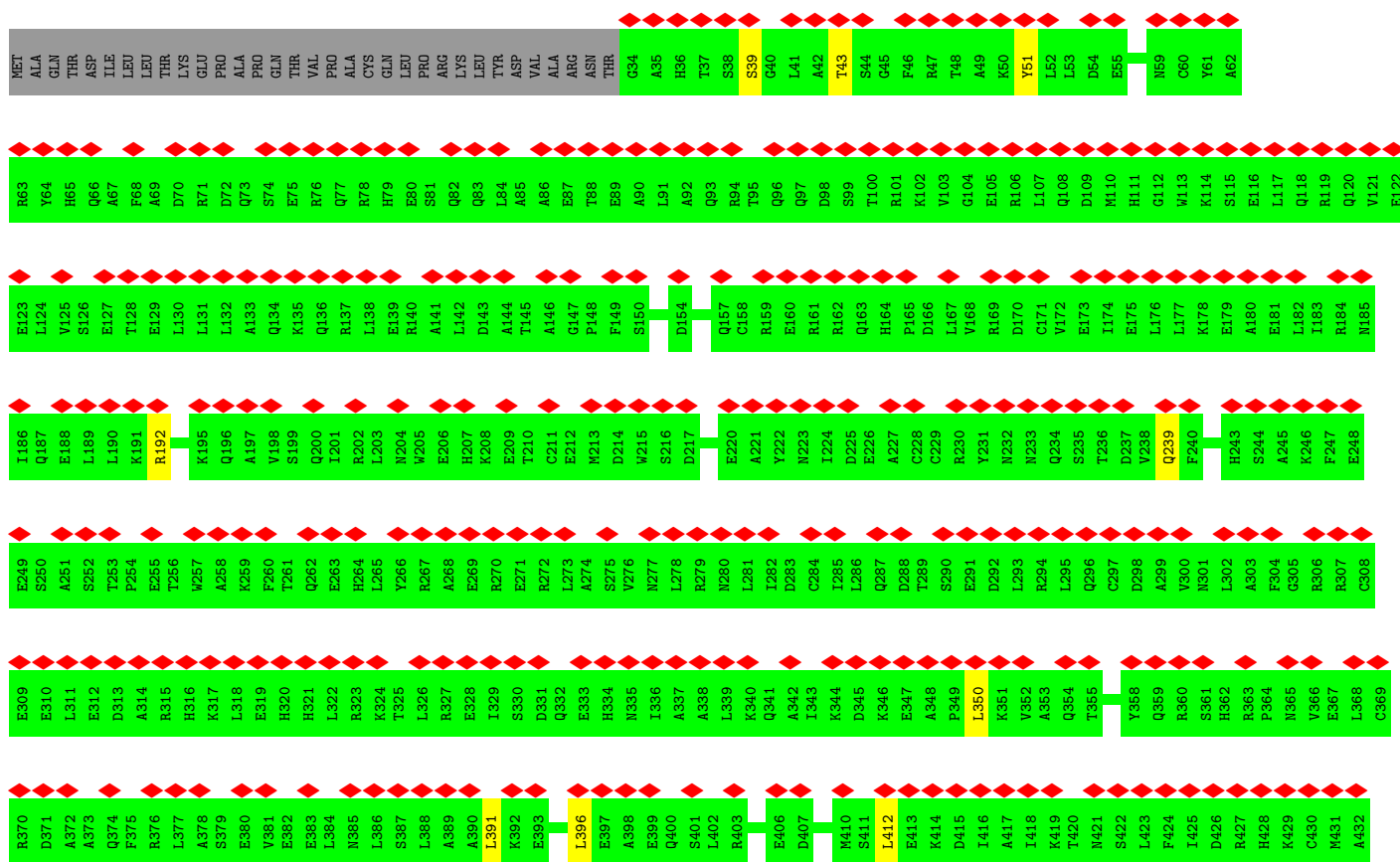
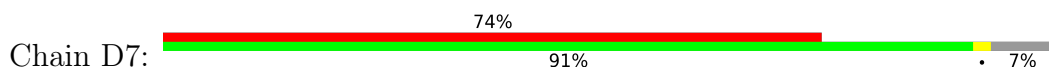


• Molecule 14: Tektin-4





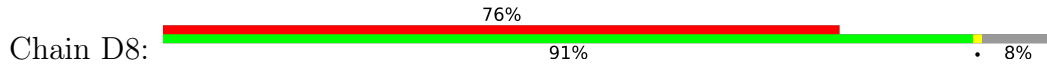
• Molecule 14: Tektin-4





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● Molecule 14: Tektin-4



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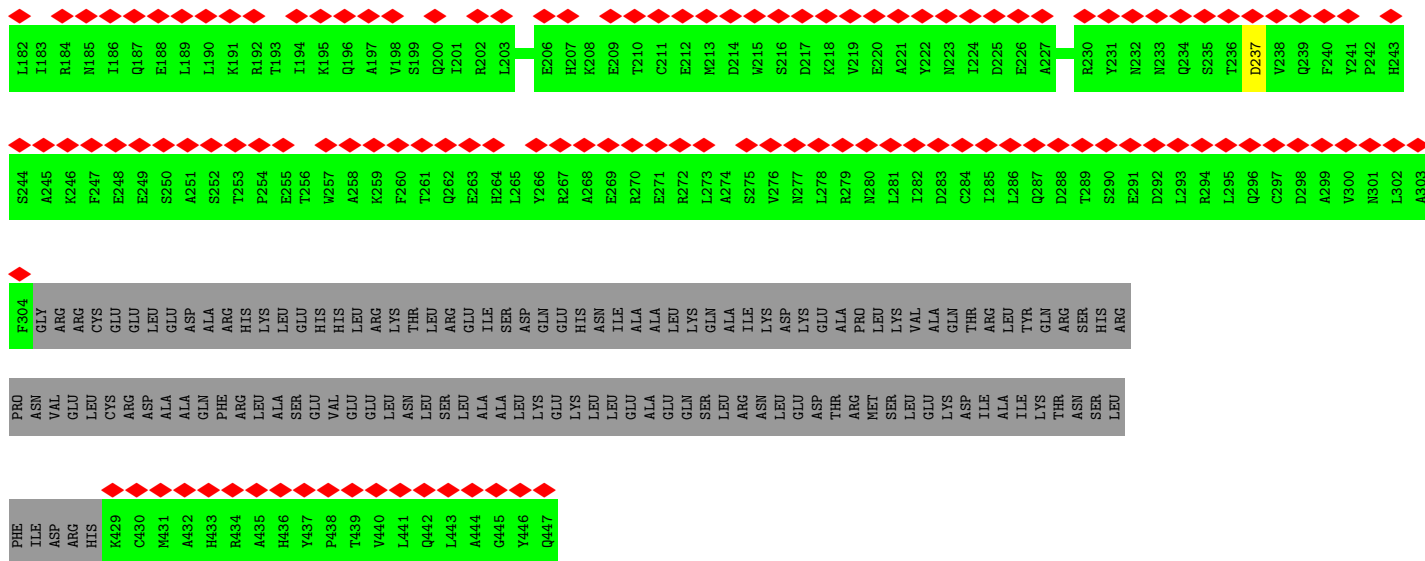
● Molecule 14: Tektin-4



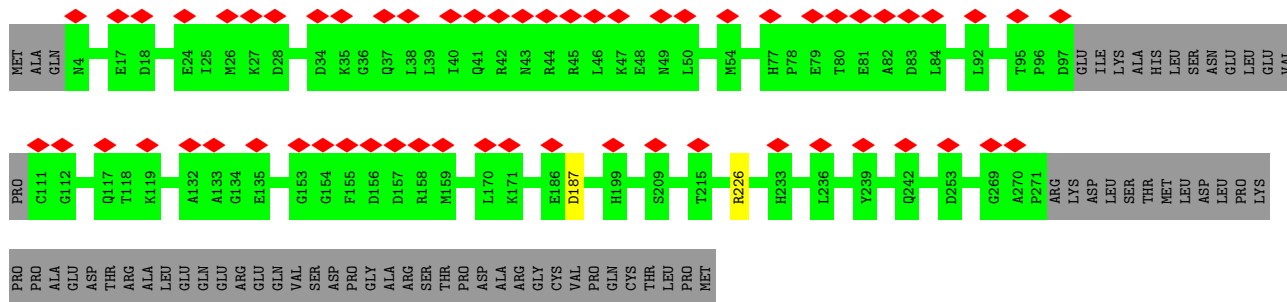
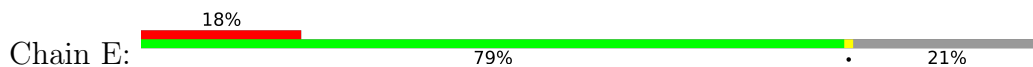
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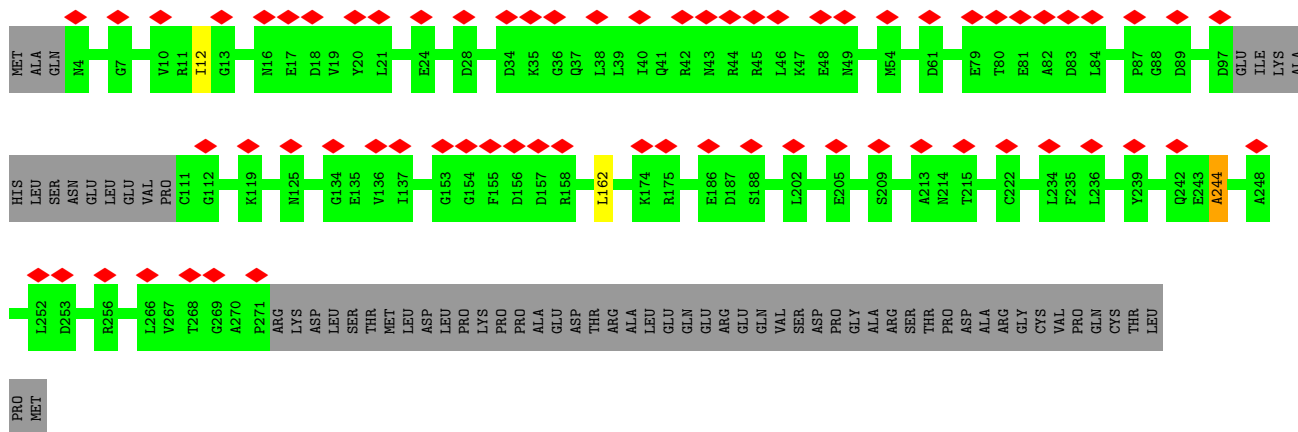
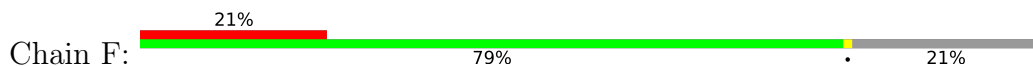
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 ◆ S115  
 ◆ E116  
 ◆ L117  
 ◆ Q118  
 ◆ R119  
 ◆ Q120  
 ◆ V121



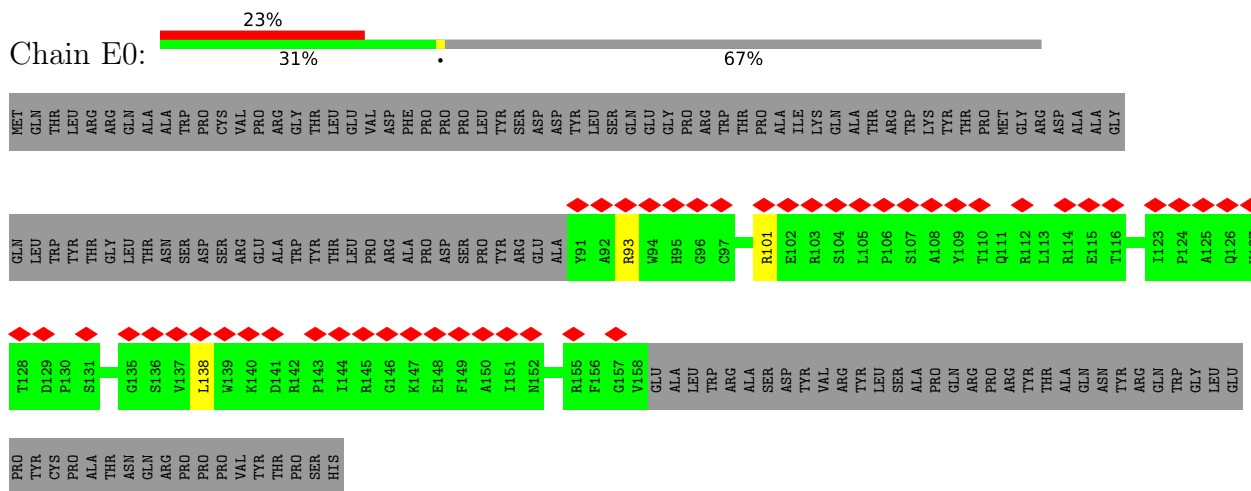
• Molecule 15: Cilia and flagella associated protein 161



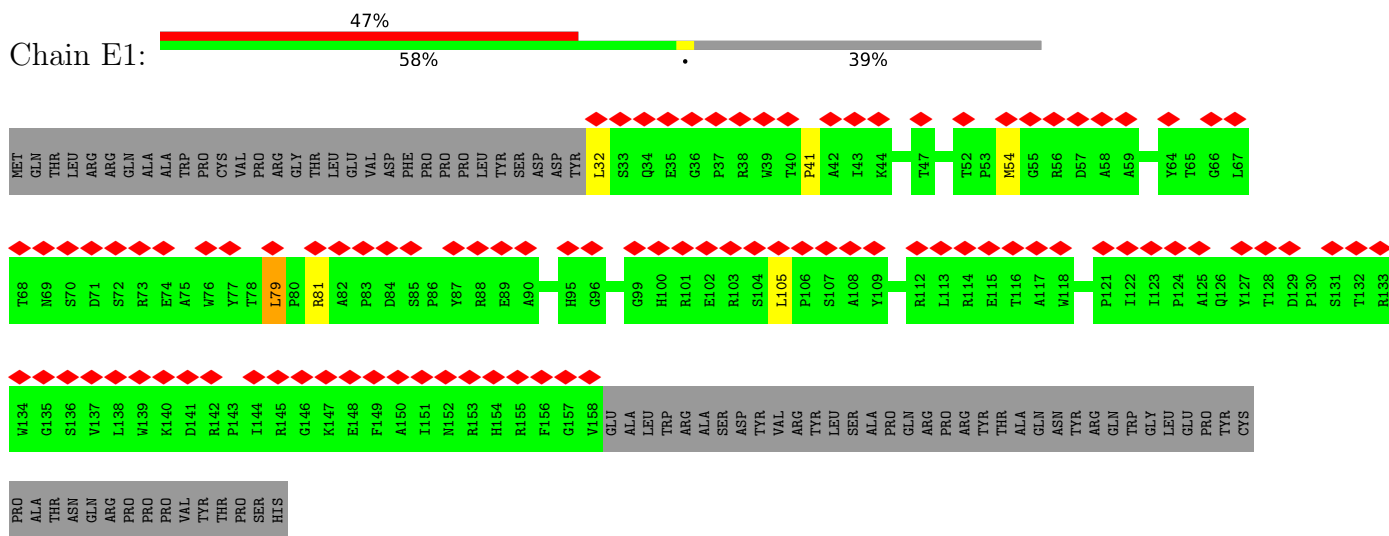
• Molecule 15: Cilia and flagella associated protein 161



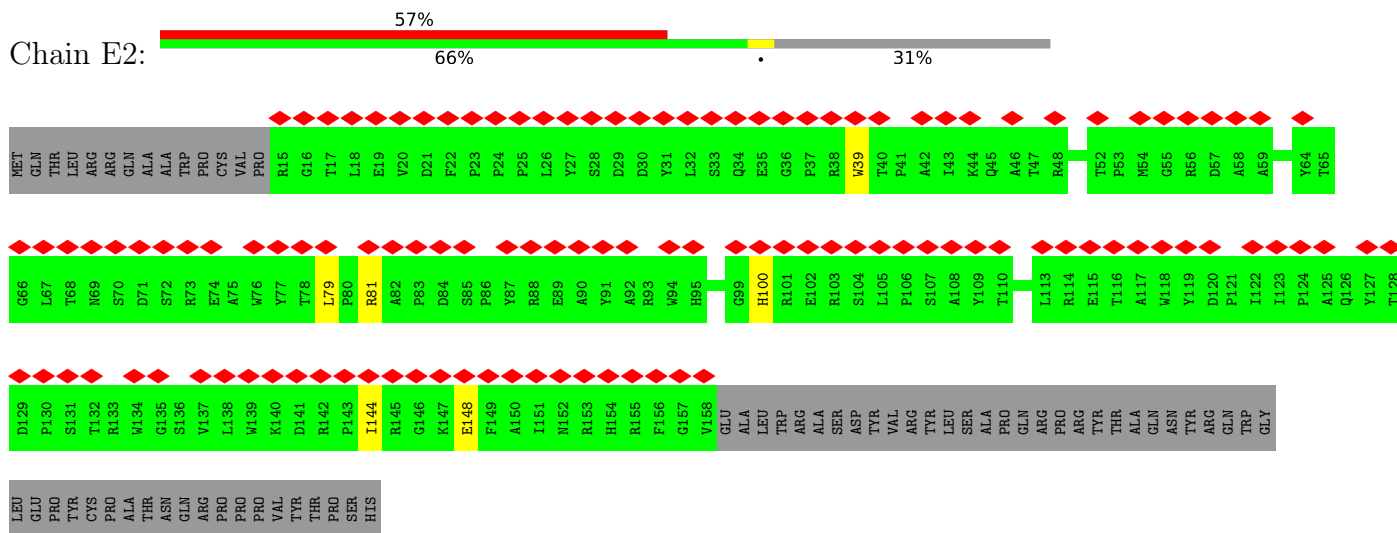
• Molecule 16: TEKTIIP1



• Molecule 16: TEKTIPT1

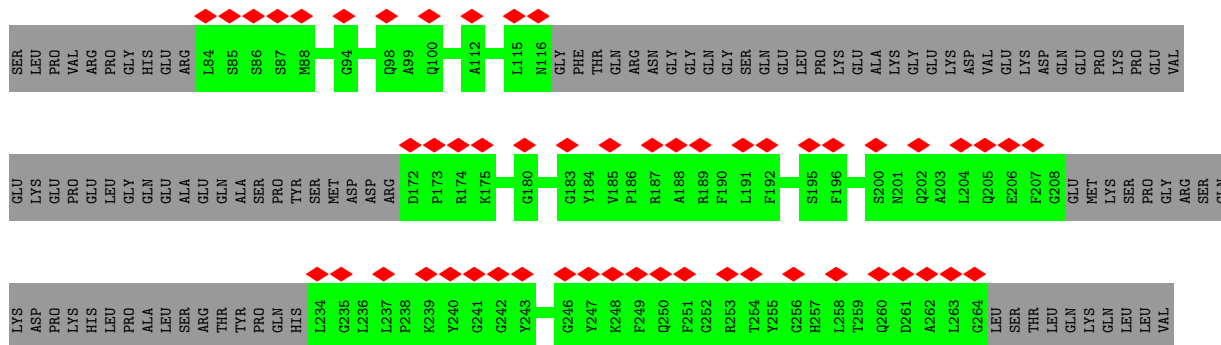


• Molecule 16: TEKTIPT1

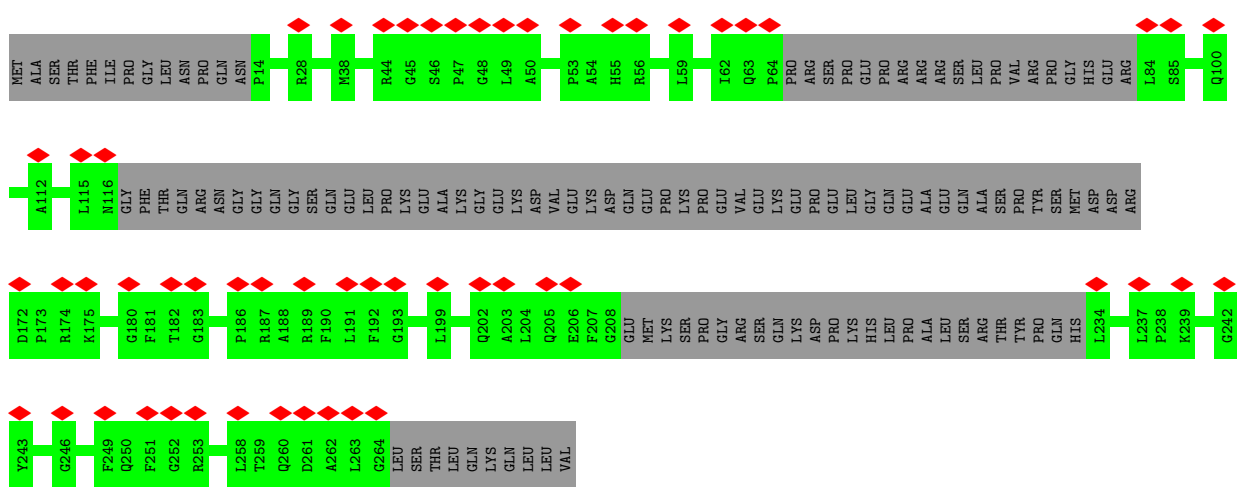


• Molecule 16: TEKTIPT1

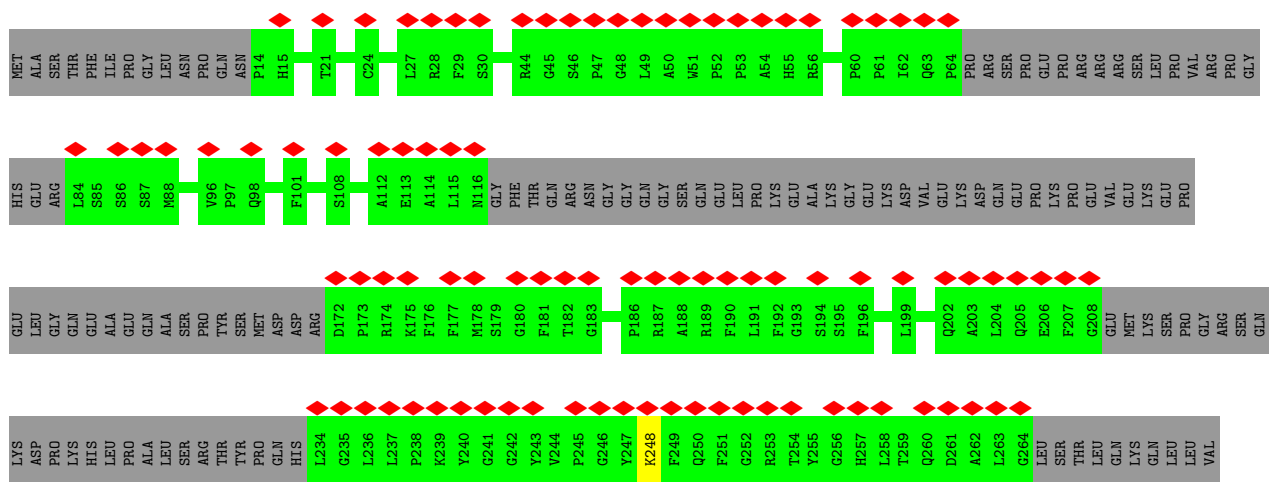




• Molecule 18: Protein FAM166B

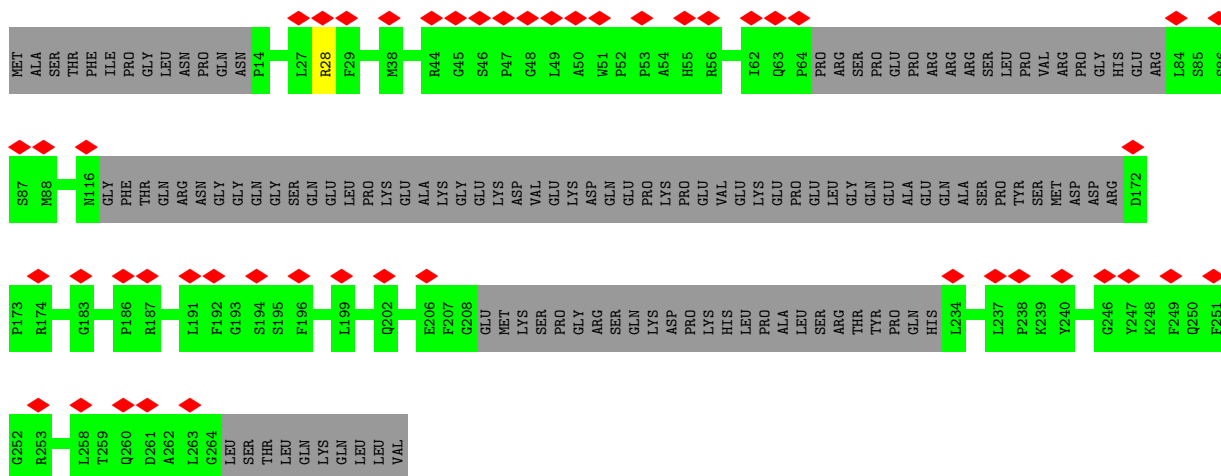


• Molecule 18: Protein FAM166B

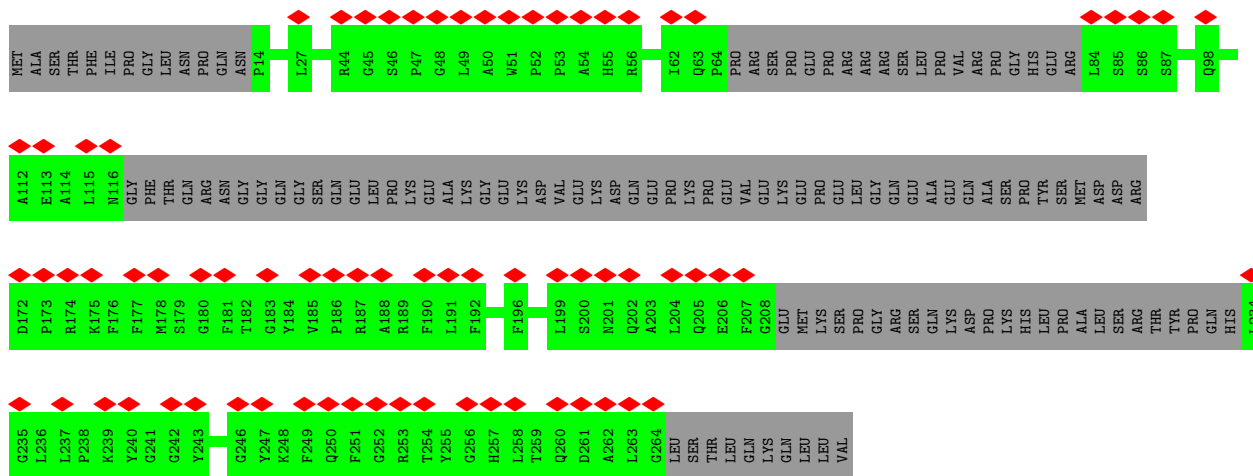


• Molecule 18: Protein FAM166B

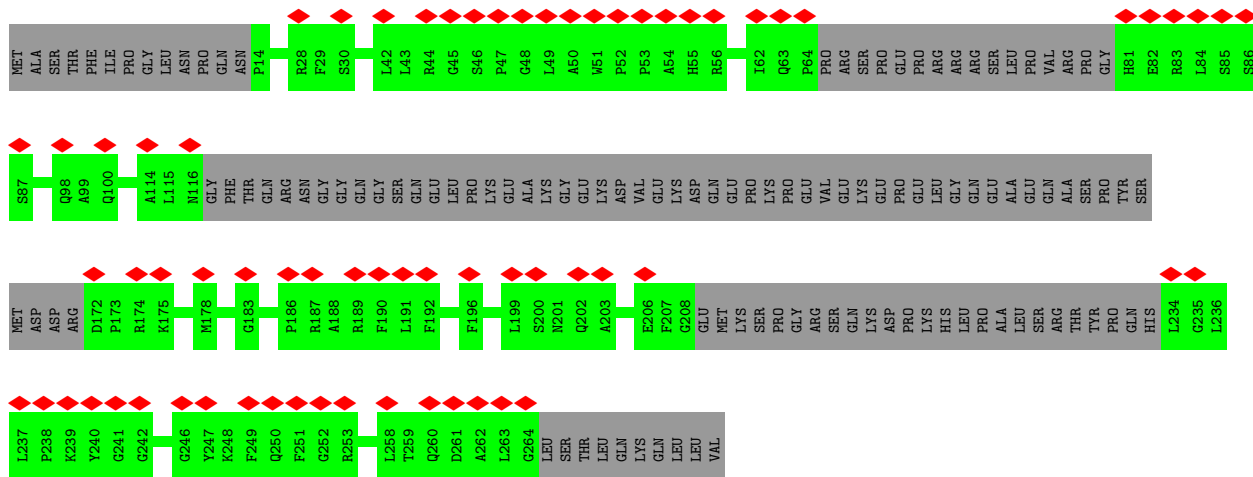




• Molecule 18: Protein FAM166B



• Molecule 18: Protein FAM166B





Residue ID	Residue Name	Residue Name	Residue Name	Residue Name	Residue Name	Residue Name	Residue Name	Residue Name	Residue Name
R235	A236	E237	K238	E239	Q242	N243	E244	L260	H261
H262	F263	L264	K265	N268	G269	D270	R271	Q272	P273
D274	S275	S276	A277	VAL	GLY	LYS	ARG	GLN	ALA
ARG	GLU	GLN	THR	LYS	THR	ALA	ARG	GLY	GLU
THR	LYS	THR	ALA	ILE	GLN	GLY	LEU	ARG	GLN
THR	GLY	LEU	LEU	THR	VAL	GLY	GLY	LEU	VAL
THR	THR	VAL	GLN	GLN	GLY	GLU	LEU	THR	ASP
THR	GLY	VAL	ASP	THR	GLN	VAL	GLU	GLY	VAL
THR	LEU	THR	VAL	THR	GLY	VAL	GLN	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

● Molecule 19: Coiled-coil domain containing 114



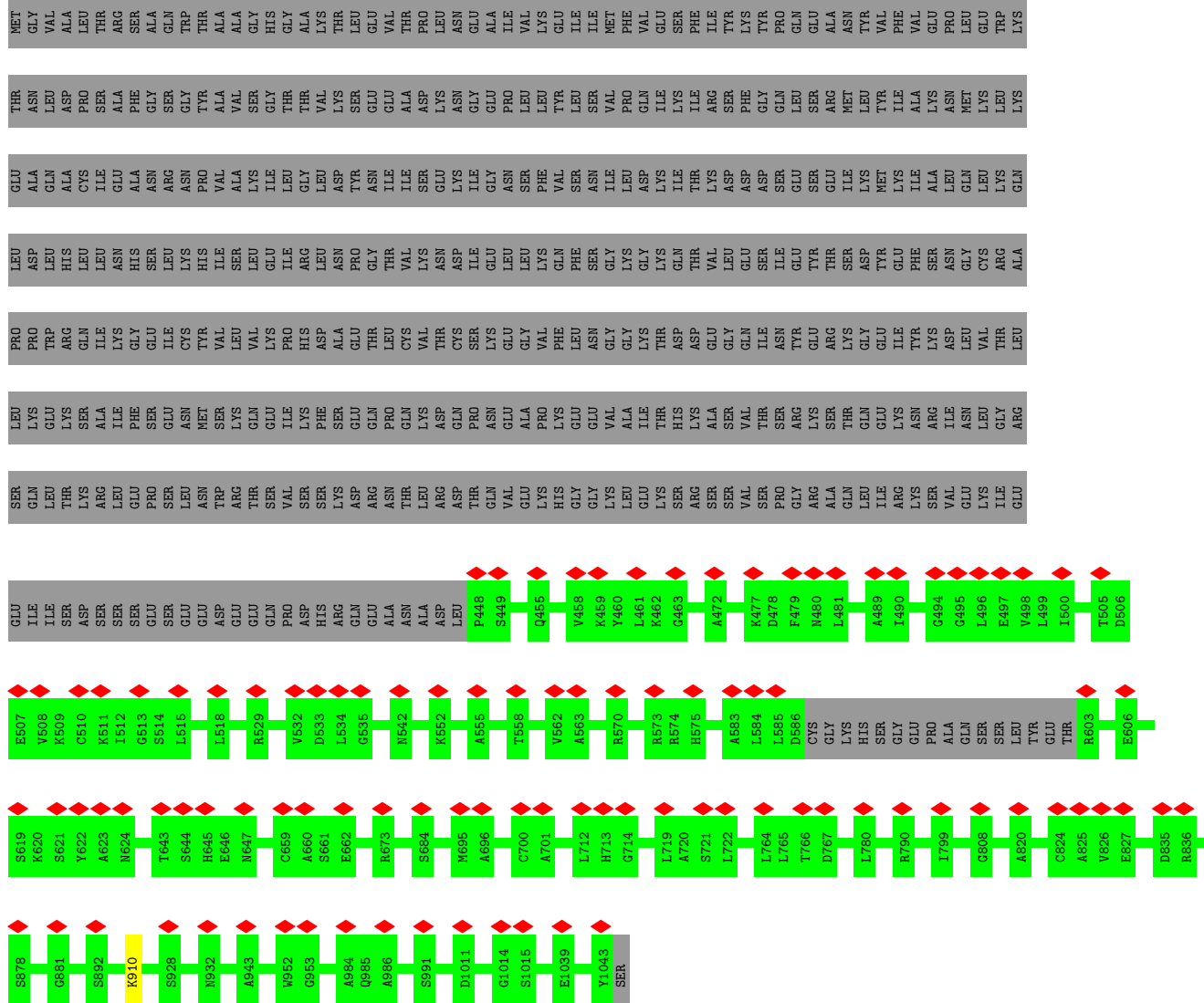
Residue ID	Residue Name	Residue Name	Residue Name	Residue Name	Residue Name	Residue Name	Residue Name	Residue Name	Residue Name
MET	PRO	PHE	GLY	GLN	ALA	GLY	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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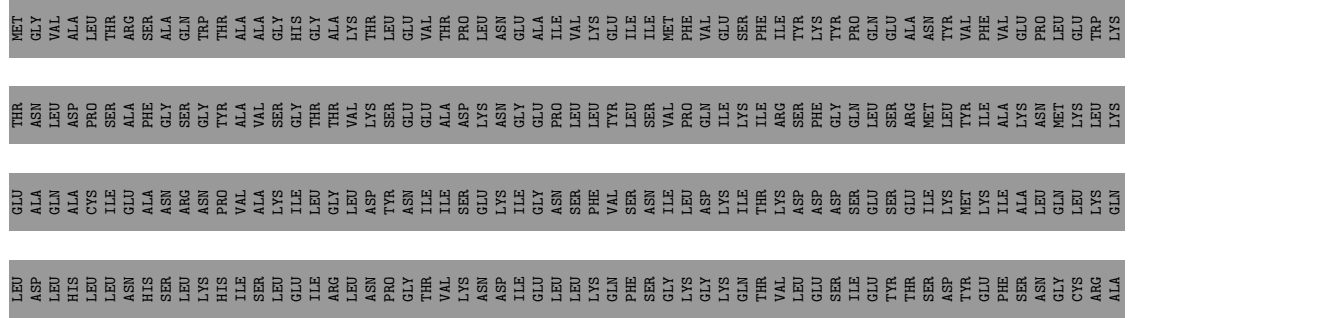


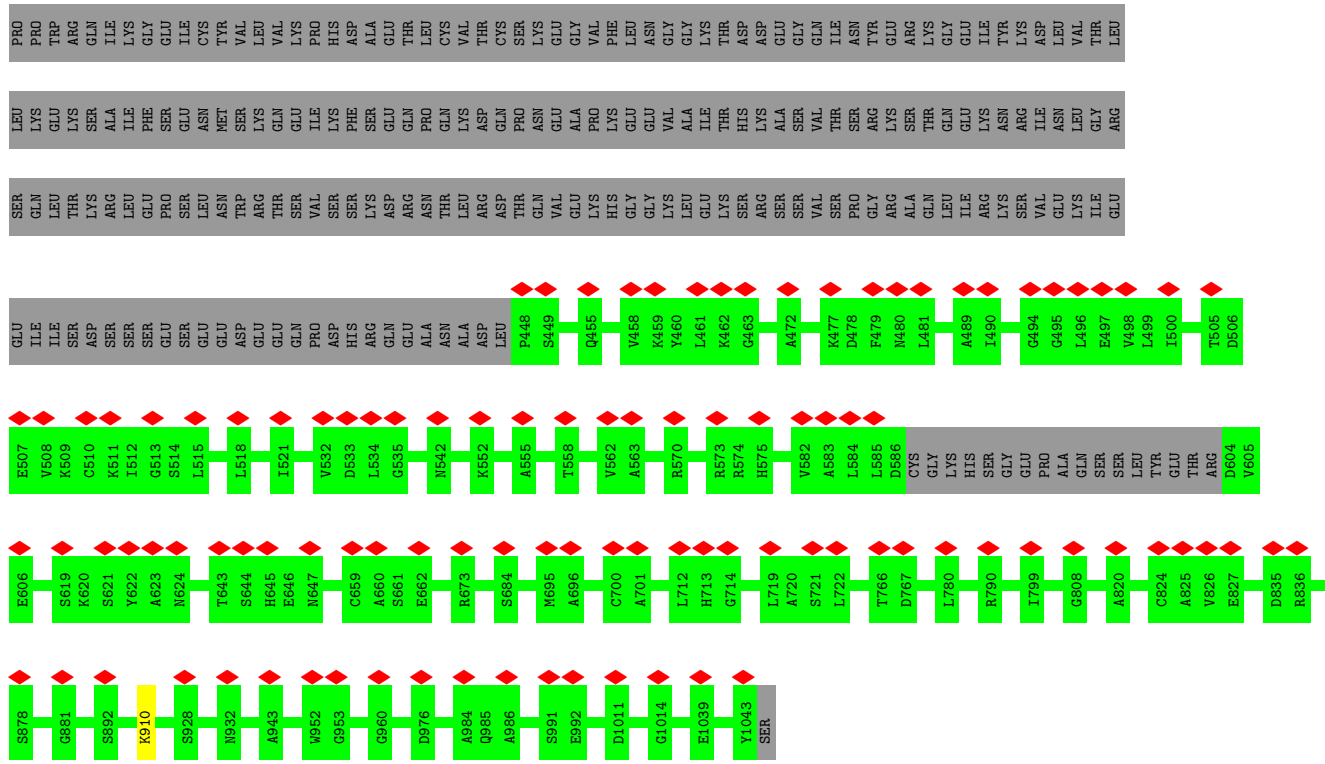


● Molecule 21: Armadillo repeat containing 4

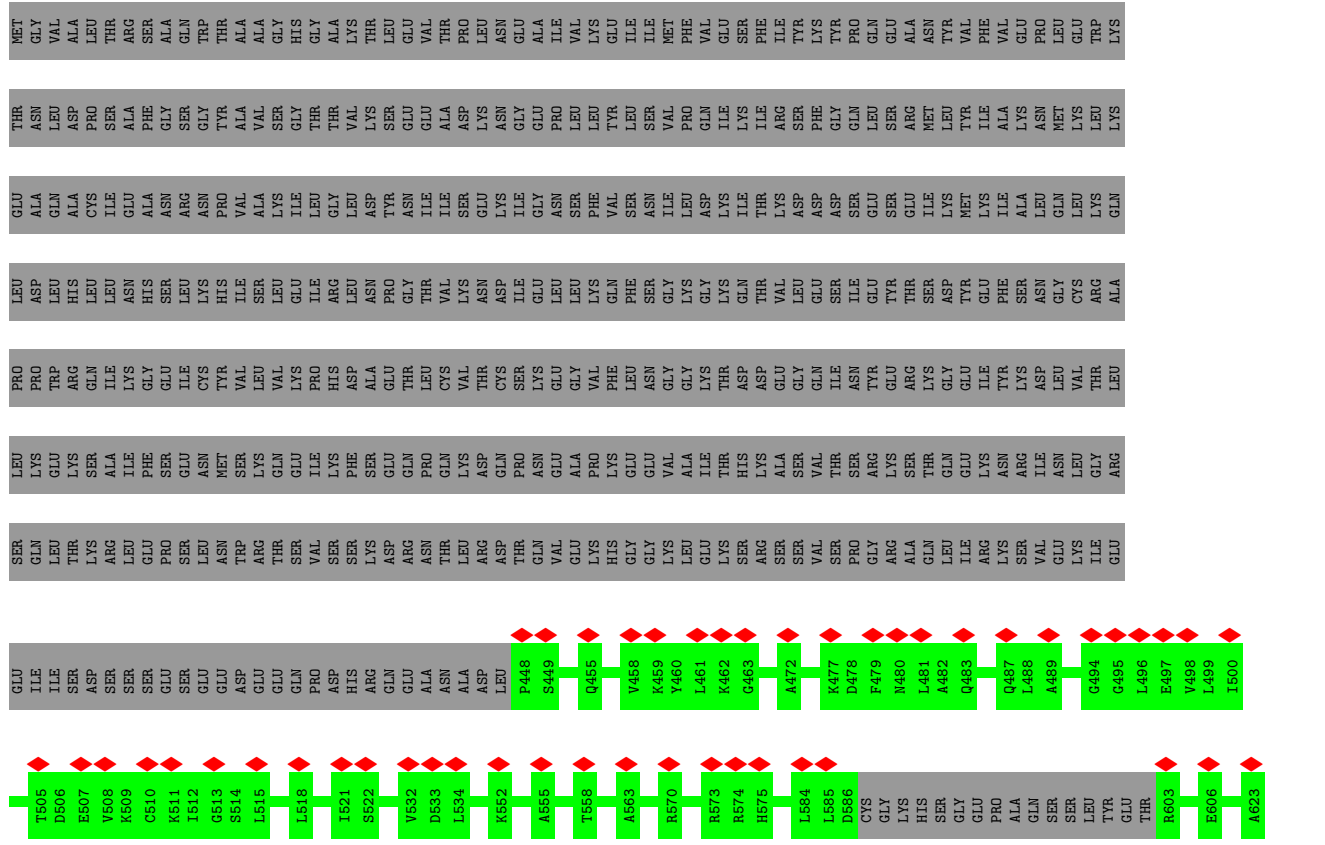


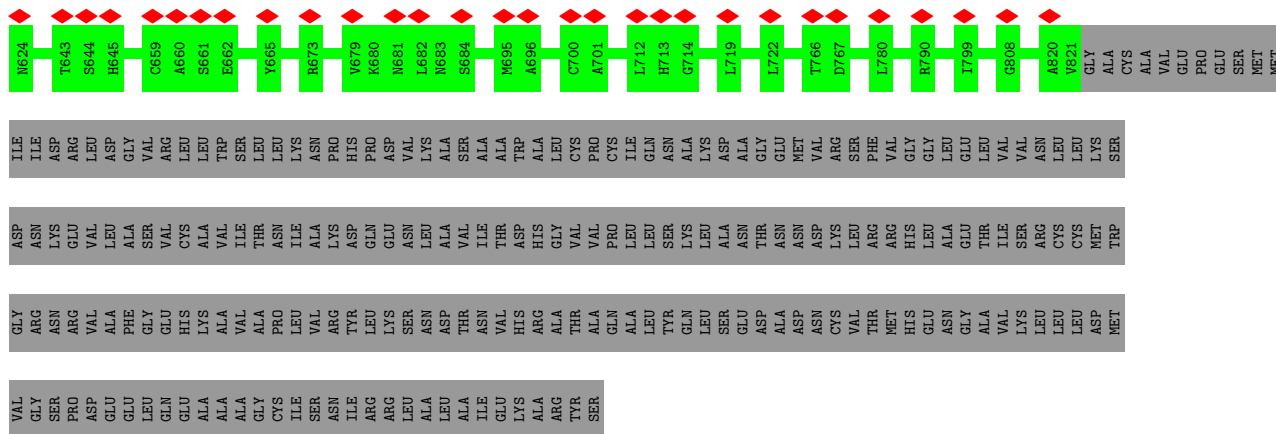
● Molecule 21: Armadillo repeat containing 4



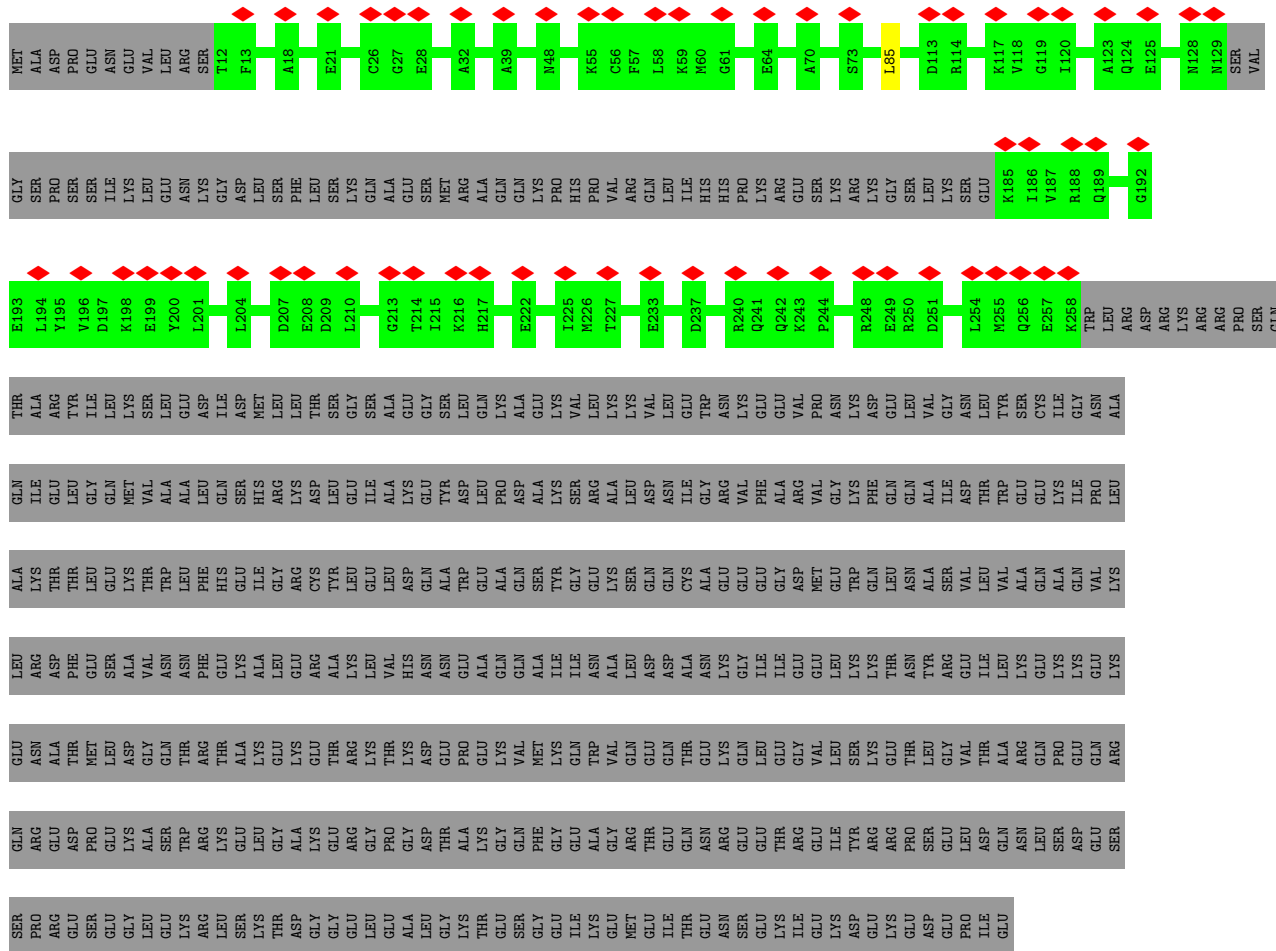


● Molecule 21: Armadillo repeat containing 4



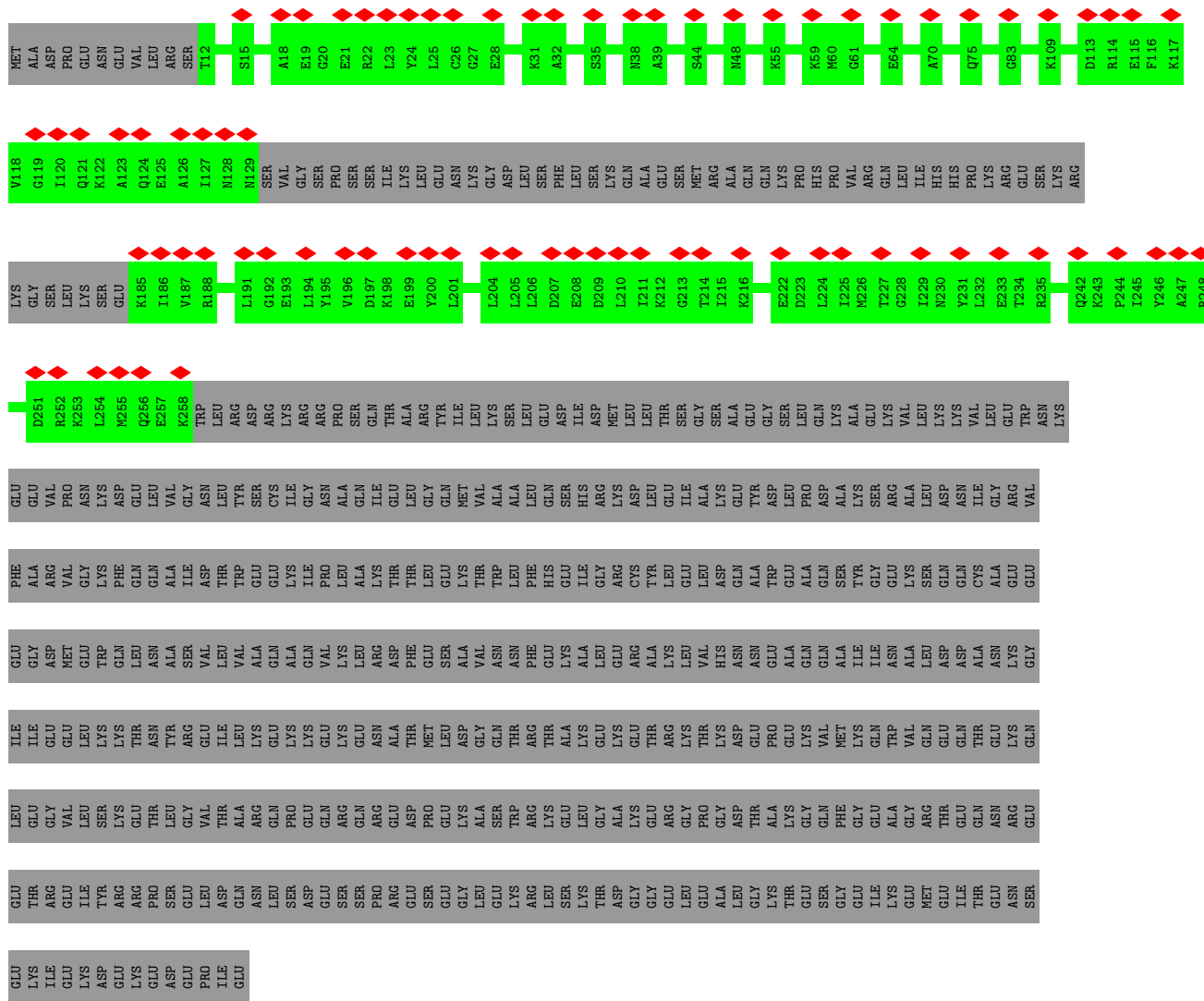


• Molecule 22: TTC25 protein

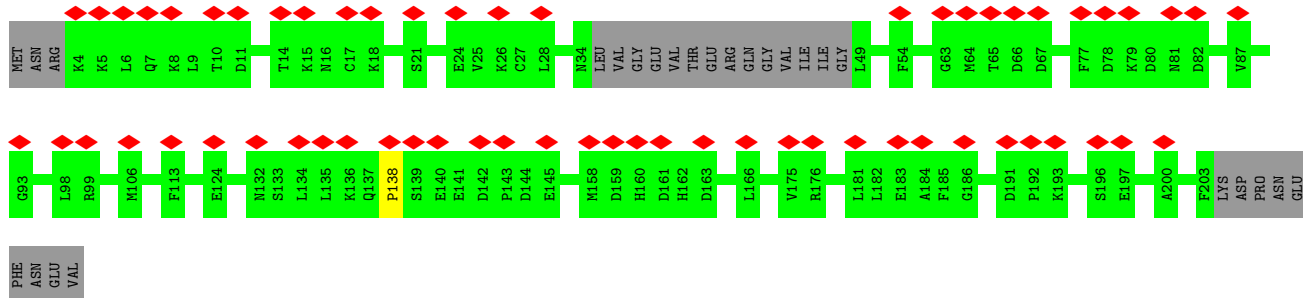
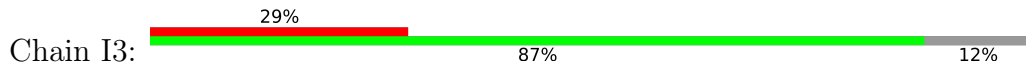


• Molecule 22: TTC25 protein

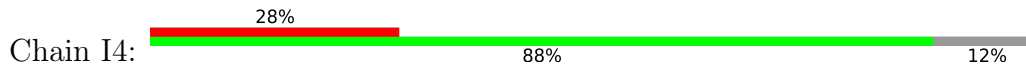


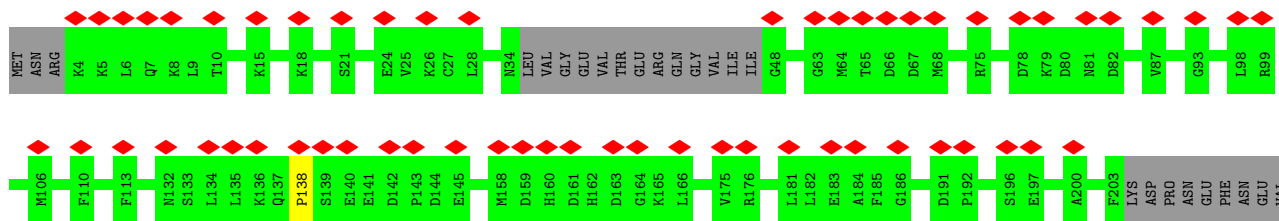


• Molecule 23: EF-hand calcium-binding domain-containing protein 1

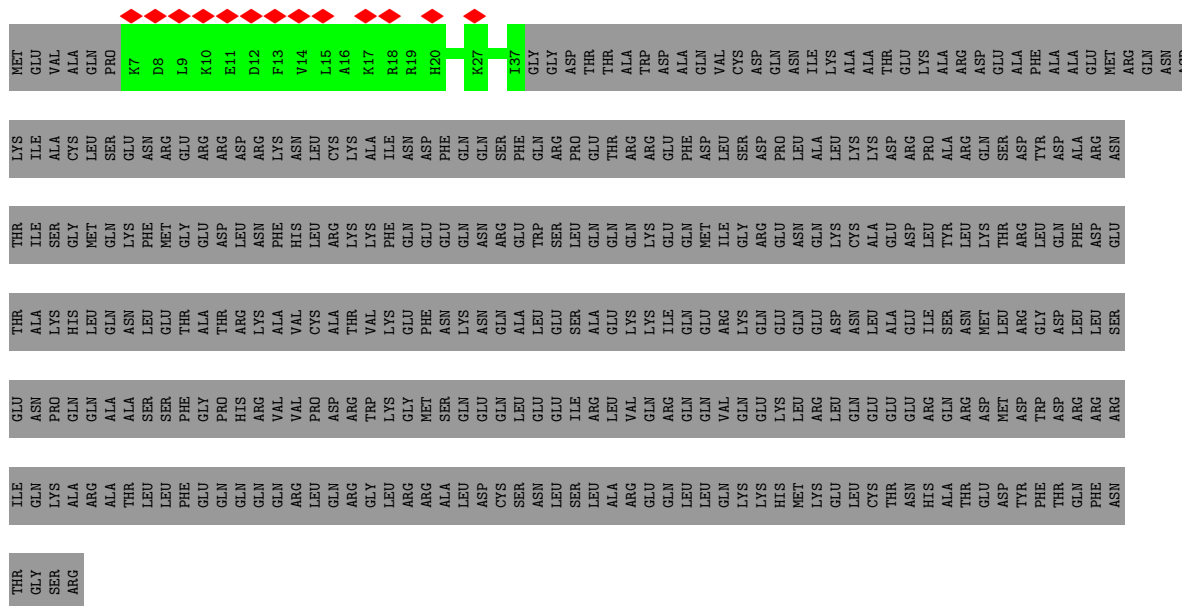


• Molecule 23: EF-hand calcium-binding domain-containing protein 1

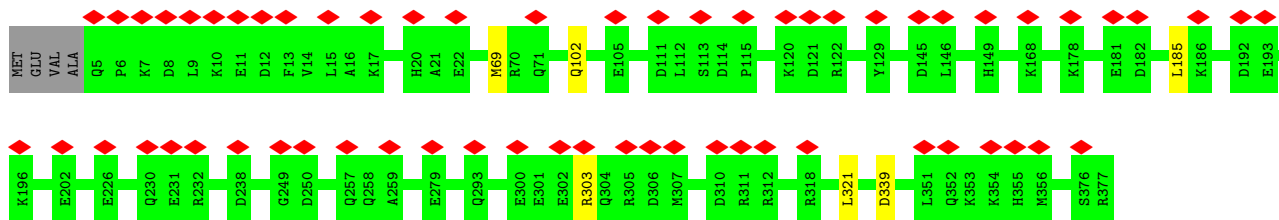




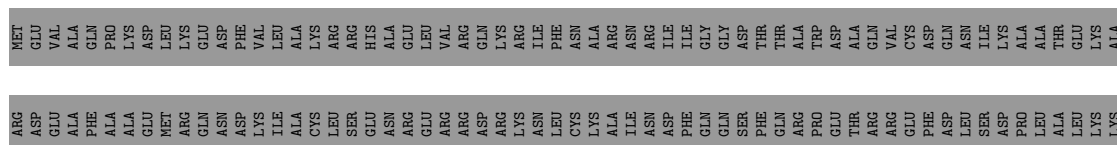
• Molecule 24: RIB43A-like with coiled-coils protein 2

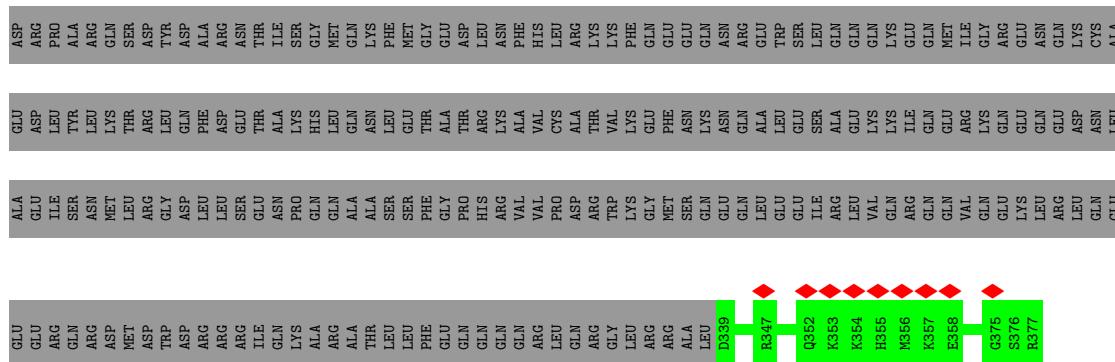


• Molecule 24: RIB43A-like with coiled-coils protein 2

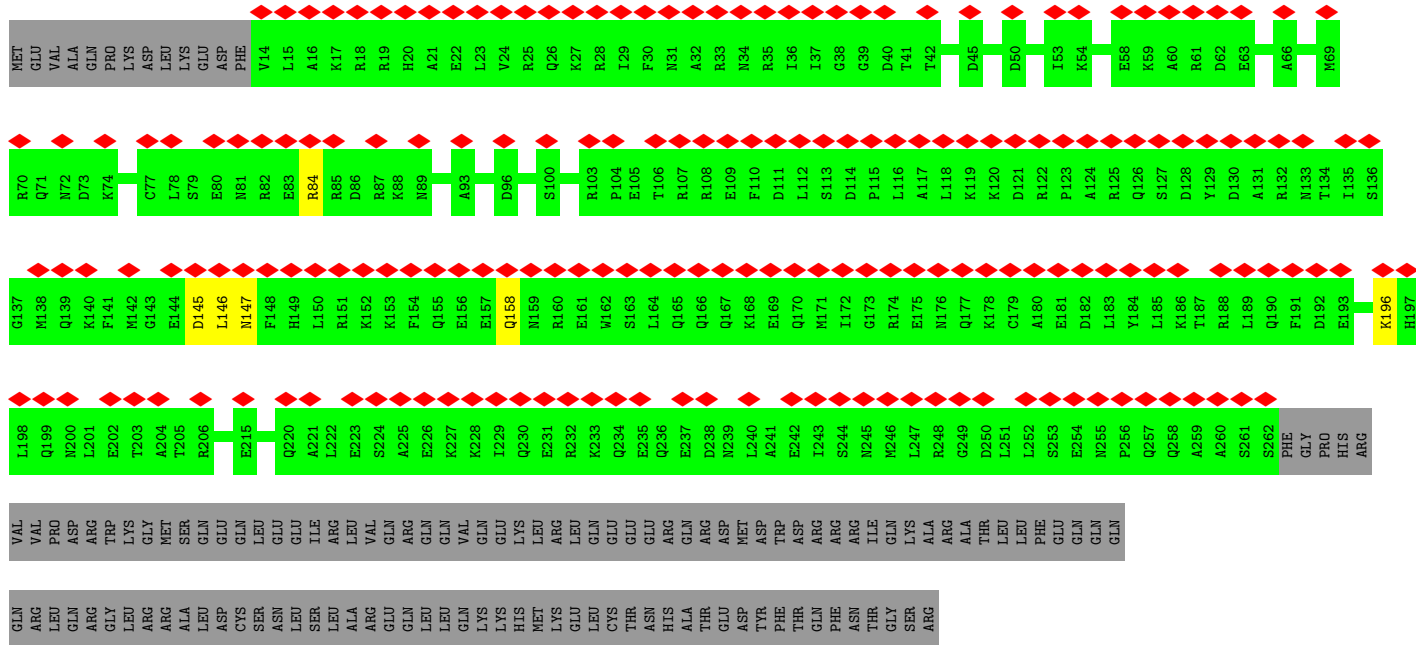


• Molecule 24: RIB43A-like with coiled-coils protein 2

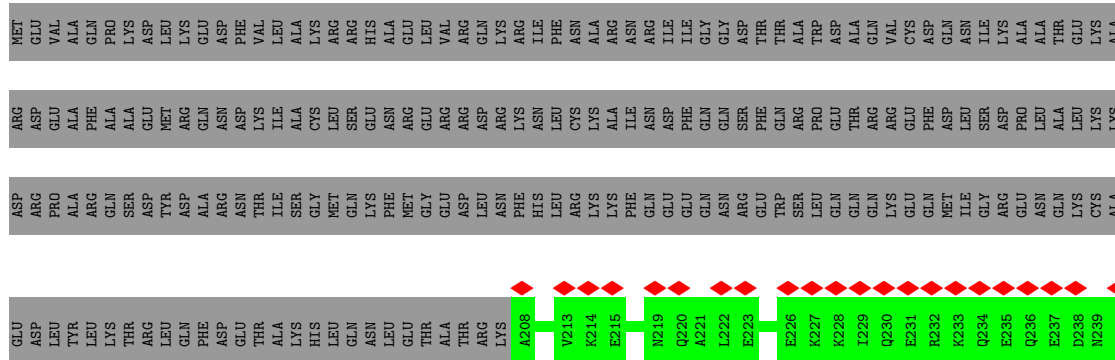




● Molecule 24: RIB43A-like with coiled-coils protein 2

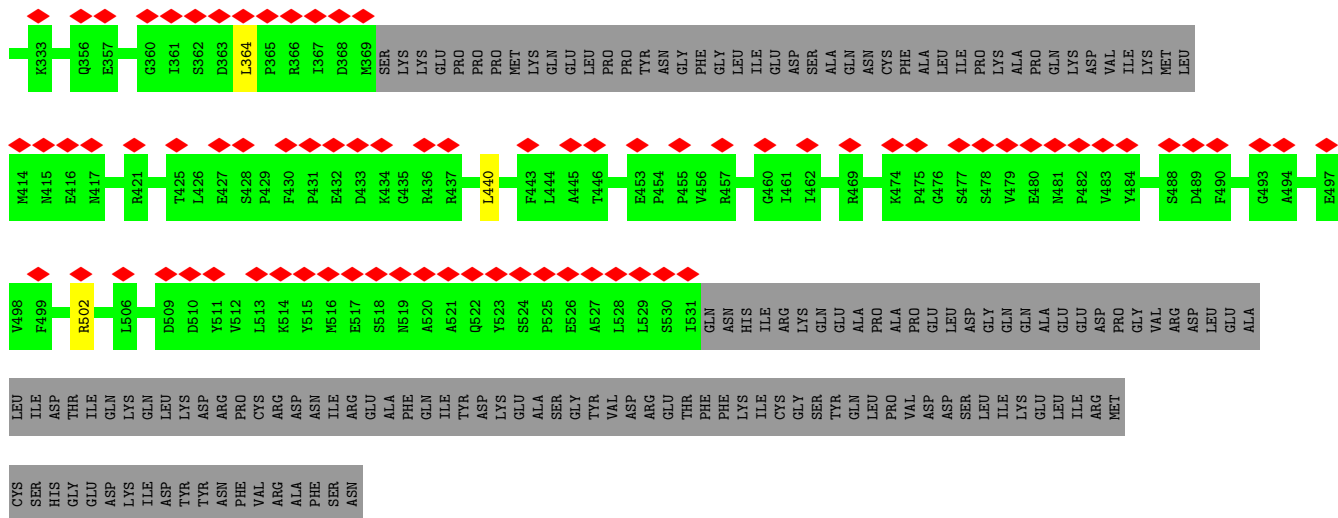


● Molecule 24: RIB43A-like with coiled-coils protein 2

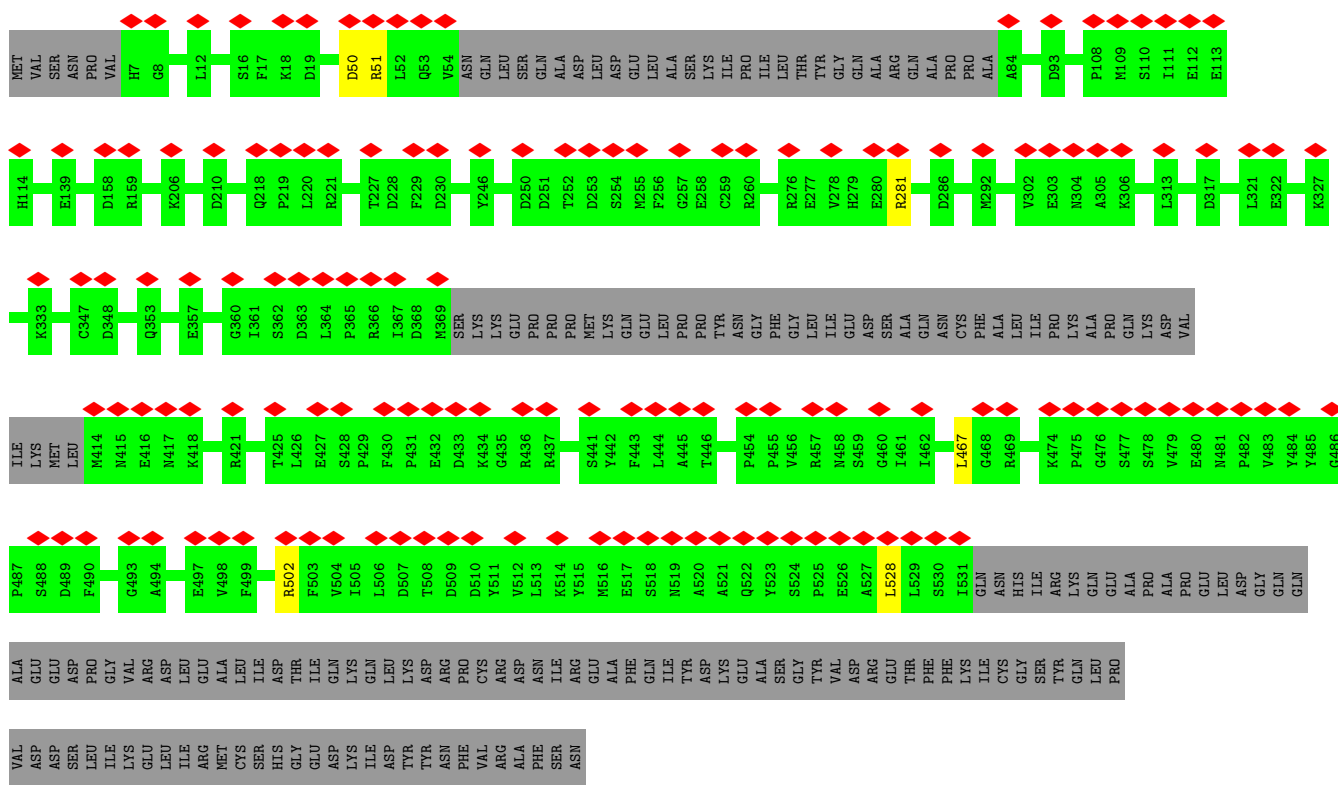




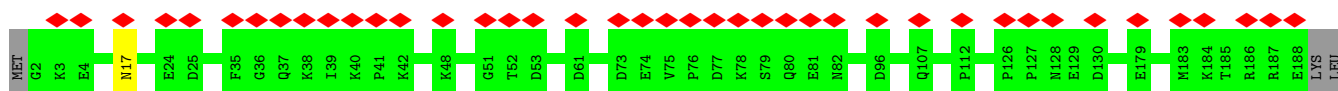
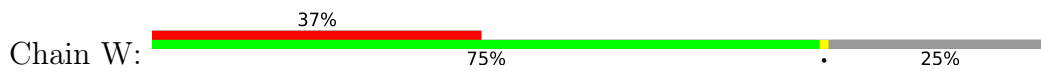


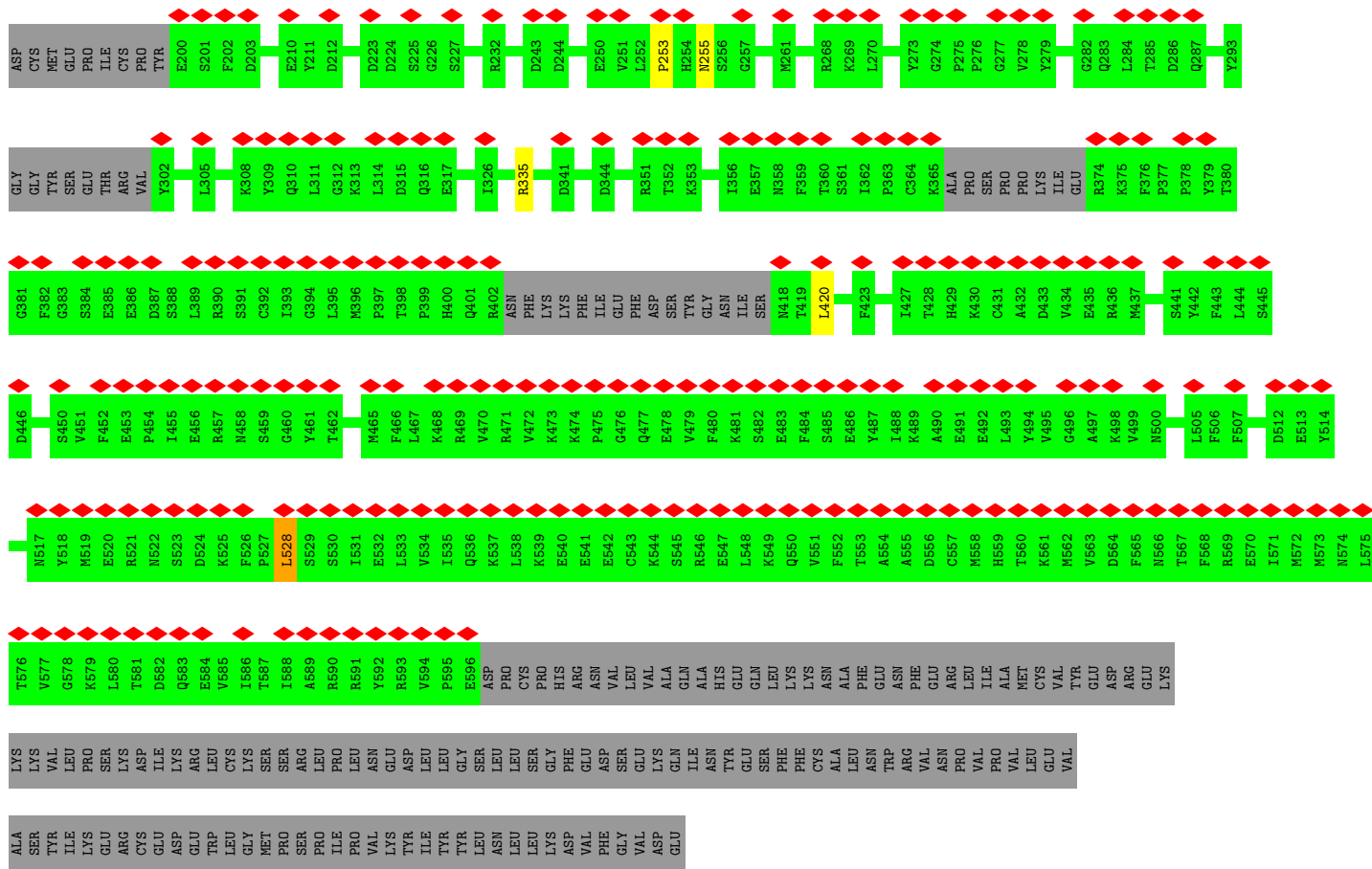


• Molecule 25: EF-hand domain containing 1

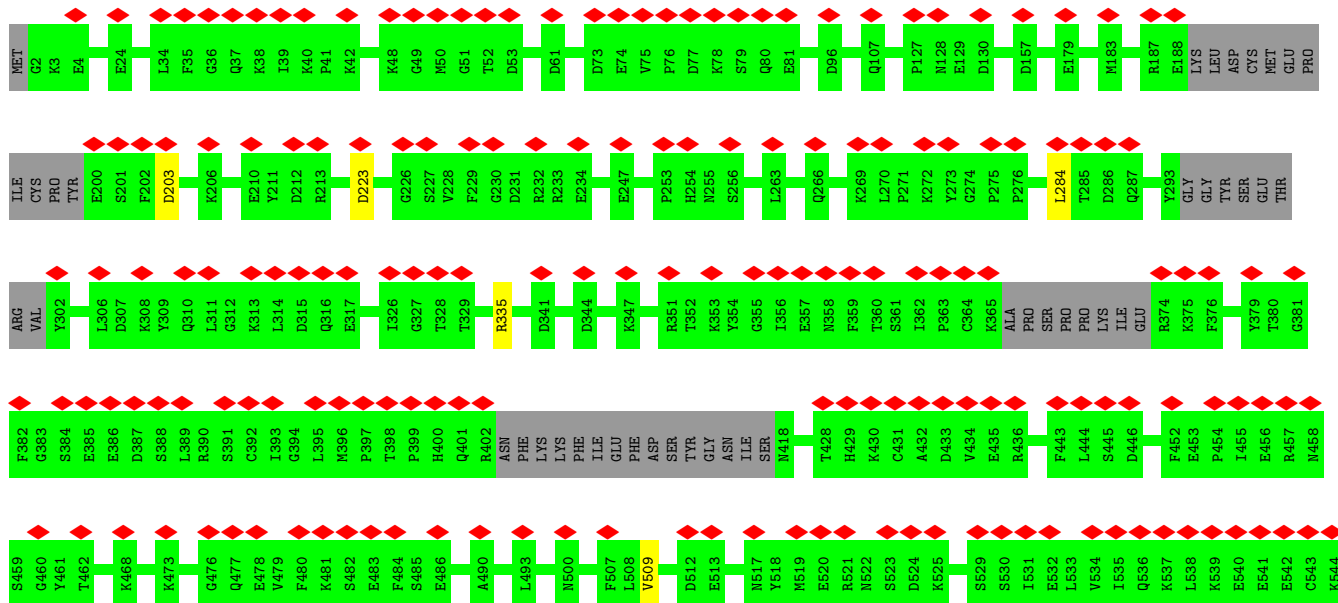
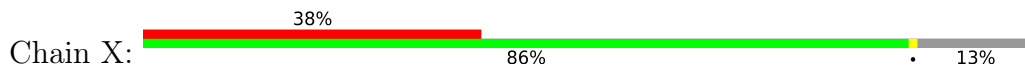


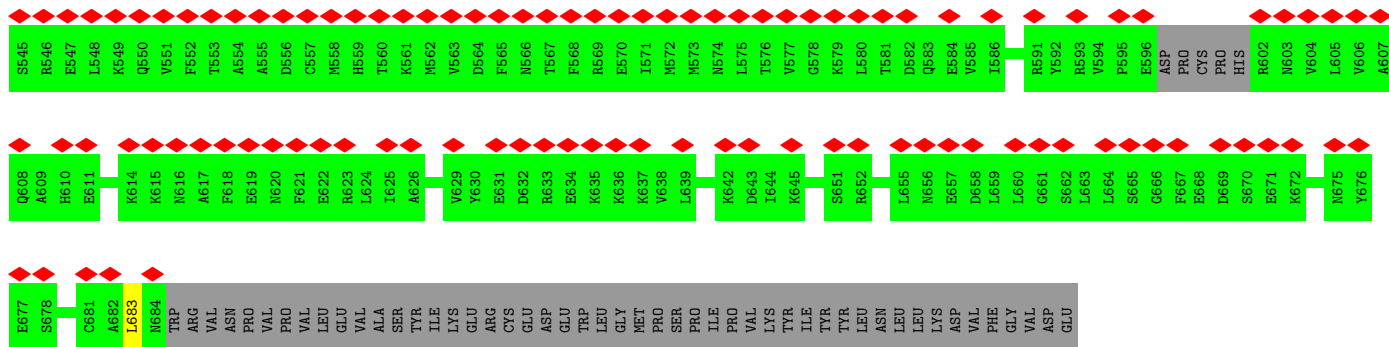
• Molecule 26: EFHC2



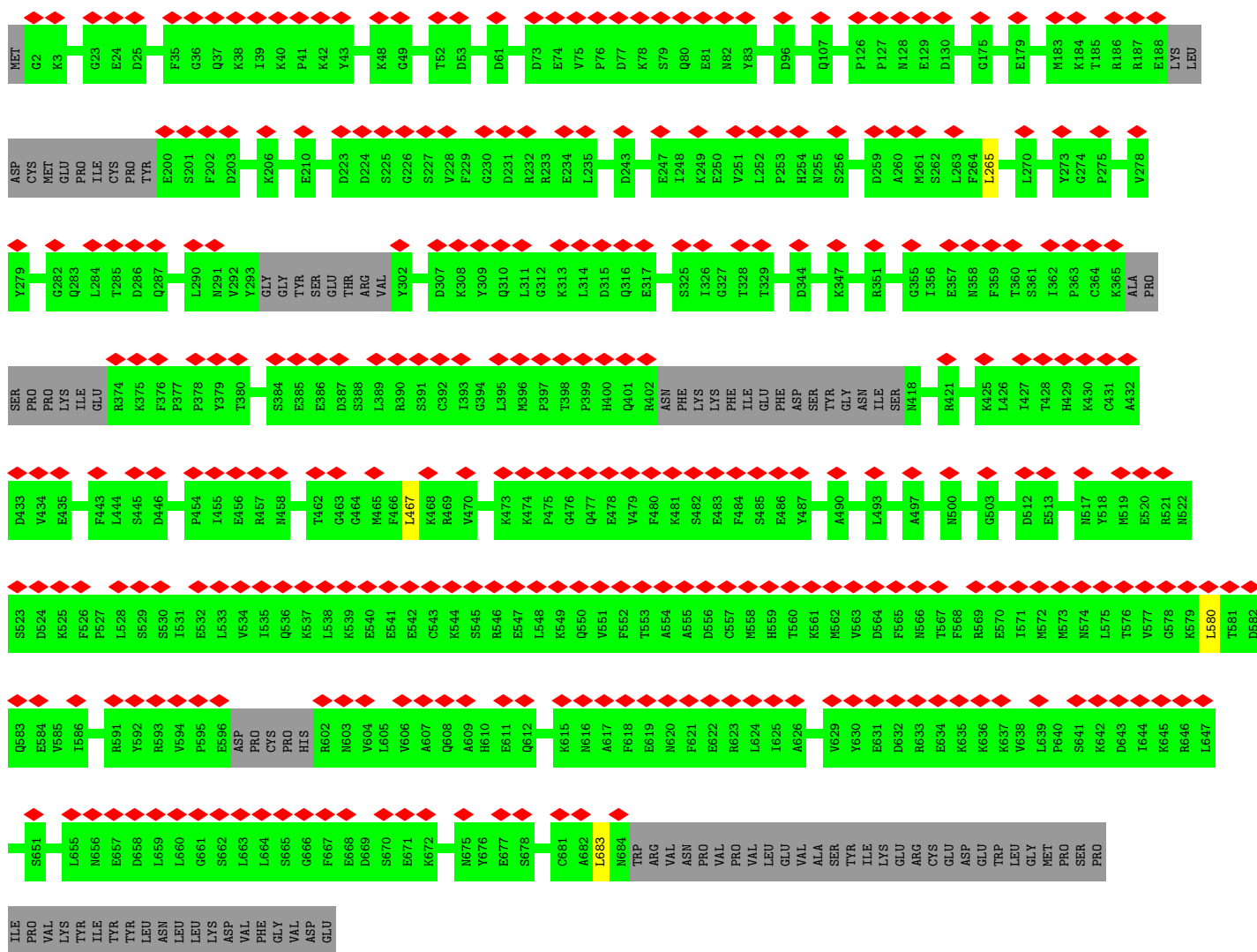
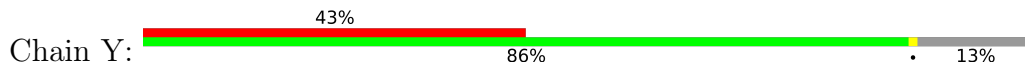


● Molecule 26: EFHC2



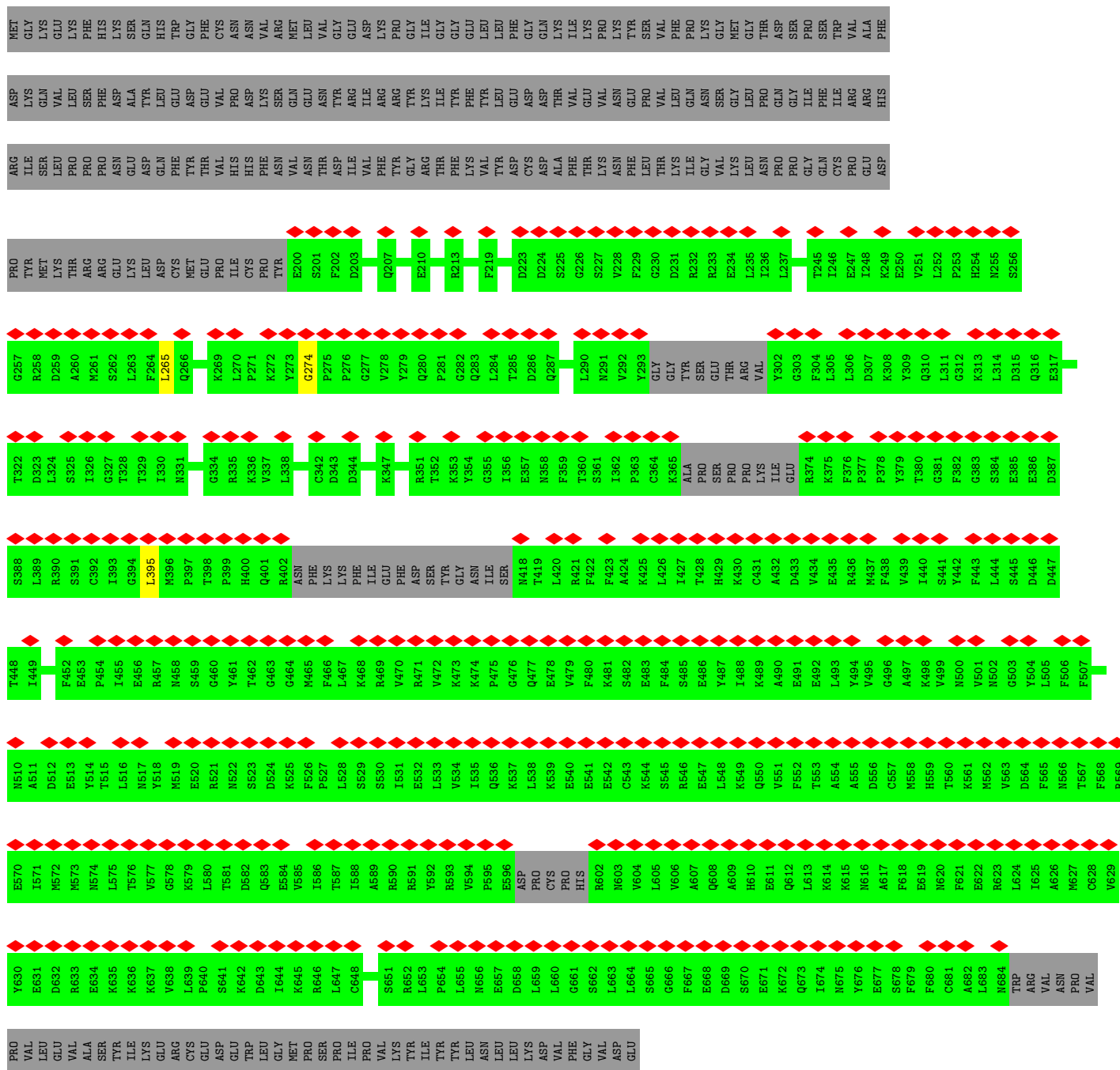


• Molecule 26: EFHC2

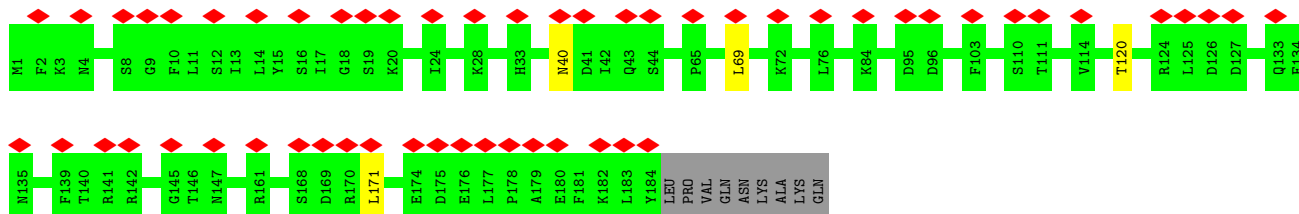


• Molecule 26: EFHC2

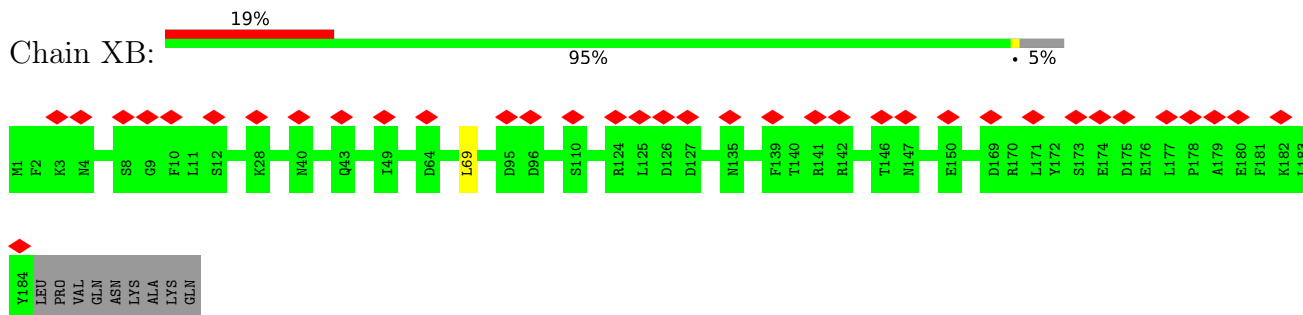




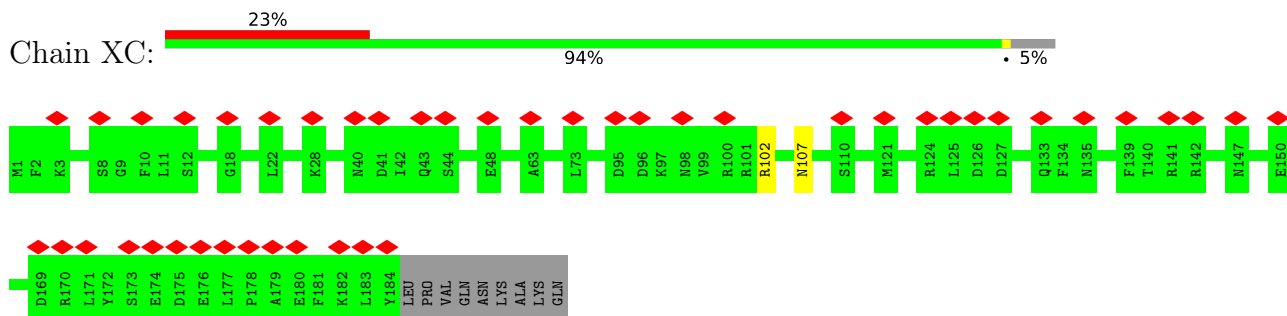
• Molecule 27: Cilia- and flagella-associated protein 20



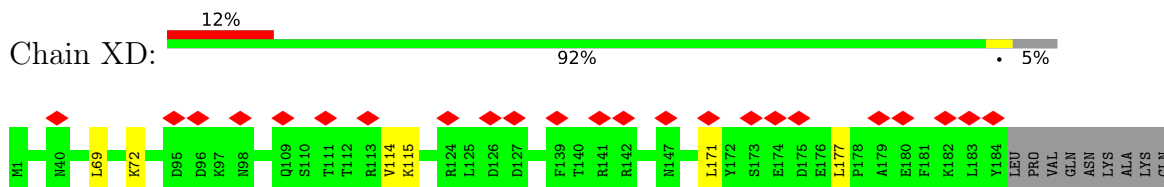
• Molecule 27: Cilia- and flagella-associated protein 20



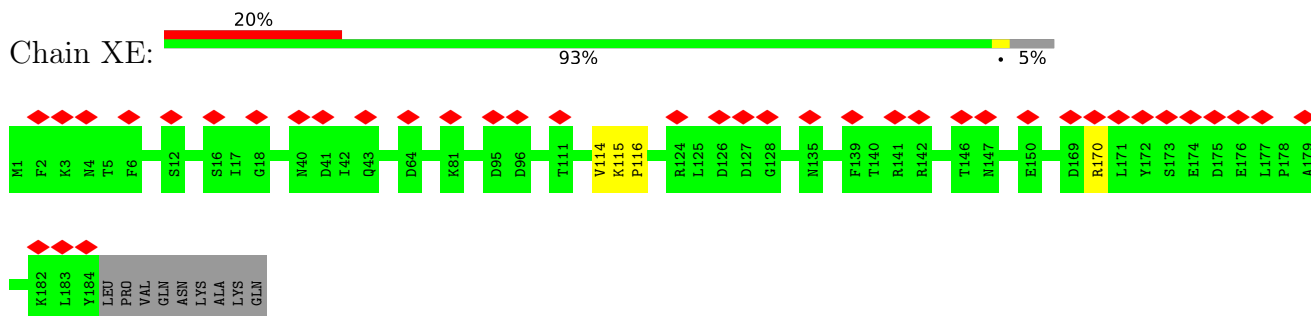
• Molecule 27: Cilia- and flagella-associated protein 20



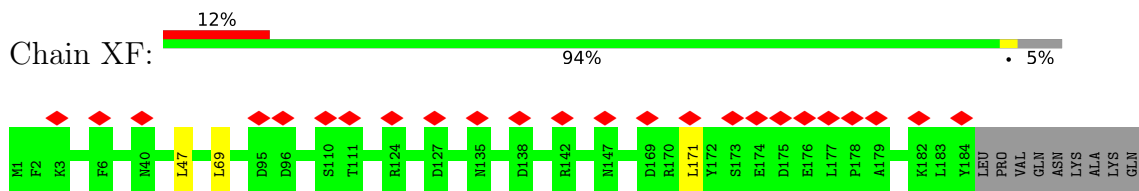
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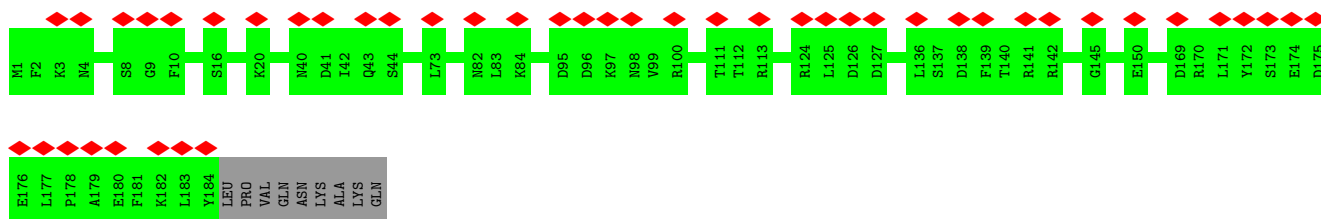
• Molecule 27: Cilia- and flagella-associated protein 20



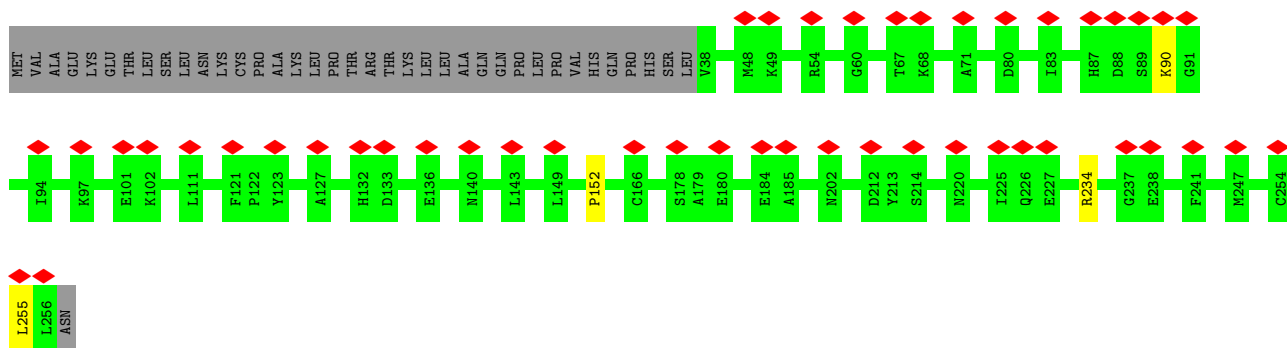
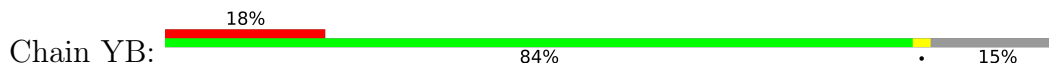
• Molecule 27: Cilia- and flagella-associated protein 20



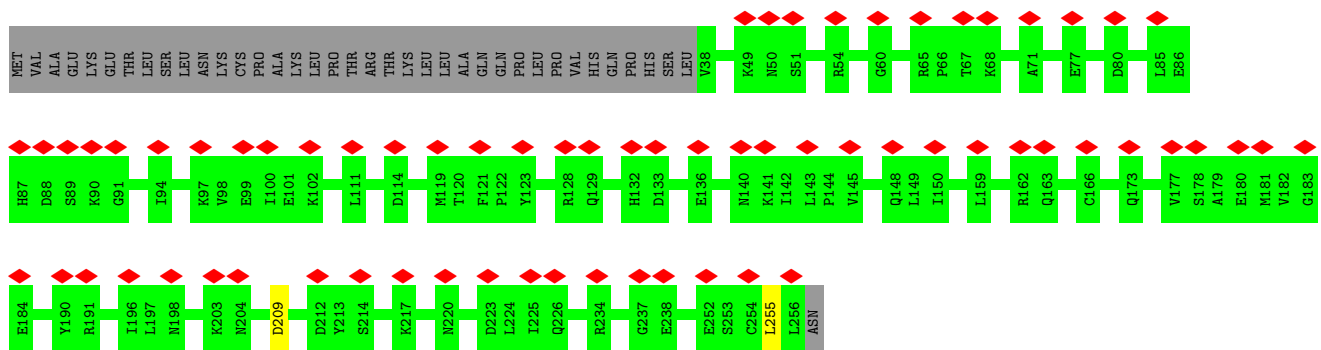
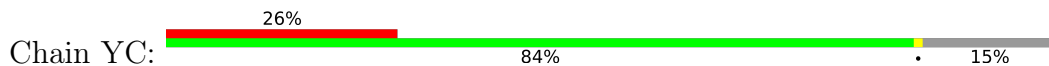
• Molecule 27: Cilia- and flagella-associated protein 20



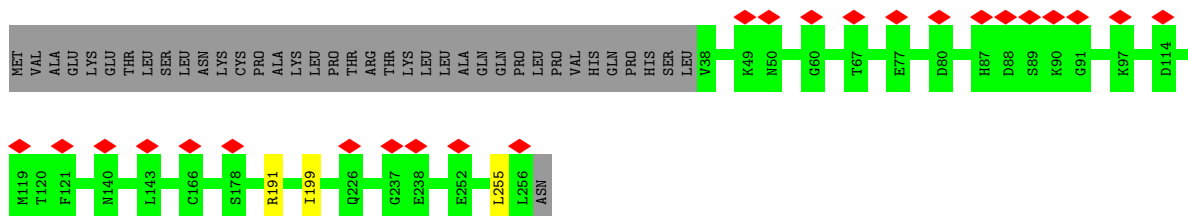
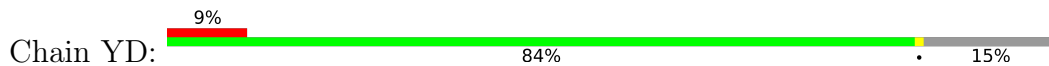
• Molecule 28: PACRG protein



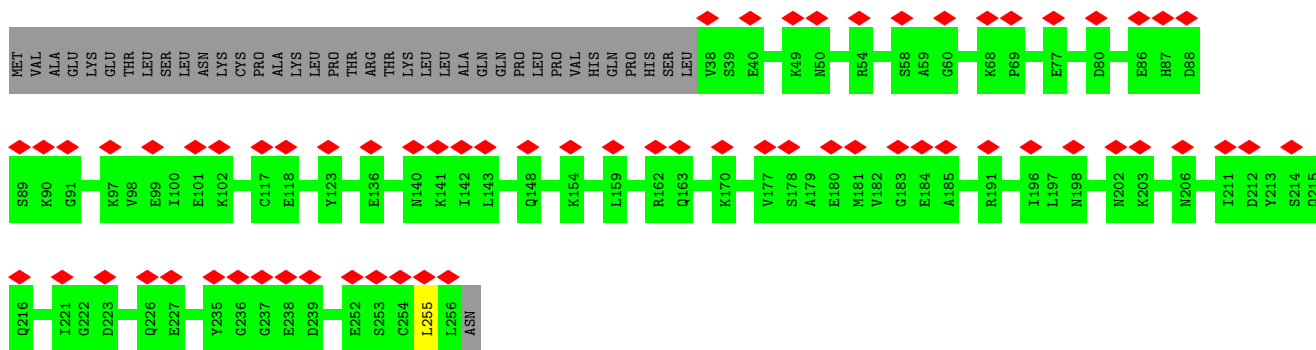
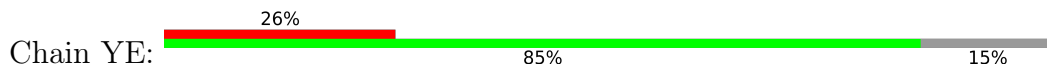
• Molecule 28: PACRG protein



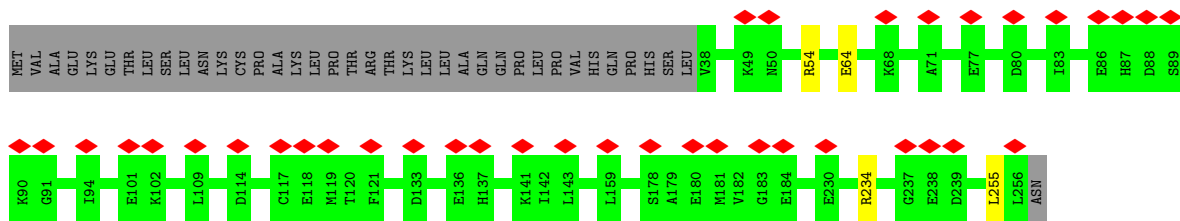
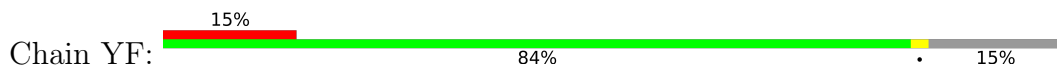
• Molecule 28: PACRG protein



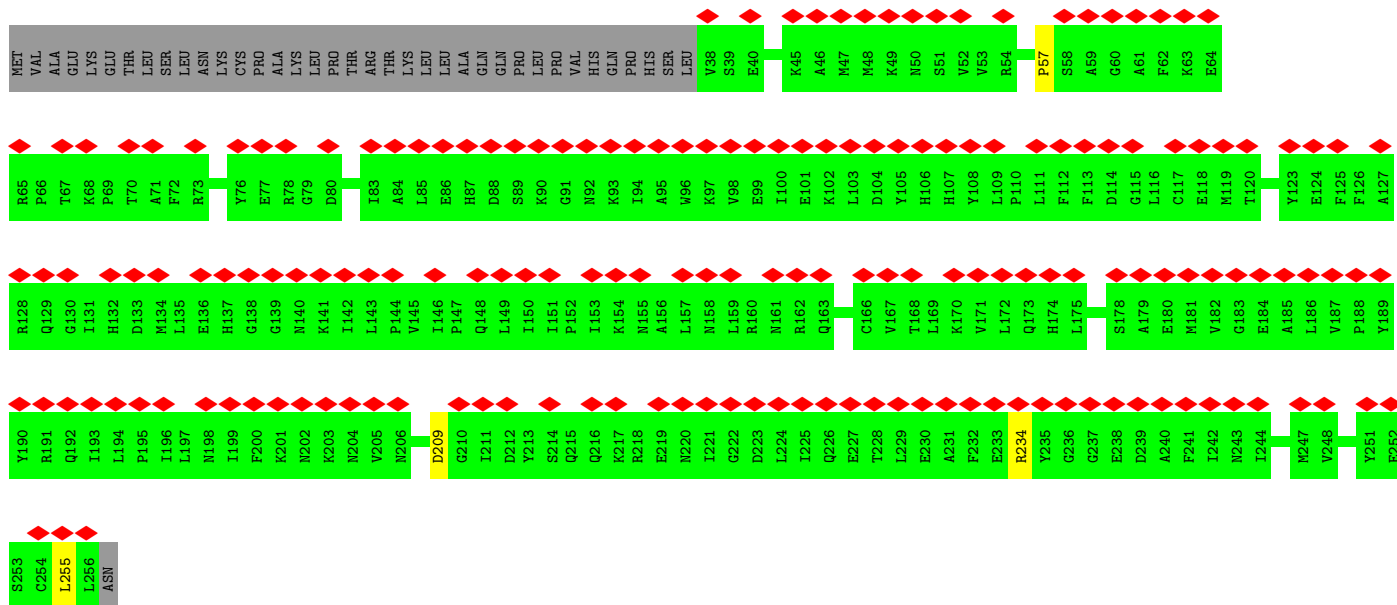
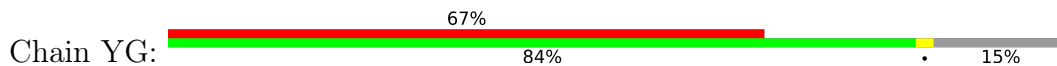
• Molecule 28: PACRG protein



• Molecule 28: PACRG protein



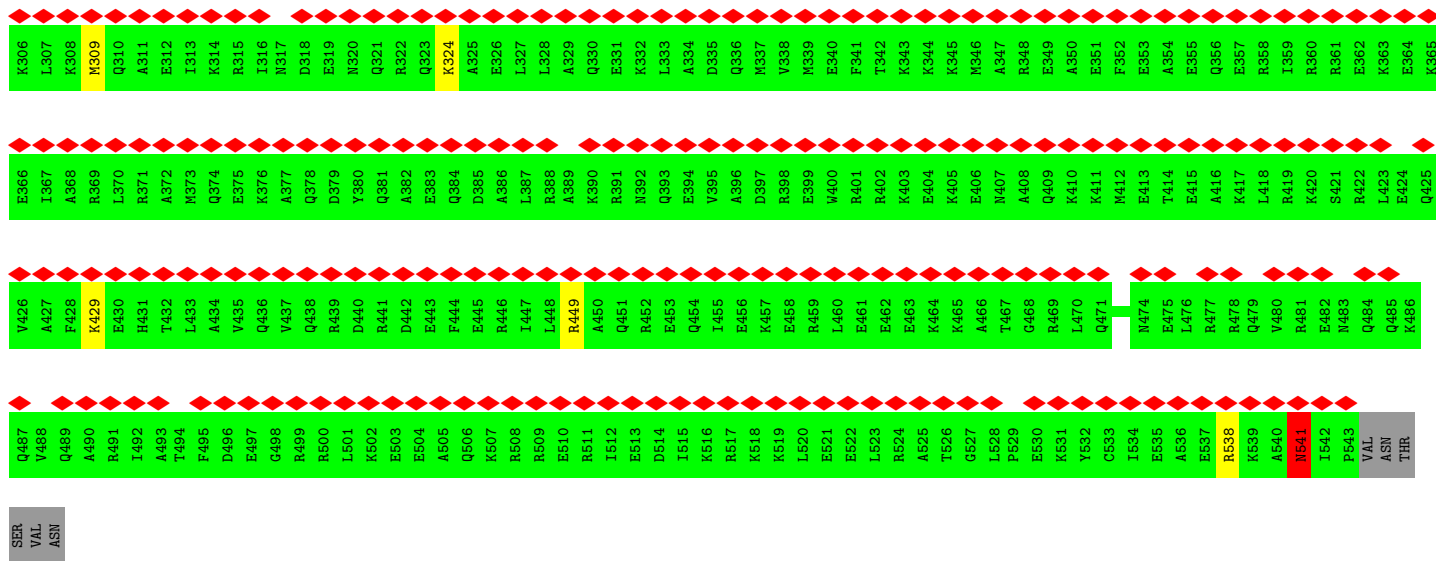
• Molecule 28: PACRG protein



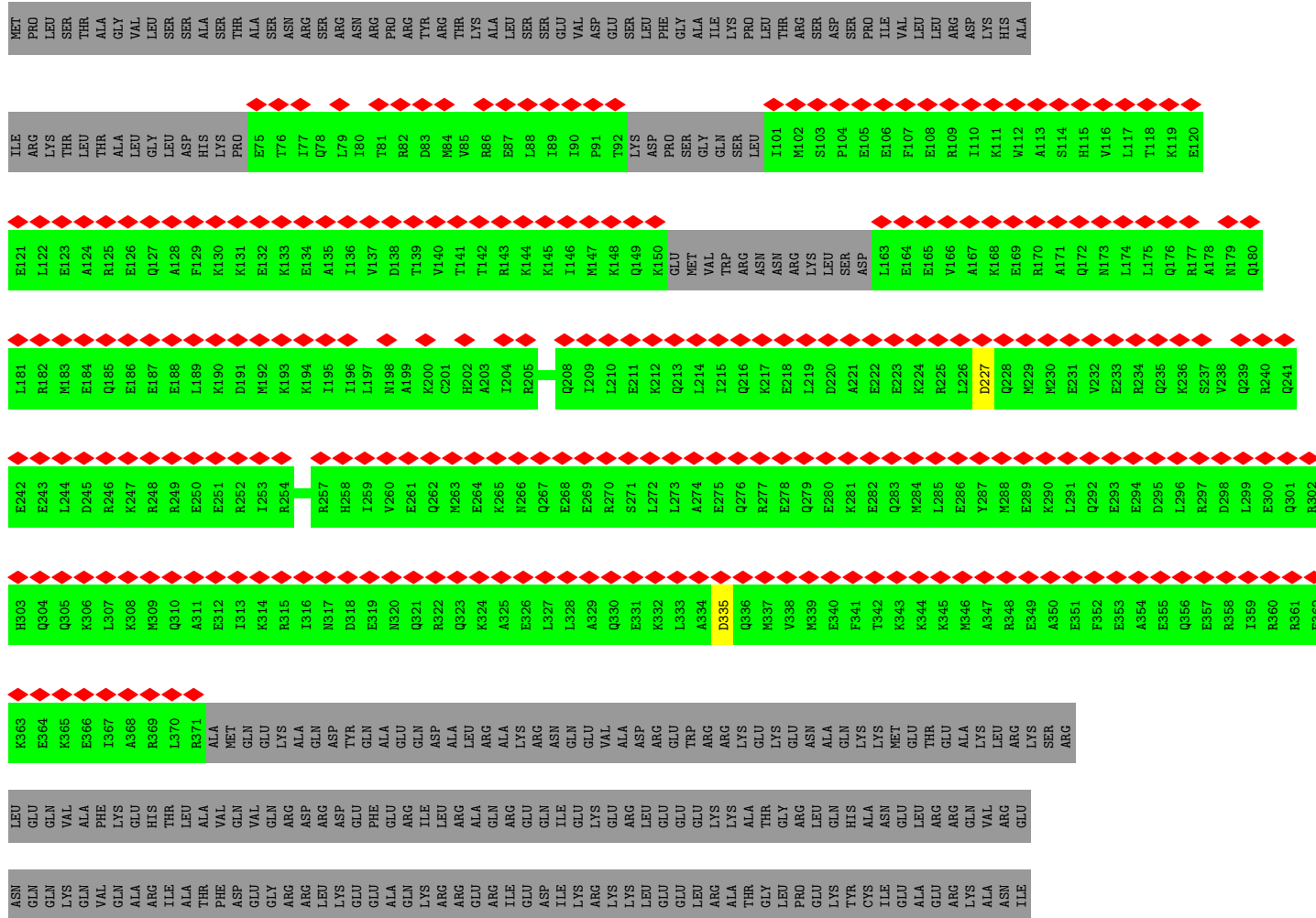
• Molecule 29: Cilia and flagella associated protein 45



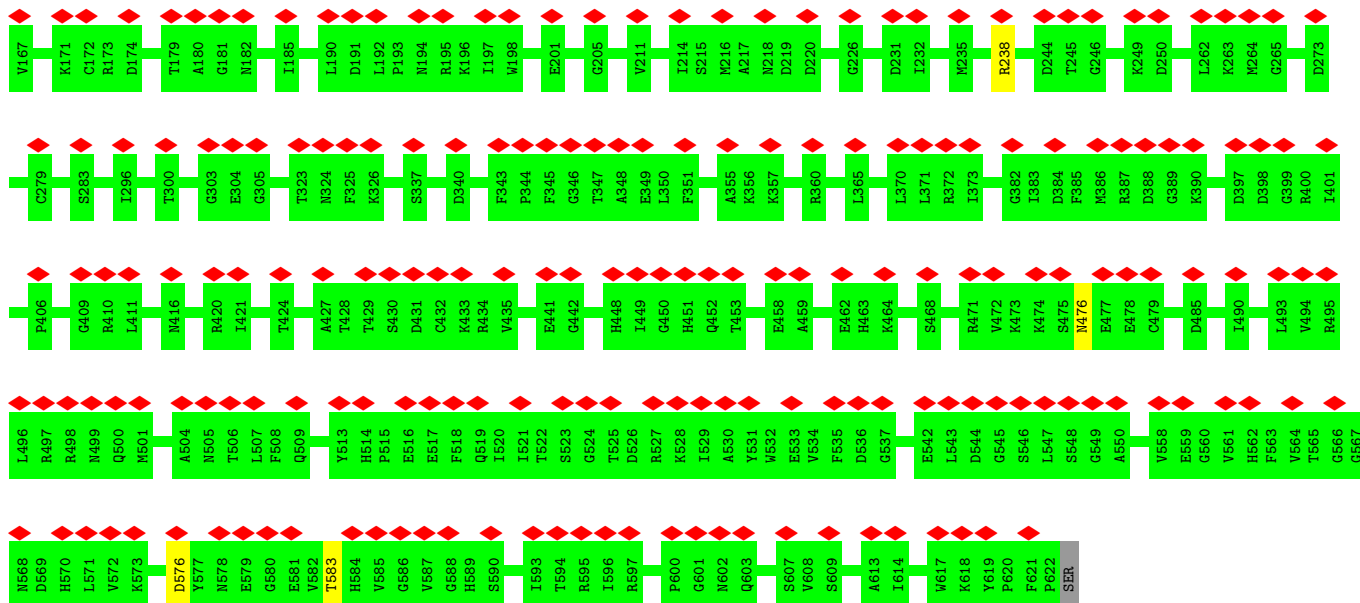




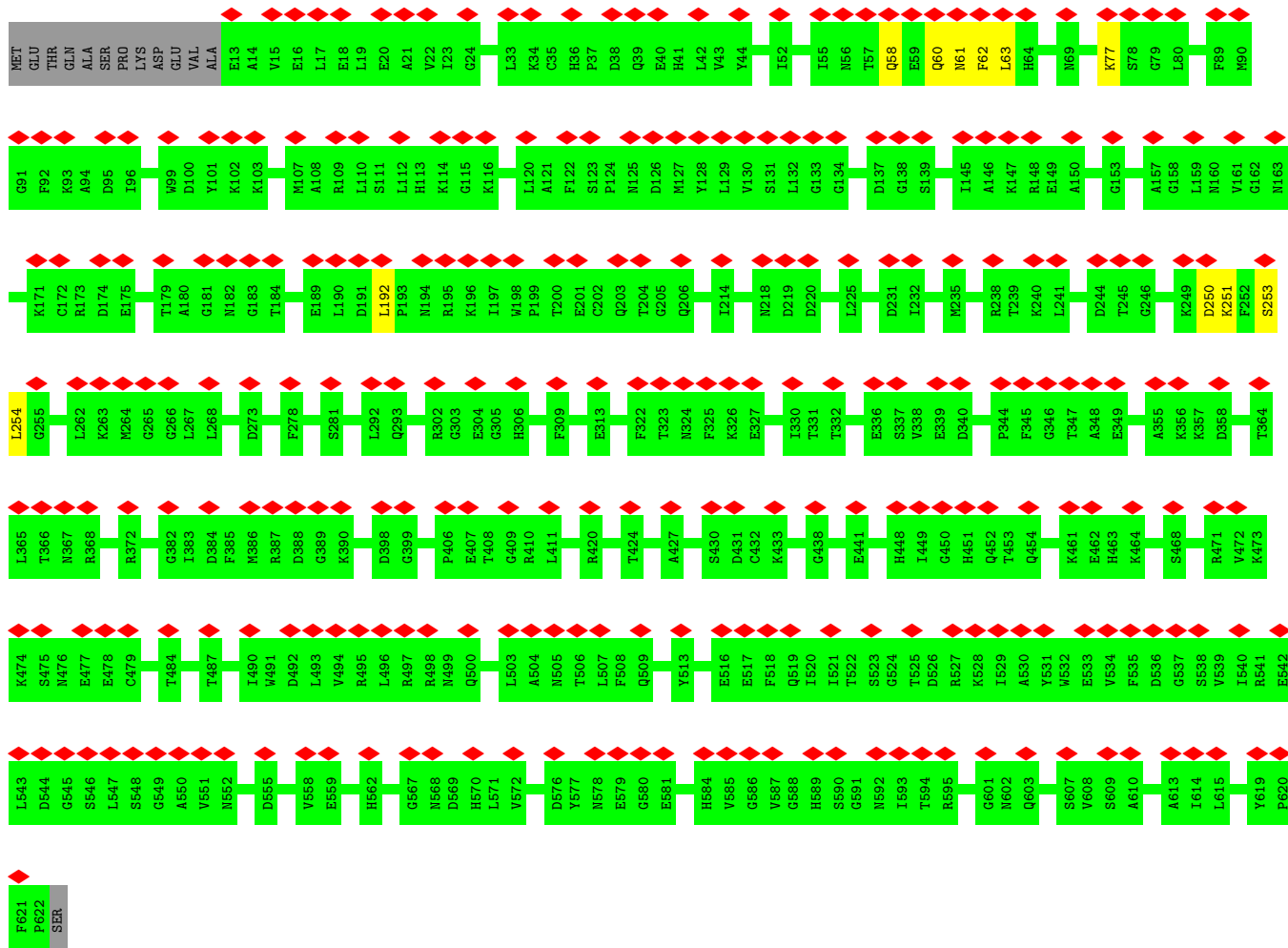
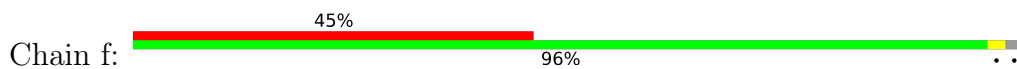
● Molecule 29: Cilia and flagella associated protein 45







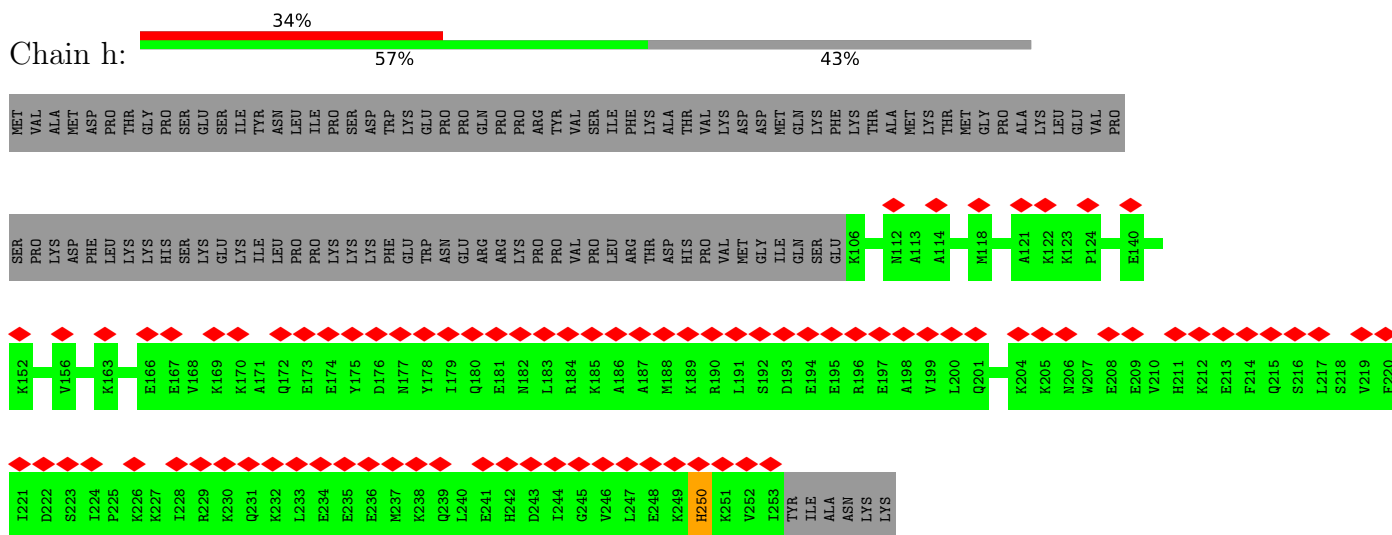
• Molecule 30: Cilia and flagella associated protein 52



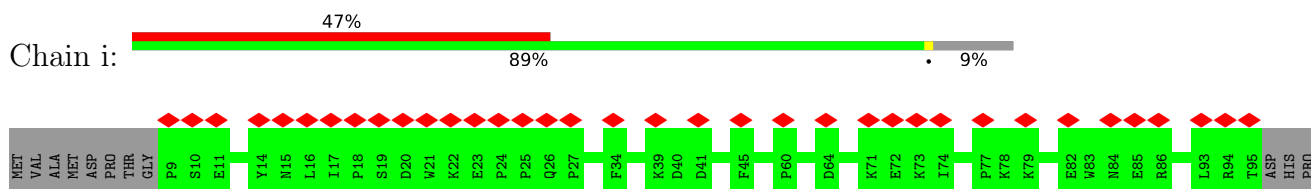
• Molecule 30: Cilia and flagella associated protein 52

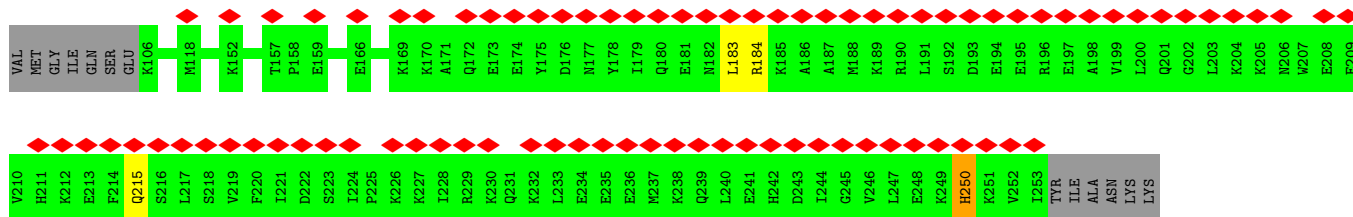


• Molecule 31: Enkurin, TRPC channel interacting protein

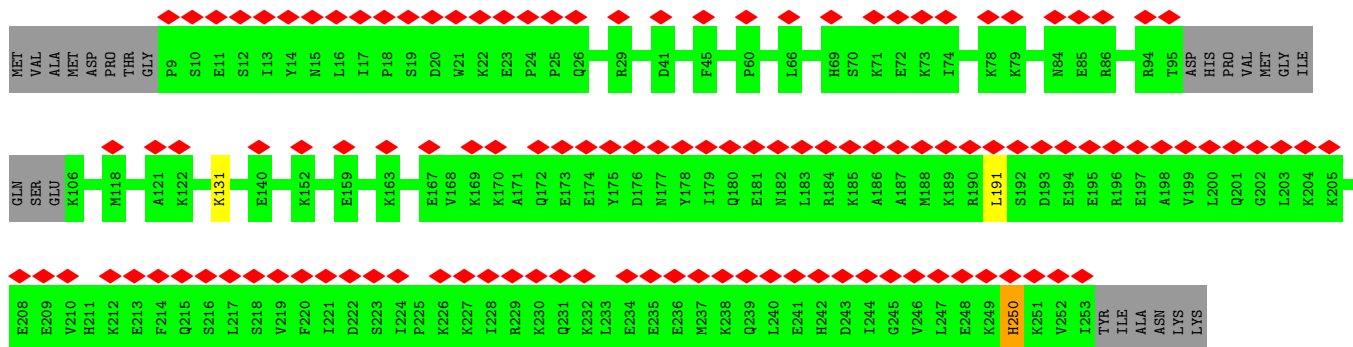
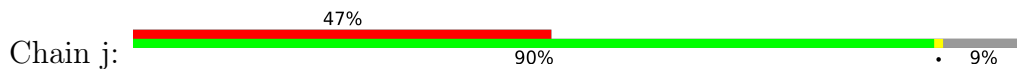


• Molecule 31: Enkurin, TRPC channel interacting protein

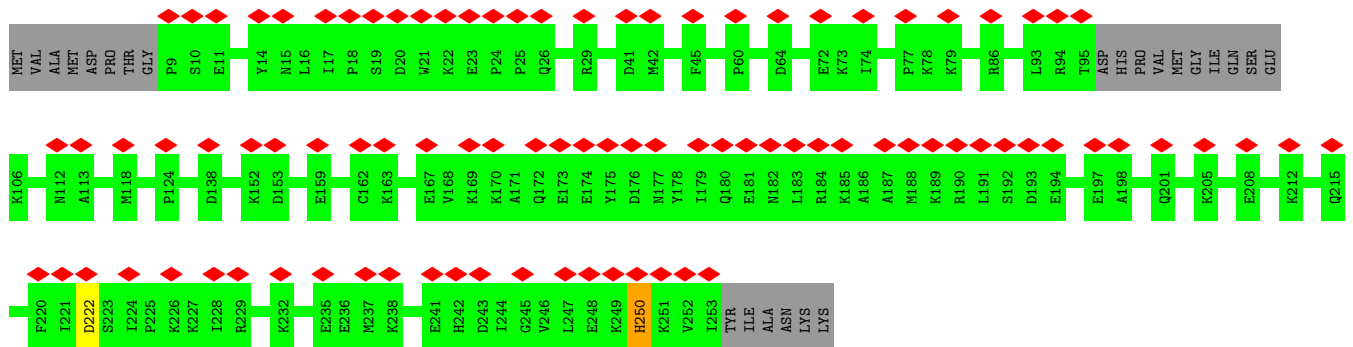
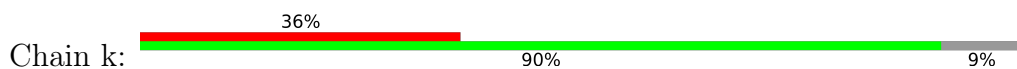




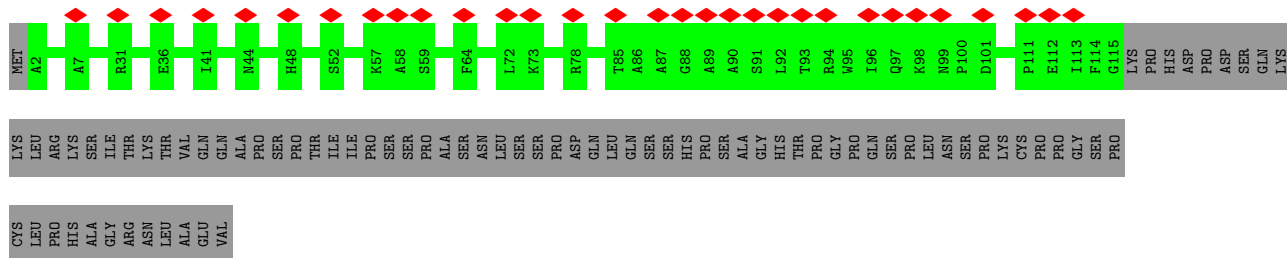
• Molecule 31: Enkurin, TRPC channel interacting protein



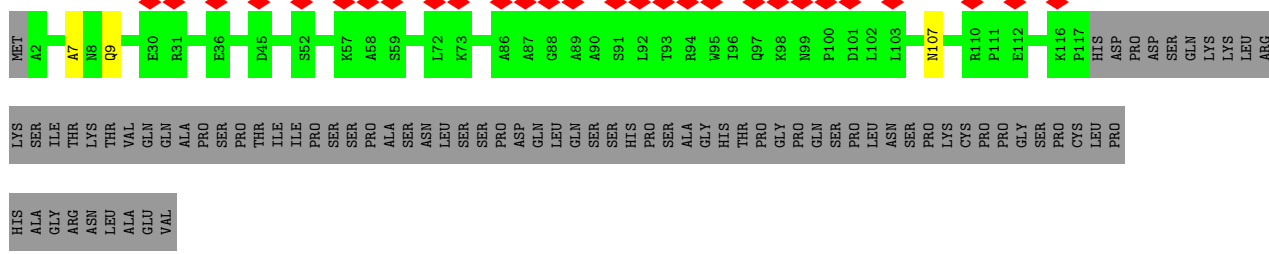
• Molecule 31: Enkurin, TRPC channel interacting protein



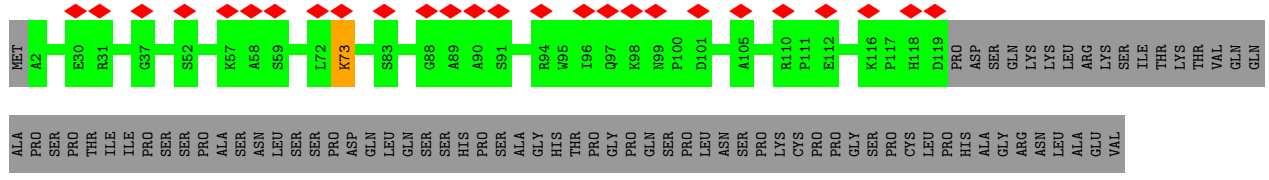
• Molecule 32: Protein Flattop



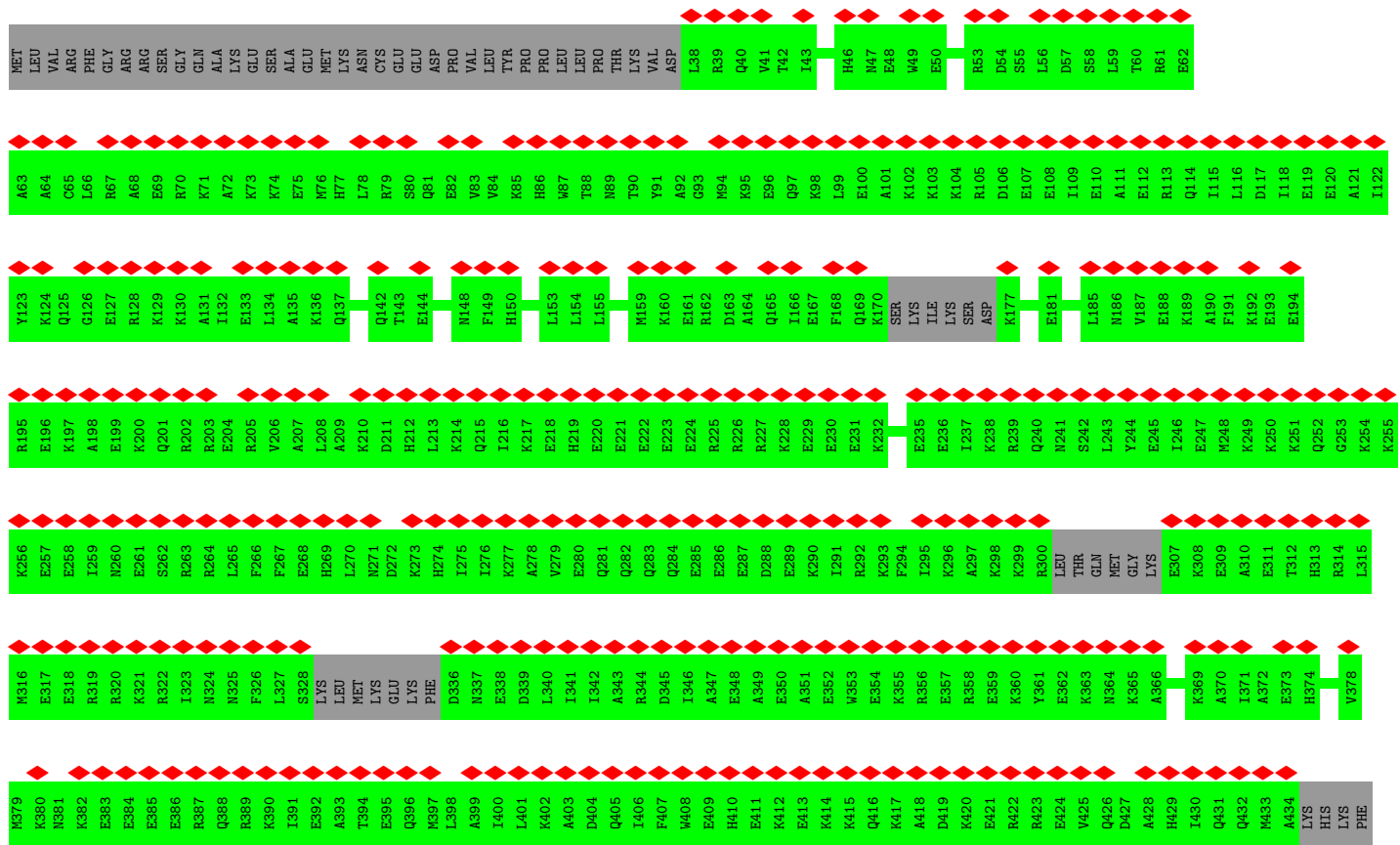
• Molecule 32: Protein Flattop



• Molecule 32: Protein Flattop



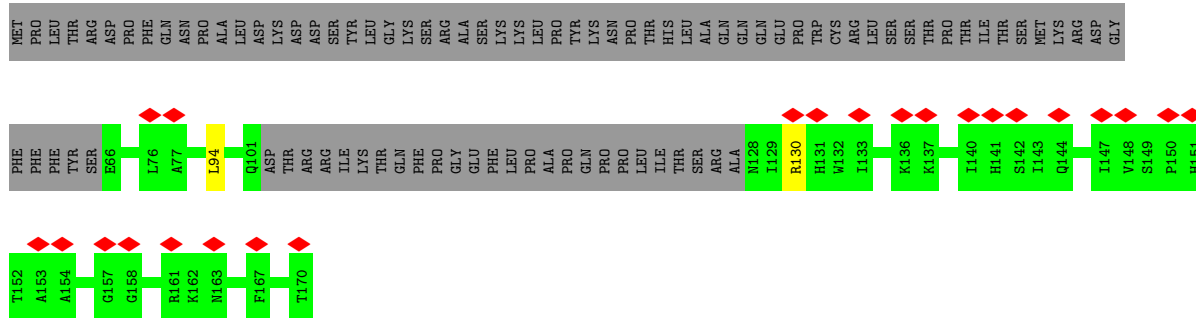
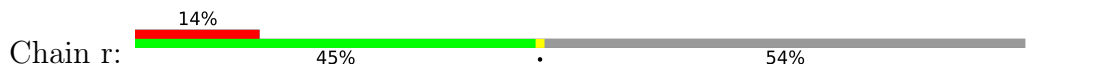
• Molecule 33: Coiled-coil domain containing 173



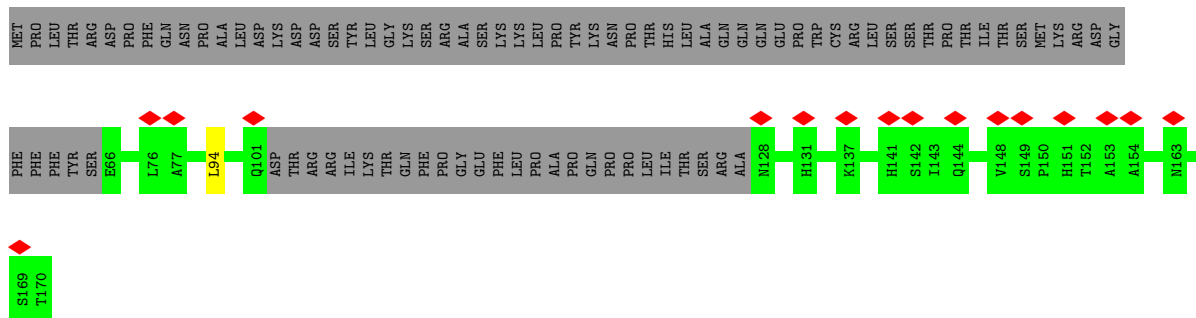




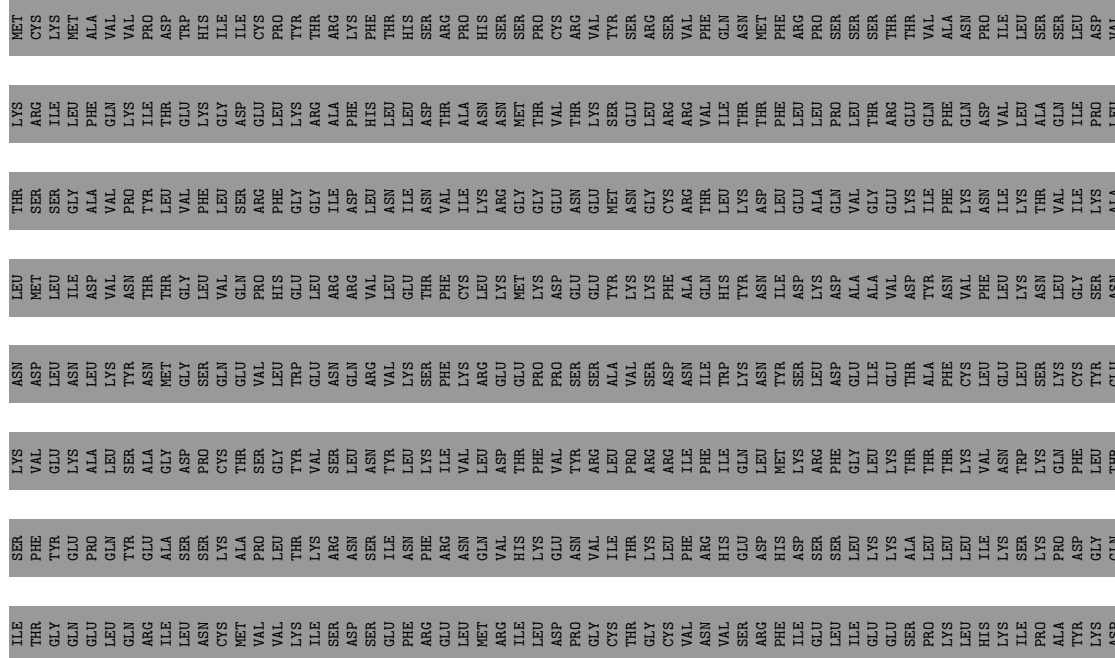
● Molecule 34: Chromosome 3 C1orf194 homolog



● Molecule 34: Chromosome 3 C1orf194 homolog



● Molecule 35: EFCAB6

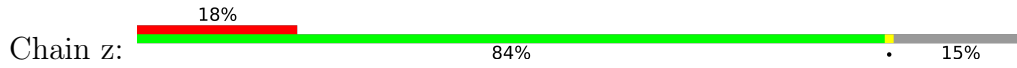




MET SER GLU TYR GLY ASP PRO LYS ALA CYS THR VAL HIS GLU PRO GLU MET P74 R86 N96 K105 D112 Y118 D119 R120 L121 R131 I134 C136 D136

GLN ALA TYR GLY SER ARG ALA PRO THR VAL HIS GLU MET P74 R86 N96 K105 D112 Y118 D119 R120 L121 R131 I134 C136 D136

● Molecule 36: Pierce1



MET SER GLU TYR GLY ASP PRO LYS ALA CYS THR VAL HIS GLU PRO GLU MET P74 R86 N96 K105 D112 Y118 D119 R120 L121 R131 I134 C136 D136 E22 K23 D26 R29 E32 D33 T49 A50 E51 F52 P53 R57 N60 Q61 A62 R66 G91 M103 E104 K105 D112 L121 R131 P132 S133 I134 C135

D136

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80503	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	49.832	Depositor
Minimum map value	0.000	Depositor
Average map value	0.284	Depositor
Map value standard deviation	1.458	Depositor
Recommended contour level	7.0	Depositor
Map size (Å)	732.48004, 732.48004, 732.48004	wwPDB
Map dimensions	672, 672, 672	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.37	0/337	0.56	0/452
1	7	0.39	0/820	0.60	1/1122 (0.1%)
2	1	0.33	0/933	0.56	0/1284
2	2	0.27	0/1528	0.48	0/2114
3	3	0.40	0/2303	0.58	2/3079 (0.1%)
3	4	0.43	0/1868	0.66	0/2471
4	5	0.33	0/2575	0.64	0/3508
4	6	0.35	0/3011	0.67	2/4065 (0.0%)
5	8	0.40	0/1671	0.74	2/2285 (0.1%)
5	9	0.34	0/294	0.54	0/398
6	A	0.38	0/1433	0.67	4/1901 (0.2%)
6	B	0.44	1/3071 (0.0%)	0.66	1/4071 (0.0%)
7	A0	0.43	0/1815	0.60	1/2442 (0.0%)
7	A1	0.44	0/3298	0.57	1/4442 (0.0%)
7	A2	0.45	0/3278	0.63	3/4415 (0.1%)
7	A3	0.43	0/2792	0.61	4/3754 (0.1%)
7	A4	0.42	0/296	0.59	0/397
8	AA	0.50	0/3500	0.73	1/4751 (0.0%)
8	AC	0.55	0/3515	0.73	4/4771 (0.1%)
8	AE	0.49	0/3515	0.70	4/4771 (0.1%)
8	AG	0.56	0/3515	0.75	6/4771 (0.1%)
8	AI	0.51	0/3515	0.67	3/4771 (0.1%)
8	AK	0.58	0/3515	0.71	3/4771 (0.1%)
8	AM	0.49	0/3508	0.66	2/4761 (0.0%)
8	BA	0.45	0/3449	0.69	1/4682 (0.0%)
8	BC	0.51	0/3515	0.69	2/4771 (0.0%)
8	BE	0.47	0/3473	0.68	1/4714 (0.0%)
8	BG	0.51	0/3515	0.72	3/4771 (0.1%)
8	BI	0.46	0/3451	0.66	0/4684
8	BK	0.53	0/3508	0.70	1/4761 (0.0%)
8	BM	0.46	0/3449	0.66	2/4681 (0.0%)
8	CA	0.40	0/3500	0.71	5/4751 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	CC	0.47	0/3502	0.69	5/4753 (0.1%)
8	CE	0.42	0/3502	0.64	0/4753
8	CG	0.49	0/3508	0.70	4/4761 (0.1%)
8	CI	0.42	0/3508	0.70	4/4761 (0.1%)
8	CK	0.45	0/3508	0.63	0/4761
8	CM	0.41	0/3508	0.67	2/4761 (0.0%)
8	DA	0.38	0/3209	0.74	7/4357 (0.2%)
8	DC	0.40	0/3443	0.68	1/4673 (0.0%)
8	DE	0.41	0/3449	0.69	2/4681 (0.0%)
8	DG	0.45	0/3456	0.74	6/4691 (0.1%)
8	DI	0.43	0/3441	0.73	4/4670 (0.1%)
8	DK	0.43	0/3449	0.72	1/4681 (0.0%)
8	DM	0.39	0/3449	0.69	3/4681 (0.1%)
8	EC	0.42	0/3508	0.70	3/4761 (0.1%)
8	EE	0.41	0/3524	0.72	3/4783 (0.1%)
8	EG	0.44	0/3494	0.72	1/4742 (0.0%)
8	EI	0.42	0/3486	0.77	7/4732 (0.1%)
8	EK	0.43	0/3515	0.76	6/4771 (0.1%)
8	EM	0.42	0/3435	0.70	2/4662 (0.0%)
8	FC	0.38	0/3456	0.70	2/4691 (0.0%)
8	FE	0.42	0/3415	0.74	5/4635 (0.1%)
8	FG	0.44	0/3423	0.78	6/4647 (0.1%)
8	FI	0.44	0/3422	0.79	2/4644 (0.0%)
8	FK	0.42	0/3401	0.76	5/4617 (0.1%)
8	FM	0.41	0/3441	0.73	4/4669 (0.1%)
8	GC	0.46	0/3515	0.66	1/4771 (0.0%)
8	GE	0.34	0/3448	0.62	0/4680
8	GG	0.42	0/3515	0.64	2/4771 (0.0%)
8	GI	0.43	0/3442	0.63	0/4672
8	GK	0.38	0/3440	0.66	4/4668 (0.1%)
8	GM	0.42	0/3508	0.65	6/4761 (0.1%)
8	HC	0.44	0/3427	0.67	2/4651 (0.0%)
8	HE	0.37	0/3451	0.63	3/4684 (0.1%)
8	HG	0.40	0/3448	0.64	1/4680 (0.0%)
8	HI	0.43	0/3448	0.64	0/4680
8	HK	0.36	0/3456	0.64	2/4691 (0.0%)
8	HM	0.42	0/3441	0.68	1/4669 (0.0%)
8	HO	0.45	0/3104	0.69	2/4206 (0.0%)
8	IC	0.41	0/3442	0.62	0/4672
8	IE	0.42	0/3465	0.66	1/4703 (0.0%)
8	IG	0.38	0/3515	0.67	3/4771 (0.1%)
8	II	0.42	0/3464	0.68	1/4702 (0.0%)
8	IK	0.39	0/3515	0.70	3/4771 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	IM	0.41	0/3455	0.70	1/4689 (0.0%)
8	IO	0.37	0/3427	0.64	1/4652 (0.0%)
8	JC	0.42	0/3460	0.69	2/4695 (0.0%)
8	JE	0.40	0/3449	0.66	0/4681
8	JG	0.39	0/3435	0.65	0/4662
8	JI	0.42	0/3443	0.70	4/4673 (0.1%)
8	JK	0.43	0/3515	0.75	6/4771 (0.1%)
8	JM	0.41	0/3449	0.69	3/4681 (0.1%)
8	KC	0.56	0/3461	0.73	2/4697 (0.0%)
8	KE	0.55	0/3457	0.71	3/4692 (0.1%)
8	KG	0.51	0/3447	0.66	0/4678
8	KI	0.56	0/3435	0.67	2/4662 (0.0%)
8	KK	0.53	0/3449	0.67	4/4681 (0.1%)
8	KM	0.58	0/3453	0.67	1/4686 (0.0%)
8	KO	0.49	0/3291	0.60	0/4462
8	LC	0.54	0/3515	0.69	5/4771 (0.1%)
8	LE	0.52	0/3515	0.67	2/4771 (0.0%)
8	LG	0.51	0/3515	0.63	2/4771 (0.0%)
8	LI	0.56	0/3515	0.67	2/4771 (0.0%)
8	LK	0.53	0/3515	0.66	1/4771 (0.0%)
8	LM	0.55	1/3455 (0.0%)	0.64	2/4689 (0.0%)
8	MC	0.47	0/3508	0.69	1/4761 (0.0%)
8	ME	0.44	0/3443	0.68	2/4673 (0.0%)
8	MG	0.44	0/3449	0.71	5/4681 (0.1%)
8	MI	0.46	0/3456	0.70	2/4691 (0.0%)
8	MK	0.45	0/3515	0.73	7/4771 (0.1%)
8	MM	0.47	0/3453	0.70	5/4687 (0.1%)
8	NA	0.36	0/3449	0.67	1/4682 (0.0%)
8	NC	0.37	0/3442	0.67	1/4672 (0.0%)
8	NE	0.38	0/3451	0.74	7/4684 (0.1%)
8	NG	0.36	0/3464	0.67	2/4702 (0.0%)
8	NI	0.35	0/3464	0.66	2/4702 (0.0%)
8	NK	0.36	0/3451	0.66	3/4684 (0.1%)
8	OA	0.37	0/3435	0.66	2/4663 (0.0%)
8	OC	0.38	0/3443	0.64	1/4673 (0.0%)
8	OE	0.35	0/3473	0.66	1/4714 (0.0%)
8	OG	0.37	0/3468	0.67	3/4707 (0.1%)
8	OI	0.35	0/3464	0.64	2/4702 (0.0%)
8	OK	0.37	0/3457	0.64	1/4692 (0.0%)
8	PA	0.33	0/3449	0.63	3/4682 (0.1%)
8	PC	0.38	0/3463	0.69	3/4700 (0.1%)
8	PE	0.36	0/3457	0.69	0/4692
8	PG	0.38	0/3448	0.68	4/4680 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	PI	0.35	0/3425	0.67	1/4648 (0.0%)
8	PK	0.38	0/3448	0.67	3/4680 (0.1%)
8	PM	0.32	0/3449	0.62	1/4681 (0.0%)
8	QA	0.33	0/3453	0.71	5/4687 (0.1%)
8	QC	0.37	0/3449	0.70	4/4681 (0.1%)
8	QE	0.33	0/3449	0.64	2/4681 (0.0%)
8	QG	0.38	0/3457	0.69	2/4692 (0.0%)
8	QI	0.34	0/3443	0.66	2/4673 (0.0%)
8	QK	0.36	0/3457	0.66	2/4692 (0.0%)
8	QM	0.33	0/3455	0.63	1/4689 (0.0%)
8	RA	0.33	0/3441	0.66	3/4671 (0.1%)
8	RC	0.36	0/3464	0.66	2/4702 (0.0%)
8	RE	0.37	0/3435	0.70	2/4662 (0.0%)
8	RG	0.36	0/3448	0.65	1/4679 (0.0%)
8	RI	0.32	0/3456	0.61	1/4691 (0.0%)
8	RK	0.38	0/3456	0.69	6/4691 (0.1%)
8	RM	0.37	0/3433	0.66	3/4660 (0.1%)
8	SA	0.32	0/3449	0.66	5/4682 (0.1%)
8	SC	0.38	0/3448	0.67	1/4679 (0.0%)
8	SE	0.36	0/3457	0.67	4/4691 (0.1%)
8	SG	0.40	0/3456	0.69	3/4691 (0.1%)
8	SI	0.36	0/3434	0.65	3/4661 (0.1%)
8	SK	0.37	0/3464	0.69	0/4702
8	SM	0.36	0/3455	0.64	2/4689 (0.0%)
8	TC	0.34	0/3448	0.68	5/4680 (0.1%)
8	TE	0.32	0/3465	0.65	3/4703 (0.1%)
8	TG	0.35	0/3448	0.71	7/4680 (0.1%)
8	TI	0.34	0/3448	0.63	1/4680 (0.0%)
8	TK	0.36	0/3464	0.70	2/4702 (0.0%)
8	TM	0.36	0/3449	0.70	3/4681 (0.1%)
8	UC	0.35	0/3470	0.62	3/4710 (0.1%)
8	UE	0.34	0/3465	0.67	1/4703 (0.0%)
8	UG	0.35	0/3470	0.63	1/4710 (0.0%)
8	UI	0.35	0/3470	0.62	0/4710
8	UK	0.38	0/3468	0.64	0/4707
8	UM	0.36	0/3455	0.66	2/4689 (0.0%)
8	VC	0.39	0/3515	0.68	4/4771 (0.1%)
8	VE	0.38	0/3473	0.65	1/4714 (0.0%)
8	VG	0.36	0/3515	0.63	0/4771
8	VI	0.38	0/3470	0.66	3/4710 (0.1%)
8	VK	0.37	0/3515	0.66	1/4771 (0.0%)
8	VM	0.40	0/3449	0.70	6/4681 (0.1%)
8	WC	0.42	0/3515	0.73	6/4771 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	WE	0.39	0/3457	0.66	4/4692 (0.1%)
8	WG	0.38	0/3508	0.69	4/4761 (0.1%)
8	WI	0.40	0/3457	0.66	1/4692 (0.0%)
8	WK	0.37	0/3502	0.62	0/4753
8	WM	0.42	0/3455	0.68	3/4689 (0.1%)
9	AB	0.55	0/3500	0.71	2/4742 (0.0%)
9	AD	0.52	0/3500	0.70	4/4742 (0.1%)
9	AF	0.57	0/3500	0.75	4/4742 (0.1%)
9	AH	0.52	0/3500	0.71	5/4742 (0.1%)
9	AJ	0.55	0/3500	0.73	7/4742 (0.1%)
9	AL	0.52	0/3492	0.70	5/4732 (0.1%)
9	BB	0.49	0/3431	0.69	2/4649 (0.0%)
9	BD	0.47	0/3431	0.69	2/4649 (0.0%)
9	BF	0.48	0/3436	0.70	3/4656 (0.1%)
9	BH	0.46	0/3431	0.64	2/4649 (0.0%)
9	BJ	0.47	0/3431	0.67	1/4649 (0.0%)
9	BL	0.48	0/3415	0.66	4/4628 (0.1%)
9	CB	0.46	0/3423	0.73	6/4638 (0.1%)
9	CD	0.47	0/3423	0.67	3/4638 (0.1%)
9	CF	0.47	0/3436	0.74	3/4656 (0.1%)
9	CH	0.49	0/3431	0.69	1/4649 (0.0%)
9	CJ	0.44	0/3436	0.67	1/4656 (0.0%)
9	CL	0.44	0/3415	0.65	2/4628 (0.0%)
9	DB	0.41	0/3423	0.70	2/4638 (0.0%)
9	DD	0.45	0/3423	0.74	5/4638 (0.1%)
9	DF	0.41	0/3423	0.74	4/4638 (0.1%)
9	DH	0.46	0/3423	0.79	7/4638 (0.2%)
9	DJ	0.40	0/3423	0.69	1/4638 (0.0%)
9	DL	0.43	0/3415	0.70	4/4628 (0.1%)
9	DN	0.35	0/3102	0.66	2/4201 (0.0%)
9	EB	0.39	0/3423	0.70	5/4638 (0.1%)
9	ED	0.43	0/3423	0.76	5/4638 (0.1%)
9	EF	0.39	0/3423	0.73	3/4638 (0.1%)
9	EH	0.44	0/3436	0.73	2/4656 (0.0%)
9	EJ	0.40	0/3423	0.72	2/4638 (0.0%)
9	EL	0.41	0/3415	0.73	4/4628 (0.1%)
9	EN	0.34	0/3423	0.69	3/4638 (0.1%)
9	FB	0.35	0/3423	0.65	1/4638 (0.0%)
9	FD	0.41	0/3431	0.72	3/4649 (0.1%)
9	FF	0.39	0/3423	0.66	1/4638 (0.0%)
9	FH	0.46	0/3423	0.78	6/4638 (0.1%)
9	FJ	0.38	0/3423	0.68	2/4638 (0.0%)
9	FL	0.41	0/3415	0.72	4/4628 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	FN	0.34	0/3436	0.64	1/4656 (0.0%)
9	GB	0.44	0/3436	0.65	1/4656 (0.0%)
9	GD	0.41	0/3431	0.68	2/4649 (0.0%)
9	GF	0.38	0/3436	0.63	2/4656 (0.0%)
9	GH	0.44	0/3436	0.70	6/4656 (0.1%)
9	GJ	0.40	0/3436	0.65	1/4656 (0.0%)
9	GL	0.36	0/3415	0.63	2/4628 (0.0%)
9	GN	0.45	0/3436	0.64	2/4656 (0.0%)
9	HB	0.42	0/3423	0.67	3/4638 (0.1%)
9	HD	0.40	0/3431	0.66	3/4649 (0.1%)
9	HF	0.36	0/3436	0.61	0/4656
9	HH	0.43	0/3431	0.68	4/4649 (0.1%)
9	HJ	0.39	0/3436	0.63	2/4656 (0.0%)
9	HL	0.36	0/3415	0.64	2/4628 (0.0%)
9	HN	0.43	0/3431	0.68	4/4649 (0.1%)
9	IB	0.38	0/2962	0.71	5/4007 (0.1%)
9	ID	0.44	0/3431	0.69	1/4649 (0.0%)
9	IF	0.38	0/3436	0.62	2/4656 (0.0%)
9	IH	0.41	0/3431	0.68	3/4649 (0.1%)
9	IJ	0.39	0/3436	0.66	1/4656 (0.0%)
9	IL	0.43	0/3423	0.67	1/4638 (0.0%)
9	IN	0.39	0/3436	0.70	1/4656 (0.0%)
9	JB	0.39	0/3423	0.67	1/4638 (0.0%)
9	JD	0.42	0/3431	0.68	2/4649 (0.0%)
9	JF	0.38	0/3423	0.67	3/4638 (0.1%)
9	JH	0.41	0/3423	0.68	2/4638 (0.0%)
9	JJ	0.40	0/3423	0.68	6/4638 (0.1%)
9	JL	0.43	0/3423	0.72	1/4638 (0.0%)
9	JN	0.39	0/3423	0.67	0/4638
9	KB	0.48	0/3232	0.72	3/4380 (0.1%)
9	KD	0.55	0/3436	0.65	2/4656 (0.0%)
9	KF	0.49	0/3431	0.65	3/4649 (0.1%)
9	KH	0.56	0/3443	0.63	1/4666 (0.0%)
9	KJ	0.50	0/3423	0.61	1/4638 (0.0%)
9	KL	0.58	0/3443	0.65	1/4666 (0.0%)
9	KN	0.51	0/3436	0.64	2/4656 (0.0%)
9	LB	0.47	0/3436	0.66	0/4656
9	LD	0.51	0/3431	0.68	2/4649 (0.0%)
9	LF	0.48	0/3436	0.65	1/4656 (0.0%)
9	LH	0.54	0/3436	0.66	3/4656 (0.1%)
9	LJ	0.50	0/3436	0.65	0/4656
9	LL	0.56	0/3423	0.70	6/4638 (0.1%)
9	LN	0.49	0/3436	0.64	3/4656 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	MB	0.44	0/3423	0.68	4/4638 (0.1%)
9	MD	0.46	0/3423	0.70	4/4638 (0.1%)
9	MF	0.40	0/3436	0.65	3/4656 (0.1%)
9	MH	0.44	0/3436	0.66	3/4656 (0.1%)
9	MJ	0.42	0/3423	0.68	3/4638 (0.1%)
9	ML	0.46	0/3423	0.75	3/4638 (0.1%)
9	MN	0.43	0/3423	0.70	2/4638 (0.0%)
9	NO	0.34	0/3431	0.63	1/4649 (0.0%)
9	NB	0.38	0/3436	0.70	2/4656 (0.0%)
9	ND	0.34	0/3431	0.66	0/4649
9	NF	0.37	0/3431	0.69	2/4649 (0.0%)
9	NH	0.33	0/3436	0.63	0/4656
9	NJ	0.36	0/3436	0.70	2/4656 (0.0%)
9	NL	0.34	0/3414	0.67	1/4626 (0.0%)
9	OO	0.38	0/3293	0.70	3/4463 (0.1%)
9	OB	0.37	0/3414	0.66	2/4626 (0.0%)
9	OD	0.34	0/3401	0.64	1/4608 (0.0%)
9	OF	0.40	0/3414	0.69	0/4626
9	OH	0.33	0/3436	0.63	1/4656 (0.0%)
9	OJ	0.36	0/3436	0.67	3/4656 (0.1%)
9	OL	0.36	0/3401	0.65	1/4608 (0.0%)
9	PB	0.36	0/3431	0.70	2/4649 (0.0%)
9	PD	0.35	0/3431	0.64	1/4649 (0.0%)
9	PF	0.38	0/3436	0.69	3/4656 (0.1%)
9	PH	0.36	0/3436	0.64	2/4656 (0.0%)
9	PJ	0.35	0/3436	0.67	3/4656 (0.1%)
9	PL	0.36	0/3415	0.72	4/4628 (0.1%)
9	QB	0.33	0/3436	0.64	1/4656 (0.0%)
9	QD	0.33	0/3431	0.64	1/4649 (0.0%)
9	QF	0.37	0/3436	0.70	4/4656 (0.1%)
9	QH	0.35	0/3436	0.67	3/4656 (0.1%)
9	QJ	0.34	0/3436	0.65	3/4656 (0.1%)
9	QL	0.35	0/3423	0.68	2/4638 (0.0%)
9	RB	0.33	0/3436	0.68	2/4656 (0.0%)
9	RD	0.34	0/3431	0.63	1/4649 (0.0%)
9	RF	0.35	0/3436	0.68	5/4656 (0.1%)
9	RH	0.36	0/3436	0.68	2/4656 (0.0%)
9	RJ	0.35	0/3436	0.69	4/4656 (0.1%)
9	RL	0.35	0/3423	0.64	1/4638 (0.0%)
9	SB	0.35	0/3436	0.66	1/4656 (0.0%)
9	SD	0.36	0/3431	0.67	4/4649 (0.1%)
9	SF	0.36	0/3436	0.68	3/4656 (0.1%)
9	SH	0.38	0/3436	0.68	0/4656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	SJ	0.34	0/3436	0.71	7/4656 (0.2%)
9	SL	0.36	0/3423	0.68	5/4638 (0.1%)
9	TB	0.32	0/3436	0.66	1/4656 (0.0%)
9	TD	0.33	0/3431	0.67	2/4649 (0.0%)
9	TF	0.34	0/3436	0.67	5/4656 (0.1%)
9	TH	0.34	0/3436	0.64	4/4656 (0.1%)
9	TJ	0.35	0/3436	0.70	4/4656 (0.1%)
9	TL	0.36	0/3423	0.67	3/4638 (0.1%)
9	UB	0.33	0/3436	0.65	2/4656 (0.0%)
9	UD	0.35	0/3431	0.62	1/4649 (0.0%)
9	UF	0.34	0/3436	0.62	0/4656
9	UH	0.36	0/3436	0.64	0/4656
9	UJ	0.33	0/3436	0.65	3/4656 (0.1%)
9	UL	0.36	0/3423	0.67	1/4638 (0.0%)
9	UN	0.34	0/3436	0.64	2/4656 (0.0%)
9	VB	0.36	0/3436	0.68	4/4656 (0.1%)
9	VD	0.37	0/3431	0.65	2/4649 (0.0%)
9	VF	0.34	0/3431	0.62	2/4649 (0.0%)
9	VH	0.38	0/3436	0.66	2/4656 (0.0%)
9	VJ	0.34	0/3436	0.61	0/4656
9	VL	0.37	0/3423	0.66	1/4638 (0.0%)
9	VN	0.35	0/3436	0.63	0/4656
9	WB	0.38	0/3436	0.67	2/4656 (0.0%)
9	WD	0.42	0/3431	0.77	8/4649 (0.2%)
9	WF	0.37	0/3423	0.65	2/4638 (0.0%)
9	WH	0.42	0/3423	0.67	0/4638
9	WJ	0.37	0/3423	0.65	1/4638 (0.0%)
9	WL	0.41	0/3423	0.71	3/4638 (0.1%)
9	WN	0.40	0/3423	0.71	3/4638 (0.1%)
10	B0	0.40	0/1559	0.58	1/2100 (0.0%)
10	B1	0.44	0/3434	0.59	1/4630 (0.0%)
10	B2	0.44	0/3434	0.59	2/4630 (0.0%)
10	B3	0.42	0/3149	0.61	1/4243 (0.0%)
10	B4	0.39	0/410	0.56	0/552
10	B5	0.39	0/423	0.65	0/570
10	B6	0.39	0/2943	0.61	2/3961 (0.1%)
10	B7	0.38	0/3415	0.64	3/4605 (0.1%)
10	B8	0.40	0/3325	0.74	9/4480 (0.2%)
10	B9	0.41	0/1544	0.76	5/2080 (0.2%)
11	C	0.42	0/801	0.78	2/1073 (0.2%)
12	C0	0.31	0/267	0.63	0/362
12	C1	0.40	0/2747	0.63	4/3704 (0.1%)
12	C2	0.41	0/3249	0.62	3/4380 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
12	C3	0.40	0/3249	0.60	2/4380 (0.0%)
12	C4	0.44	0/1761	0.70	3/2370 (0.1%)
12	C5	0.37	0/914	0.55	0/1231
12	C6	0.38	0/3170	0.58	4/4272 (0.1%)
12	C7	0.39	0/3403	0.60	1/4589 (0.0%)
12	C8	0.38	0/3354	0.60	1/4523 (0.0%)
12	C9	0.35	0/942	0.62	1/1273 (0.1%)
12	F0	0.37	0/1186	0.61	0/1610
12	F1	0.42	0/3486	0.63	3/4708 (0.1%)
12	F2	0.43	0/3486	0.63	3/4708 (0.1%)
12	F3	0.41	0/3100	0.63	1/4176 (0.0%)
12	F4	0.42	0/815	0.67	2/1097 (0.2%)
13	D	0.33	0/961	0.59	1/1323 (0.1%)
14	D0	0.42	0/2416	0.57	1/3260 (0.0%)
14	D1	0.45	1/3537 (0.0%)	0.57	0/4765
14	D2	0.44	0/3537	0.61	1/4765 (0.0%)
14	D3	0.44	0/2627	0.62	2/3537 (0.1%)
14	D5	0.26	0/78	0.64	0/104
14	D6	0.39	0/2653	0.64	4/3571 (0.1%)
14	D7	0.41	0/3442	0.64	4/4637 (0.1%)
14	D8	0.37	0/3433	0.64	3/4625 (0.1%)
14	D9	0.38	0/2296	0.64	2/3098 (0.1%)
15	E	0.40	0/2105	0.67	1/2851 (0.0%)
15	F	0.42	0/2105	0.72	3/2851 (0.1%)
16	E0	0.41	0/603	0.77	2/819 (0.2%)
16	E1	0.35	0/1102	0.68	4/1503 (0.3%)
16	E2	0.33	0/1248	0.62	0/1705
16	E3	0.34	0/1248	0.63	0/1705
17	G	0.40	0/802	0.71	1/1094 (0.1%)
18	H	0.39	0/671	0.63	0/916
18	I	0.36	0/1230	0.66	1/1667 (0.1%)
18	J	0.40	0/1230	0.66	0/1667
18	K	0.37	0/1230	0.66	0/1667
18	L	0.39	0/1230	0.65	0/1667
18	M	0.35	0/1230	0.63	0/1667
18	N	0.38	0/1261	0.61	0/1708
19	H1	0.41	0/1584	0.71	3/2120 (0.1%)
19	H2	0.38	0/2085	0.74	6/2785 (0.2%)
19	H3	0.43	0/886	0.64	1/1180 (0.1%)
20	H4	0.41	0/1644	0.67	1/2200 (0.0%)
20	H5	0.39	0/2120	0.71	2/2840 (0.1%)
20	H6	0.41	0/1073	0.68	1/1440 (0.1%)
21	H7	0.29	0/2865	0.42	0/3988

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
21	H8	0.28	0/2860	0.41	0/3981
21	H9	0.24	0/1766	0.37	0/2456
22	I1	0.37	0/1318	0.61	1/1783 (0.1%)
22	I2	0.45	0/1318	0.70	0/1783
23	I3	0.25	0/919	0.39	0/1278
23	I4	0.25	0/923	0.38	0/1283
24	O	0.30	0/272	0.65	0/359
24	P	0.41	0/3142	0.68	7/4198 (0.2%)
24	Q	0.42	0/321	0.61	0/429
24	R	0.40	0/2063	0.61	2/2756 (0.1%)
24	S	0.37	0/1427	0.60	0/1907
25	T	0.46	0/3823	0.64	2/5172 (0.0%)
25	U	0.47	0/3823	0.70	4/5172 (0.1%)
25	V	0.44	0/3823	0.64	4/5172 (0.1%)
26	W	0.40	0/4670	0.67	2/6296 (0.0%)
26	X	0.40	0/5355	0.68	5/7211 (0.1%)
26	Y	0.40	0/5355	0.66	4/7211 (0.1%)
26	Z	0.36	0/3766	0.67	3/5063 (0.1%)
27	XA	0.43	0/1565	0.76	3/2111 (0.1%)
27	XB	0.50	0/1565	0.77	1/2111 (0.0%)
27	XC	0.42	0/1565	0.73	1/2111 (0.0%)
27	XD	0.45	0/1565	0.73	3/2111 (0.1%)
27	XE	0.39	0/1565	0.67	0/2111
27	XF	0.48	0/1565	0.72	3/2111 (0.1%)
27	XG	0.38	0/1565	0.68	0/2111
28	YB	0.44	0/1810	0.76	3/2446 (0.1%)
28	YC	0.40	0/1810	0.72	3/2446 (0.1%)
28	YD	0.44	0/1810	0.73	3/2446 (0.1%)
28	YE	0.40	0/1810	0.70	1/2446 (0.0%)
28	YF	0.43	0/1810	0.74	4/2446 (0.2%)
28	YG	0.36	0/1810	0.73	3/2446 (0.1%)
29	a	0.37	0/1432	0.63	0/1899
29	b	0.38	0/2869	0.67	2/3794 (0.1%)
29	c	0.38	0/2371	0.66	2/3139 (0.1%)
29	d	0.37	0/1842	0.59	2/2438 (0.1%)
30	e	0.37	0/4821	0.70	3/6527 (0.0%)
30	f	0.37	0/4821	0.69	2/6527 (0.0%)
30	g	0.39	0/4821	0.70	3/6527 (0.0%)
31	h	0.39	0/1239	0.69	1/1657 (0.1%)
31	i	0.36	0/1982	0.63	2/2659 (0.1%)
31	j	0.36	0/1982	0.64	3/2659 (0.1%)
31	k	0.37	0/1982	0.67	2/2659 (0.1%)
32	l	0.46	0/921	0.66	0/1253

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	m	0.48	0/938	0.70	1/1276 (0.1%)
32	n	0.43	0/957	0.62	1/1302 (0.1%)
33	o	0.33	0/2072	0.36	0/2868
33	p	0.39	0/847	0.63	1/1131 (0.1%)
34	q	0.40	0/646	0.68	1/871 (0.1%)
34	r	0.36	0/646	0.66	1/871 (0.1%)
34	s	0.39	0/646	0.74	1/871 (0.1%)
35	t	0.24	0/881	0.41	0/1227
36	y	0.41	0/530	0.62	0/718
36	z	0.41	0/981	0.67	1/1334 (0.1%)
All	All	0.41	3/1294189 (0.0%)	0.67	964/1753471 (0.1%)

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	7	0	1
11	C	0	1
29	b	0	1
31	h	0	1
31	i	0	1
31	j	0	1
31	k	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D1	212	GLU	CB-CG	-6.00	1.40	1.52
8	LM	295	CYS	CB-SG	-5.89	1.72	1.81
6	B	462	TYR	CD2-CE2	-5.29	1.31	1.39

The worst 5 of 964 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	k	250	HIS	O-C-N	-12.58	102.58	122.70
31	i	250	HIS	O-C-N	-12.16	103.25	122.70
5	8	124	LEU	CB-CG-CD2	-10.99	92.31	111.00
8	AG	396	ASP	CB-CG-OD2	10.58	127.82	118.30
9	WL	118	ASP	CB-CG-OD1	10.46	127.71	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	7	162	PRO	Mainchain
11	C	100	ARG	Mainchain
29	b	541	ASN	Mainchain
31	h	250	HIS	Mainchain
31	i	250	HIS	Mainchain

## 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	0	38/232 (16%)	36 (95%)	2 (5%)	0	100	100
1	7	117/232 (50%)	104 (89%)	11 (9%)	2 (2%)	9	34
2	1	148/877 (17%)	142 (96%)	6 (4%)	0	100	100
2	2	288/877 (33%)	258 (90%)	30 (10%)	0	100	100
3	3	304/514 (59%)	304 (100%)	0	0	100	100
3	4	215/514 (42%)	215 (100%)	0	0	100	100
4	5	370/377 (98%)	347 (94%)	23 (6%)	0	100	100
4	6	370/377 (98%)	348 (94%)	22 (6%)	0	100	100
5	8	189/196 (96%)	159 (84%)	29 (15%)	1 (0%)	29	61
5	9	33/196 (17%)	30 (91%)	3 (9%)	0	100	100
6	A	168/494 (34%)	167 (99%)	1 (1%)	0	100	100
6	B	352/494 (71%)	349 (99%)	3 (1%)	0	100	100
7	A0	217/418 (52%)	209 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	A1	394/418 (94%)	383 (97%)	10 (2%)	1 (0%)	41	72
7	A2	391/418 (94%)	383 (98%)	7 (2%)	1 (0%)	41	72
7	A3	330/418 (79%)	320 (97%)	10 (3%)	0	100	100
7	A4	32/418 (8%)	31 (97%)	1 (3%)	0	100	100
8	AA	436/452 (96%)	399 (92%)	37 (8%)	0	100	100
8	AC	438/452 (97%)	407 (93%)	31 (7%)	0	100	100
8	AE	438/452 (97%)	413 (94%)	25 (6%)	0	100	100
8	AG	438/452 (97%)	413 (94%)	25 (6%)	0	100	100
8	AI	438/452 (97%)	408 (93%)	30 (7%)	0	100	100
8	AK	438/452 (97%)	410 (94%)	27 (6%)	1 (0%)	47	78
8	AM	437/452 (97%)	418 (96%)	19 (4%)	0	100	100
8	BA	426/452 (94%)	391 (92%)	35 (8%)	0	100	100
8	BC	438/452 (97%)	409 (93%)	29 (7%)	0	100	100
8	BE	429/452 (95%)	396 (92%)	33 (8%)	0	100	100
8	BG	438/452 (97%)	398 (91%)	40 (9%)	0	100	100
8	BI	426/452 (94%)	390 (92%)	36 (8%)	0	100	100
8	BK	437/452 (97%)	394 (90%)	43 (10%)	0	100	100
8	BM	426/452 (94%)	391 (92%)	35 (8%)	0	100	100
8	CA	436/452 (96%)	406 (93%)	30 (7%)	0	100	100
8	CC	436/452 (96%)	406 (93%)	30 (7%)	0	100	100
8	CE	436/452 (96%)	399 (92%)	37 (8%)	0	100	100
8	CG	437/452 (97%)	405 (93%)	32 (7%)	0	100	100
8	CI	437/452 (97%)	408 (93%)	29 (7%)	0	100	100
8	CK	437/452 (97%)	410 (94%)	27 (6%)	0	100	100
8	CM	437/452 (97%)	410 (94%)	27 (6%)	0	100	100
8	DA	393/452 (87%)	359 (91%)	34 (9%)	0	100	100
8	DC	425/452 (94%)	392 (92%)	33 (8%)	0	100	100
8	DE	426/452 (94%)	379 (89%)	47 (11%)	0	100	100
8	DG	427/452 (94%)	378 (88%)	49 (12%)	0	100	100
8	DI	425/452 (94%)	396 (93%)	29 (7%)	0	100	100
8	DK	426/452 (94%)	388 (91%)	38 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	DM	426/452 (94%)	400 (94%)	26 (6%)	0	100	100
8	EC	437/452 (97%)	395 (90%)	42 (10%)	0	100	100
8	EE	439/452 (97%)	395 (90%)	44 (10%)	0	100	100
8	EG	435/452 (96%)	390 (90%)	45 (10%)	0	100	100
8	EI	434/452 (96%)	387 (89%)	47 (11%)	0	100	100
8	EK	438/452 (97%)	383 (87%)	54 (12%)	1 (0%)	47	78
8	EM	424/452 (94%)	379 (89%)	44 (10%)	1 (0%)	47	78
8	FC	427/452 (94%)	395 (92%)	32 (8%)	0	100	100
8	FE	421/452 (93%)	372 (88%)	49 (12%)	0	100	100
8	FG	422/452 (93%)	381 (90%)	40 (10%)	1 (0%)	47	78
8	FI	423/452 (94%)	383 (90%)	40 (10%)	0	100	100
8	FK	420/452 (93%)	377 (90%)	43 (10%)	0	100	100
8	FM	425/452 (94%)	384 (90%)	41 (10%)	0	100	100
8	GC	438/452 (97%)	411 (94%)	27 (6%)	0	100	100
8	GE	426/452 (94%)	409 (96%)	17 (4%)	0	100	100
8	GG	438/452 (97%)	410 (94%)	28 (6%)	0	100	100
8	GI	425/452 (94%)	401 (94%)	24 (6%)	0	100	100
8	GK	425/452 (94%)	396 (93%)	27 (6%)	2 (0%)	29	61
8	GM	437/452 (97%)	405 (93%)	31 (7%)	1 (0%)	47	78
8	HC	423/452 (94%)	401 (95%)	22 (5%)	0	100	100
8	HE	426/452 (94%)	402 (94%)	24 (6%)	0	100	100
8	HG	426/452 (94%)	396 (93%)	30 (7%)	0	100	100
8	HI	426/452 (94%)	398 (93%)	28 (7%)	0	100	100
8	HK	427/452 (94%)	392 (92%)	35 (8%)	0	100	100
8	HM	425/452 (94%)	403 (95%)	22 (5%)	0	100	100
8	HO	376/452 (83%)	355 (94%)	21 (6%)	0	100	100
8	IC	425/452 (94%)	390 (92%)	35 (8%)	0	100	100
8	IE	428/452 (95%)	396 (92%)	32 (8%)	0	100	100
8	IG	438/452 (97%)	404 (92%)	34 (8%)	0	100	100
8	II	428/452 (95%)	381 (89%)	47 (11%)	0	100	100
8	IK	438/452 (97%)	391 (89%)	47 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	IM	427/452 (94%)	378 (88%)	49 (12%)	0	100	100
8	IO	423/452 (94%)	396 (94%)	27 (6%)	0	100	100
8	JC	428/452 (95%)	394 (92%)	34 (8%)	0	100	100
8	JE	426/452 (94%)	399 (94%)	27 (6%)	0	100	100
8	JG	424/452 (94%)	391 (92%)	33 (8%)	0	100	100
8	JI	425/452 (94%)	394 (93%)	31 (7%)	0	100	100
8	JK	438/452 (97%)	399 (91%)	39 (9%)	0	100	100
8	JM	426/452 (94%)	379 (89%)	47 (11%)	0	100	100
8	KC	428/452 (95%)	394 (92%)	34 (8%)	0	100	100
8	KE	427/452 (94%)	394 (92%)	33 (8%)	0	100	100
8	KG	426/452 (94%)	404 (95%)	22 (5%)	0	100	100
8	KI	424/452 (94%)	396 (93%)	28 (7%)	0	100	100
8	KK	426/452 (94%)	405 (95%)	21 (5%)	0	100	100
8	KM	428/452 (95%)	399 (93%)	29 (7%)	0	100	100
8	KO	400/452 (88%)	371 (93%)	29 (7%)	0	100	100
8	LC	438/452 (97%)	407 (93%)	31 (7%)	0	100	100
8	LE	438/452 (97%)	406 (93%)	32 (7%)	0	100	100
8	LG	438/452 (97%)	407 (93%)	31 (7%)	0	100	100
8	LI	438/452 (97%)	405 (92%)	33 (8%)	0	100	100
8	LK	438/452 (97%)	413 (94%)	25 (6%)	0	100	100
8	LM	427/452 (94%)	398 (93%)	29 (7%)	0	100	100
8	MC	437/452 (97%)	393 (90%)	44 (10%)	0	100	100
8	ME	425/452 (94%)	398 (94%)	27 (6%)	0	100	100
8	MG	426/452 (94%)	396 (93%)	30 (7%)	0	100	100
8	MI	427/452 (94%)	385 (90%)	42 (10%)	0	100	100
8	MK	438/452 (97%)	398 (91%)	40 (9%)	0	100	100
8	MM	427/452 (94%)	384 (90%)	43 (10%)	0	100	100
8	NA	426/452 (94%)	393 (92%)	33 (8%)	0	100	100
8	NC	425/452 (94%)	391 (92%)	34 (8%)	0	100	100
8	NE	426/452 (94%)	397 (93%)	28 (7%)	1 (0%)	47	78
8	NG	428/452 (95%)	382 (89%)	46 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	NI	428/452 (95%)	391 (91%)	37 (9%)	0	100	100
8	NK	426/452 (94%)	400 (94%)	26 (6%)	0	100	100
8	OA	424/452 (94%)	401 (95%)	23 (5%)	0	100	100
8	OC	425/452 (94%)	395 (93%)	30 (7%)	0	100	100
8	OE	429/452 (95%)	398 (93%)	31 (7%)	0	100	100
8	OG	429/452 (95%)	394 (92%)	35 (8%)	0	100	100
8	OI	428/452 (95%)	397 (93%)	31 (7%)	0	100	100
8	OK	427/452 (94%)	402 (94%)	25 (6%)	0	100	100
8	PA	426/452 (94%)	401 (94%)	25 (6%)	0	100	100
8	PC	428/452 (95%)	392 (92%)	36 (8%)	0	100	100
8	PE	427/452 (94%)	403 (94%)	24 (6%)	0	100	100
8	PG	426/452 (94%)	383 (90%)	42 (10%)	1 (0%)	47	78
8	PI	423/452 (94%)	399 (94%)	24 (6%)	0	100	100
8	PK	426/452 (94%)	399 (94%)	27 (6%)	0	100	100
8	PM	426/452 (94%)	401 (94%)	25 (6%)	0	100	100
8	QA	427/452 (94%)	396 (93%)	31 (7%)	0	100	100
8	QC	426/452 (94%)	396 (93%)	30 (7%)	0	100	100
8	QE	426/452 (94%)	398 (93%)	28 (7%)	0	100	100
8	QG	427/452 (94%)	393 (92%)	33 (8%)	1 (0%)	47	78
8	QI	425/452 (94%)	394 (93%)	30 (7%)	1 (0%)	47	78
8	QK	427/452 (94%)	392 (92%)	35 (8%)	0	100	100
8	QM	427/452 (94%)	397 (93%)	30 (7%)	0	100	100
8	RA	425/452 (94%)	395 (93%)	30 (7%)	0	100	100
8	RC	428/452 (95%)	393 (92%)	34 (8%)	1 (0%)	47	78
8	RE	424/452 (94%)	393 (93%)	31 (7%)	0	100	100
8	RG	426/452 (94%)	387 (91%)	39 (9%)	0	100	100
8	RI	427/452 (94%)	397 (93%)	30 (7%)	0	100	100
8	RK	427/452 (94%)	396 (93%)	31 (7%)	0	100	100
8	RM	424/452 (94%)	398 (94%)	26 (6%)	0	100	100
8	SA	426/452 (94%)	394 (92%)	32 (8%)	0	100	100
8	SC	426/452 (94%)	388 (91%)	38 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	SE	427/452 (94%)	402 (94%)	25 (6%)	0	100	100
8	SG	427/452 (94%)	388 (91%)	39 (9%)	0	100	100
8	SI	421/452 (93%)	385 (91%)	36 (9%)	0	100	100
8	SK	428/452 (95%)	397 (93%)	30 (7%)	1 (0%)	47	78
8	SM	427/452 (94%)	397 (93%)	30 (7%)	0	100	100
8	TC	426/452 (94%)	384 (90%)	42 (10%)	0	100	100
8	TE	428/452 (95%)	392 (92%)	36 (8%)	0	100	100
8	TG	426/452 (94%)	384 (90%)	42 (10%)	0	100	100
8	TI	426/452 (94%)	397 (93%)	29 (7%)	0	100	100
8	TK	428/452 (95%)	400 (94%)	28 (6%)	0	100	100
8	TM	426/452 (94%)	382 (90%)	44 (10%)	0	100	100
8	UC	429/452 (95%)	400 (93%)	29 (7%)	0	100	100
8	UE	428/452 (95%)	400 (94%)	28 (6%)	0	100	100
8	UG	429/452 (95%)	398 (93%)	31 (7%)	0	100	100
8	UI	429/452 (95%)	399 (93%)	30 (7%)	0	100	100
8	UK	429/452 (95%)	407 (95%)	22 (5%)	0	100	100
8	UM	427/452 (94%)	400 (94%)	27 (6%)	0	100	100
8	VC	438/452 (97%)	400 (91%)	38 (9%)	0	100	100
8	VE	429/452 (95%)	401 (94%)	28 (6%)	0	100	100
8	VG	438/452 (97%)	398 (91%)	40 (9%)	0	100	100
8	VI	429/452 (95%)	401 (94%)	28 (6%)	0	100	100
8	VK	438/452 (97%)	406 (93%)	32 (7%)	0	100	100
8	VM	426/452 (94%)	394 (92%)	32 (8%)	0	100	100
8	WC	438/452 (97%)	394 (90%)	43 (10%)	1 (0%)	47	78
8	WE	427/452 (94%)	391 (92%)	36 (8%)	0	100	100
8	WG	437/452 (97%)	403 (92%)	34 (8%)	0	100	100
8	WI	427/452 (94%)	400 (94%)	27 (6%)	0	100	100
8	WK	436/452 (96%)	404 (93%)	32 (7%)	0	100	100
8	WM	427/452 (94%)	397 (93%)	30 (7%)	0	100	100
9	AB	434/445 (98%)	404 (93%)	30 (7%)	0	100	100
9	AD	434/445 (98%)	402 (93%)	32 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AF	434/445 (98%)	409 (94%)	25 (6%)	0	100	100
9	AH	434/445 (98%)	404 (93%)	30 (7%)	0	100	100
9	AJ	434/445 (98%)	408 (94%)	26 (6%)	0	100	100
9	AL	433/445 (97%)	411 (95%)	22 (5%)	0	100	100
9	BB	425/445 (96%)	398 (94%)	27 (6%)	0	100	100
9	BD	425/445 (96%)	393 (92%)	32 (8%)	0	100	100
9	BF	426/445 (96%)	391 (92%)	35 (8%)	0	100	100
9	BH	425/445 (96%)	398 (94%)	27 (6%)	0	100	100
9	BJ	425/445 (96%)	395 (93%)	30 (7%)	0	100	100
9	BL	423/445 (95%)	395 (93%)	28 (7%)	0	100	100
9	CB	424/445 (95%)	386 (91%)	37 (9%)	1 (0%)	47	78
9	CD	424/445 (95%)	392 (92%)	32 (8%)	0	100	100
9	CF	426/445 (96%)	393 (92%)	33 (8%)	0	100	100
9	CH	425/445 (96%)	390 (92%)	35 (8%)	0	100	100
9	CJ	426/445 (96%)	396 (93%)	30 (7%)	0	100	100
9	CL	423/445 (95%)	397 (94%)	25 (6%)	1 (0%)	47	78
9	DB	424/445 (95%)	393 (93%)	31 (7%)	0	100	100
9	DD	424/445 (95%)	384 (91%)	40 (9%)	0	100	100
9	DF	424/445 (95%)	383 (90%)	41 (10%)	0	100	100
9	DH	424/445 (95%)	375 (88%)	48 (11%)	1 (0%)	47	78
9	DJ	424/445 (95%)	387 (91%)	37 (9%)	0	100	100
9	DL	423/445 (95%)	391 (92%)	32 (8%)	0	100	100
9	DN	381/445 (86%)	358 (94%)	23 (6%)	0	100	100
9	EB	424/445 (95%)	392 (92%)	32 (8%)	0	100	100
9	ED	424/445 (95%)	383 (90%)	41 (10%)	0	100	100
9	EF	424/445 (95%)	379 (89%)	45 (11%)	0	100	100
9	EH	426/445 (96%)	377 (88%)	47 (11%)	2 (0%)	29	61
9	EJ	424/445 (95%)	386 (91%)	37 (9%)	1 (0%)	47	78
9	EL	423/445 (95%)	378 (89%)	45 (11%)	0	100	100
9	EN	424/445 (95%)	385 (91%)	39 (9%)	0	100	100
9	FB	424/445 (95%)	391 (92%)	33 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	FD	425/445 (96%)	388 (91%)	37 (9%)	0	100	100
9	FF	424/445 (95%)	373 (88%)	49 (12%)	2 (0%)	29	61
9	FH	424/445 (95%)	369 (87%)	53 (12%)	2 (0%)	29	61
9	FJ	424/445 (95%)	397 (94%)	27 (6%)	0	100	100
9	FL	423/445 (95%)	386 (91%)	37 (9%)	0	100	100
9	FN	426/445 (96%)	390 (92%)	36 (8%)	0	100	100
9	GB	426/445 (96%)	397 (93%)	29 (7%)	0	100	100
9	GD	425/445 (96%)	399 (94%)	26 (6%)	0	100	100
9	GF	426/445 (96%)	398 (93%)	28 (7%)	0	100	100
9	GH	426/445 (96%)	389 (91%)	37 (9%)	0	100	100
9	GJ	426/445 (96%)	398 (93%)	28 (7%)	0	100	100
9	GL	423/445 (95%)	394 (93%)	29 (7%)	0	100	100
9	GN	426/445 (96%)	400 (94%)	26 (6%)	0	100	100
9	HB	424/445 (95%)	397 (94%)	27 (6%)	0	100	100
9	HD	425/445 (96%)	397 (93%)	28 (7%)	0	100	100
9	HF	426/445 (96%)	405 (95%)	21 (5%)	0	100	100
9	HH	425/445 (96%)	393 (92%)	31 (7%)	1 (0%)	47	78
9	HJ	426/445 (96%)	402 (94%)	24 (6%)	0	100	100
9	HL	423/445 (95%)	395 (93%)	27 (6%)	1 (0%)	47	78
9	HN	425/445 (96%)	399 (94%)	26 (6%)	0	100	100
9	IB	360/445 (81%)	338 (94%)	22 (6%)	0	100	100
9	ID	425/445 (96%)	391 (92%)	34 (8%)	0	100	100
9	IF	426/445 (96%)	394 (92%)	32 (8%)	0	100	100
9	IH	425/445 (96%)	388 (91%)	35 (8%)	2 (0%)	29	61
9	IJ	426/445 (96%)	391 (92%)	34 (8%)	1 (0%)	47	78
9	IL	424/445 (95%)	384 (91%)	39 (9%)	1 (0%)	47	78
9	IN	426/445 (96%)	391 (92%)	35 (8%)	0	100	100
9	JB	424/445 (95%)	383 (90%)	41 (10%)	0	100	100
9	JD	425/445 (96%)	384 (90%)	41 (10%)	0	100	100
9	JF	424/445 (95%)	393 (93%)	31 (7%)	0	100	100
9	JH	424/445 (95%)	389 (92%)	35 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	JJ	424/445 (95%)	392 (92%)	32 (8%)	0	100	100
9	JL	424/445 (95%)	376 (89%)	47 (11%)	1 (0%)	47	78
9	JN	424/445 (95%)	390 (92%)	34 (8%)	0	100	100
9	KB	397/445 (89%)	378 (95%)	19 (5%)	0	100	100
9	KD	426/445 (96%)	397 (93%)	29 (7%)	0	100	100
9	KF	425/445 (96%)	398 (94%)	27 (6%)	0	100	100
9	KH	427/445 (96%)	406 (95%)	21 (5%)	0	100	100
9	KJ	424/445 (95%)	397 (94%)	27 (6%)	0	100	100
9	KL	427/445 (96%)	399 (93%)	28 (7%)	0	100	100
9	KN	426/445 (96%)	412 (97%)	14 (3%)	0	100	100
9	LB	426/445 (96%)	403 (95%)	23 (5%)	0	100	100
9	LD	425/445 (96%)	397 (93%)	28 (7%)	0	100	100
9	LF	426/445 (96%)	401 (94%)	25 (6%)	0	100	100
9	LH	426/445 (96%)	398 (93%)	28 (7%)	0	100	100
9	LJ	426/445 (96%)	401 (94%)	25 (6%)	0	100	100
9	LL	424/445 (95%)	398 (94%)	26 (6%)	0	100	100
9	LN	426/445 (96%)	401 (94%)	25 (6%)	0	100	100
9	MB	424/445 (95%)	390 (92%)	34 (8%)	0	100	100
9	MD	424/445 (95%)	384 (91%)	40 (9%)	0	100	100
9	MF	426/445 (96%)	392 (92%)	34 (8%)	0	100	100
9	MH	426/445 (96%)	395 (93%)	31 (7%)	0	100	100
9	MJ	424/445 (95%)	390 (92%)	34 (8%)	0	100	100
9	ML	424/445 (95%)	387 (91%)	37 (9%)	0	100	100
9	MN	424/445 (95%)	383 (90%)	41 (10%)	0	100	100
9	NO	425/445 (96%)	398 (94%)	27 (6%)	0	100	100
9	NB	426/445 (96%)	386 (91%)	40 (9%)	0	100	100
9	ND	425/445 (96%)	394 (93%)	31 (7%)	0	100	100
9	NF	425/445 (96%)	387 (91%)	38 (9%)	0	100	100
9	NH	426/445 (96%)	393 (92%)	32 (8%)	1 (0%)	47	78
9	NJ	426/445 (96%)	396 (93%)	30 (7%)	0	100	100
9	NL	423/445 (95%)	398 (94%)	25 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	O0	408/445 (92%)	383 (94%)	25 (6%)	0	100	100
9	OB	423/445 (95%)	395 (93%)	28 (7%)	0	100	100
9	OD	422/445 (95%)	402 (95%)	20 (5%)	0	100	100
9	OF	423/445 (95%)	390 (92%)	33 (8%)	0	100	100
9	OH	426/445 (96%)	399 (94%)	27 (6%)	0	100	100
9	OJ	426/445 (96%)	398 (93%)	28 (7%)	0	100	100
9	OL	422/445 (95%)	390 (92%)	32 (8%)	0	100	100
9	PB	425/445 (96%)	393 (92%)	31 (7%)	1 (0%)	47	78
9	PD	425/445 (96%)	395 (93%)	30 (7%)	0	100	100
9	PF	426/445 (96%)	400 (94%)	26 (6%)	0	100	100
9	PH	426/445 (96%)	397 (93%)	29 (7%)	0	100	100
9	PJ	426/445 (96%)	399 (94%)	27 (6%)	0	100	100
9	PL	423/445 (95%)	394 (93%)	29 (7%)	0	100	100
9	QB	426/445 (96%)	396 (93%)	30 (7%)	0	100	100
9	QD	425/445 (96%)	399 (94%)	26 (6%)	0	100	100
9	QF	426/445 (96%)	389 (91%)	37 (9%)	0	100	100
9	QH	426/445 (96%)	386 (91%)	39 (9%)	1 (0%)	47	78
9	QJ	426/445 (96%)	392 (92%)	34 (8%)	0	100	100
9	QL	424/445 (95%)	399 (94%)	25 (6%)	0	100	100
9	RB	426/445 (96%)	384 (90%)	42 (10%)	0	100	100
9	RD	425/445 (96%)	394 (93%)	31 (7%)	0	100	100
9	RF	426/445 (96%)	390 (92%)	36 (8%)	0	100	100
9	RH	426/445 (96%)	397 (93%)	29 (7%)	0	100	100
9	RJ	426/445 (96%)	397 (93%)	29 (7%)	0	100	100
9	RL	424/445 (95%)	386 (91%)	38 (9%)	0	100	100
9	SB	426/445 (96%)	385 (90%)	40 (9%)	1 (0%)	47	78
9	SD	425/445 (96%)	394 (93%)	31 (7%)	0	100	100
9	SF	426/445 (96%)	393 (92%)	33 (8%)	0	100	100
9	SH	426/445 (96%)	396 (93%)	29 (7%)	1 (0%)	47	78
9	SJ	426/445 (96%)	398 (93%)	28 (7%)	0	100	100
9	SL	424/445 (95%)	391 (92%)	33 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	TB	426/445 (96%)	393 (92%)	33 (8%)	0	100	100
9	TD	425/445 (96%)	394 (93%)	31 (7%)	0	100	100
9	TF	426/445 (96%)	392 (92%)	34 (8%)	0	100	100
9	TH	426/445 (96%)	405 (95%)	21 (5%)	0	100	100
9	TJ	426/445 (96%)	383 (90%)	43 (10%)	0	100	100
9	TL	424/445 (95%)	389 (92%)	35 (8%)	0	100	100
9	UB	426/445 (96%)	393 (92%)	33 (8%)	0	100	100
9	UD	425/445 (96%)	392 (92%)	33 (8%)	0	100	100
9	UF	426/445 (96%)	396 (93%)	30 (7%)	0	100	100
9	UH	426/445 (96%)	399 (94%)	27 (6%)	0	100	100
9	UJ	426/445 (96%)	392 (92%)	34 (8%)	0	100	100
9	UL	424/445 (95%)	383 (90%)	41 (10%)	0	100	100
9	UN	426/445 (96%)	404 (95%)	22 (5%)	0	100	100
9	VB	426/445 (96%)	384 (90%)	42 (10%)	0	100	100
9	VD	425/445 (96%)	393 (92%)	32 (8%)	0	100	100
9	VF	425/445 (96%)	395 (93%)	30 (7%)	0	100	100
9	VH	426/445 (96%)	400 (94%)	26 (6%)	0	100	100
9	VJ	426/445 (96%)	396 (93%)	30 (7%)	0	100	100
9	VL	424/445 (95%)	384 (91%)	40 (9%)	0	100	100
9	VN	426/445 (96%)	400 (94%)	26 (6%)	0	100	100
9	WB	426/445 (96%)	381 (89%)	45 (11%)	0	100	100
9	WD	425/445 (96%)	388 (91%)	37 (9%)	0	100	100
9	WF	424/445 (95%)	396 (93%)	28 (7%)	0	100	100
9	WH	424/445 (95%)	391 (92%)	33 (8%)	0	100	100
9	WJ	424/445 (95%)	399 (94%)	25 (6%)	0	100	100
9	WL	424/445 (95%)	386 (91%)	38 (9%)	0	100	100
9	WN	424/445 (95%)	397 (94%)	27 (6%)	0	100	100
10	B0	185/430 (43%)	181 (98%)	4 (2%)	0	100	100
10	B1	414/430 (96%)	406 (98%)	8 (2%)	0	100	100
10	B2	414/430 (96%)	397 (96%)	17 (4%)	0	100	100
10	B3	381/430 (89%)	367 (96%)	13 (3%)	1 (0%)	41	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	B4	47/430 (11%)	46 (98%)	1 (2%)	0	100	100
10	B5	49/430 (11%)	46 (94%)	3 (6%)	0	100	100
10	B6	356/430 (83%)	354 (99%)	2 (1%)	0	100	100
10	B7	412/430 (96%)	402 (98%)	10 (2%)	0	100	100
10	B8	401/430 (93%)	390 (97%)	11 (3%)	0	100	100
10	B9	183/430 (43%)	176 (96%)	7 (4%)	0	100	100
11	C	89/101 (88%)	89 (100%)	0	0	100	100
12	C0	28/490 (6%)	28 (100%)	0	0	100	100
12	C1	330/490 (67%)	320 (97%)	10 (3%)	0	100	100
12	C2	392/490 (80%)	387 (99%)	5 (1%)	0	100	100
12	C3	392/490 (80%)	378 (96%)	14 (4%)	0	100	100
12	C4	211/490 (43%)	203 (96%)	7 (3%)	1 (0%)	29	61
12	C5	111/490 (23%)	109 (98%)	2 (2%)	0	100	100
12	C6	383/490 (78%)	376 (98%)	7 (2%)	0	100	100
12	C7	411/490 (84%)	402 (98%)	8 (2%)	1 (0%)	47	78
12	C8	403/490 (82%)	395 (98%)	7 (2%)	1 (0%)	47	78
12	C9	108/490 (22%)	107 (99%)	1 (1%)	0	100	100
12	F0	133/490 (27%)	127 (96%)	6 (4%)	0	100	100
12	F1	417/490 (85%)	402 (96%)	15 (4%)	0	100	100
12	F2	417/490 (85%)	403 (97%)	14 (3%)	0	100	100
12	F3	376/490 (77%)	369 (98%)	7 (2%)	0	100	100
12	F4	97/490 (20%)	92 (95%)	5 (5%)	0	100	100
13	D	141/484 (29%)	128 (91%)	13 (9%)	0	100	100
14	D0	285/447 (64%)	280 (98%)	5 (2%)	0	100	100
14	D1	423/447 (95%)	409 (97%)	14 (3%)	0	100	100
14	D2	423/447 (95%)	413 (98%)	10 (2%)	0	100	100
14	D3	312/447 (70%)	308 (99%)	4 (1%)	0	100	100
14	D5	7/447 (2%)	7 (100%)	0	0	100	100
14	D6	315/447 (70%)	307 (98%)	8 (2%)	0	100	100
14	D7	412/447 (92%)	397 (96%)	14 (3%)	1 (0%)	47	78
14	D8	411/447 (92%)	401 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	D9	271/447 (61%)	261 (96%)	10 (4%)	0	100	100
15	E	251/321 (78%)	230 (92%)	21 (8%)	0	100	100
15	F	251/321 (78%)	220 (88%)	30 (12%)	1 (0%)	34	67
16	E0	66/208 (32%)	60 (91%)	6 (9%)	0	100	100
16	E1	125/208 (60%)	112 (90%)	12 (10%)	1 (1%)	19	51
16	E2	142/208 (68%)	129 (91%)	12 (8%)	1 (1%)	22	55
16	E3	142/208 (68%)	129 (91%)	12 (8%)	1 (1%)	22	55
17	G	94/120 (78%)	86 (92%)	8 (8%)	0	100	100
18	H	80/274 (29%)	70 (88%)	10 (12%)	0	100	100
18	I	144/274 (53%)	139 (96%)	5 (4%)	0	100	100
18	J	144/274 (53%)	131 (91%)	13 (9%)	0	100	100
18	K	144/274 (53%)	131 (91%)	13 (9%)	0	100	100
18	L	144/274 (53%)	137 (95%)	7 (5%)	0	100	100
18	M	144/274 (53%)	136 (94%)	8 (6%)	0	100	100
18	N	147/274 (54%)	135 (92%)	12 (8%)	0	100	100
19	H1	190/687 (28%)	188 (99%)	2 (1%)	0	100	100
19	H2	248/687 (36%)	243 (98%)	5 (2%)	0	100	100
19	H3	103/687 (15%)	102 (99%)	1 (1%)	0	100	100
20	H4	191/621 (31%)	186 (97%)	5 (3%)	0	100	100
20	H5	247/621 (40%)	246 (100%)	1 (0%)	0	100	100
20	H6	123/621 (20%)	121 (98%)	2 (2%)	0	100	100
21	H7	576/1044 (55%)	541 (94%)	34 (6%)	1 (0%)	47	78
21	H8	575/1044 (55%)	543 (94%)	31 (5%)	1 (0%)	47	78
21	H9	354/1044 (34%)	338 (96%)	16 (4%)	0	100	100
22	I1	188/683 (28%)	176 (94%)	12 (6%)	0	100	100
22	I2	188/683 (28%)	181 (96%)	7 (4%)	0	100	100
23	I3	182/212 (86%)	174 (96%)	7 (4%)	1 (0%)	29	61
23	I4	183/212 (86%)	175 (96%)	7 (4%)	1 (0%)	29	61
24	O	29/377 (8%)	29 (100%)	0	0	100	100
24	P	371/377 (98%)	359 (97%)	12 (3%)	0	100	100
24	Q	37/377 (10%)	34 (92%)	3 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	R	247/377 (66%)	240 (97%)	7 (3%)	0	100	100
24	S	168/377 (45%)	167 (99%)	1 (1%)	0	100	100
25	T	446/640 (70%)	404 (91%)	41 (9%)	1 (0%)	47	78
25	U	446/640 (70%)	396 (89%)	50 (11%)	0	100	100
25	V	446/640 (70%)	405 (91%)	41 (9%)	0	100	100
26	W	543/733 (74%)	484 (89%)	58 (11%)	1 (0%)	47	78
26	X	624/733 (85%)	560 (90%)	64 (10%)	0	100	100
26	Y	624/733 (85%)	567 (91%)	57 (9%)	0	100	100
26	Z	439/733 (60%)	400 (91%)	39 (9%)	0	100	100
27	XA	182/193 (94%)	168 (92%)	14 (8%)	0	100	100
27	XB	182/193 (94%)	162 (89%)	20 (11%)	0	100	100
27	XC	182/193 (94%)	163 (90%)	19 (10%)	0	100	100
27	XD	182/193 (94%)	167 (92%)	15 (8%)	0	100	100
27	XE	182/193 (94%)	168 (92%)	13 (7%)	1 (0%)	29	61
27	XF	182/193 (94%)	165 (91%)	17 (9%)	0	100	100
27	XG	182/193 (94%)	168 (92%)	14 (8%)	0	100	100
28	YB	217/257 (84%)	194 (89%)	23 (11%)	0	100	100
28	YC	217/257 (84%)	196 (90%)	21 (10%)	0	100	100
28	YD	217/257 (84%)	196 (90%)	21 (10%)	0	100	100
28	YE	217/257 (84%)	202 (93%)	15 (7%)	0	100	100
28	YF	217/257 (84%)	201 (93%)	16 (7%)	0	100	100
28	YG	217/257 (84%)	198 (91%)	18 (8%)	1 (0%)	29	61
29	a	163/549 (30%)	162 (99%)	1 (1%)	0	100	100
29	b	330/549 (60%)	327 (99%)	3 (1%)	0	100	100
29	c	271/549 (49%)	271 (100%)	0	0	100	100
29	d	213/549 (39%)	209 (98%)	4 (2%)	0	100	100
30	e	608/623 (98%)	541 (89%)	67 (11%)	0	100	100
30	f	608/623 (98%)	530 (87%)	77 (13%)	1 (0%)	47	78
30	g	608/623 (98%)	536 (88%)	70 (12%)	2 (0%)	41	72
31	h	146/259 (56%)	139 (95%)	7 (5%)	0	100	100
31	i	231/259 (89%)	222 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	j	231/259 (89%)	219 (95%)	12 (5%)	0	100	100
31	k	231/259 (89%)	224 (97%)	7 (3%)	0	100	100
32	l	112/196 (57%)	102 (91%)	10 (9%)	0	100	100
32	m	114/196 (58%)	106 (93%)	8 (7%)	0	100	100
32	n	116/196 (59%)	108 (93%)	8 (7%)	0	100	100
33	o	370/547 (68%)	367 (99%)	3 (1%)	0	100	100
33	p	98/547 (18%)	96 (98%)	2 (2%)	0	100	100
34	q	75/170 (44%)	70 (93%)	5 (7%)	0	100	100
34	r	75/170 (44%)	68 (91%)	7 (9%)	0	100	100
34	s	75/170 (44%)	67 (89%)	8 (11%)	0	100	100
35	t	176/1497 (12%)	162 (92%)	14 (8%)	0	100	100
36	y	61/136 (45%)	55 (90%)	6 (10%)	0	100	100
36	z	113/136 (83%)	108 (96%)	5 (4%)	0	100	100
All	All	160251/190211 (84%)	148753 (93%)	11437 (7%)	61 (0%)	100	100

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	EH	180	VAL
8	GK	224	TYR
8	GM	130	THR
9	QH	393	ALA
8	SK	268	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	0	36/208 (17%)	36 (100%)	0	100	100
1	7	57/208 (27%)	56 (98%)	1 (2%)	59	79
2	1	47/750 (6%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	20/750 (3%)	20 (100%)	0	100	100
3	3	199/469 (42%)	199 (100%)	0	100	100
3	4	200/469 (43%)	198 (99%)	2 (1%)	76	88
4	5	191/324 (59%)	186 (97%)	5 (3%)	46	72
4	6	319/324 (98%)	313 (98%)	6 (2%)	57	78
5	8	177/182 (97%)	172 (97%)	5 (3%)	43	70
5	9	33/182 (18%)	33 (100%)	0	100	100
6	A	151/451 (34%)	150 (99%)	1 (1%)	84	92
6	B	321/451 (71%)	319 (99%)	2 (1%)	86	94
7	A0	201/382 (53%)	200 (100%)	1 (0%)	88	94
7	A1	366/382 (96%)	364 (100%)	2 (0%)	88	94
7	A2	364/382 (95%)	361 (99%)	3 (1%)	81	91
7	A3	311/382 (81%)	311 (100%)	0	100	100
7	A4	29/382 (8%)	29 (100%)	0	100	100
8	AA	368/379 (97%)	367 (100%)	1 (0%)	92	97
8	AC	370/379 (98%)	368 (100%)	2 (0%)	88	94
8	AE	370/379 (98%)	370 (100%)	0	100	100
8	AG	370/379 (98%)	370 (100%)	0	100	100
8	AI	370/379 (98%)	368 (100%)	2 (0%)	88	94
8	AK	370/379 (98%)	370 (100%)	0	100	100
8	AM	369/379 (97%)	367 (100%)	2 (0%)	88	94
8	BA	363/379 (96%)	363 (100%)	0	100	100
8	BC	370/379 (98%)	369 (100%)	1 (0%)	92	97
8	BE	366/379 (97%)	366 (100%)	0	100	100
8	BG	370/379 (98%)	369 (100%)	1 (0%)	92	97
8	BI	363/379 (96%)	363 (100%)	0	100	100
8	BK	369/379 (97%)	367 (100%)	2 (0%)	88	94
8	BM	363/379 (96%)	361 (99%)	2 (1%)	86	94
8	CA	368/379 (97%)	366 (100%)	2 (0%)	88	94
8	CC	368/379 (97%)	366 (100%)	2 (0%)	88	94
8	CE	368/379 (97%)	367 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CG	369/379 (97%)	366 (99%)	3 (1%)	81	91
8	CI	369/379 (97%)	369 (100%)	0	100	100
8	CK	369/379 (97%)	369 (100%)	0	100	100
8	CM	369/379 (97%)	368 (100%)	1 (0%)	92	97
8	DA	341/379 (90%)	340 (100%)	1 (0%)	92	97
8	DC	362/379 (96%)	360 (99%)	2 (1%)	86	94
8	DE	363/379 (96%)	362 (100%)	1 (0%)	92	97
8	DG	364/379 (96%)	364 (100%)	0	100	100
8	DI	362/379 (96%)	362 (100%)	0	100	100
8	DK	363/379 (96%)	363 (100%)	0	100	100
8	DM	363/379 (96%)	357 (98%)	6 (2%)	60	80
8	EC	369/379 (97%)	367 (100%)	2 (0%)	88	94
8	EE	371/379 (98%)	368 (99%)	3 (1%)	81	91
8	EG	367/379 (97%)	366 (100%)	1 (0%)	92	97
8	EI	366/379 (97%)	359 (98%)	7 (2%)	57	78
8	EK	370/379 (98%)	360 (97%)	10 (3%)	44	70
8	EM	361/379 (95%)	358 (99%)	3 (1%)	81	91
8	FC	364/379 (96%)	362 (100%)	2 (0%)	88	94
8	FE	359/379 (95%)	358 (100%)	1 (0%)	92	97
8	FG	360/379 (95%)	358 (99%)	2 (1%)	86	94
8	FI	360/379 (95%)	359 (100%)	1 (0%)	92	97
8	FK	358/379 (94%)	356 (99%)	2 (1%)	86	94
8	FM	362/379 (96%)	362 (100%)	0	100	100
8	GC	370/379 (98%)	368 (100%)	2 (0%)	88	94
8	GE	363/379 (96%)	363 (100%)	0	100	100
8	GG	370/379 (98%)	369 (100%)	1 (0%)	92	97
8	GI	362/379 (96%)	362 (100%)	0	100	100
8	GK	362/379 (96%)	359 (99%)	3 (1%)	81	91
8	GM	369/379 (97%)	367 (100%)	2 (0%)	88	94
8	HC	360/379 (95%)	358 (99%)	2 (1%)	86	94
8	HE	363/379 (96%)	362 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	HG	363/379 (96%)	360 (99%)	3 (1%)	81	91
8	HI	363/379 (96%)	362 (100%)	1 (0%)	92	97
8	HK	364/379 (96%)	363 (100%)	1 (0%)	92	97
8	HM	362/379 (96%)	360 (99%)	2 (1%)	86	94
8	HO	326/379 (86%)	326 (100%)	0	100	100
8	IC	362/379 (96%)	361 (100%)	1 (0%)	92	97
8	IE	365/379 (96%)	365 (100%)	0	100	100
8	IG	370/379 (98%)	370 (100%)	0	100	100
8	II	365/379 (96%)	362 (99%)	3 (1%)	81	91
8	IK	370/379 (98%)	368 (100%)	2 (0%)	88	94
8	IM	364/379 (96%)	364 (100%)	0	100	100
8	IO	360/379 (95%)	360 (100%)	0	100	100
8	JC	364/379 (96%)	364 (100%)	0	100	100
8	JE	363/379 (96%)	361 (99%)	2 (1%)	86	94
8	JG	361/379 (95%)	360 (100%)	1 (0%)	92	97
8	JI	362/379 (96%)	361 (100%)	1 (0%)	92	97
8	JK	370/379 (98%)	369 (100%)	1 (0%)	92	97
8	JM	363/379 (96%)	361 (99%)	2 (1%)	86	94
8	KC	364/379 (96%)	363 (100%)	1 (0%)	92	97
8	KE	364/379 (96%)	363 (100%)	1 (0%)	92	97
8	KG	362/379 (96%)	362 (100%)	0	100	100
8	KI	361/379 (95%)	357 (99%)	4 (1%)	73	86
8	KK	363/379 (96%)	363 (100%)	0	100	100
8	KM	362/379 (96%)	362 (100%)	0	100	100
8	KO	346/379 (91%)	345 (100%)	1 (0%)	92	97
8	LC	370/379 (98%)	369 (100%)	1 (0%)	92	97
8	LE	370/379 (98%)	368 (100%)	2 (0%)	88	94
8	LG	370/379 (98%)	370 (100%)	0	100	100
8	LI	370/379 (98%)	369 (100%)	1 (0%)	92	97
8	LK	370/379 (98%)	370 (100%)	0	100	100
8	LM	364/379 (96%)	364 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	MC	369/379 (97%)	367 (100%)	2 (0%)	88	94
8	ME	362/379 (96%)	362 (100%)	0	100	100
8	MG	363/379 (96%)	362 (100%)	1 (0%)	92	97
8	MI	364/379 (96%)	363 (100%)	1 (0%)	92	97
8	MK	370/379 (98%)	368 (100%)	2 (0%)	88	94
8	MM	363/379 (96%)	362 (100%)	1 (0%)	92	97
8	NA	363/379 (96%)	361 (99%)	2 (1%)	86	94
8	NC	362/379 (96%)	361 (100%)	1 (0%)	92	97
8	NE	363/379 (96%)	361 (99%)	2 (1%)	86	94
8	NG	365/379 (96%)	364 (100%)	1 (0%)	92	97
8	NI	365/379 (96%)	363 (100%)	2 (0%)	88	94
8	NK	363/379 (96%)	363 (100%)	0	100	100
8	OA	361/379 (95%)	358 (99%)	3 (1%)	81	91
8	OC	362/379 (96%)	358 (99%)	4 (1%)	73	86
8	OE	366/379 (97%)	365 (100%)	1 (0%)	92	97
8	OG	365/379 (96%)	364 (100%)	1 (0%)	92	97
8	OI	365/379 (96%)	361 (99%)	4 (1%)	73	86
8	OK	364/379 (96%)	361 (99%)	3 (1%)	81	91
8	PA	363/379 (96%)	360 (99%)	3 (1%)	81	91
8	PC	365/379 (96%)	364 (100%)	1 (0%)	92	97
8	PE	364/379 (96%)	359 (99%)	5 (1%)	67	83
8	PG	363/379 (96%)	362 (100%)	1 (0%)	92	97
8	PI	360/379 (95%)	358 (99%)	2 (1%)	86	94
8	PK	363/379 (96%)	360 (99%)	3 (1%)	81	91
8	PM	363/379 (96%)	361 (99%)	2 (1%)	86	94
8	QA	363/379 (96%)	359 (99%)	4 (1%)	73	86
8	QC	363/379 (96%)	361 (99%)	2 (1%)	86	94
8	QE	363/379 (96%)	361 (99%)	2 (1%)	86	94
8	QG	364/379 (96%)	363 (100%)	1 (0%)	92	97
8	QI	362/379 (96%)	359 (99%)	3 (1%)	81	91
8	QK	364/379 (96%)	362 (100%)	2 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QM	364/379 (96%)	358 (98%)	6 (2%)	62	81
8	RA	362/379 (96%)	362 (100%)	0	100	100
8	RC	365/379 (96%)	363 (100%)	2 (0%)	88	94
8	RE	361/379 (95%)	358 (99%)	3 (1%)	81	91
8	RG	363/379 (96%)	360 (99%)	3 (1%)	81	91
8	RI	364/379 (96%)	363 (100%)	1 (0%)	92	97
8	RK	364/379 (96%)	361 (99%)	3 (1%)	81	91
8	RM	361/379 (95%)	359 (99%)	2 (1%)	86	94
8	SA	363/379 (96%)	362 (100%)	1 (0%)	92	97
8	SC	363/379 (96%)	360 (99%)	3 (1%)	81	91
8	SE	364/379 (96%)	362 (100%)	2 (0%)	88	94
8	SG	364/379 (96%)	361 (99%)	3 (1%)	81	91
8	SI	363/379 (96%)	362 (100%)	1 (0%)	92	97
8	SK	365/379 (96%)	365 (100%)	0	100	100
8	SM	364/379 (96%)	362 (100%)	2 (0%)	88	94
8	TC	363/379 (96%)	358 (99%)	5 (1%)	67	83
8	TE	365/379 (96%)	363 (100%)	2 (0%)	88	94
8	TG	363/379 (96%)	363 (100%)	0	100	100
8	TI	363/379 (96%)	361 (99%)	2 (1%)	86	94
8	TK	365/379 (96%)	363 (100%)	2 (0%)	88	94
8	TM	363/379 (96%)	362 (100%)	1 (0%)	92	97
8	UC	366/379 (97%)	364 (100%)	2 (0%)	88	94
8	UE	365/379 (96%)	364 (100%)	1 (0%)	92	97
8	UG	366/379 (97%)	364 (100%)	2 (0%)	88	94
8	UI	366/379 (97%)	362 (99%)	4 (1%)	73	86
8	UK	365/379 (96%)	364 (100%)	1 (0%)	92	97
8	UM	364/379 (96%)	363 (100%)	1 (0%)	92	97
8	VC	370/379 (98%)	370 (100%)	0	100	100
8	VE	366/379 (97%)	363 (99%)	3 (1%)	81	91
8	VG	370/379 (98%)	363 (98%)	7 (2%)	57	78
8	VI	366/379 (97%)	365 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	VK	370/379 (98%)	369 (100%)	1 (0%)	92	97
8	VM	363/379 (96%)	362 (100%)	1 (0%)	92	97
8	WC	370/379 (98%)	368 (100%)	2 (0%)	88	94
8	WE	364/379 (96%)	363 (100%)	1 (0%)	92	97
8	WG	369/379 (97%)	368 (100%)	1 (0%)	92	97
8	WI	364/379 (96%)	361 (99%)	3 (1%)	81	91
8	WK	368/379 (97%)	366 (100%)	2 (0%)	88	94
8	WM	364/379 (96%)	362 (100%)	2 (0%)	88	94
9	AB	373/380 (98%)	372 (100%)	1 (0%)	92	97
9	AD	373/380 (98%)	370 (99%)	3 (1%)	81	91
9	AF	373/380 (98%)	369 (99%)	4 (1%)	73	86
9	AH	373/380 (98%)	373 (100%)	0	100	100
9	AJ	373/380 (98%)	364 (98%)	9 (2%)	49	74
9	AL	372/380 (98%)	370 (100%)	2 (0%)	88	94
9	BB	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	BD	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	BF	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	BH	367/380 (97%)	361 (98%)	6 (2%)	62	81
9	BJ	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	BL	365/380 (96%)	364 (100%)	1 (0%)	92	97
9	CB	366/380 (96%)	366 (100%)	0	100	100
9	CD	366/380 (96%)	366 (100%)	0	100	100
9	CF	367/380 (97%)	367 (100%)	0	100	100
9	CH	367/380 (97%)	361 (98%)	6 (2%)	62	81
9	CJ	367/380 (97%)	359 (98%)	8 (2%)	52	75
9	CL	365/380 (96%)	361 (99%)	4 (1%)	73	86
9	DB	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	DD	366/380 (96%)	366 (100%)	0	100	100
9	DF	366/380 (96%)	366 (100%)	0	100	100
9	DH	366/380 (96%)	359 (98%)	7 (2%)	57	78
9	DJ	366/380 (96%)	365 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	DL	365/380 (96%)	363 (100%)	2 (0%)	88	94
9	DN	330/380 (87%)	328 (99%)	2 (1%)	86	94
9	EB	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	ED	366/380 (96%)	362 (99%)	4 (1%)	73	86
9	EF	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	EH	367/380 (97%)	363 (99%)	4 (1%)	73	86
9	EJ	366/380 (96%)	362 (99%)	4 (1%)	73	86
9	EL	365/380 (96%)	362 (99%)	3 (1%)	81	91
9	EN	366/380 (96%)	364 (100%)	2 (0%)	88	94
9	FB	366/380 (96%)	366 (100%)	0	100	100
9	FD	367/380 (97%)	367 (100%)	0	100	100
9	FF	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	FH	366/380 (96%)	364 (100%)	2 (0%)	88	94
9	FJ	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	FL	365/380 (96%)	360 (99%)	5 (1%)	67	83
9	FN	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	GB	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	GD	367/380 (97%)	367 (100%)	0	100	100
9	GF	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	GH	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	GJ	367/380 (97%)	367 (100%)	0	100	100
9	GL	365/380 (96%)	364 (100%)	1 (0%)	92	97
9	GN	367/380 (97%)	367 (100%)	0	100	100
9	HB	366/380 (96%)	366 (100%)	0	100	100
9	HD	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	HF	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	HH	367/380 (97%)	367 (100%)	0	100	100
9	HJ	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	HL	365/380 (96%)	361 (99%)	4 (1%)	73	86
9	HN	367/380 (97%)	367 (100%)	0	100	100
9	IB	322/380 (85%)	321 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	ID	367/380 (97%)	363 (99%)	4 (1%)	73	86
9	IF	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	IH	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	IJ	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	IL	366/380 (96%)	360 (98%)	6 (2%)	62	81
9	IN	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	JB	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	JD	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	JF	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	JH	366/380 (96%)	364 (100%)	2 (0%)	88	94
9	JJ	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	JL	366/380 (96%)	362 (99%)	4 (1%)	73	86
9	JN	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	KB	350/380 (92%)	350 (100%)	0	100	100
9	KD	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	KF	367/380 (97%)	367 (100%)	0	100	100
9	KH	368/380 (97%)	367 (100%)	1 (0%)	92	97
9	KJ	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	KL	368/380 (97%)	368 (100%)	0	100	100
9	KN	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	LB	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	LD	367/380 (97%)	367 (100%)	0	100	100
9	LF	367/380 (97%)	367 (100%)	0	100	100
9	LH	367/380 (97%)	367 (100%)	0	100	100
9	LJ	367/380 (97%)	367 (100%)	0	100	100
9	LL	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	LN	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	MB	366/380 (96%)	359 (98%)	7 (2%)	57	78
9	MD	366/380 (96%)	366 (100%)	0	100	100
9	MF	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	MH	367/380 (97%)	367 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	MJ	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	ML	366/380 (96%)	362 (99%)	4 (1%)	73	86
9	MN	366/380 (96%)	365 (100%)	1 (0%)	92	97
9	NO	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	NB	367/380 (97%)	354 (96%)	13 (4%)	36	65
9	ND	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	NF	367/380 (97%)	360 (98%)	7 (2%)	57	78
9	NH	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	NJ	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	NL	365/380 (96%)	360 (99%)	5 (1%)	67	83
9	OO	354/380 (93%)	353 (100%)	1 (0%)	92	97
9	OB	365/380 (96%)	365 (100%)	0	100	100
9	OD	364/380 (96%)	362 (100%)	2 (0%)	88	94
9	OF	365/380 (96%)	365 (100%)	0	100	100
9	OH	367/380 (97%)	367 (100%)	0	100	100
9	OJ	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	OL	364/380 (96%)	364 (100%)	0	100	100
9	PB	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	PD	367/380 (97%)	367 (100%)	0	100	100
9	PF	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	PH	367/380 (97%)	367 (100%)	0	100	100
9	PJ	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	PL	365/380 (96%)	358 (98%)	7 (2%)	57	78
9	QB	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	QD	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	QF	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	QH	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	QJ	367/380 (97%)	367 (100%)	0	100	100
9	QL	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	RB	367/380 (97%)	367 (100%)	0	100	100
9	RD	367/380 (97%)	366 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	RF	367/380 (97%)	363 (99%)	4 (1%)	73	86
9	RH	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	RJ	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	RL	366/380 (96%)	361 (99%)	5 (1%)	67	83
9	SB	367/380 (97%)	361 (98%)	6 (2%)	62	81
9	SD	367/380 (97%)	367 (100%)	0	100	100
9	SF	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	SH	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	SJ	367/380 (97%)	367 (100%)	0	100	100
9	SL	366/380 (96%)	366 (100%)	0	100	100
9	TB	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	TD	367/380 (97%)	363 (99%)	4 (1%)	73	86
9	TF	367/380 (97%)	367 (100%)	0	100	100
9	TH	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	TJ	367/380 (97%)	367 (100%)	0	100	100
9	TL	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	UB	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	UD	367/380 (97%)	367 (100%)	0	100	100
9	UF	367/380 (97%)	364 (99%)	3 (1%)	81	91
9	UH	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	UJ	367/380 (97%)	360 (98%)	7 (2%)	57	78
9	UL	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	UN	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	VB	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	VD	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	VF	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	VH	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	VJ	367/380 (97%)	367 (100%)	0	100	100
9	VL	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	VN	367/380 (97%)	365 (100%)	2 (0%)	88	94
9	WB	367/380 (97%)	365 (100%)	2 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	WD	367/380 (97%)	366 (100%)	1 (0%)	92	97
9	WF	366/380 (96%)	363 (99%)	3 (1%)	81	91
9	WH	366/380 (96%)	366 (100%)	0	100	100
9	WJ	366/380 (96%)	364 (100%)	2 (0%)	88	94
9	WL	366/380 (96%)	366 (100%)	0	100	100
9	WN	366/380 (96%)	364 (100%)	2 (0%)	88	94
10	B0	171/386 (44%)	171 (100%)	0	100	100
10	B1	373/386 (97%)	370 (99%)	3 (1%)	81	91
10	B2	373/386 (97%)	370 (99%)	3 (1%)	81	91
10	B3	344/386 (89%)	343 (100%)	1 (0%)	92	97
10	B4	44/386 (11%)	44 (100%)	0	100	100
10	B5	45/386 (12%)	45 (100%)	0	100	100
10	B6	319/386 (83%)	318 (100%)	1 (0%)	92	97
10	B7	371/386 (96%)	367 (99%)	4 (1%)	73	86
10	B8	360/386 (93%)	356 (99%)	4 (1%)	73	86
10	B9	169/386 (44%)	169 (100%)	0	100	100
11	C	83/92 (90%)	83 (100%)	0	100	100
12	C0	30/444 (7%)	30 (100%)	0	100	100
12	C1	300/444 (68%)	299 (100%)	1 (0%)	92	97
12	C2	356/444 (80%)	355 (100%)	1 (0%)	92	97
12	C3	356/444 (80%)	355 (100%)	1 (0%)	92	97
12	C4	196/444 (44%)	196 (100%)	0	100	100
12	C5	101/444 (23%)	101 (100%)	0	100	100
12	C6	347/444 (78%)	346 (100%)	1 (0%)	92	97
12	C7	375/444 (84%)	371 (99%)	4 (1%)	73	86
12	C8	369/444 (83%)	368 (100%)	1 (0%)	92	97
12	C9	107/444 (24%)	105 (98%)	2 (2%)	57	78
12	F0	129/444 (29%)	129 (100%)	0	100	100
12	F1	381/444 (86%)	378 (99%)	3 (1%)	81	91
12	F2	381/444 (86%)	380 (100%)	1 (0%)	92	97
12	F3	340/444 (77%)	337 (99%)	3 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	F4	91/444 (20%)	91 (100%)	0	100	100
13	D	65/397 (16%)	65 (100%)	0	100	100
14	D0	255/394 (65%)	255 (100%)	0	100	100
14	D1	375/394 (95%)	375 (100%)	0	100	100
14	D2	375/394 (95%)	374 (100%)	1 (0%)	92	97
14	D3	283/394 (72%)	282 (100%)	1 (0%)	91	95
14	D5	9/394 (2%)	9 (100%)	0	100	100
14	D6	286/394 (73%)	283 (99%)	3 (1%)	76	88
14	D7	365/394 (93%)	361 (99%)	4 (1%)	73	86
14	D8	364/394 (92%)	362 (100%)	2 (0%)	88	94
14	D9	242/394 (61%)	241 (100%)	1 (0%)	91	95
15	E	223/281 (79%)	222 (100%)	1 (0%)	91	95
15	F	223/281 (79%)	223 (100%)	0	100	100
16	E0	58/178 (33%)	57 (98%)	1 (2%)	60	80
16	E1	106/178 (60%)	104 (98%)	2 (2%)	57	78
16	E2	122/178 (68%)	117 (96%)	5 (4%)	30	59
16	E3	122/178 (68%)	121 (99%)	1 (1%)	81	91
17	G	91/114 (80%)	90 (99%)	1 (1%)	73	86
18	H	69/231 (30%)	69 (100%)	0	100	100
18	I	123/231 (53%)	123 (100%)	0	100	100
18	J	123/231 (53%)	123 (100%)	0	100	100
18	K	123/231 (53%)	122 (99%)	1 (1%)	81	91
18	L	123/231 (53%)	122 (99%)	1 (1%)	81	91
18	M	123/231 (53%)	123 (100%)	0	100	100
18	N	126/231 (54%)	126 (100%)	0	100	100
19	H1	174/611 (28%)	171 (98%)	3 (2%)	60	80
19	H2	229/611 (38%)	227 (99%)	2 (1%)	78	90
19	H3	97/611 (16%)	97 (100%)	0	100	100
20	H4	174/551 (32%)	170 (98%)	4 (2%)	50	74
20	H5	226/551 (41%)	224 (99%)	2 (1%)	78	90
20	H6	115/551 (21%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	I1	97/593 (16%)	97 (100%)	0	100	100
22	I2	97/593 (16%)	97 (100%)	0	100	100
24	O	28/335 (8%)	28 (100%)	0	100	100
24	P	332/335 (99%)	332 (100%)	0	100	100
24	Q	36/335 (11%)	36 (100%)	0	100	100
24	R	217/335 (65%)	213 (98%)	4 (2%)	59	79
24	S	153/335 (46%)	153 (100%)	0	100	100
25	T	409/574 (71%)	404 (99%)	5 (1%)	71	85
25	U	409/574 (71%)	408 (100%)	1 (0%)	93	98
25	V	409/574 (71%)	407 (100%)	2 (0%)	88	94
26	W	506/672 (75%)	502 (99%)	4 (1%)	81	91
26	X	582/672 (87%)	581 (100%)	1 (0%)	93	98
26	Y	582/672 (87%)	582 (100%)	0	100	100
26	Z	412/672 (61%)	412 (100%)	0	100	100
27	XA	172/180 (96%)	171 (99%)	1 (1%)	86	94
27	XB	172/180 (96%)	172 (100%)	0	100	100
27	XC	172/180 (96%)	171 (99%)	1 (1%)	86	94
27	XD	172/180 (96%)	169 (98%)	3 (2%)	60	80
27	XE	172/180 (96%)	169 (98%)	3 (2%)	60	80
27	XF	172/180 (96%)	172 (100%)	0	100	100
27	XG	172/180 (96%)	172 (100%)	0	100	100
28	YB	192/227 (85%)	191 (100%)	1 (0%)	88	94
28	YC	192/227 (85%)	192 (100%)	0	100	100
28	YD	192/227 (85%)	192 (100%)	0	100	100
28	YE	192/227 (85%)	192 (100%)	0	100	100
28	YF	192/227 (85%)	192 (100%)	0	100	100
28	YG	192/227 (85%)	192 (100%)	0	100	100
29	a	157/495 (32%)	155 (99%)	2 (1%)	69	84
29	b	299/495 (60%)	293 (98%)	6 (2%)	55	77
29	c	256/495 (52%)	256 (100%)	0	100	100
29	d	187/495 (38%)	183 (98%)	4 (2%)	53	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	e	516/527 (98%)	514 (100%)	2 (0%)	91	95
30	f	516/527 (98%)	508 (98%)	8 (2%)	62	81
30	g	516/527 (98%)	510 (99%)	6 (1%)	71	85
31	h	135/238 (57%)	135 (100%)	0	100	100
31	i	218/238 (92%)	216 (99%)	2 (1%)	78	90
31	j	218/238 (92%)	218 (100%)	0	100	100
31	k	218/238 (92%)	218 (100%)	0	100	100
32	l	95/168 (56%)	95 (100%)	0	100	100
32	m	97/168 (58%)	95 (98%)	2 (2%)	53	76
32	n	99/168 (59%)	98 (99%)	1 (1%)	76	88
33	o	49/486 (10%)	49 (100%)	0	100	100
33	p	88/486 (18%)	88 (100%)	0	100	100
34	q	69/152 (45%)	67 (97%)	2 (3%)	42	69
34	r	69/152 (45%)	68 (99%)	1 (1%)	67	83
34	s	69/152 (45%)	69 (100%)	0	100	100
36	y	59/122 (48%)	58 (98%)	1 (2%)	60	80
36	z	105/122 (86%)	105 (100%)	0	100	100
All	All	135879/158917 (86%)	135160 (100%)	719 (0%)	89	94

5 of 719 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	PI	221	ARG
8	TC	2	ARG
8	PM	308	ARG
8	PG	216	ASN
9	RF	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 315 such sidechains are listed below:

Mol	Chain	Res	Type
8	SC	139	HIS
9	WF	334	GLN
9	SJ	15	GLN
9	UJ	6	HIS

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Mol	Chain	Res	Type
30	f	41	HIS

### 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 451 ligands modelled in this entry, 149 are monoatomic - leaving 302 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
37	GTP	MG	501	-	26,34,34	1.23	1 (3%)	32,54,54	1.59	6 (18%)
37	GTP	WC	501	-	26,34,34	1.21	2 (7%)	32,54,54	1.55	7 (21%)
39	GDP	WB	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.27	4 (13%)
39	GDP	SL	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.34	4 (13%)
37	GTP	JG	501	-	26,34,34	1.32	3 (11%)	32,54,54	1.57	7 (21%)
37	GTP	HO	501	-	26,34,34	1.24	2 (7%)	32,54,54	1.80	7 (21%)
37	GTP	LE	501	-	26,34,34	1.40	2 (7%)	32,54,54	1.67	6 (18%)
39	GDP	FJ	502	-	24,30,30	1.05	1 (4%)	30,47,47	1.52	7 (23%)
39	GDP	IH	502	-	24,30,30	1.09	1 (4%)	30,47,47	1.38	5 (16%)
39	GDP	AH	502	-	24,30,30	1.11	1 (4%)	30,47,47	1.51	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	GTP	GM	501	-	26,34,34	1.32	3 (11%)	32,54,54	1.81	7 (21%)
37	GTP	HK	501	-	26,34,34	1.26	2 (7%)	32,54,54	1.60	6 (18%)
39	GDP	HN	502	-	24,30,30	1.01	1 (4%)	30,47,47	1.58	5 (16%)
37	GTP	ME	501	-	26,34,34	1.37	2 (7%)	32,54,54	1.77	6 (18%)
37	GTP	IO	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.86	6 (18%)
37	GTP	OG	501	-	26,34,34	1.27	2 (7%)	32,54,54	1.77	8 (25%)
37	GTP	AG	501	-	26,34,34	1.39	4 (15%)	32,54,54	1.63	8 (25%)
39	GDP	SD	502	-	24,30,30	1.01	1 (4%)	30,47,47	1.34	4 (13%)
37	GTP	SE	501	-	26,34,34	1.29	3 (11%)	32,54,54	1.73	7 (21%)
39	GDP	PL	502	-	24,30,30	1.02	2 (8%)	30,47,47	1.30	3 (10%)
39	GDP	UN	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.33	4 (13%)
37	GTP	SI	501	-	26,34,34	1.22	1 (3%)	32,54,54	1.84	6 (18%)
39	GDP	FD	502	-	24,30,30	1.08	1 (4%)	30,47,47	1.36	3 (10%)
39	GDP	EJ	502	-	24,30,30	1.06	1 (4%)	30,47,47	1.43	3 (10%)
37	GTP	KC	501	-	26,34,34	1.55	3 (11%)	32,54,54	1.83	7 (21%)
37	GTP	QG	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.54	6 (18%)
37	GTP	BA	501	-	26,34,34	1.32	2 (7%)	32,54,54	1.78	7 (21%)
39	GDP	CB	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.46	5 (16%)
39	GDP	RJ	502	-	24,30,30	1.01	1 (4%)	30,47,47	1.43	5 (16%)
37	GTP	DM	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.59	6 (18%)
39	GDP	LL	502	-	24,30,30	1.12	1 (4%)	30,47,47	1.24	5 (16%)
39	GDP	UB	502	-	24,30,30	1.04	2 (8%)	30,47,47	1.38	3 (10%)
37	GTP	LG	501	-	26,34,34	1.42	1 (3%)	32,54,54	1.61	6 (18%)
37	GTP	PG	501	-	26,34,34	1.22	2 (7%)	32,54,54	1.61	10 (31%)
37	GTP	HI	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.66	7 (21%)
37	GTP	VK	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.66	7 (21%)
39	GDP	TL	502	-	24,30,30	0.98	1 (4%)	30,47,47	1.17	4 (13%)
39	GDP	AL	502	-	24,30,30	1.07	1 (4%)	30,47,47	1.42	5 (16%)
37	GTP	LI	501	-	26,34,34	1.43	2 (7%)	32,54,54	1.63	6 (18%)
37	GTP	EE	501	-	26,34,34	1.30	1 (3%)	32,54,54	1.57	6 (18%)
37	GTP	LK	501	-	26,34,34	1.39	2 (7%)	32,54,54	1.57	6 (18%)
37	GTP	PM	501	-	26,34,34	1.32	2 (7%)	32,54,54	1.58	7 (21%)
37	GTP	QI	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.67	9 (28%)
37	GTP	IG	501	-	26,34,34	1.17	1 (3%)	32,54,54	1.89	8 (25%)
37	GTP	HM	501	-	26,34,34	1.21	2 (7%)	32,54,54	1.67	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	GTP	FI	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.91	8 (25%)
37	GTP	KE	501	-	26,34,34	1.51	3 (11%)	32,54,54	1.49	5 (15%)
37	GTP	QM	501	-	26,34,34	1.25	2 (7%)	32,54,54	1.53	7 (21%)
37	GTP	AC	501	-	26,34,34	1.42	3 (11%)	32,54,54	1.69	7 (21%)
37	GTP	TM	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.52	8 (25%)
37	GTP	KG	501	-	26,34,34	1.55	3 (11%)	32,54,54	1.75	9 (28%)
37	GTP	LC	501	-	26,34,34	1.31	2 (7%)	32,54,54	1.71	7 (21%)
37	GTP	OE	501	-	26,34,34	1.25	2 (7%)	32,54,54	1.67	7 (21%)
37	GTP	GG	501	-	26,34,34	1.38	2 (7%)	32,54,54	1.84	7 (21%)
39	GDP	CD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.52	4 (13%)
39	GDP	O0	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.39	4 (13%)
39	GDP	IN	502	-	24,30,30	1.04	1 (4%)	30,47,47	1.31	6 (20%)
39	GDP	MJ	502	-	24,30,30	1.06	1 (4%)	30,47,47	1.46	5 (16%)
37	GTP	IE	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.66	7 (21%)
39	GDP	HB	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.54	4 (13%)
39	GDP	AJ	502	-	24,30,30	1.13	1 (4%)	30,47,47	1.45	5 (16%)
39	GDP	HH	502	-	24,30,30	0.98	1 (4%)	30,47,47	1.37	3 (10%)
37	GTP	HC	501	-	26,34,34	1.28	2 (7%)	32,54,54	1.72	7 (21%)
37	GTP	CK	501	-	26,34,34	1.21	1 (3%)	32,54,54	1.66	6 (18%)
37	GTP	UC	501	-	26,34,34	1.26	2 (7%)	32,54,54	1.73	6 (18%)
39	GDP	BF	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.37	5 (16%)
39	GDP	RF	502	-	24,30,30	1.07	1 (4%)	30,47,47	1.21	3 (10%)
37	GTP	RC	501	-	26,34,34	1.31	2 (7%)	32,54,54	1.64	7 (21%)
39	GDP	MF	502	-	24,30,30	1.06	1 (4%)	30,47,47	1.29	3 (10%)
39	GDP	UD	502	-	24,30,30	0.98	1 (4%)	30,47,47	1.35	4 (13%)
39	GDP	WJ	502	-	24,30,30	1.03	1 (4%)	30,47,47	1.29	3 (10%)
39	GDP	EH	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.30	4 (13%)
37	GTP	JM	501	-	26,34,34	1.26	2 (7%)	32,54,54	1.56	7 (21%)
37	GTP	CC	501	-	26,34,34	1.24	3 (11%)	32,54,54	1.74	7 (21%)
37	GTP	GK	501	-	26,34,34	1.31	2 (7%)	32,54,54	1.82	7 (21%)
39	GDP	OF	502	-	24,30,30	0.89	0	30,47,47	1.33	6 (20%)
39	GDP	PD	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	5 (16%)
39	GDP	LN	502	-	24,30,30	1.09	2 (8%)	30,47,47	1.32	3 (10%)
37	GTP	NE	501	-	26,34,34	1.22	2 (7%)	32,54,54	1.72	7 (21%)
39	GDP	JL	502	-	24,30,30	1.06	1 (4%)	30,47,47	1.29	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	GDP	RH	502	-	24,30,30	1.03	1 (4%)	30,47,47	1.40	5 (16%)
37	GTP	NA	501	-	26,34,34	1.27	1 (3%)	32,54,54	1.63	7 (21%)
39	GDP	CL	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.42	4 (13%)
37	GTP	CI	501	-	26,34,34	1.25	3 (11%)	32,54,54	1.74	7 (21%)
39	GDP	KB	502	-	24,30,30	1.07	1 (4%)	30,47,47	1.39	3 (10%)
39	GDP	JF	502	-	24,30,30	1.08	1 (4%)	30,47,47	1.26	4 (13%)
39	GDP	TH	502	-	24,30,30	1.03	1 (4%)	30,47,47	1.27	4 (13%)
39	GDP	GH	502	-	24,30,30	1.04	1 (4%)	30,47,47	1.48	4 (13%)
37	GTP	WG	501	-	26,34,34	1.21	2 (7%)	32,54,54	1.66	7 (21%)
39	GDP	HF	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.39	4 (13%)
39	GDP	VJ	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.26	4 (13%)
37	GTP	BM	501	-	26,34,34	1.36	3 (11%)	32,54,54	1.64	6 (18%)
37	GTP	CG	501	-	26,34,34	1.22	2 (7%)	32,54,54	1.78	7 (21%)
37	GTP	RK	501	-	26,34,34	1.33	3 (11%)	32,54,54	1.55	7 (21%)
37	GTP	UK	501	-	26,34,34	1.23	2 (7%)	32,54,54	1.55	8 (25%)
37	GTP	KM	501	-	26,34,34	1.49	4 (15%)	32,54,54	1.57	6 (18%)
37	GTP	MK	501	-	26,34,34	1.38	2 (7%)	32,54,54	1.74	9 (28%)
39	GDP	DJ	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.27	5 (16%)
39	GDP	SJ	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.50	5 (16%)
37	GTP	OK	501	-	26,34,34	1.30	3 (11%)	32,54,54	1.71	8 (25%)
37	GTP	OI	501	-	26,34,34	1.22	2 (7%)	32,54,54	1.76	7 (21%)
37	GTP	AA	501	-	26,34,34	1.35	3 (11%)	32,54,54	1.64	9 (28%)
37	GTP	FM	501	-	26,34,34	1.26	3 (11%)	32,54,54	1.69	10 (31%)
39	GDP	DF	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.37	4 (13%)
39	GDP	NH	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.44	4 (13%)
37	GTP	EG	501	-	26,34,34	1.26	1 (3%)	32,54,54	1.67	7 (21%)
39	GDP	OB	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	4 (13%)
37	GTP	FG	501	-	26,34,34	1.20	2 (7%)	32,54,54	1.60	7 (21%)
39	GDP	FN	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.23	3 (10%)
39	GDP	QH	502	-	24,30,30	0.98	1 (4%)	30,47,47	1.33	4 (13%)
37	GTP	JK	501	-	26,34,34	1.31	2 (7%)	32,54,54	1.72	7 (21%)
39	GDP	BB	502	-	24,30,30	0.87	0	30,47,47	1.78	8 (26%)
37	GTP	IC	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.63	7 (21%)
39	GDP	ID	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.44	4 (13%)
39	GDP	LJ	502	-	24,30,30	1.09	1 (4%)	30,47,47	1.41	5 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	GDP	ML	502	-	24,30,30	1.18	2 (8%)	30,47,47	1.32	4 (13%)
37	GTP	HE	501	-	26,34,34	1.29	2 (7%)	32,54,54	1.73	7 (21%)
37	GTP	GE	501	-	26,34,34	1.27	1 (3%)	32,54,54	1.79	7 (21%)
39	GDP	EL	502	-	24,30,30	1.13	1 (4%)	30,47,47	1.32	4 (13%)
39	GDP	MN	502	-	24,30,30	1.09	1 (4%)	30,47,47	1.34	4 (13%)
37	GTP	CE	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.64	6 (18%)
37	GTP	BK	501	-	26,34,34	1.37	4 (15%)	32,54,54	1.70	7 (21%)
39	GDP	BJ	502	-	24,30,30	1.06	1 (4%)	30,47,47	1.47	4 (13%)
37	GTP	WM	501	-	26,34,34	1.24	1 (3%)	32,54,54	1.61	6 (18%)
37	GTP	AI	501	-	26,34,34	1.37	3 (11%)	32,54,54	1.62	6 (18%)
39	GDP	PF	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.39	4 (13%)
39	GDP	TD	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.26	4 (13%)
37	GTP	EK	501	-	26,34,34	1.25	1 (3%)	32,54,54	1.56	6 (18%)
39	GDP	UL	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.41	3 (10%)
39	GDP	GJ	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.37	4 (13%)
39	GDP	OD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
39	GDP	TF	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.42	4 (13%)
39	GDP	WF	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.33	4 (13%)
37	GTP	GC	501	-	26,34,34	1.40	4 (15%)	32,54,54	1.85	7 (21%)
37	GTP	QA	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.57	7 (21%)
39	GDP	CJ	502	-	24,30,30	1.03	1 (4%)	30,47,47	1.53	6 (20%)
37	GTP	RA	501	-	26,34,34	1.21	2 (7%)	32,54,54	1.64	7 (21%)
39	GDP	DD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
39	GDP	CF	502	-	24,30,30	1.07	1 (4%)	30,47,47	1.40	5 (16%)
39	GDP	RL	502	-	24,30,30	1.01	1 (4%)	30,47,47	1.39	5 (16%)
39	GDP	VF	502	-	24,30,30	1.01	1 (4%)	30,47,47	1.38	4 (13%)
37	GTP	VG	501	-	26,34,34	1.21	2 (7%)	32,54,54	1.67	7 (21%)
37	GTP	PK	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.71	8 (25%)
39	GDP	LH	502	-	24,30,30	1.11	1 (4%)	30,47,47	1.40	4 (13%)
37	GTP	FC	501	-	26,34,34	1.24	1 (3%)	32,54,54	1.63	7 (21%)
37	GTP	PE	501	-	26,34,34	1.23	2 (7%)	32,54,54	1.82	7 (21%)
37	GTP	MC	501	-	26,34,34	1.43	3 (11%)	32,54,54	1.70	6 (18%)
37	GTP	MI	501	-	26,34,34	1.35	2 (7%)	32,54,54	1.79	9 (28%)
39	GDP	QF	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
39	GDP	LF	502	-	24,30,30	1.09	1 (4%)	30,47,47	1.29	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	GDP	WD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.39	6 (20%)
39	GDP	WH	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.55	5 (16%)
37	GTP	WK	501	-	26,34,34	1.17	1 (3%)	32,54,54	1.62	6 (18%)
39	GDP	LD	502	-	24,30,30	1.15	1 (4%)	30,47,47	1.34	3 (10%)
37	GTP	NG	501	-	26,34,34	1.26	1 (3%)	32,54,54	1.54	9 (28%)
39	GDP	QL	502	-	24,30,30	1.05	1 (4%)	30,47,47	1.39	5 (16%)
39	GDP	KN	502	-	24,30,30	1.07	1 (4%)	30,47,47	1.44	4 (13%)
39	GDP	SB	502	-	24,30,30	1.03	1 (4%)	30,47,47	1.34	5 (16%)
37	GTP	NI	501	-	26,34,34	1.24	2 (7%)	32,54,54	1.64	7 (21%)
37	GTP	JC	501	-	26,34,34	1.25	2 (7%)	32,54,54	1.70	8 (25%)
37	GTP	OC	501	-	26,34,34	1.35	4 (15%)	32,54,54	1.80	7 (21%)
37	GTP	VM	501	-	26,34,34	1.25	2 (7%)	32,54,54	1.82	7 (21%)
39	GDP	JJ	502	-	24,30,30	0.98	1 (4%)	30,47,47	1.35	5 (16%)
39	GDP	UF	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.39	4 (13%)
39	GDP	PB	502	-	24,30,30	1.01	1 (4%)	30,47,47	1.38	4 (13%)
39	GDP	GF	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.30	4 (13%)
39	GDP	EN	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.26	4 (13%)
39	GDP	UJ	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.43	5 (16%)
39	GDP	BH	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.46	4 (13%)
37	GTP	IM	501	-	26,34,34	1.30	2 (7%)	32,54,54	1.75	8 (25%)
37	GTP	QK	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.49	5 (15%)
37	GTP	DA	501	-	26,34,34	1.11	2 (7%)	32,54,54	1.56	5 (15%)
39	GDP	DB	502	-	24,30,30	1.07	1 (4%)	30,47,47	1.45	6 (20%)
39	GDP	SF	502	-	24,30,30	1.01	1 (4%)	30,47,47	1.43	5 (16%)
39	GDP	VH	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.29	5 (16%)
39	GDP	HD	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.41	5 (16%)
37	GTP	OA	501	-	26,34,34	1.23	2 (7%)	32,54,54	1.64	7 (21%)
37	GTP	LM	501	-	26,34,34	1.45	4 (15%)	32,54,54	1.66	7 (21%)
37	GTP	UG	501	-	26,34,34	1.29	1 (3%)	32,54,54	1.65	7 (21%)
39	GDP	ED	502	-	24,30,30	1.05	1 (4%)	30,47,47	1.41	4 (13%)
39	GDP	BD	502	-	24,30,30	1.04	1 (4%)	30,47,47	1.46	4 (13%)
39	GDP	JB	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.28	3 (10%)
39	GDP	MD	502	-	24,30,30	1.14	1 (4%)	30,47,47	1.29	2 (6%)
39	GDP	NL	502	-	24,30,30	0.92	1 (4%)	30,47,47	1.44	4 (13%)
39	GDP	VL	502	-	24,30,30	1.01	1 (4%)	30,47,47	1.36	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	GTP	DI	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
37	GTP	DK	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.51	6 (18%)
39	GDP	DL	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.34	4 (13%)
37	GTP	PC	501	-	26,34,34	1.20	2 (7%)	32,54,54	1.53	6 (18%)
39	GDP	HL	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.41	4 (13%)
37	GTP	VI	501	-	26,34,34	1.20	2 (7%)	32,54,54	1.92	6 (18%)
39	GDP	FB	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.29	3 (10%)
39	GDP	DN	502	-	24,30,30	1.02	2 (8%)	30,47,47	1.34	4 (13%)
39	GDP	AB	502	-	24,30,30	1.07	1 (4%)	30,47,47	1.35	4 (13%)
39	GDP	CH	502	-	24,30,30	1.04	1 (4%)	30,47,47	1.58	5 (16%)
39	GDP	MH	502	-	24,30,30	1.05	1 (4%)	30,47,47	1.35	4 (13%)
37	GTP	WE	501	-	26,34,34	1.27	2 (7%)	32,54,54	1.66	6 (18%)
37	GTP	RG	501	-	26,34,34	1.34	3 (11%)	32,54,54	1.64	6 (18%)
39	GDP	DH	502	-	24,30,30	1.06	1 (4%)	30,47,47	1.26	3 (10%)
37	GTP	SM	501	-	26,34,34	1.33	1 (3%)	32,54,54	1.68	7 (21%)
39	GDP	FF	502	-	24,30,30	1.05	1 (4%)	30,47,47	1.35	4 (13%)
39	GDP	VB	502	-	24,30,30	0.90	0	30,47,47	1.51	4 (13%)
37	GTP	EM	501	-	26,34,34	1.32	3 (11%)	32,54,54	1.68	6 (18%)
37	GTP	NK	501	-	26,34,34	1.22	2 (7%)	32,54,54	1.62	8 (25%)
37	GTP	RM	501	-	26,34,34	1.24	1 (3%)	32,54,54	1.73	7 (21%)
37	GTP	DC	501	-	26,34,34	1.22	2 (7%)	32,54,54	1.48	6 (18%)
39	GDP	QJ	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.32	4 (13%)
37	GTP	BI	501	-	26,34,34	1.35	2 (7%)	32,54,54	1.67	8 (25%)
37	GTP	CM	501	-	26,34,34	1.24	2 (7%)	32,54,54	1.82	7 (21%)
37	GTP	AM	501	-	26,34,34	1.44	4 (15%)	32,54,54	1.62	6 (18%)
39	GDP	QD	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.26	4 (13%)
37	GTP	PI	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.80	6 (18%)
37	GTP	QE	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.85	7 (21%)
39	GDP	GN	502	-	24,30,30	0.98	1 (4%)	30,47,47	1.47	4 (13%)
37	GTP	EC	501	-	26,34,34	1.28	1 (3%)	32,54,54	1.76	6 (18%)
39	GDP	HJ	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.31	4 (13%)
37	GTP	KO	501	-	26,34,34	1.41	3 (11%)	32,54,54	1.57	7 (21%)
37	GTP	QC	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.59	7 (21%)
39	GDP	TJ	502	-	24,30,30	0.92	1 (4%)	30,47,47	1.26	4 (13%)
37	GTP	TE	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.45	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	GDP	OJ	502	-	24,30,30	0.97	1 (4%)	30,47,47	1.36	4 (13%)
37	GTP	TK	501	-	26,34,34	1.25	1 (3%)	32,54,54	1.49	7 (21%)
37	GTP	MM	501	-	26,34,34	1.37	1 (3%)	32,54,54	1.51	7 (21%)
37	GTP	KK	501	-	26,34,34	1.48	4 (15%)	32,54,54	1.65	7 (21%)
39	GDP	MB	502	-	24,30,30	0.98	1 (4%)	30,47,47	1.64	6 (20%)
37	GTP	PA	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.71	8 (25%)
39	GDP	EF	502	-	24,30,30	1.12	1 (4%)	30,47,47	1.26	4 (13%)
37	GTP	RI	501	-	26,34,34	1.20	2 (7%)	32,54,54	1.81	9 (28%)
37	GTP	JE	501	-	26,34,34	1.28	2 (7%)	32,54,54	1.61	6 (18%)
37	GTP	SG	501	-	26,34,34	1.28	3 (11%)	32,54,54	1.44	5 (15%)
39	GDP	JH	502	-	24,30,30	1.05	1 (4%)	30,47,47	1.30	3 (10%)
39	GDP	PJ	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.37	4 (13%)
37	GTP	EI	501	-	26,34,34	1.35	3 (11%)	32,54,54	1.87	8 (25%)
37	GTP	TG	501	-	26,34,34	1.18	1 (3%)	32,54,54	1.46	8 (25%)
37	GTP	NC	501	-	26,34,34	1.22	2 (7%)	32,54,54	1.65	7 (21%)
37	GTP	UM	501	-	26,34,34	1.21	2 (7%)	32,54,54	1.79	7 (21%)
37	GTP	TI	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.44	6 (18%)
37	GTP	AK	501	-	26,34,34	1.40	3 (11%)	32,54,54	1.70	7 (21%)
37	GTP	AE	501	-	26,34,34	1.41	3 (11%)	32,54,54	1.65	7 (21%)
39	GDP	IF	502	-	24,30,30	1.07	1 (4%)	30,47,47	1.37	5 (16%)
39	GDP	JD	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.32	6 (20%)
37	GTP	IK	501	-	26,34,34	1.24	2 (7%)	32,54,54	1.64	7 (21%)
39	GDP	OH	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.43	5 (16%)
39	GDP	KJ	502	-	24,30,30	1.06	1 (4%)	30,47,47	1.37	4 (13%)
37	GTP	DE	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.65	8 (25%)
37	GTP	SA	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.68	7 (21%)
37	GTP	II	501	-	26,34,34	1.19	1 (3%)	32,54,54	1.68	7 (21%)
39	GDP	FH	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.23	4 (13%)
39	GDP	RB	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
37	GTP	GI	501	-	26,34,34	1.27	1 (3%)	32,54,54	1.76	7 (21%)
37	GTP	JI	501	-	26,34,34	1.34	2 (7%)	32,54,54	1.69	7 (21%)
39	GDP	QB	502	-	24,30,30	1.03	1 (4%)	30,47,47	1.28	4 (13%)
39	GDP	EB	502	-	24,30,30	0.98	1 (4%)	30,47,47	1.40	4 (13%)
37	GTP	FK	501	-	26,34,34	1.27	2 (7%)	32,54,54	1.67	8 (25%)
39	GDP	JN	502	-	24,30,30	1.07	1 (4%)	30,47,47	1.38	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	GTP	FE	501	-	26,34,34	1.23	3 (11%)	32,54,54	1.95	8 (25%)
37	GTP	UE	501	-	26,34,34	1.20	1 (3%)	32,54,54	1.72	6 (18%)
39	GDP	VD	502	-	24,30,30	1.04	1 (4%)	30,47,47	1.51	5 (16%)
37	GTP	SC	501	-	26,34,34	1.30	2 (7%)	32,54,54	1.66	7 (21%)
37	GTP	BC	501	-	26,34,34	1.35	2 (7%)	32,54,54	1.71	7 (21%)
39	GDP	AF	502	-	24,30,30	1.16	2 (8%)	30,47,47	1.41	4 (13%)
37	GTP	DG	501	-	26,34,34	1.25	2 (7%)	32,54,54	1.72	7 (21%)
37	GTP	VC	501	-	26,34,34	1.22	2 (7%)	32,54,54	1.83	7 (21%)
39	GDP	LB	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.45	4 (13%)
39	GDP	VN	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.41	4 (13%)
39	GDP	GD	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.40	4 (13%)
39	GDP	WN	502	-	24,30,30	1.08	1 (4%)	30,47,47	1.41	4 (13%)
39	GDP	UH	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.47	3 (10%)
39	GDP	N0	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	4 (13%)
39	GDP	GL	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.41	4 (13%)
39	GDP	IJ	502	-	24,30,30	1.04	1 (4%)	30,47,47	1.56	4 (13%)
37	GTP	SK	501	-	26,34,34	1.32	3 (11%)	32,54,54	1.82	6 (18%)
39	GDP	FL	502	-	24,30,30	1.05	1 (4%)	30,47,47	1.38	4 (13%)
37	GTP	BG	501	-	26,34,34	1.35	2 (7%)	32,54,54	1.78	8 (25%)
37	GTP	RE	501	-	26,34,34	1.22	1 (3%)	32,54,54	1.76	7 (21%)
37	GTP	VE	501	-	26,34,34	1.26	2 (7%)	32,54,54	1.87	7 (21%)
37	GTP	WI	501	-	26,34,34	1.26	2 (7%)	32,54,54	1.61	5 (15%)
39	GDP	BL	502	-	24,30,30	1.05	1 (4%)	30,47,47	1.38	4 (13%)
39	GDP	IB	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.38	4 (13%)
39	GDP	AD	502	-	24,30,30	0.97	2 (8%)	30,47,47	1.47	5 (16%)
39	GDP	KF	502	-	24,30,30	1.08	1 (4%)	30,47,47	1.31	4 (13%)
39	GDP	NF	502	-	24,30,30	0.91	0	30,47,47	1.47	4 (13%)
39	GDP	OL	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.56	5 (16%)
37	GTP	CA	501	-	26,34,34	1.25	2 (7%)	32,54,54	1.75	7 (21%)
37	GTP	UI	501	-	26,34,34	1.25	2 (7%)	32,54,54	1.76	7 (21%)
39	GDP	SH	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.47	4 (13%)
39	GDP	TB	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.30	4 (13%)
39	GDP	KH	502	-	24,30,30	1.09	1 (4%)	30,47,47	1.43	4 (13%)
39	GDP	NJ	502	-	24,30,30	0.98	1 (4%)	30,47,47	1.36	4 (13%)
39	GDP	WL	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.44	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	GDP	GB	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.46	4 (13%)
37	GTP	KI	501	-	26,34,34	1.50	3 (11%)	32,54,54	1.63	8 (25%)
39	GDP	IL	502	-	24,30,30	1.12	1 (4%)	30,47,47	1.45	6 (20%)
39	GDP	KD	502	-	24,30,30	1.12	1 (4%)	30,47,47	1.31	4 (13%)
39	GDP	KL	502	-	24,30,30	1.04	1 (4%)	30,47,47	1.35	4 (13%)
37	GTP	HG	501	-	26,34,34	1.22	2 (7%)	32,54,54	1.73	7 (21%)
37	GTP	TC	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.67	7 (21%)
39	GDP	ND	502	-	24,30,30	0.98	1 (4%)	30,47,47	1.48	4 (13%)
39	GDP	PH	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.35	5 (16%)
39	GDP	RD	502	-	24,30,30	1.02	1 (4%)	30,47,47	1.39	4 (13%)
37	GTP	BE	501	-	26,34,34	1.37	3 (11%)	32,54,54	1.69	7 (21%)
39	GDP	NB	502	-	24,30,30	1.00	1 (4%)	30,47,47	1.41	4 (13%)

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
37	GTP	MG	501	-	-	4/18/38/38	0/3/3/3
37	GTP	WC	501	-	-	1/18/38/38	0/3/3/3
39	GDP	WB	502	-	-	1/12/32/32	0/3/3/3
39	GDP	SL	502	-	-	3/12/32/32	0/3/3/3
37	GTP	JG	501	-	-	6/18/38/38	0/3/3/3
37	GTP	HO	501	-	-	6/18/38/38	0/3/3/3
37	GTP	LE	501	-	-	6/18/38/38	0/3/3/3
39	GDP	FJ	502	-	-	3/12/32/32	0/3/3/3
39	GDP	IH	502	-	-	6/12/32/32	0/3/3/3
39	GDP	AH	502	-	-	1/12/32/32	0/3/3/3
37	GTP	GM	501	-	-	5/18/38/38	0/3/3/3
37	GTP	HK	501	-	-	5/18/38/38	0/3/3/3
39	GDP	HN	502	-	-	1/12/32/32	0/3/3/3
37	GTP	ME	501	-	-	4/18/38/38	0/3/3/3
37	GTP	IO	501	-	-	3/18/38/38	0/3/3/3
37	GTP	OG	501	-	-	0/18/38/38	0/3/3/3
37	GTP	AG	501	-	-	5/18/38/38	0/3/3/3
39	GDP	SD	502	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	GTP	SE	501	-	-	6/18/38/38	0/3/3/3
39	GDP	PL	502	-	-	7/12/32/32	0/3/3/3
39	GDP	UN	502	-	-	2/12/32/32	0/3/3/3
37	GTP	SI	501	-	-	3/18/38/38	0/3/3/3
39	GDP	FD	502	-	-	6/12/32/32	0/3/3/3
39	GDP	EJ	502	-	-	4/12/32/32	0/3/3/3
37	GTP	KC	501	-	-	10/18/38/38	0/3/3/3
37	GTP	QG	501	-	-	3/18/38/38	0/3/3/3
37	GTP	BA	501	-	-	6/18/38/38	0/3/3/3
39	GDP	CB	502	-	-	3/12/32/32	0/3/3/3
39	GDP	RJ	502	-	-	2/12/32/32	0/3/3/3
37	GTP	DM	501	-	-	2/18/38/38	0/3/3/3
39	GDP	LL	502	-	-	3/12/32/32	0/3/3/3
39	GDP	UB	502	-	-	5/12/32/32	0/3/3/3
37	GTP	LG	501	-	-	4/18/38/38	0/3/3/3
37	GTP	PG	501	-	-	4/18/38/38	0/3/3/3
37	GTP	HI	501	-	-	4/18/38/38	0/3/3/3
37	GTP	VK	501	-	-	5/18/38/38	0/3/3/3
39	GDP	TL	502	-	-	3/12/32/32	0/3/3/3
39	GDP	AL	502	-	-	1/12/32/32	0/3/3/3
37	GTP	LI	501	-	-	7/18/38/38	0/3/3/3
37	GTP	EE	501	-	-	6/18/38/38	0/3/3/3
37	GTP	LK	501	-	-	9/18/38/38	0/3/3/3
37	GTP	PM	501	-	-	3/18/38/38	0/3/3/3
37	GTP	QI	501	-	-	3/18/38/38	0/3/3/3
37	GTP	IG	501	-	-	3/18/38/38	0/3/3/3
37	GTP	HM	501	-	-	1/18/38/38	0/3/3/3
37	GTP	FI	501	-	-	5/18/38/38	0/3/3/3
37	GTP	KE	501	-	-	5/18/38/38	0/3/3/3
37	GTP	QM	501	-	-	3/18/38/38	0/3/3/3
37	GTP	AC	501	-	-	4/18/38/38	0/3/3/3
37	GTP	TM	501	-	-	5/18/38/38	0/3/3/3
37	GTP	KG	501	-	-	5/18/38/38	0/3/3/3
37	GTP	LC	501	-	-	1/18/38/38	0/3/3/3
37	GTP	OE	501	-	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	GTP	GG	501	-	-	7/18/38/38	0/3/3/3
39	GDP	CD	502	-	-	2/12/32/32	0/3/3/3
39	GDP	O0	502	-	-	1/12/32/32	0/3/3/3
39	GDP	IN	502	-	-	4/12/32/32	0/3/3/3
39	GDP	MJ	502	-	-	2/12/32/32	0/3/3/3
37	GTP	IE	501	-	-	2/18/38/38	0/3/3/3
39	GDP	HB	502	-	-	3/12/32/32	0/3/3/3
39	GDP	AJ	502	-	-	3/12/32/32	0/3/3/3
39	GDP	HH	502	-	-	6/12/32/32	0/3/3/3
37	GTP	HC	501	-	-	5/18/38/38	0/3/3/3
37	GTP	CK	501	-	-	5/18/38/38	0/3/3/3
37	GTP	UC	501	-	-	5/18/38/38	0/3/3/3
39	GDP	BF	502	-	-	5/12/32/32	0/3/3/3
39	GDP	RF	502	-	-	1/12/32/32	0/3/3/3
37	GTP	RC	501	-	-	6/18/38/38	0/3/3/3
39	GDP	MF	502	-	-	2/12/32/32	0/3/3/3
39	GDP	UD	502	-	-	2/12/32/32	0/3/3/3
39	GDP	WJ	502	-	-	4/12/32/32	0/3/3/3
39	GDP	EH	502	-	-	6/12/32/32	0/3/3/3
37	GTP	JM	501	-	-	2/18/38/38	0/3/3/3
37	GTP	CC	501	-	-	4/18/38/38	0/3/3/3
37	GTP	GK	501	-	-	4/18/38/38	0/3/3/3
39	GDP	OF	502	-	-	3/12/32/32	0/3/3/3
39	GDP	PD	502	-	-	4/12/32/32	0/3/3/3
39	GDP	LN	502	-	-	3/12/32/32	0/3/3/3
37	GTP	NE	501	-	-	6/18/38/38	0/3/3/3
39	GDP	JL	502	-	-	2/12/32/32	0/3/3/3
39	GDP	RH	502	-	-	1/12/32/32	0/3/3/3
37	GTP	NA	501	-	-	7/18/38/38	0/3/3/3
39	GDP	CL	502	-	-	5/12/32/32	0/3/3/3
37	GTP	CI	501	-	-	7/18/38/38	0/3/3/3
39	GDP	KB	502	-	-	3/12/32/32	0/3/3/3
39	GDP	JF	502	-	-	0/12/32/32	0/3/3/3
39	GDP	TH	502	-	-	2/12/32/32	0/3/3/3
39	GDP	GH	502	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	GTP	WG	501	-	-	5/18/38/38	0/3/3/3
39	GDP	HF	502	-	-	1/12/32/32	0/3/3/3
39	GDP	VJ	502	-	-	3/12/32/32	0/3/3/3
37	GTP	BM	501	-	-	3/18/38/38	0/3/3/3
37	GTP	CG	501	-	-	4/18/38/38	0/3/3/3
37	GTP	RK	501	-	-	2/18/38/38	0/3/3/3
37	GTP	UK	501	-	-	2/18/38/38	0/3/3/3
37	GTP	KM	501	-	-	4/18/38/38	0/3/3/3
37	GTP	MK	501	-	-	6/18/38/38	0/3/3/3
39	GDP	DJ	502	-	-	2/12/32/32	0/3/3/3
39	GDP	SJ	502	-	-	2/12/32/32	0/3/3/3
37	GTP	OK	501	-	-	6/18/38/38	0/3/3/3
37	GTP	OI	501	-	-	6/18/38/38	0/3/3/3
37	GTP	AA	501	-	-	4/18/38/38	0/3/3/3
37	GTP	FM	501	-	-	5/18/38/38	0/3/3/3
39	GDP	DF	502	-	-	4/12/32/32	0/3/3/3
39	GDP	NH	502	-	-	4/12/32/32	0/3/3/3
37	GTP	EG	501	-	-	8/18/38/38	0/3/3/3
39	GDP	OB	502	-	-	4/12/32/32	0/3/3/3
37	GTP	FG	501	-	-	5/18/38/38	0/3/3/3
39	GDP	FN	502	-	-	2/12/32/32	0/3/3/3
39	GDP	QH	502	-	-	0/12/32/32	0/3/3/3
37	GTP	JK	501	-	-	4/18/38/38	0/3/3/3
39	GDP	BB	502	-	-	5/12/32/32	0/3/3/3
37	GTP	IC	501	-	-	7/18/38/38	0/3/3/3
39	GDP	ID	502	-	-	6/12/32/32	0/3/3/3
39	GDP	LJ	502	-	-	5/12/32/32	0/3/3/3
39	GDP	ML	502	-	-	3/12/32/32	0/3/3/3
37	GTP	HE	501	-	-	6/18/38/38	0/3/3/3
37	GTP	GE	501	-	-	6/18/38/38	0/3/3/3
39	GDP	EL	502	-	-	4/12/32/32	0/3/3/3
39	GDP	MN	502	-	-	3/12/32/32	0/3/3/3
37	GTP	CE	501	-	-	4/18/38/38	0/3/3/3
37	GTP	BK	501	-	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	BJ	502	-	-	7/12/32/32	0/3/3/3
37	GTP	WM	501	-	-	6/18/38/38	0/3/3/3
37	GTP	AI	501	-	-	1/18/38/38	0/3/3/3
39	GDP	PF	502	-	-	3/12/32/32	0/3/3/3
39	GDP	TD	502	-	-	2/12/32/32	0/3/3/3
37	GTP	EK	501	-	-	6/18/38/38	0/3/3/3
39	GDP	UL	502	-	-	3/12/32/32	0/3/3/3
39	GDP	GJ	502	-	-	2/12/32/32	0/3/3/3
39	GDP	OD	502	-	-	1/12/32/32	0/3/3/3
39	GDP	TF	502	-	-	1/12/32/32	0/3/3/3
39	GDP	WF	502	-	-	2/12/32/32	0/3/3/3
37	GTP	GC	501	-	-	6/18/38/38	0/3/3/3
37	GTP	QA	501	-	-	5/18/38/38	0/3/3/3
39	GDP	CJ	502	-	-	6/12/32/32	0/3/3/3
37	GTP	RA	501	-	-	7/18/38/38	0/3/3/3
39	GDP	DD	502	-	-	7/12/32/32	0/3/3/3
39	GDP	CF	502	-	-	6/12/32/32	0/3/3/3
39	GDP	RL	502	-	-	2/12/32/32	0/3/3/3
39	GDP	VF	502	-	-	3/12/32/32	0/3/3/3
37	GTP	VG	501	-	-	3/18/38/38	0/3/3/3
37	GTP	PK	501	-	-	7/18/38/38	0/3/3/3
39	GDP	LH	502	-	-	5/12/32/32	0/3/3/3
37	GTP	FC	501	-	-	8/18/38/38	0/3/3/3
37	GTP	PE	501	-	-	6/18/38/38	0/3/3/3
37	GTP	MC	501	-	-	5/18/38/38	0/3/3/3
37	GTP	MI	501	-	-	8/18/38/38	0/3/3/3
39	GDP	QF	502	-	-	0/12/32/32	0/3/3/3
39	GDP	LF	502	-	-	2/12/32/32	0/3/3/3
39	GDP	WD	502	-	-	4/12/32/32	0/3/3/3
39	GDP	WH	502	-	-	2/12/32/32	0/3/3/3
37	GTP	WK	501	-	-	8/18/38/38	0/3/3/3
39	GDP	LD	502	-	-	7/12/32/32	0/3/3/3
37	GTP	NG	501	-	-	4/18/38/38	0/3/3/3
39	GDP	QL	502	-	-	1/12/32/32	0/3/3/3
39	GDP	KN	502	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	SB	502	-	-	1/12/32/32	0/3/3/3
37	GTP	NI	501	-	-	7/18/38/38	0/3/3/3
37	GTP	JC	501	-	-	0/18/38/38	0/3/3/3
37	GTP	OC	501	-	-	6/18/38/38	0/3/3/3
37	GTP	VM	501	-	-	3/18/38/38	0/3/3/3
39	GDP	JJ	502	-	-	0/12/32/32	0/3/3/3
39	GDP	UF	502	-	-	4/12/32/32	0/3/3/3
39	GDP	PB	502	-	-	5/12/32/32	0/3/3/3
39	GDP	GF	502	-	-	6/12/32/32	0/3/3/3
39	GDP	EN	502	-	-	5/12/32/32	0/3/3/3
39	GDP	UJ	502	-	-	5/12/32/32	0/3/3/3
39	GDP	BH	502	-	-	4/12/32/32	0/3/3/3
37	GTP	IM	501	-	-	6/18/38/38	0/3/3/3
37	GTP	QK	501	-	-	7/18/38/38	0/3/3/3
37	GTP	DA	501	-	-	3/18/38/38	0/3/3/3
39	GDP	DB	502	-	-	1/12/32/32	0/3/3/3
39	GDP	SF	502	-	-	0/12/32/32	0/3/3/3
39	GDP	VH	502	-	-	4/12/32/32	0/3/3/3
39	GDP	HD	502	-	-	2/12/32/32	0/3/3/3
37	GTP	OA	501	-	-	6/18/38/38	0/3/3/3
37	GTP	LM	501	-	-	4/18/38/38	0/3/3/3
37	GTP	UG	501	-	-	6/18/38/38	0/3/3/3
39	GDP	ED	502	-	-	4/12/32/32	0/3/3/3
39	GDP	BD	502	-	-	5/12/32/32	0/3/3/3
39	GDP	JB	502	-	-	1/12/32/32	0/3/3/3
39	GDP	MD	502	-	-	4/12/32/32	0/3/3/3
39	GDP	NL	502	-	-	3/12/32/32	0/3/3/3
39	GDP	VL	502	-	-	4/12/32/32	0/3/3/3
37	GTP	DI	501	-	-	6/18/38/38	0/3/3/3
37	GTP	DK	501	-	-	3/18/38/38	0/3/3/3
39	GDP	DL	502	-	-	3/12/32/32	0/3/3/3
37	GTP	PC	501	-	-	1/18/38/38	0/3/3/3
39	GDP	HL	502	-	-	1/12/32/32	0/3/3/3
37	GTP	VI	501	-	-	4/18/38/38	0/3/3/3
39	GDP	FB	502	-	-	3/12/32/32	0/3/3/3
39	GDP	DN	502	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	AB	502	-	-	4/12/32/32	0/3/3/3
39	GDP	CH	502	-	-	4/12/32/32	0/3/3/3
39	GDP	MH	502	-	-	3/12/32/32	0/3/3/3
37	GTP	WE	501	-	-	6/18/38/38	0/3/3/3
37	GTP	RG	501	-	-	3/18/38/38	0/3/3/3
39	GDP	DH	502	-	-	3/12/32/32	0/3/3/3
37	GTP	SM	501	-	-	7/18/38/38	0/3/3/3
39	GDP	FF	502	-	-	0/12/32/32	0/3/3/3
39	GDP	VB	502	-	-	5/12/32/32	0/3/3/3
37	GTP	EM	501	-	-	6/18/38/38	0/3/3/3
37	GTP	NK	501	-	-	1/18/38/38	0/3/3/3
37	GTP	RM	501	-	-	3/18/38/38	0/3/3/3
37	GTP	DC	501	-	-	6/18/38/38	0/3/3/3
39	GDP	QJ	502	-	-	3/12/32/32	0/3/3/3
37	GTP	BI	501	-	-	4/18/38/38	0/3/3/3
37	GTP	CM	501	-	-	7/18/38/38	0/3/3/3
37	GTP	AM	501	-	-	4/18/38/38	0/3/3/3
39	GDP	QD	502	-	-	2/12/32/32	0/3/3/3
37	GTP	PI	501	-	-	5/18/38/38	0/3/3/3
37	GTP	QE	501	-	-	3/18/38/38	0/3/3/3
39	GDP	GN	502	-	-	4/12/32/32	0/3/3/3
37	GTP	EC	501	-	-	6/18/38/38	0/3/3/3
39	GDP	HJ	502	-	-	3/12/32/32	0/3/3/3
37	GTP	KO	501	-	-	5/18/38/38	0/3/3/3
37	GTP	QC	501	-	-	3/18/38/38	0/3/3/3
39	GDP	TJ	502	-	-	2/12/32/32	0/3/3/3
37	GTP	TE	501	-	-	3/18/38/38	0/3/3/3
39	GDP	OJ	502	-	-	2/12/32/32	0/3/3/3
37	GTP	TK	501	-	-	5/18/38/38	0/3/3/3
37	GTP	MM	501	-	-	7/18/38/38	0/3/3/3
37	GTP	KK	501	-	-	7/18/38/38	0/3/3/3
39	GDP	MB	502	-	-	0/12/32/32	0/3/3/3
37	GTP	PA	501	-	-	7/18/38/38	0/3/3/3
39	GDP	EF	502	-	-	5/12/32/32	0/3/3/3
37	GTP	RI	501	-	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	GTP	JE	501	-	-	2/18/38/38	0/3/3/3
37	GTP	SG	501	-	-	7/18/38/38	0/3/3/3
39	GDP	JH	502	-	-	2/12/32/32	0/3/3/3
39	GDP	PJ	502	-	-	4/12/32/32	0/3/3/3
37	GTP	EI	501	-	-	6/18/38/38	0/3/3/3
37	GTP	TG	501	-	-	7/18/38/38	0/3/3/3
37	GTP	NC	501	-	-	6/18/38/38	0/3/3/3
37	GTP	UM	501	-	-	2/18/38/38	0/3/3/3
37	GTP	TI	501	-	-	5/18/38/38	0/3/3/3
37	GTP	AK	501	-	-	2/18/38/38	0/3/3/3
37	GTP	AE	501	-	-	4/18/38/38	0/3/3/3
39	GDP	IF	502	-	-	0/12/32/32	0/3/3/3
39	GDP	JD	502	-	-	1/12/32/32	0/3/3/3
37	GTP	IK	501	-	-	5/18/38/38	0/3/3/3
39	GDP	OH	502	-	-	2/12/32/32	0/3/3/3
39	GDP	KJ	502	-	-	3/12/32/32	0/3/3/3
37	GTP	DE	501	-	-	8/18/38/38	0/3/3/3
37	GTP	SA	501	-	-	3/18/38/38	0/3/3/3
37	GTP	II	501	-	-	4/18/38/38	0/3/3/3
39	GDP	FH	502	-	-	4/12/32/32	0/3/3/3
39	GDP	RB	502	-	-	4/12/32/32	0/3/3/3
37	GTP	GI	501	-	-	4/18/38/38	0/3/3/3
37	GTP	JI	501	-	-	4/18/38/38	0/3/3/3
39	GDP	QB	502	-	-	5/12/32/32	0/3/3/3
39	GDP	EB	502	-	-	4/12/32/32	0/3/3/3
37	GTP	FK	501	-	-	8/18/38/38	0/3/3/3
39	GDP	JN	502	-	-	3/12/32/32	0/3/3/3
37	GTP	FE	501	-	-	5/18/38/38	0/3/3/3
37	GTP	UE	501	-	-	5/18/38/38	0/3/3/3
39	GDP	VD	502	-	-	2/12/32/32	0/3/3/3
37	GTP	SC	501	-	-	4/18/38/38	0/3/3/3
37	GTP	BC	501	-	-	7/18/38/38	0/3/3/3
39	GDP	AF	502	-	-	6/12/32/32	0/3/3/3
37	GTP	DG	501	-	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	GTP	VC	501	-	-	6/18/38/38	0/3/3/3
39	GDP	LB	502	-	-	1/12/32/32	0/3/3/3
39	GDP	VN	502	-	-	0/12/32/32	0/3/3/3
39	GDP	GD	502	-	-	1/12/32/32	0/3/3/3
39	GDP	WN	502	-	-	7/12/32/32	0/3/3/3
39	GDP	UH	502	-	-	4/12/32/32	0/3/3/3
39	GDP	N0	502	-	-	5/12/32/32	0/3/3/3
39	GDP	GL	502	-	-	1/12/32/32	0/3/3/3
39	GDP	IJ	502	-	-	3/12/32/32	0/3/3/3
37	GTP	SK	501	-	-	6/18/38/38	0/3/3/3
39	GDP	FL	502	-	-	5/12/32/32	0/3/3/3
37	GTP	BG	501	-	-	6/18/38/38	0/3/3/3
37	GTP	RE	501	-	-	3/18/38/38	0/3/3/3
37	GTP	VE	501	-	-	4/18/38/38	0/3/3/3
37	GTP	WI	501	-	-	6/18/38/38	0/3/3/3
39	GDP	BL	502	-	-	1/12/32/32	0/3/3/3
39	GDP	IB	502	-	-	6/12/32/32	0/3/3/3
39	GDP	AD	502	-	-	3/12/32/32	0/3/3/3
39	GDP	KF	502	-	-	3/12/32/32	0/3/3/3
39	GDP	NF	502	-	-	4/12/32/32	0/3/3/3
39	GDP	OL	502	-	-	3/12/32/32	0/3/3/3
37	GTP	CA	501	-	-	3/18/38/38	0/3/3/3
37	GTP	UI	501	-	-	6/18/38/38	0/3/3/3
39	GDP	SH	502	-	-	0/12/32/32	0/3/3/3
39	GDP	TB	502	-	-	6/12/32/32	0/3/3/3
39	GDP	KH	502	-	-	4/12/32/32	0/3/3/3
39	GDP	NJ	502	-	-	2/12/32/32	0/3/3/3
39	GDP	WL	502	-	-	5/12/32/32	0/3/3/3
39	GDP	GB	502	-	-	2/12/32/32	0/3/3/3
37	GTP	KI	501	-	-	8/18/38/38	0/3/3/3
39	GDP	IL	502	-	-	0/12/32/32	0/3/3/3
39	GDP	KD	502	-	-	5/12/32/32	0/3/3/3
39	GDP	KL	502	-	-	1/12/32/32	0/3/3/3
37	GTP	HG	501	-	-	4/18/38/38	0/3/3/3
37	GTP	TC	501	-	-	9/18/38/38	0/3/3/3
39	GDP	ND	502	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	PH	502	-	-	0/12/32/32	0/3/3/3
39	GDP	RD	502	-	-	2/12/32/32	0/3/3/3
37	GTP	BE	501	-	-	4/18/38/38	0/3/3/3
39	GDP	NB	502	-	-	3/12/32/32	0/3/3/3

The worst 5 of 472 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	KC	501	GTP	C5-C6	-5.53	1.36	1.47
37	KG	501	GTP	C5-C6	-5.44	1.36	1.47
37	KE	501	GTP	C5-C6	-5.19	1.36	1.47
37	KI	501	GTP	C5-C6	-5.14	1.37	1.47
37	KM	501	GTP	C5-C6	-5.14	1.37	1.47

The worst 5 of 1688 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	GC	501	GTP	PA-O3A-PB	-5.48	114.03	132.83
37	IG	501	GTP	PA-O3A-PB	-5.45	114.12	132.83
39	IJ	502	GDP	PA-O3A-PB	-5.44	114.15	132.83
37	VI	501	GTP	PA-O3A-PB	-5.40	114.31	132.83
39	HN	502	GDP	PA-O3A-PB	-5.37	114.41	132.83

There are no chirality outliers.

5 of 1189 torsion outliers are listed below:

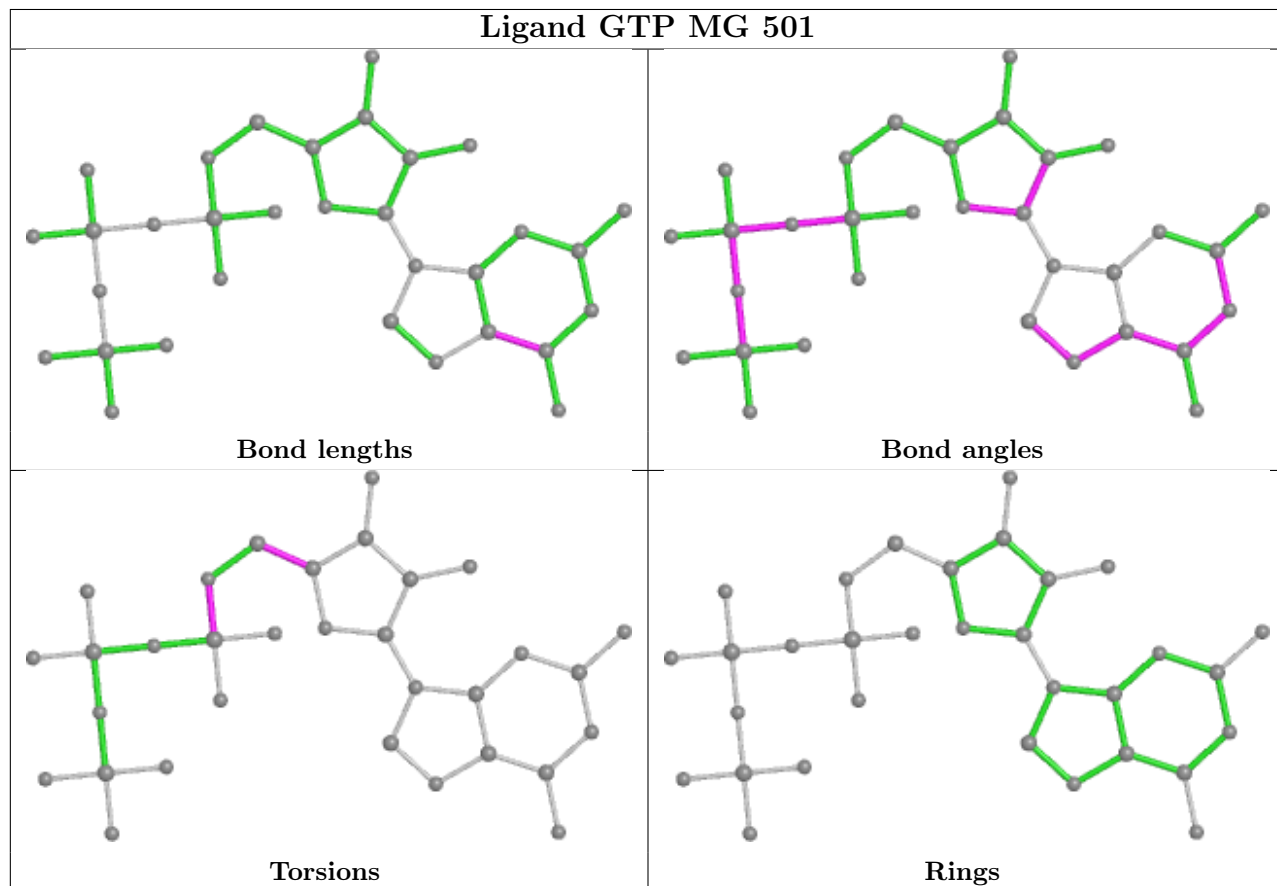
Mol	Chain	Res	Type	Atoms
37	AA	501	GTP	C5'-O5'-PA-O1A
37	AA	501	GTP	C5'-O5'-PA-O2A
37	AC	501	GTP	C5'-O5'-PA-O3A
37	AE	501	GTP	C5'-O5'-PA-O3A
37	AG	501	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

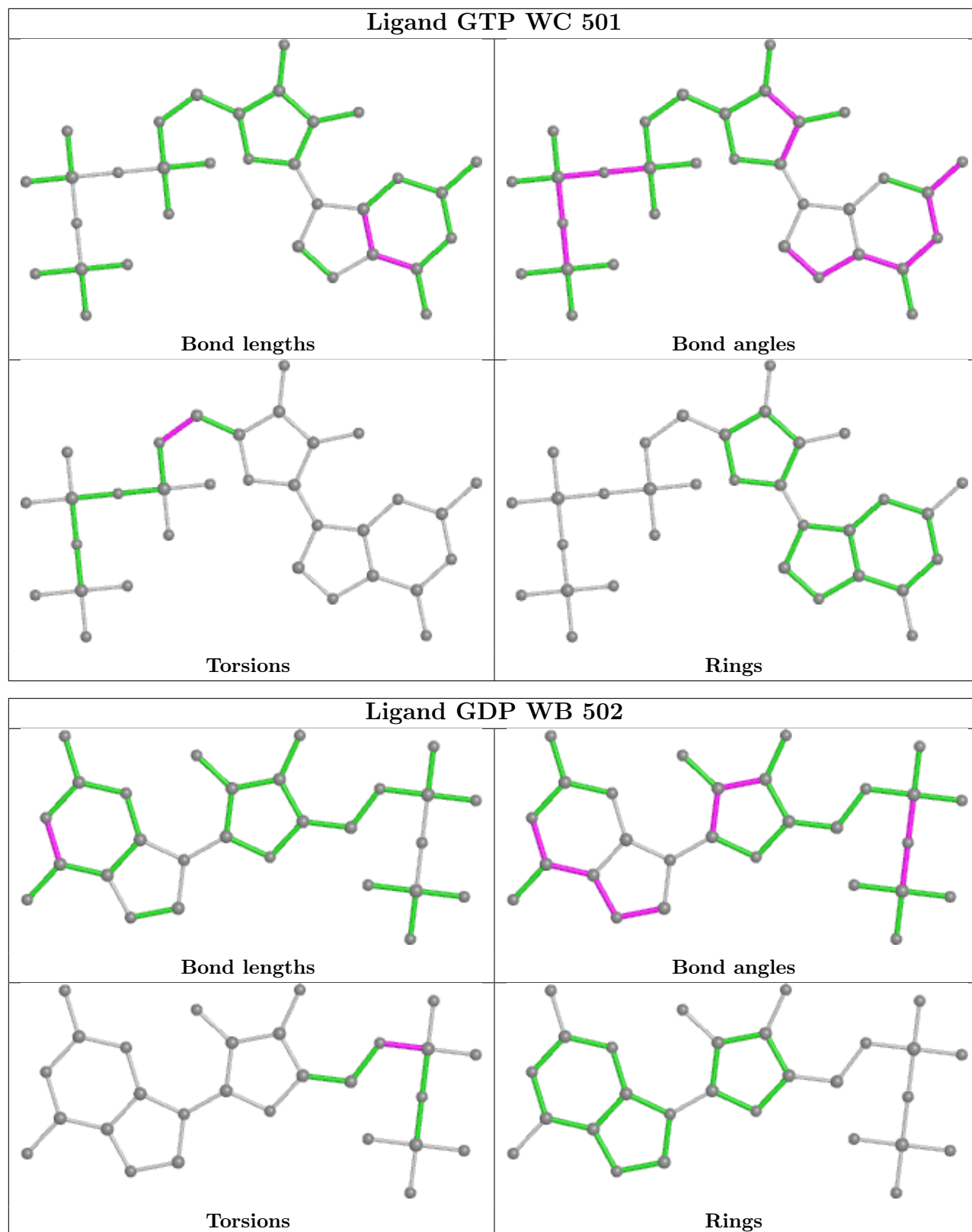
No monomer is involved in short contacts.

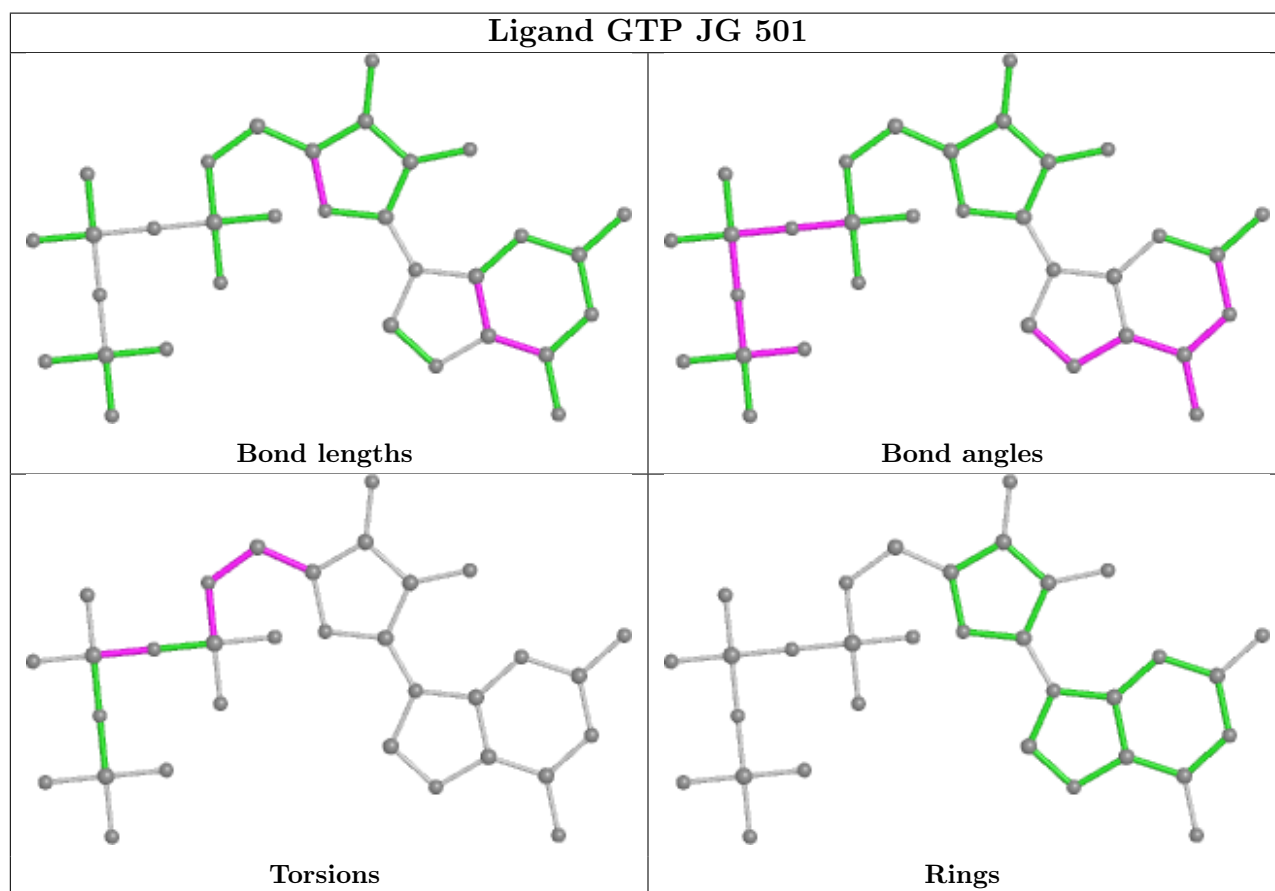
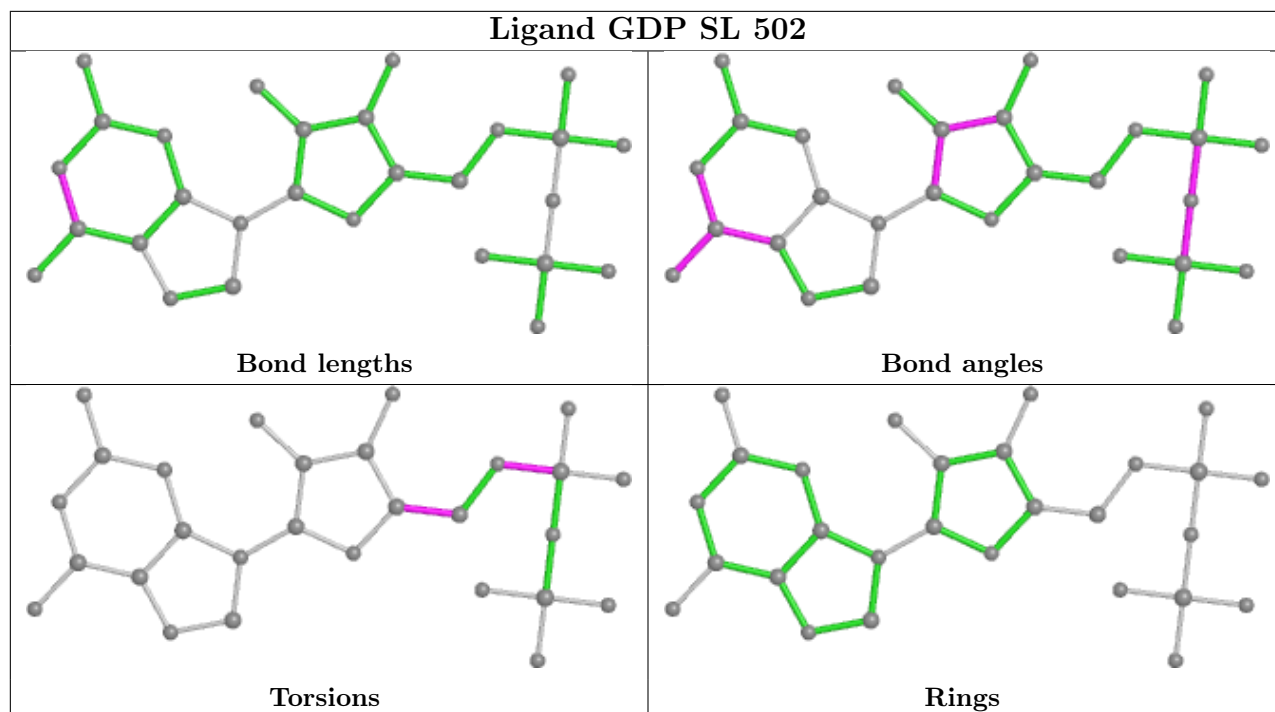
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

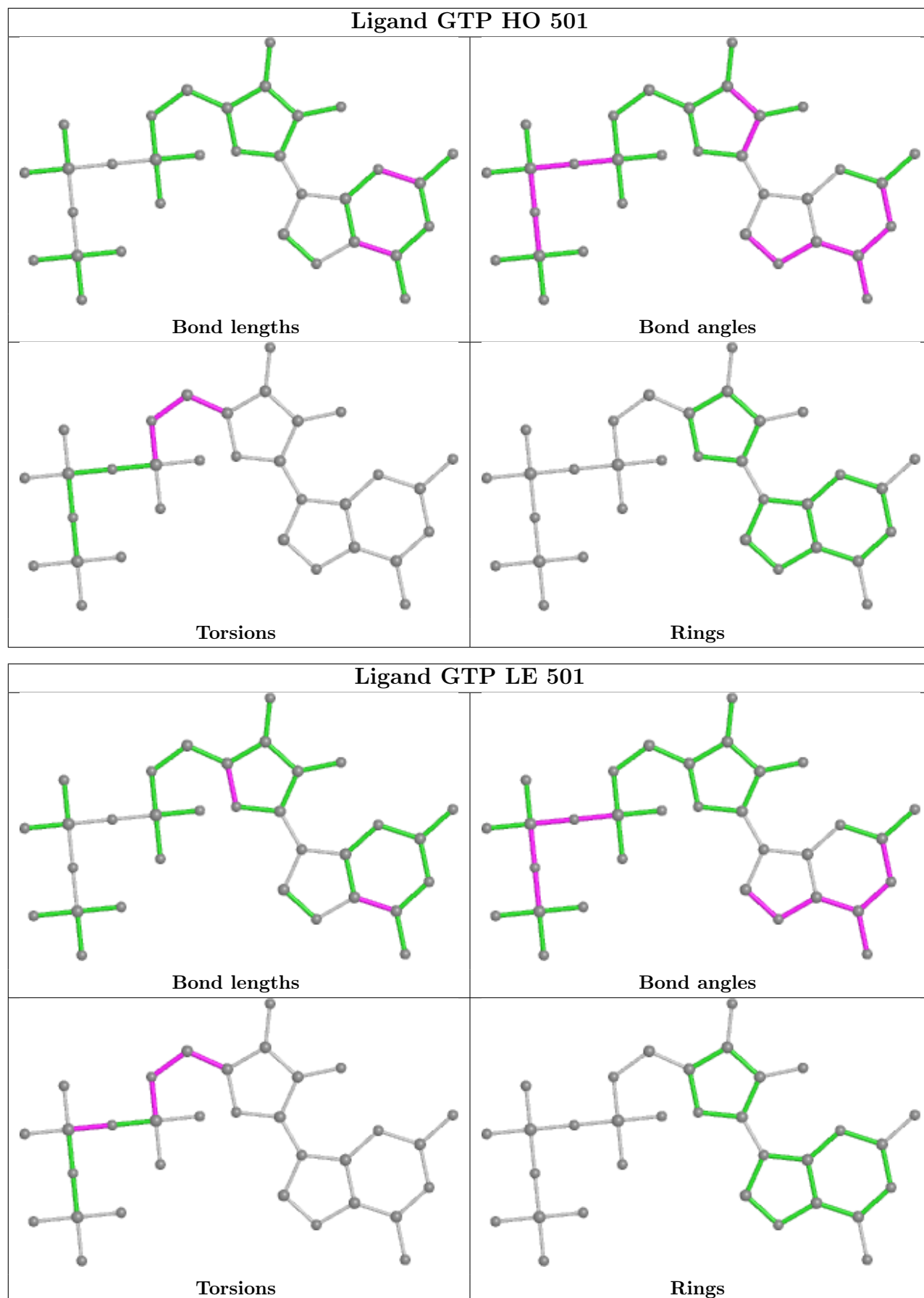
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

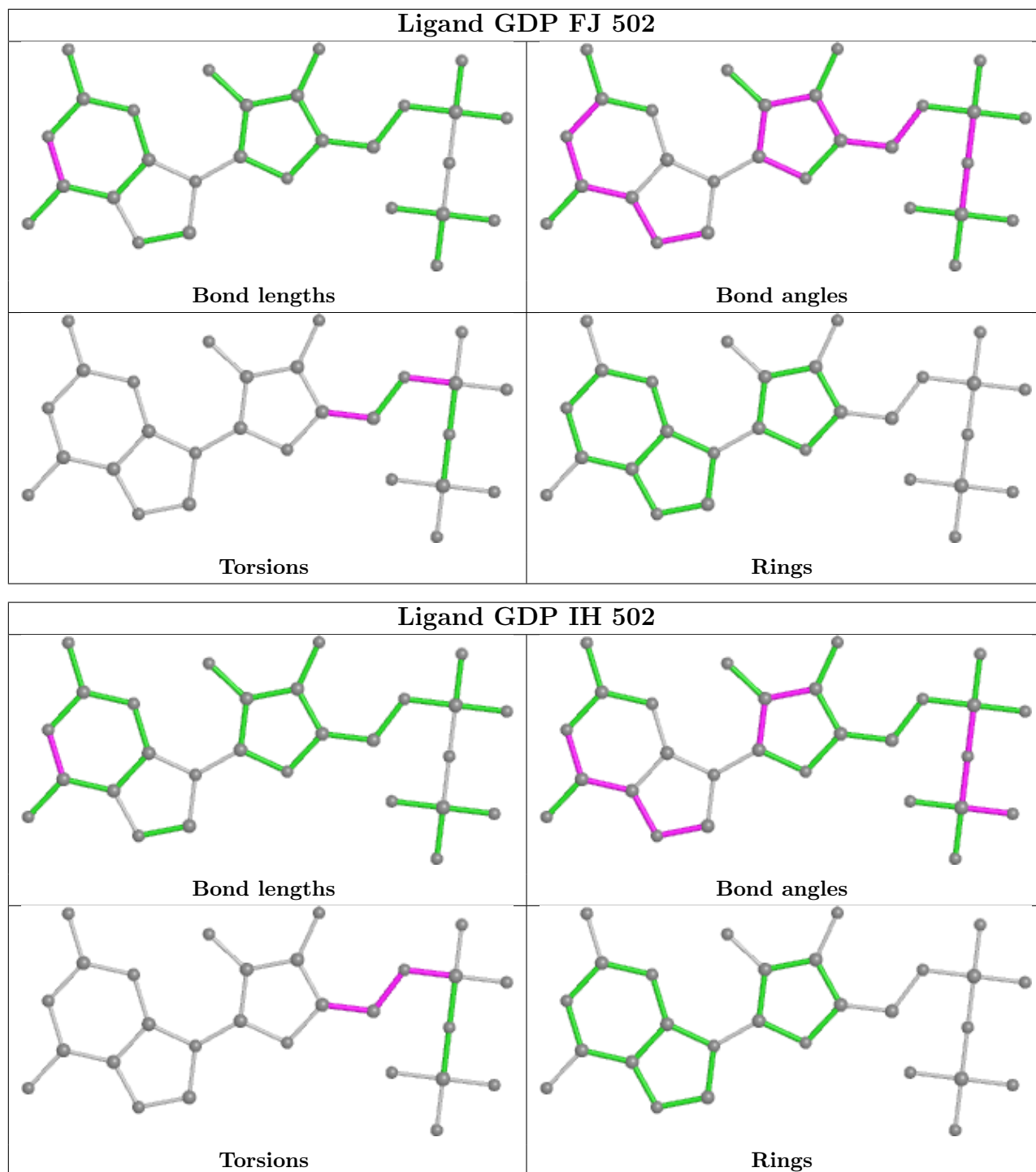


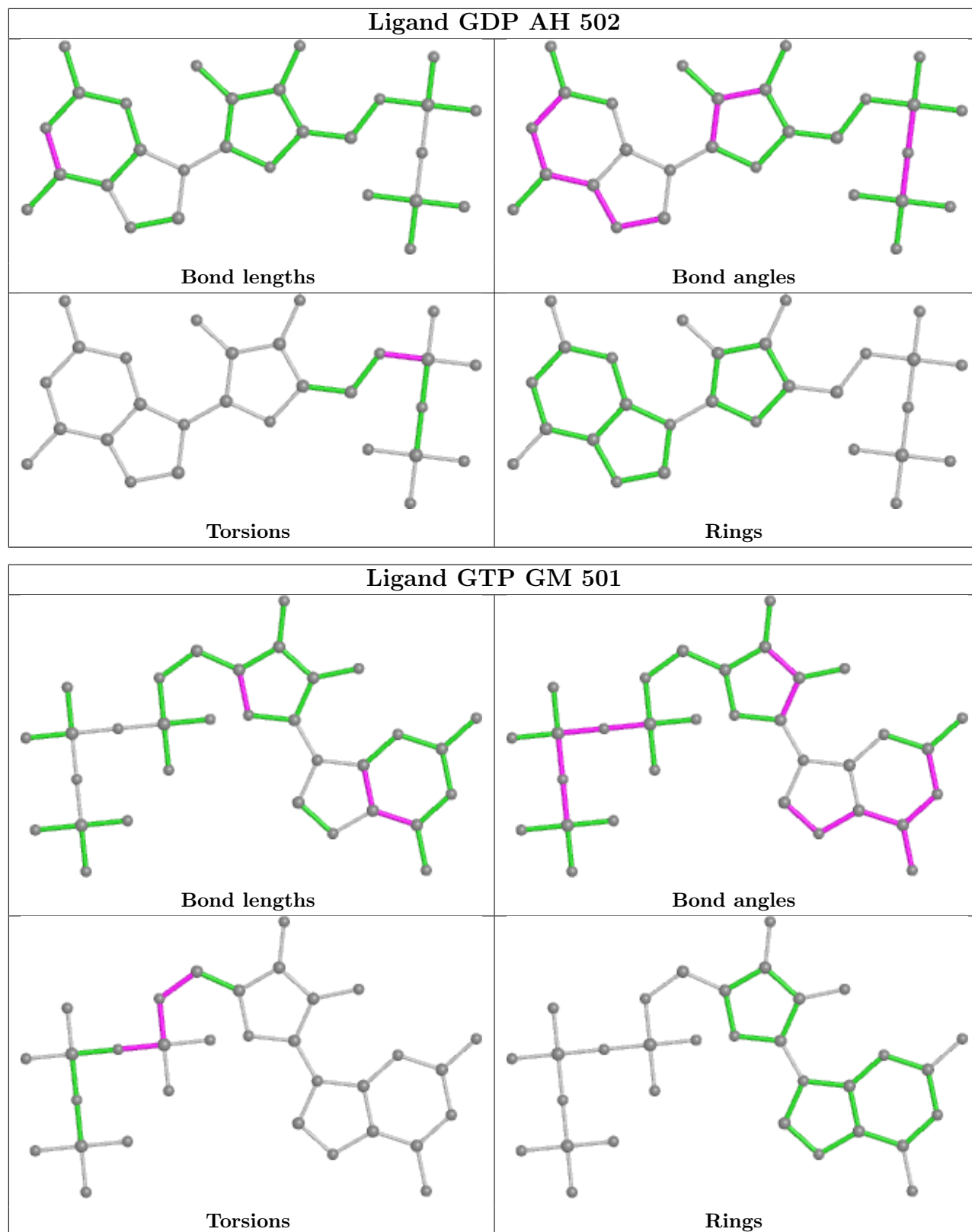


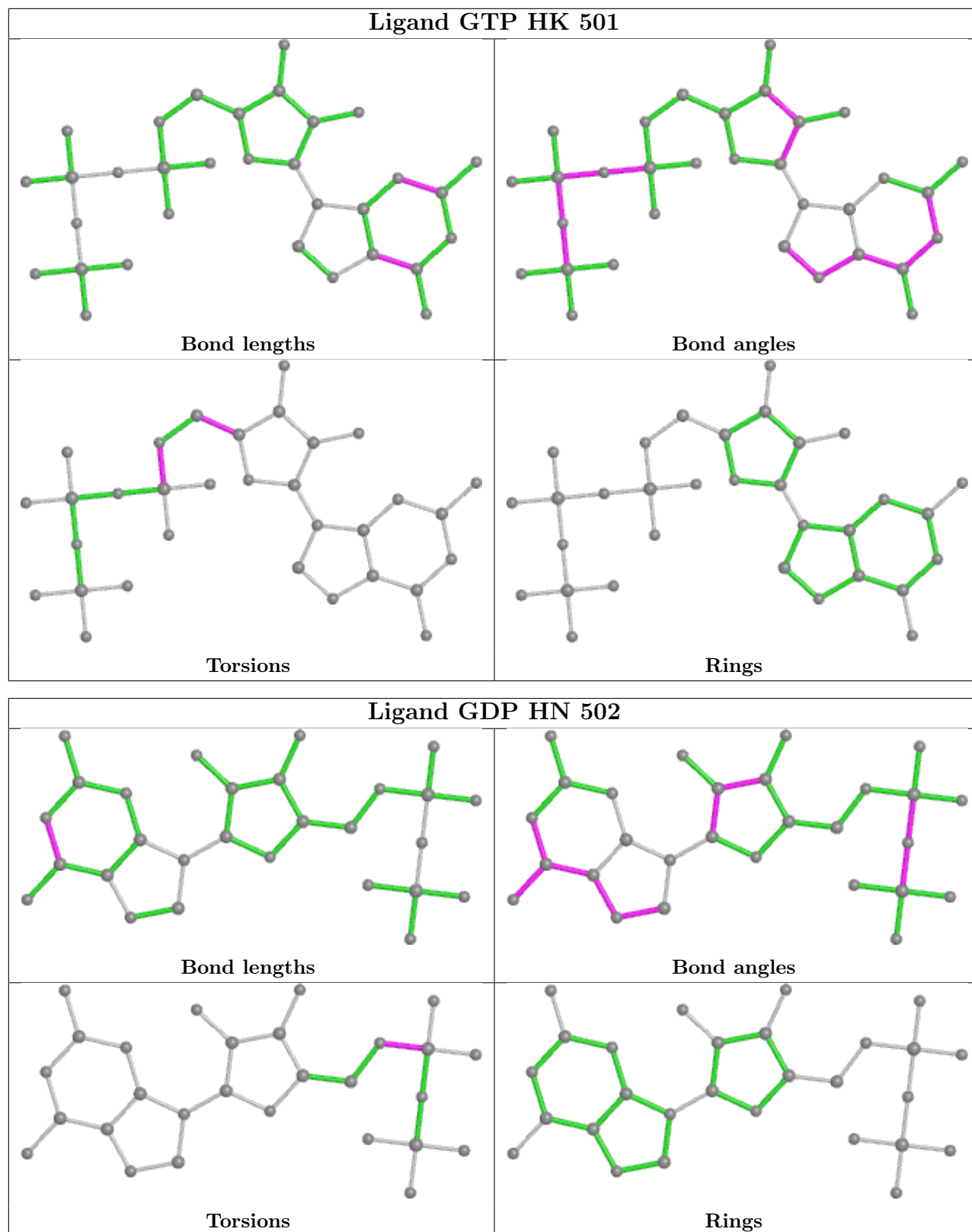


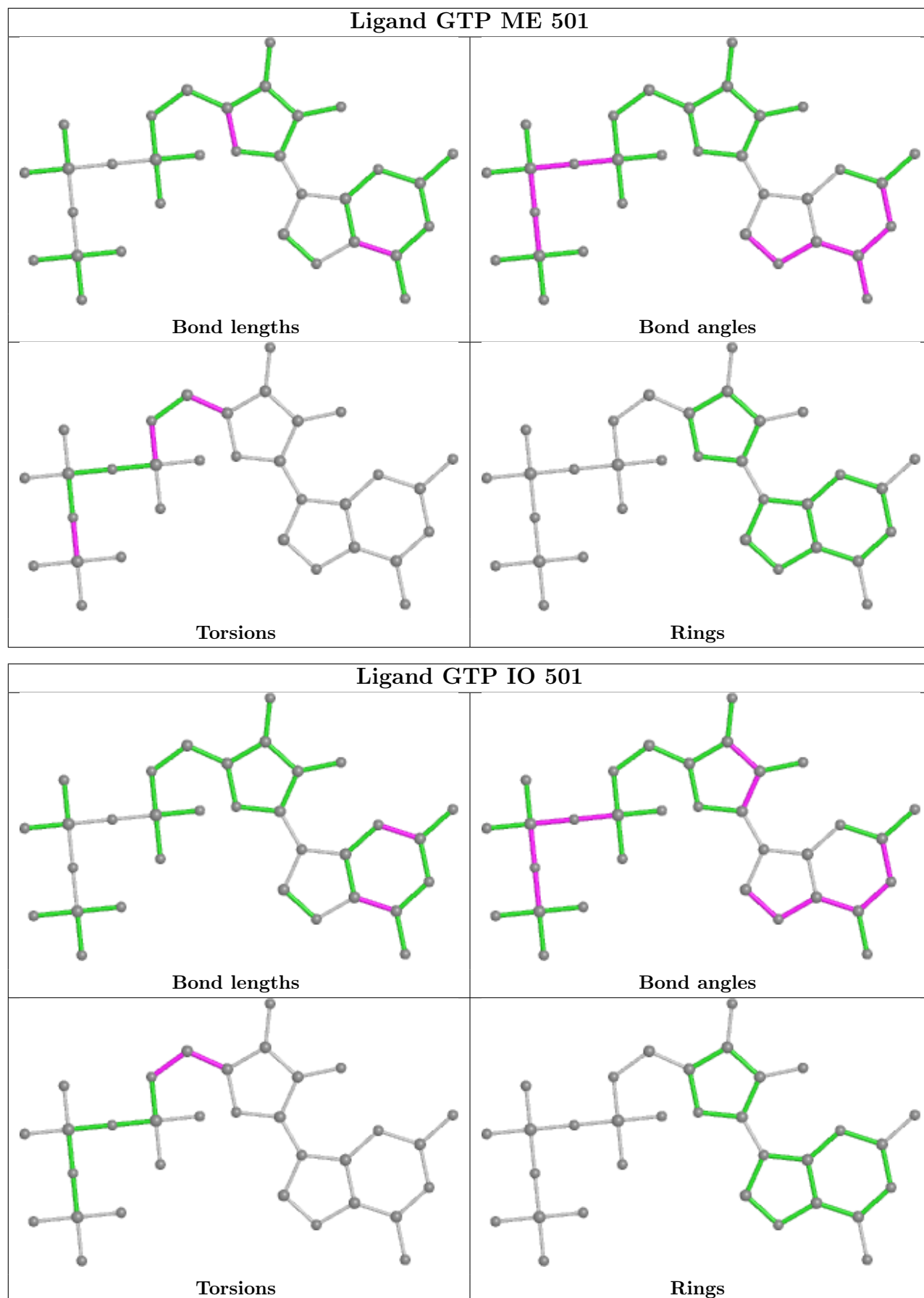


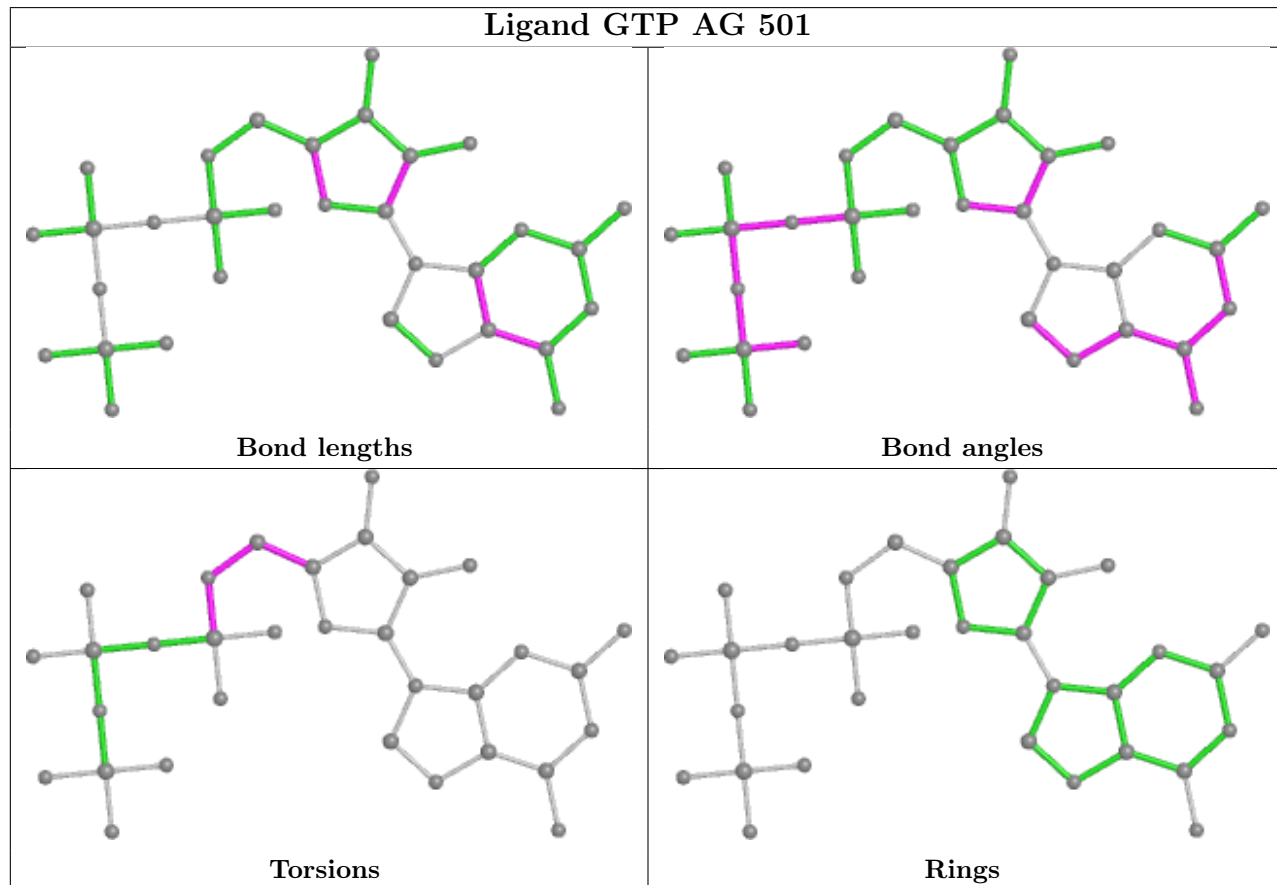
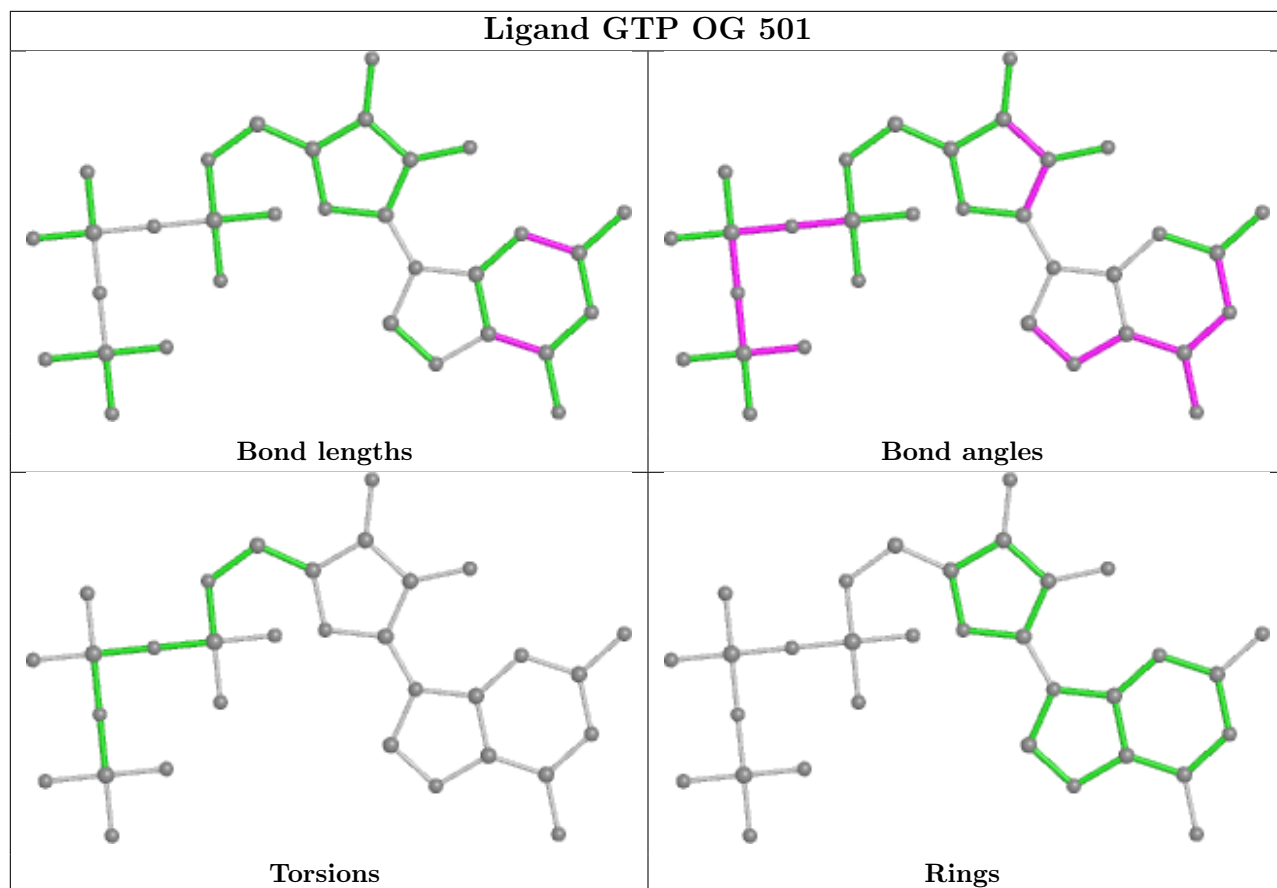




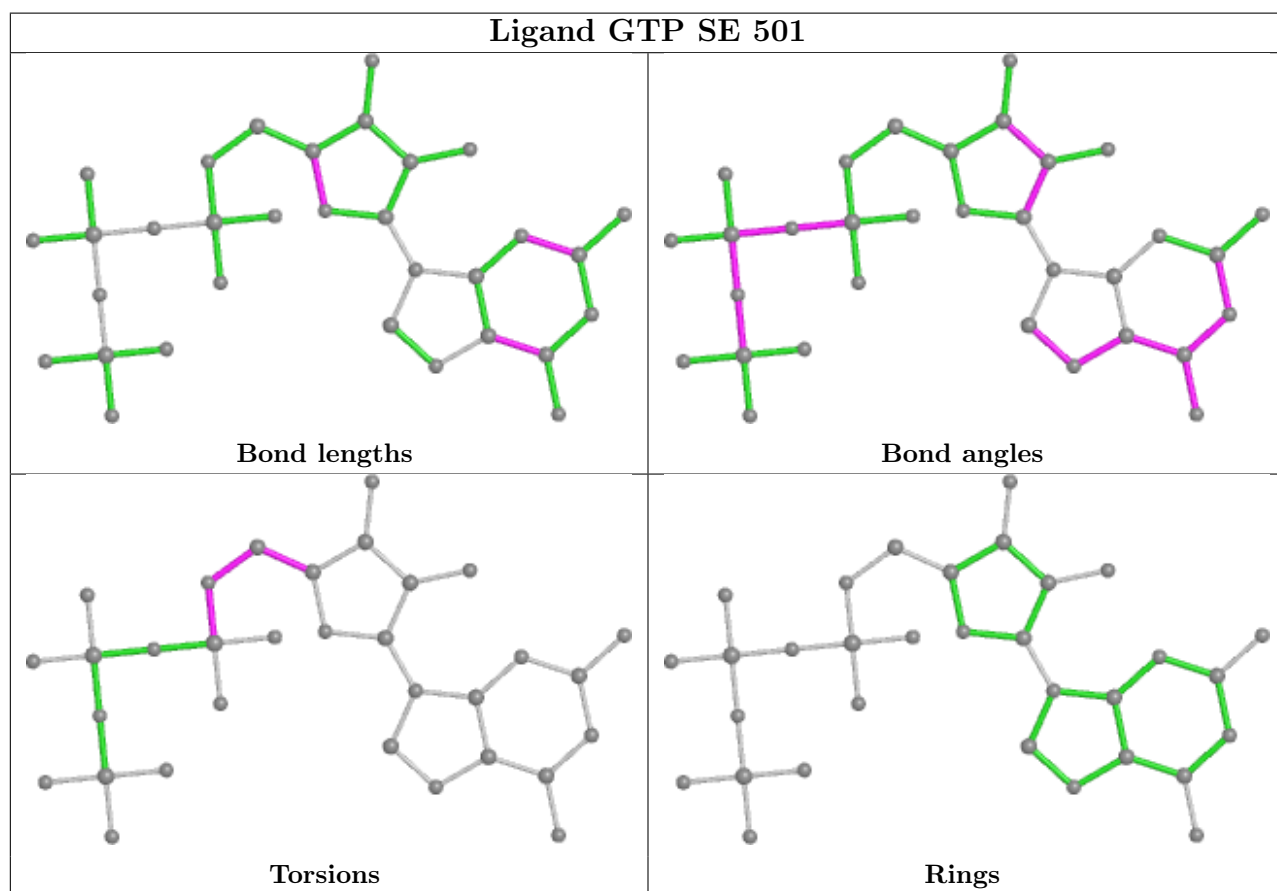
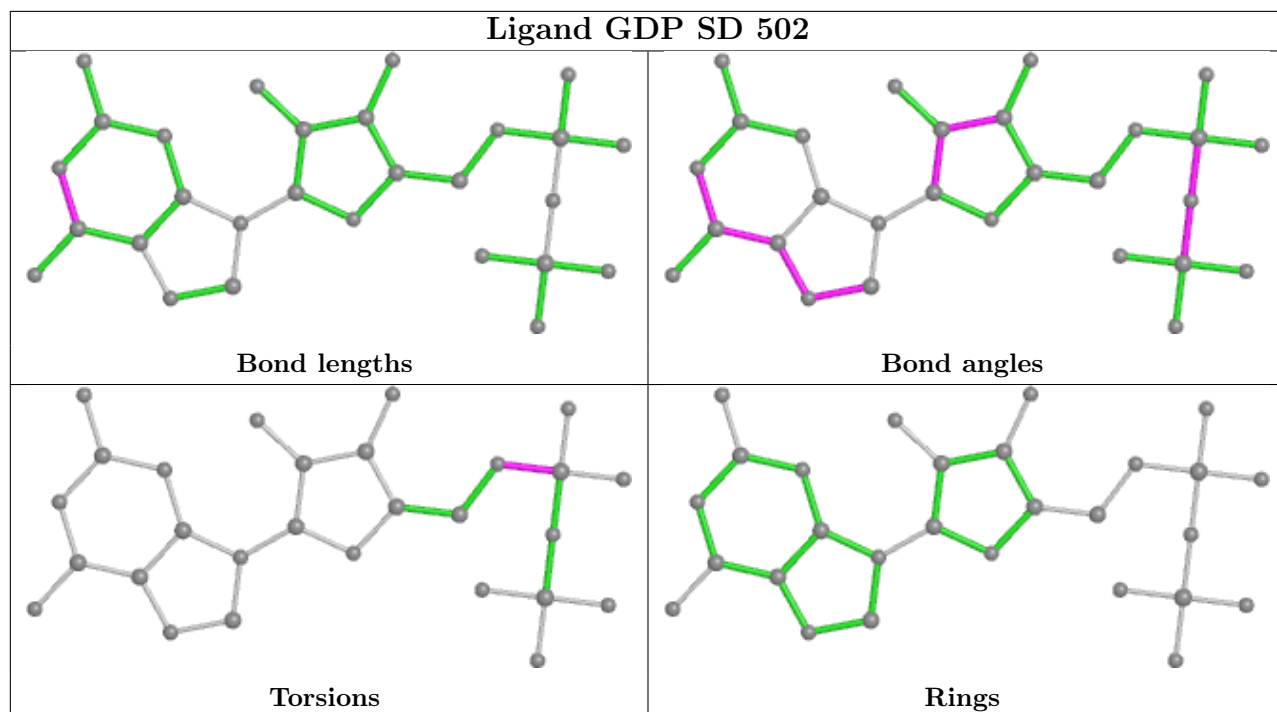


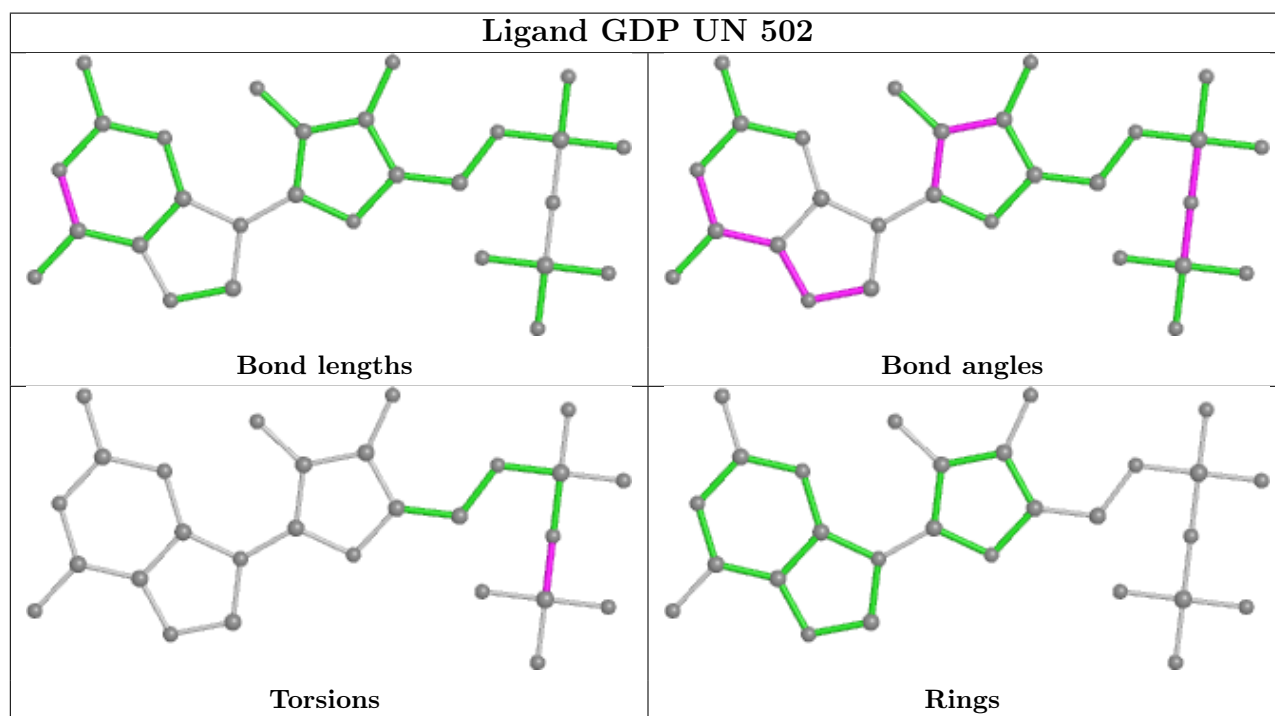
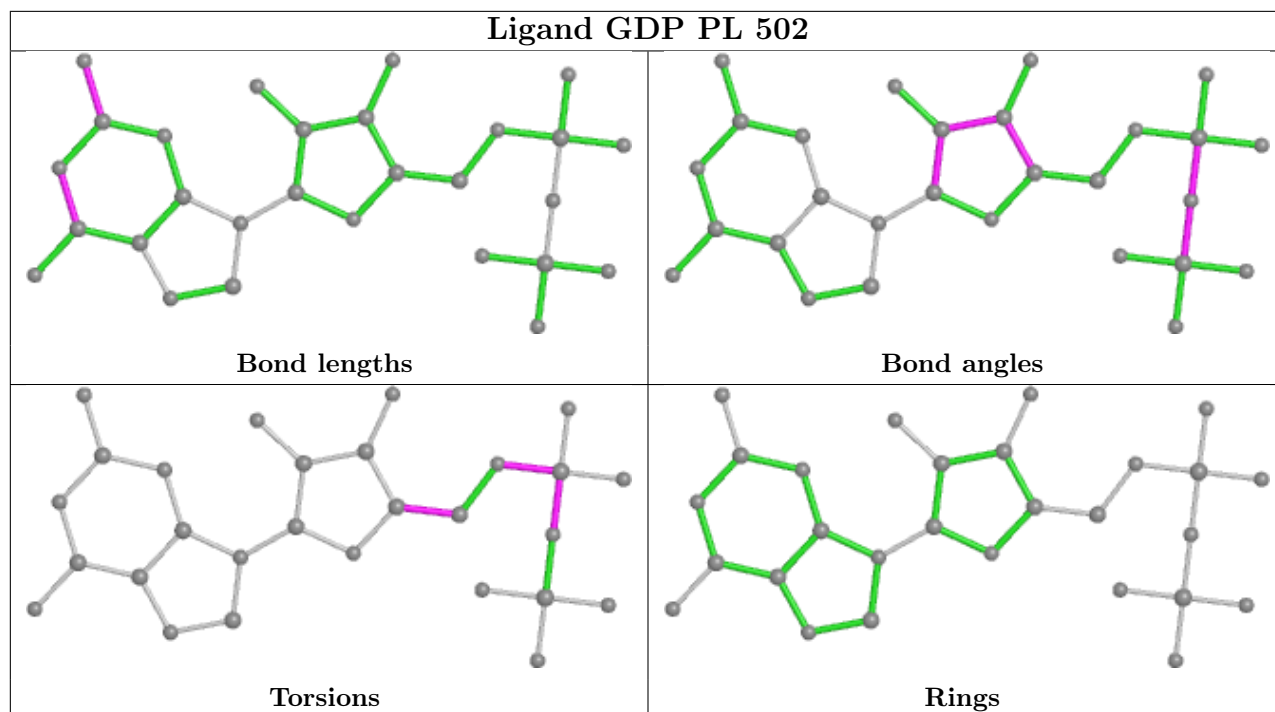


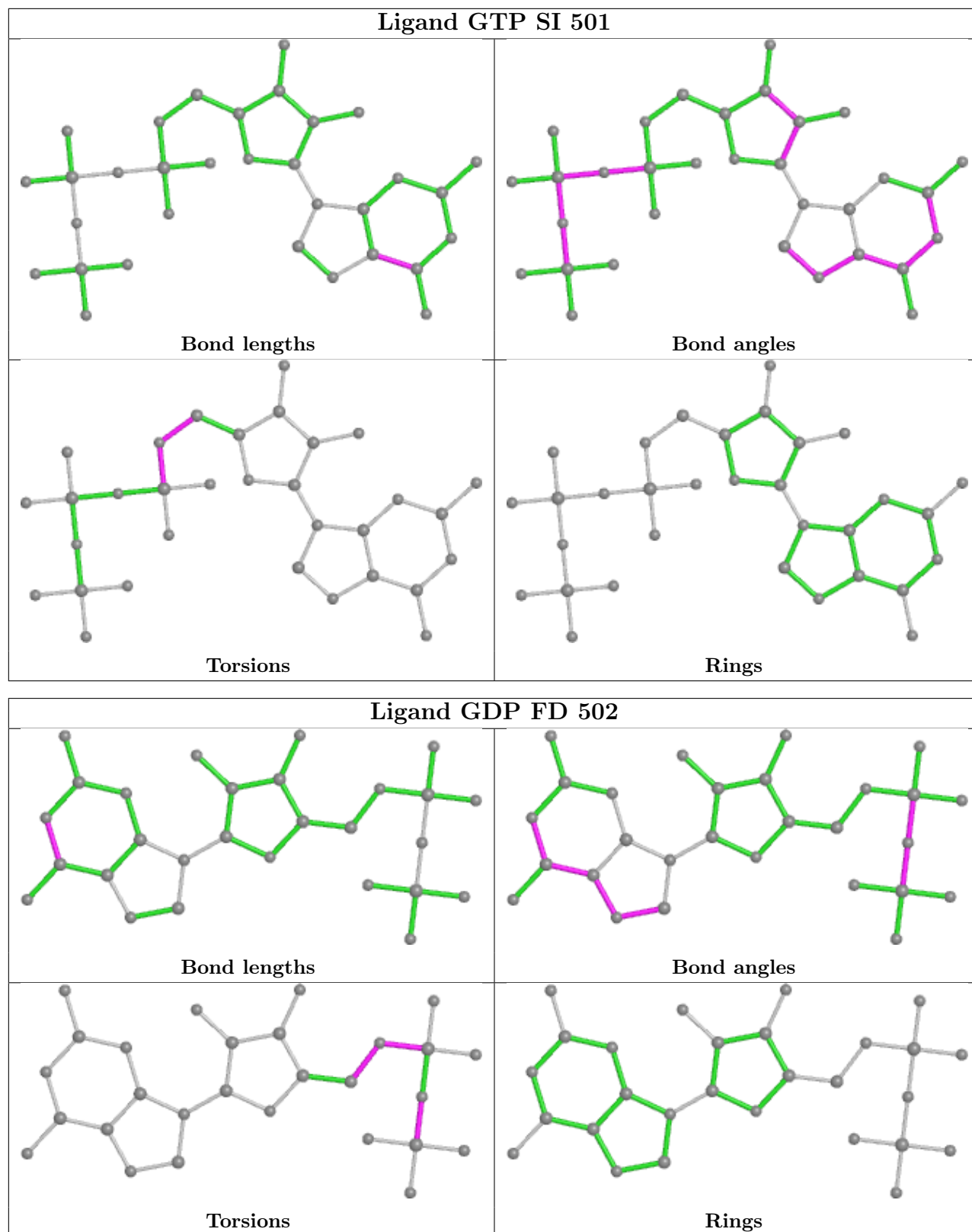


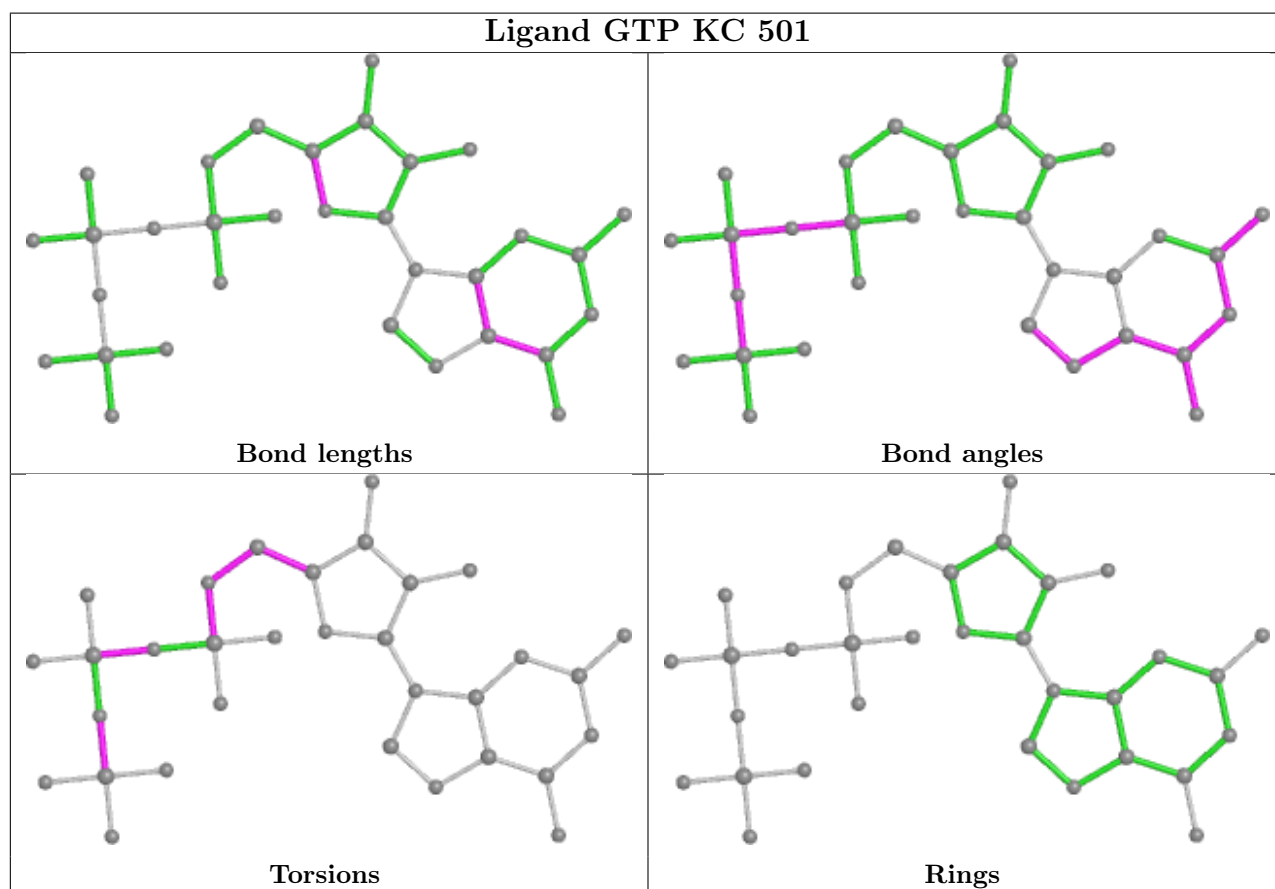
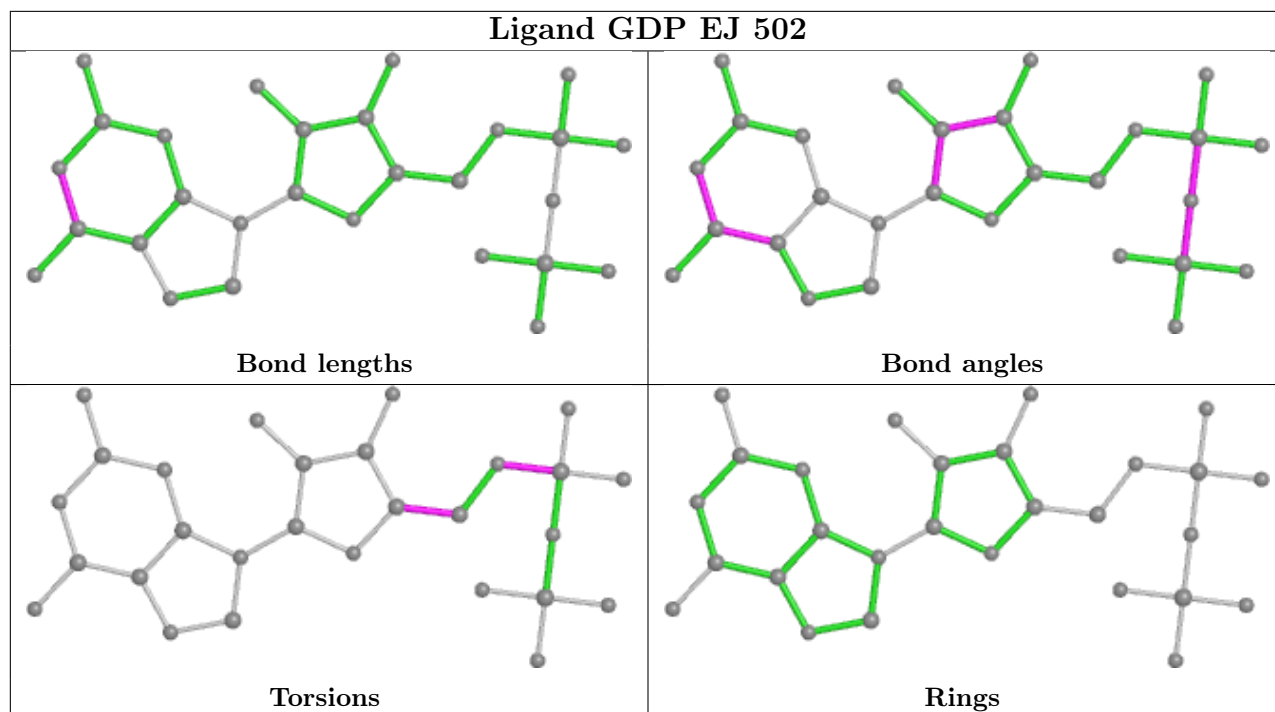


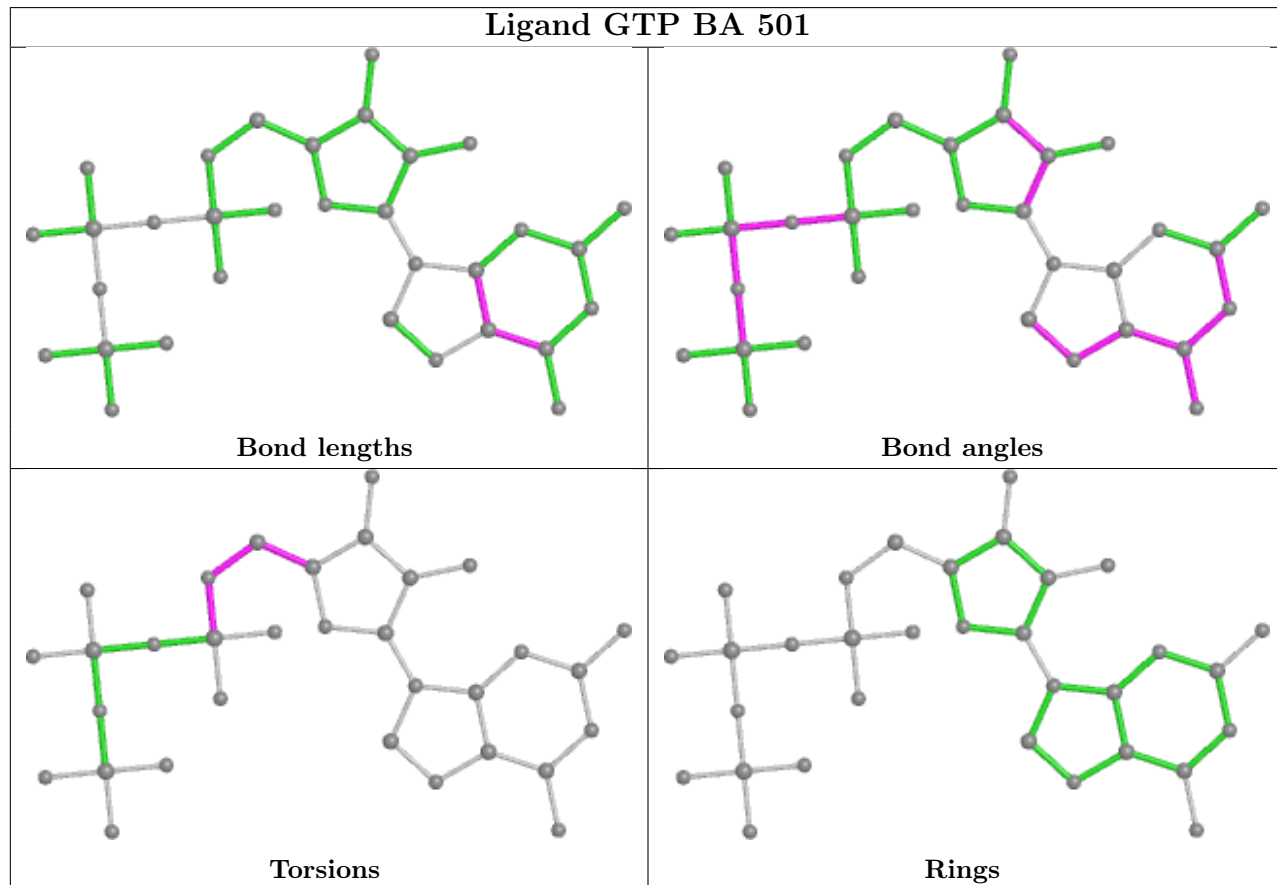
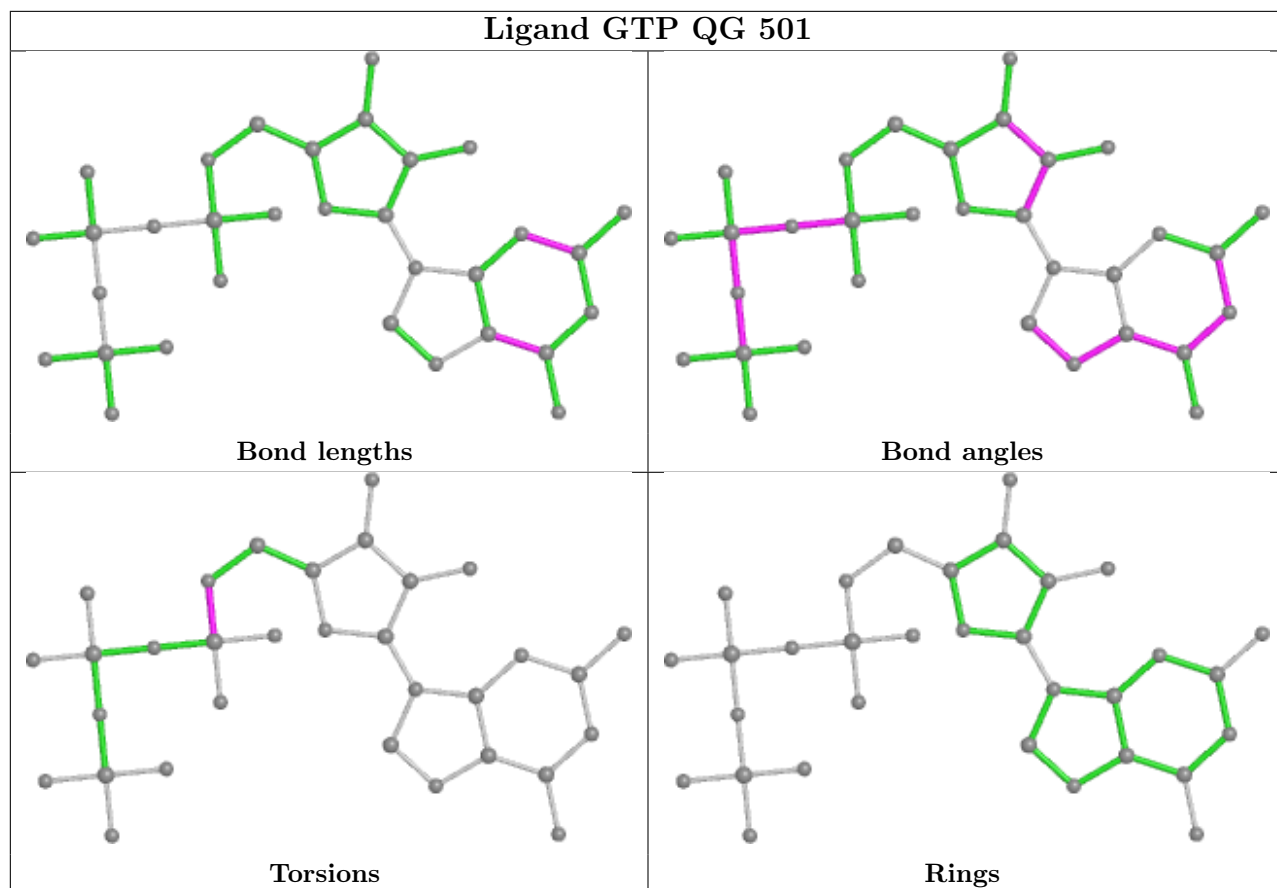


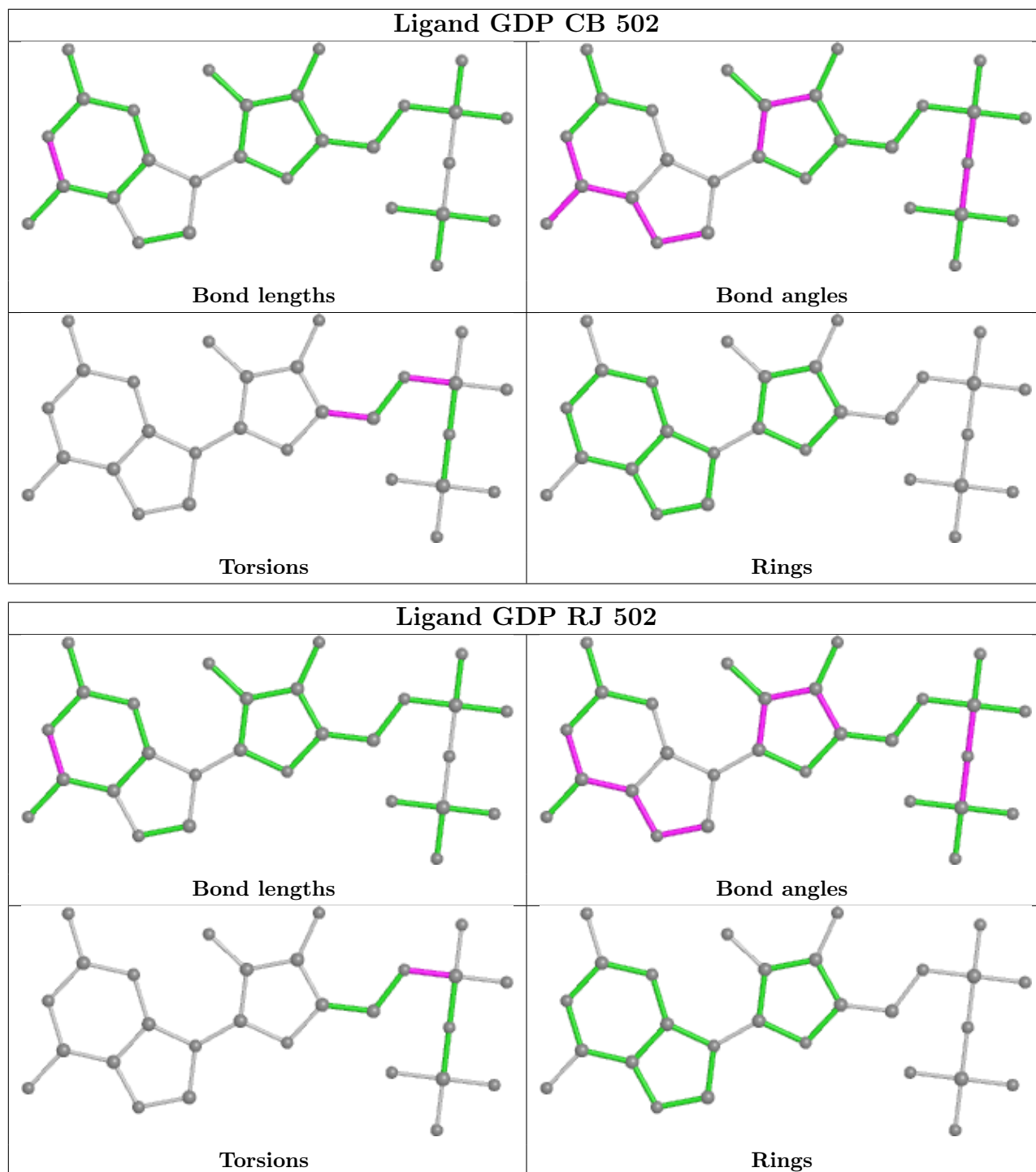


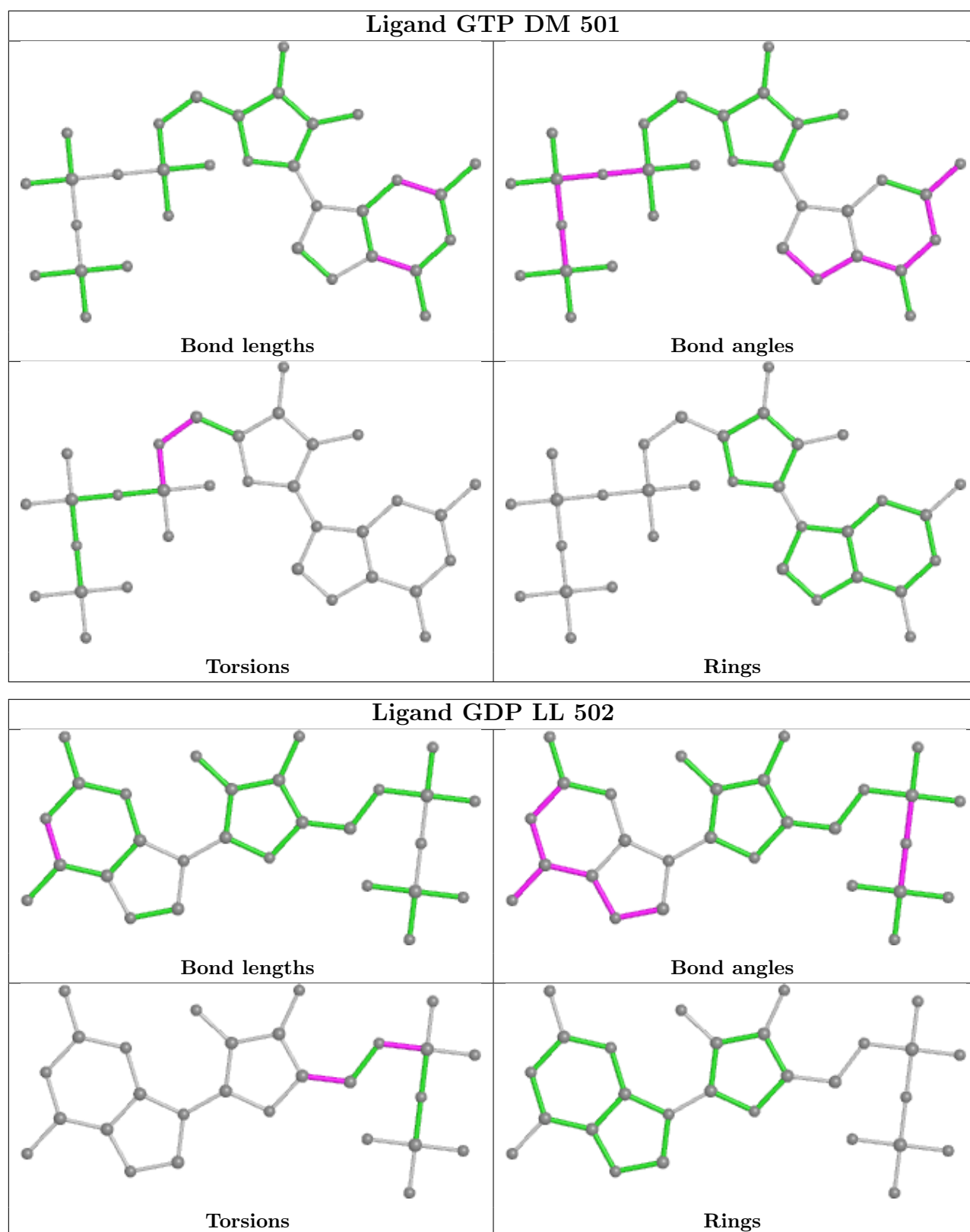


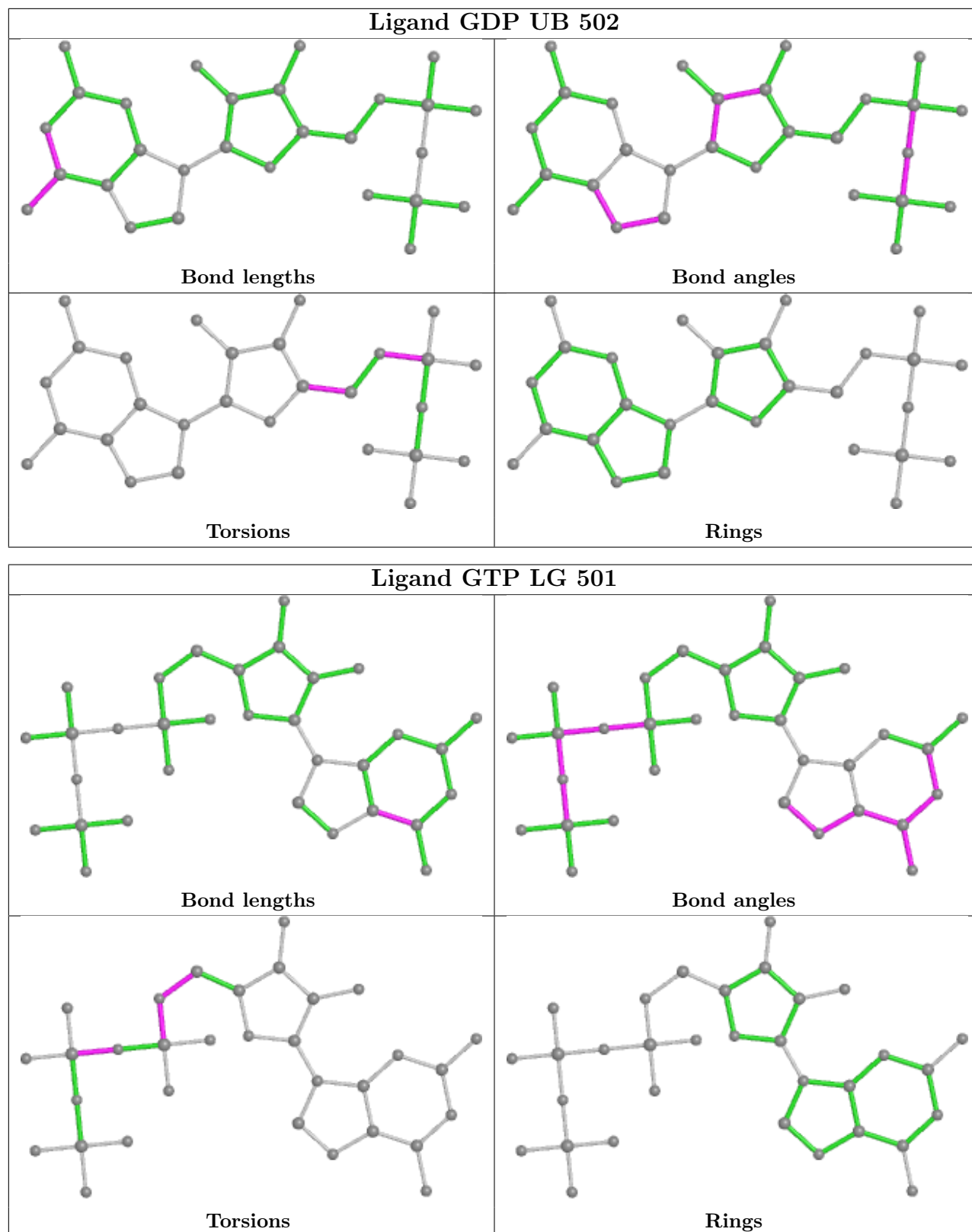




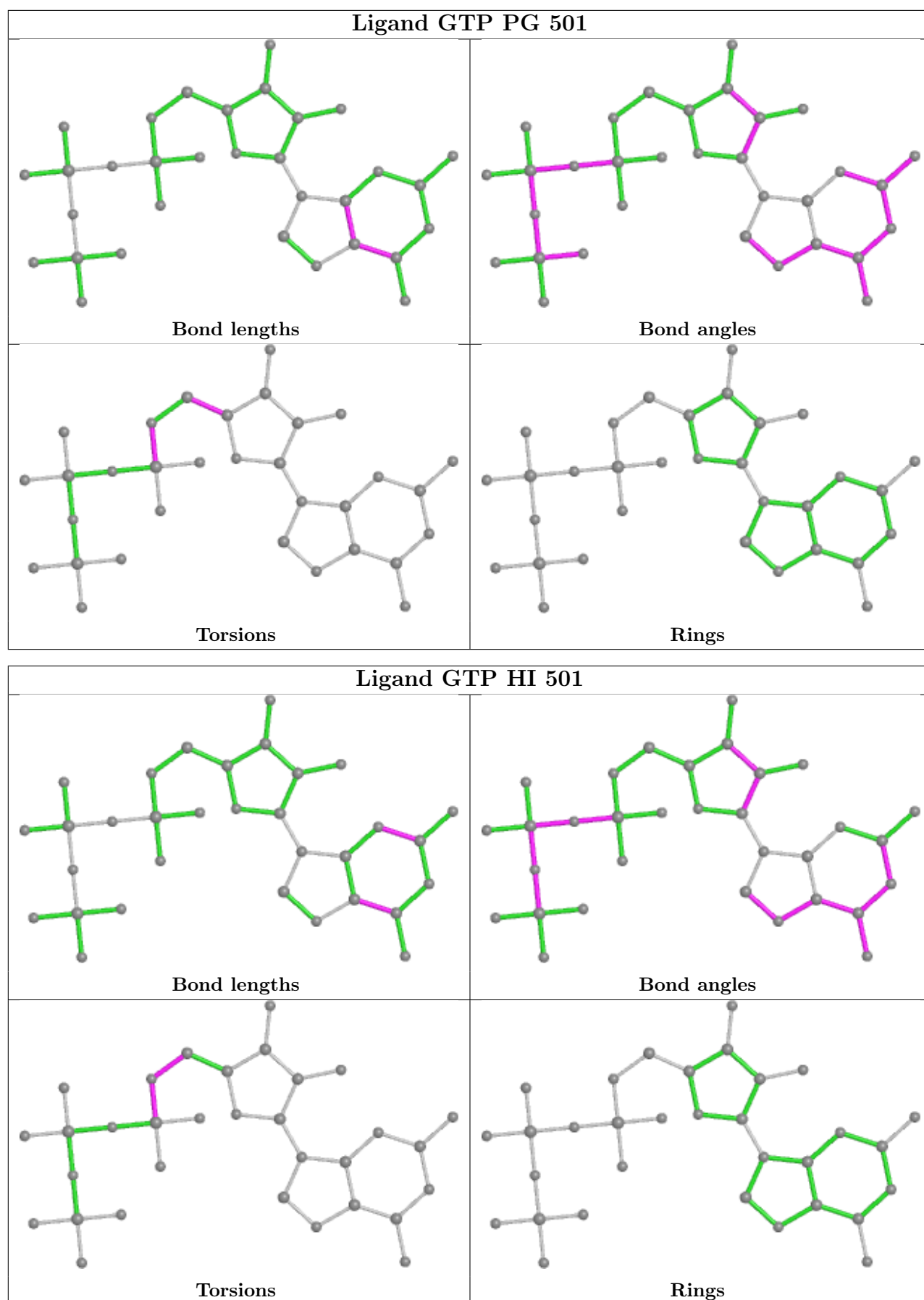


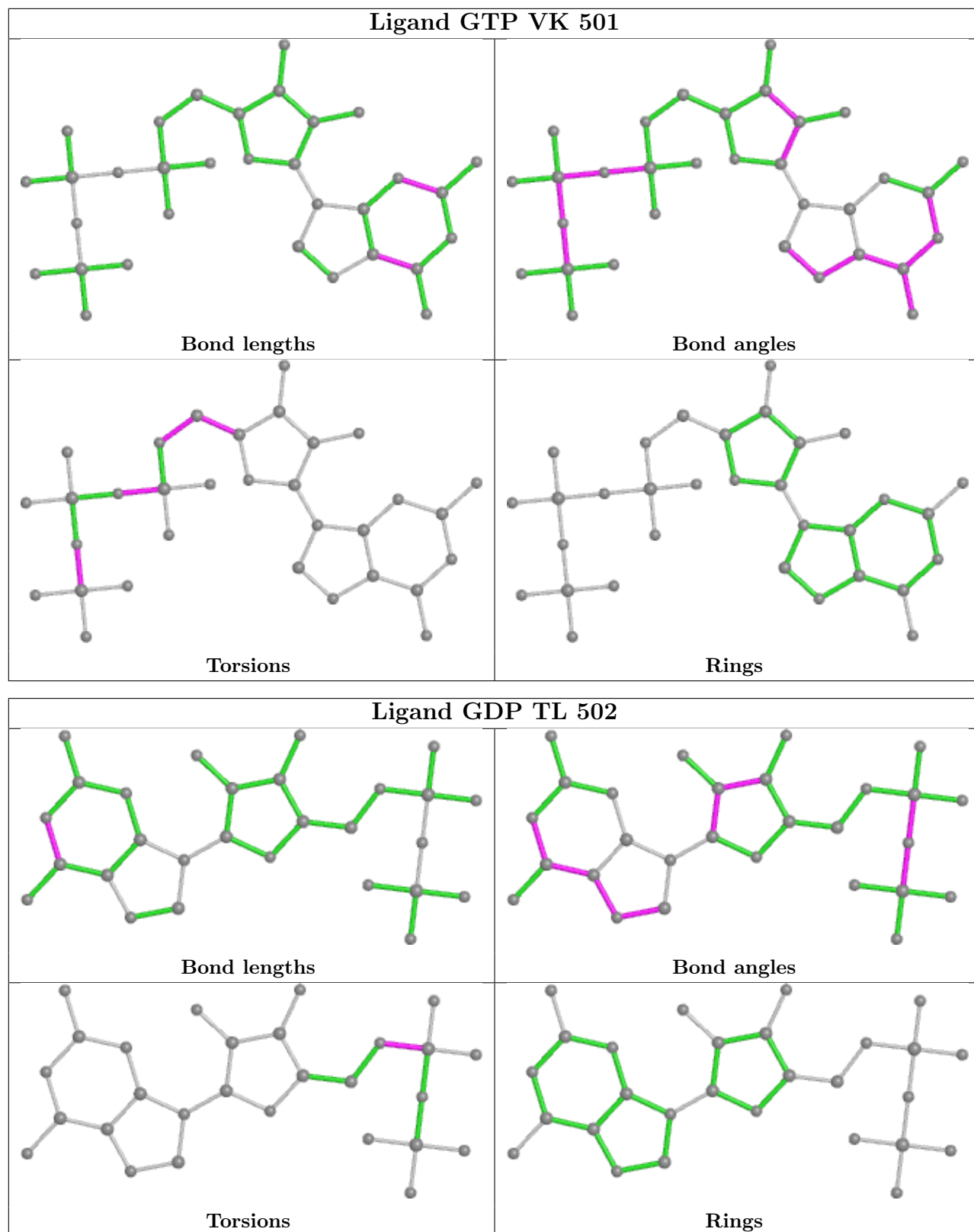


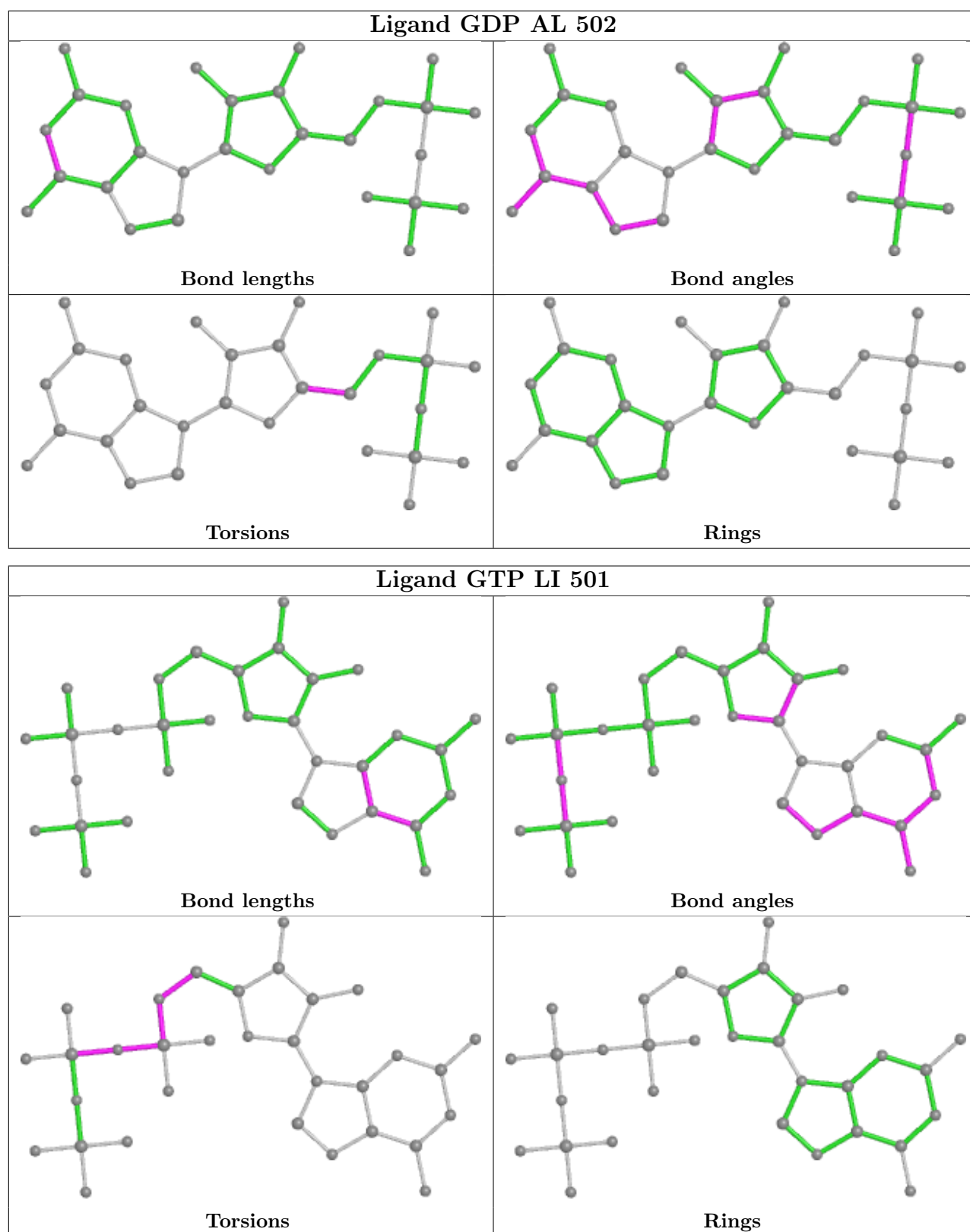


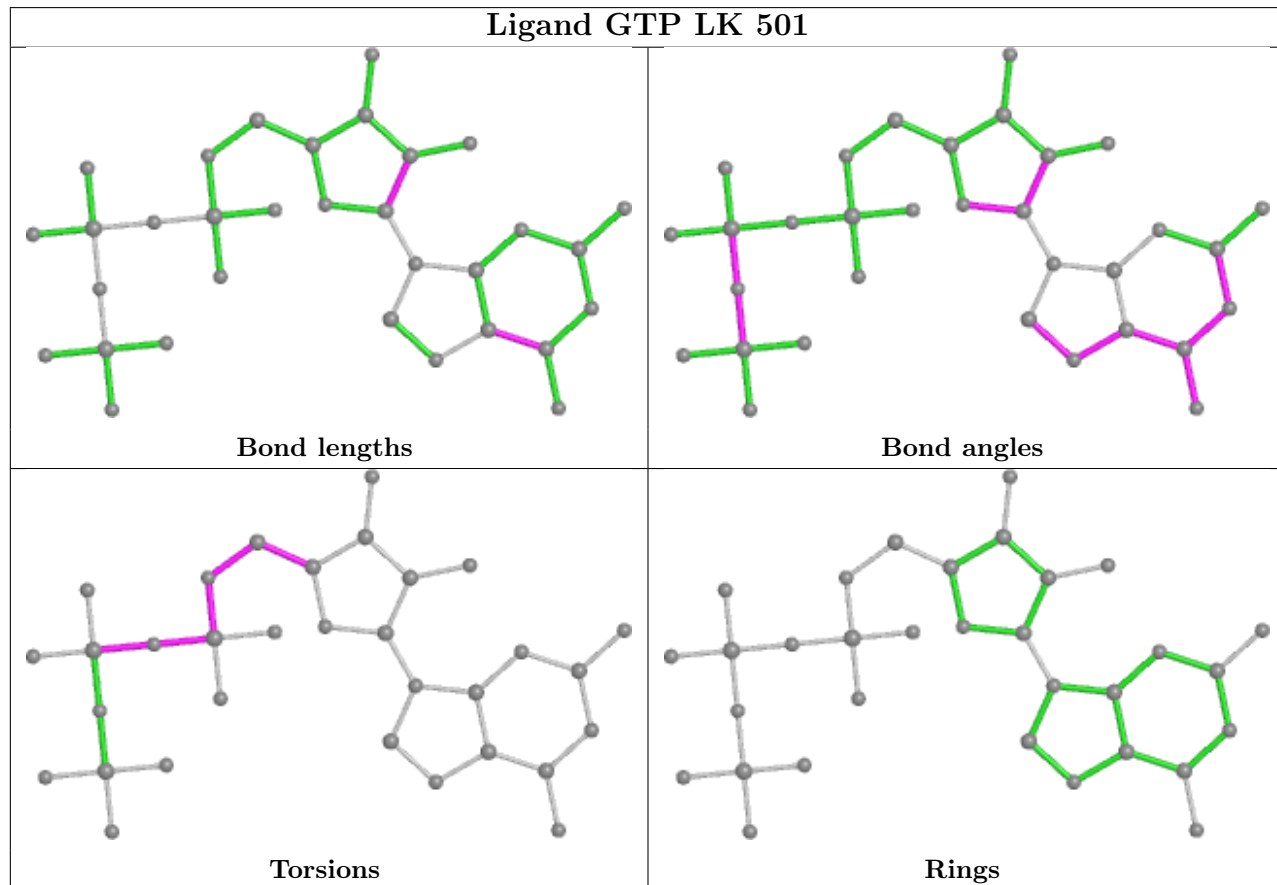
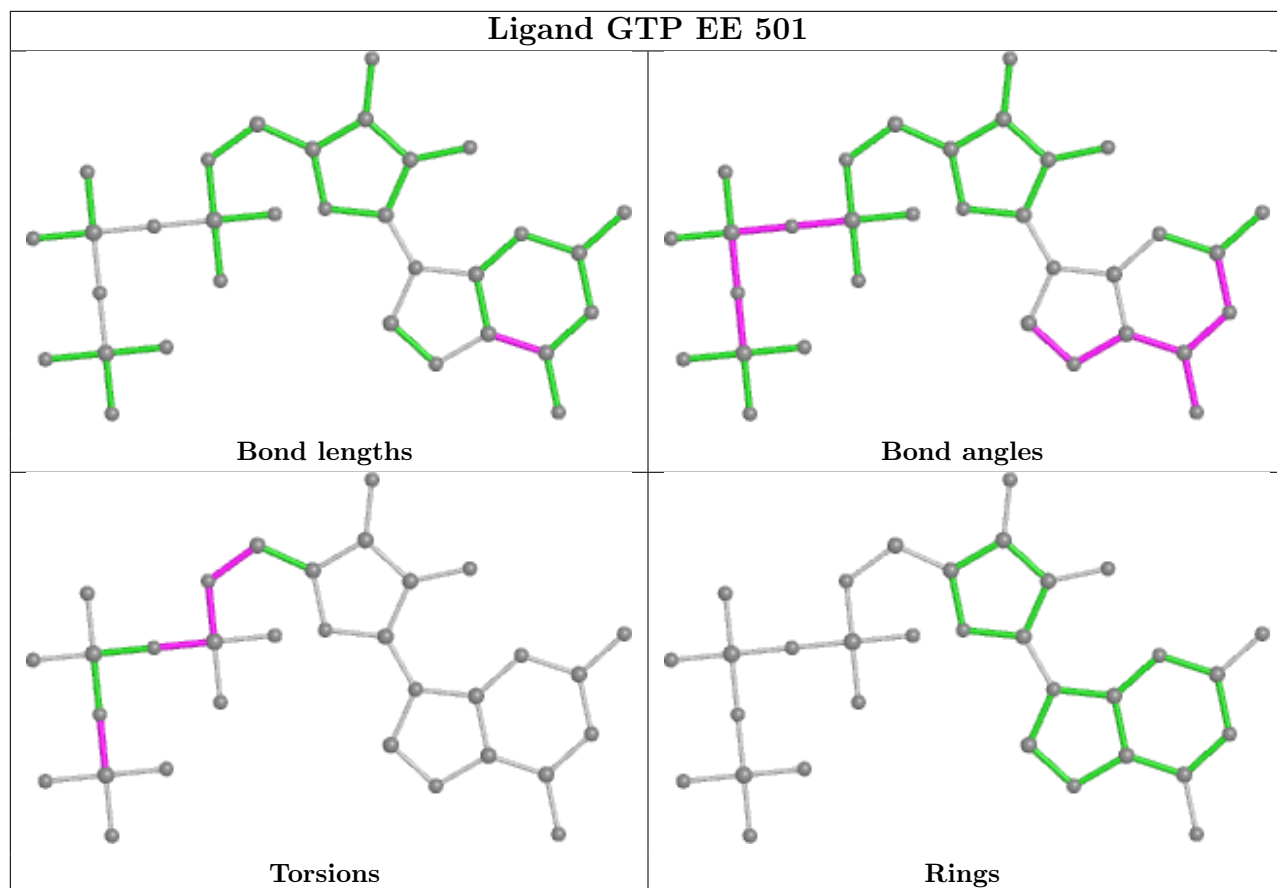


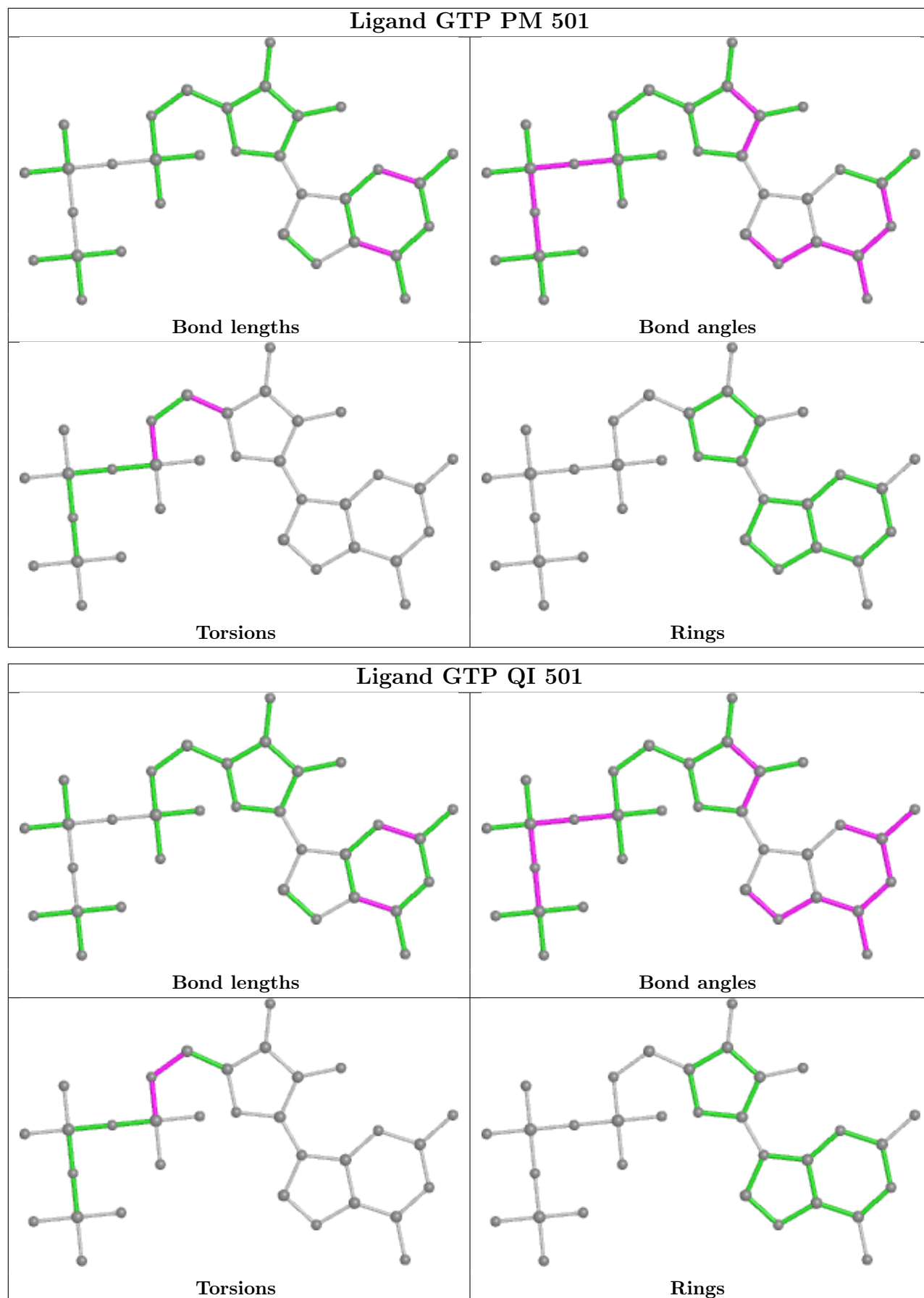


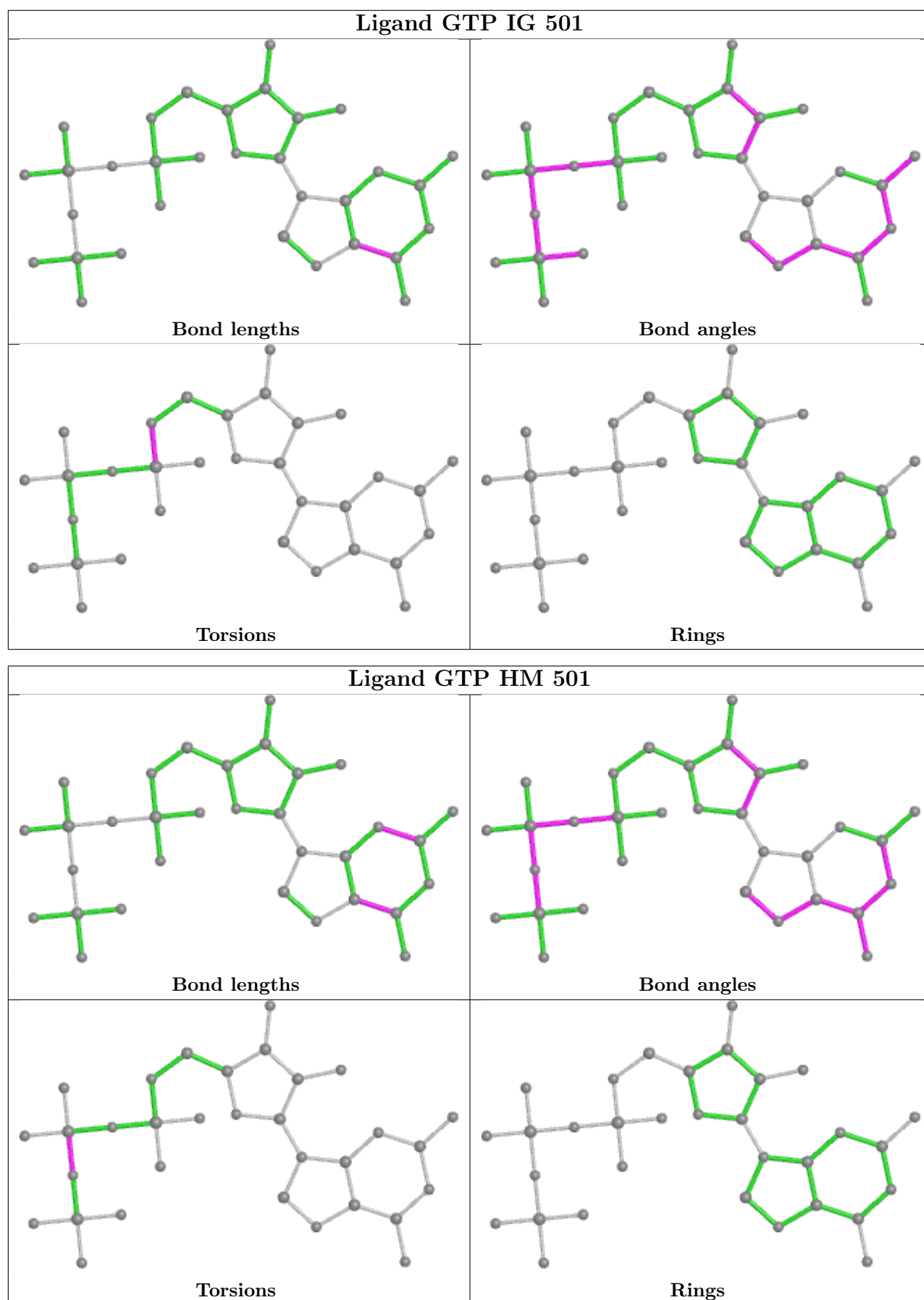


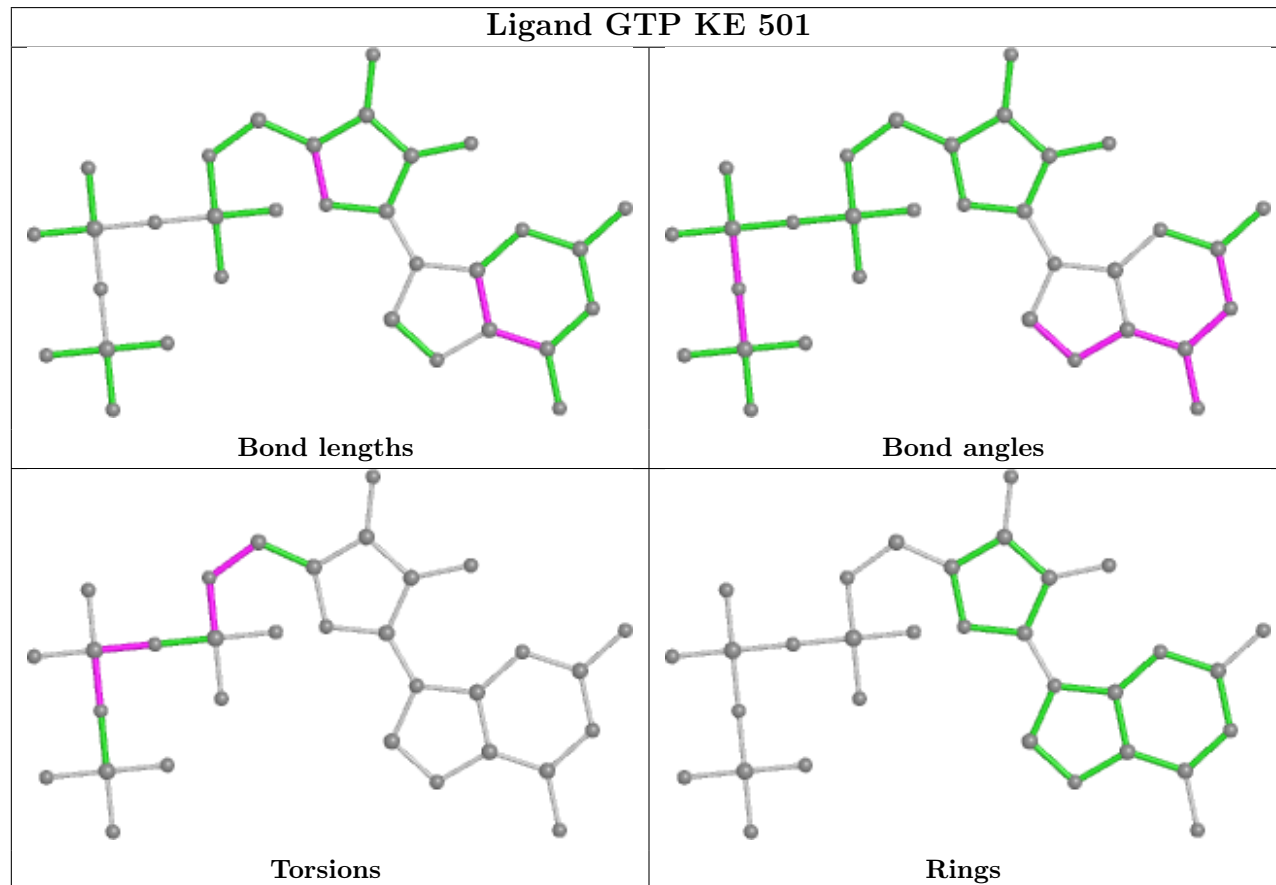
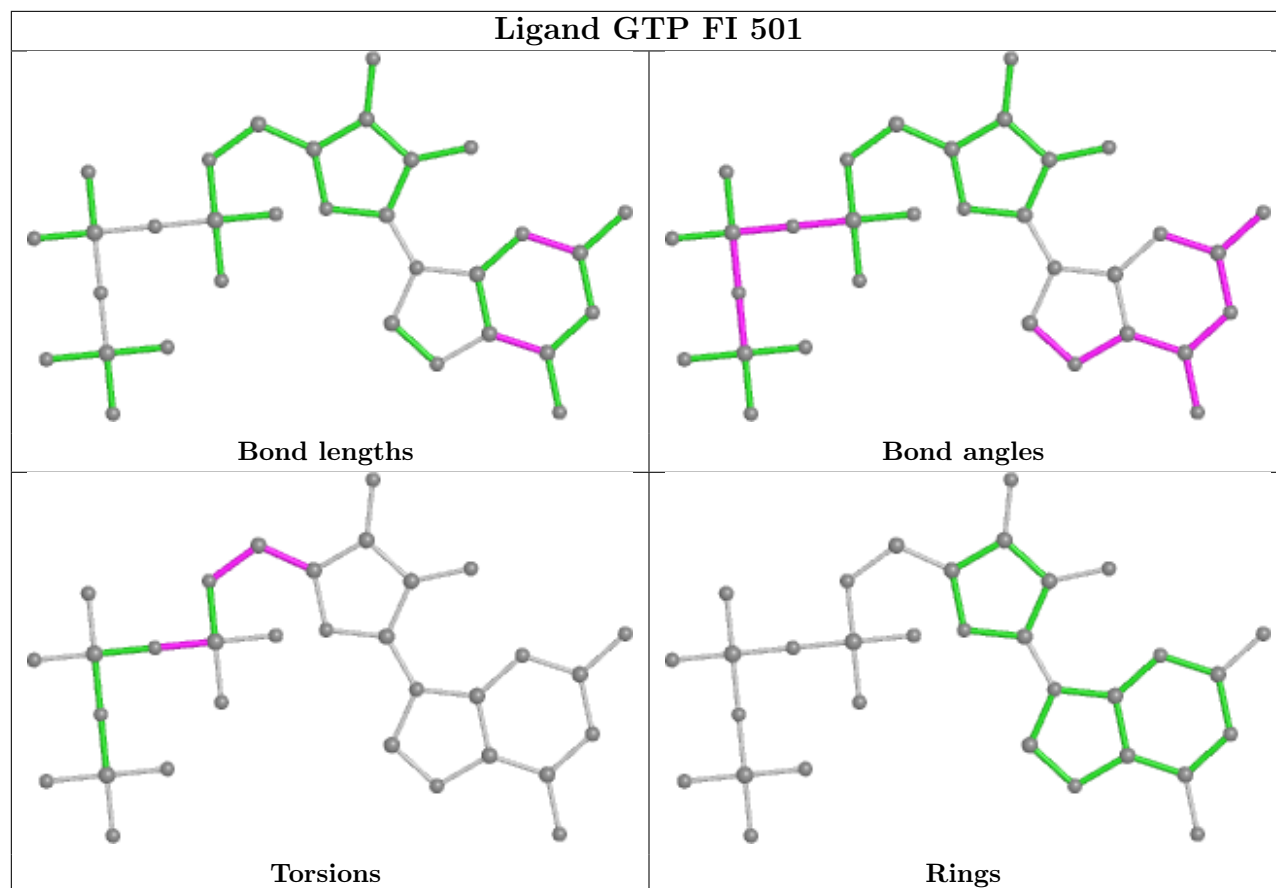


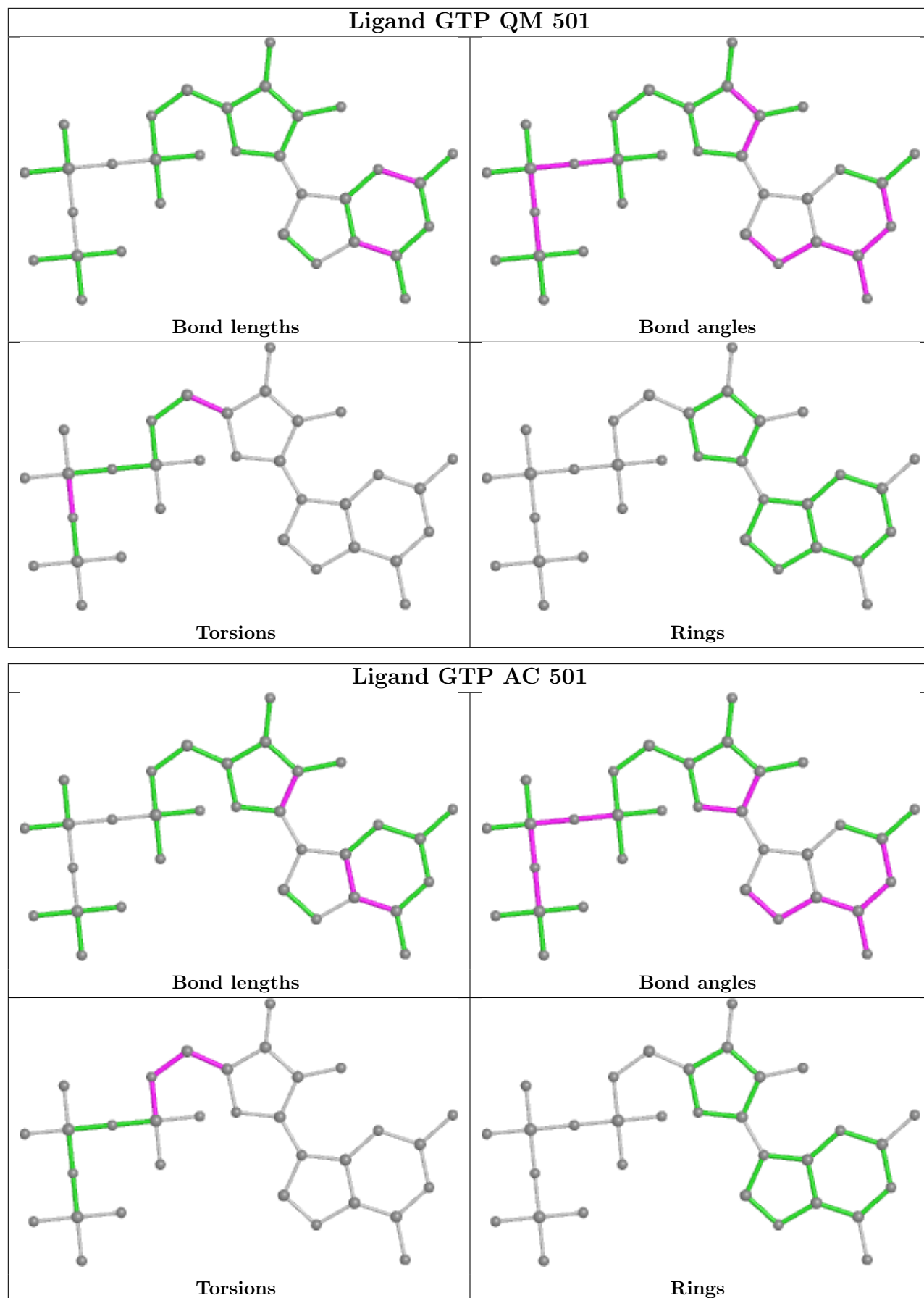




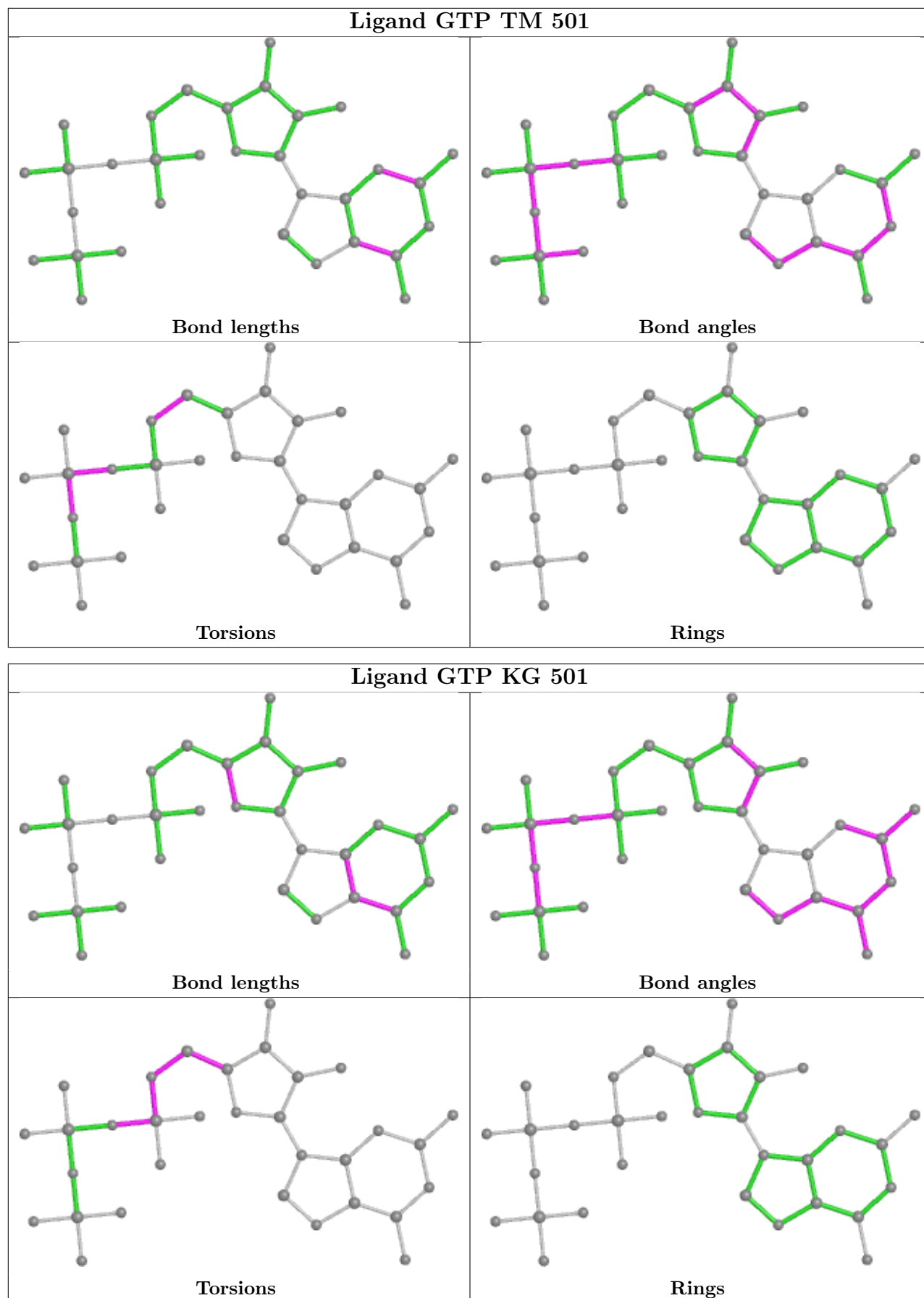


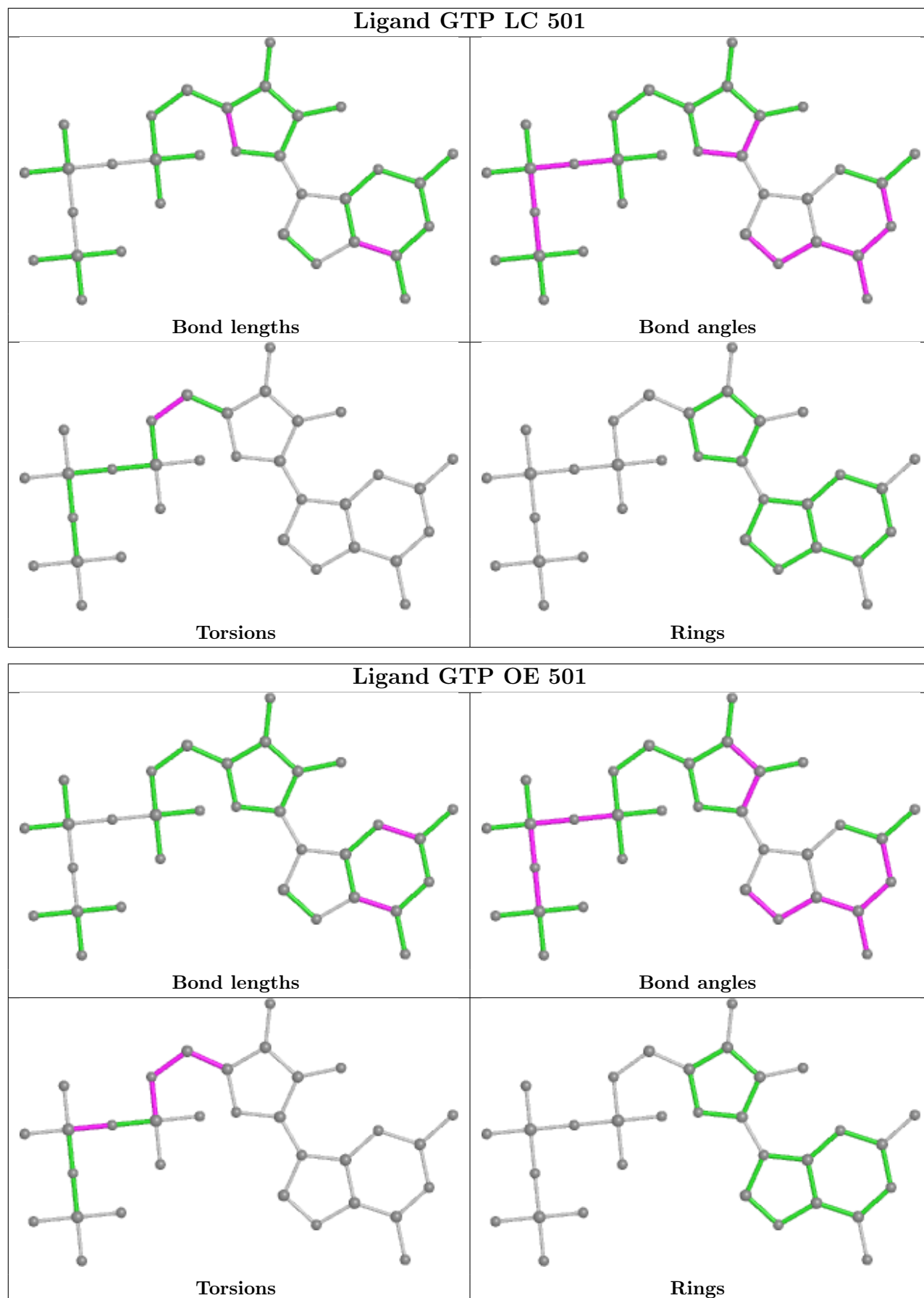


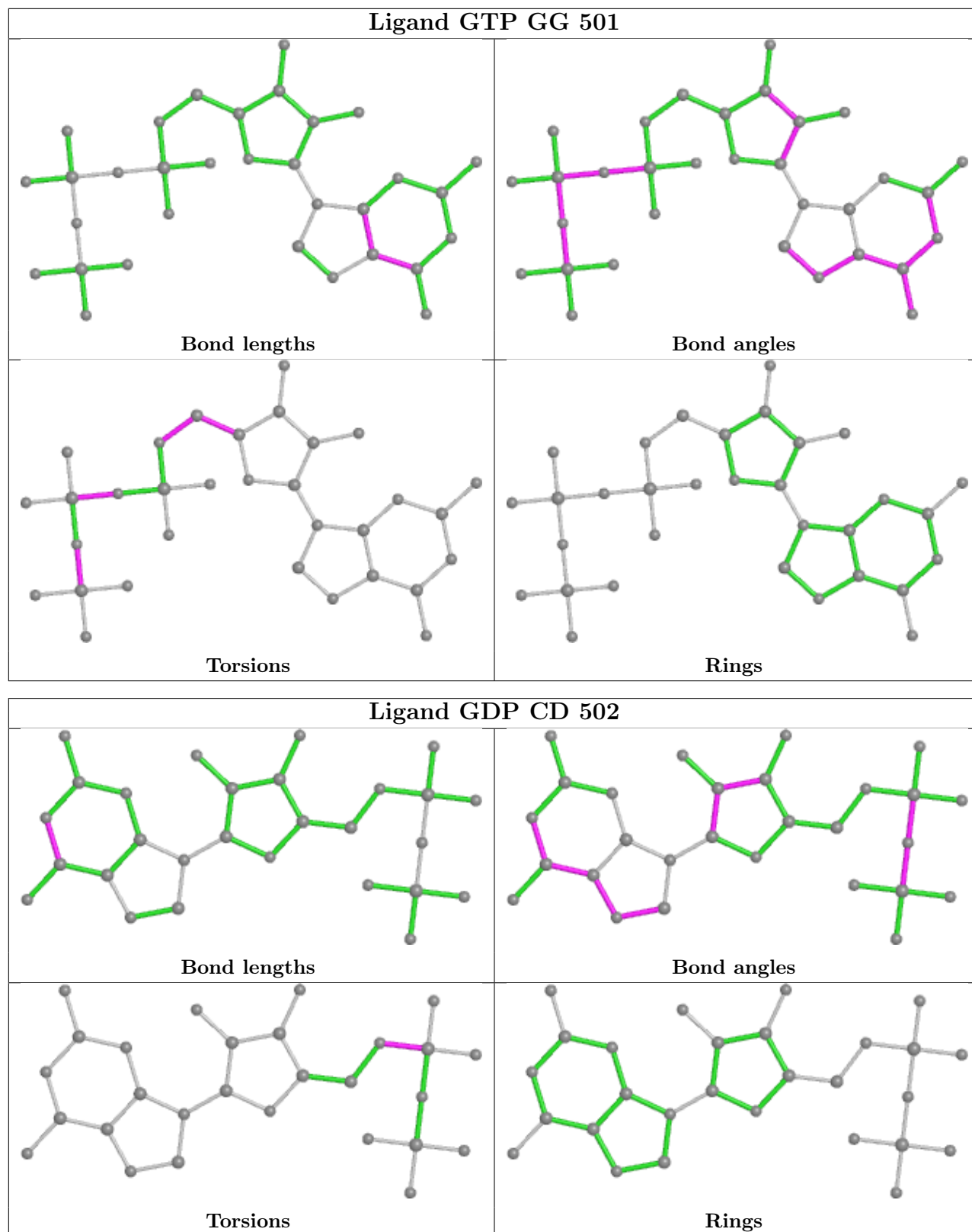


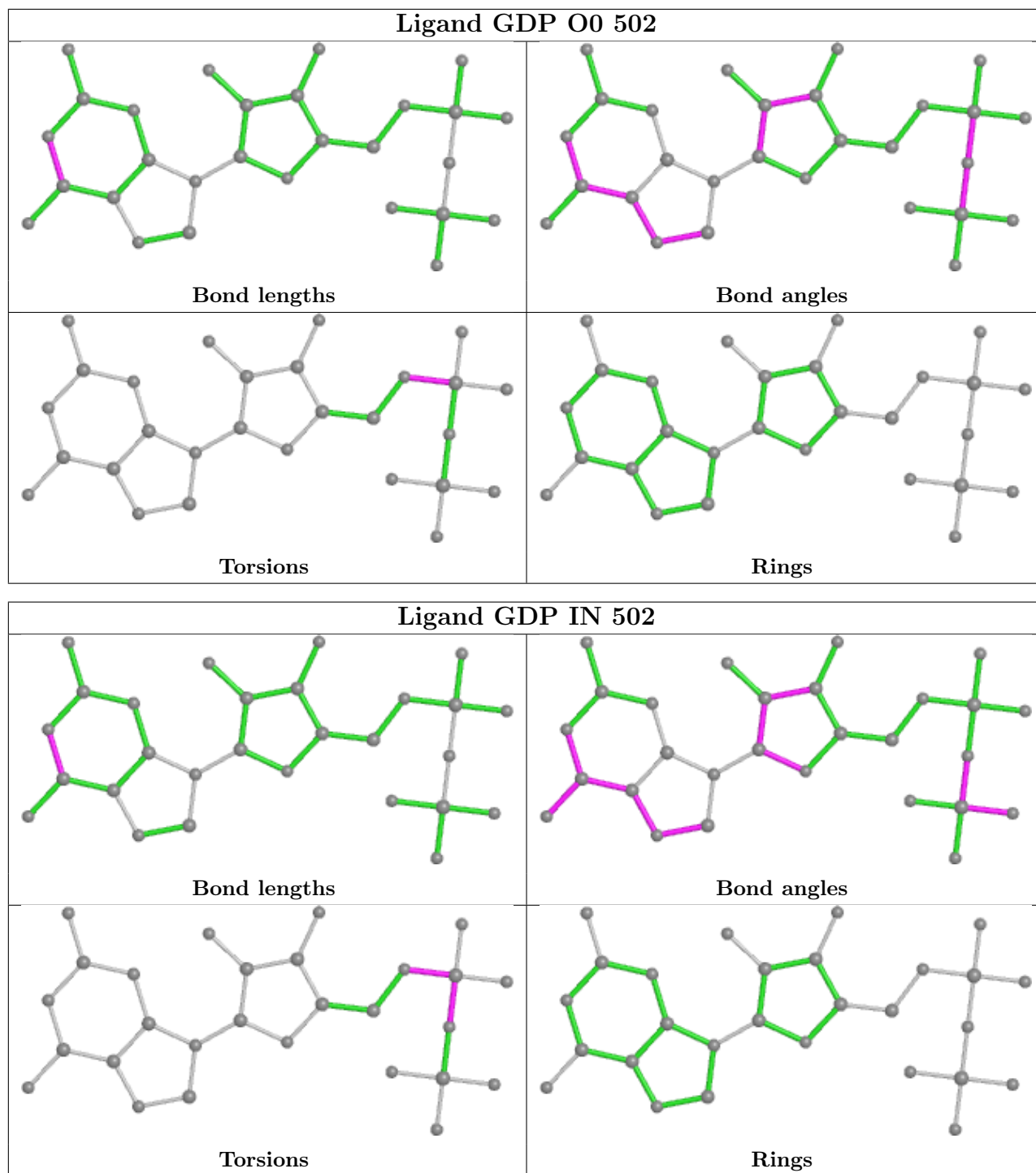


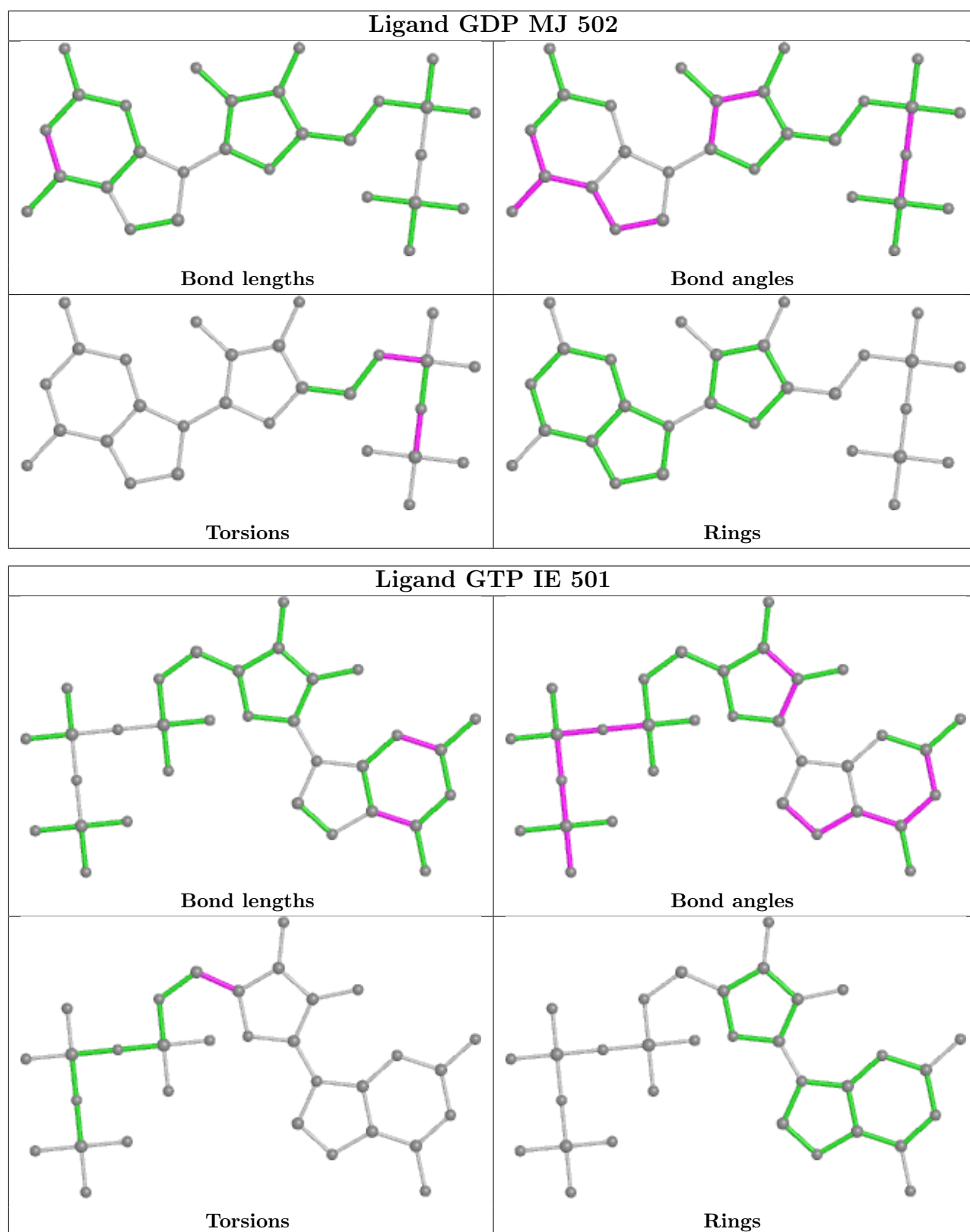


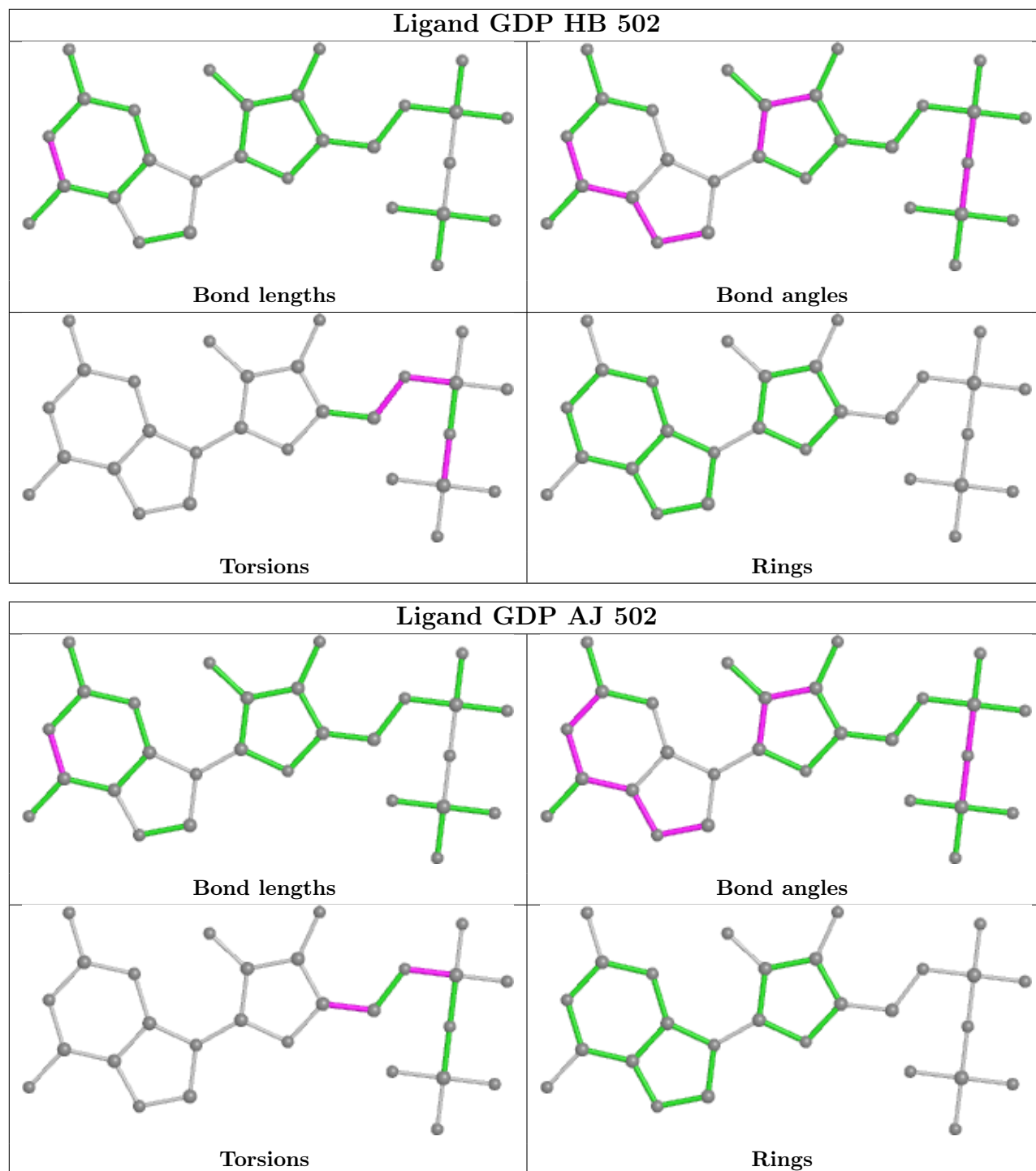


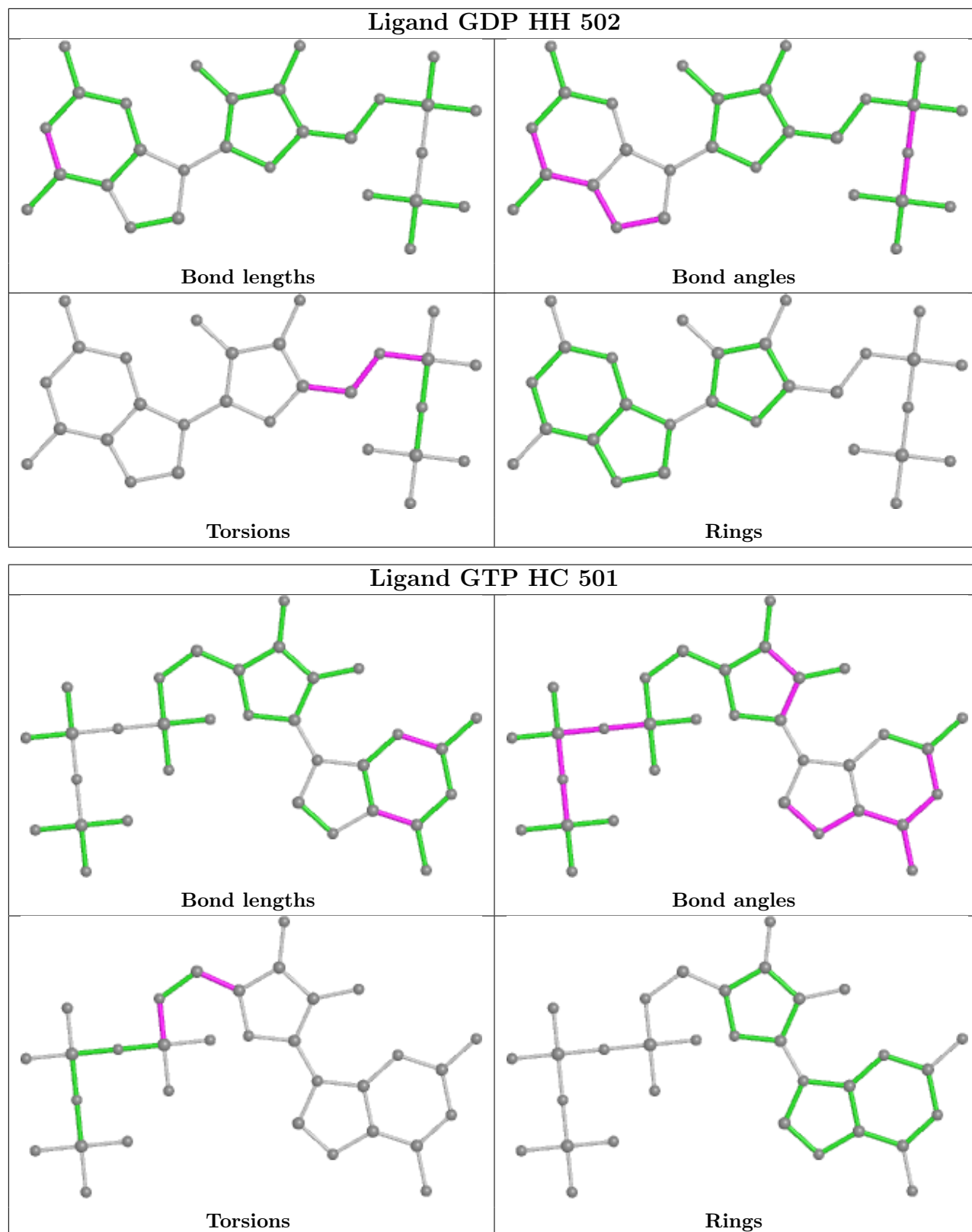


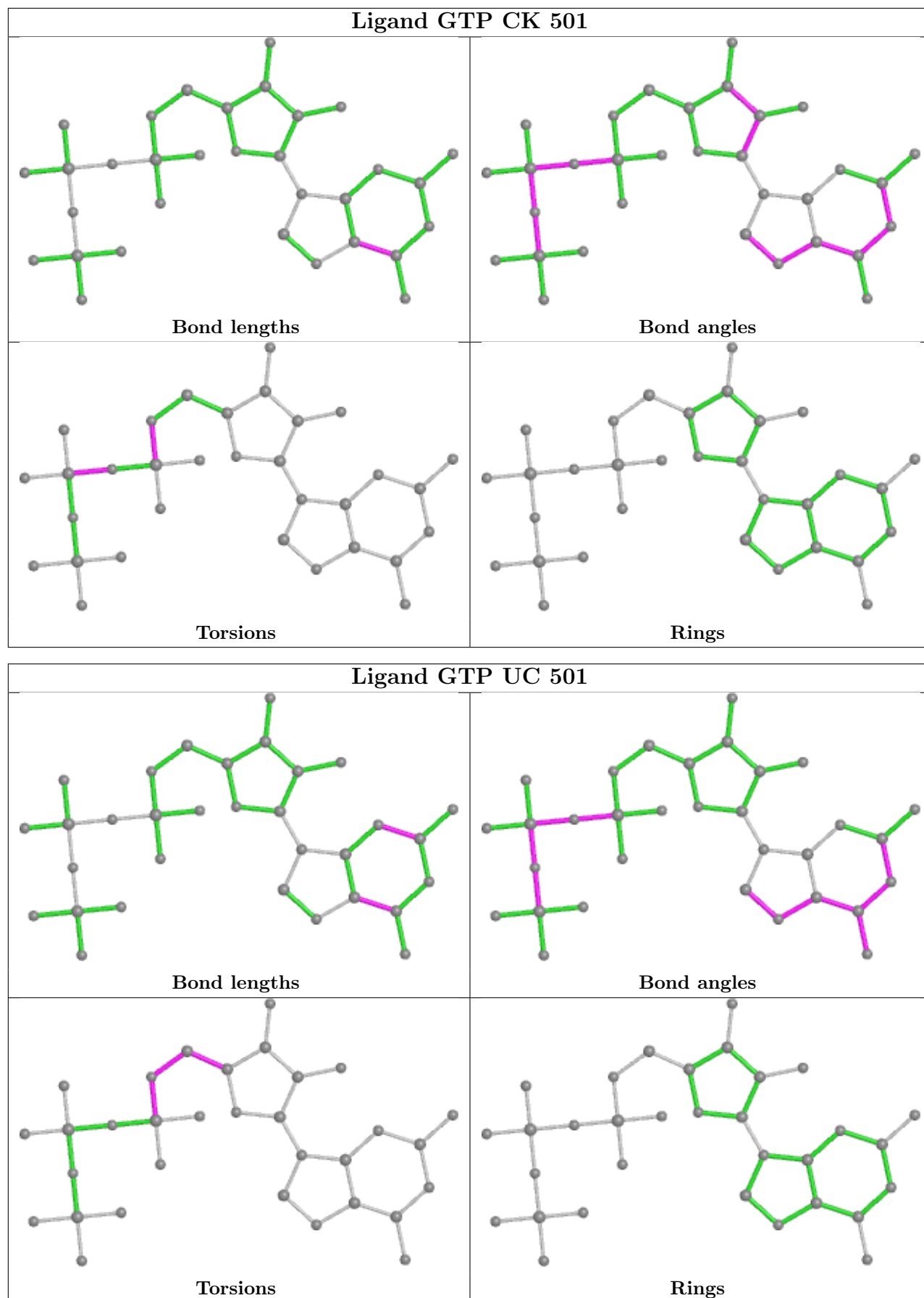




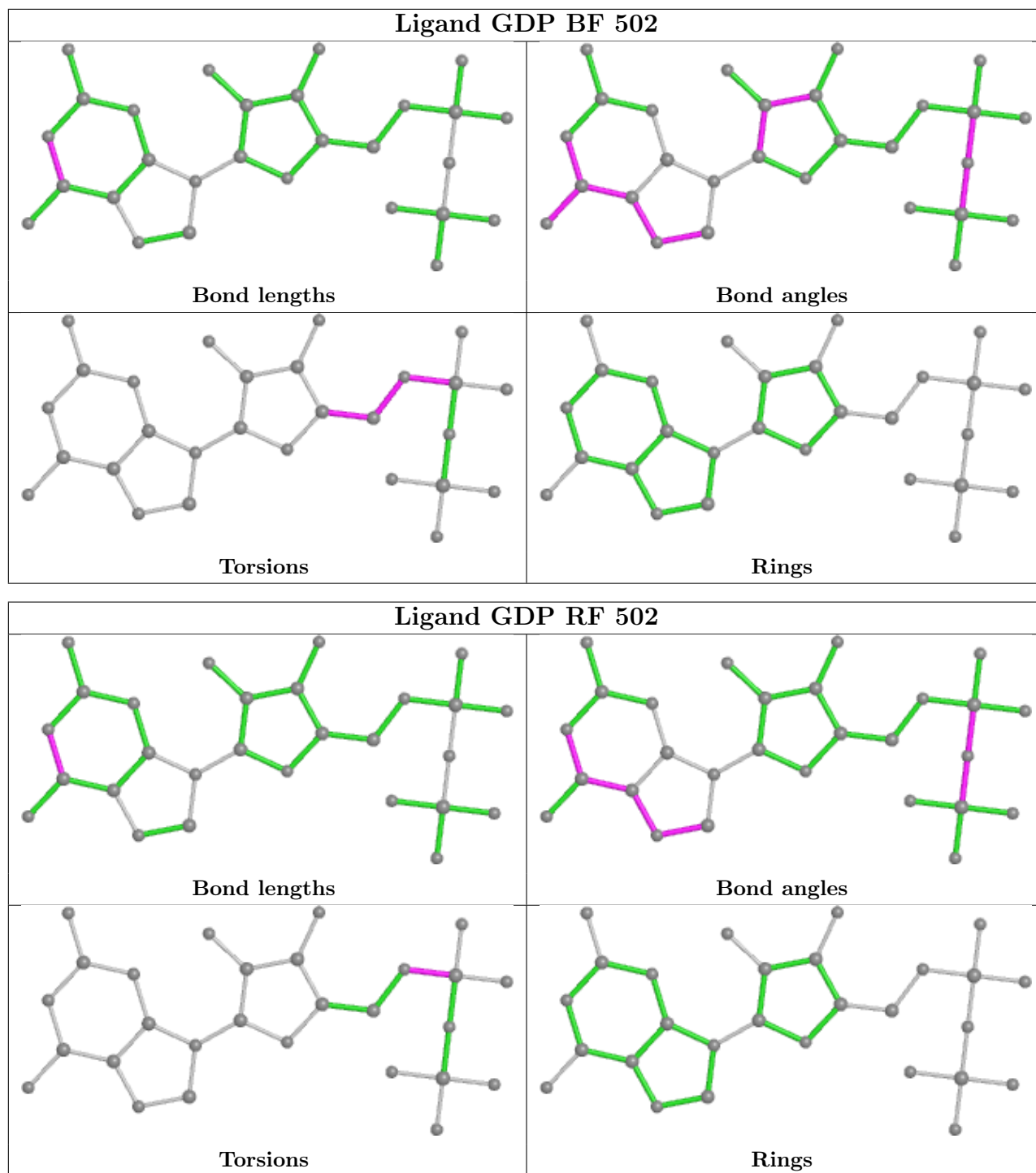


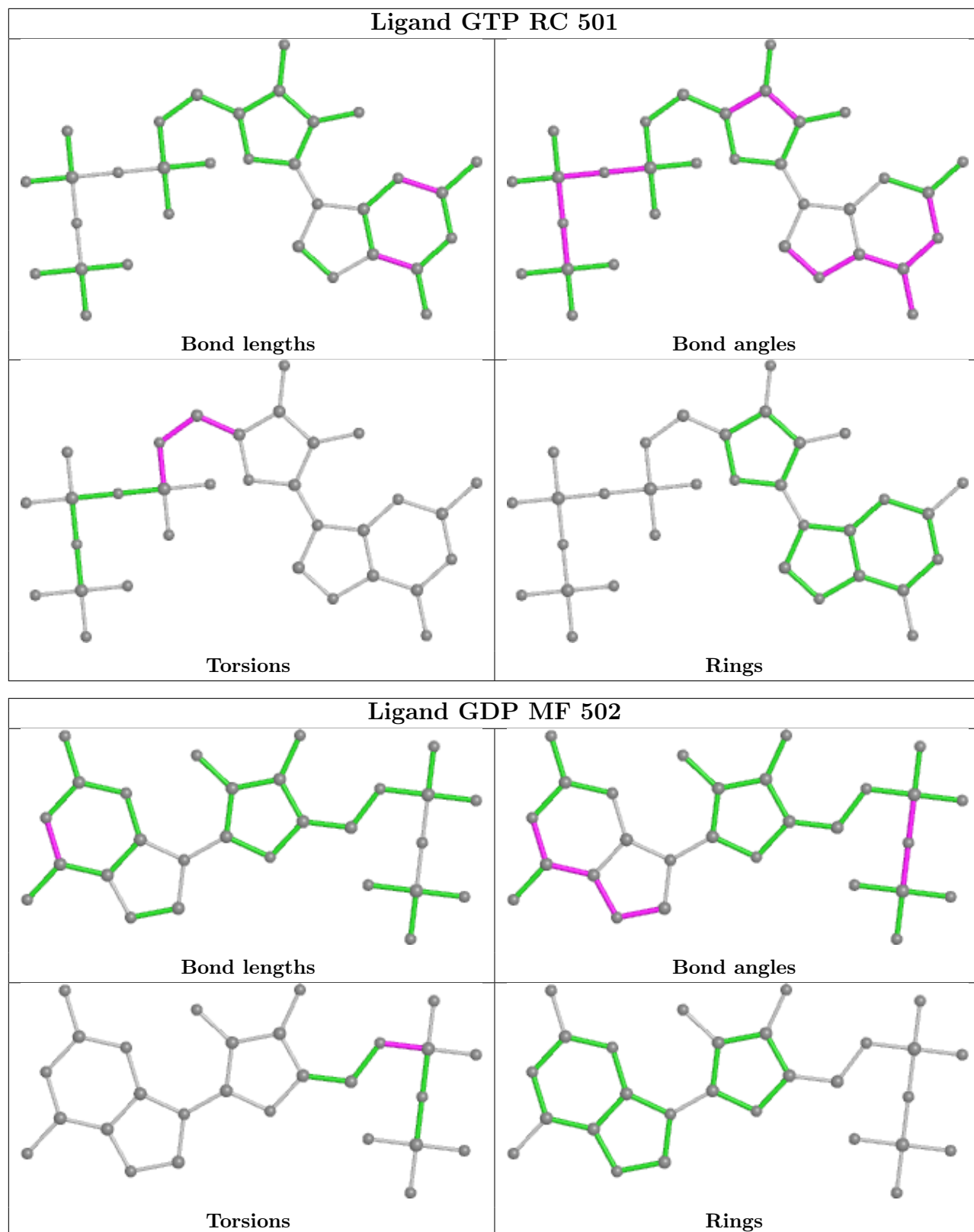


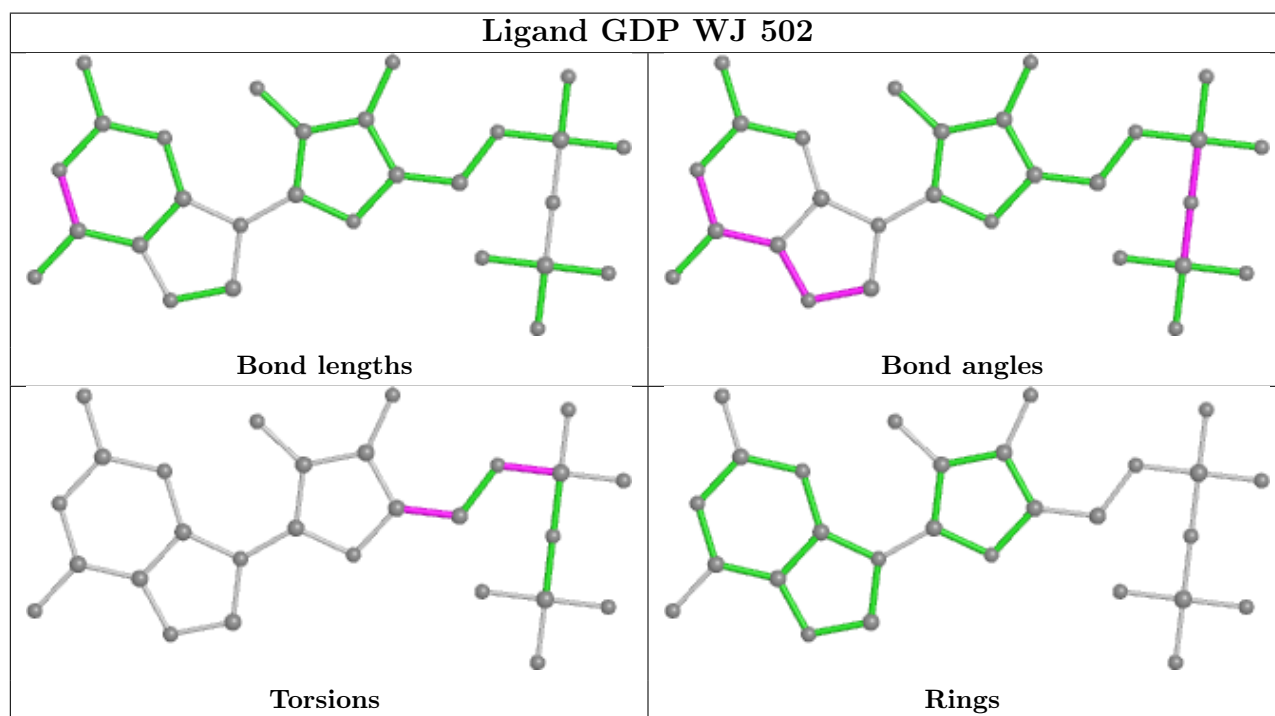
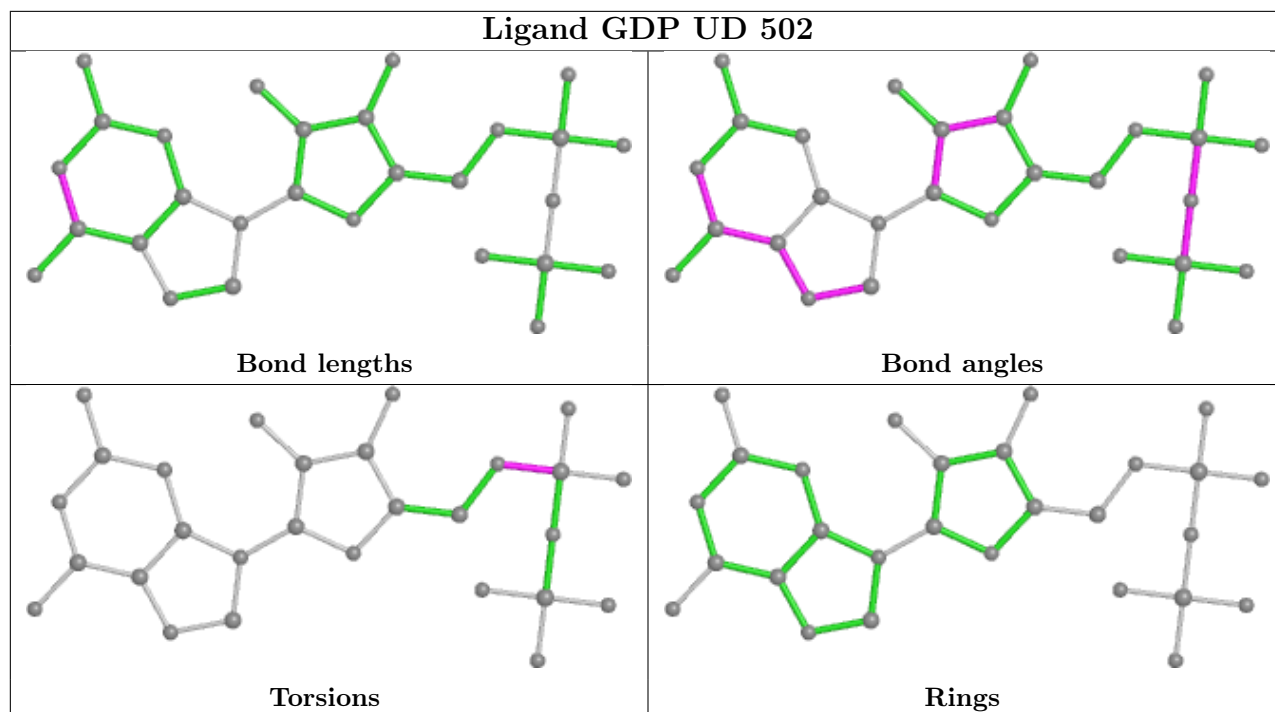


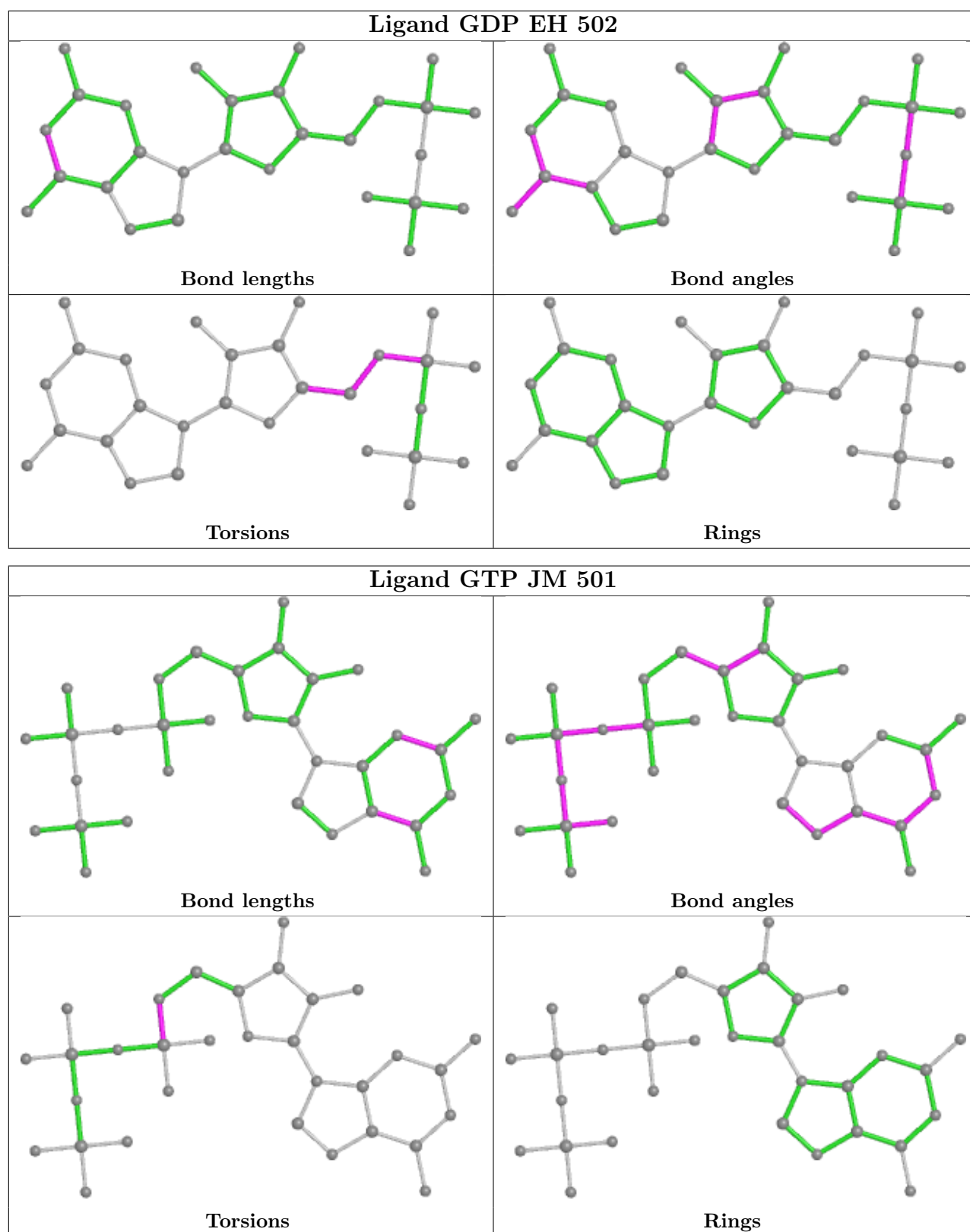


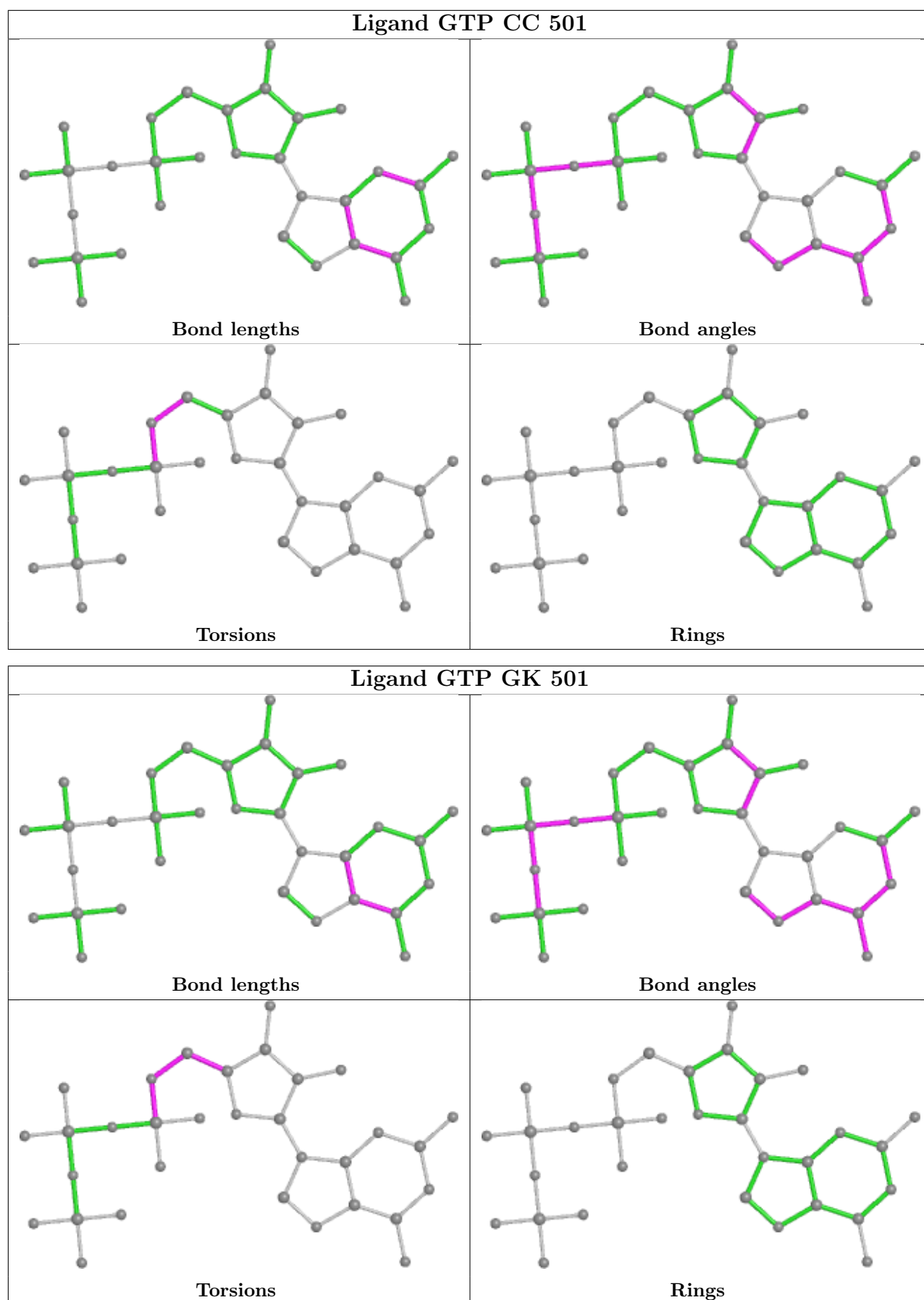


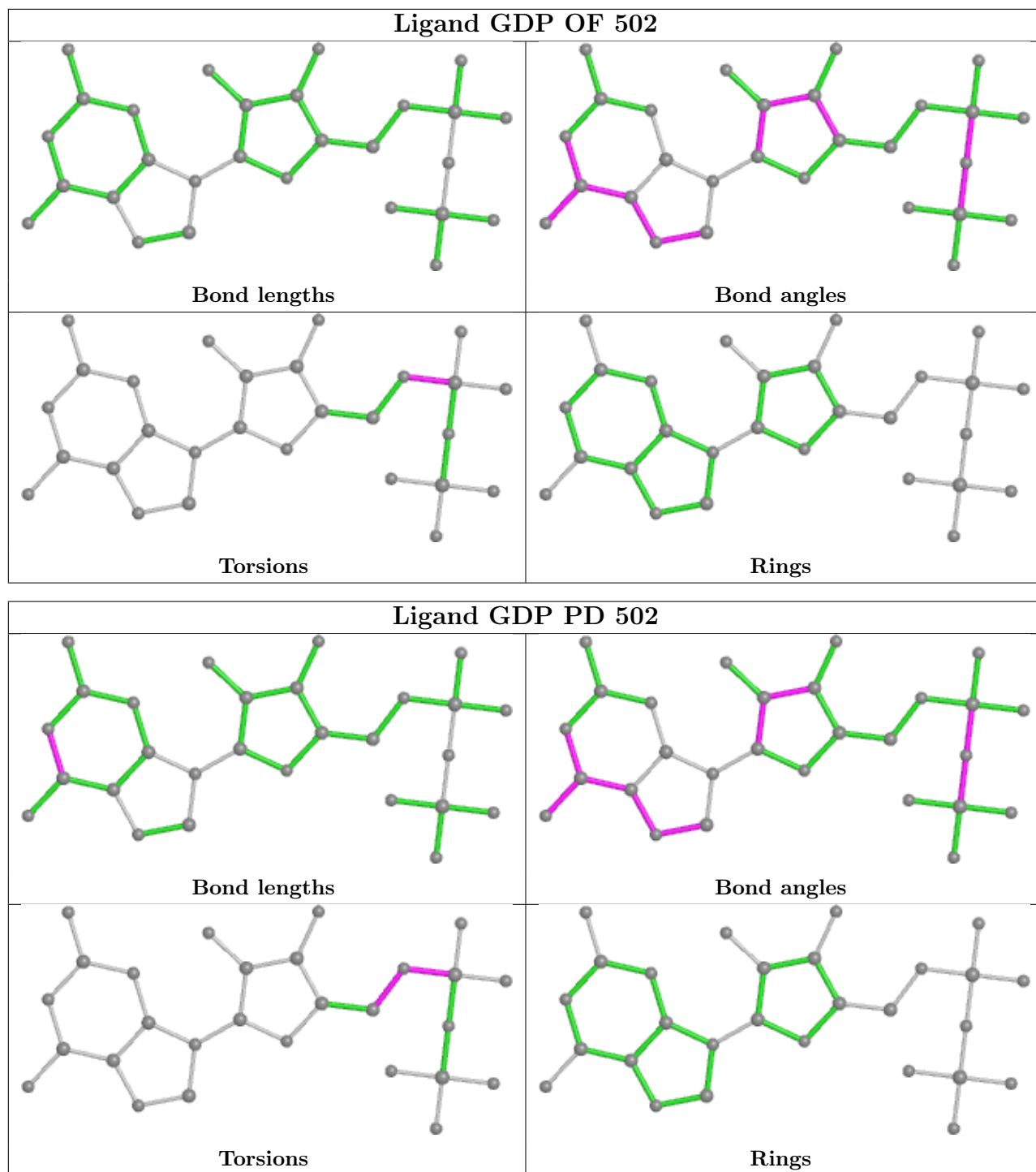


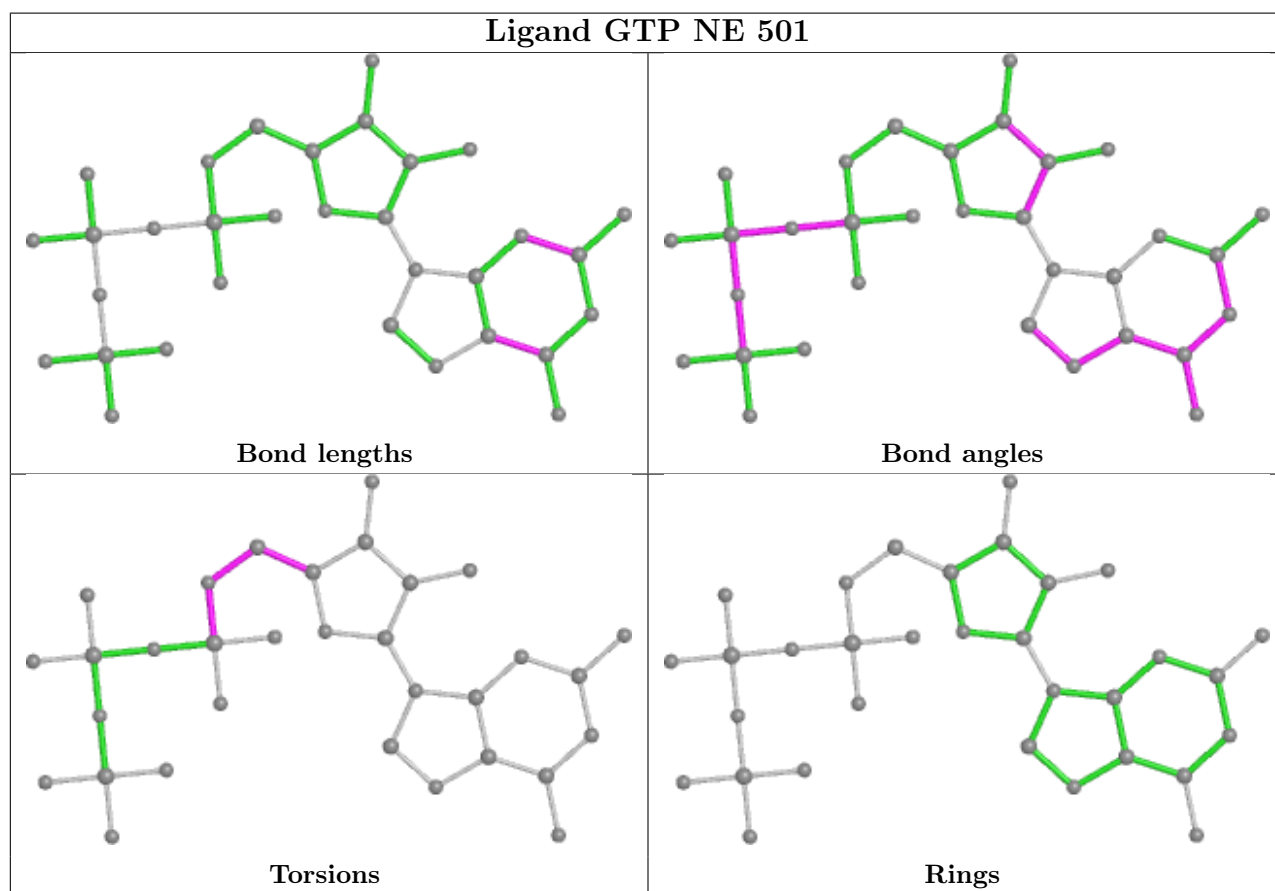
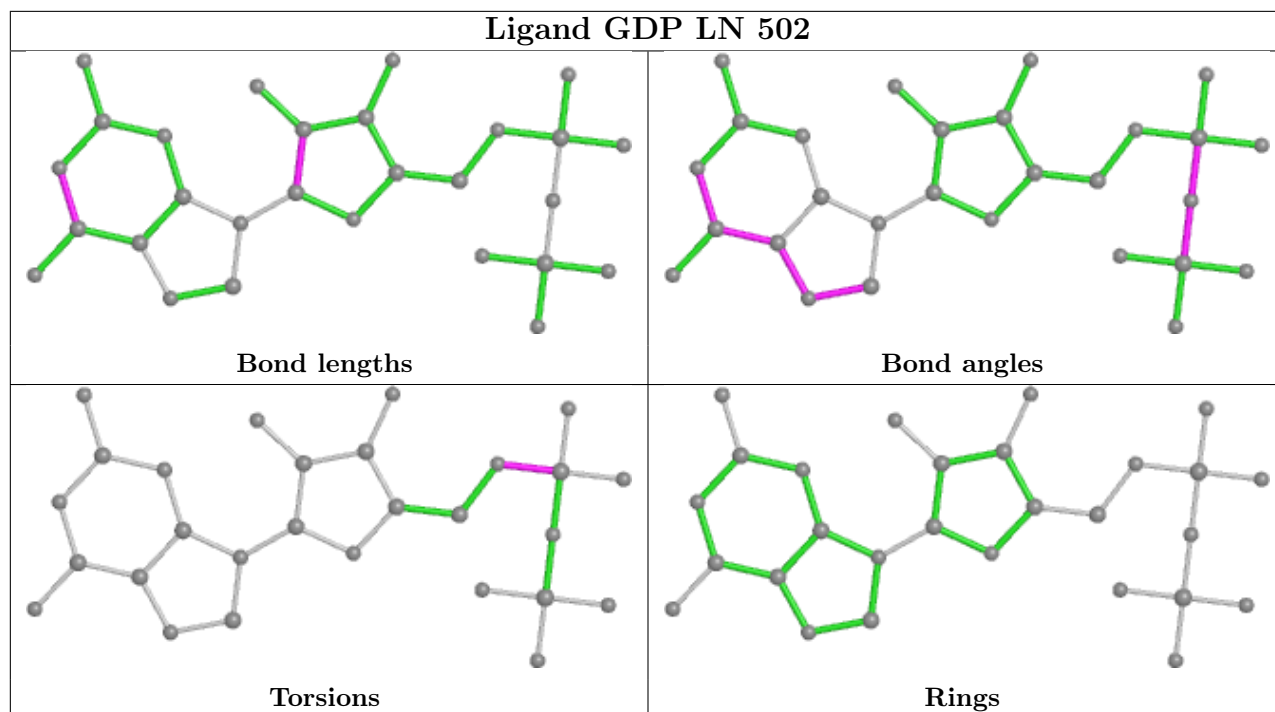


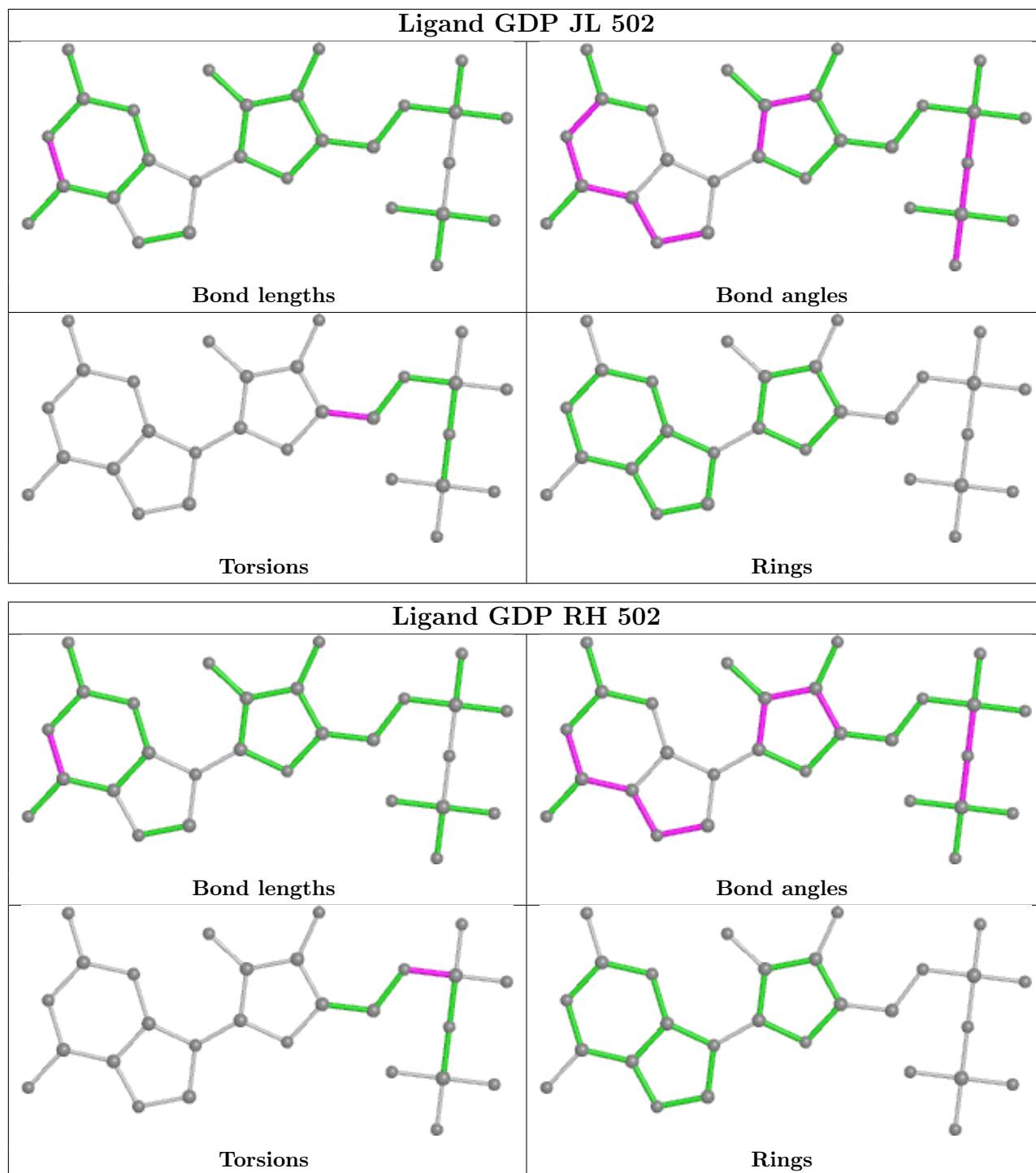




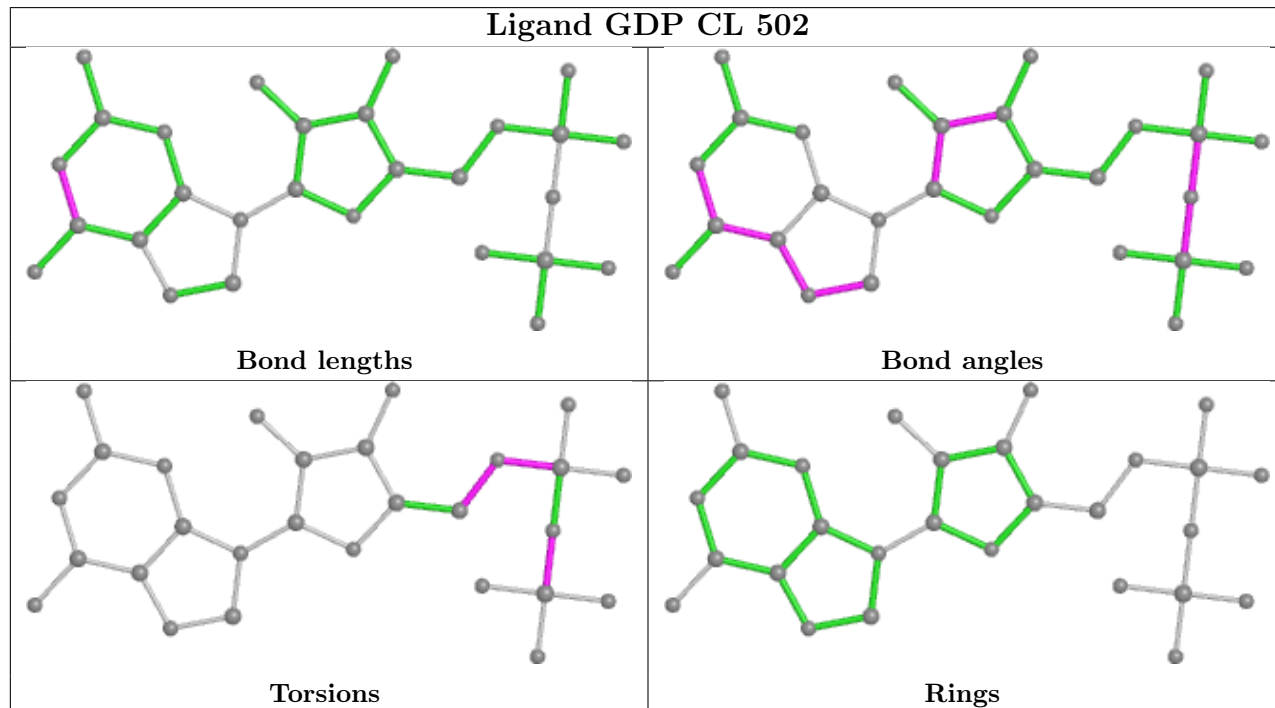
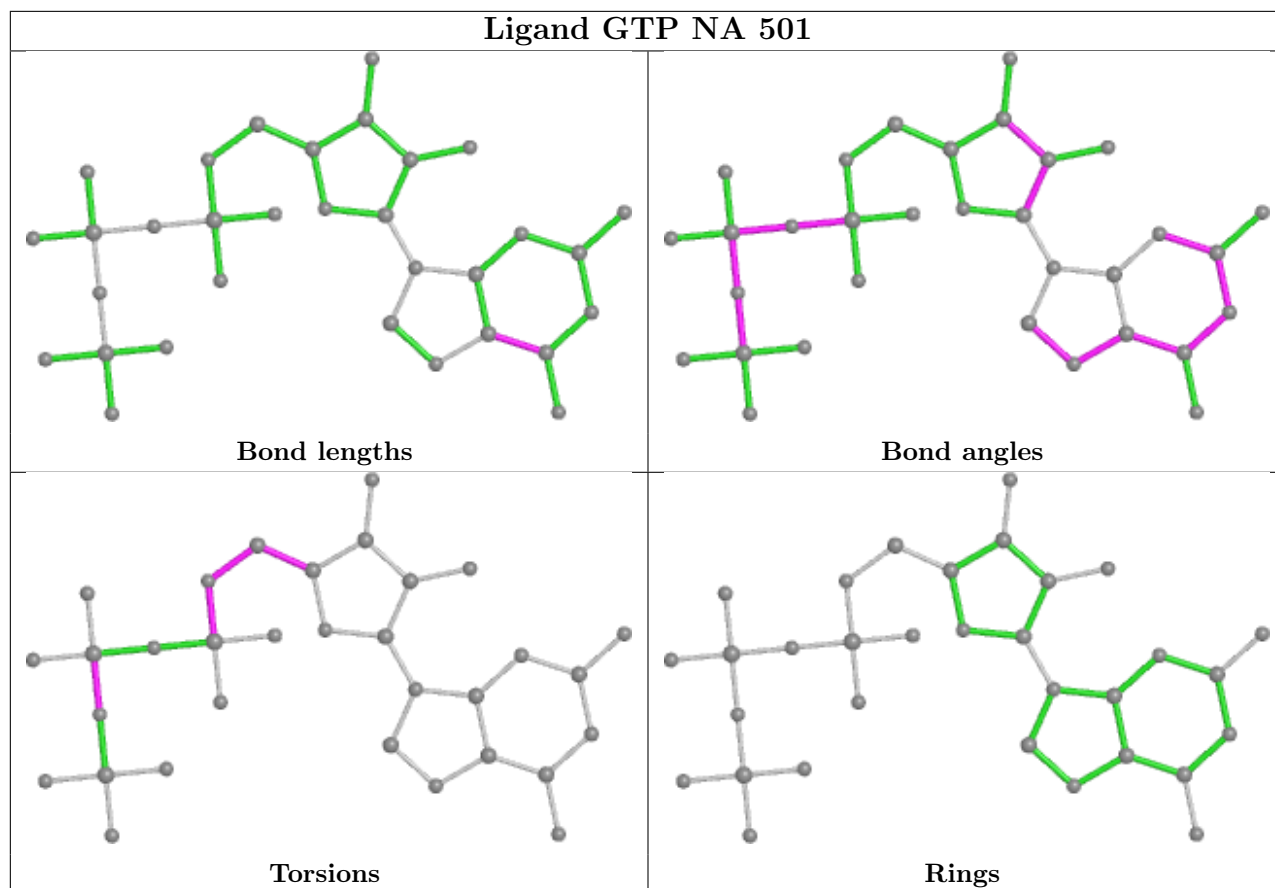


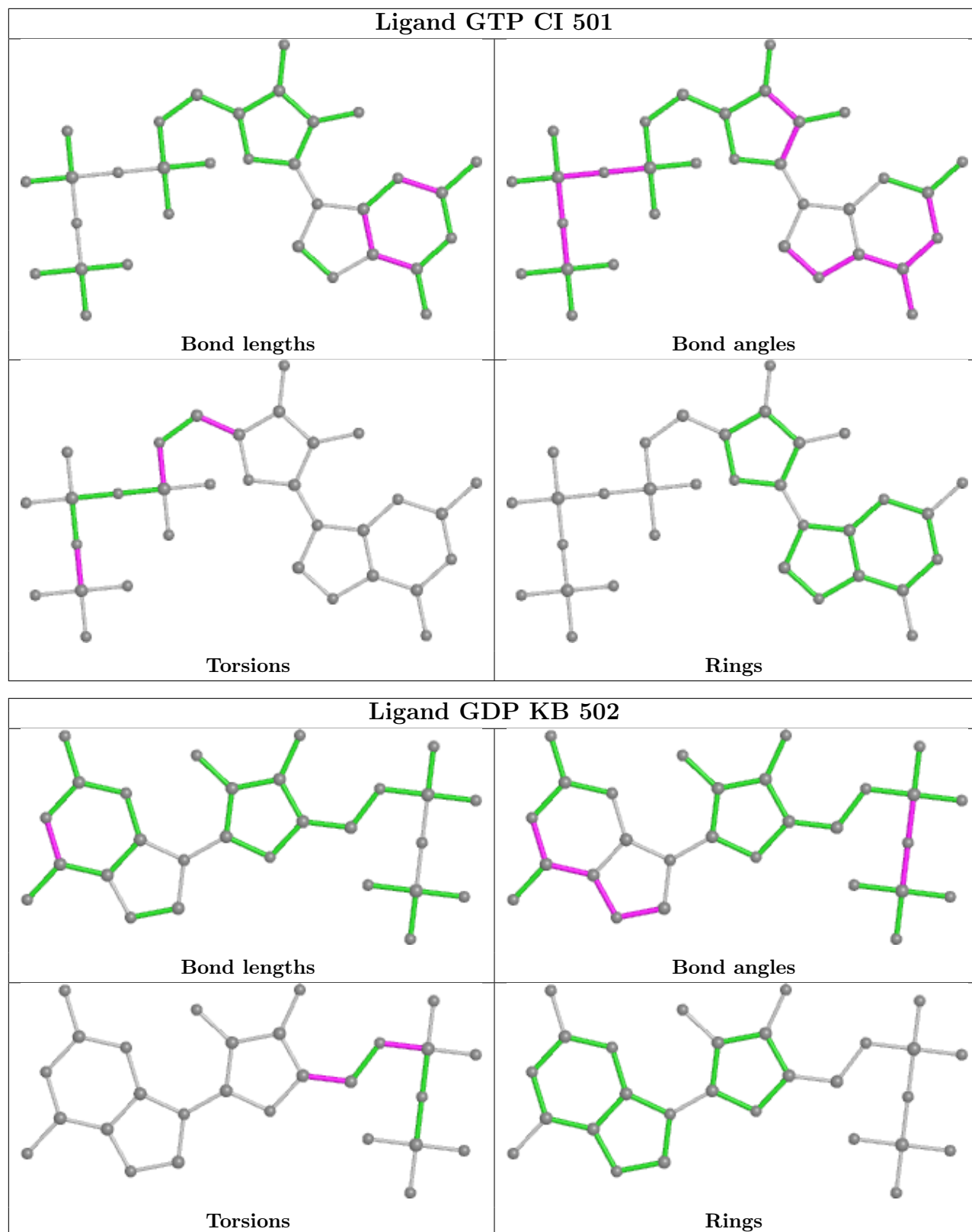


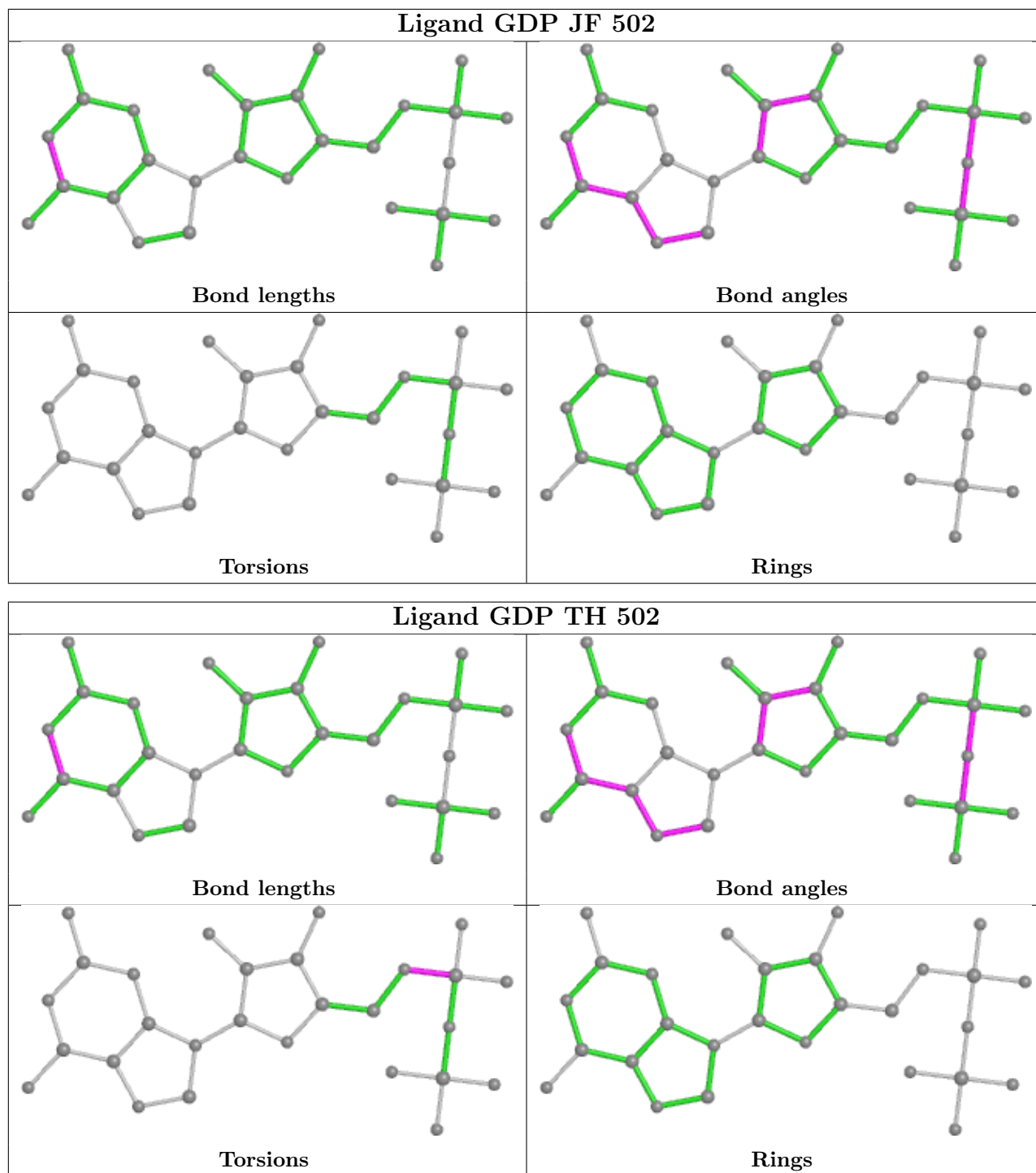


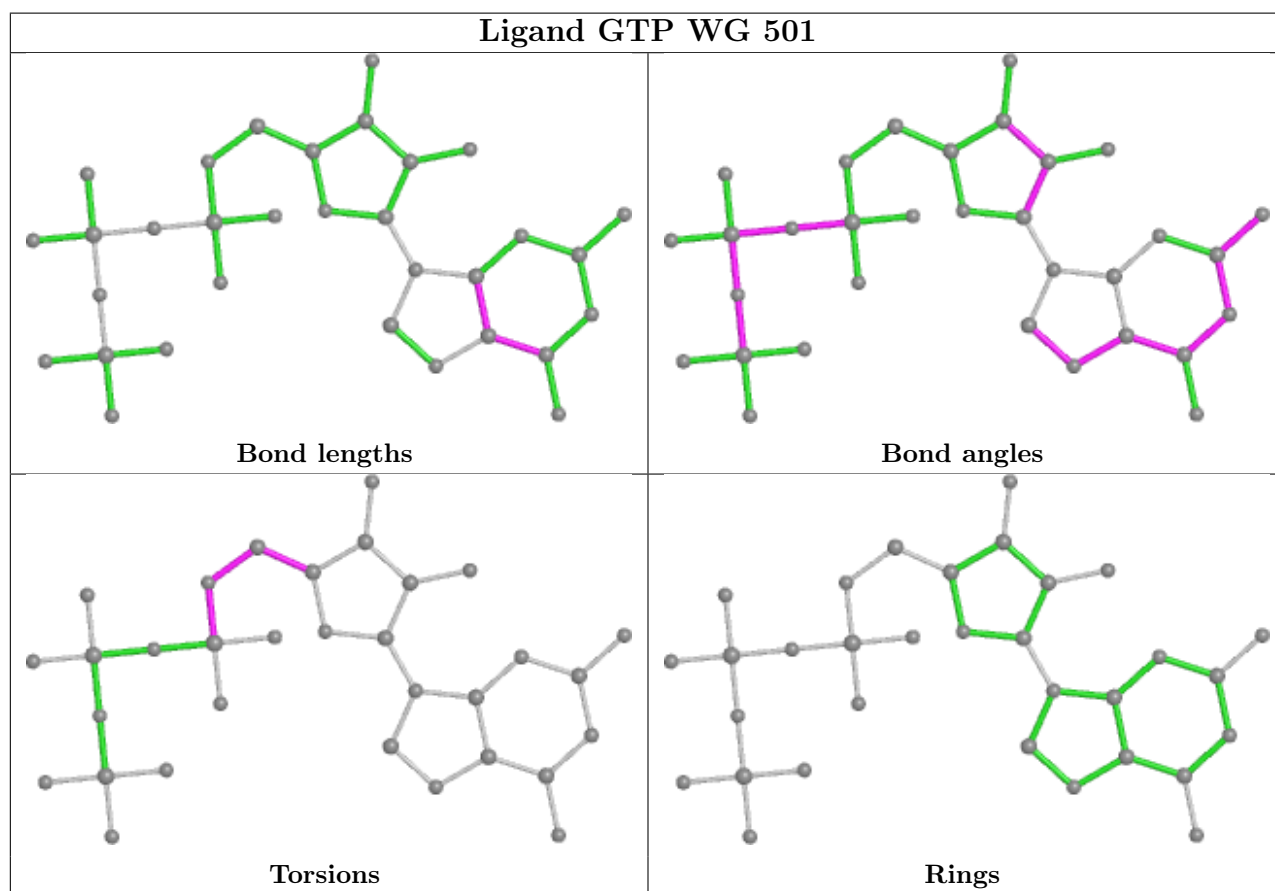
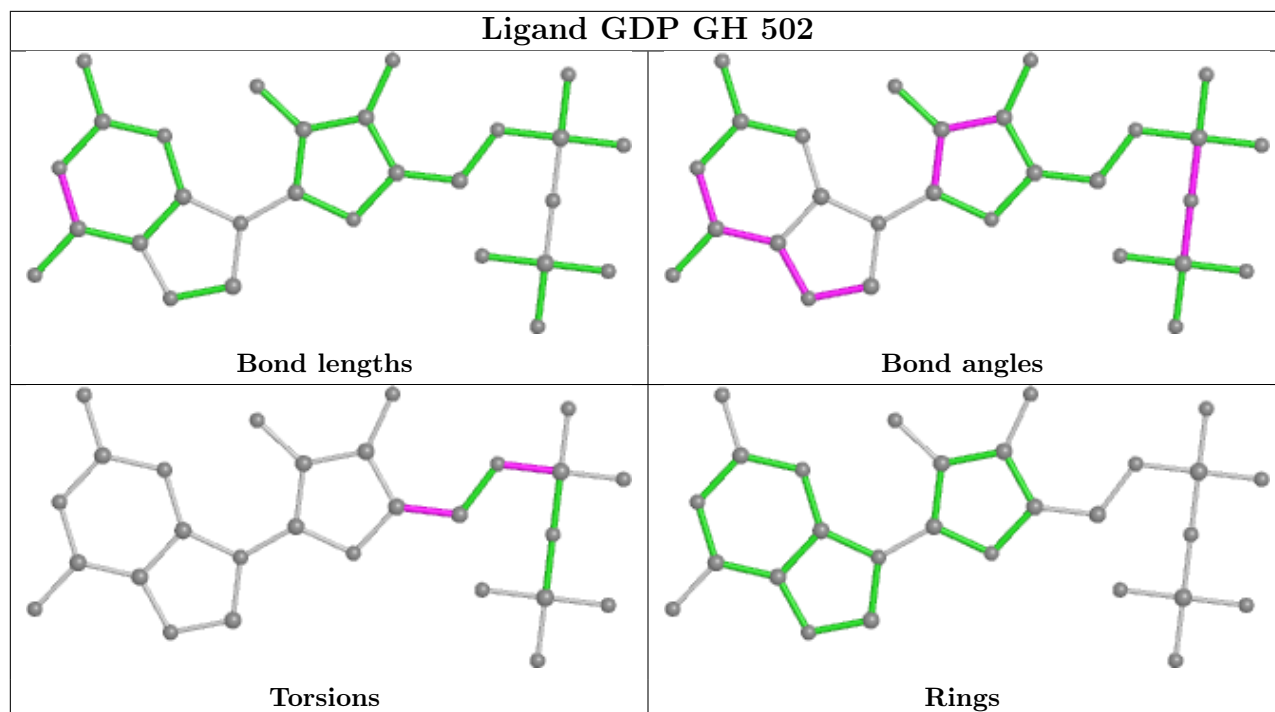


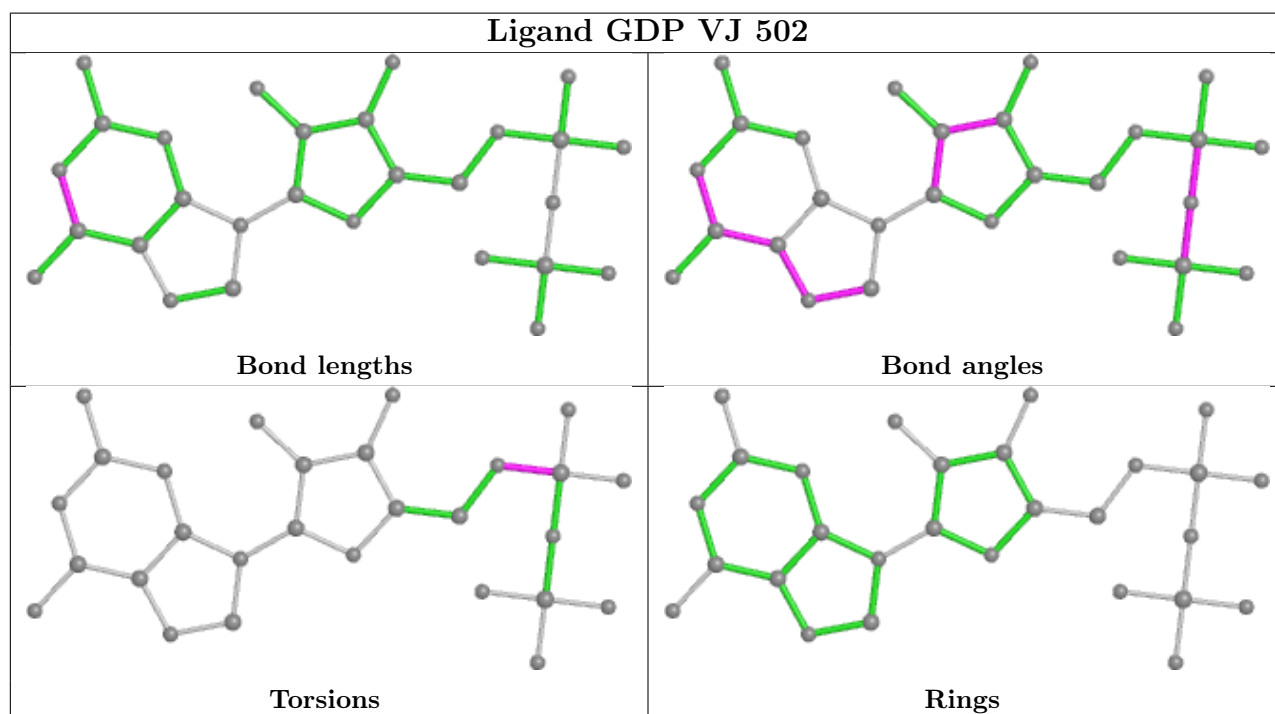
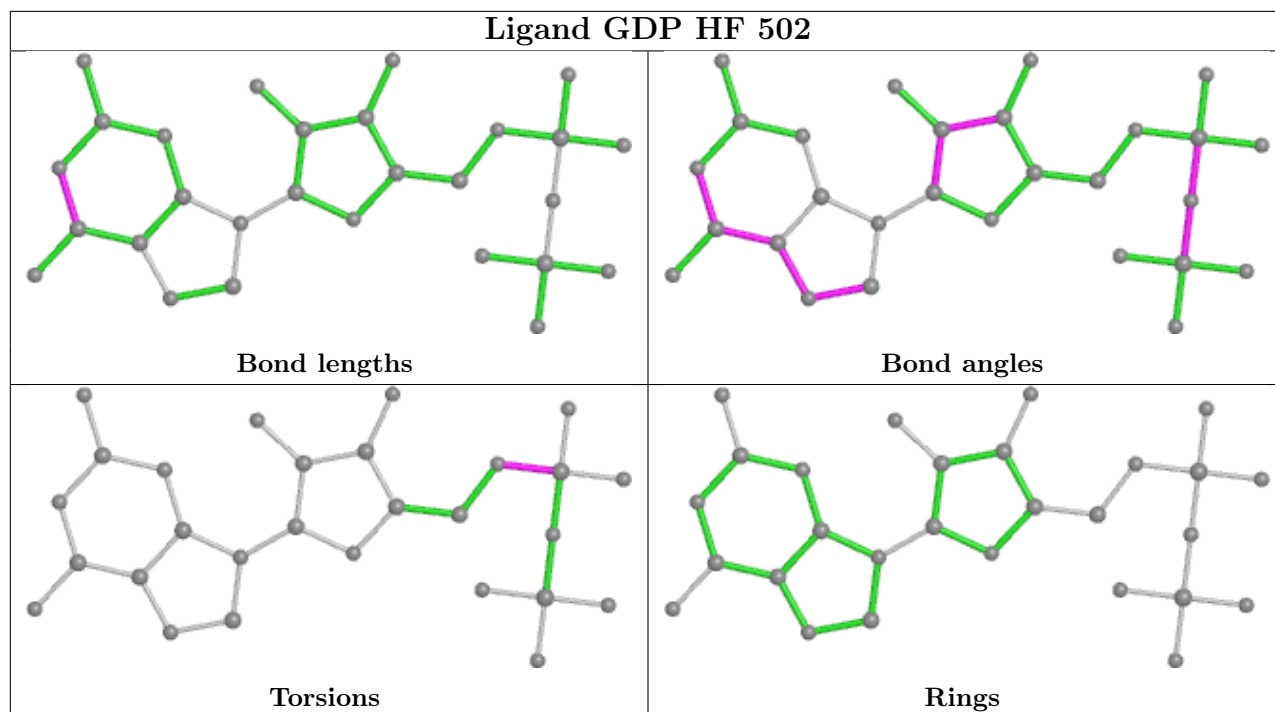


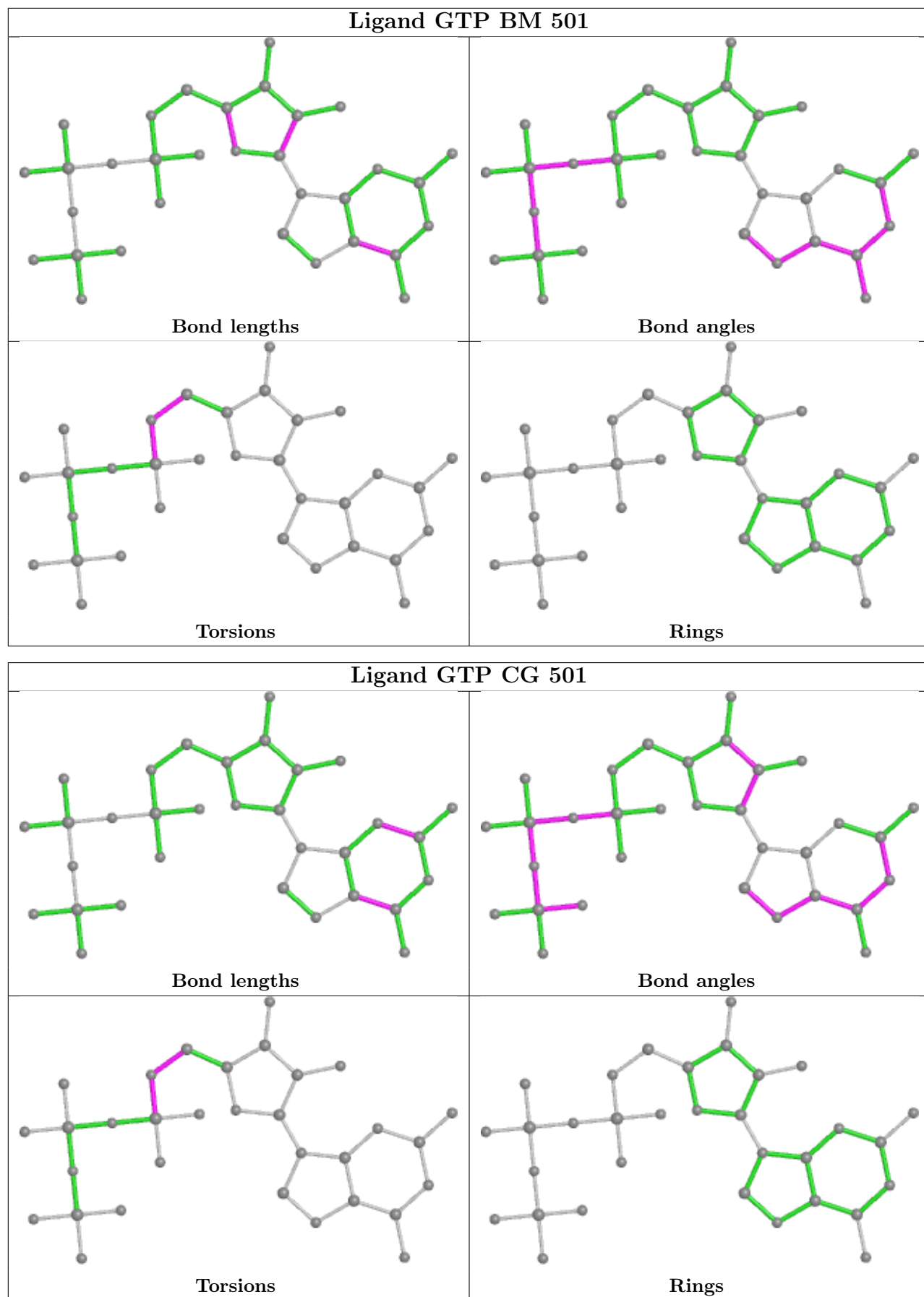


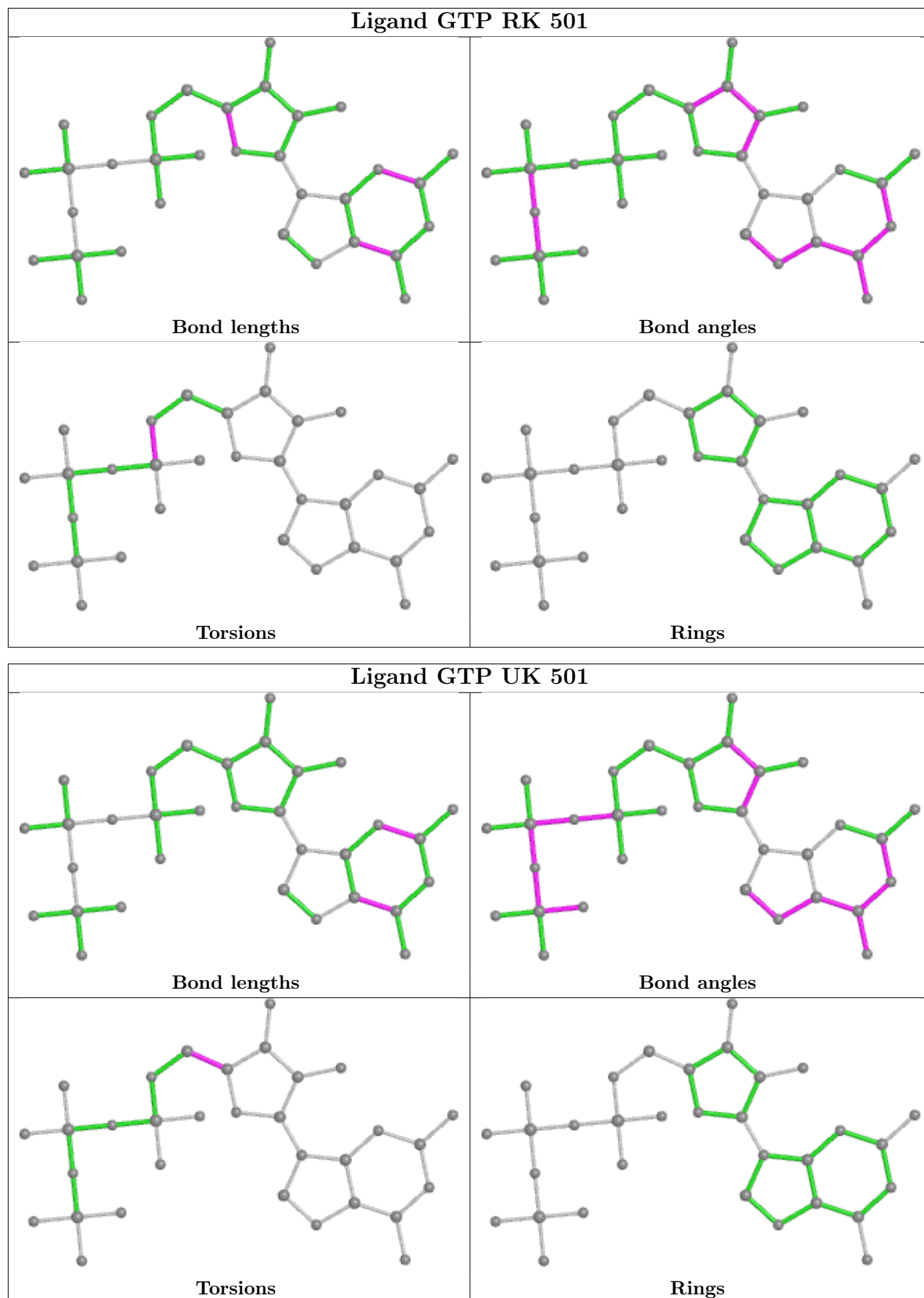


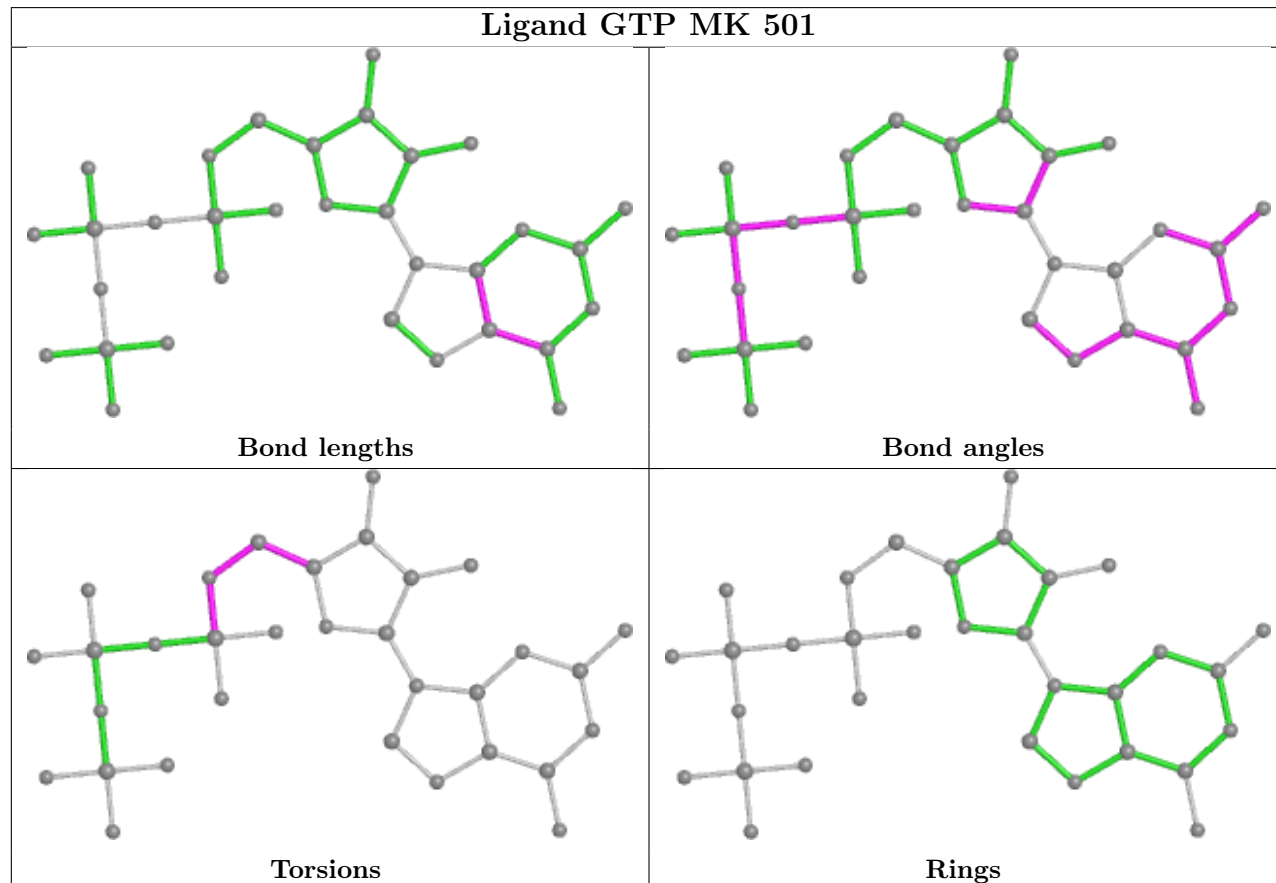
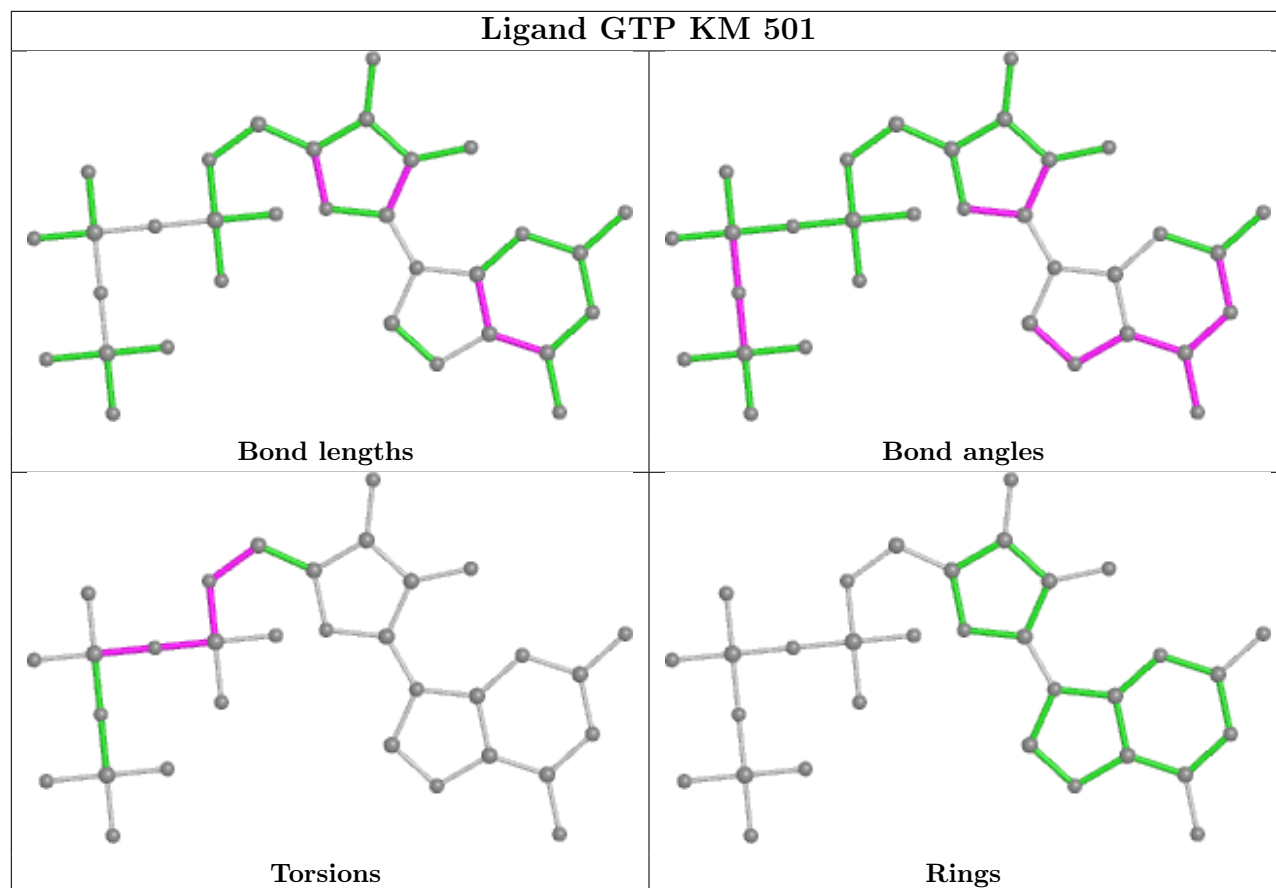




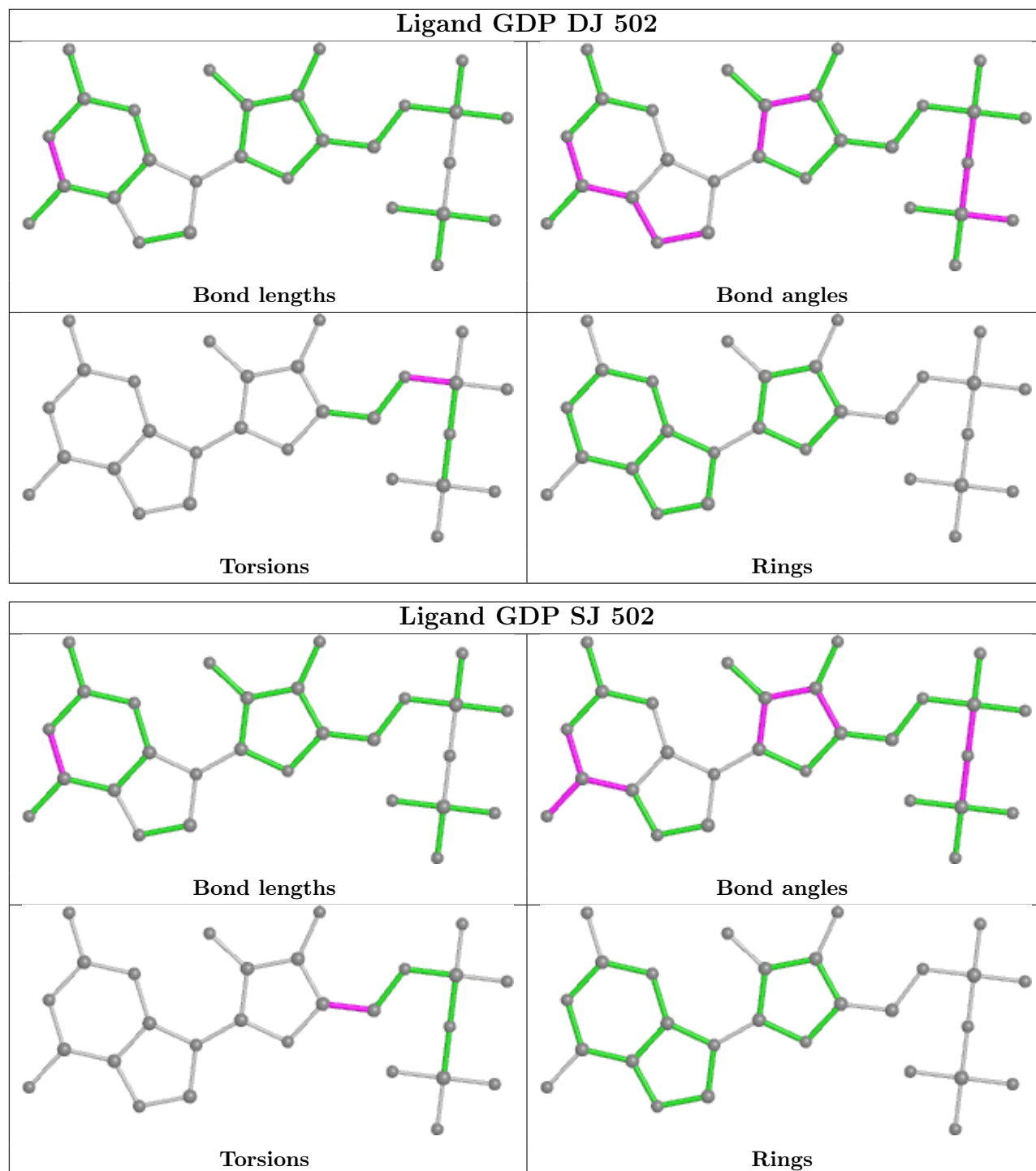


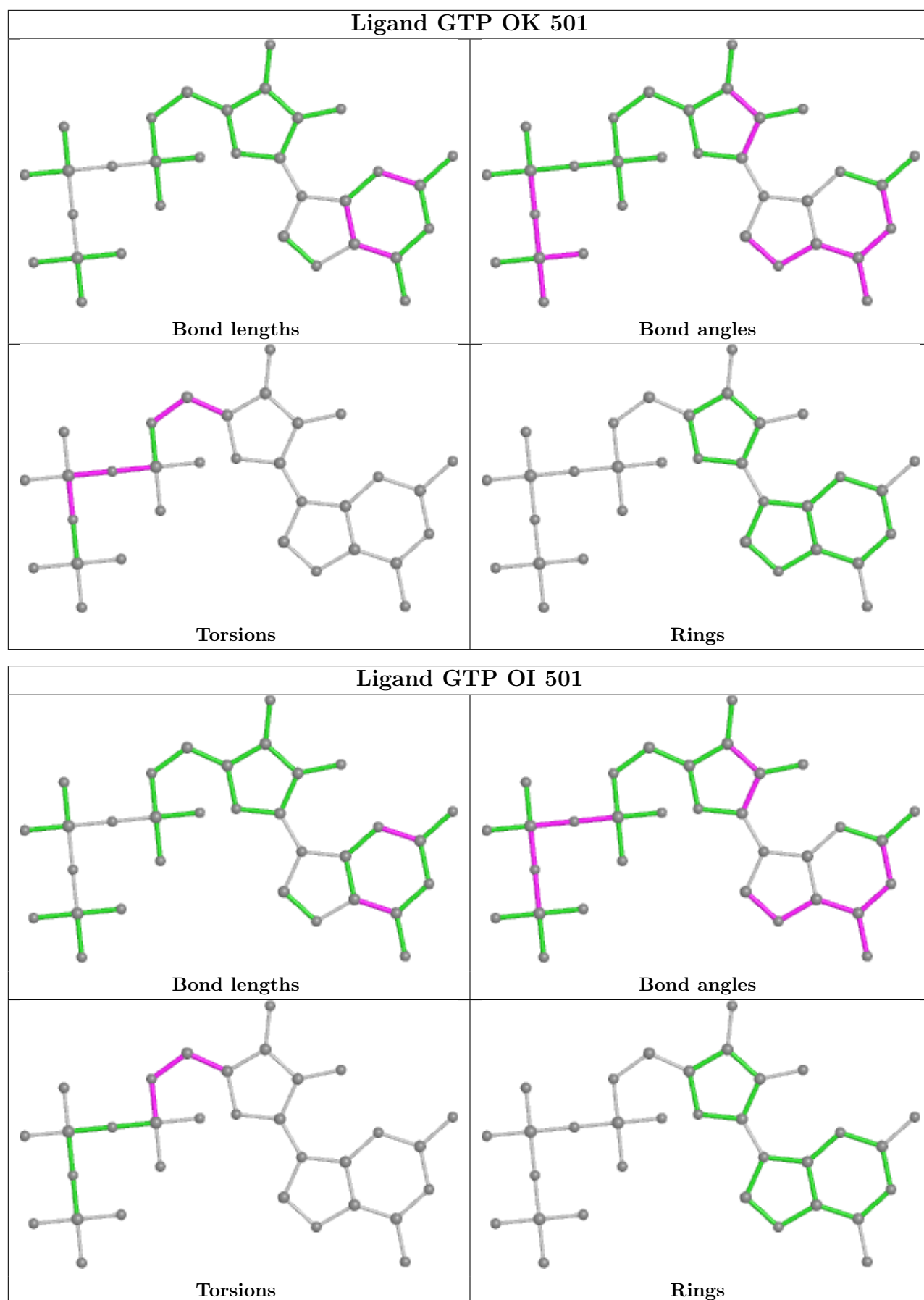


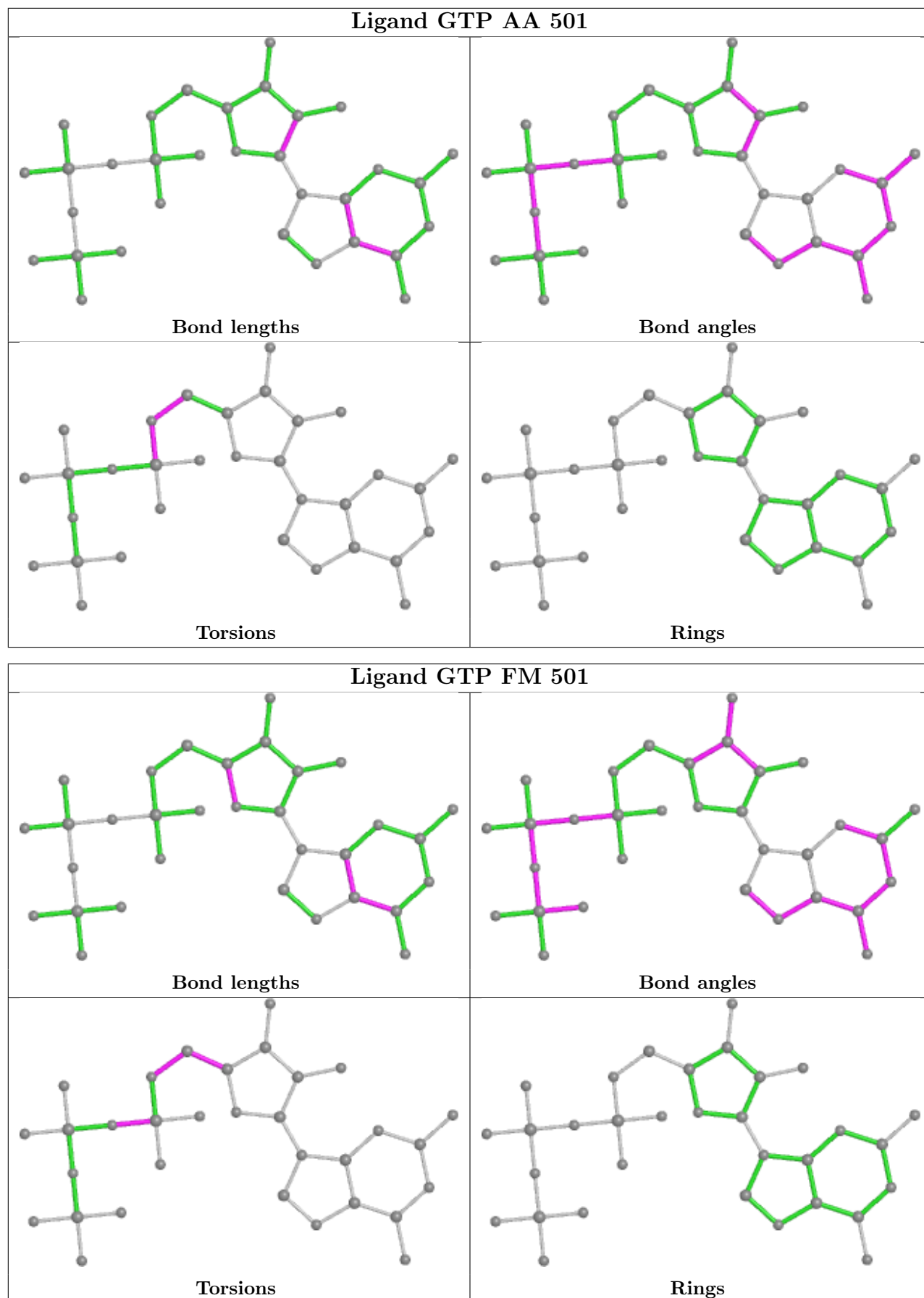


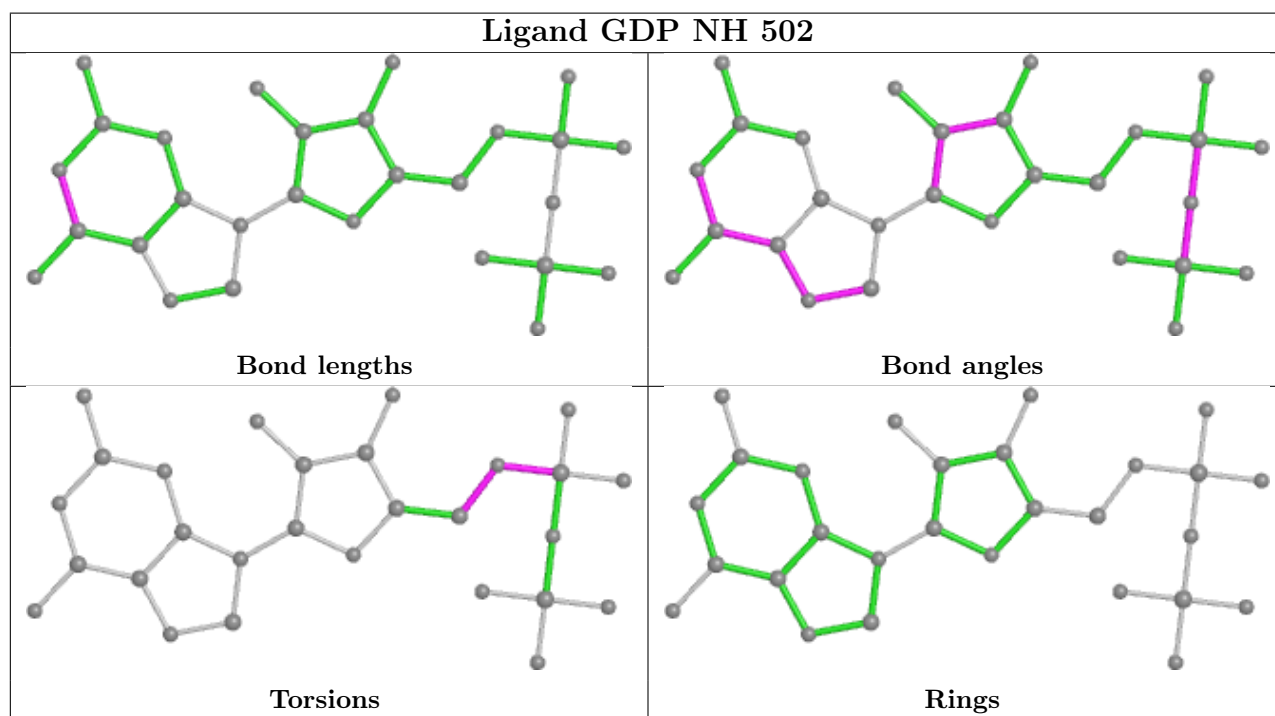
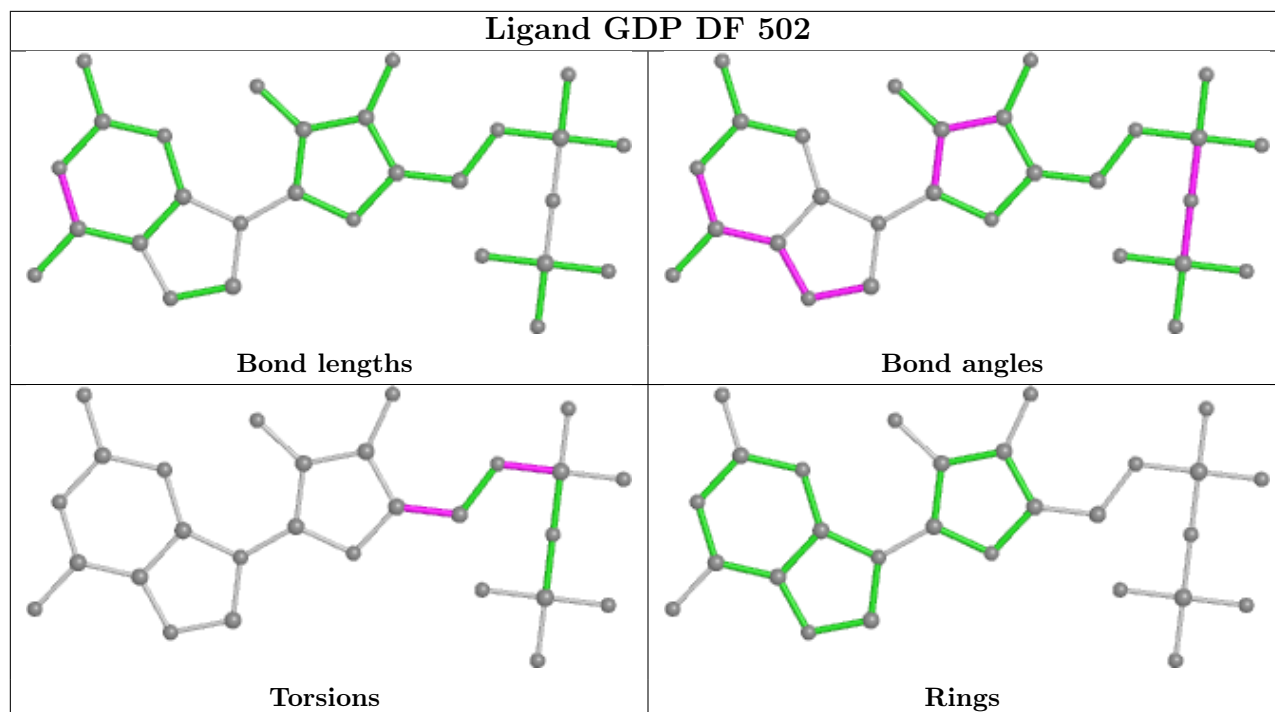


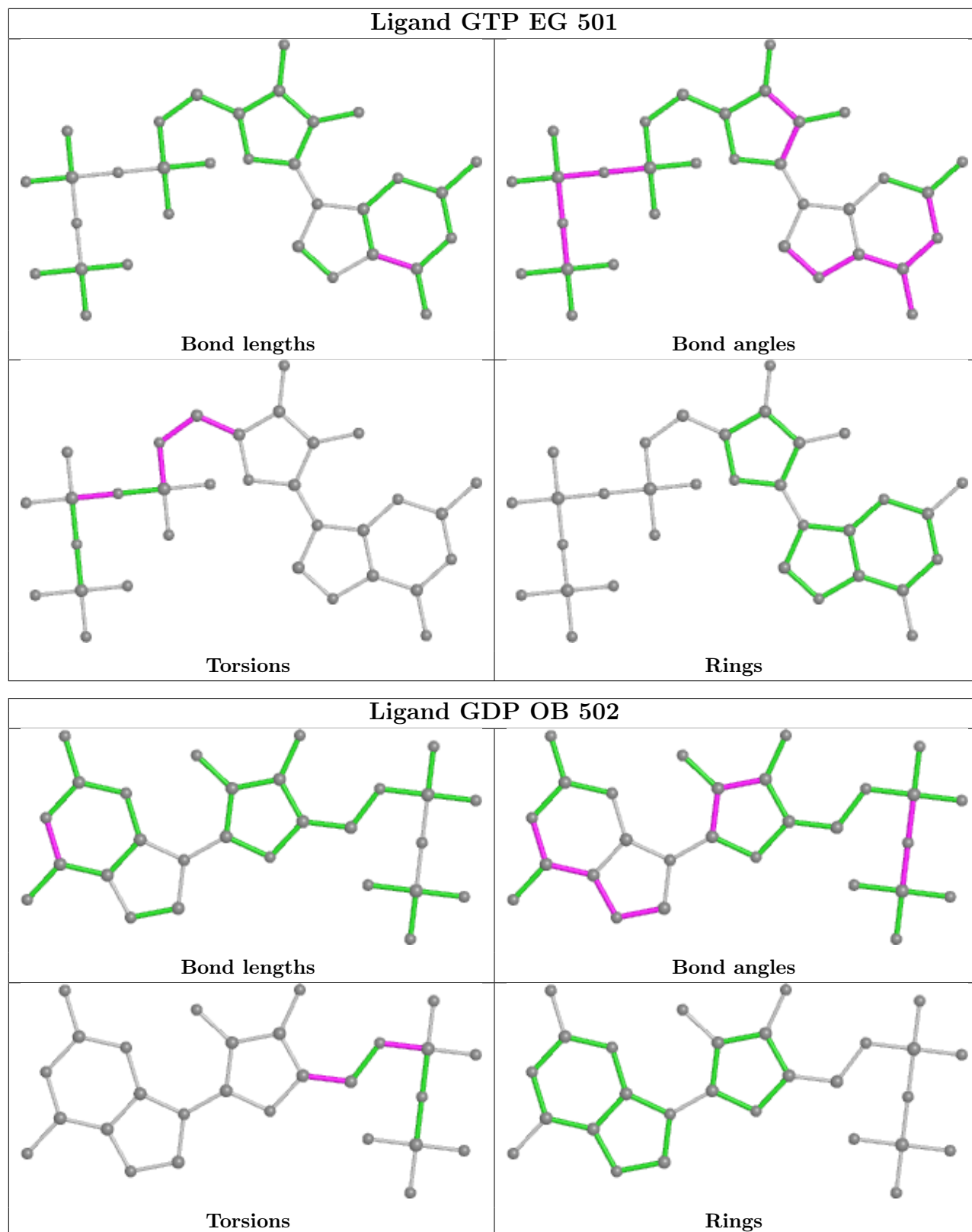


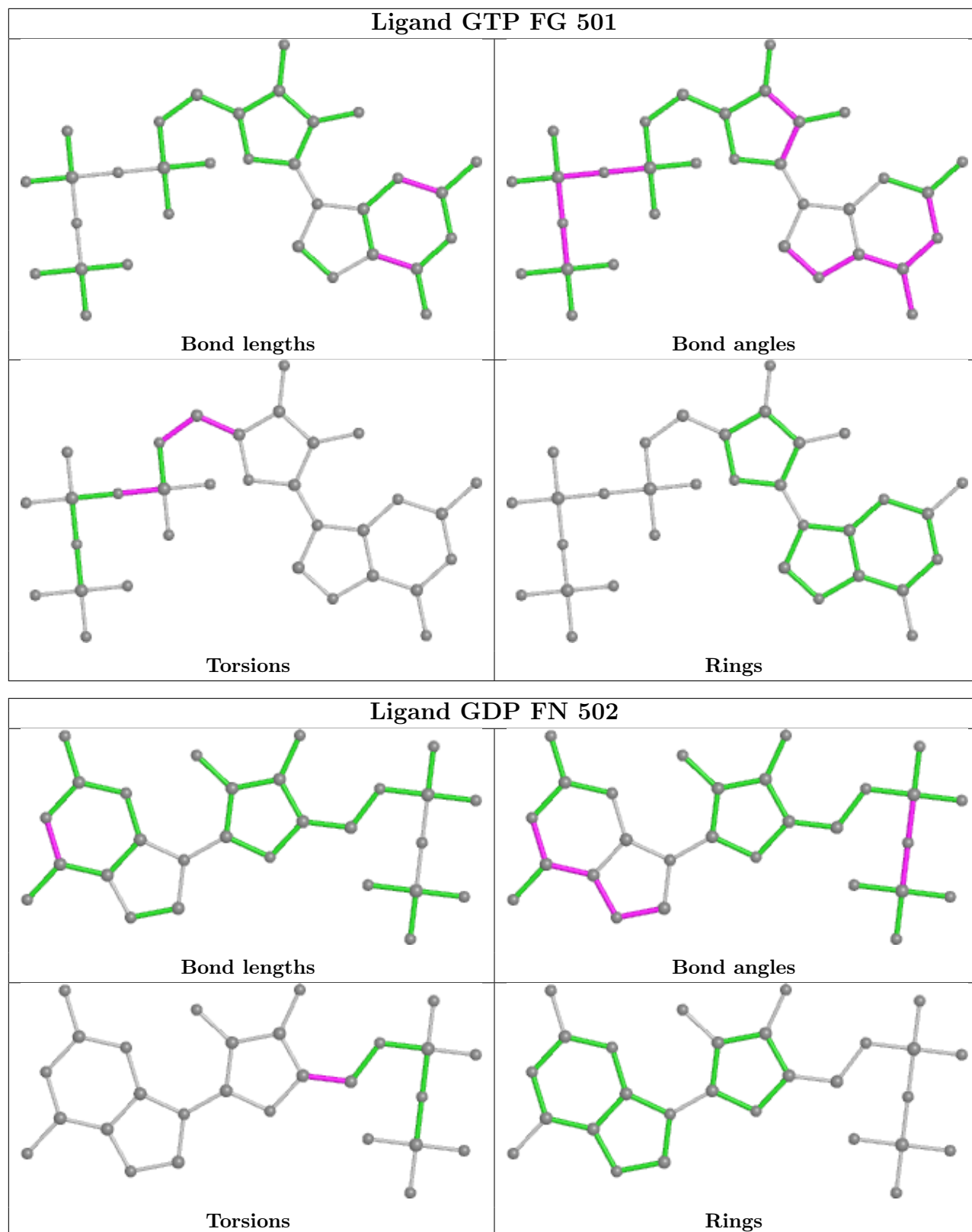


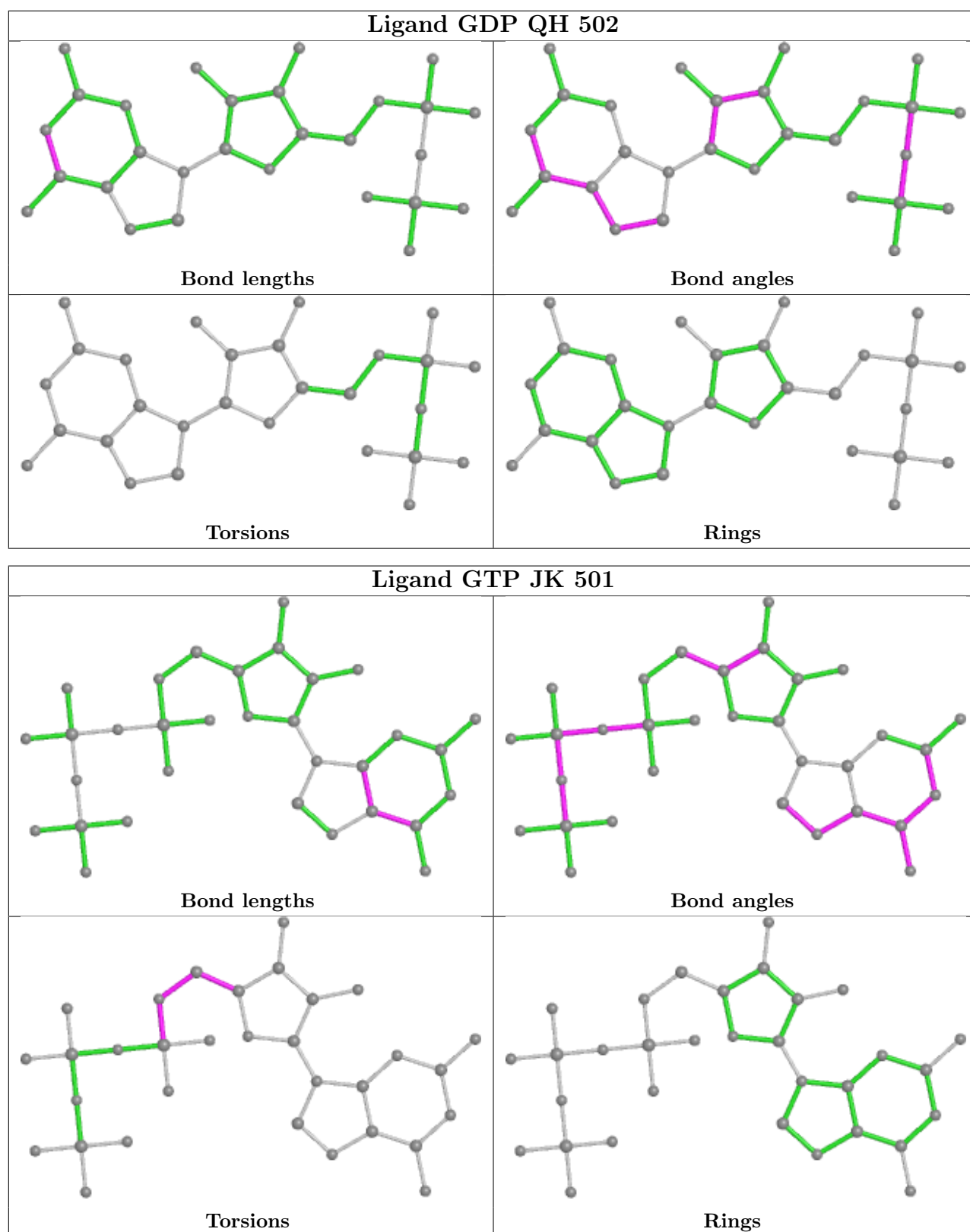


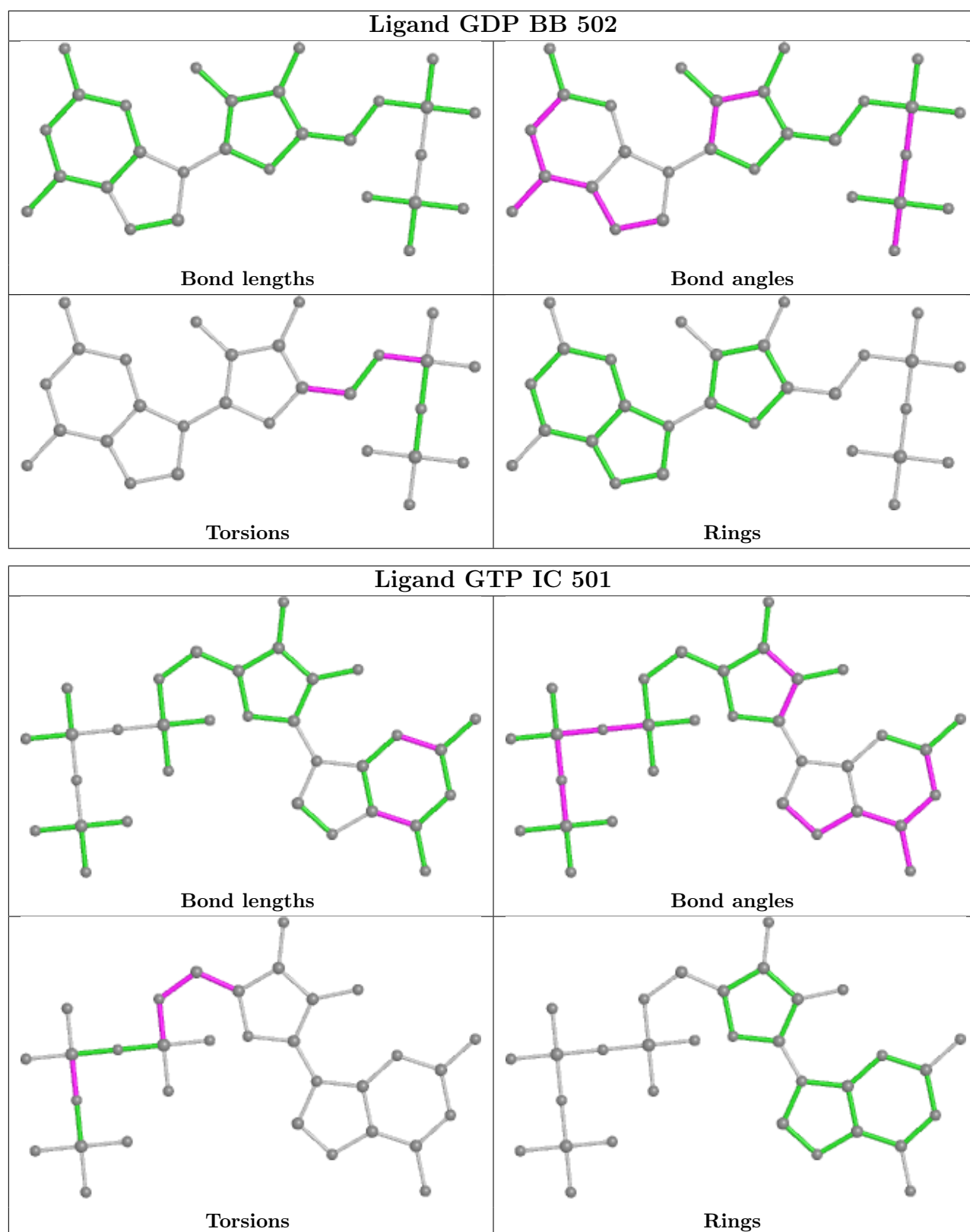




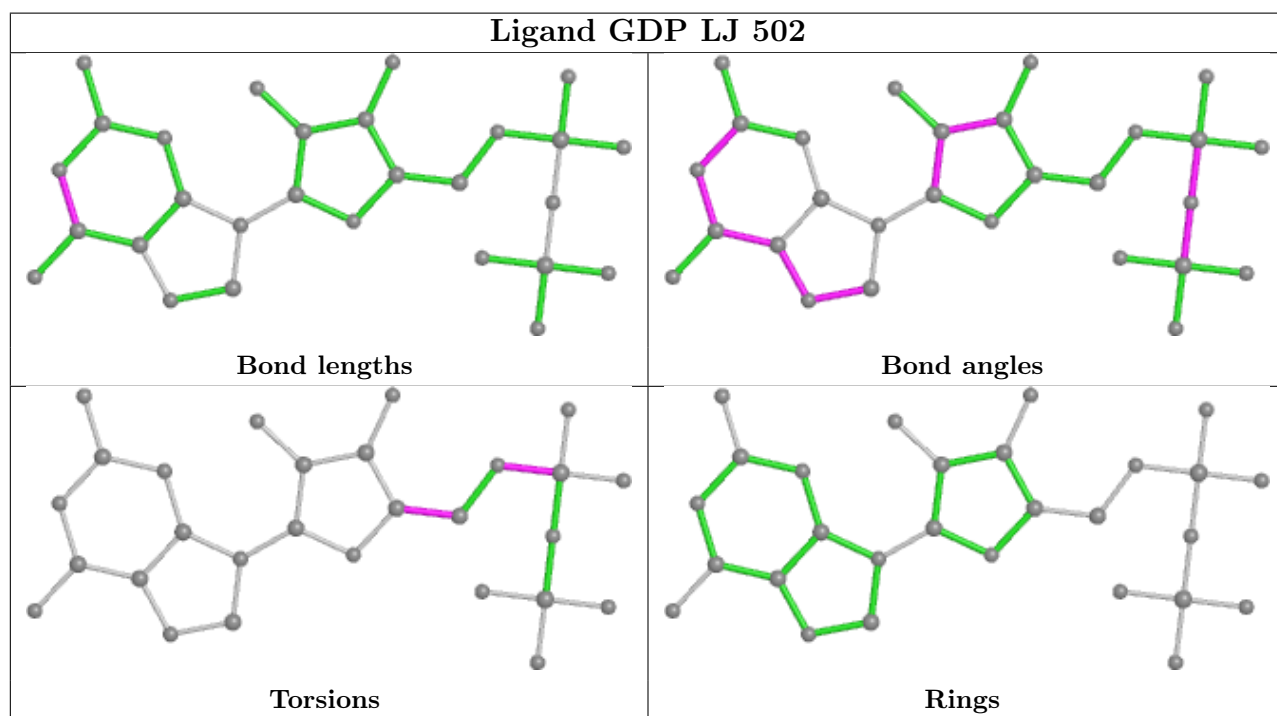
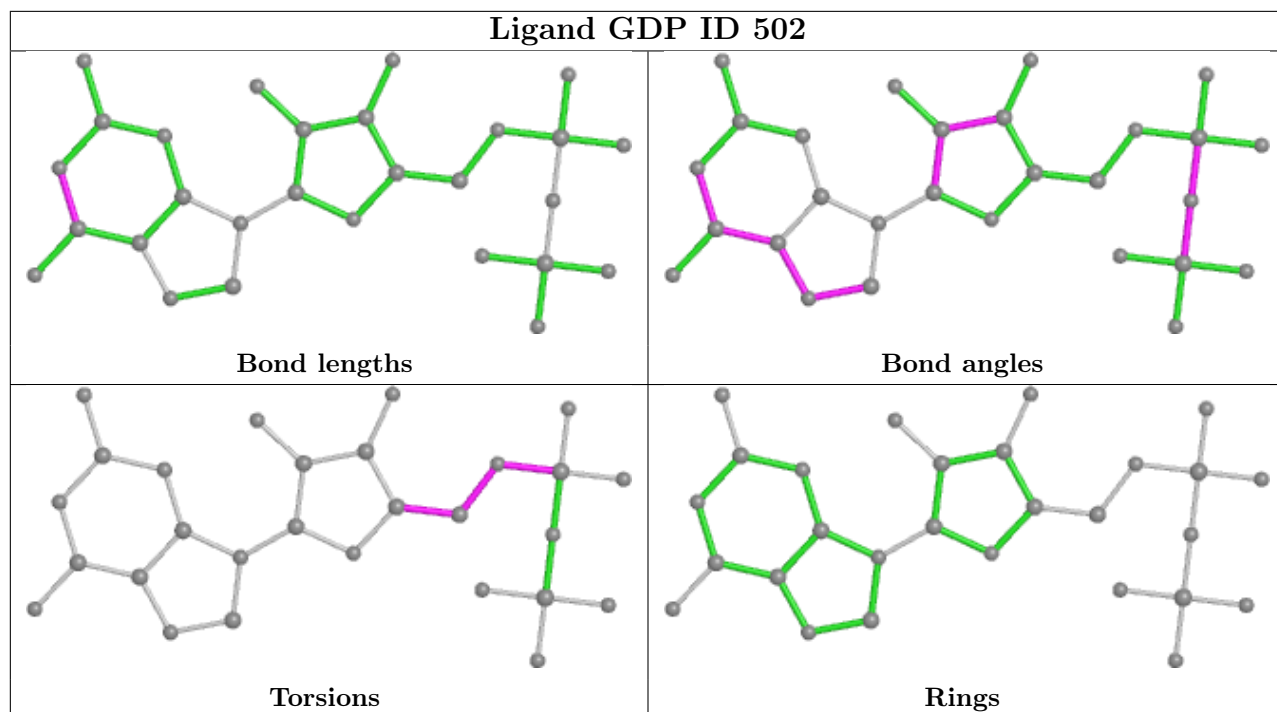


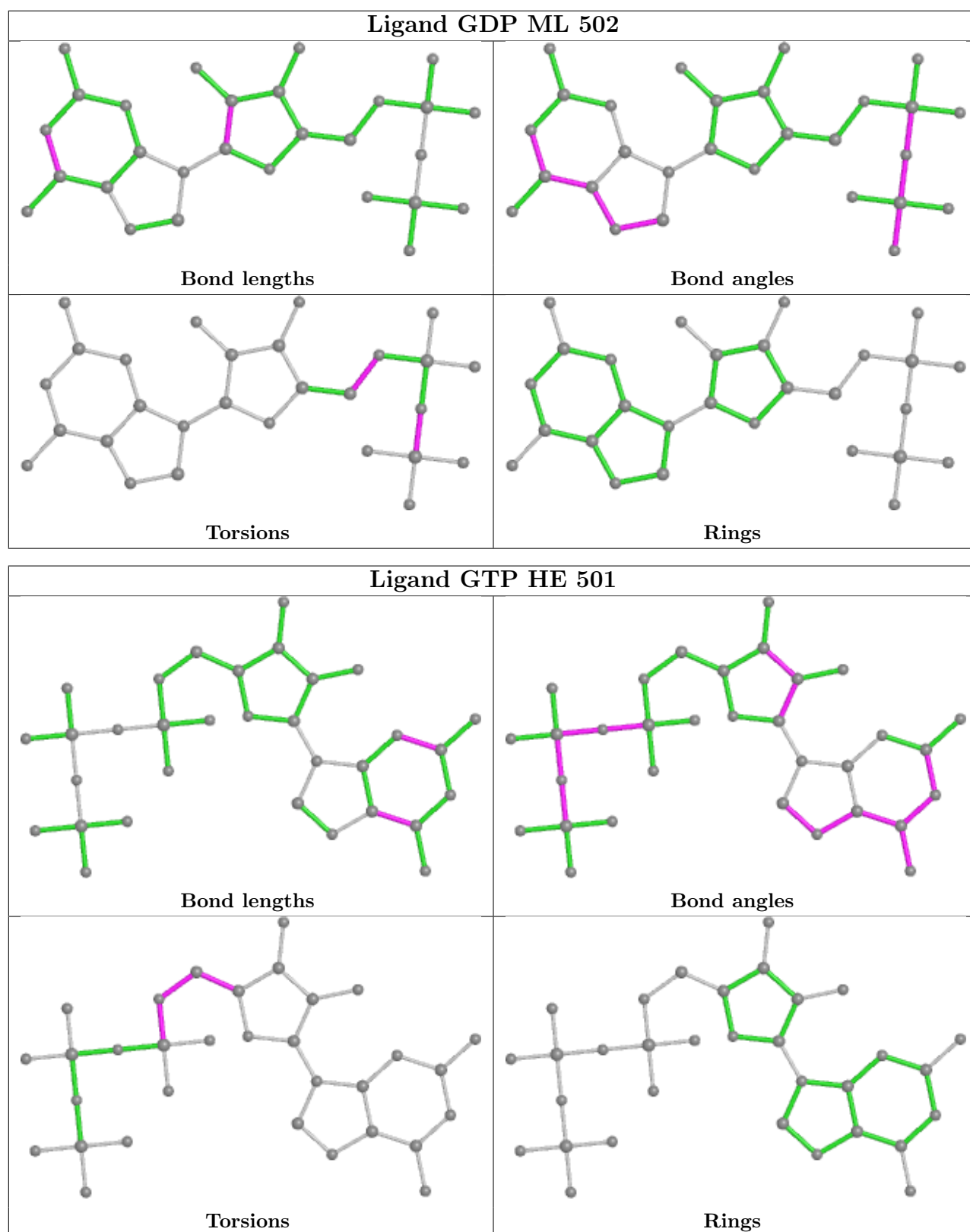


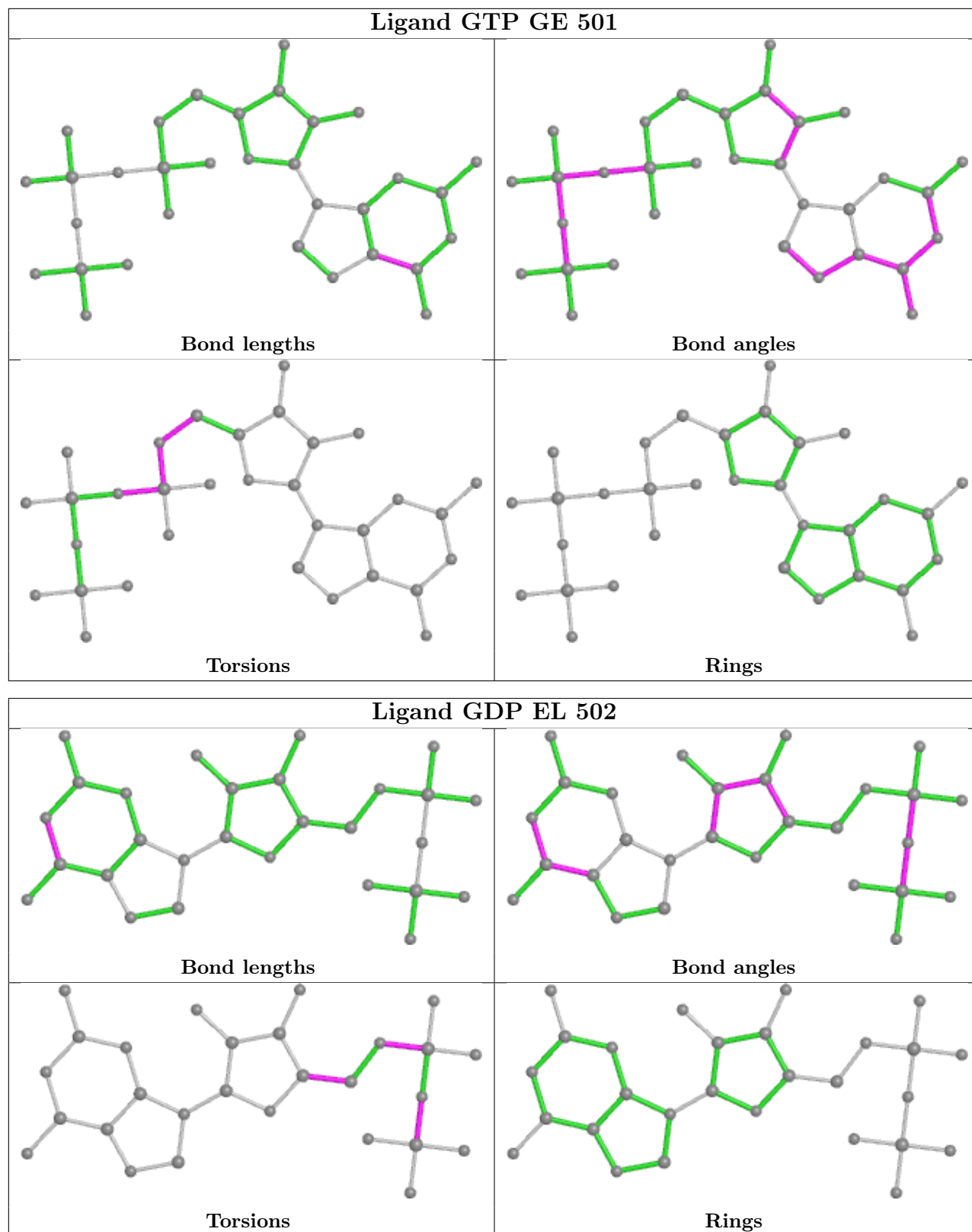


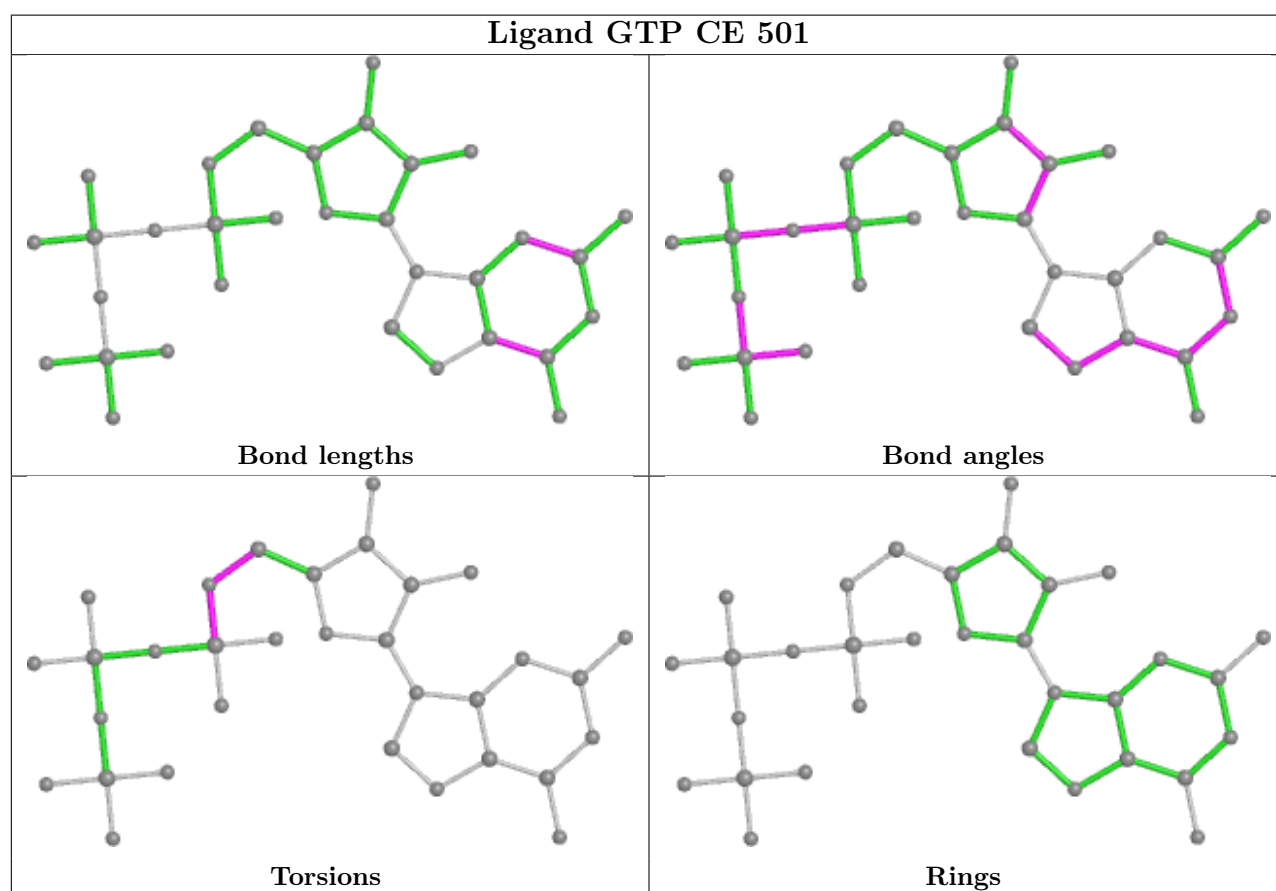
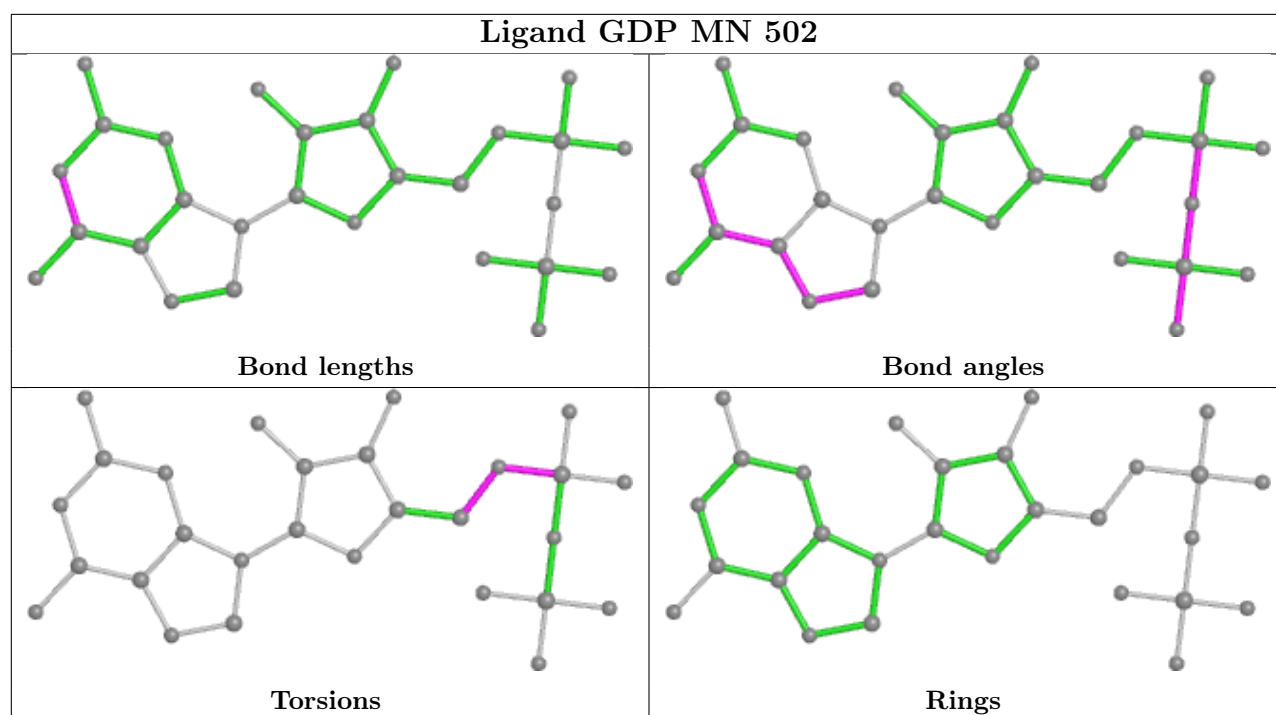


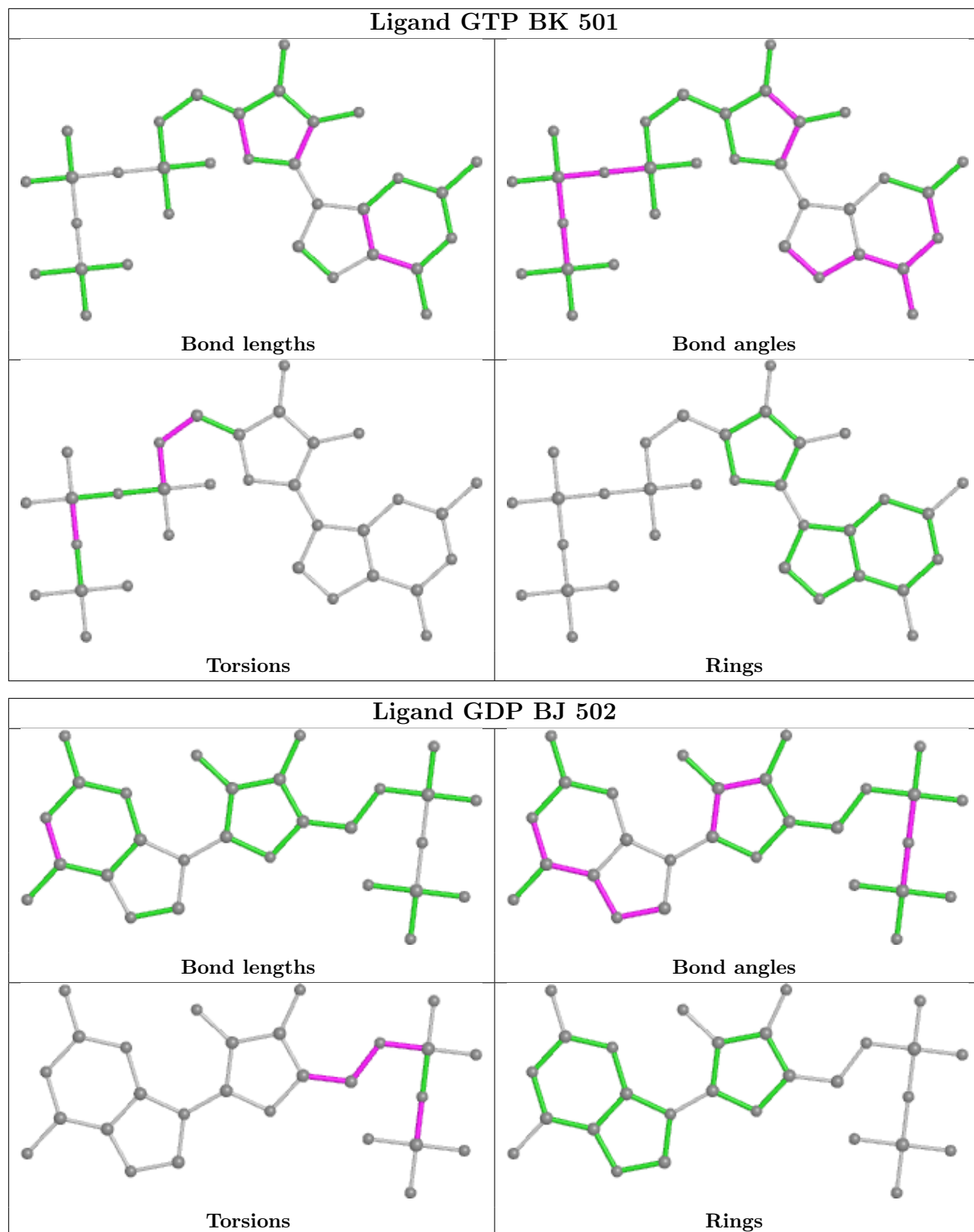


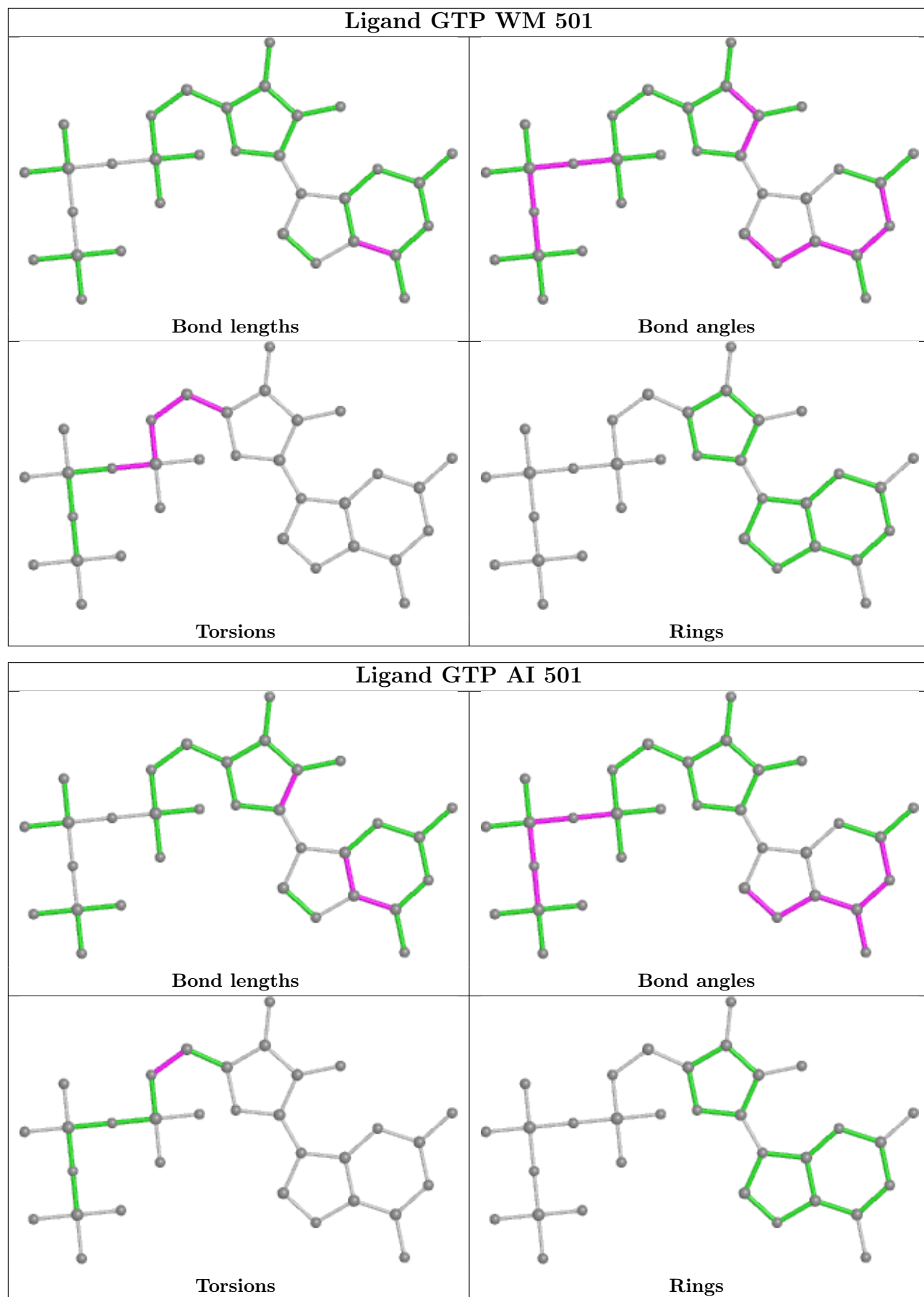


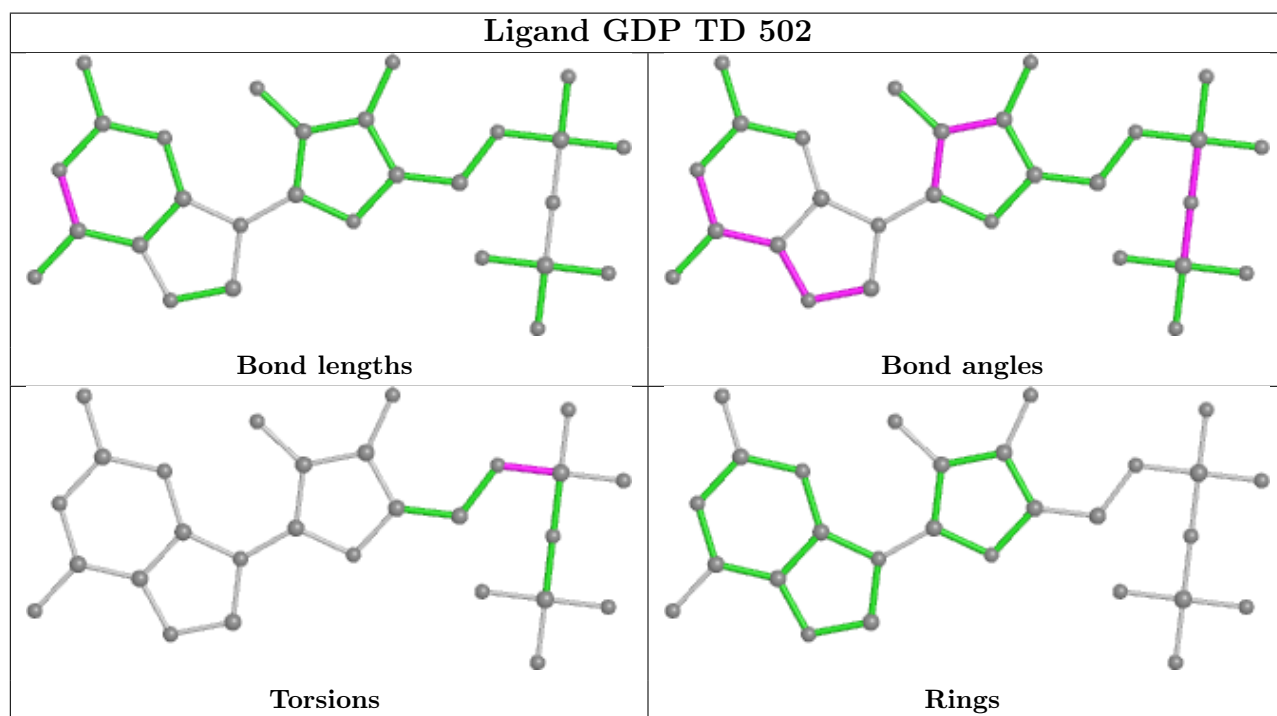
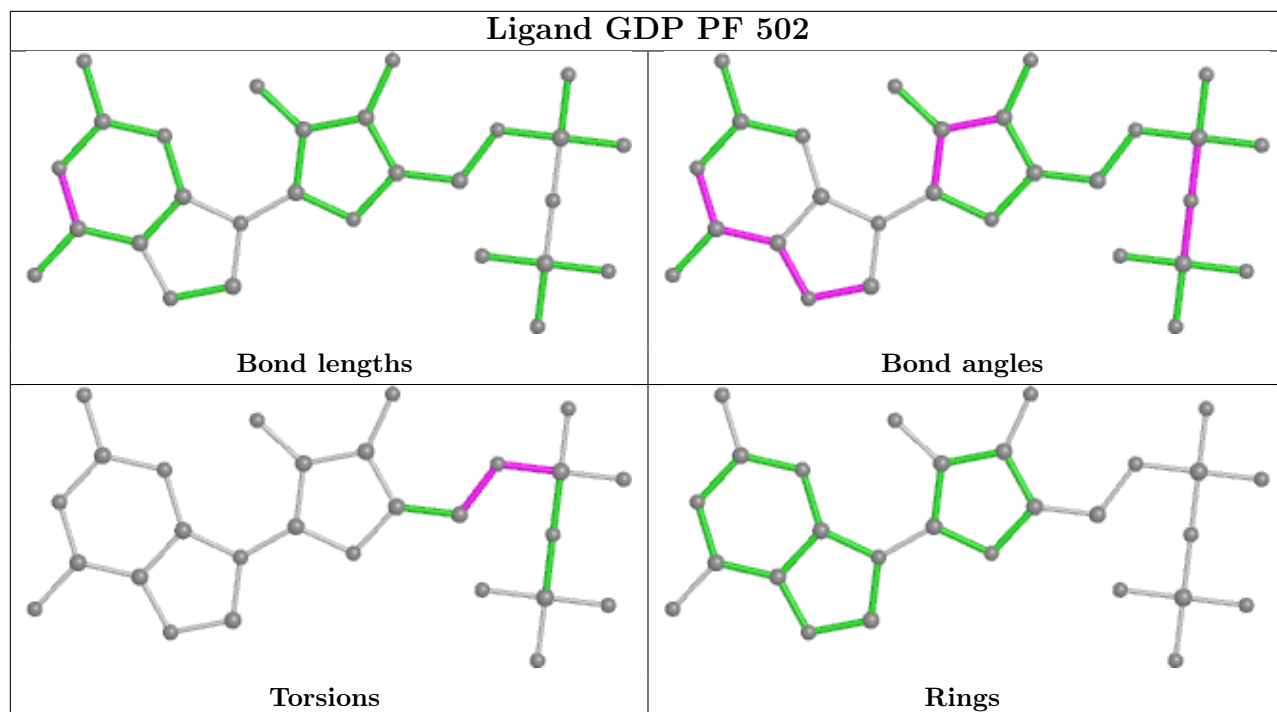


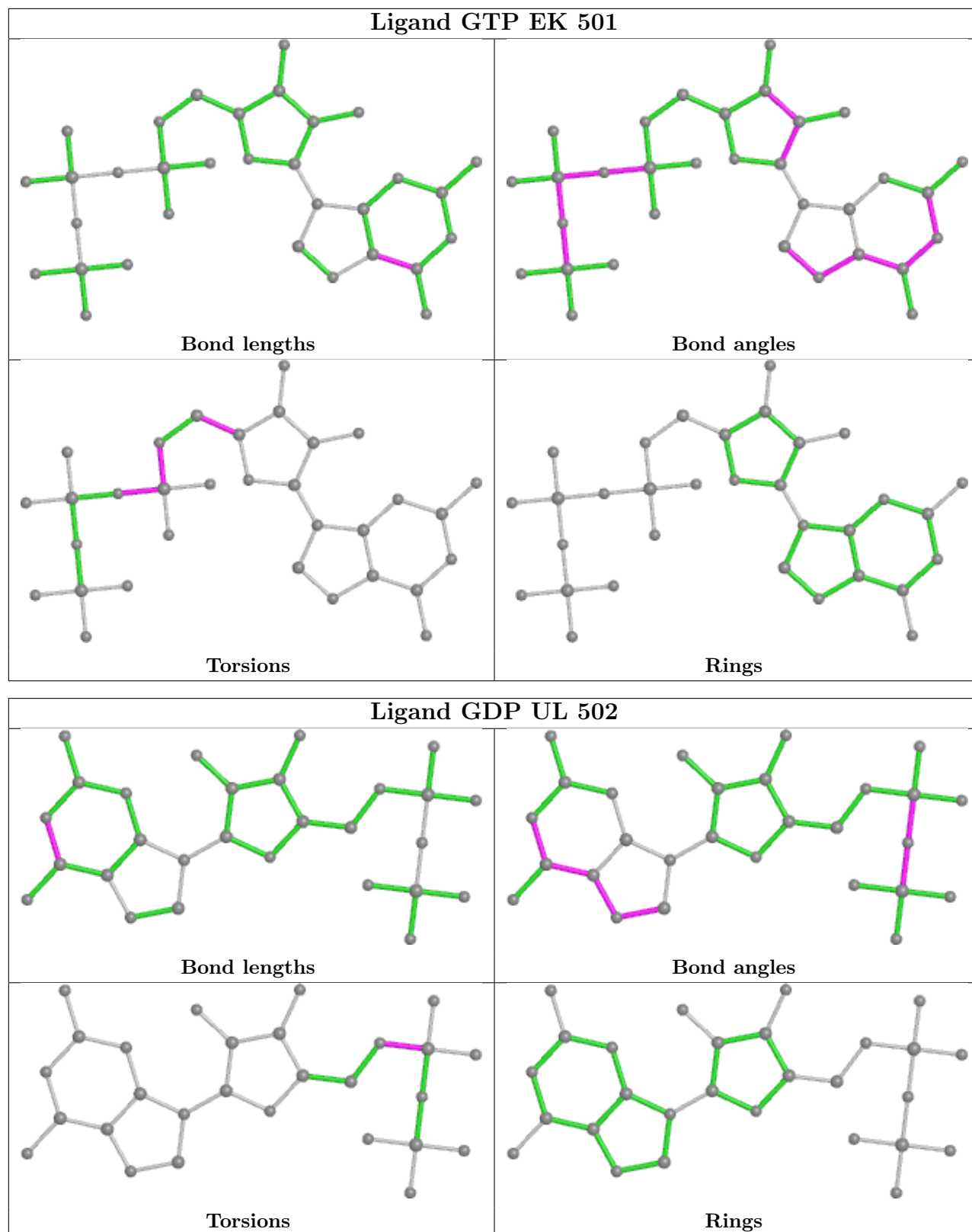




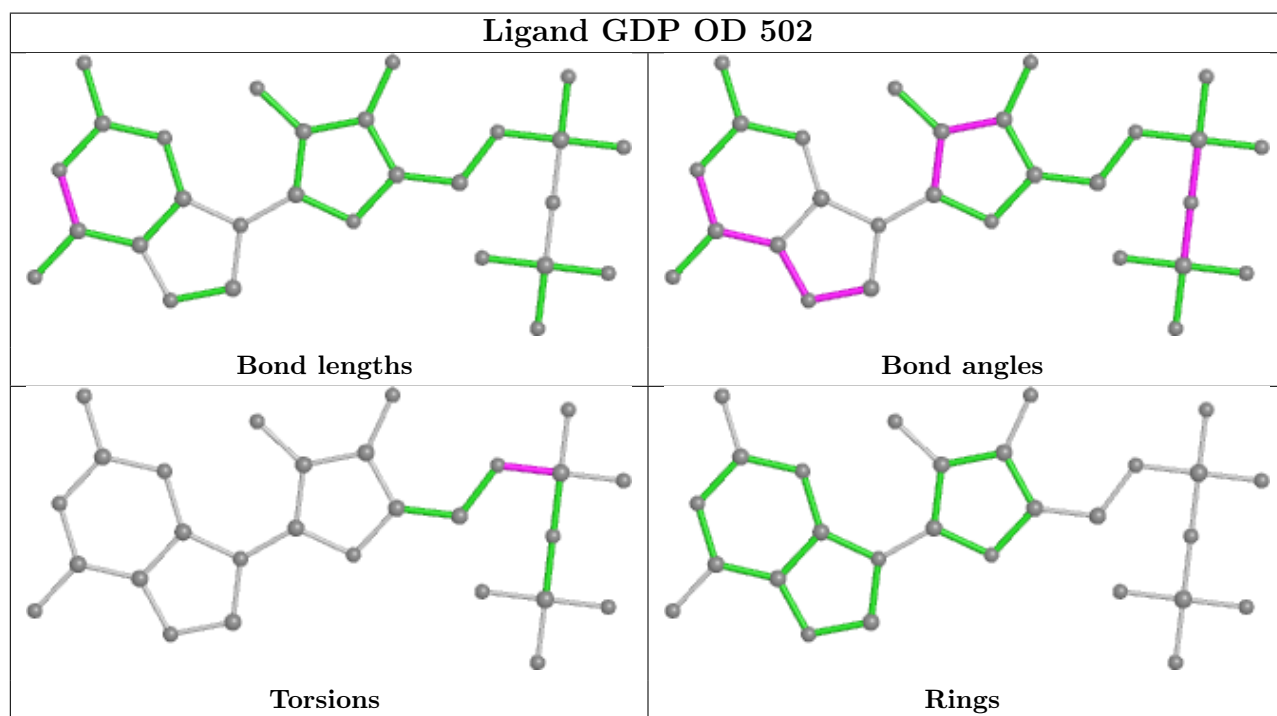
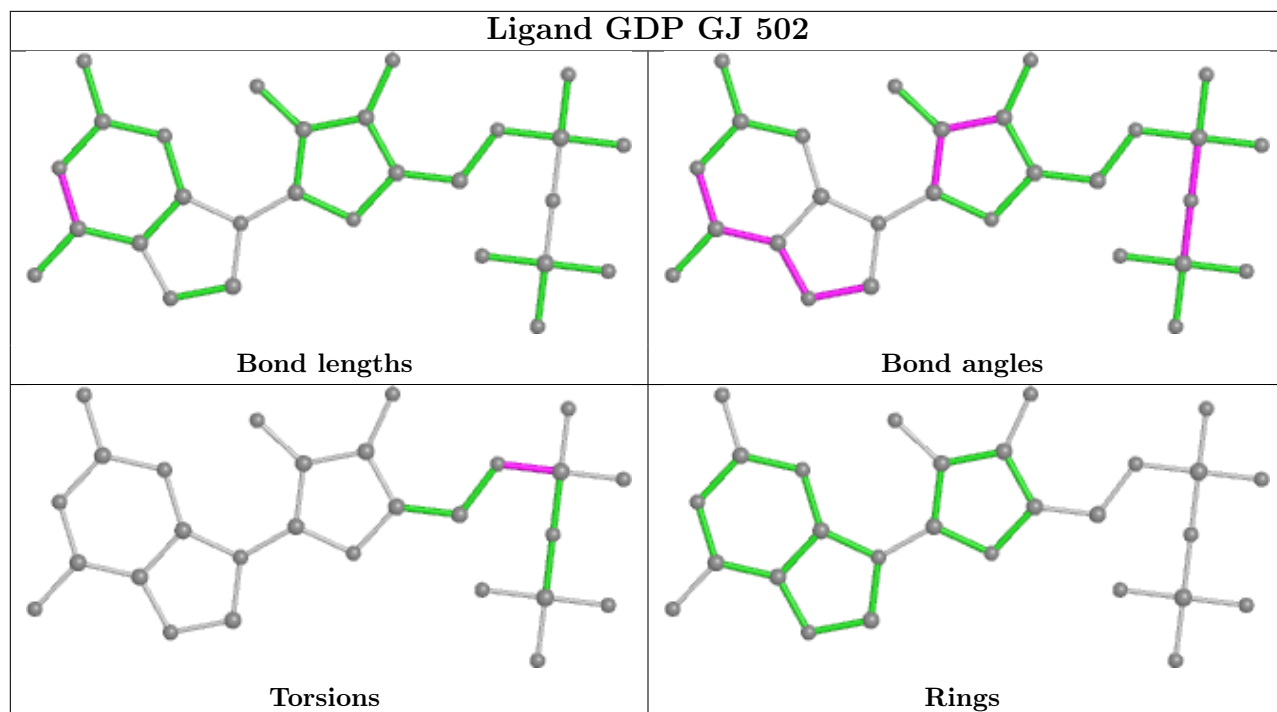


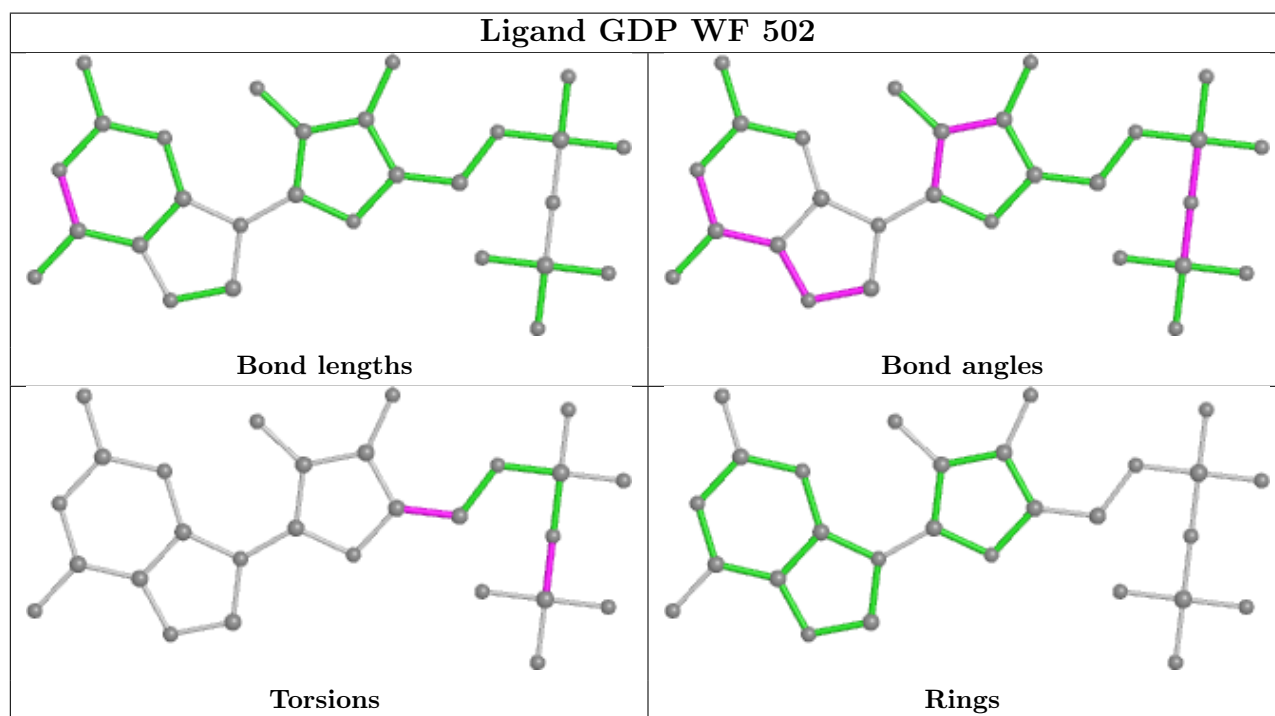
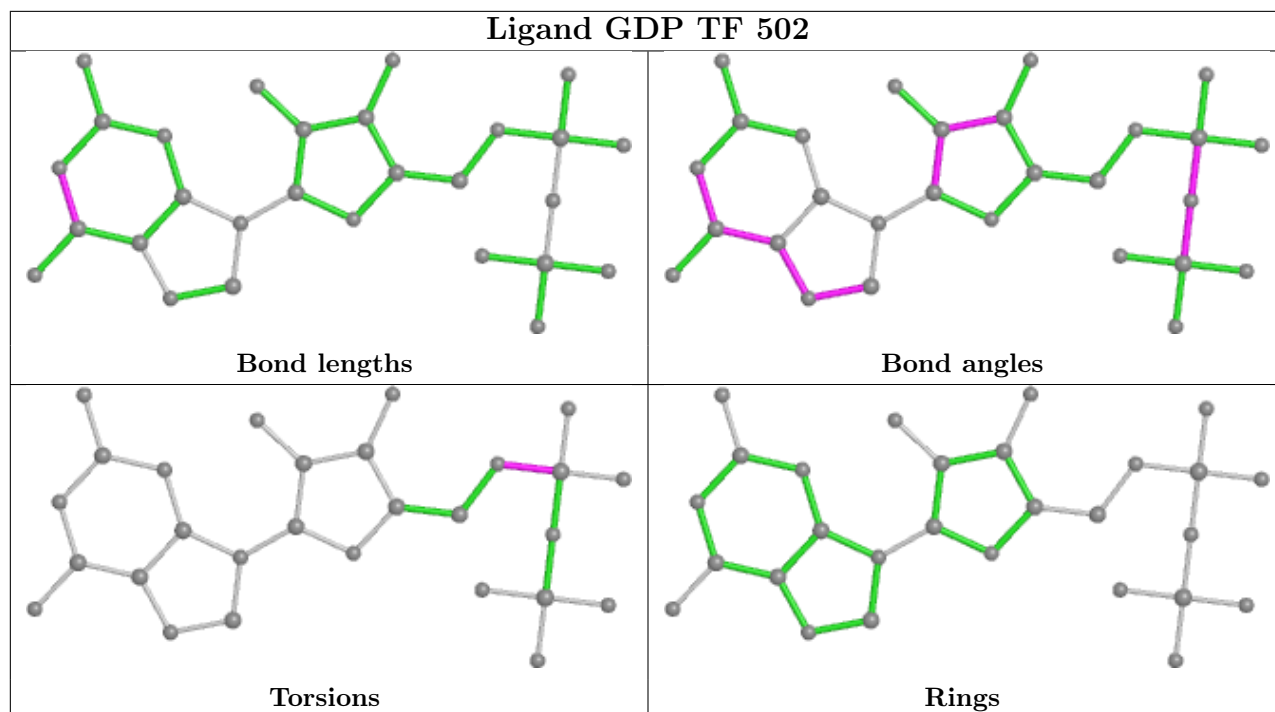


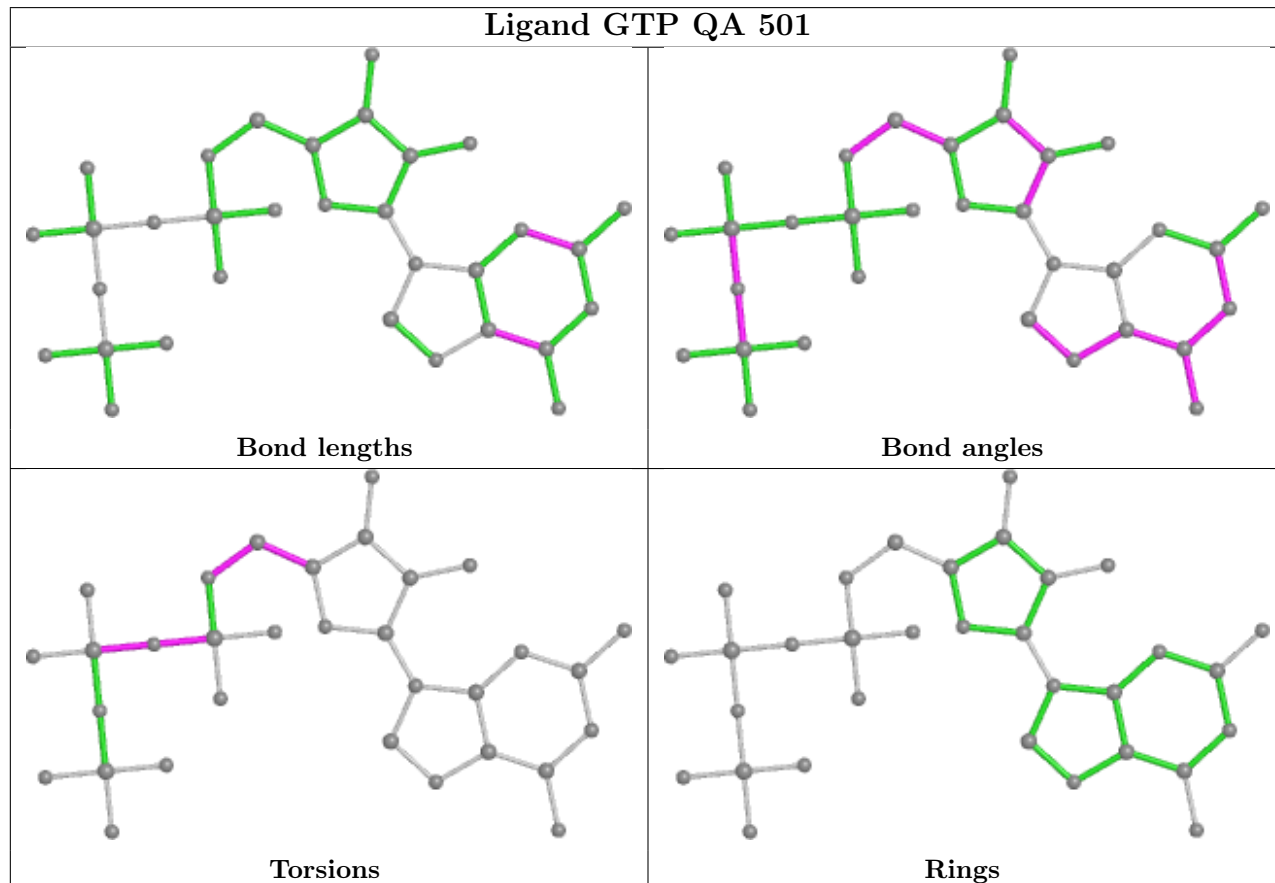
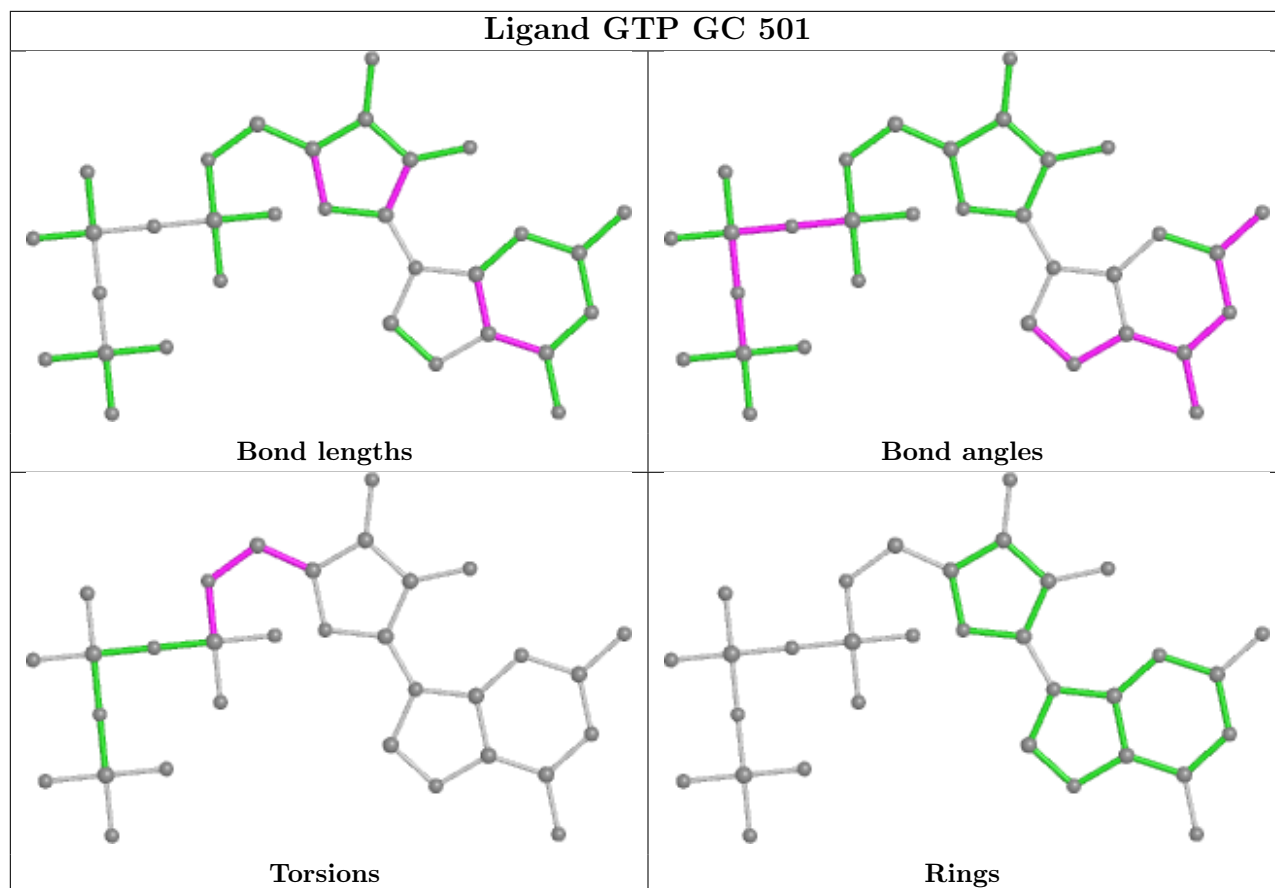


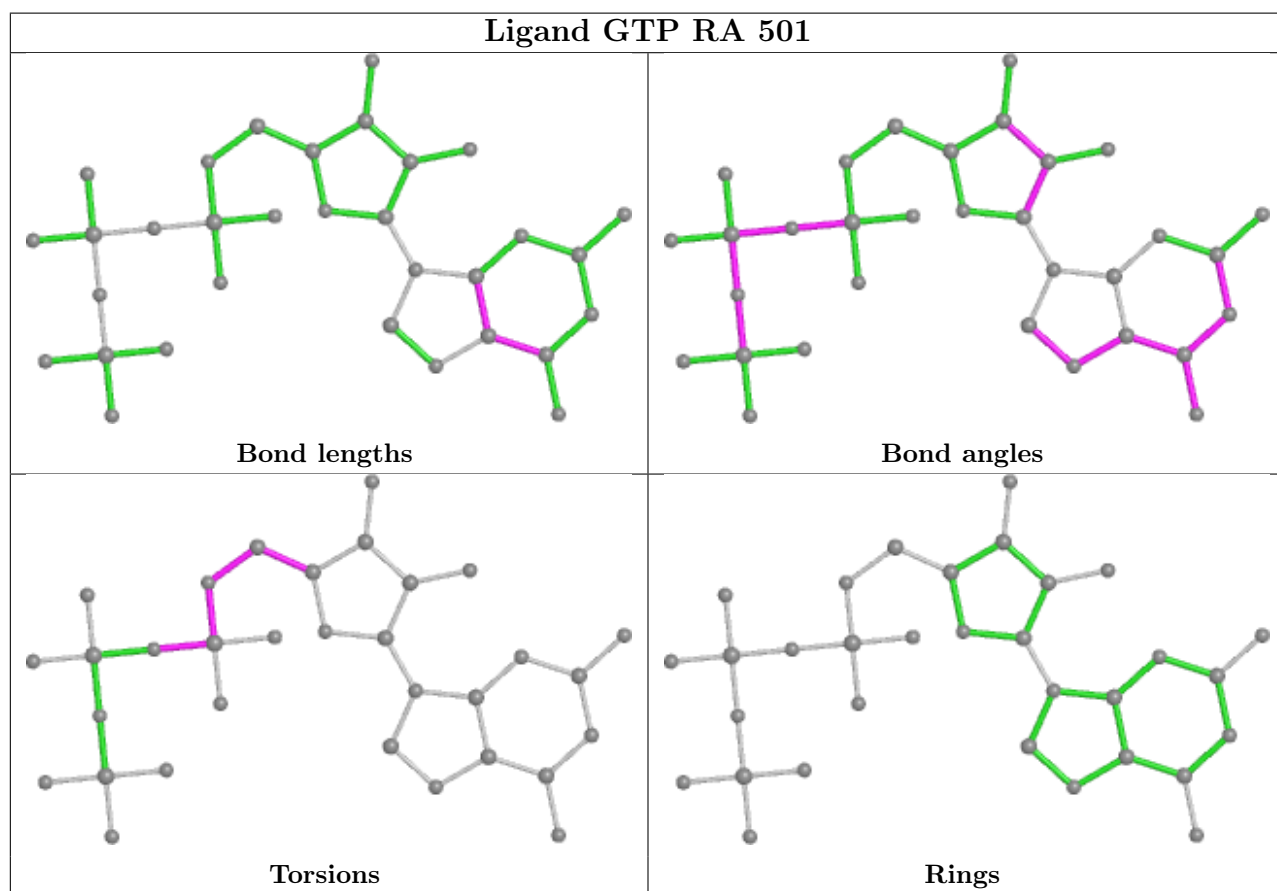
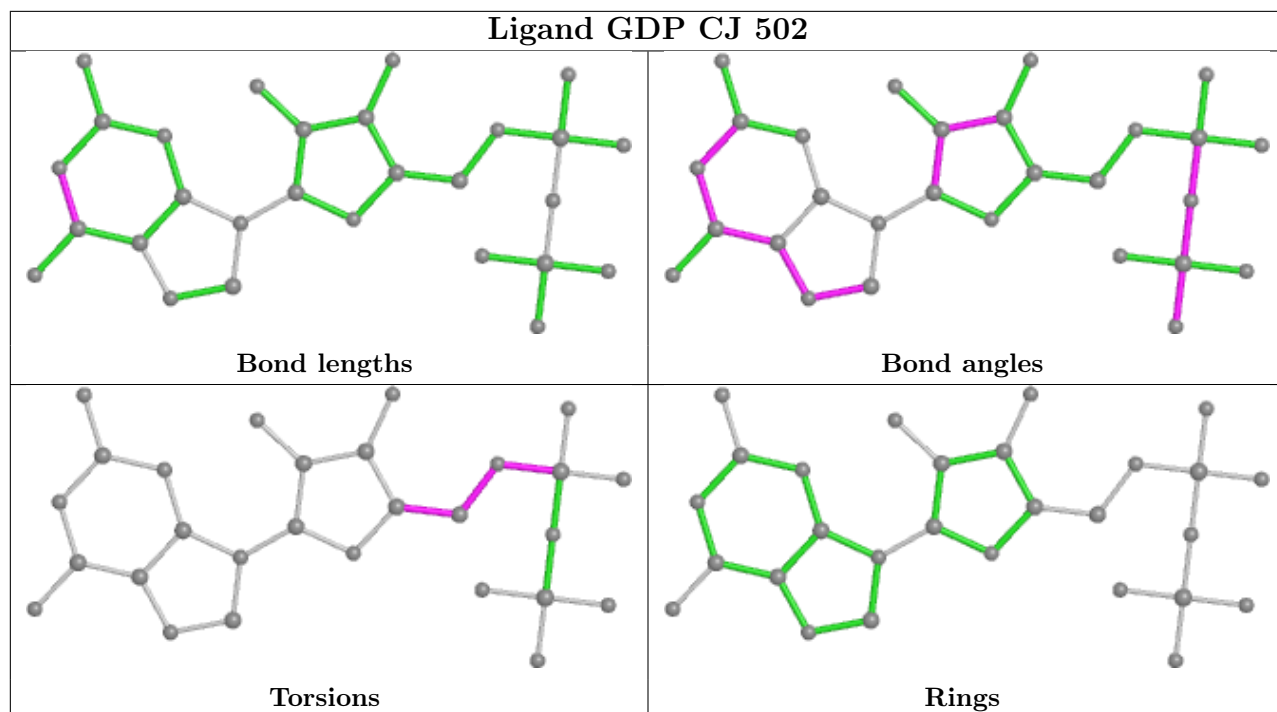


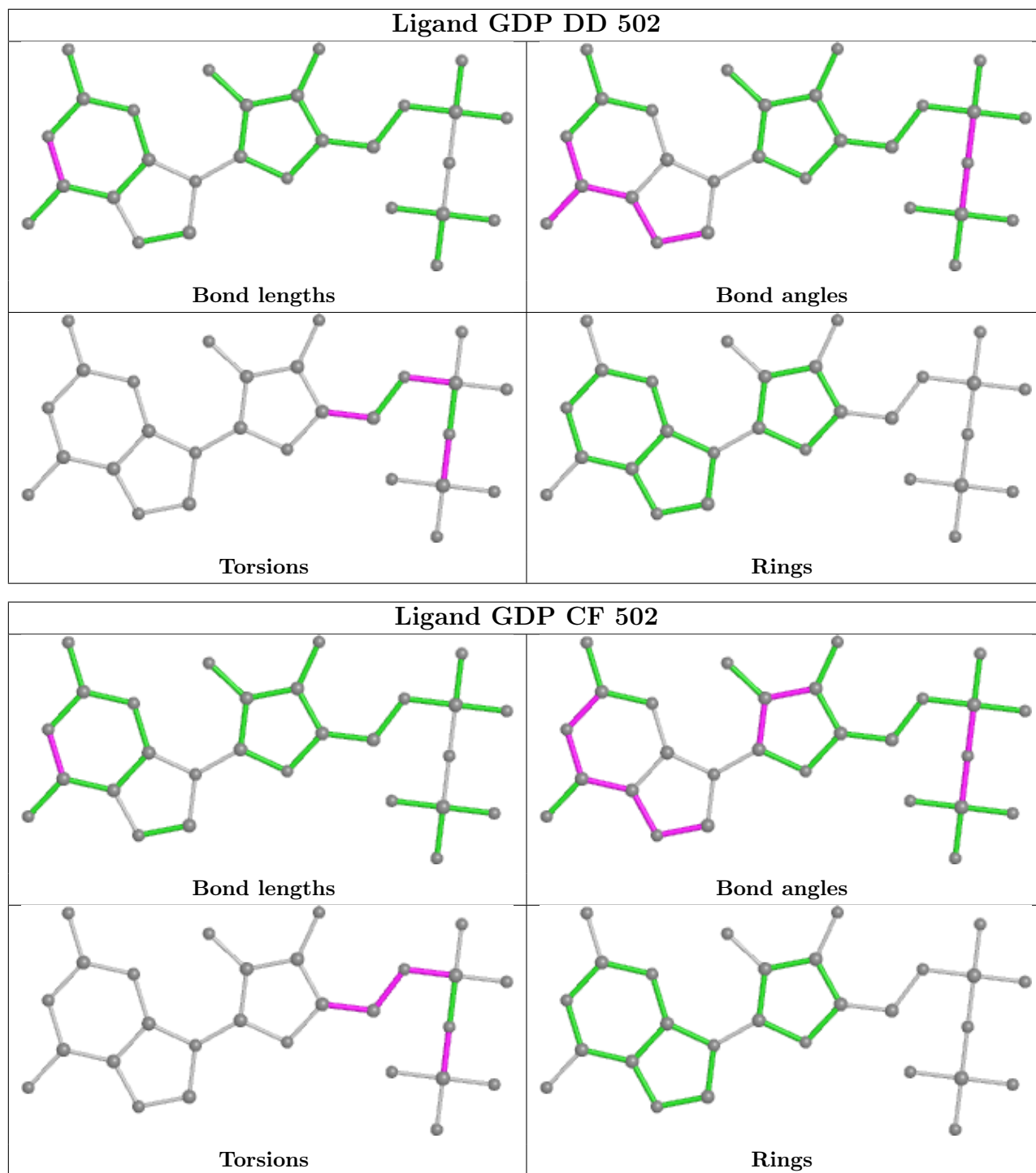


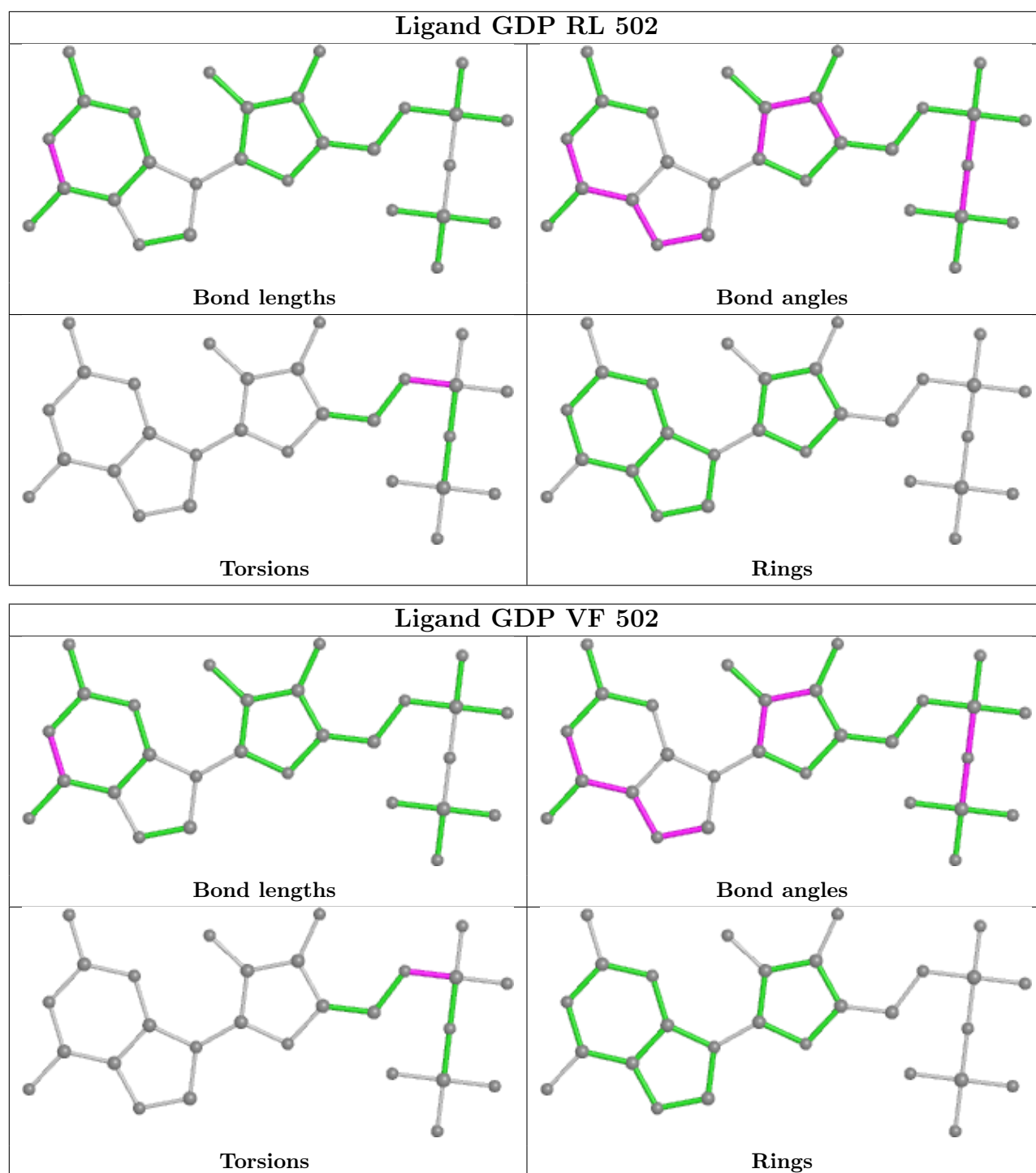


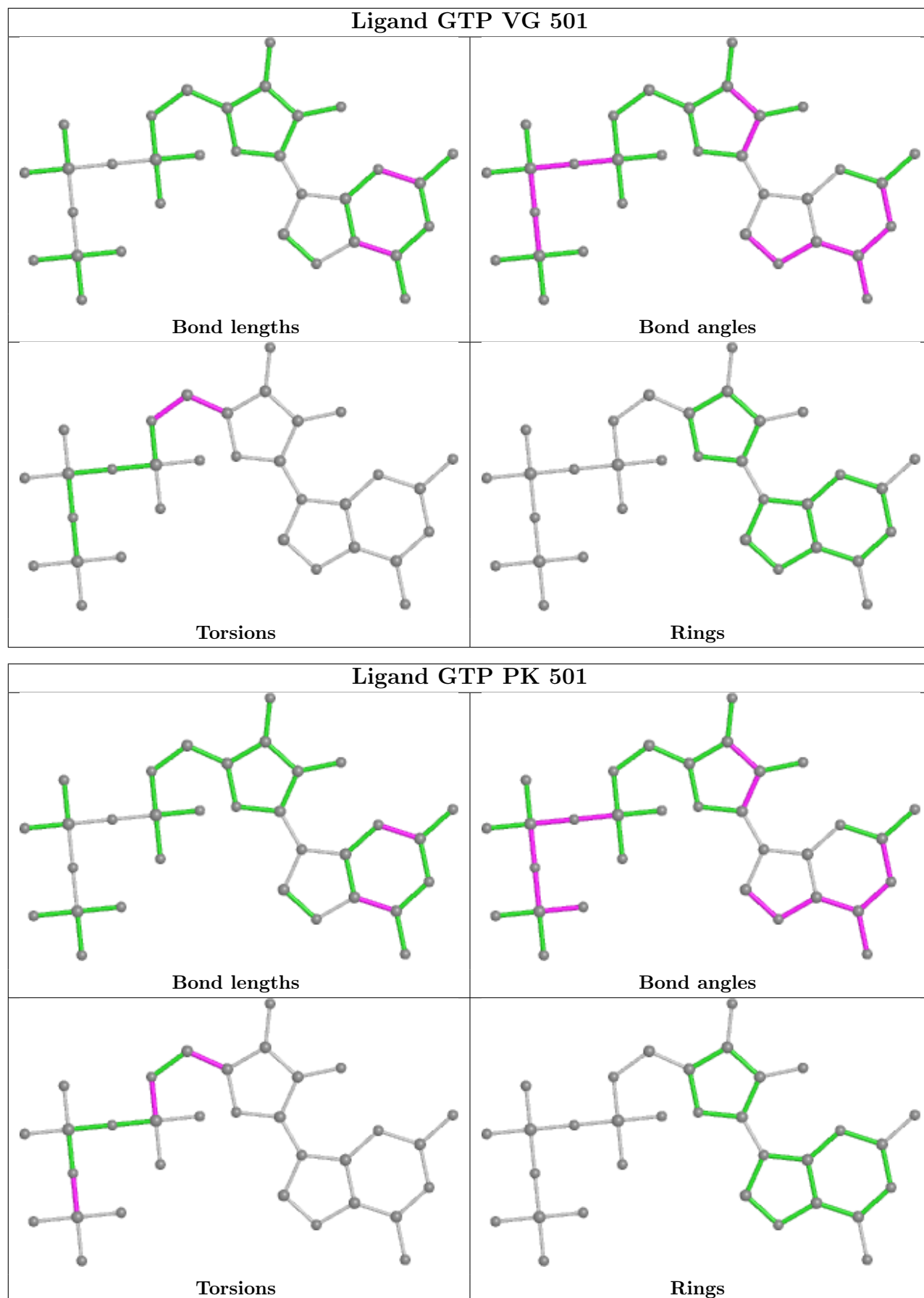


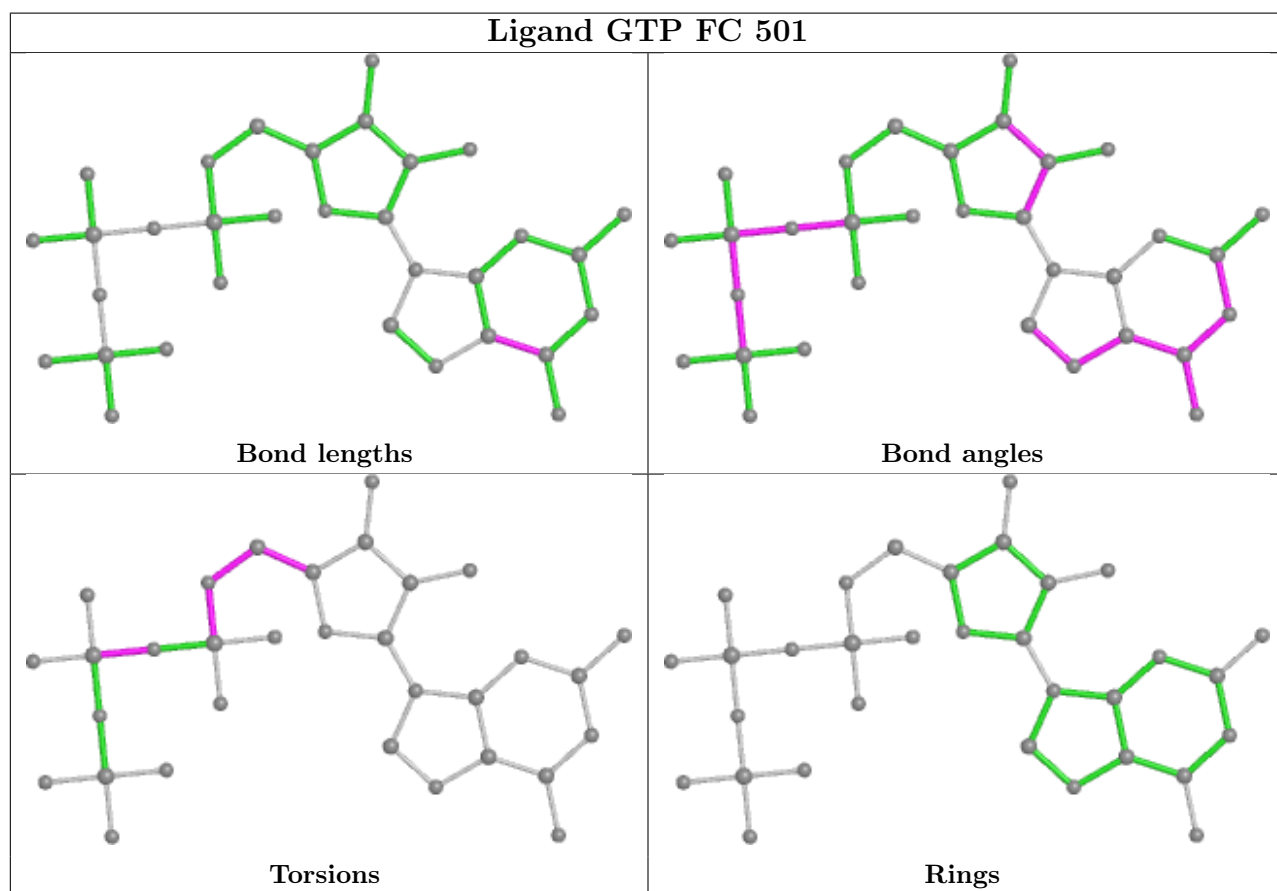
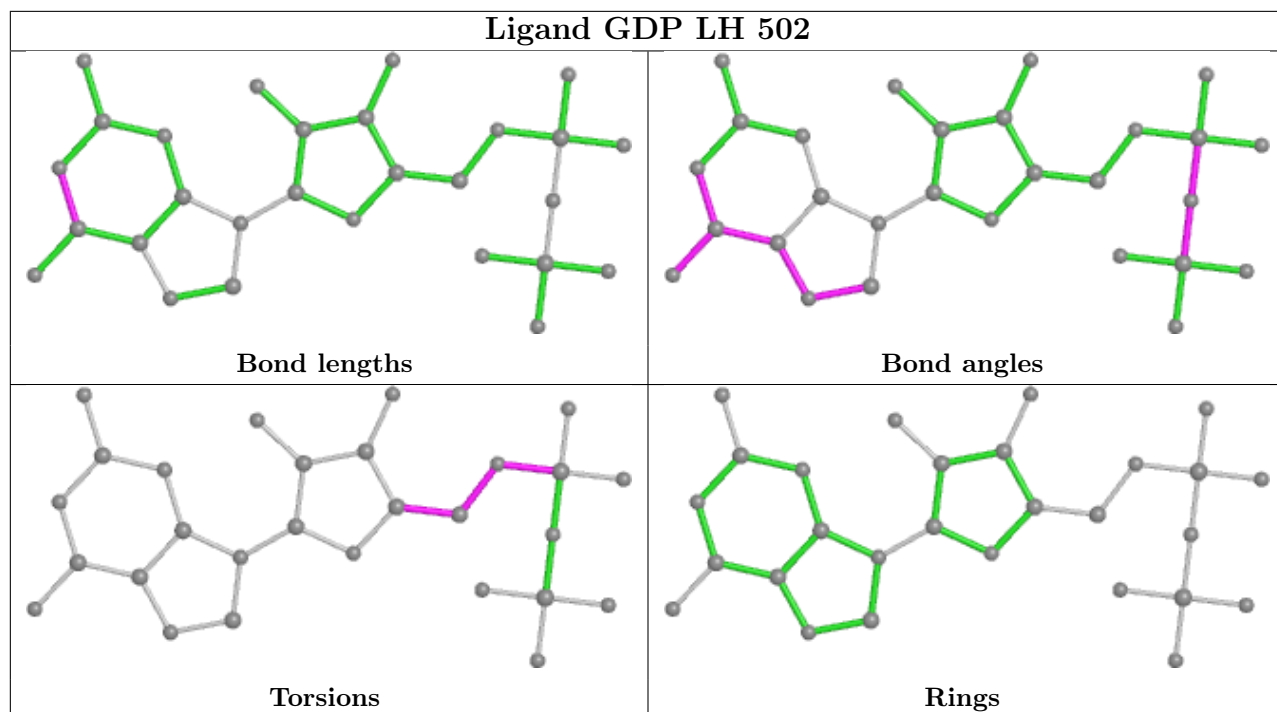




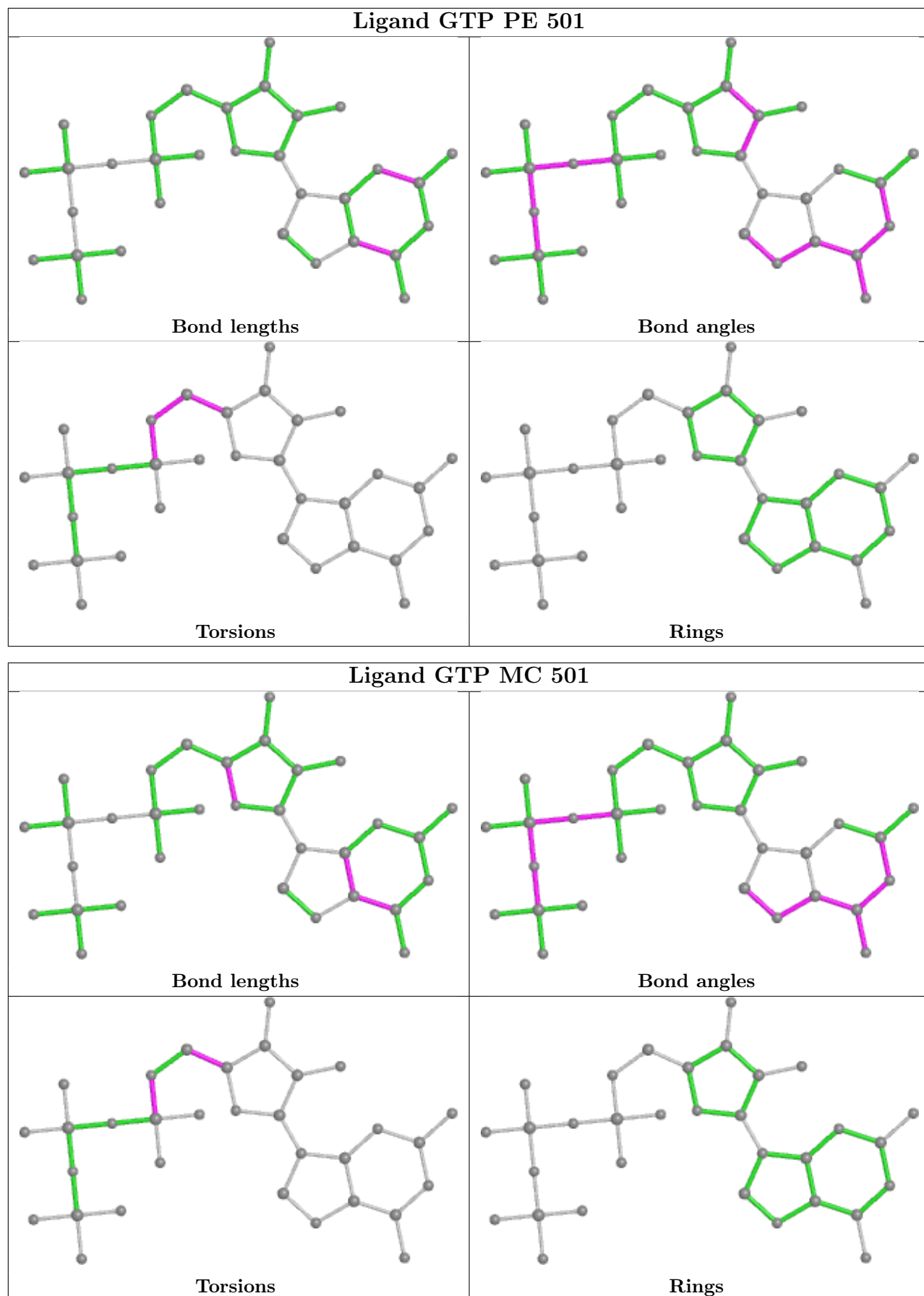


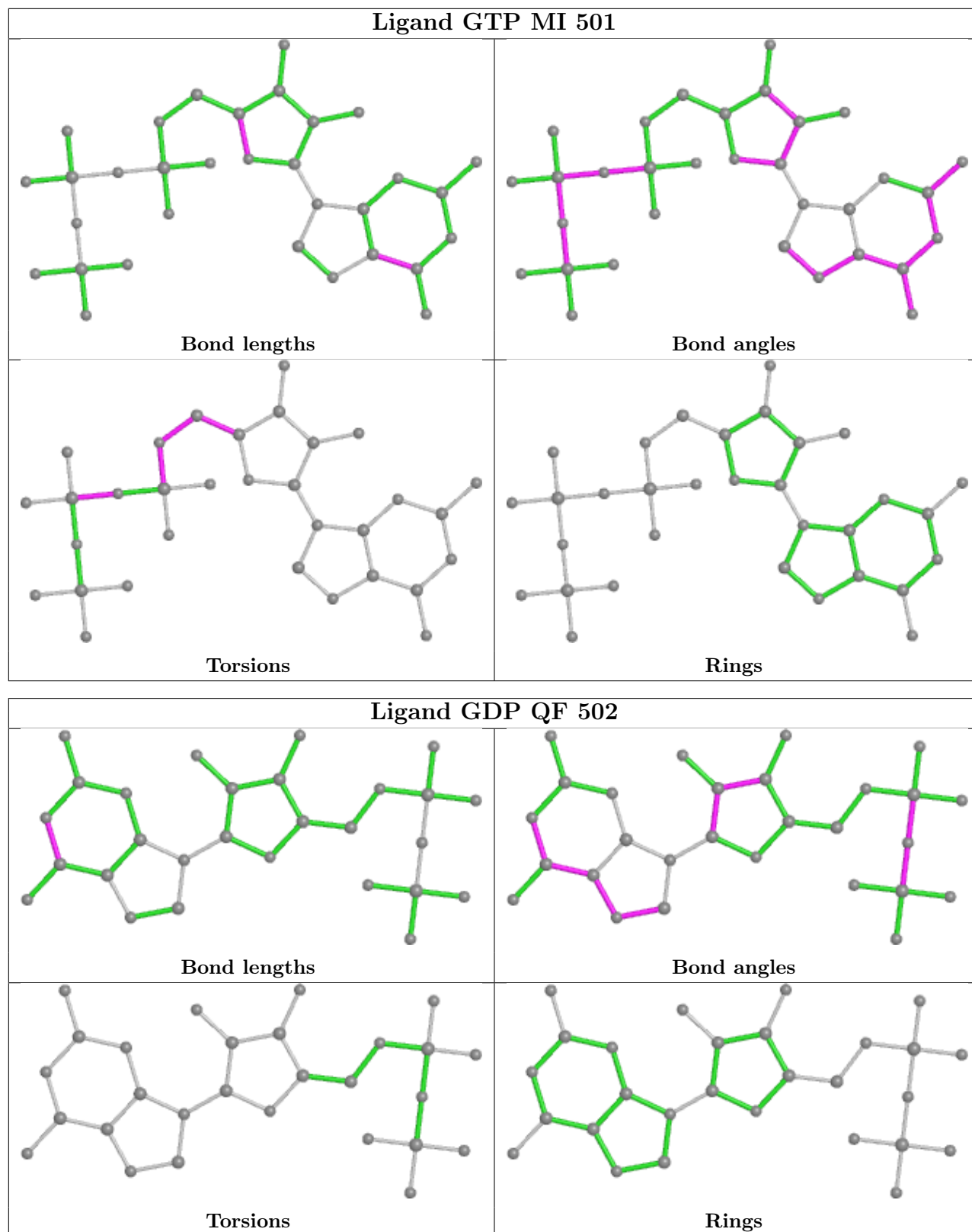


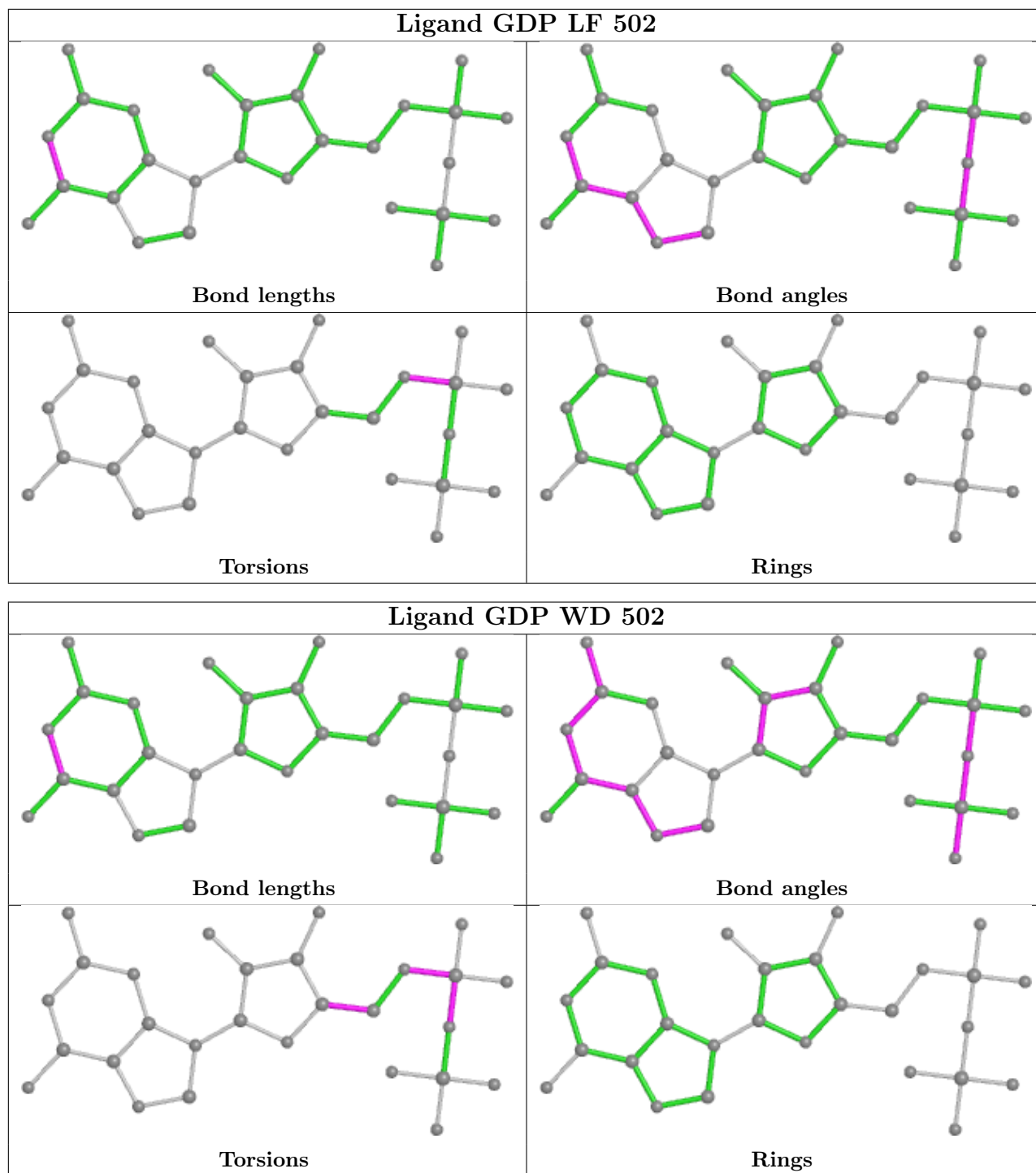


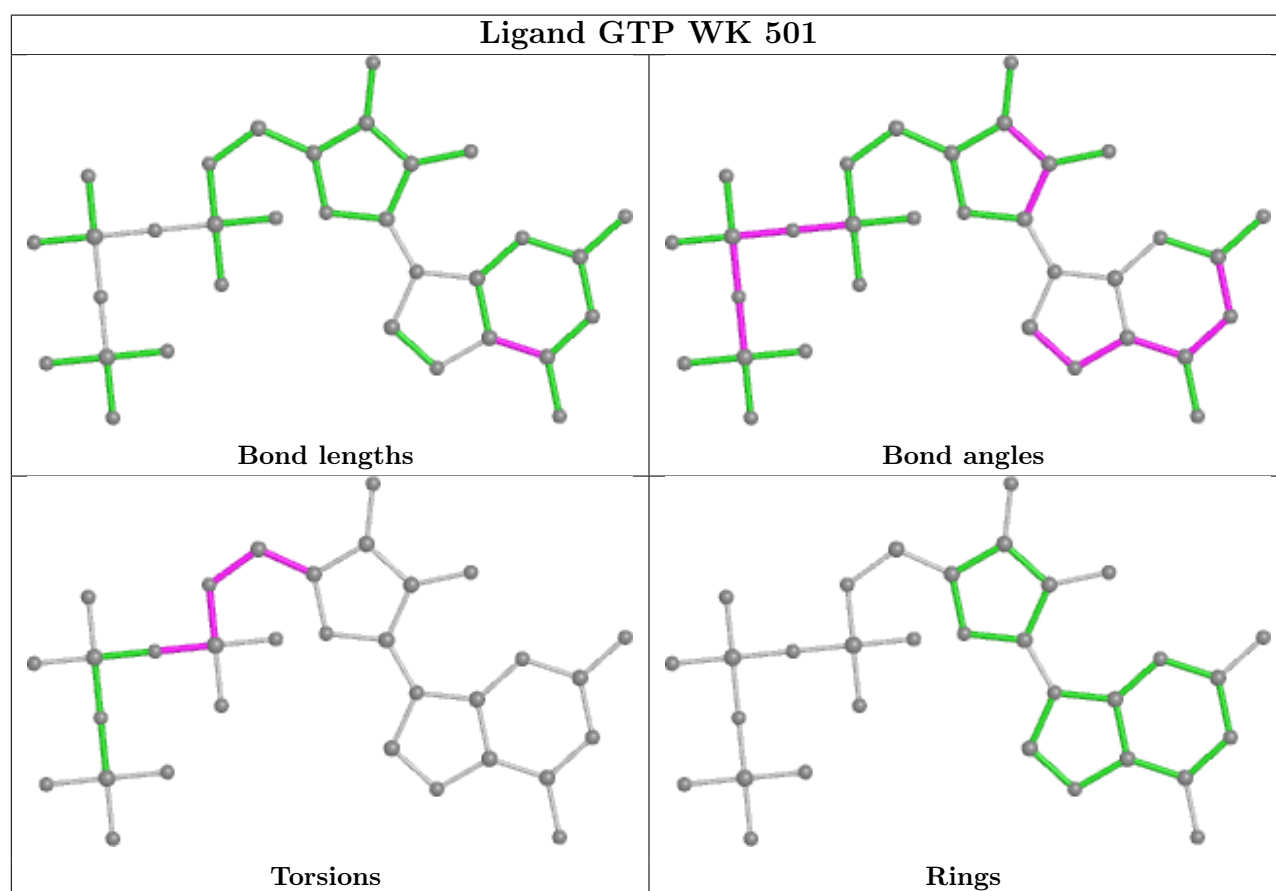
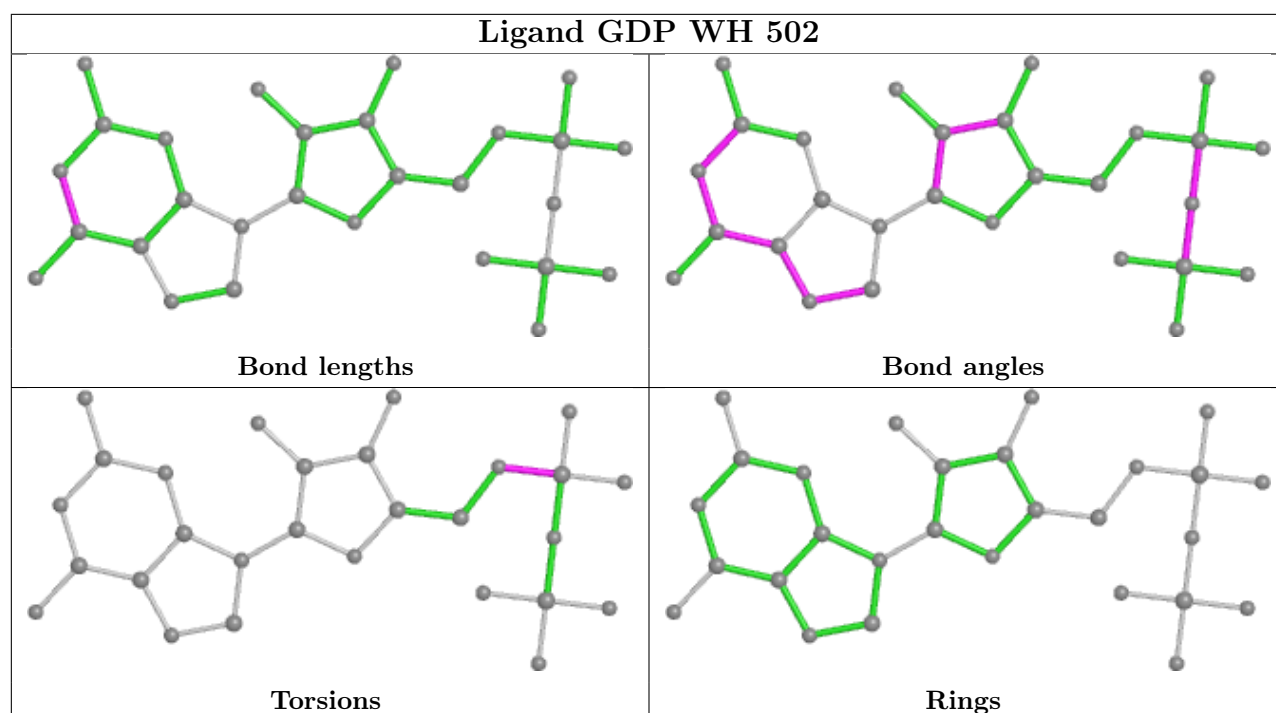


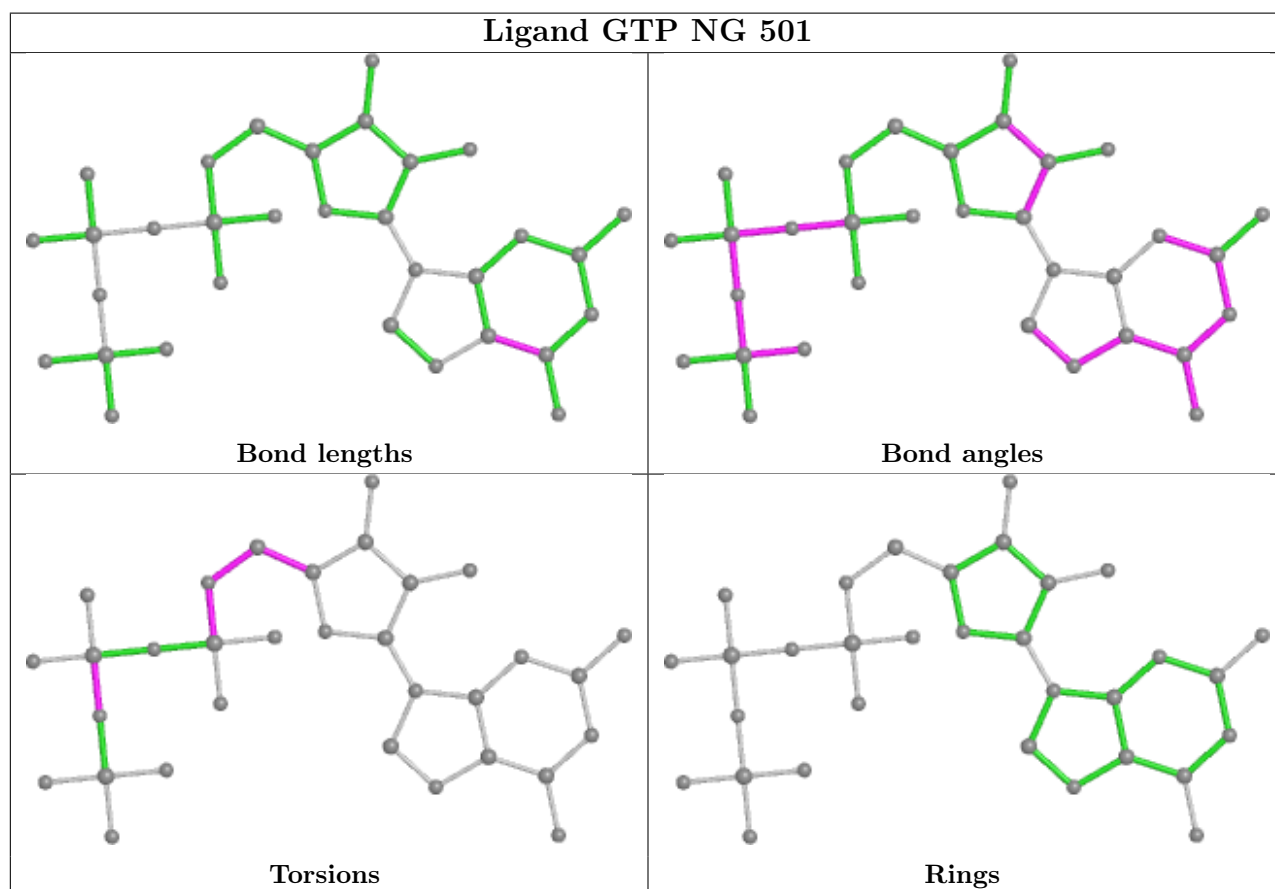
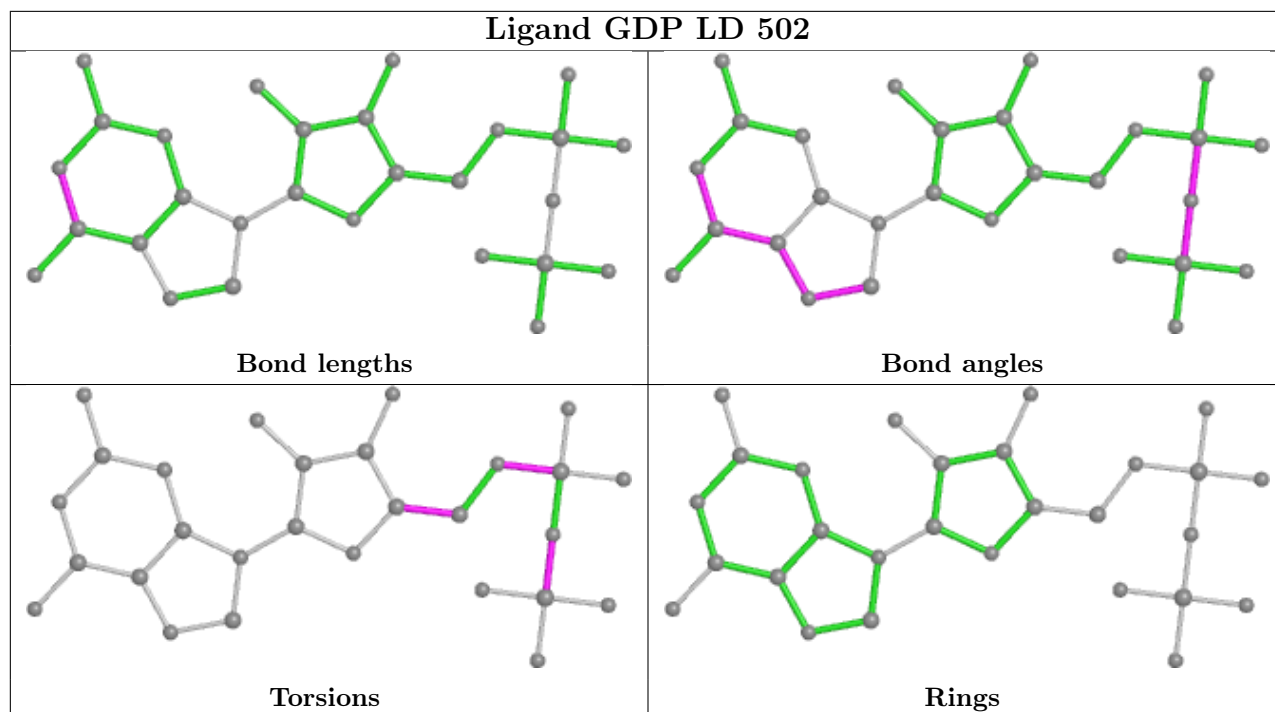


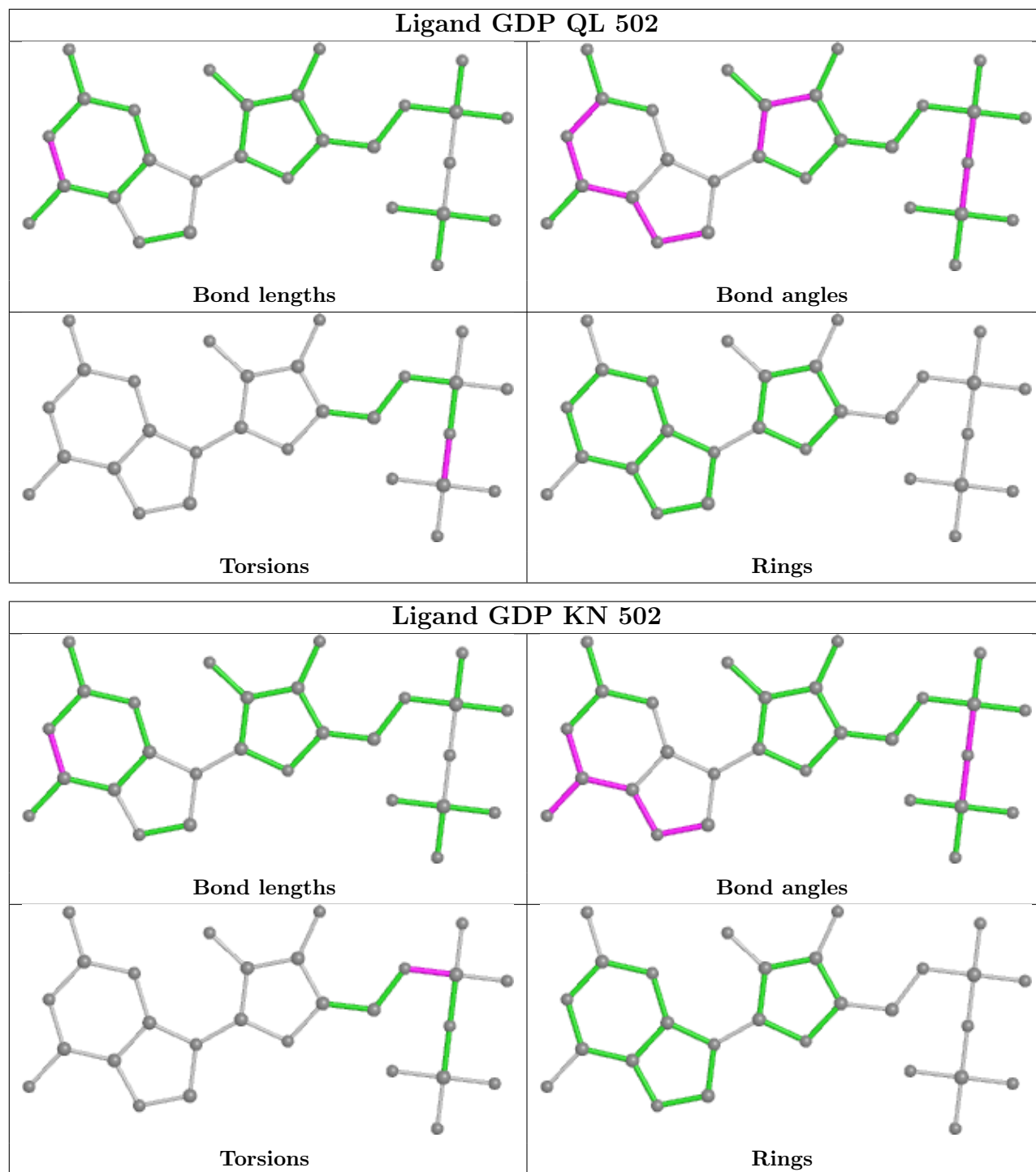


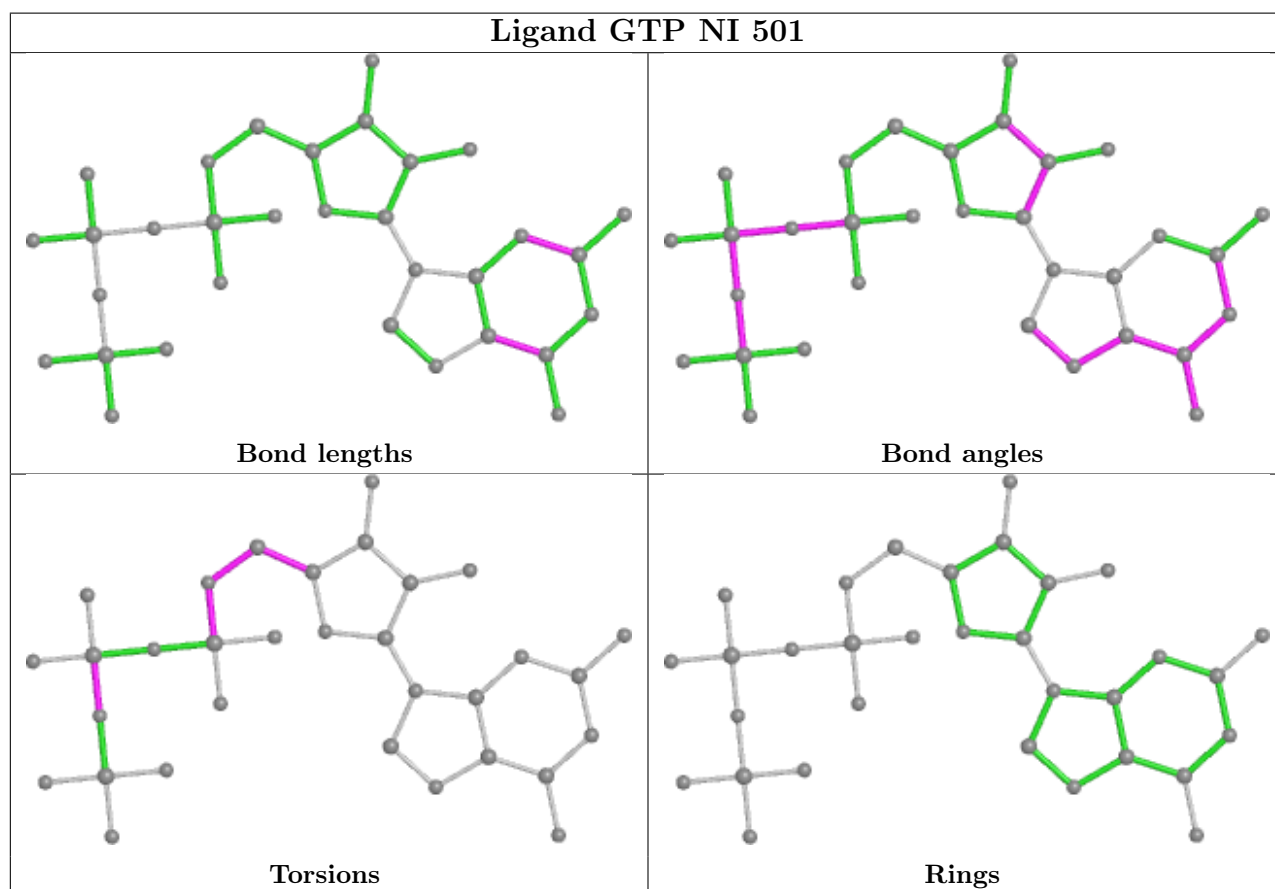
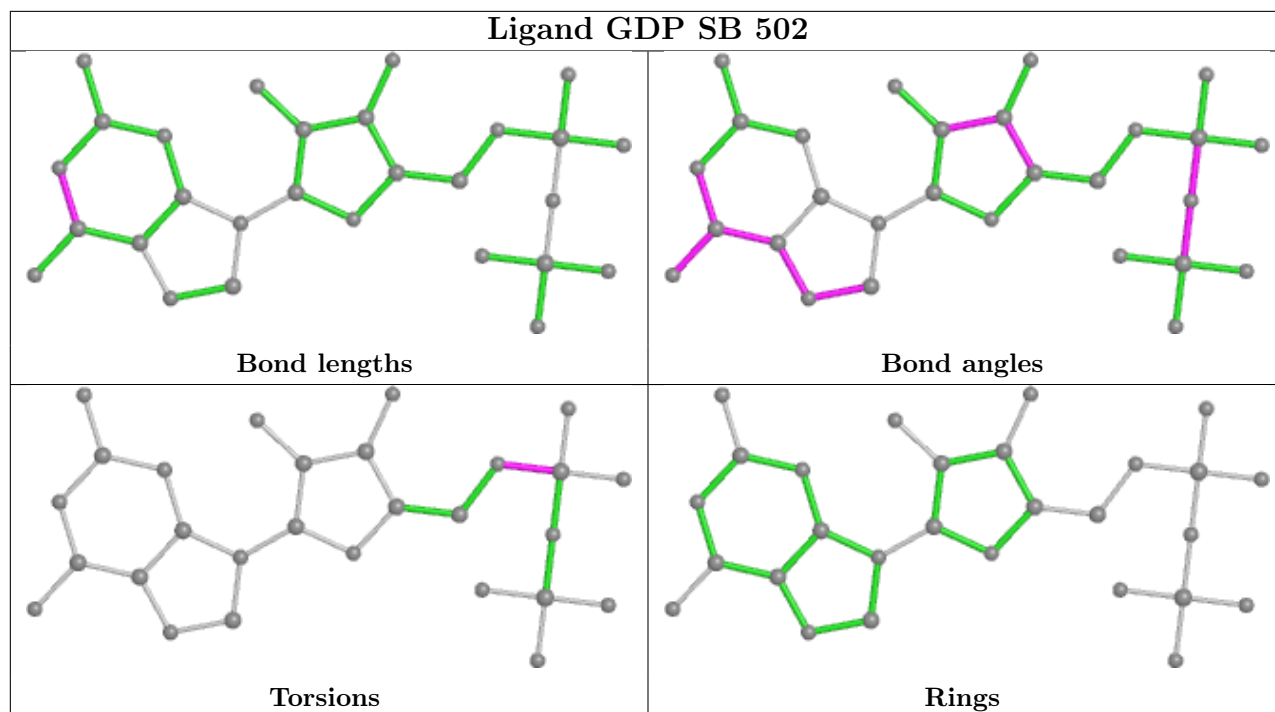


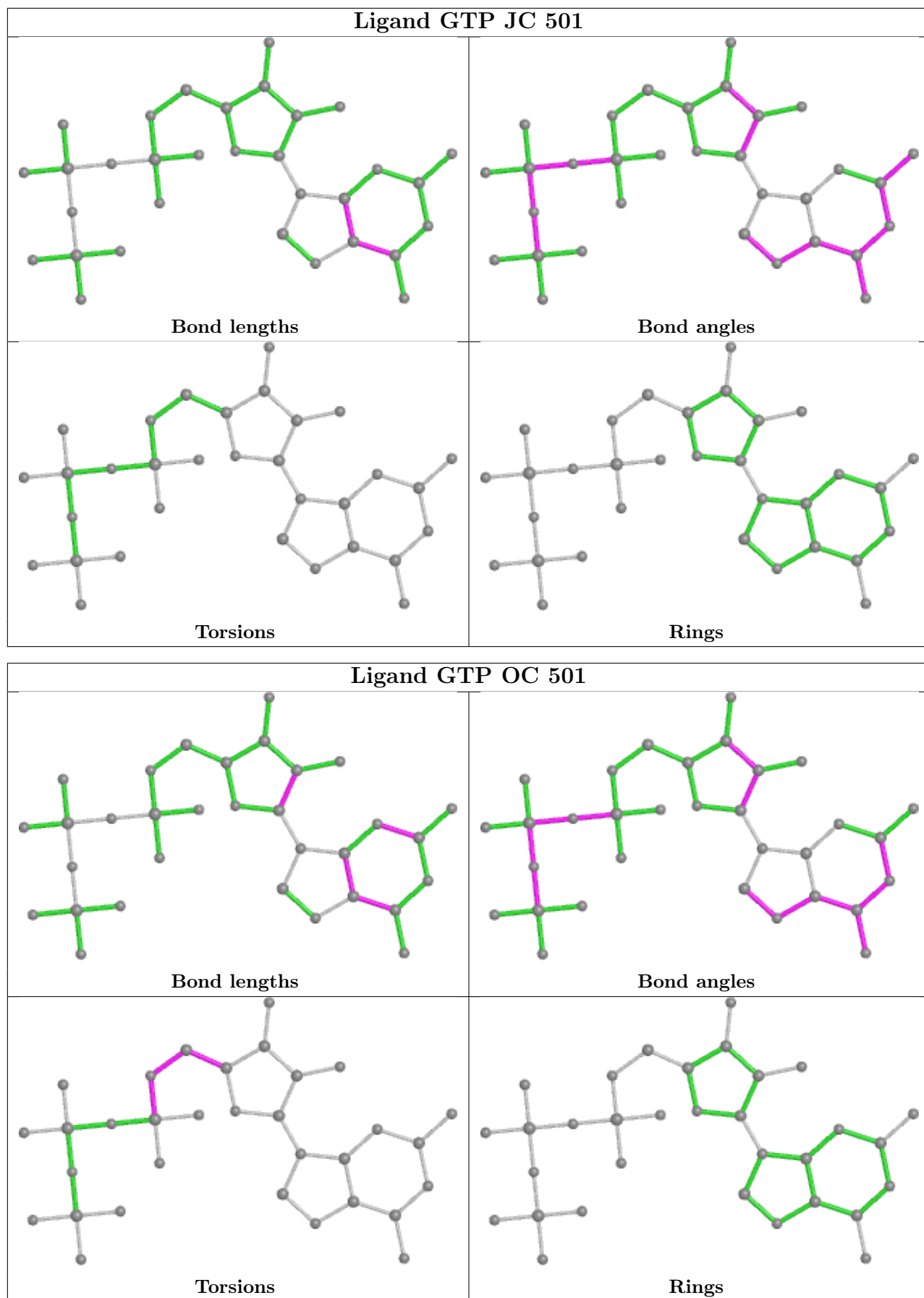




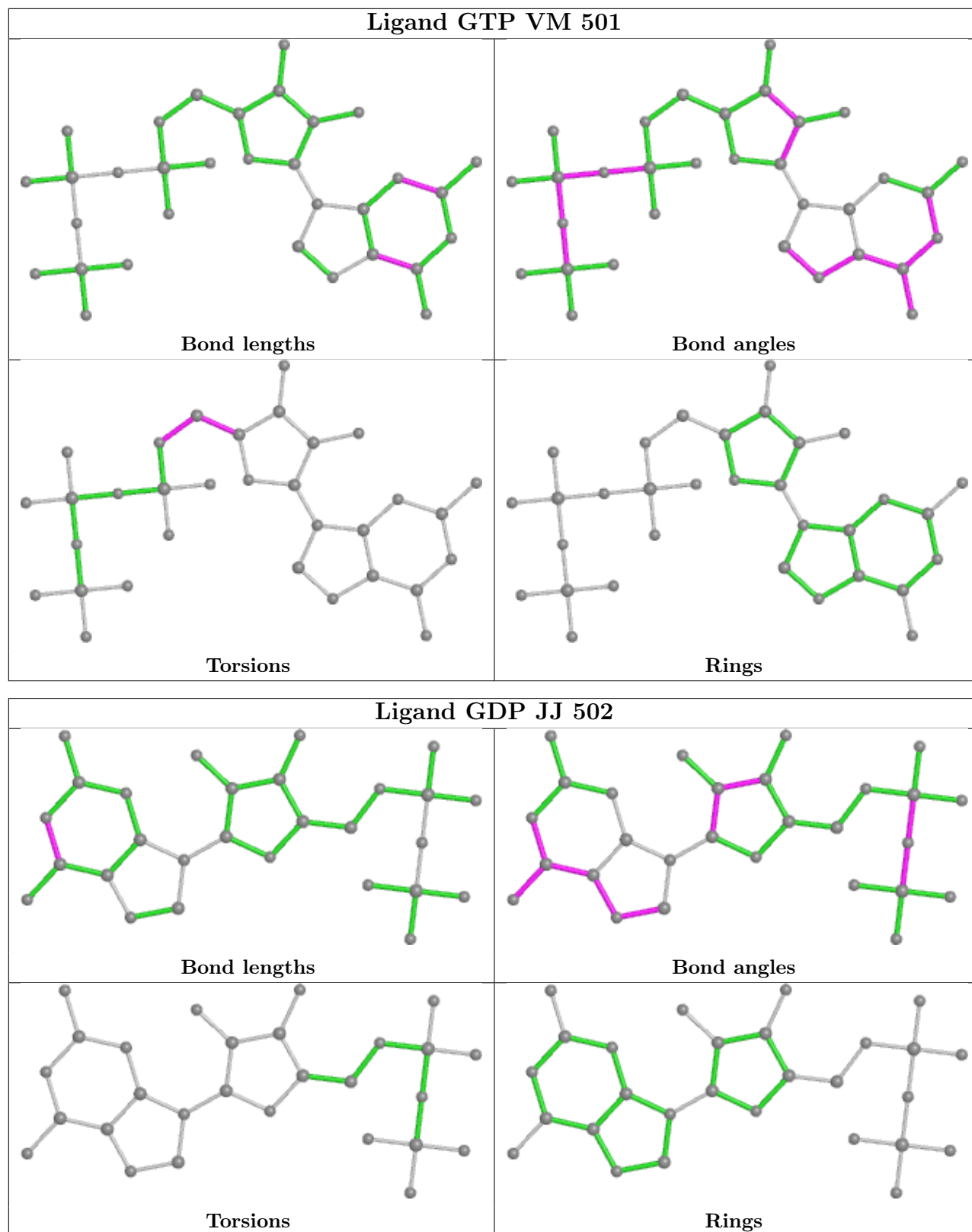


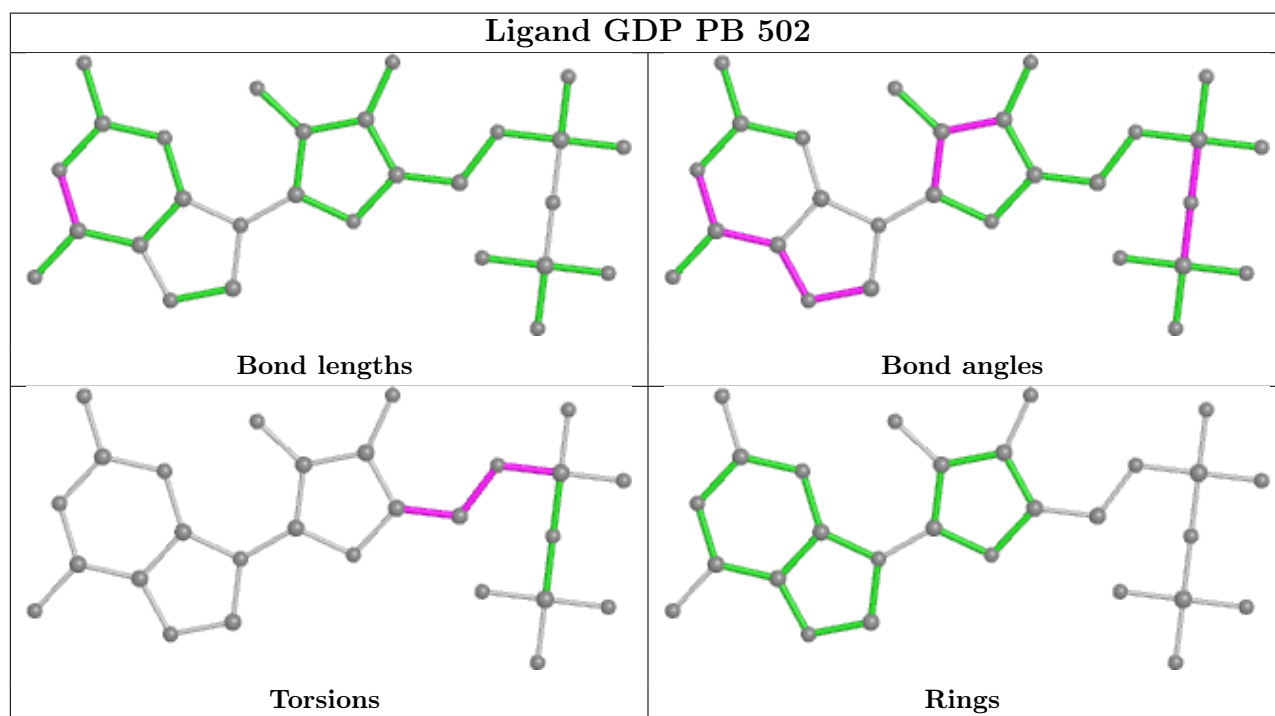
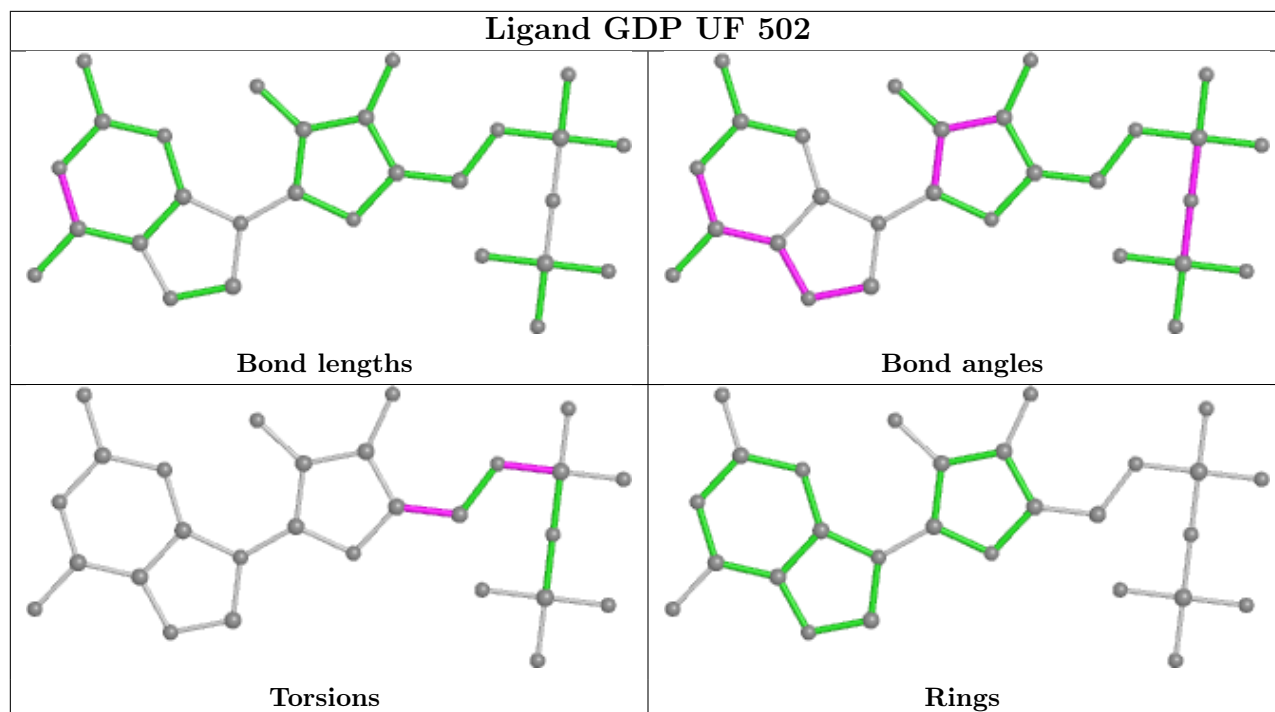


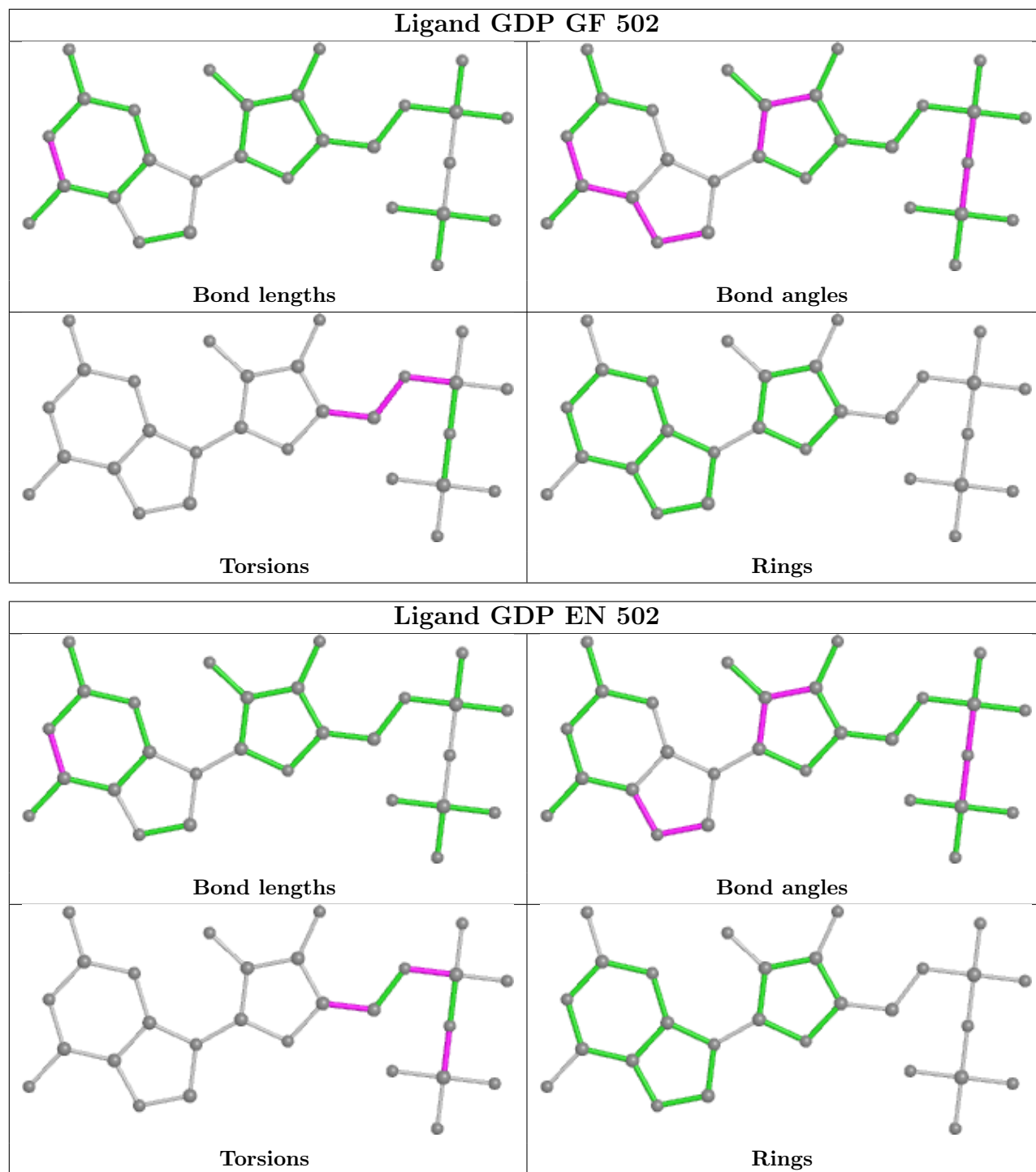


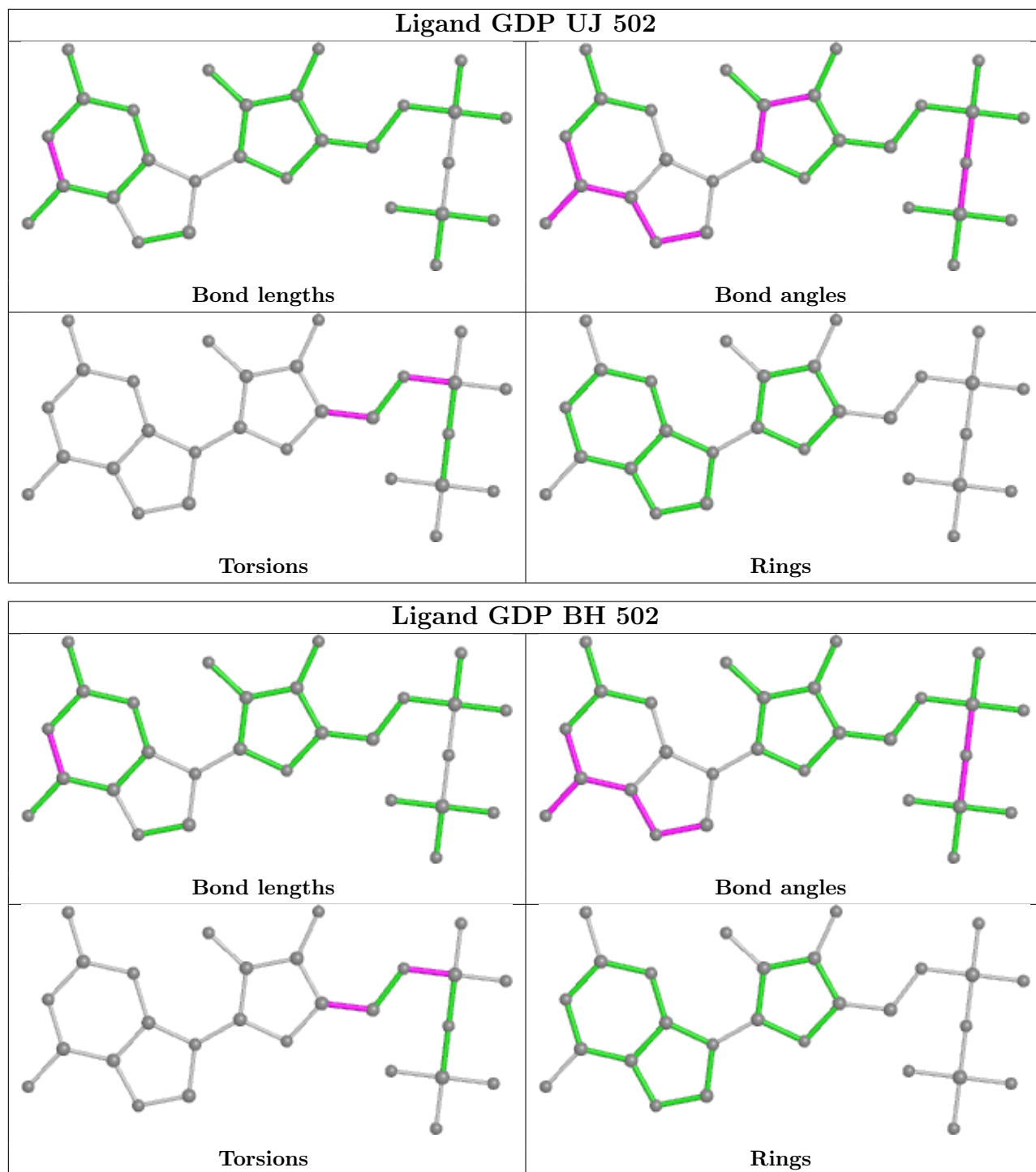


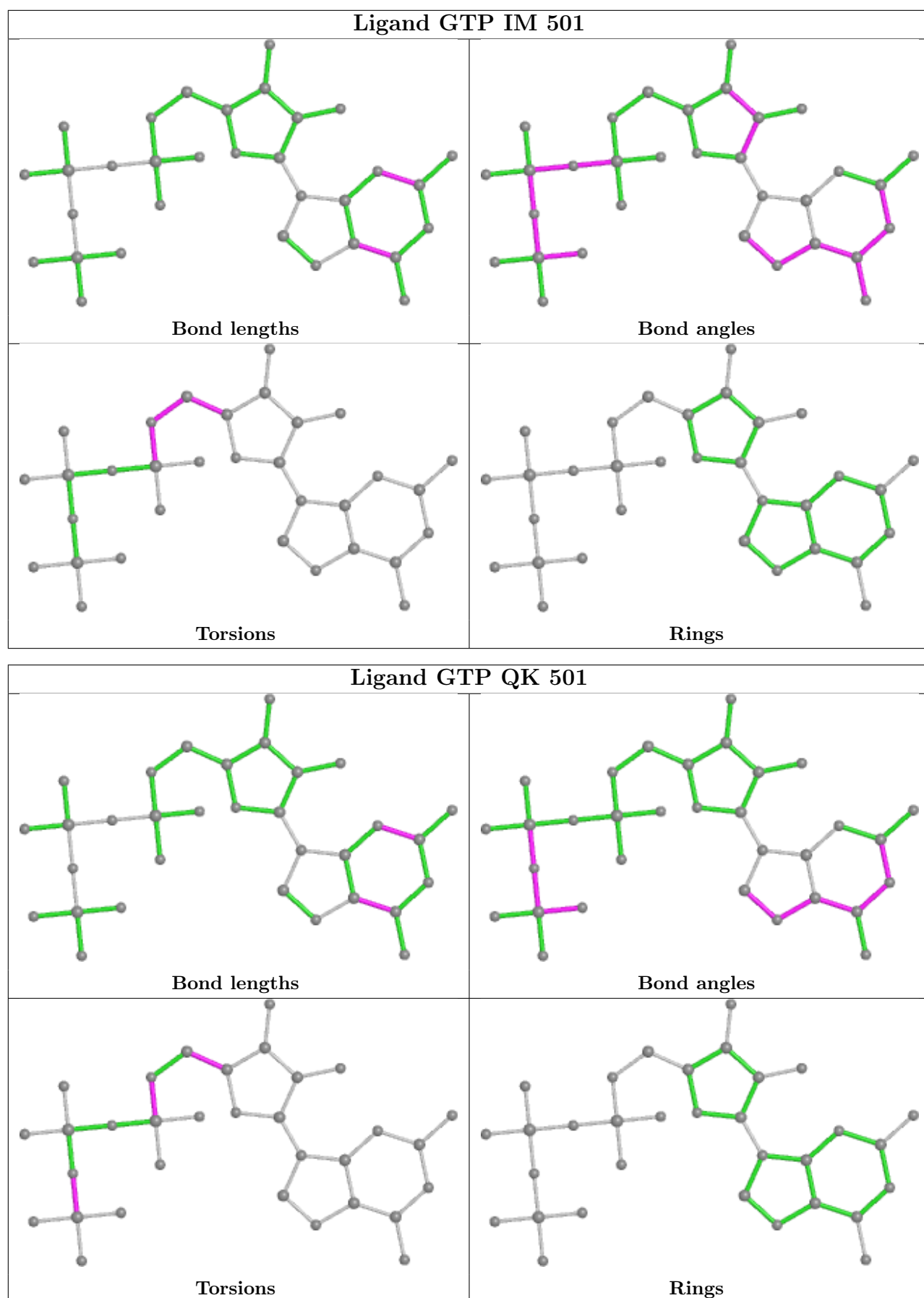


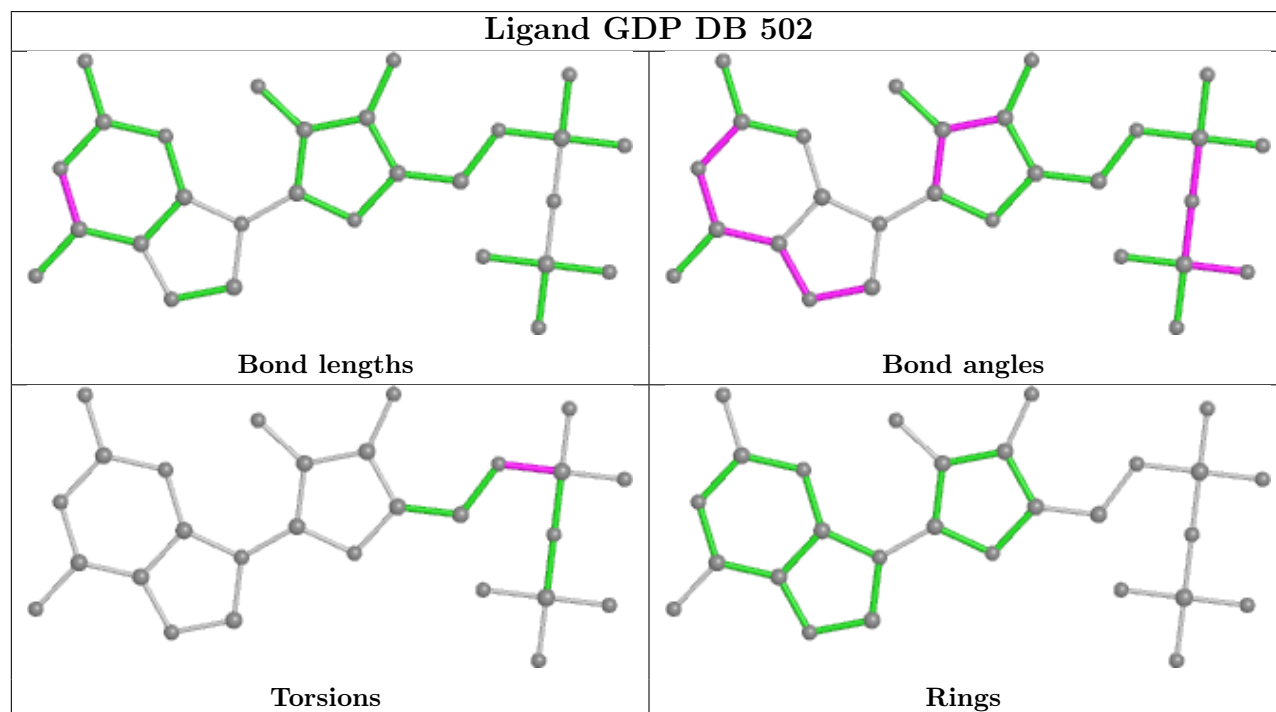
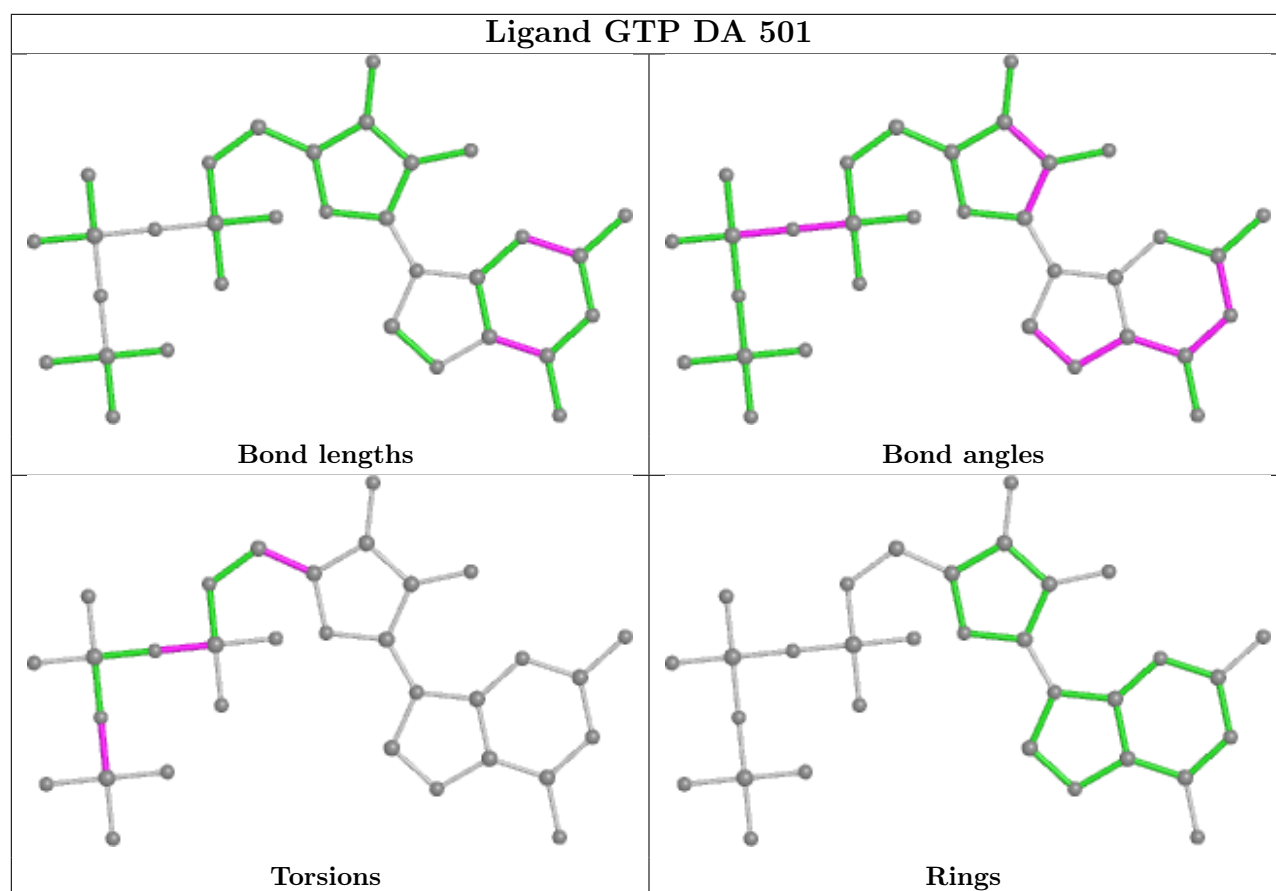


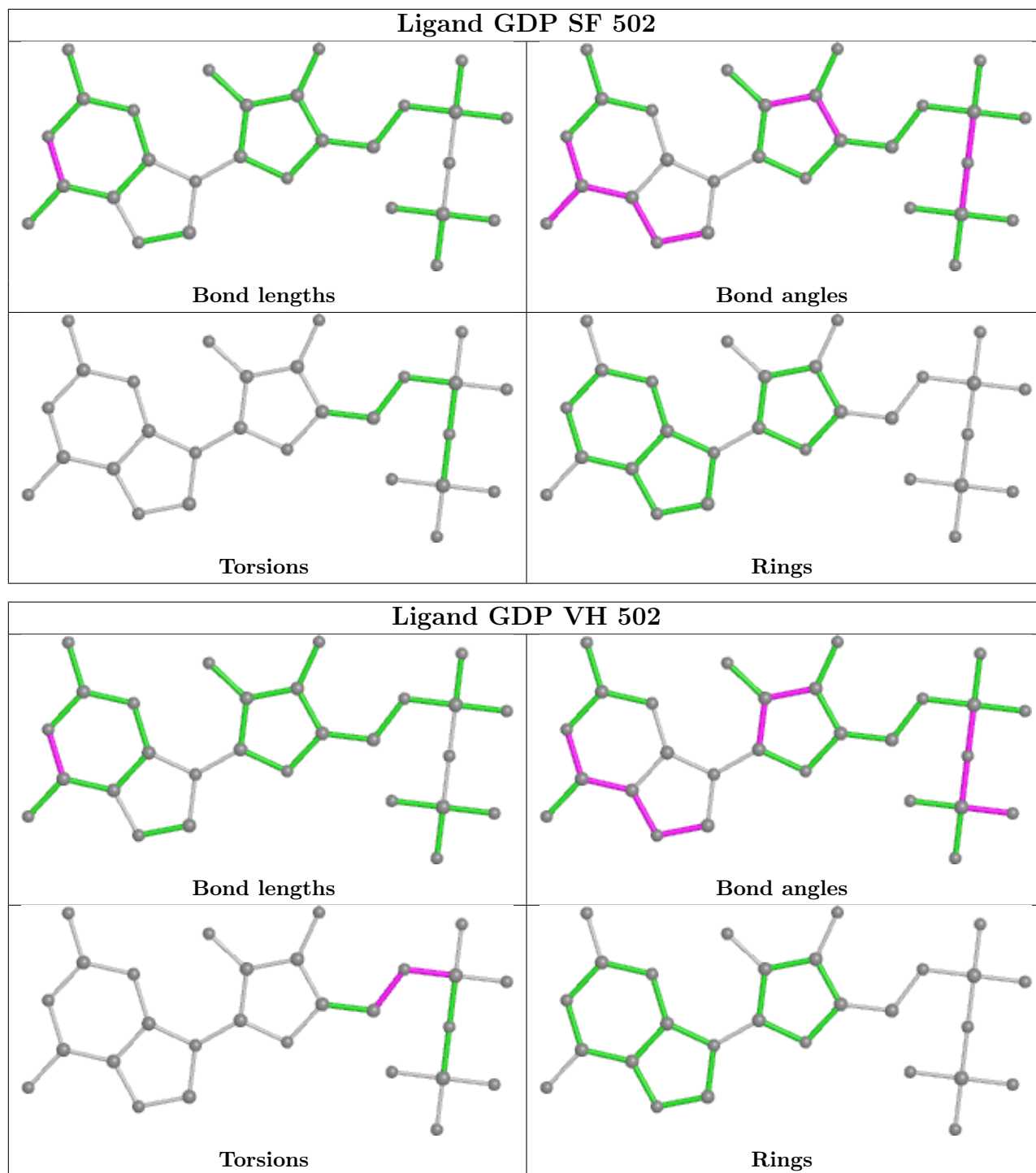


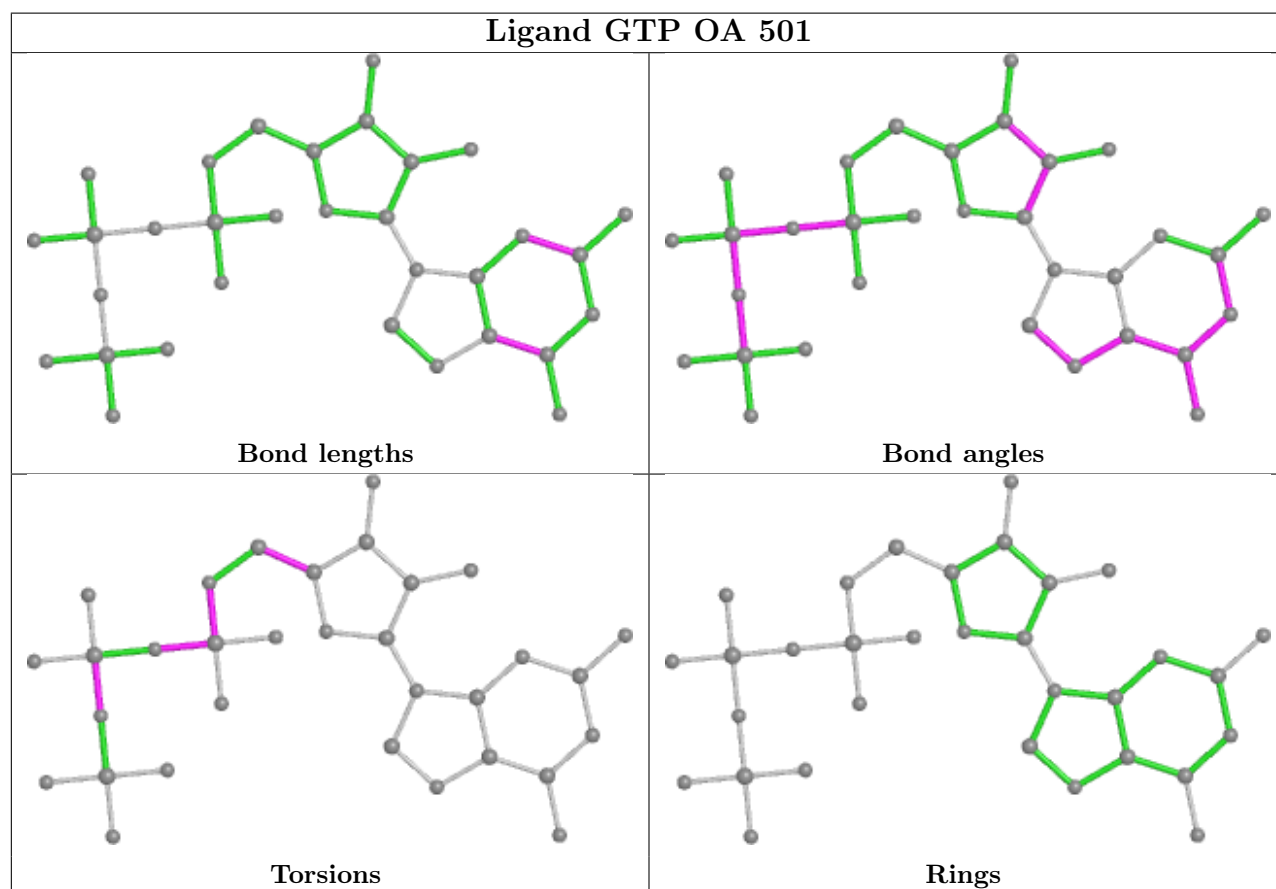
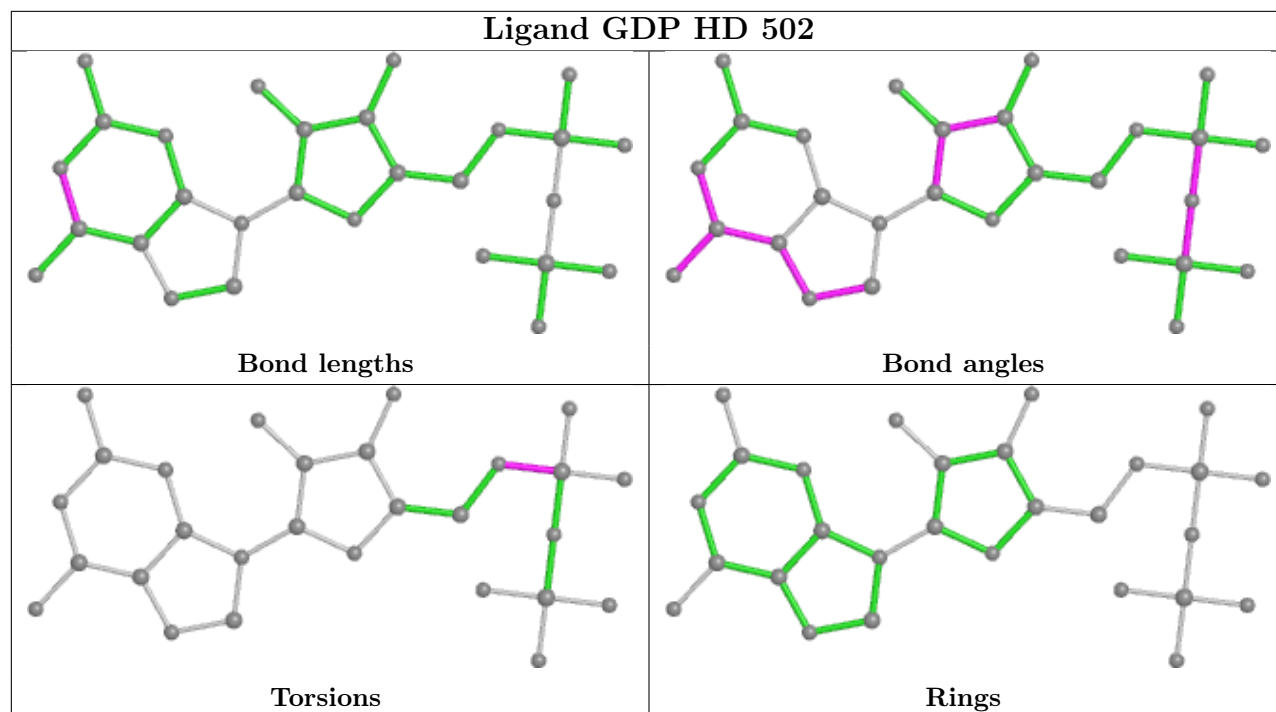




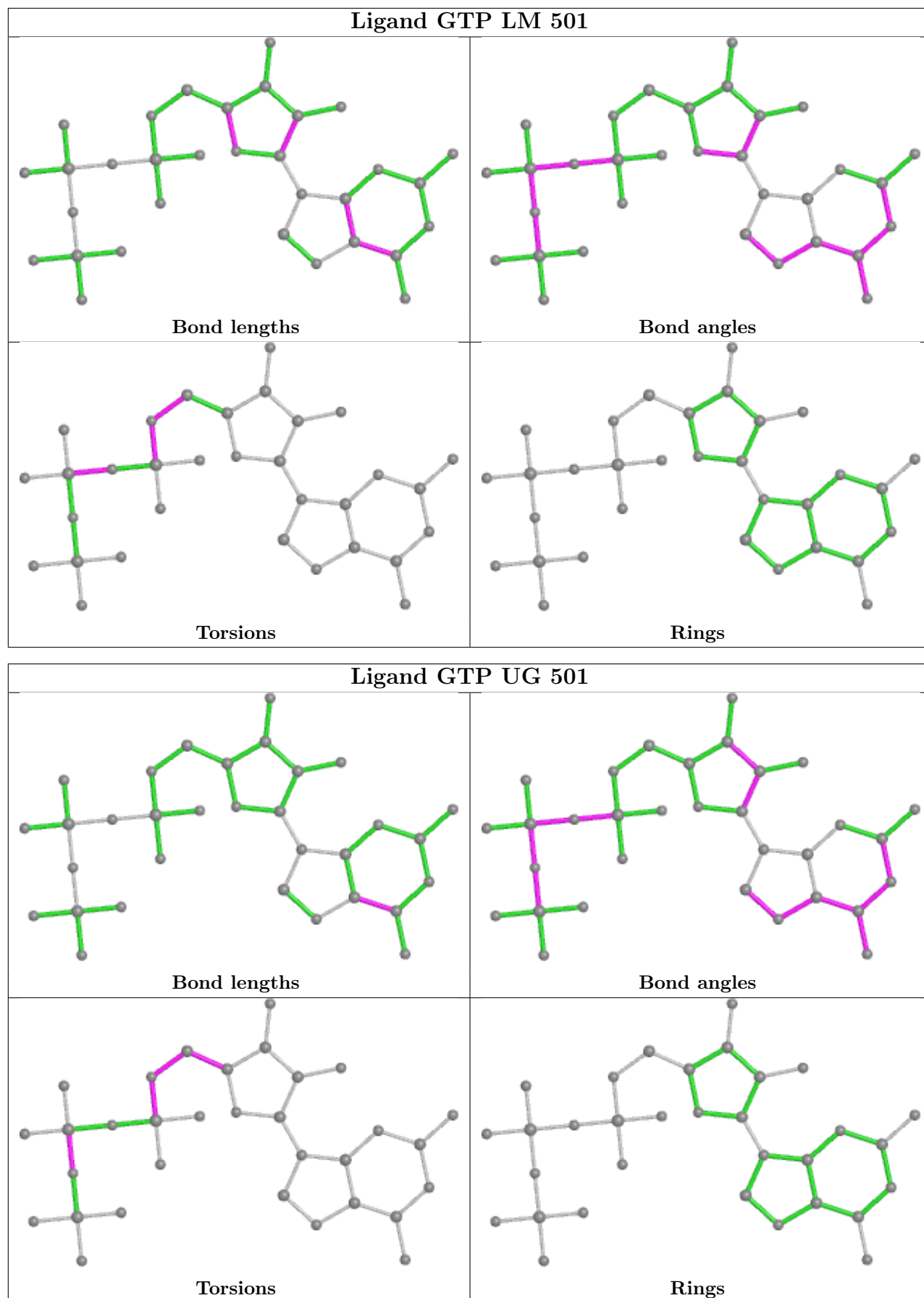


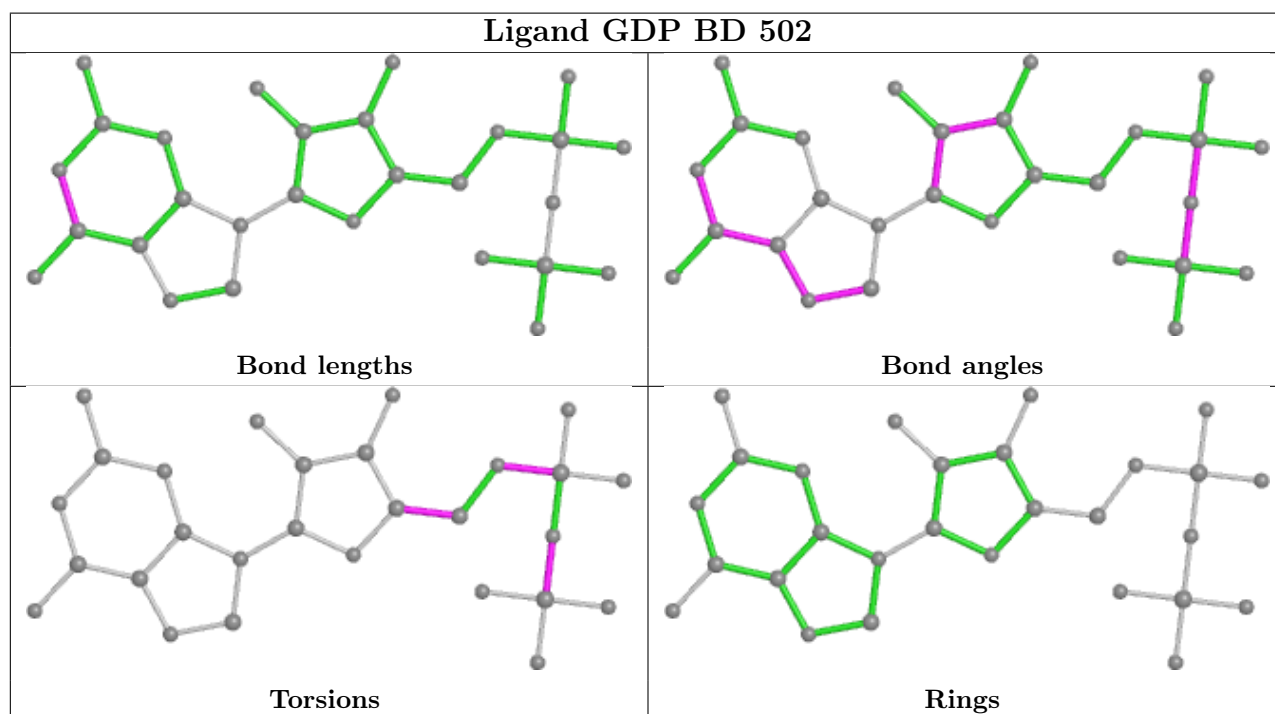
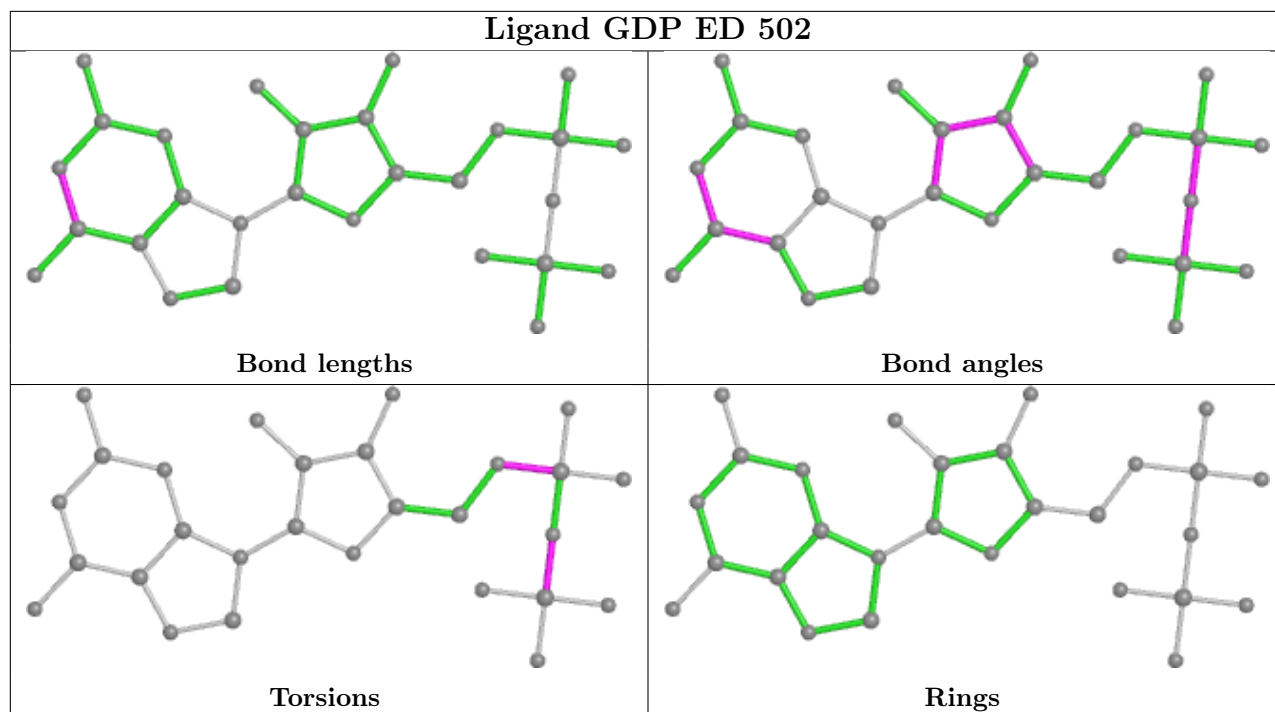


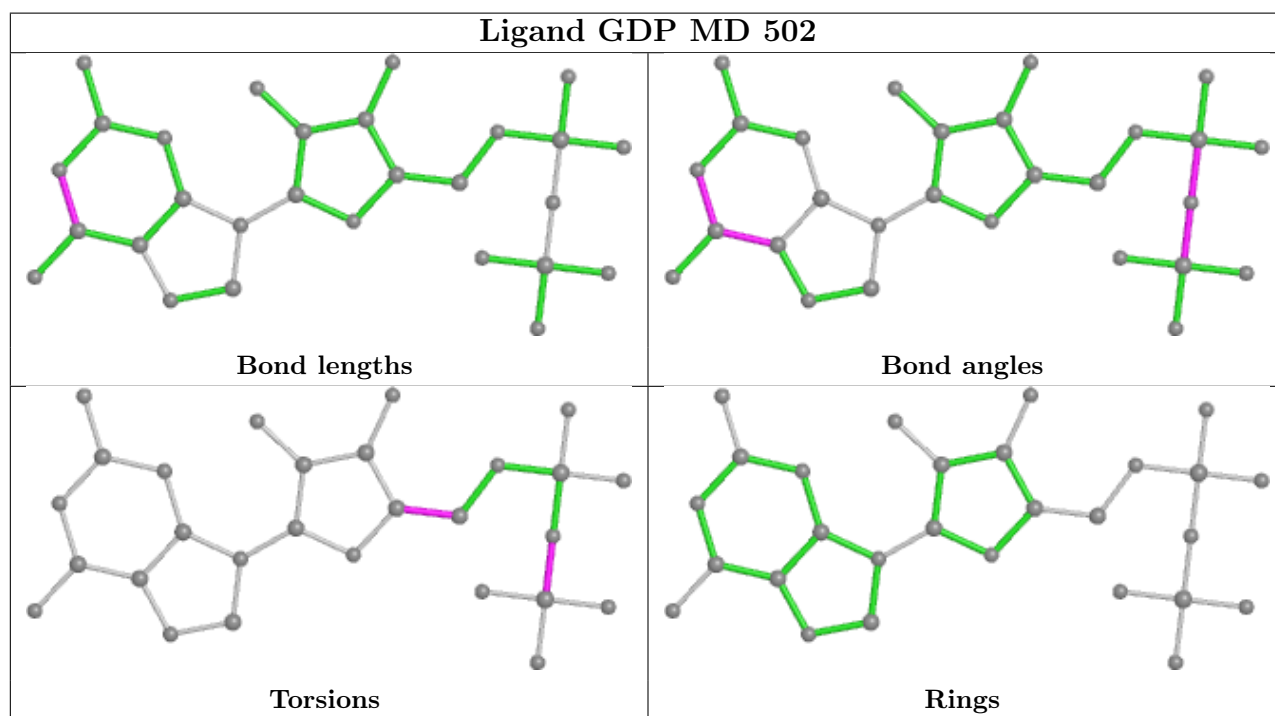
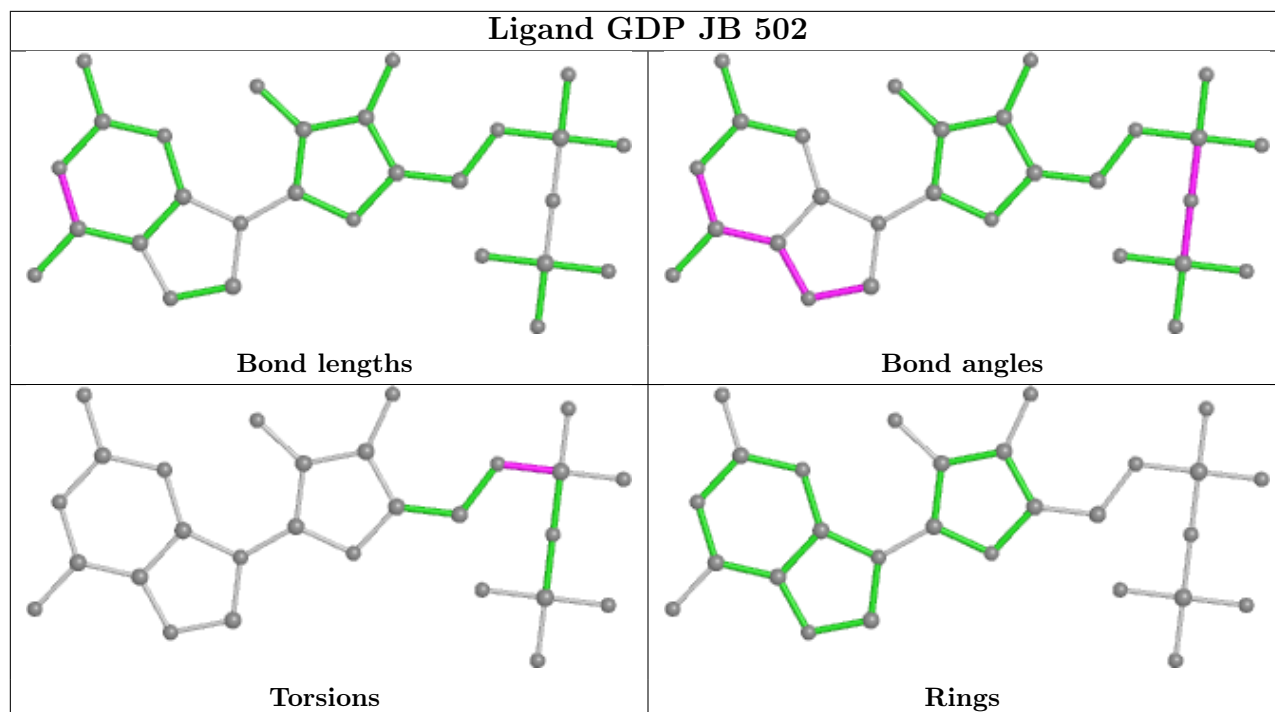


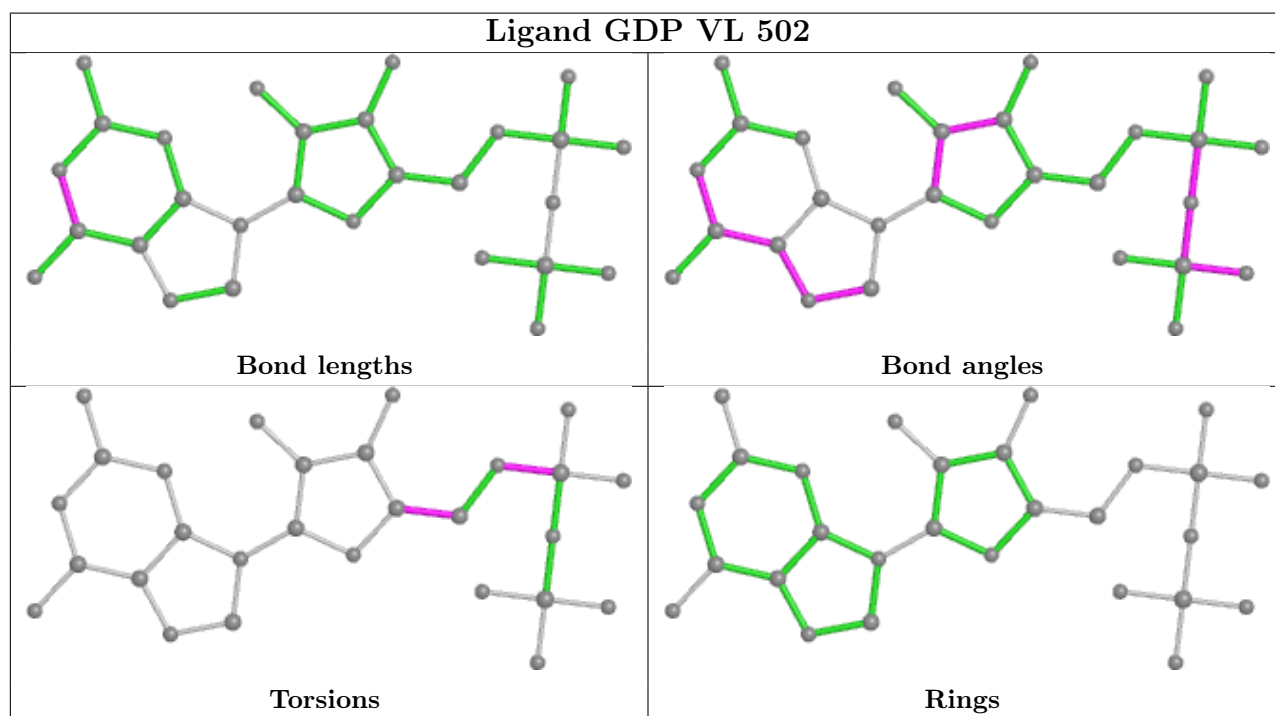
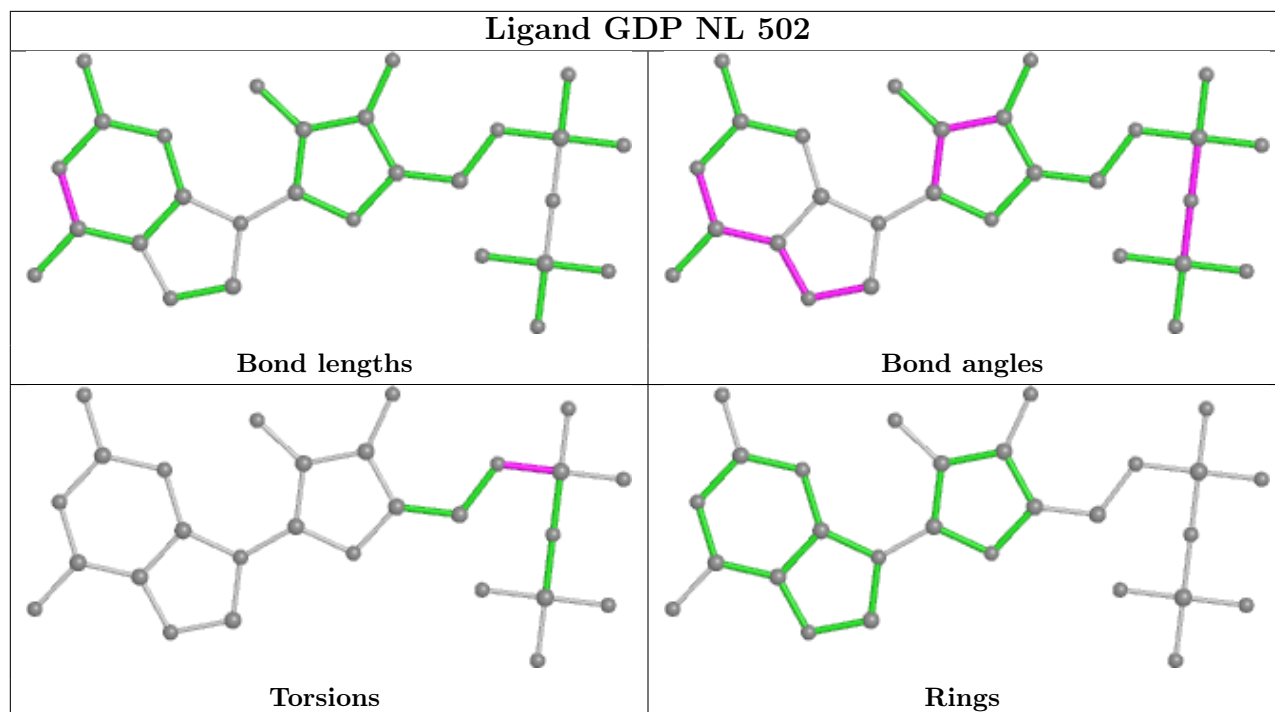


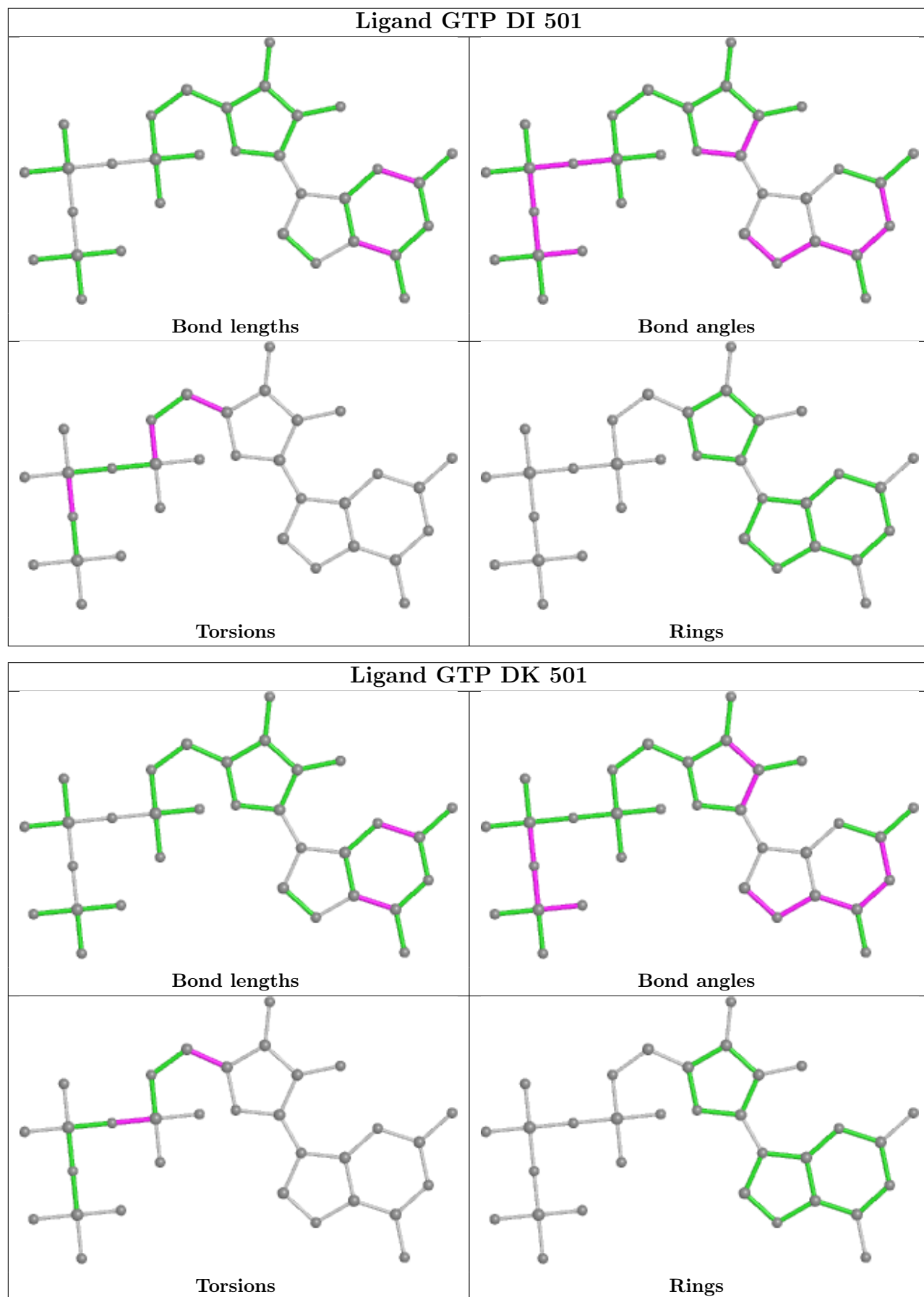


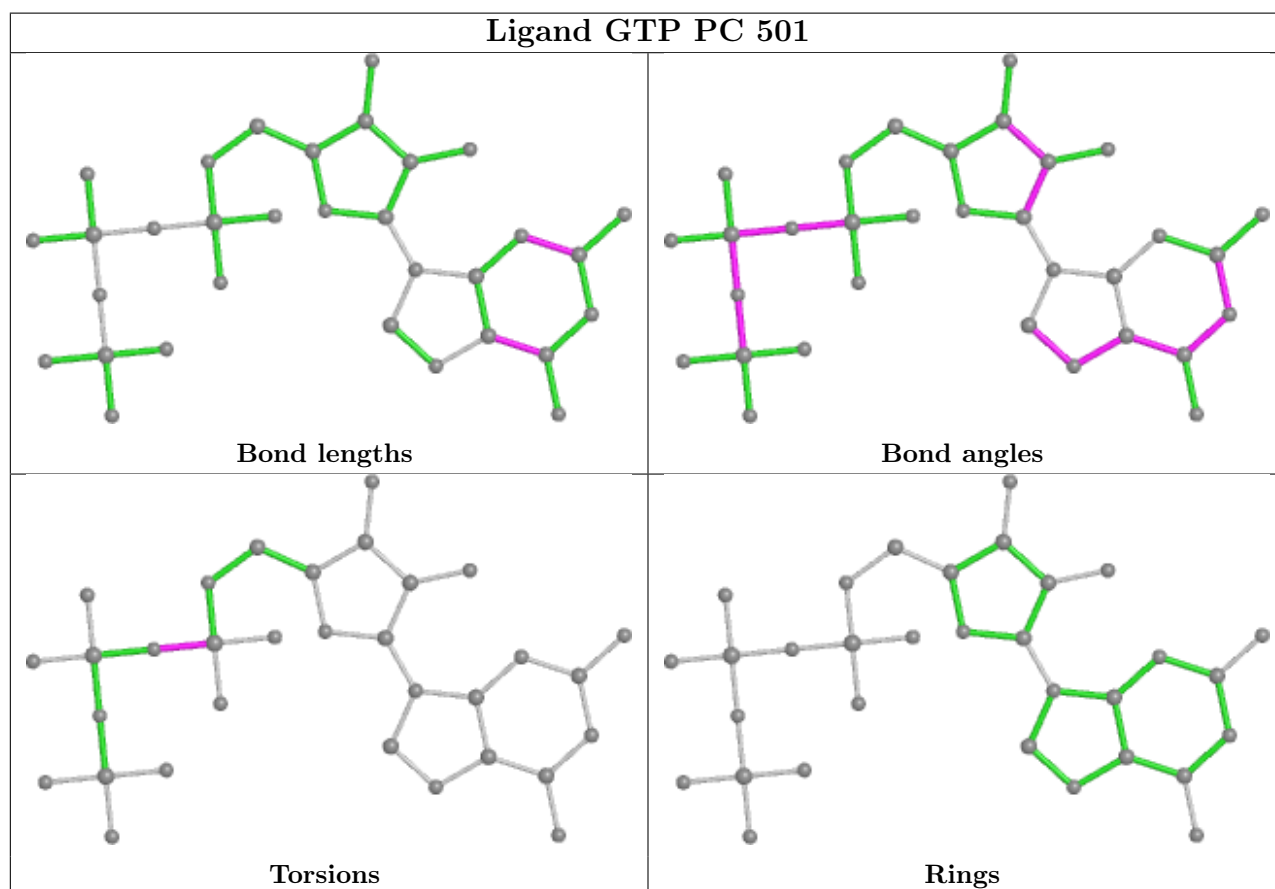
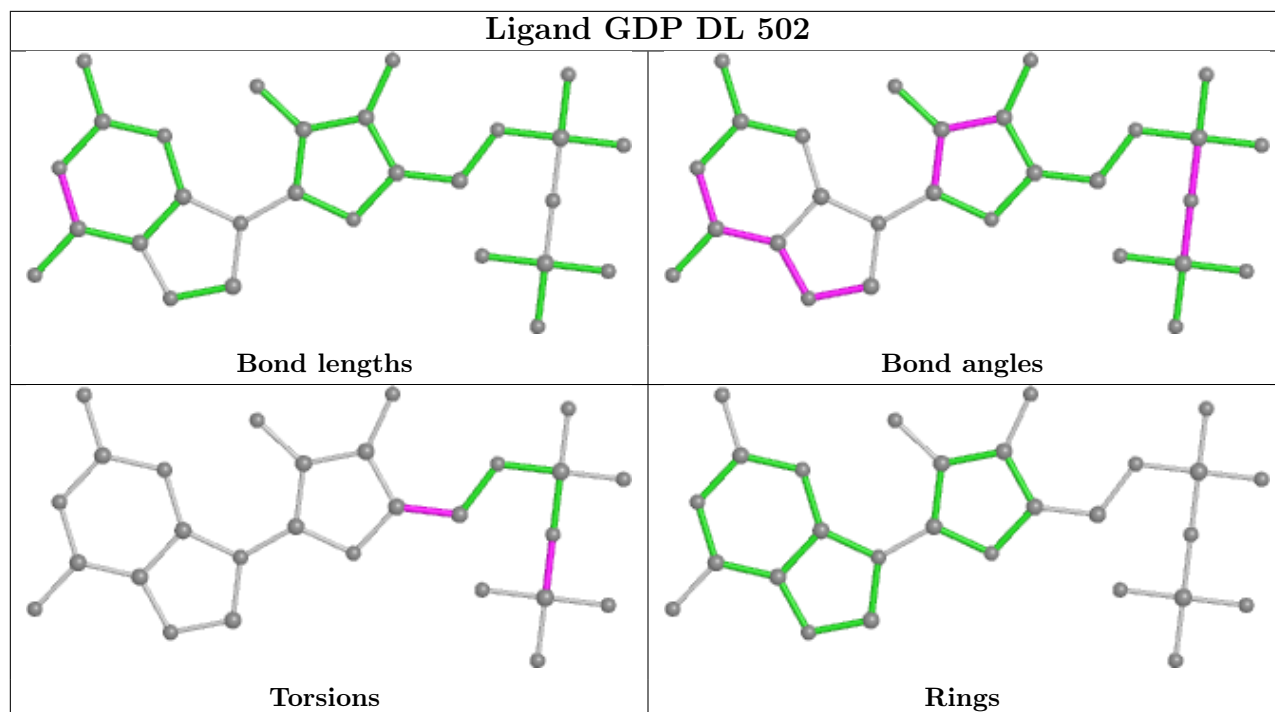


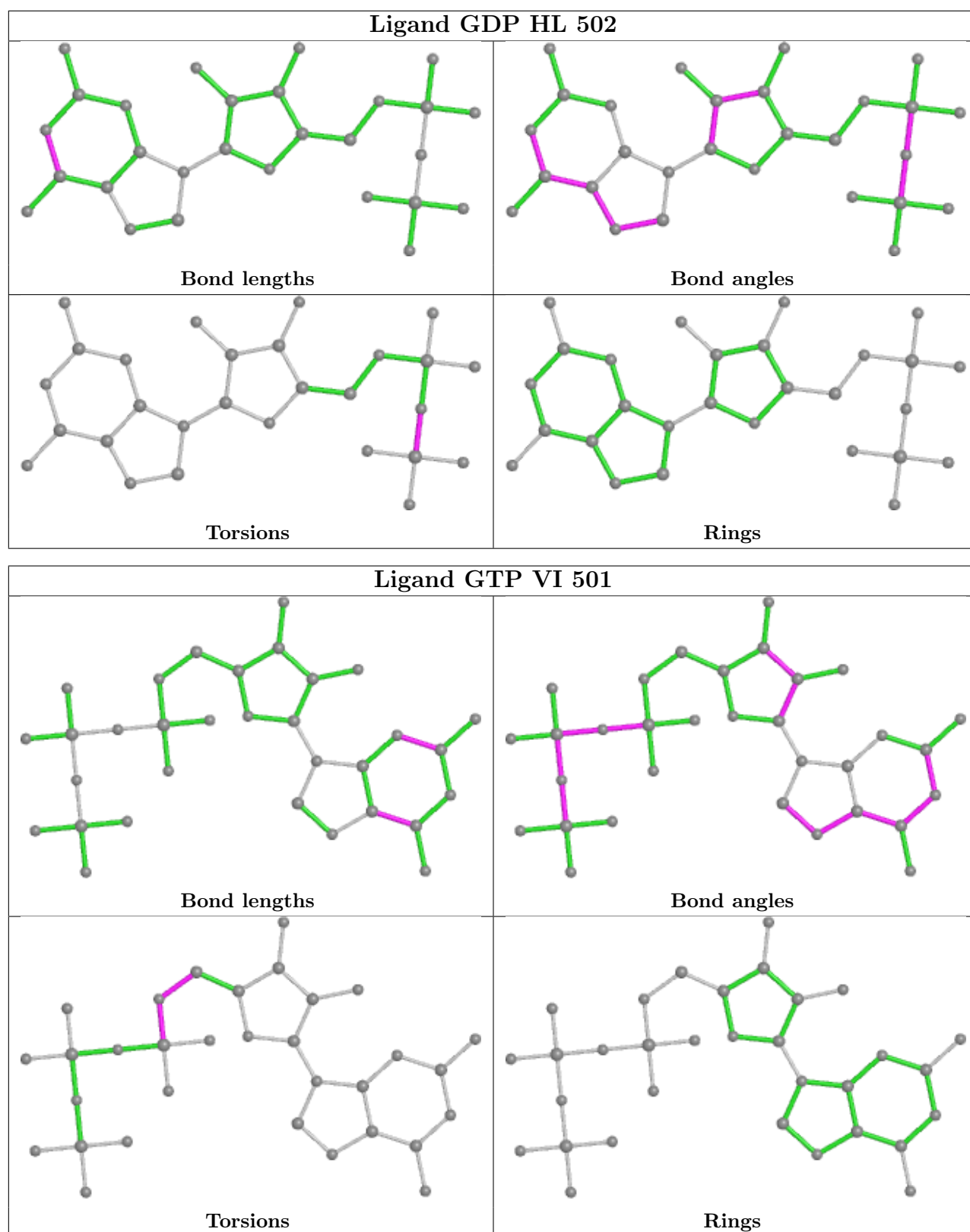


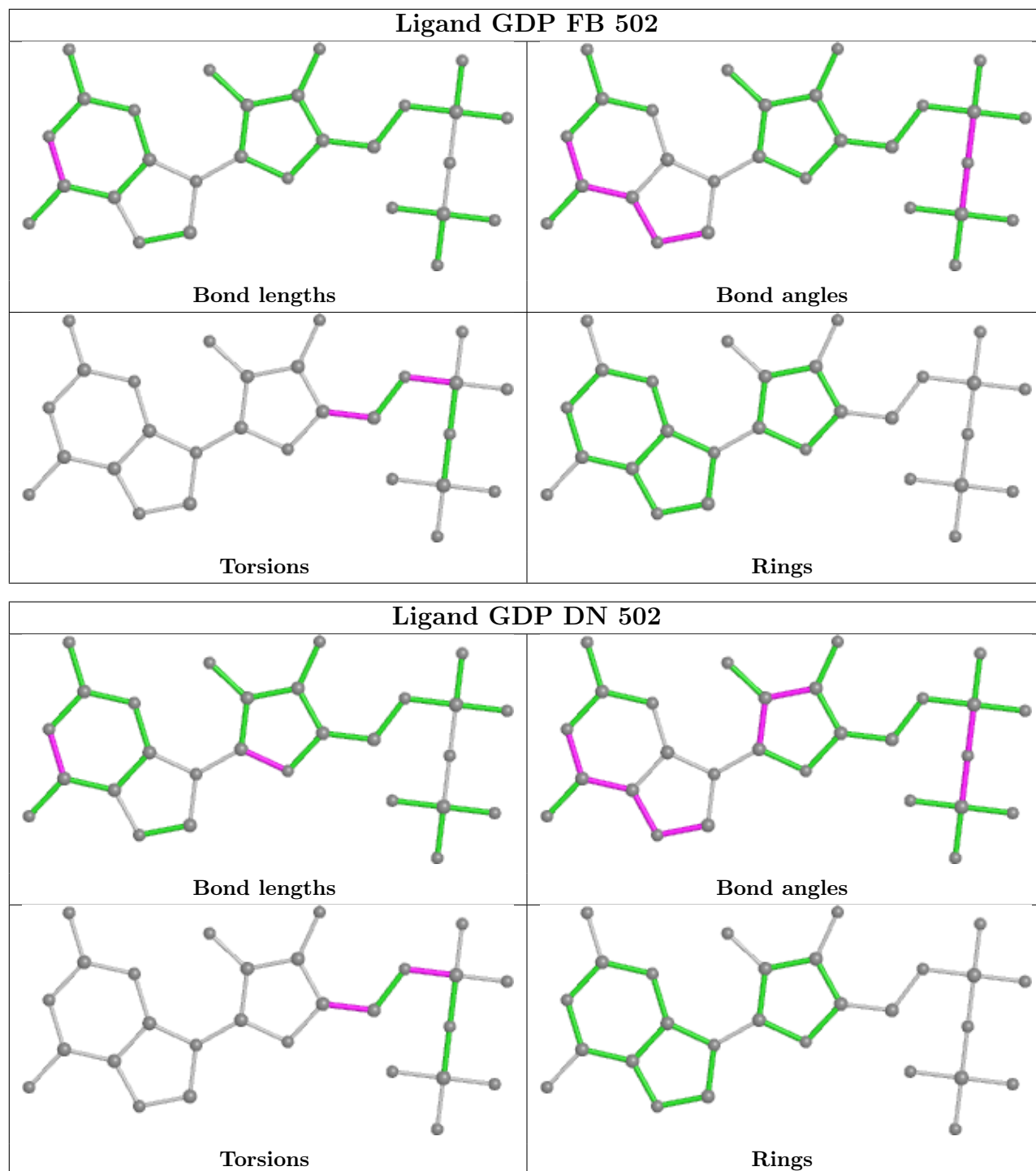




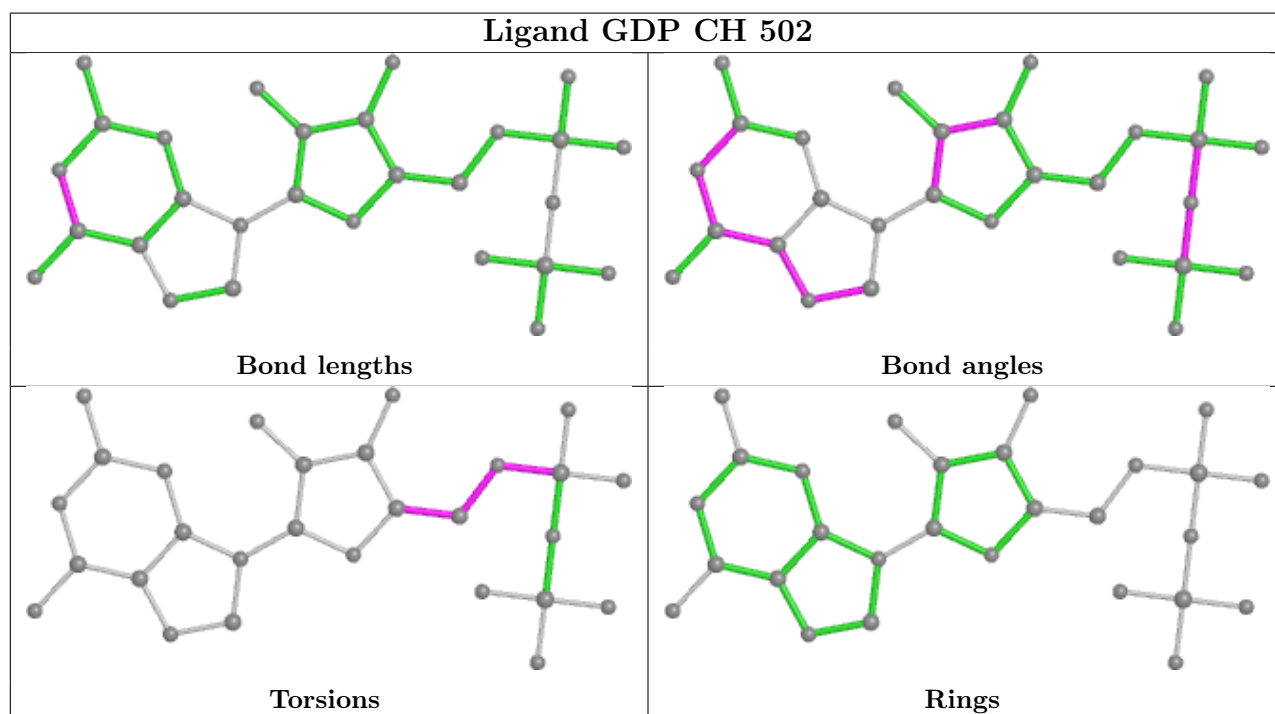
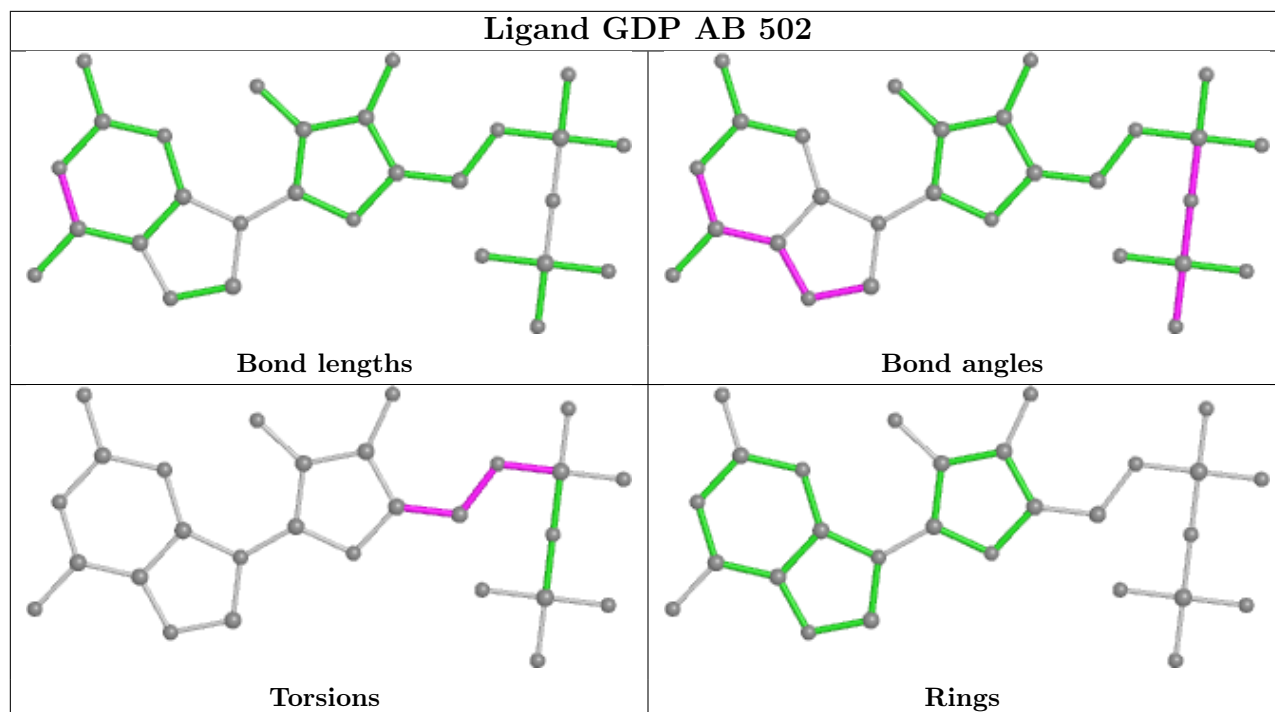


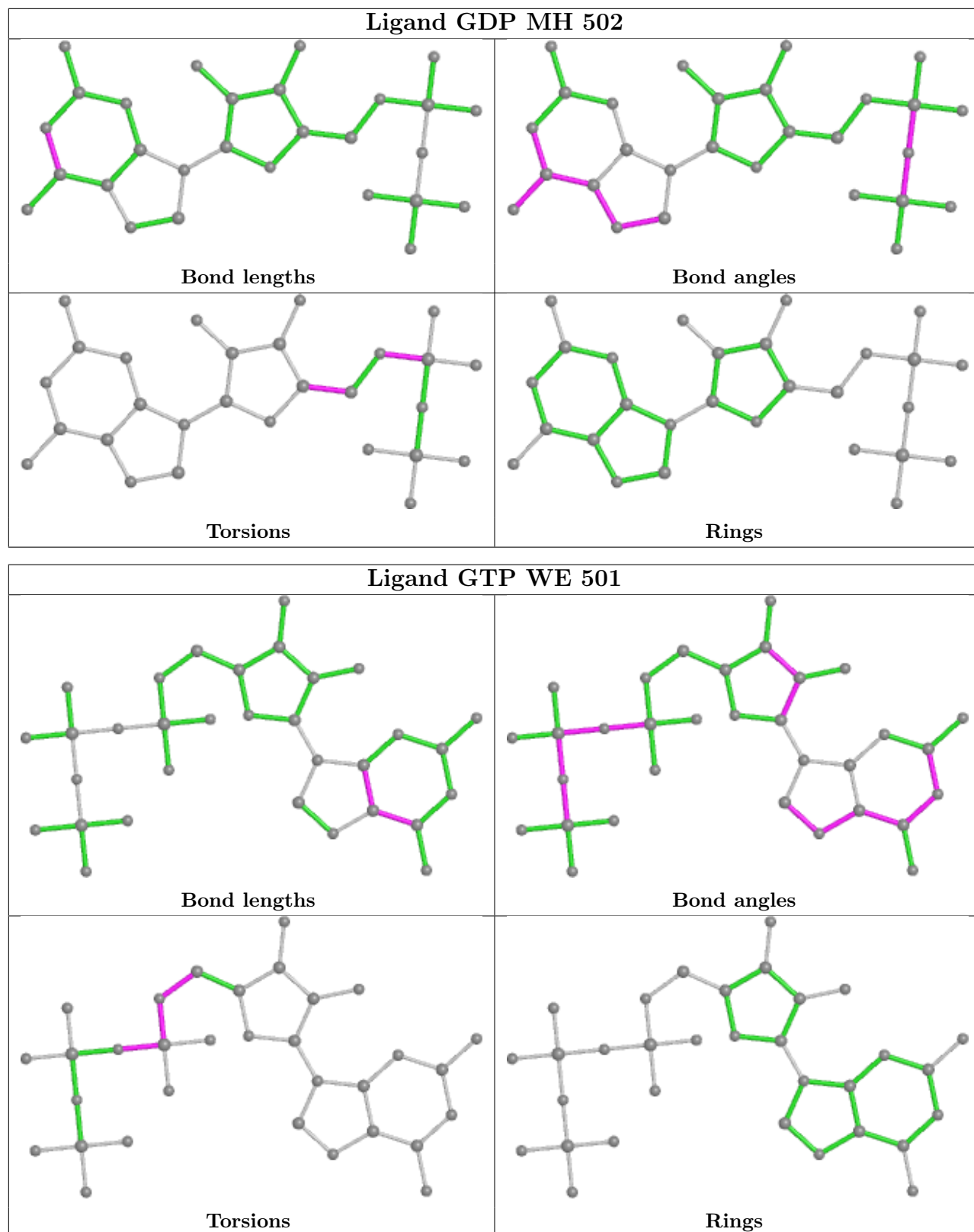


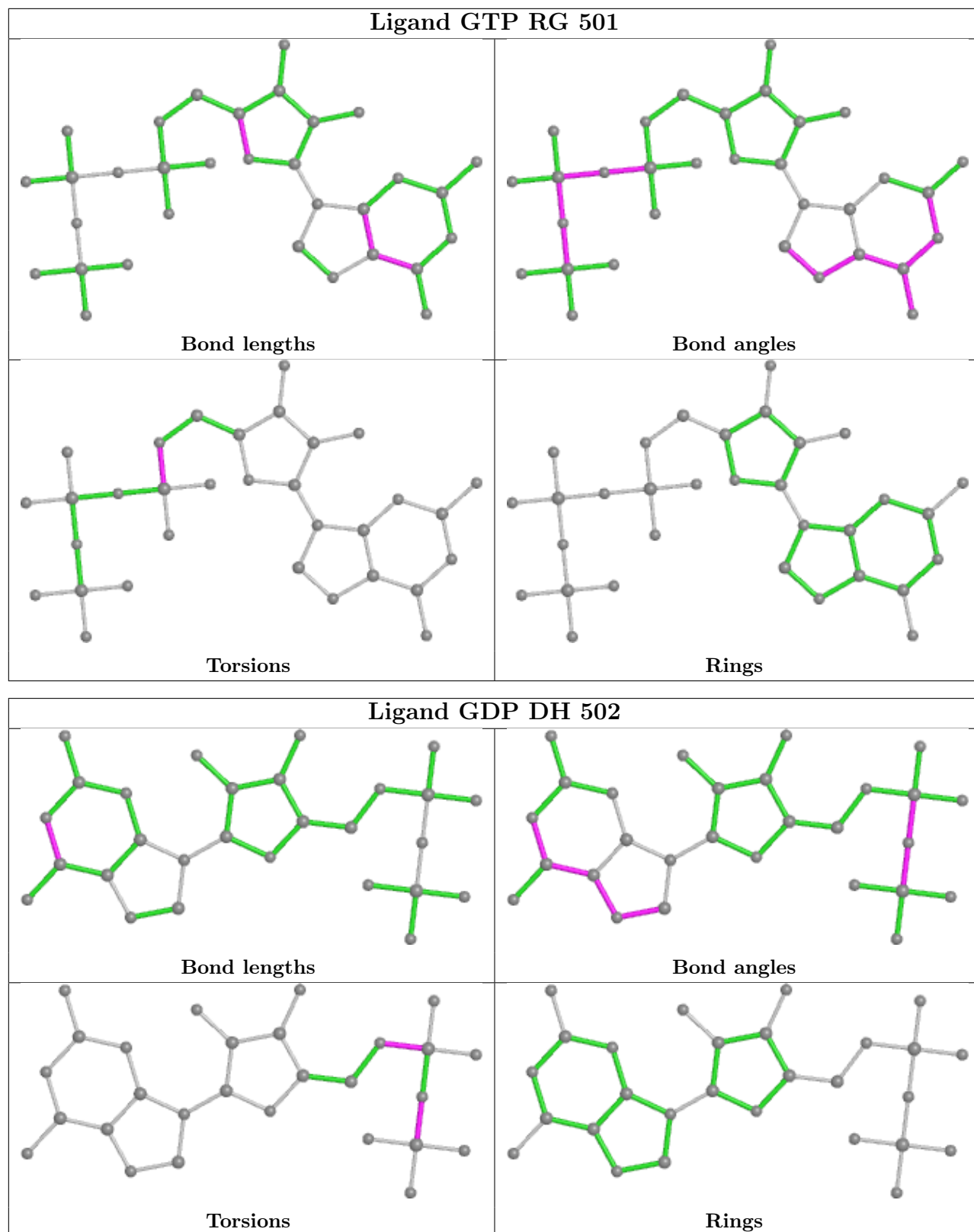


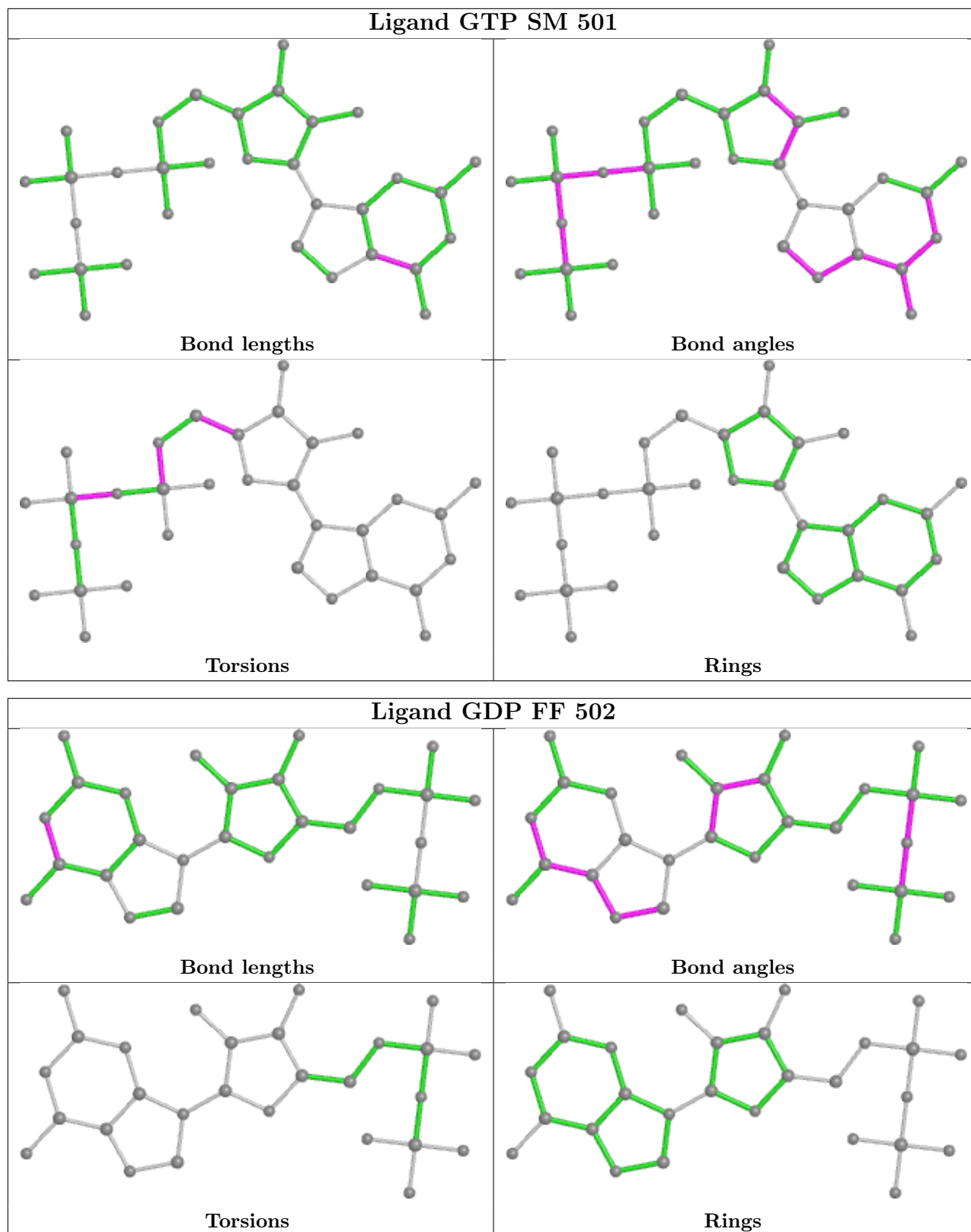


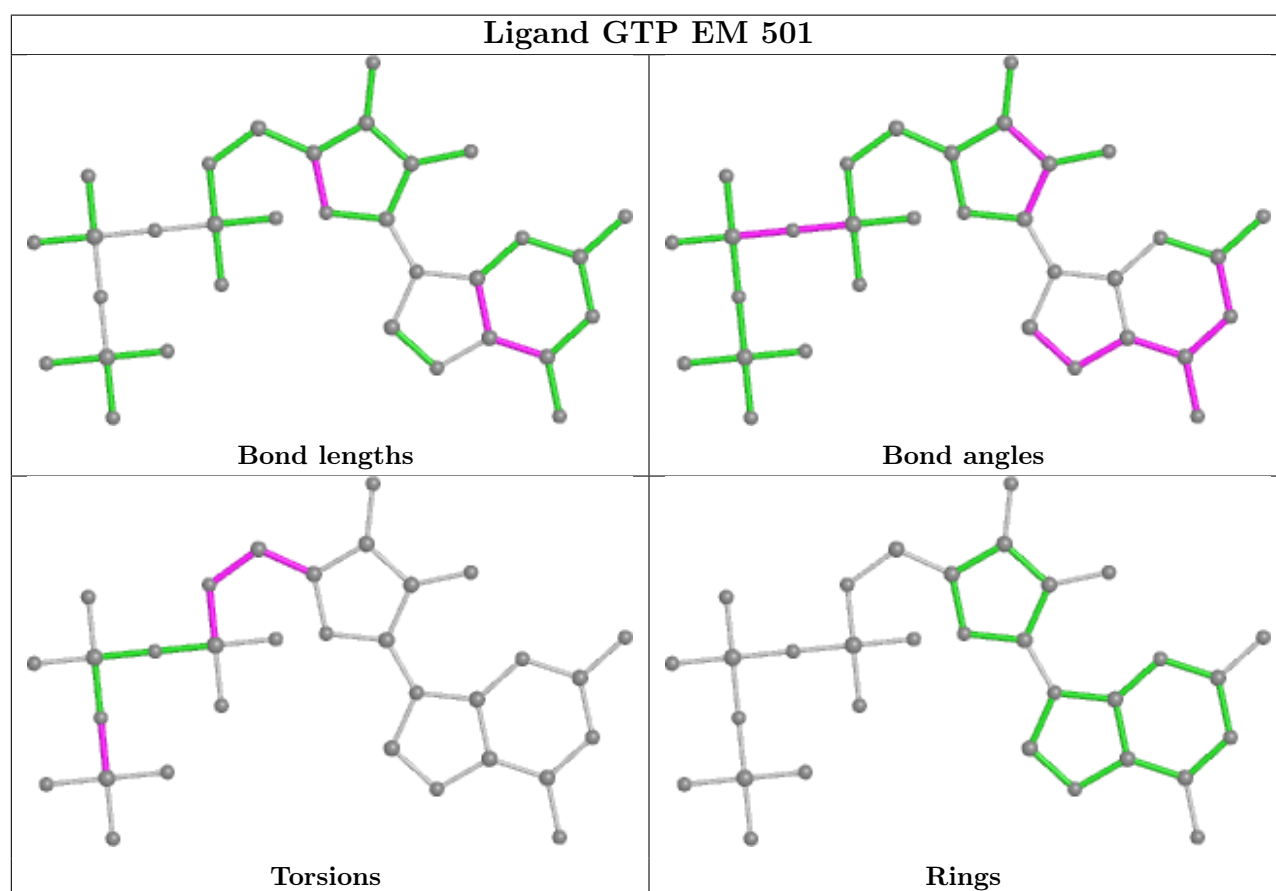
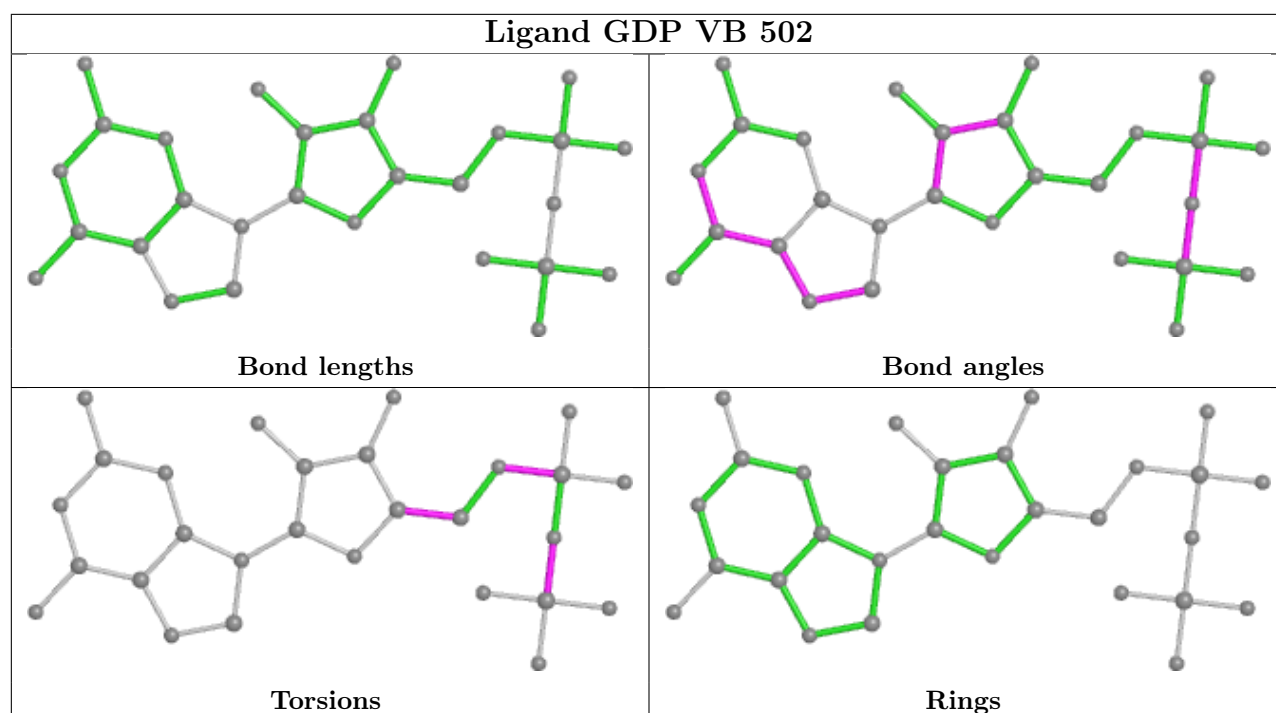


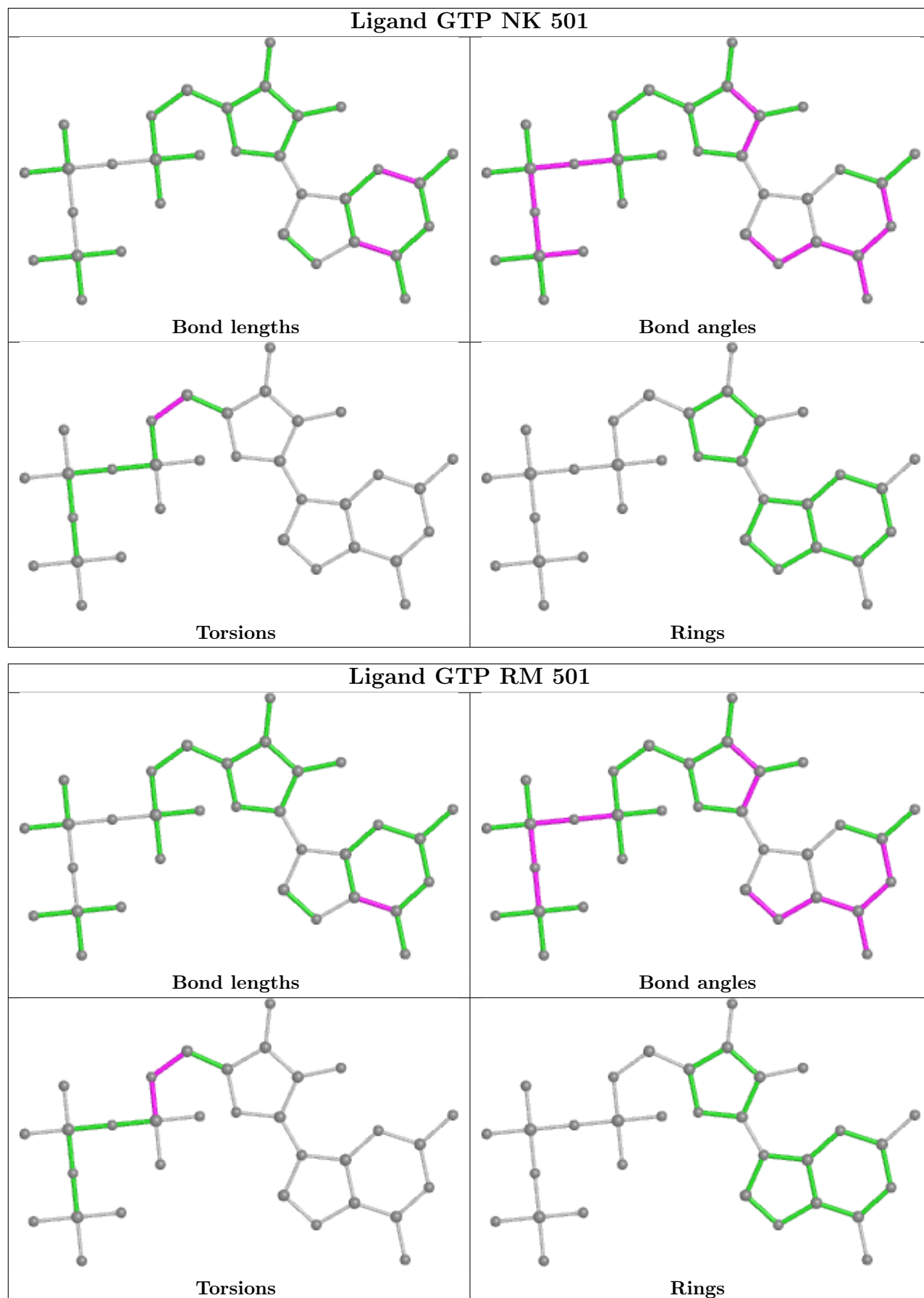


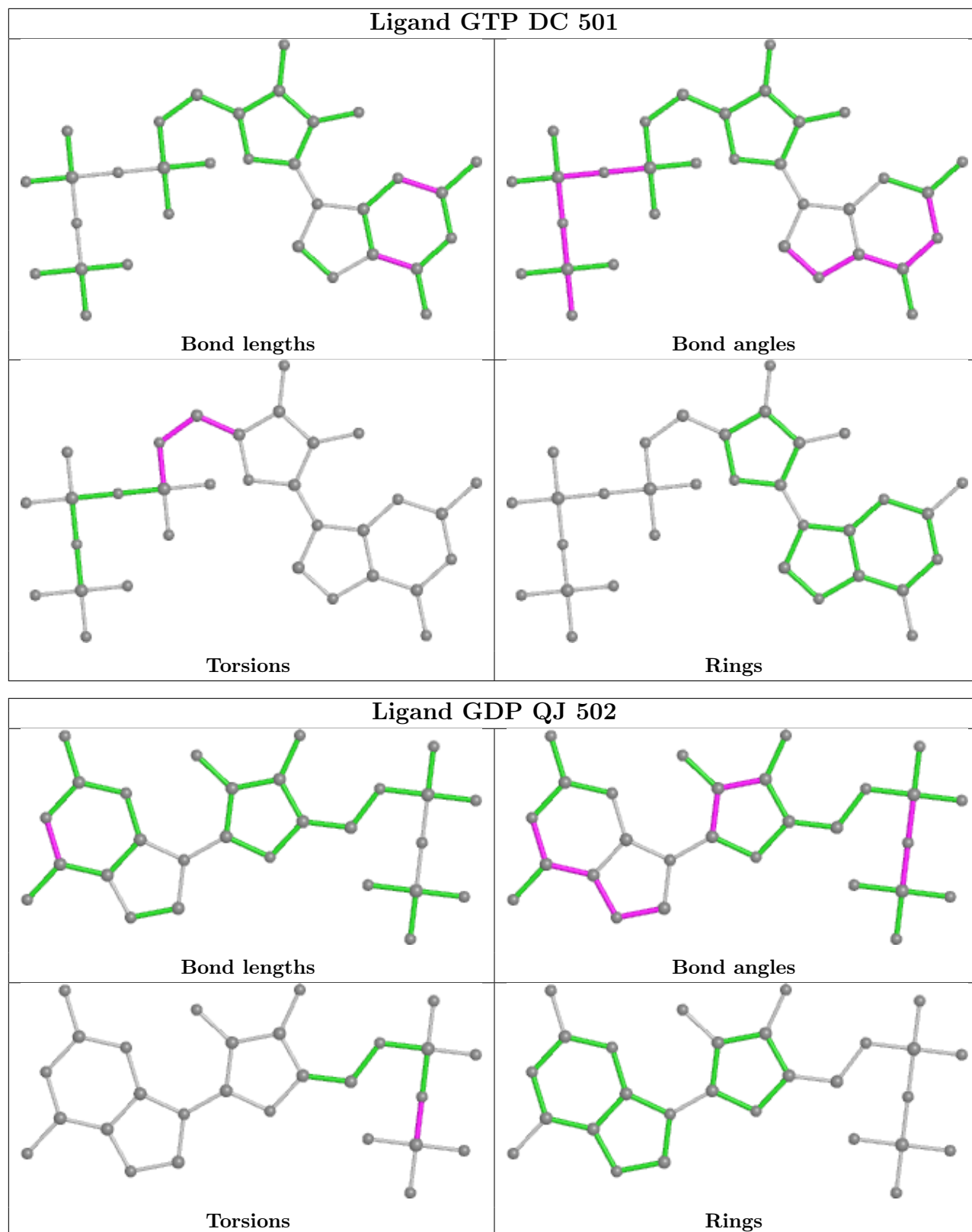


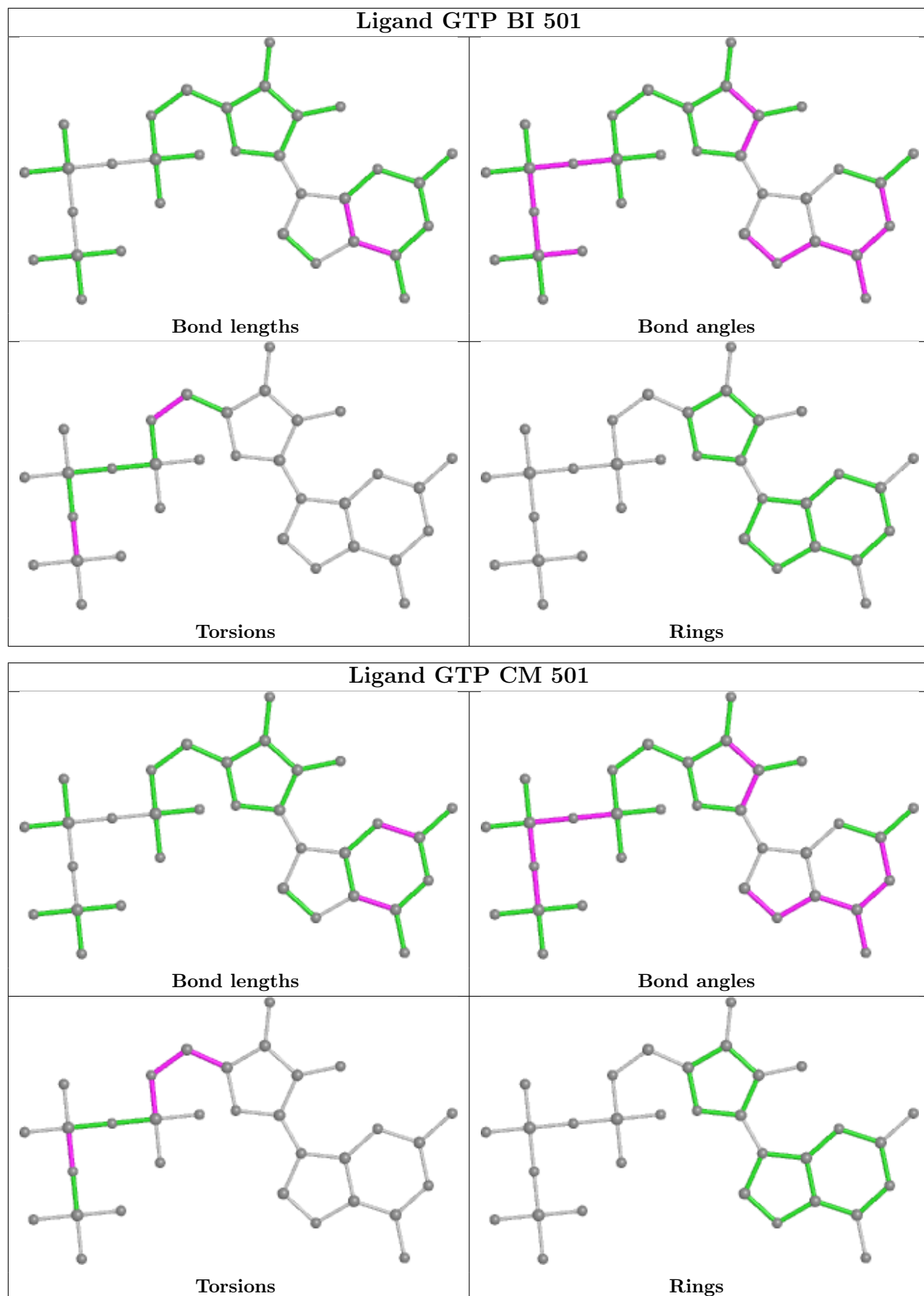




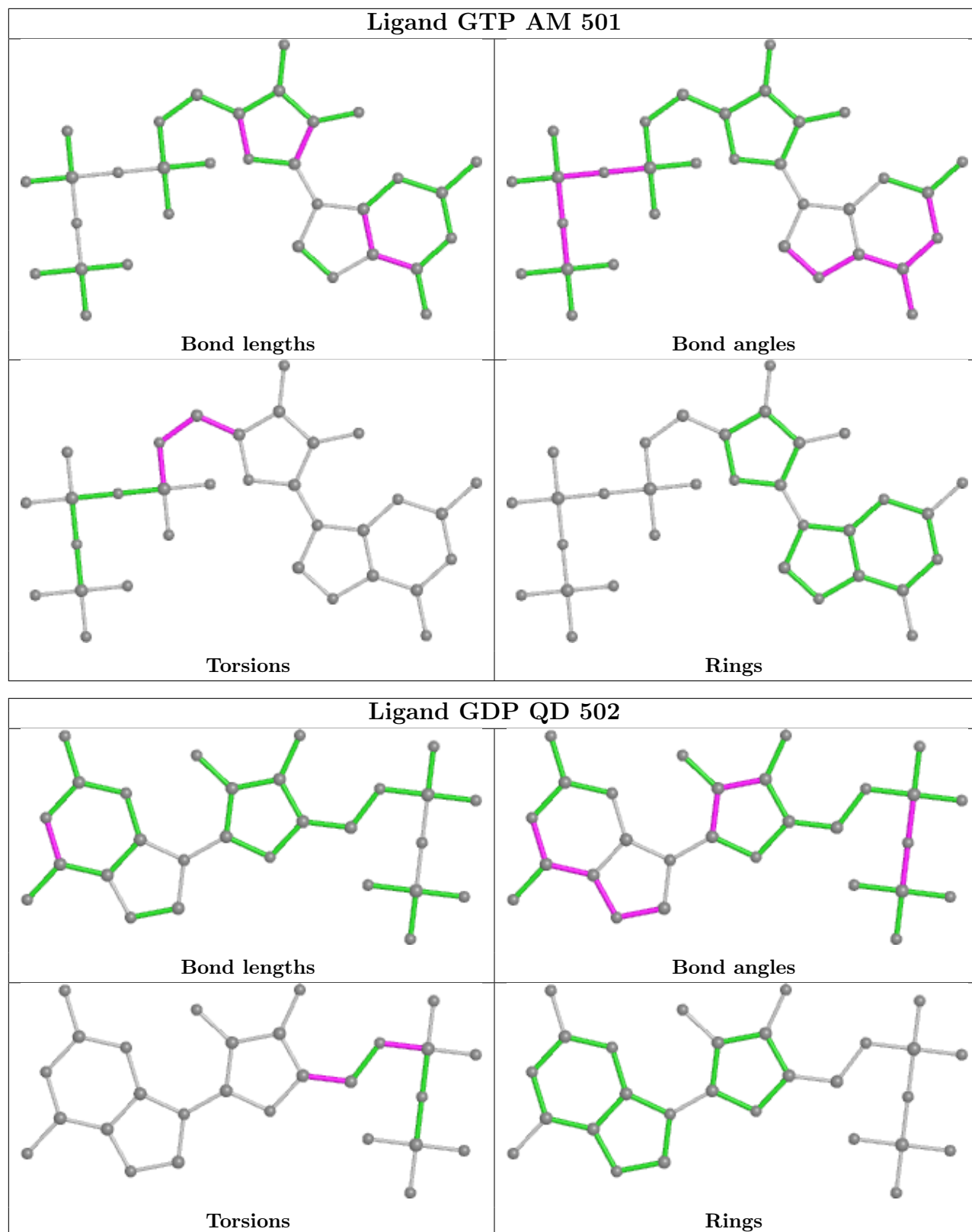


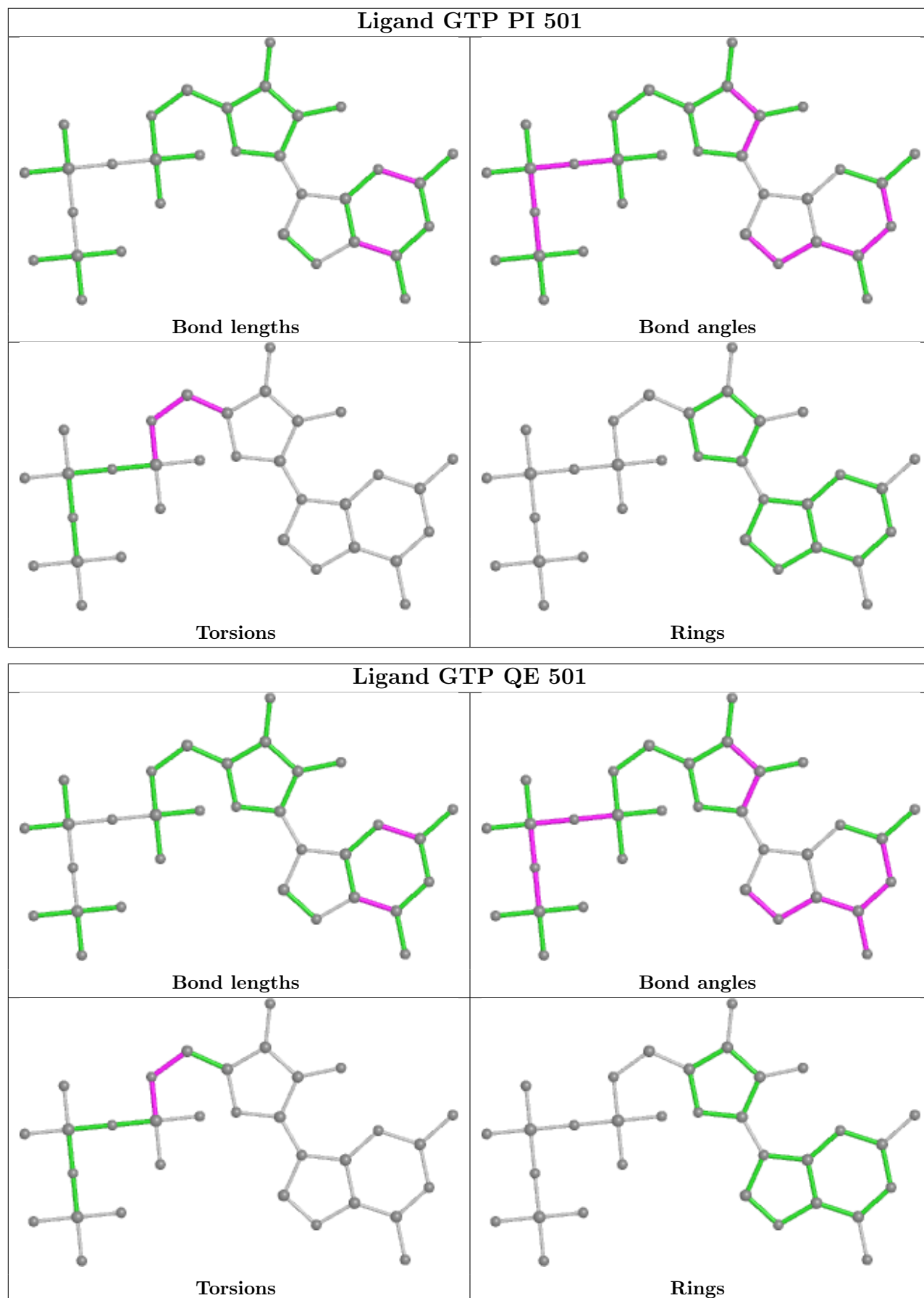


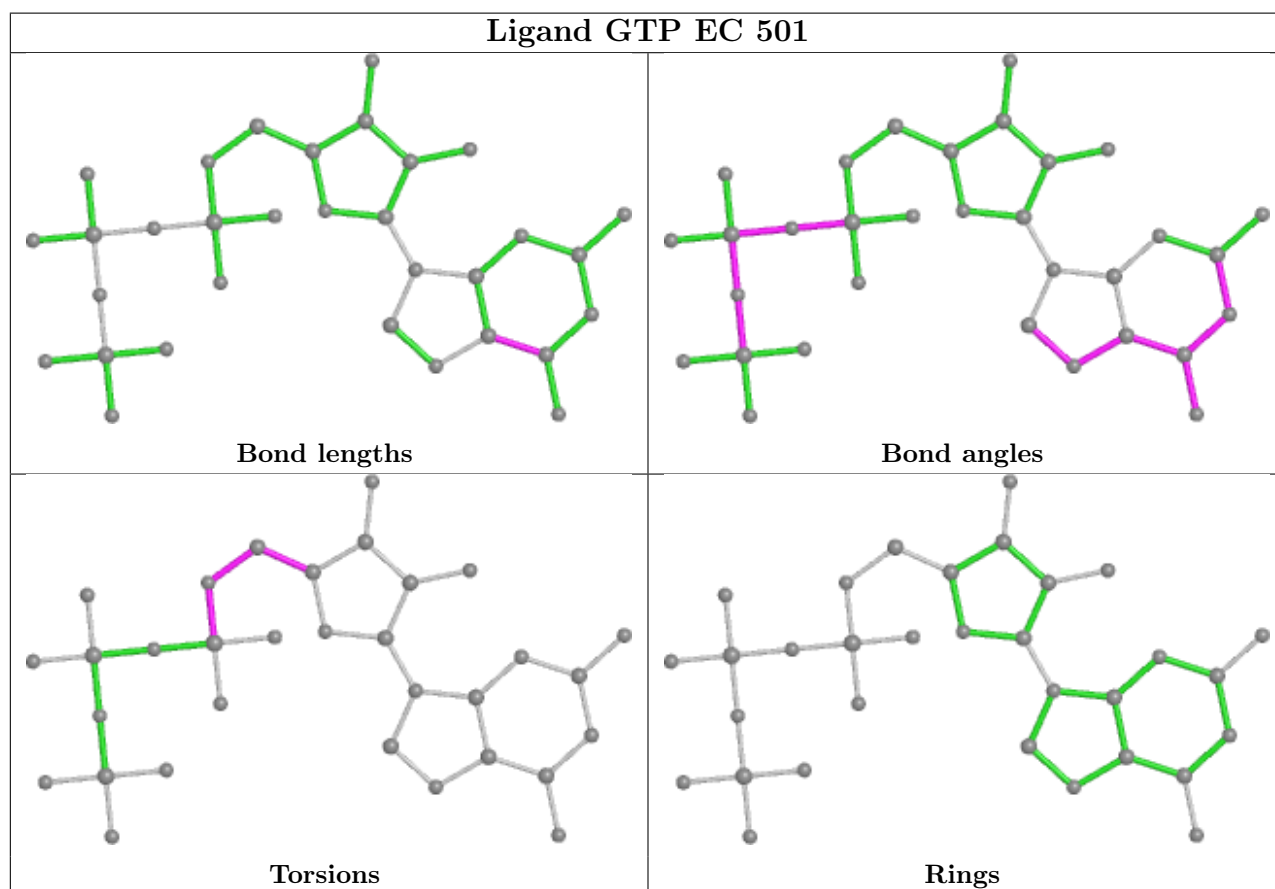
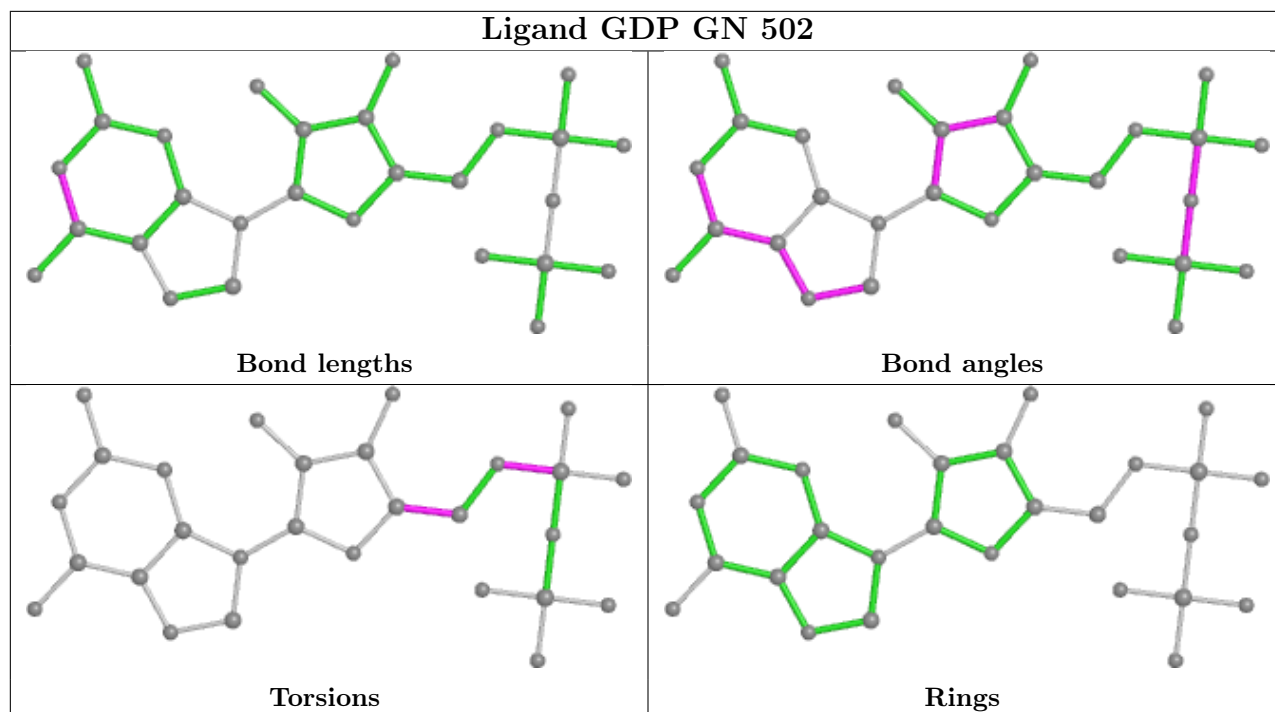


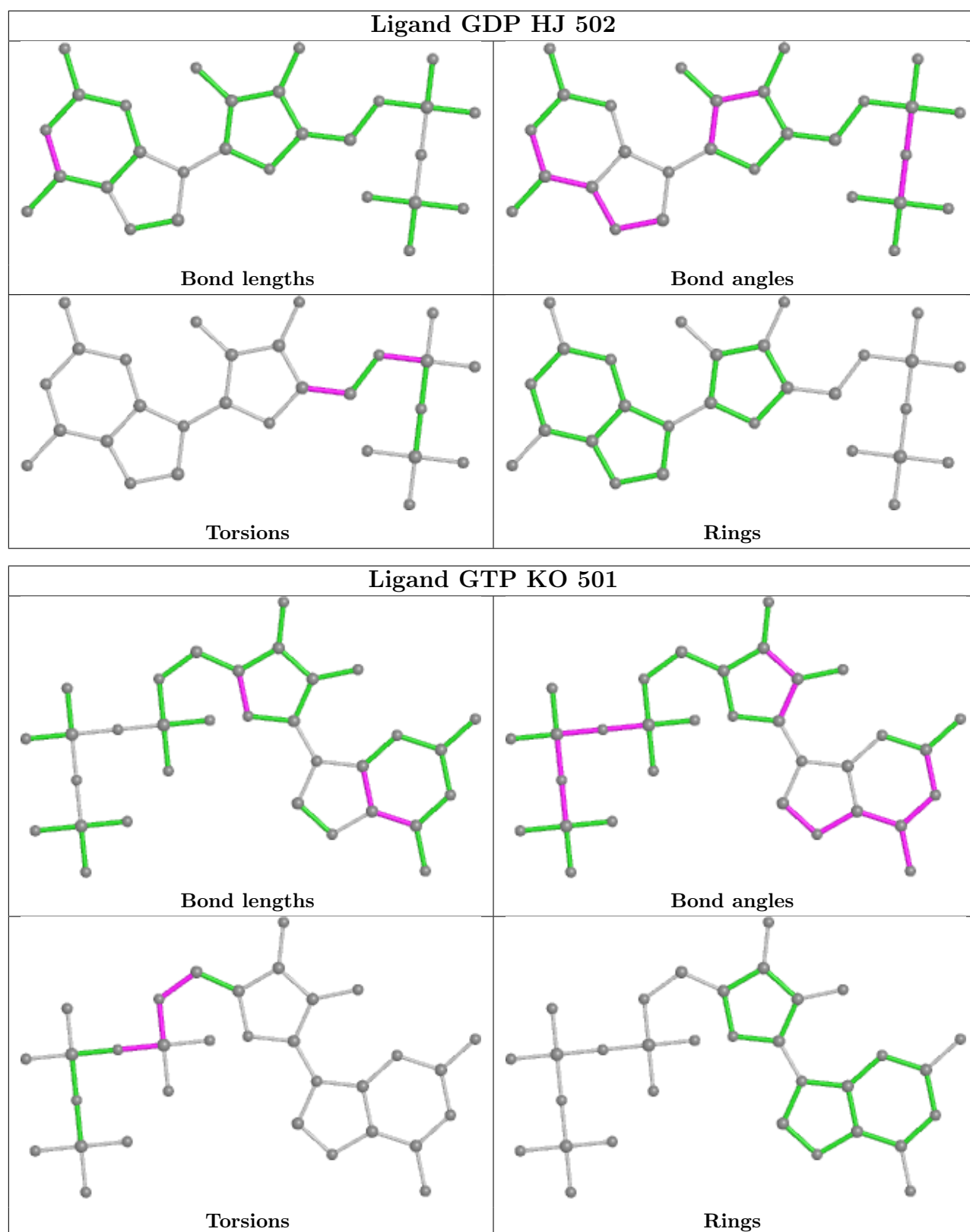


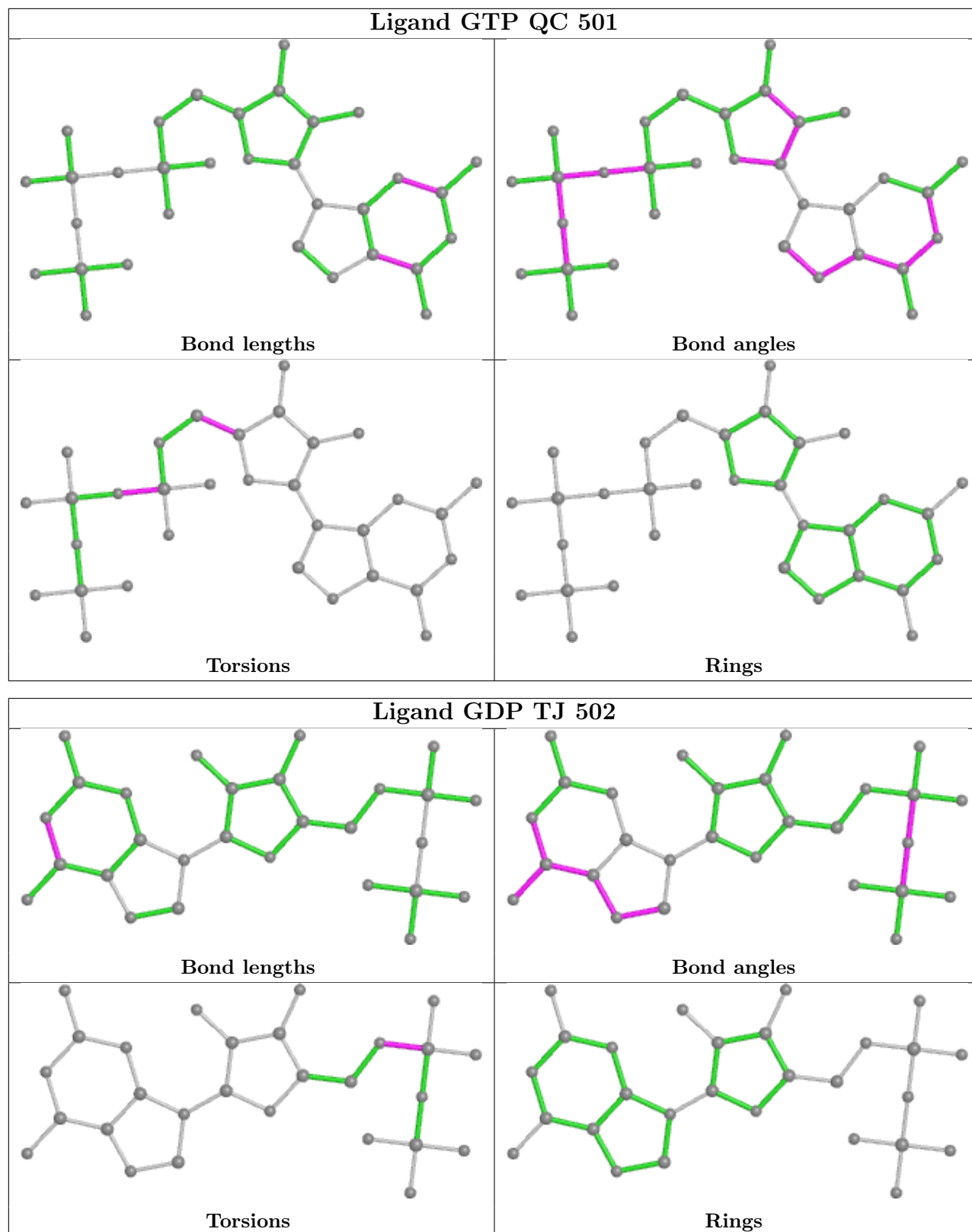


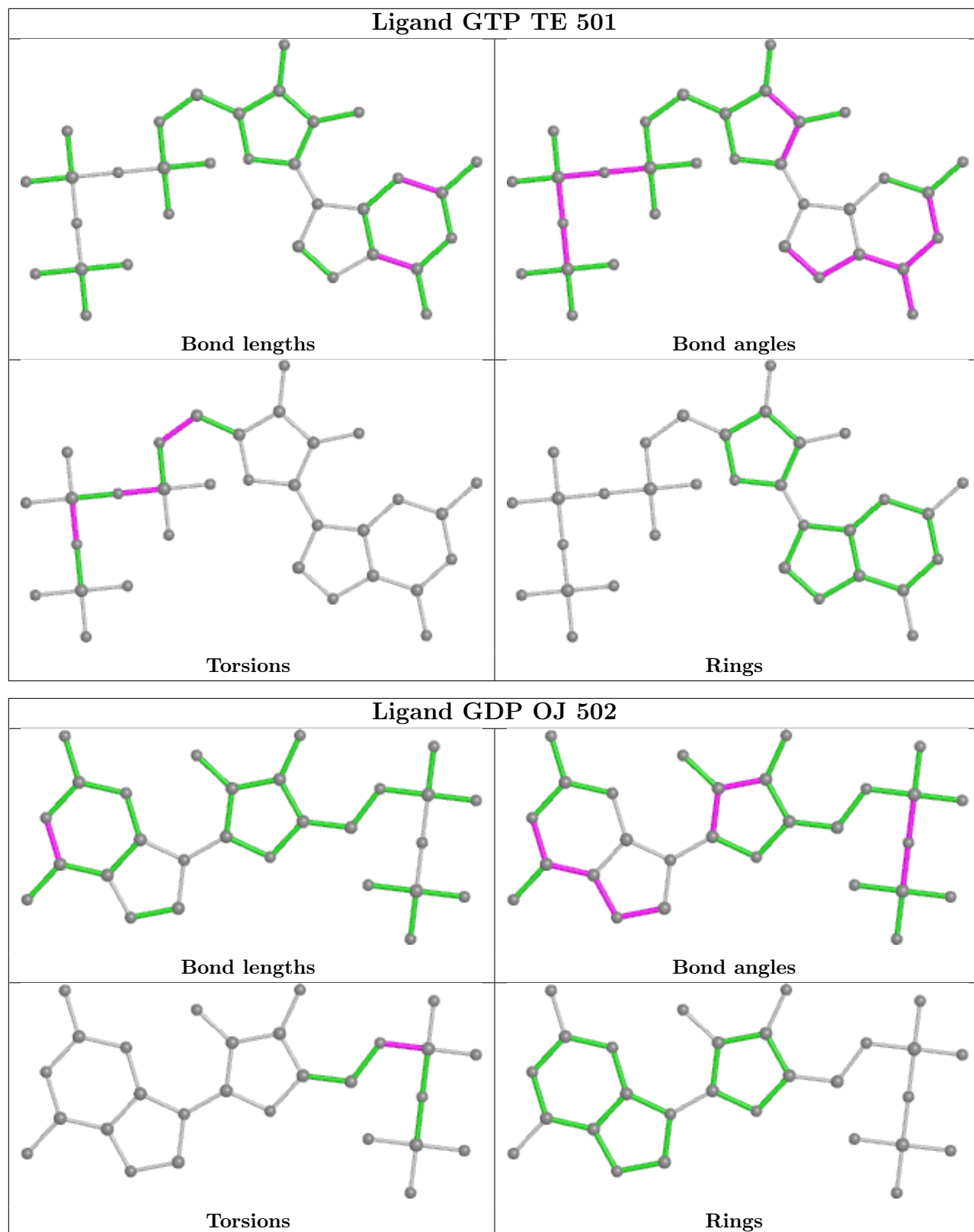


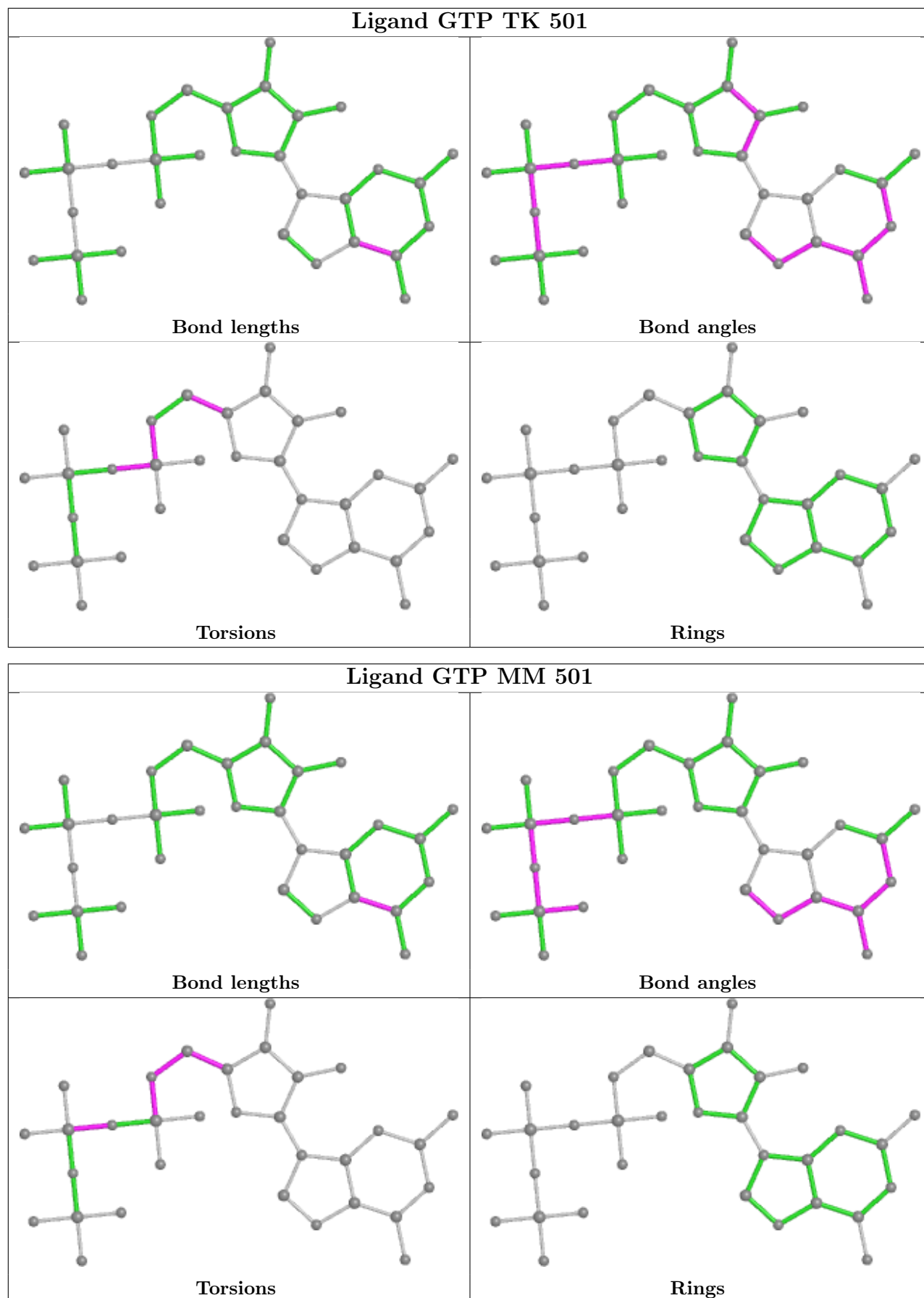


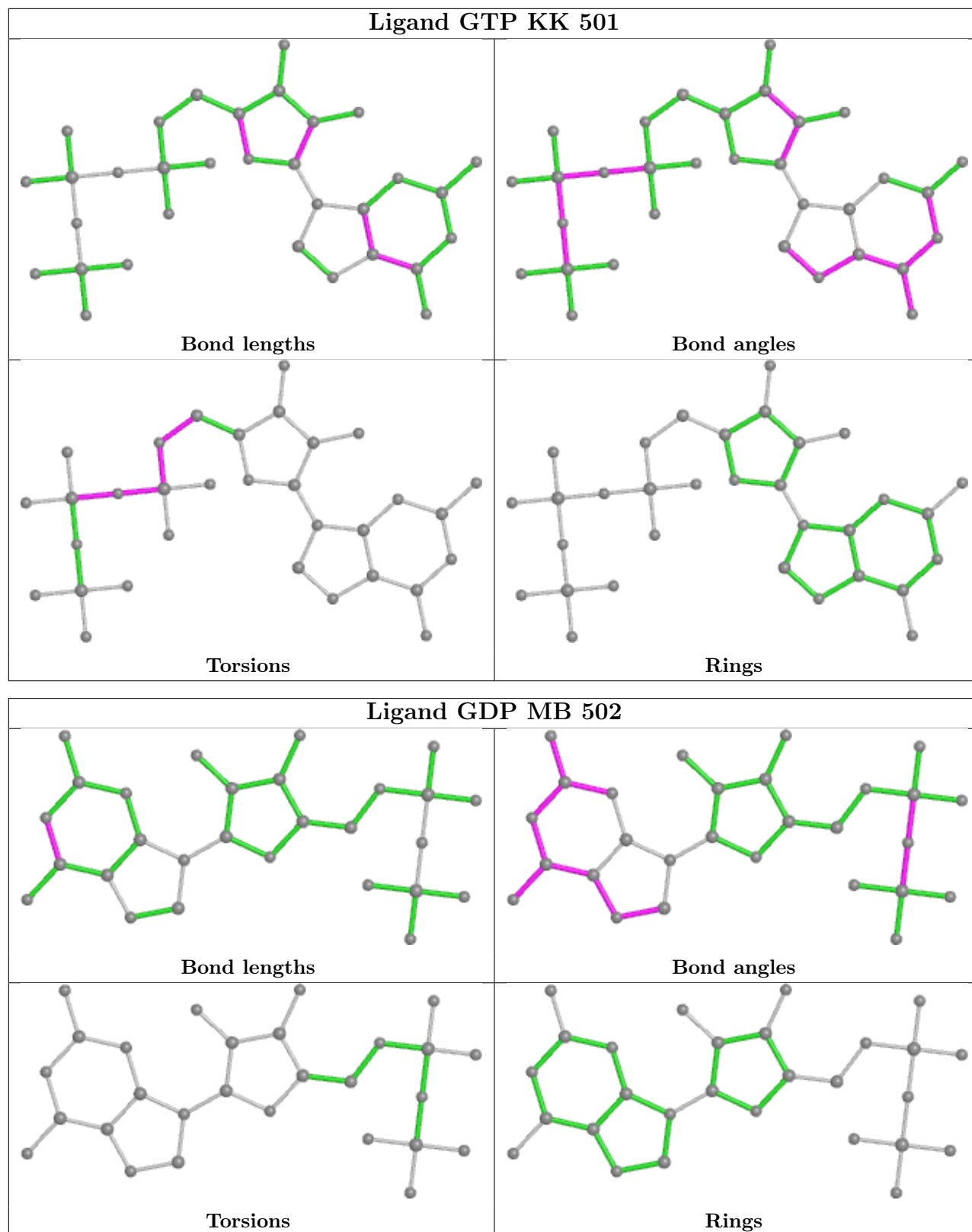




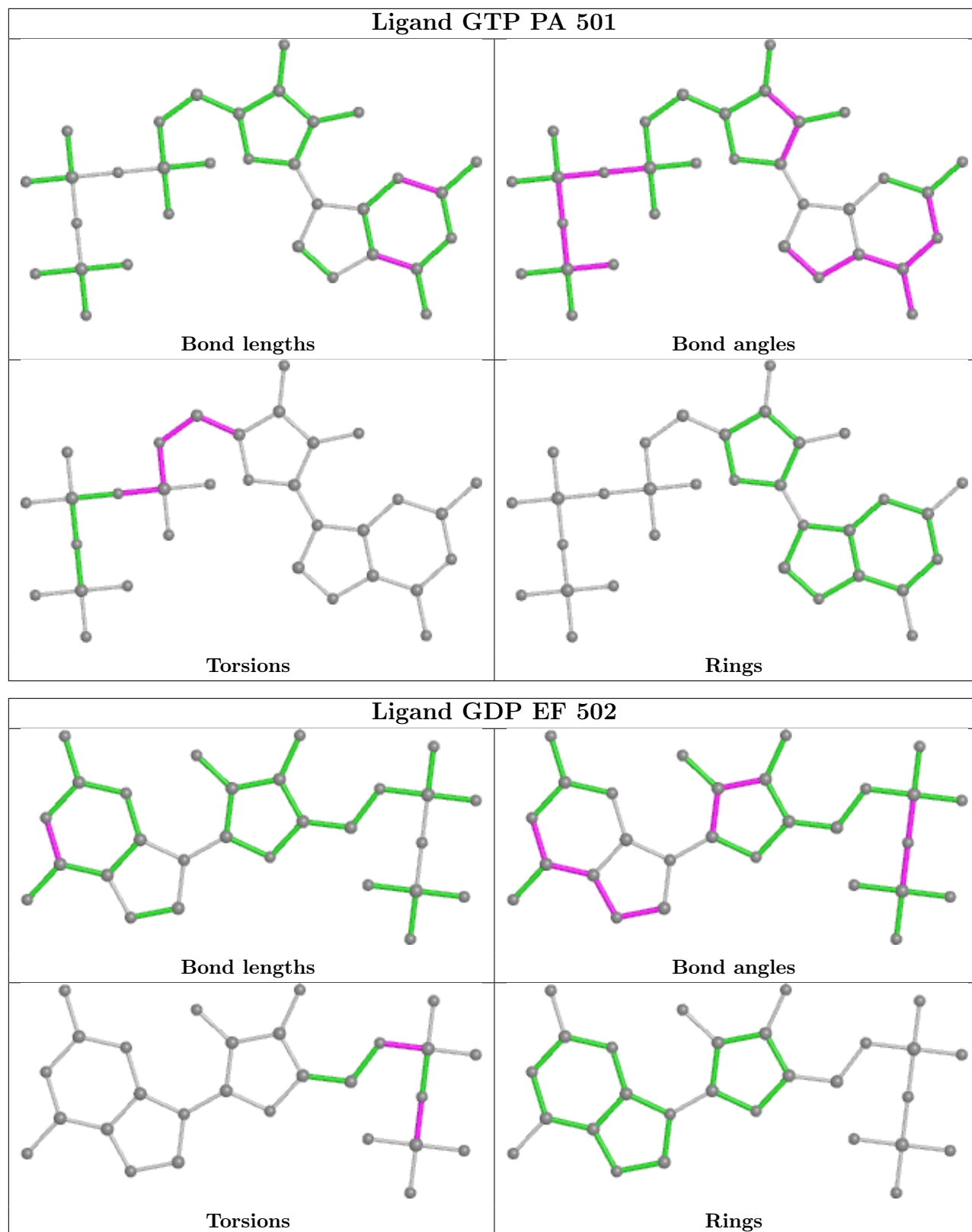


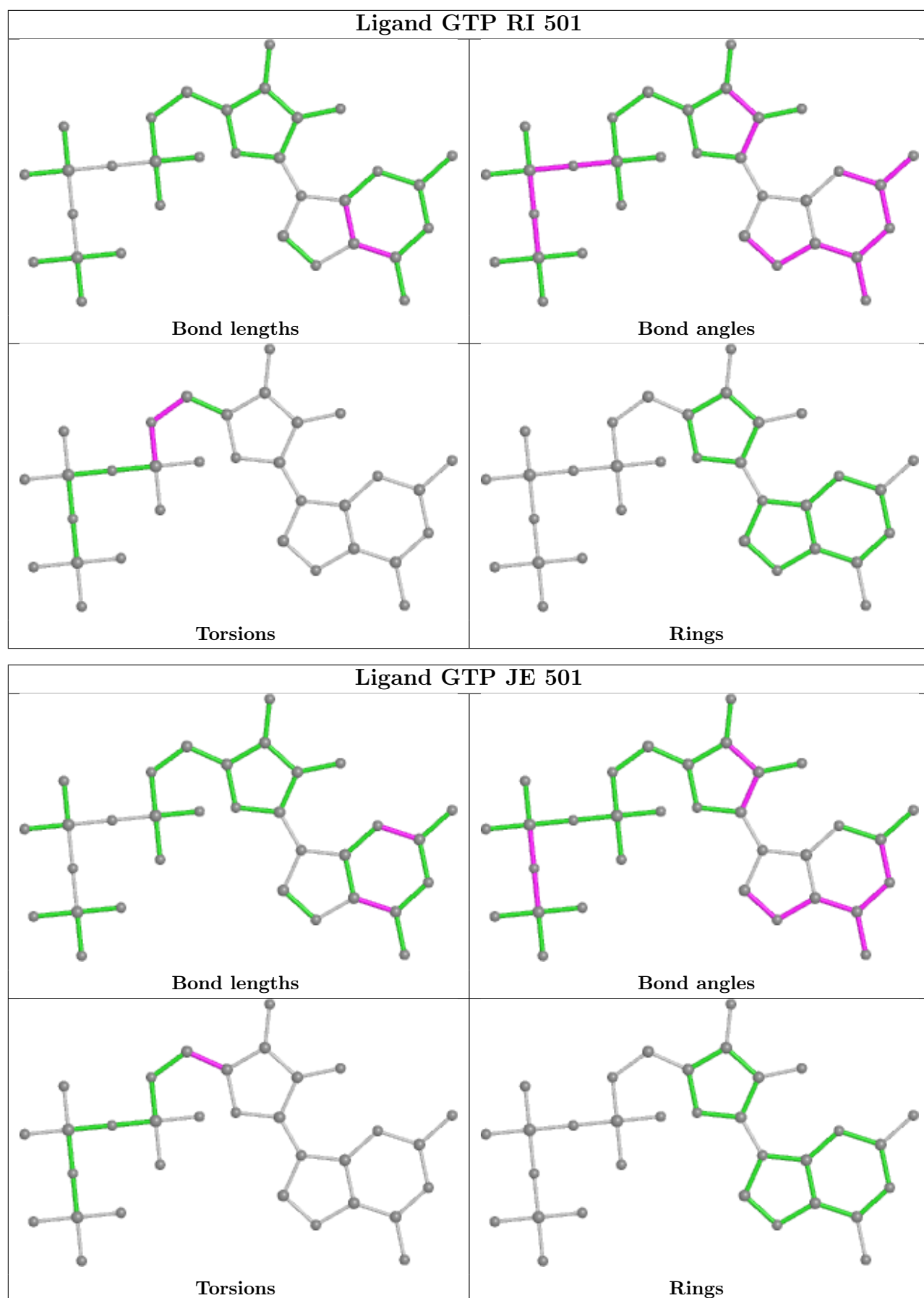


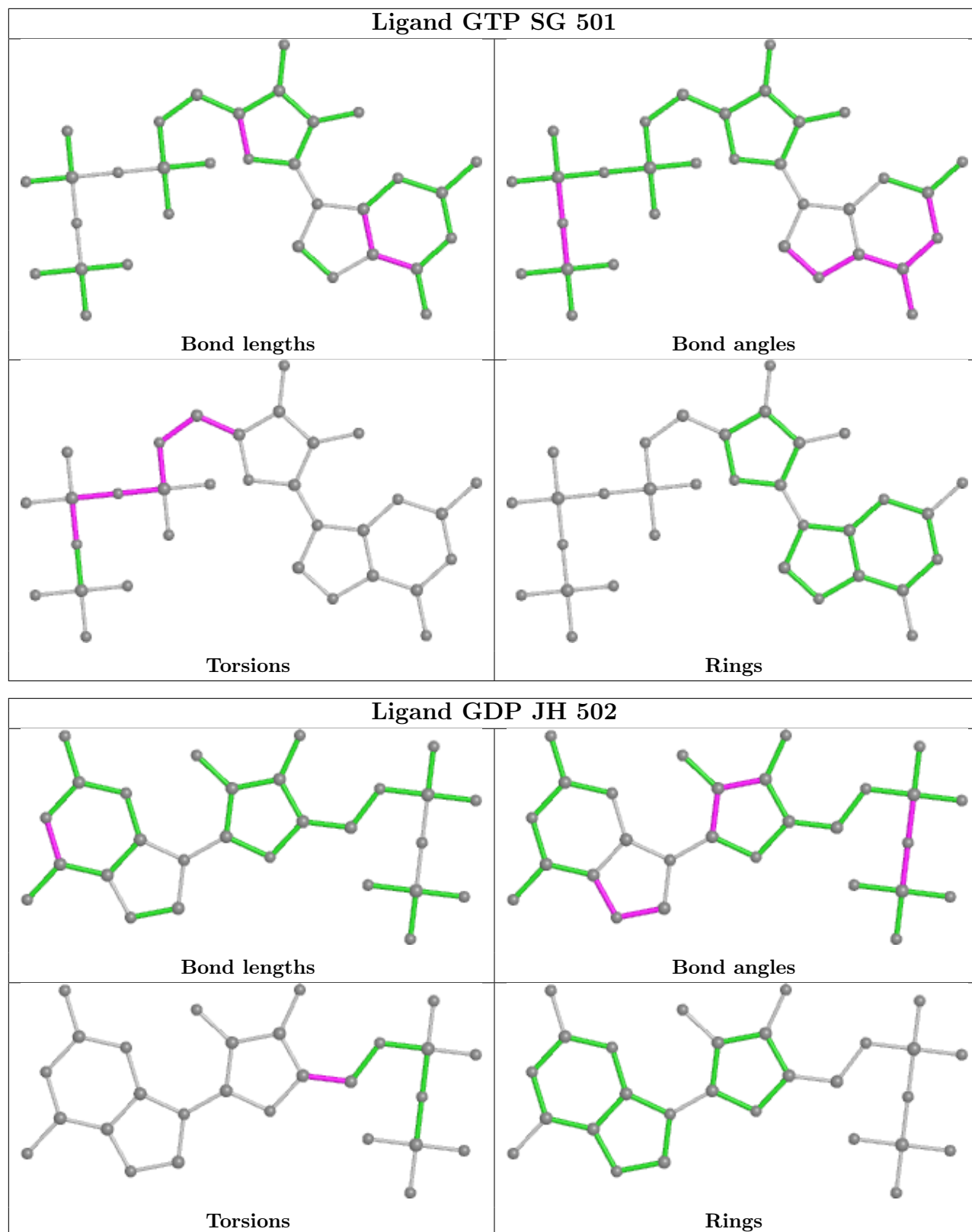


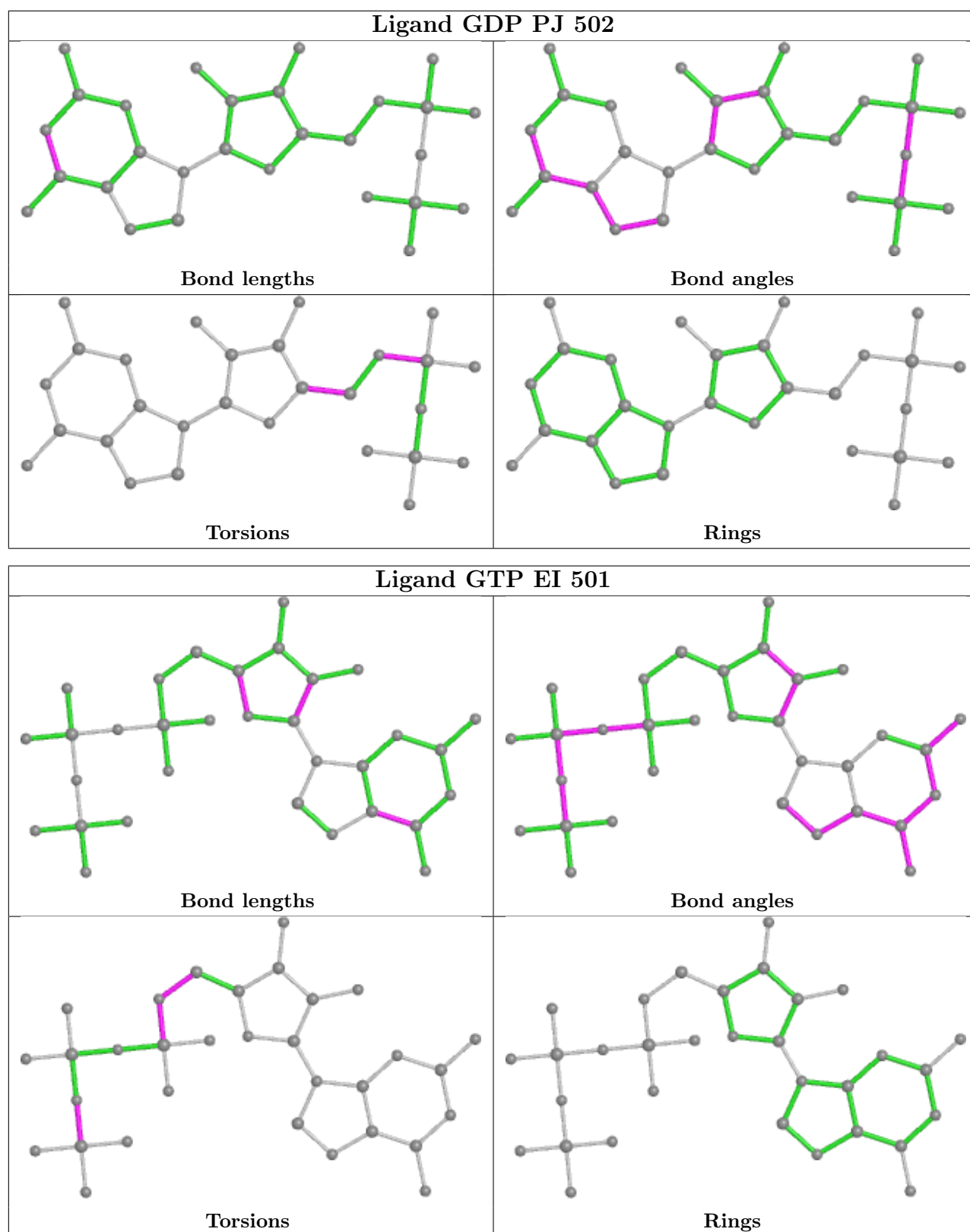


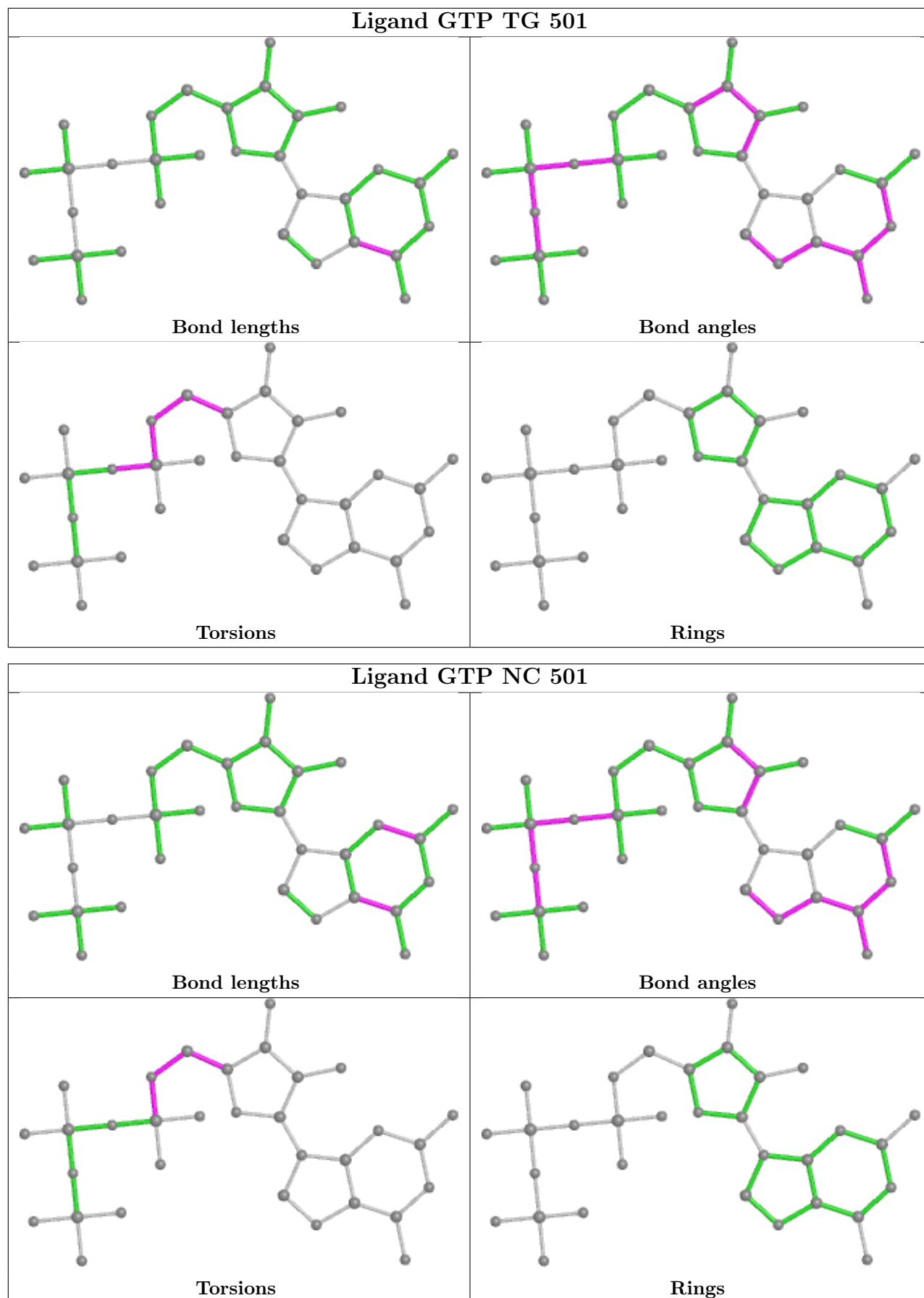


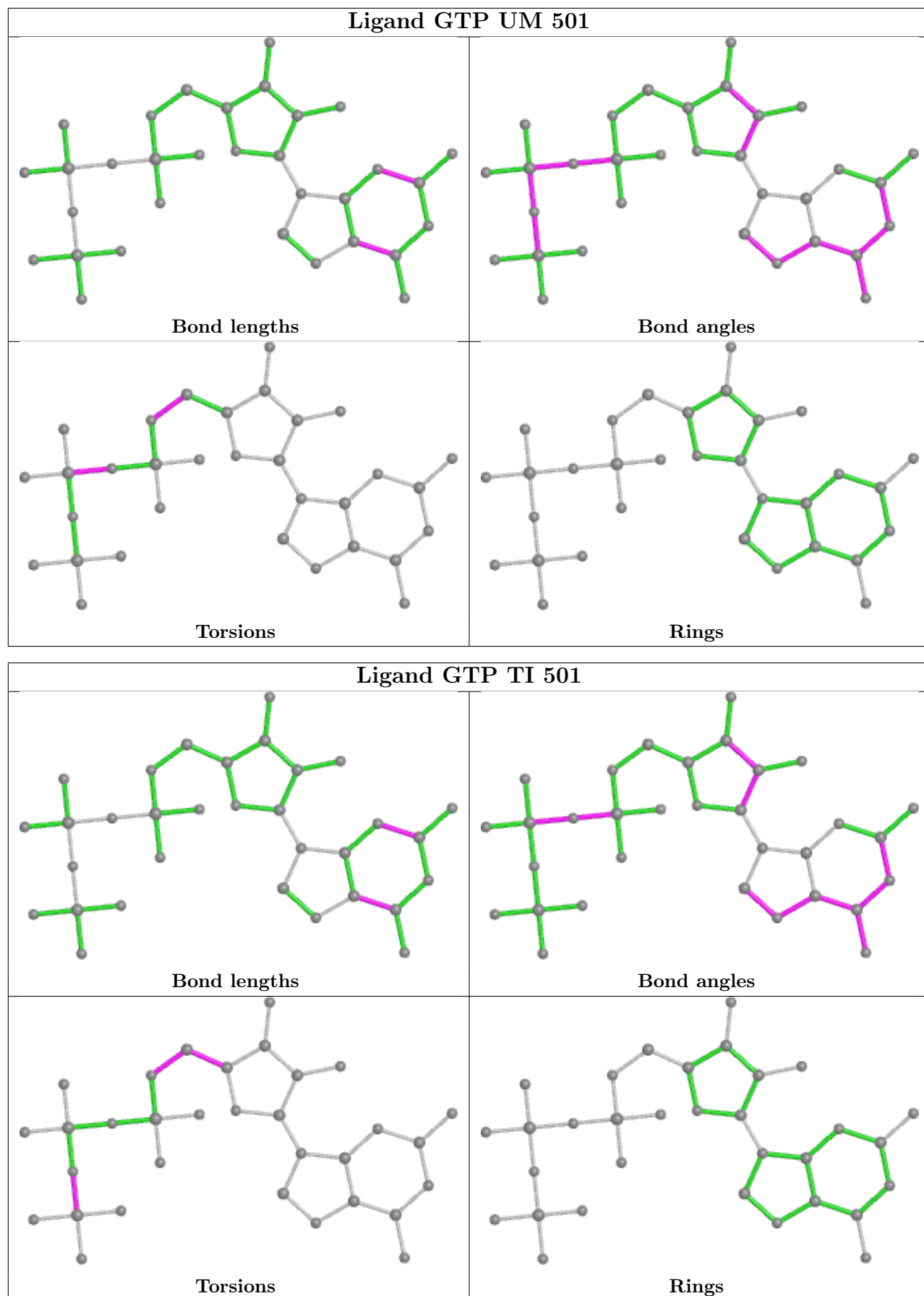


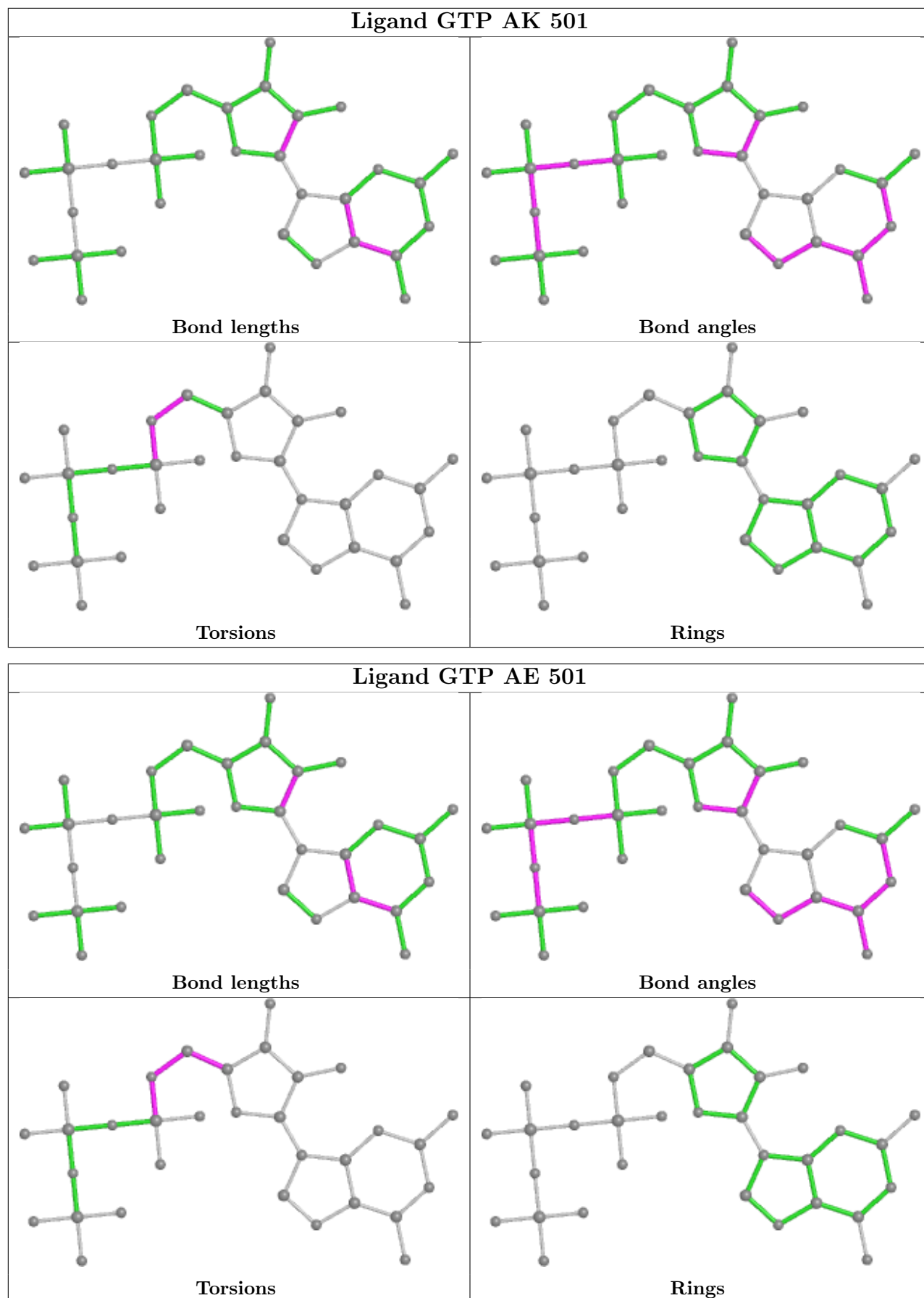


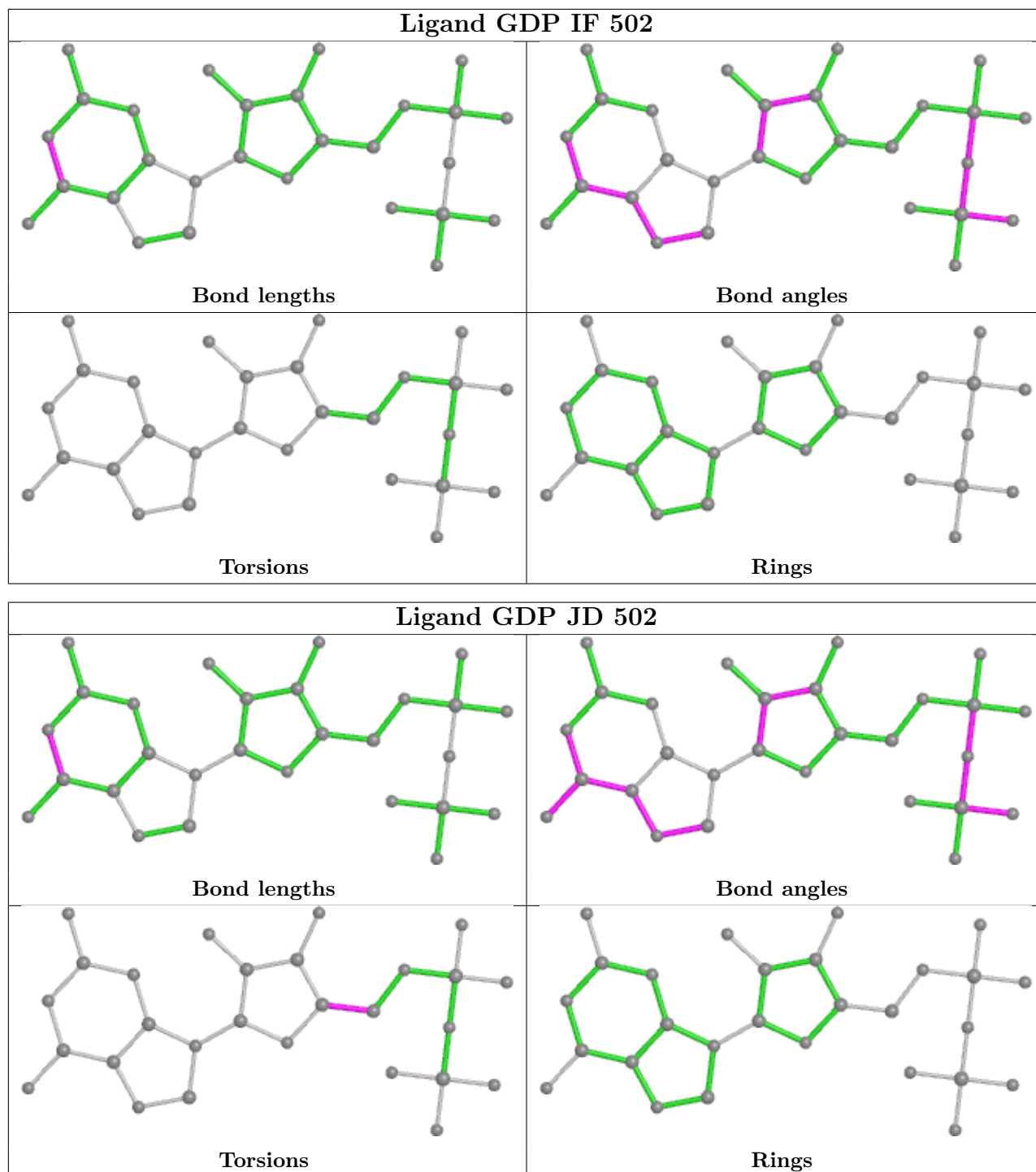




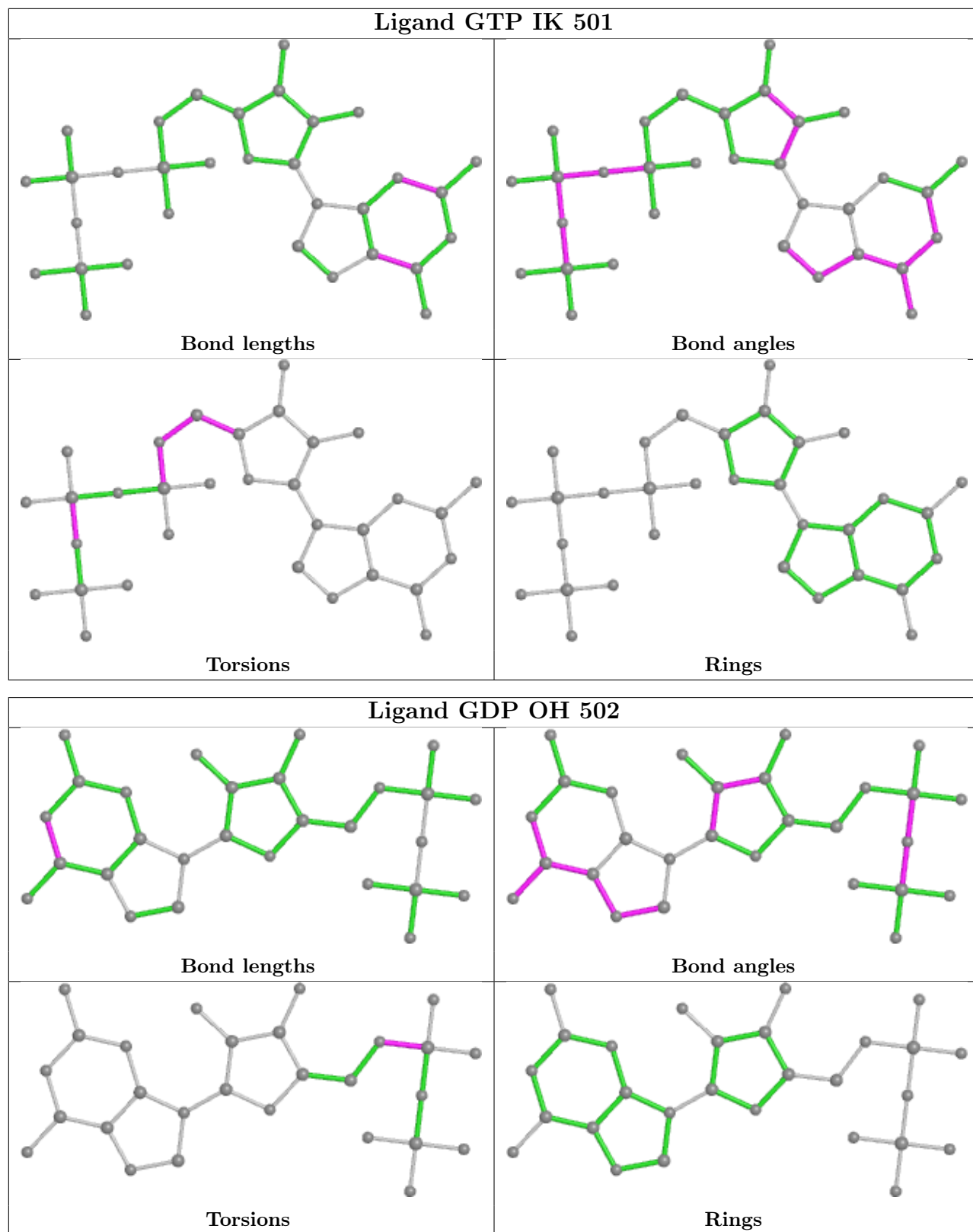


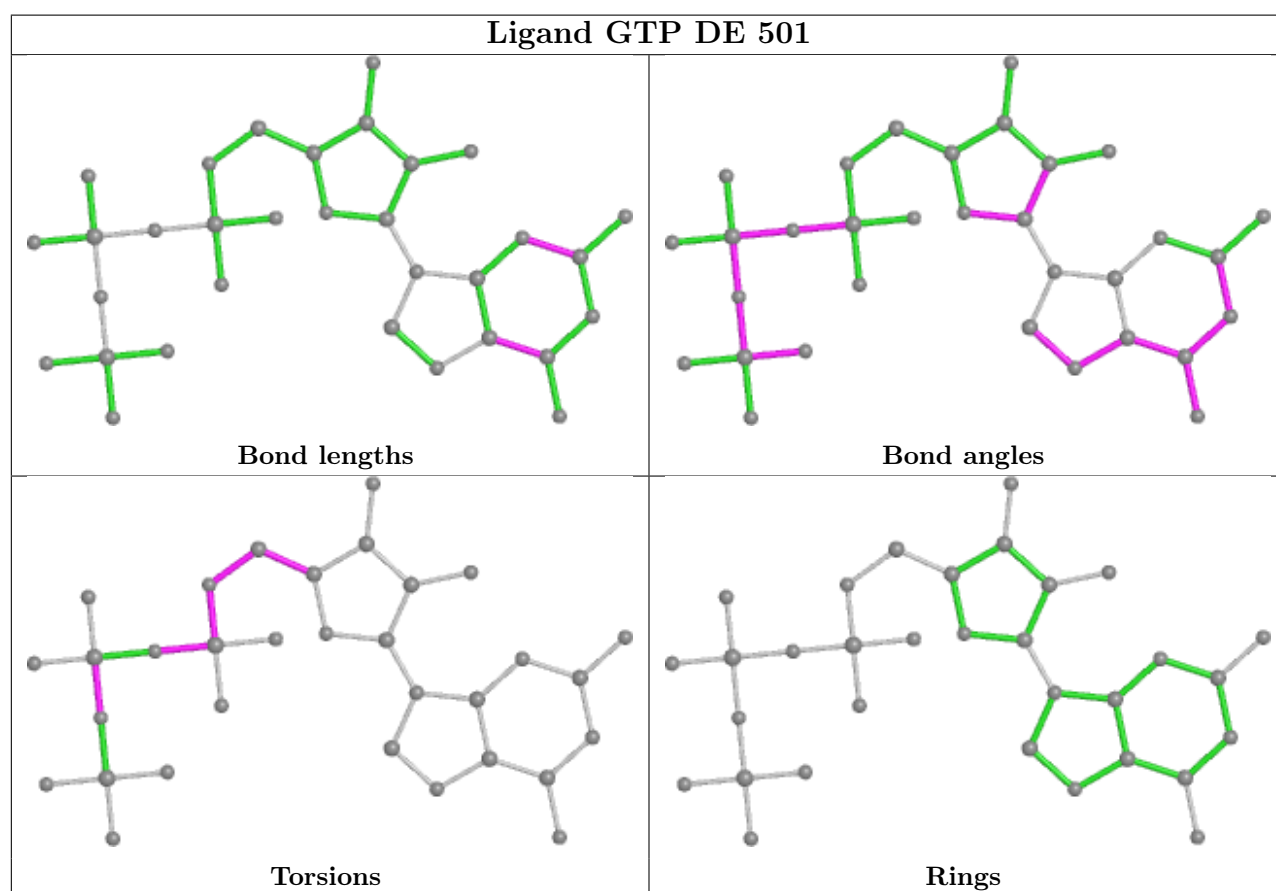
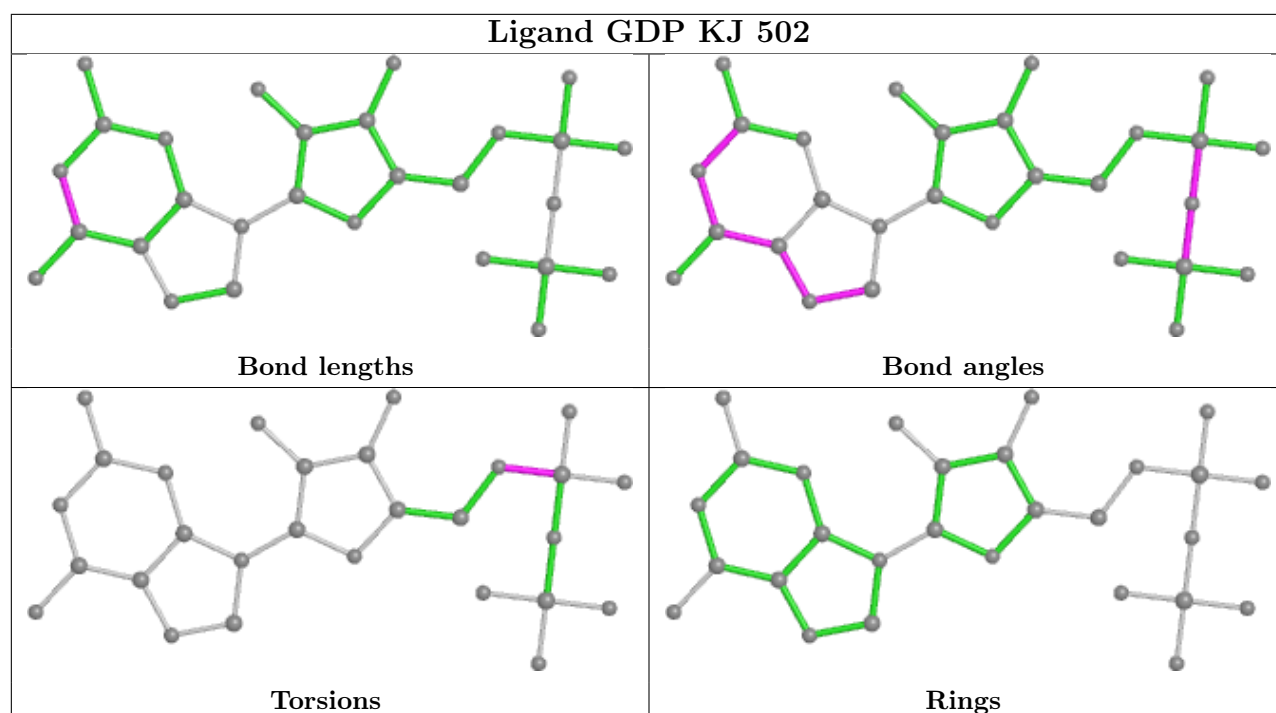


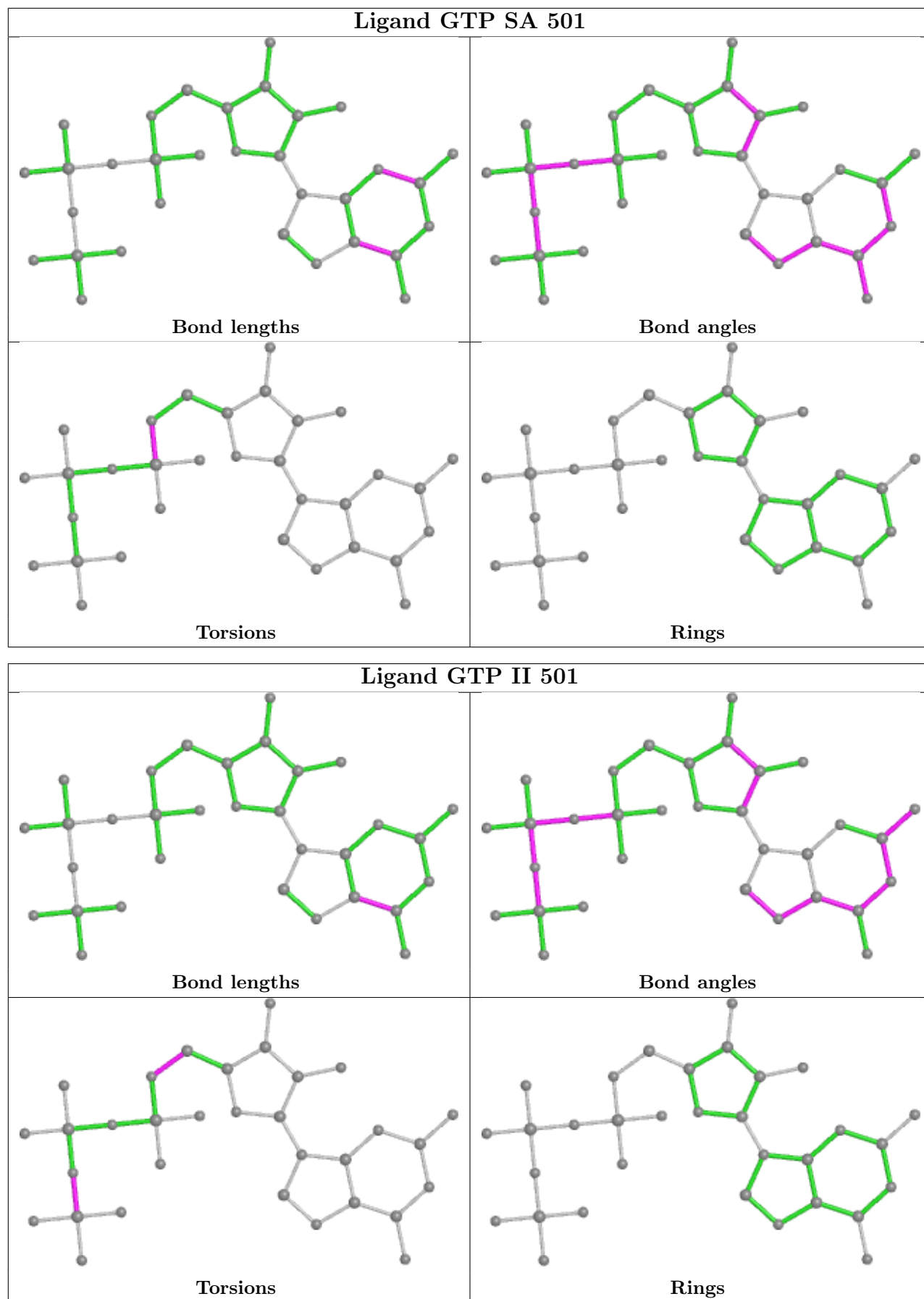


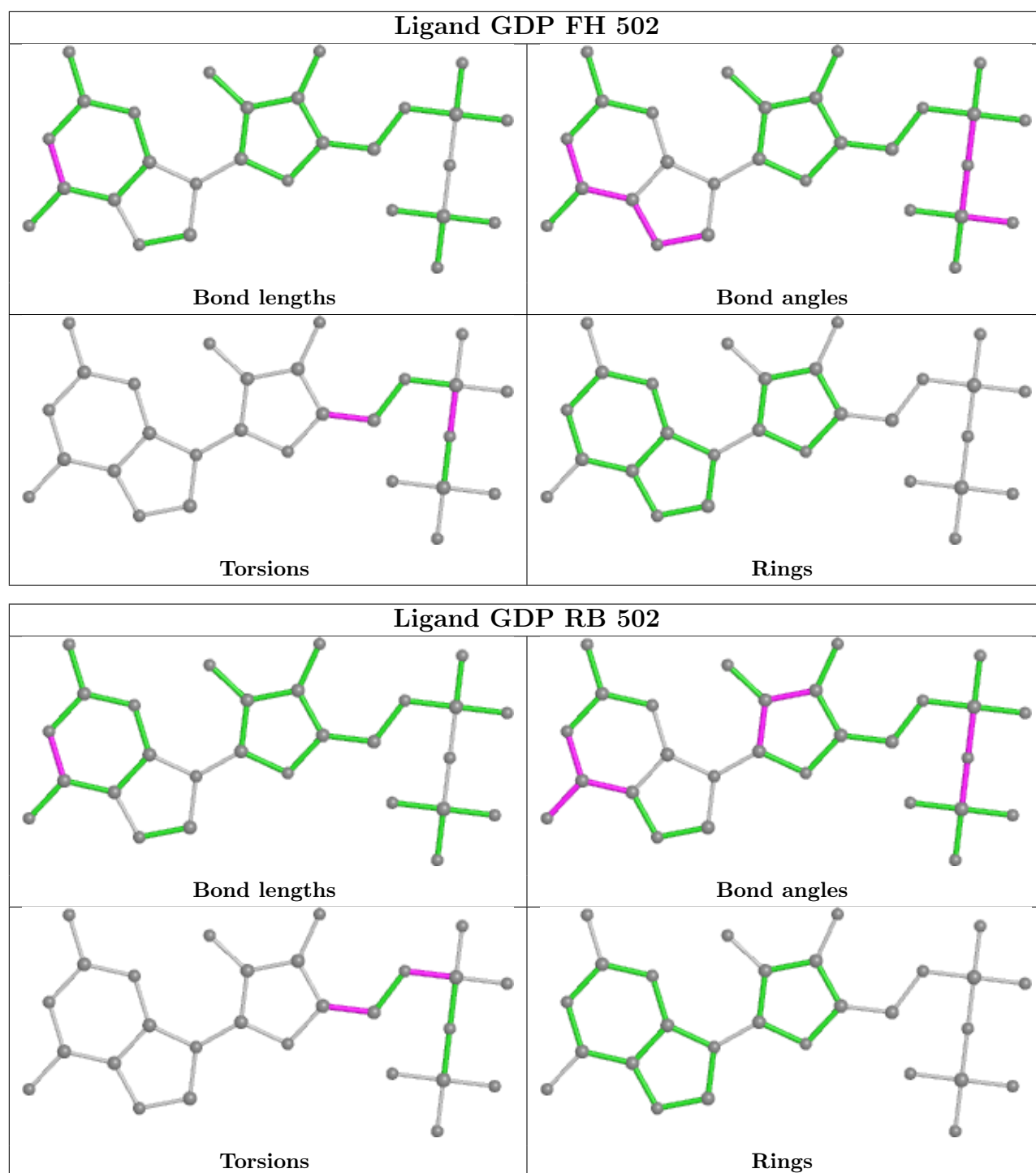


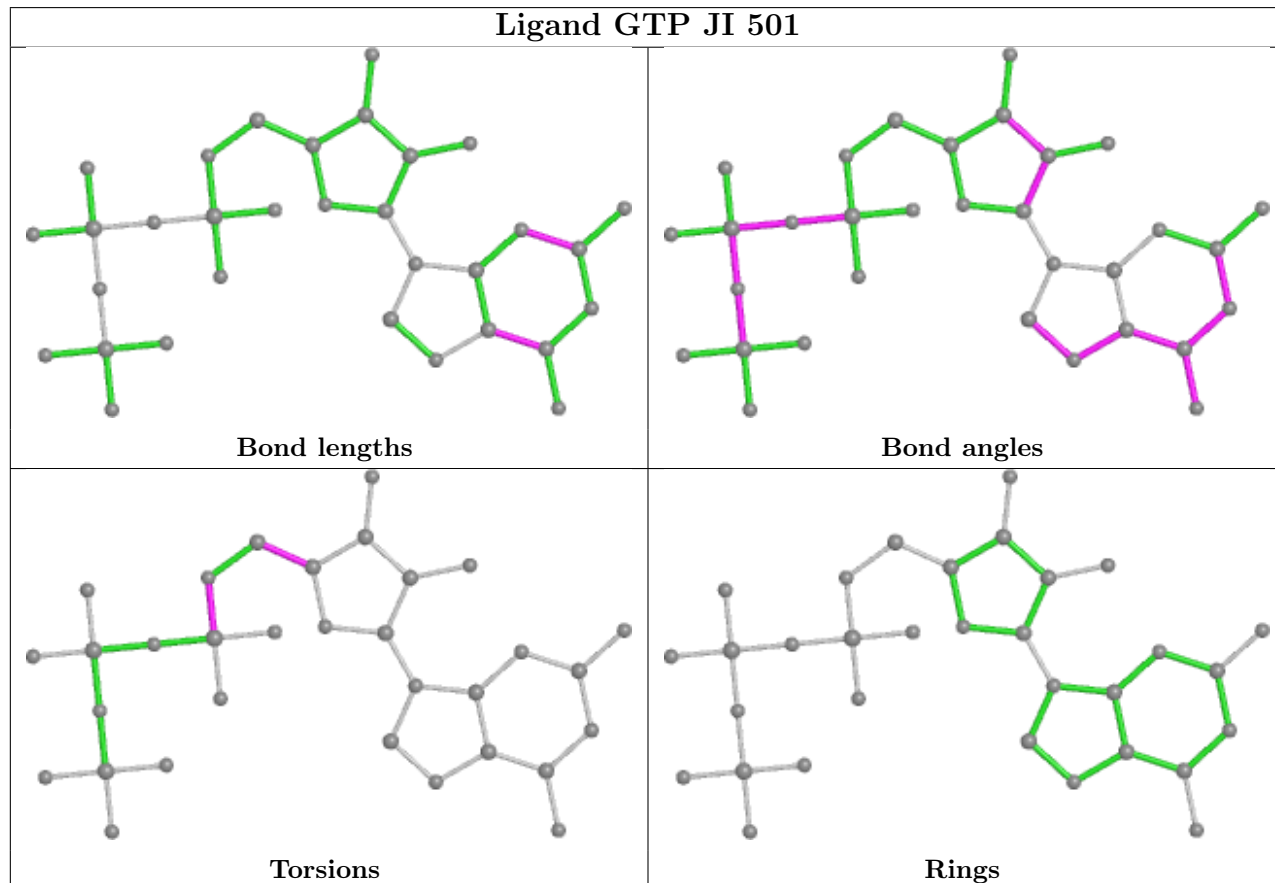
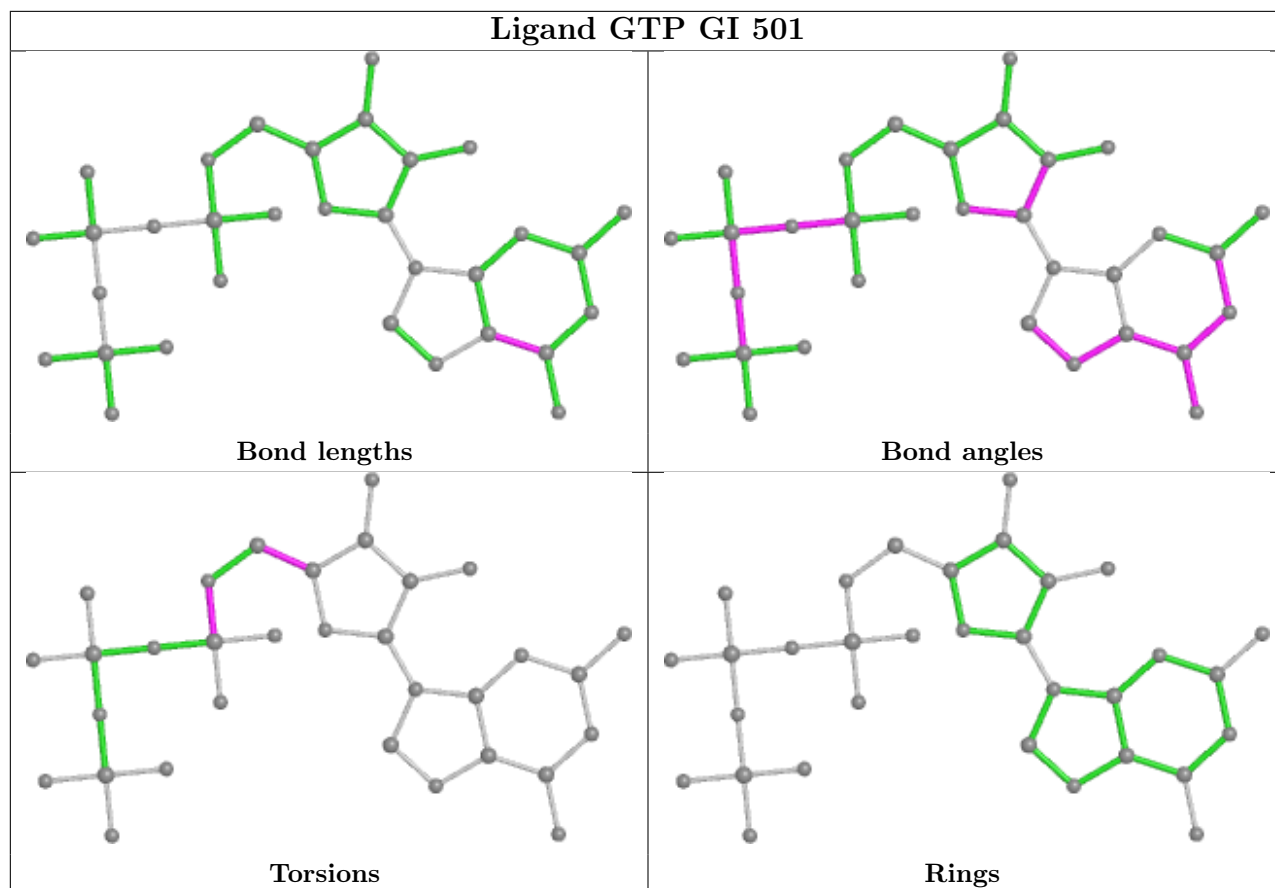


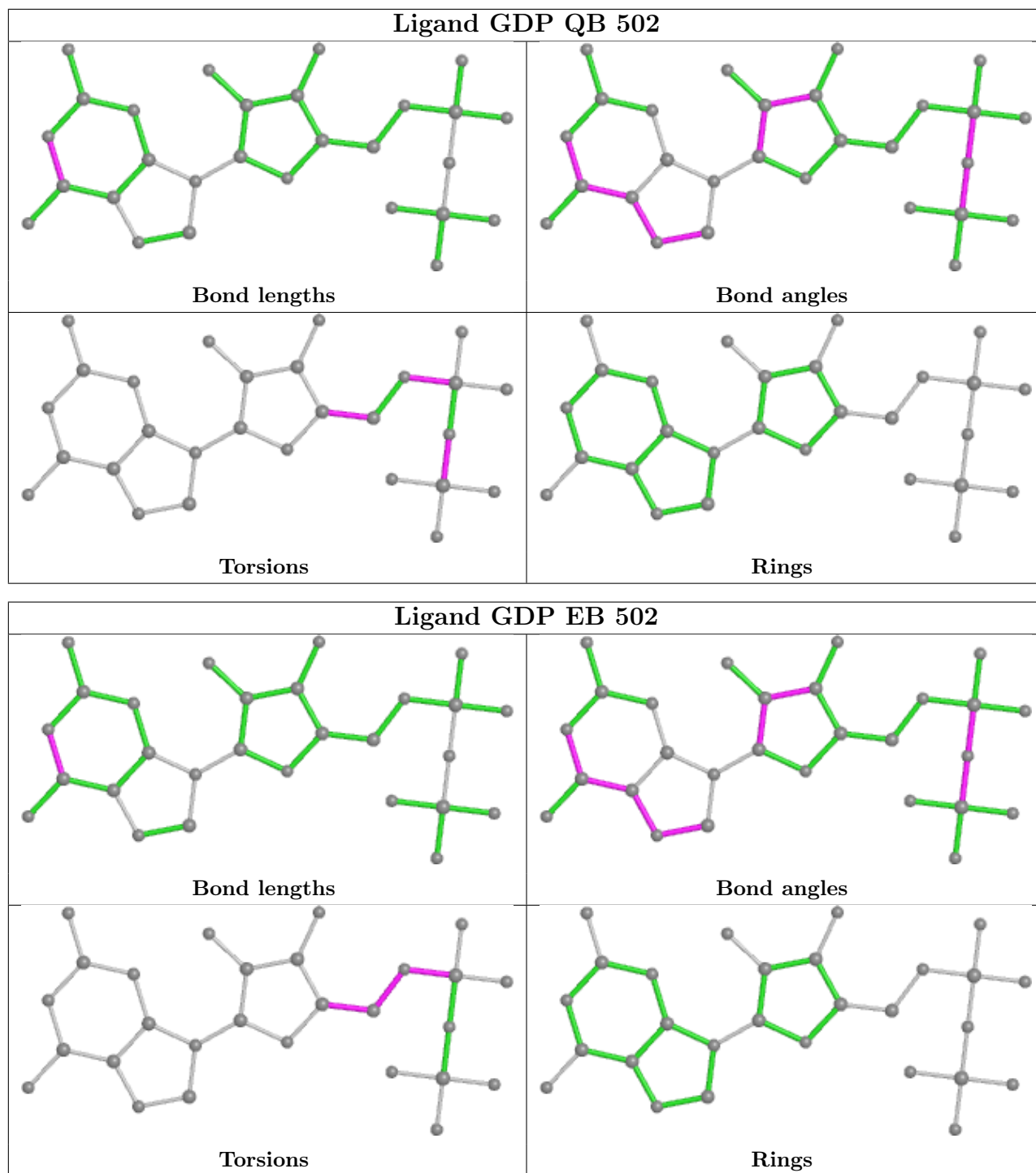


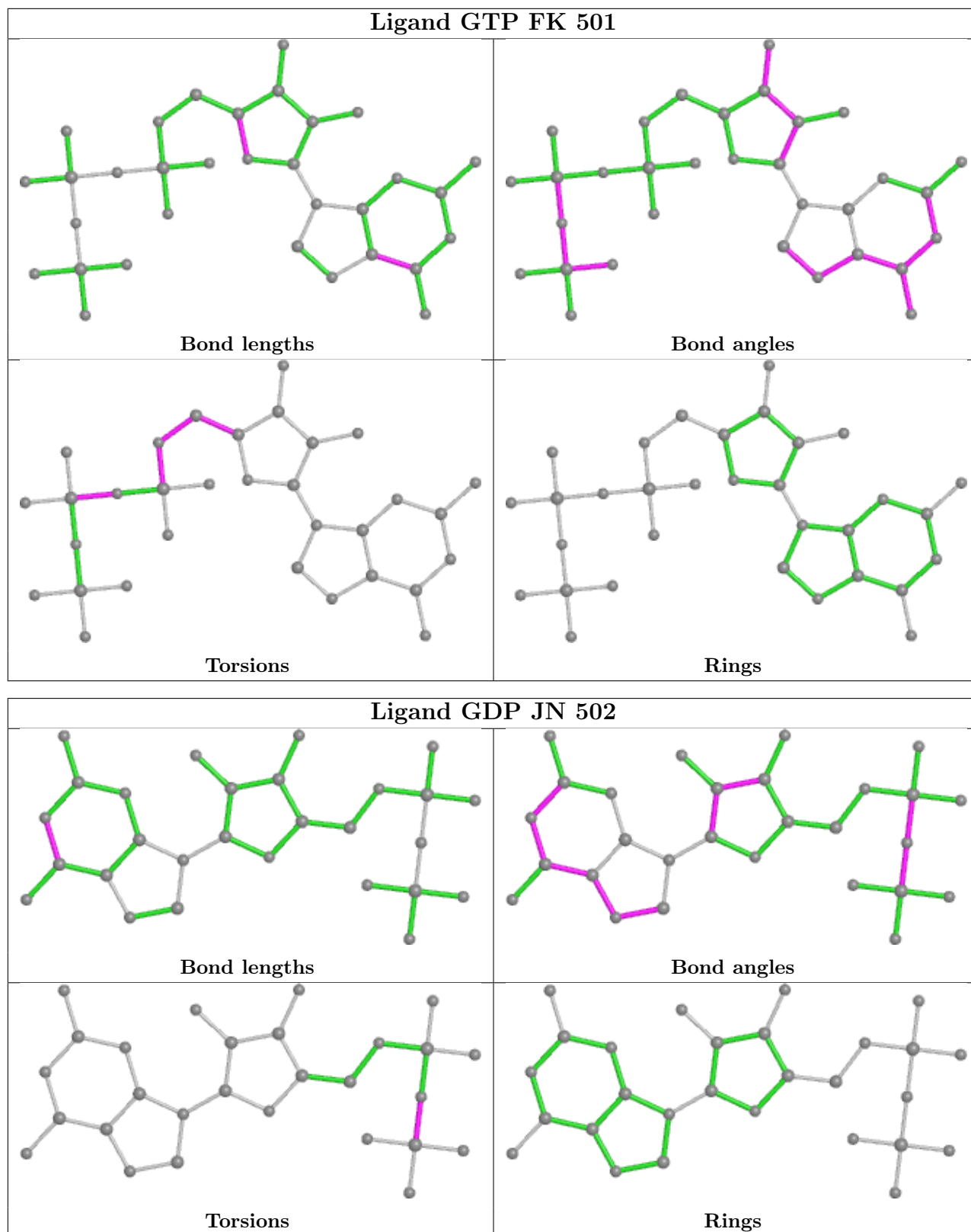


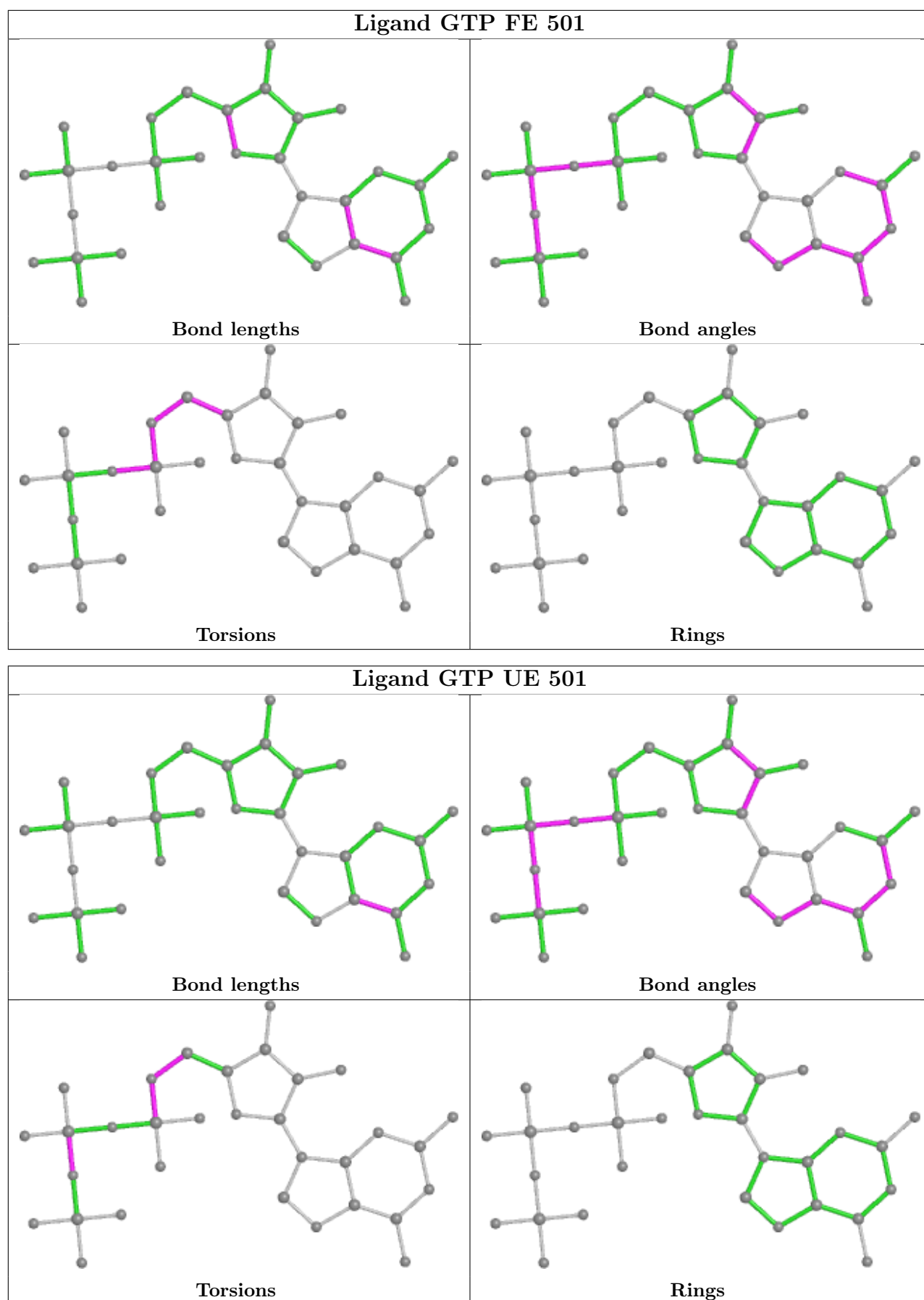




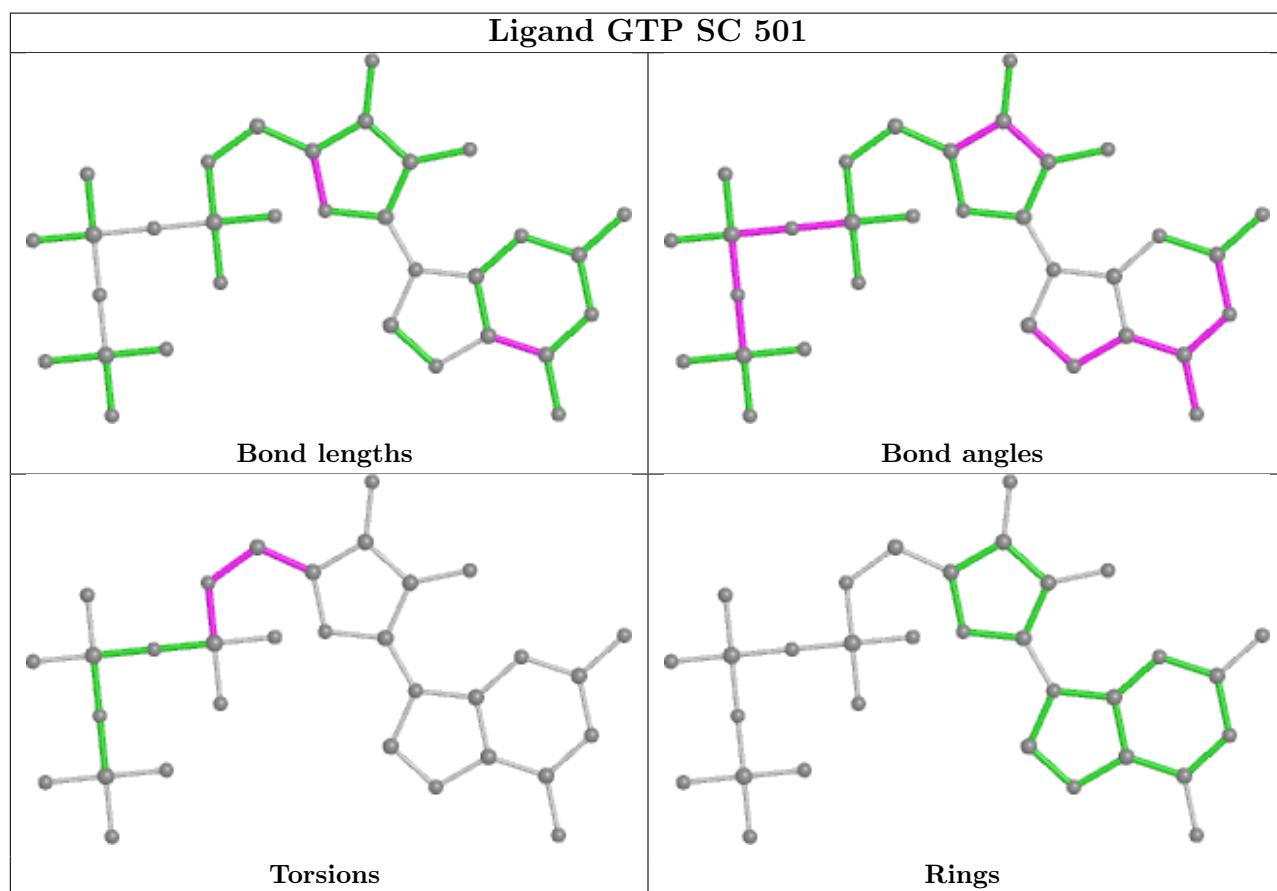
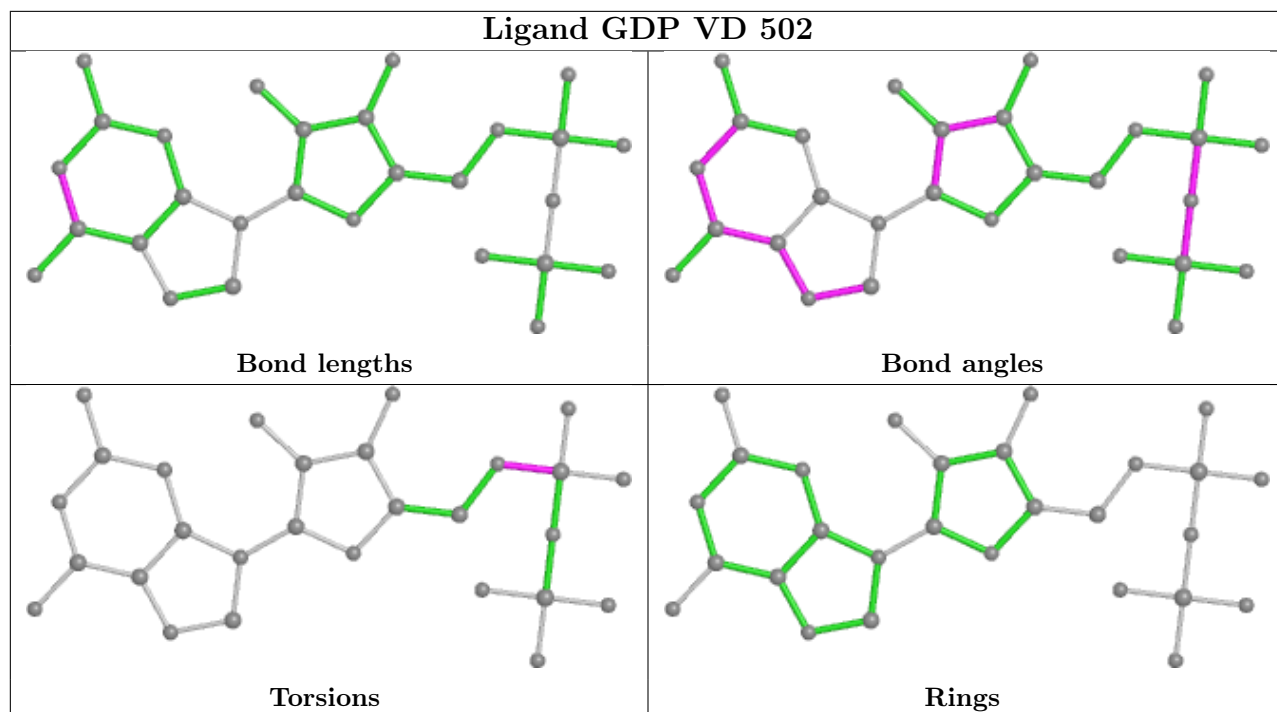


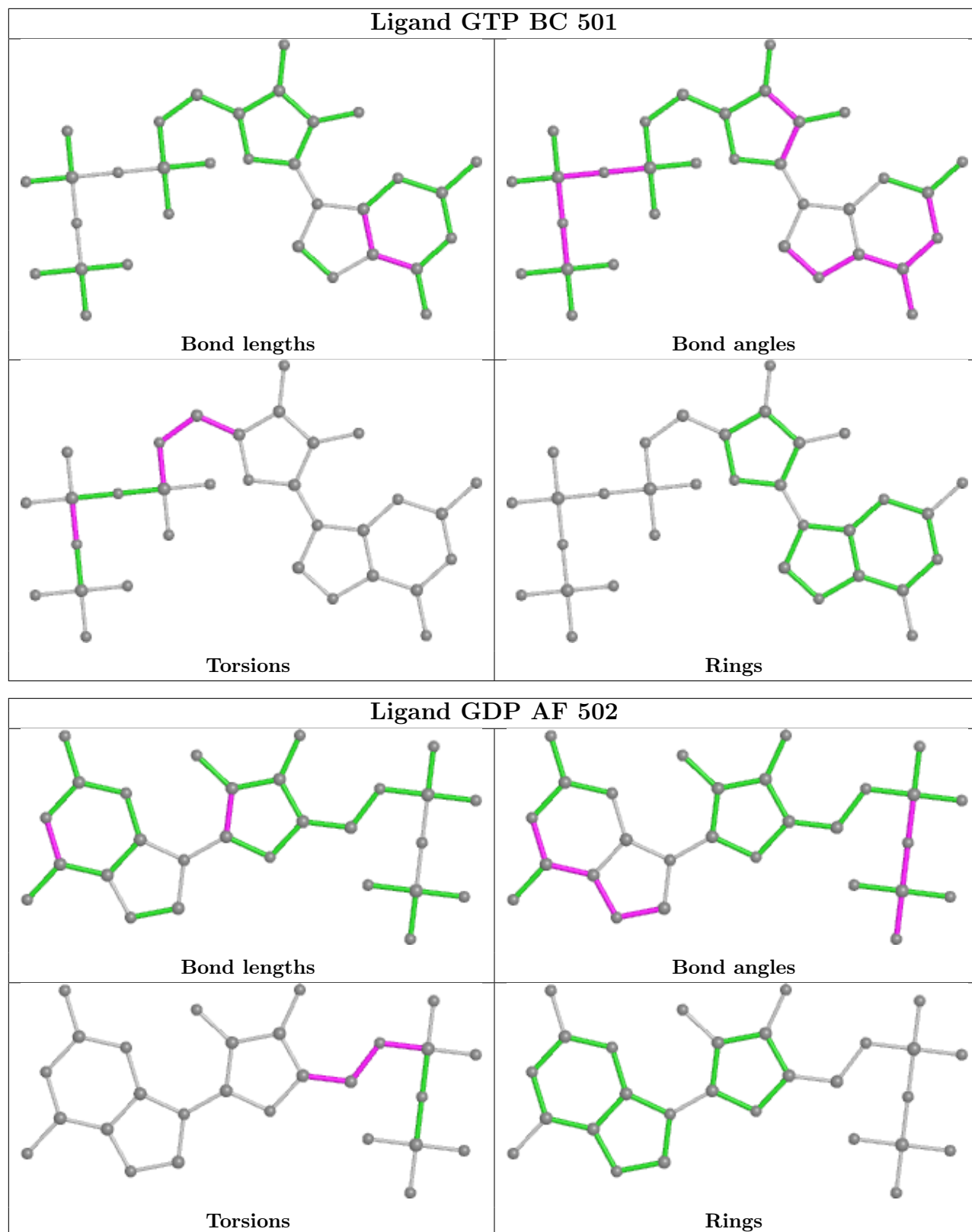


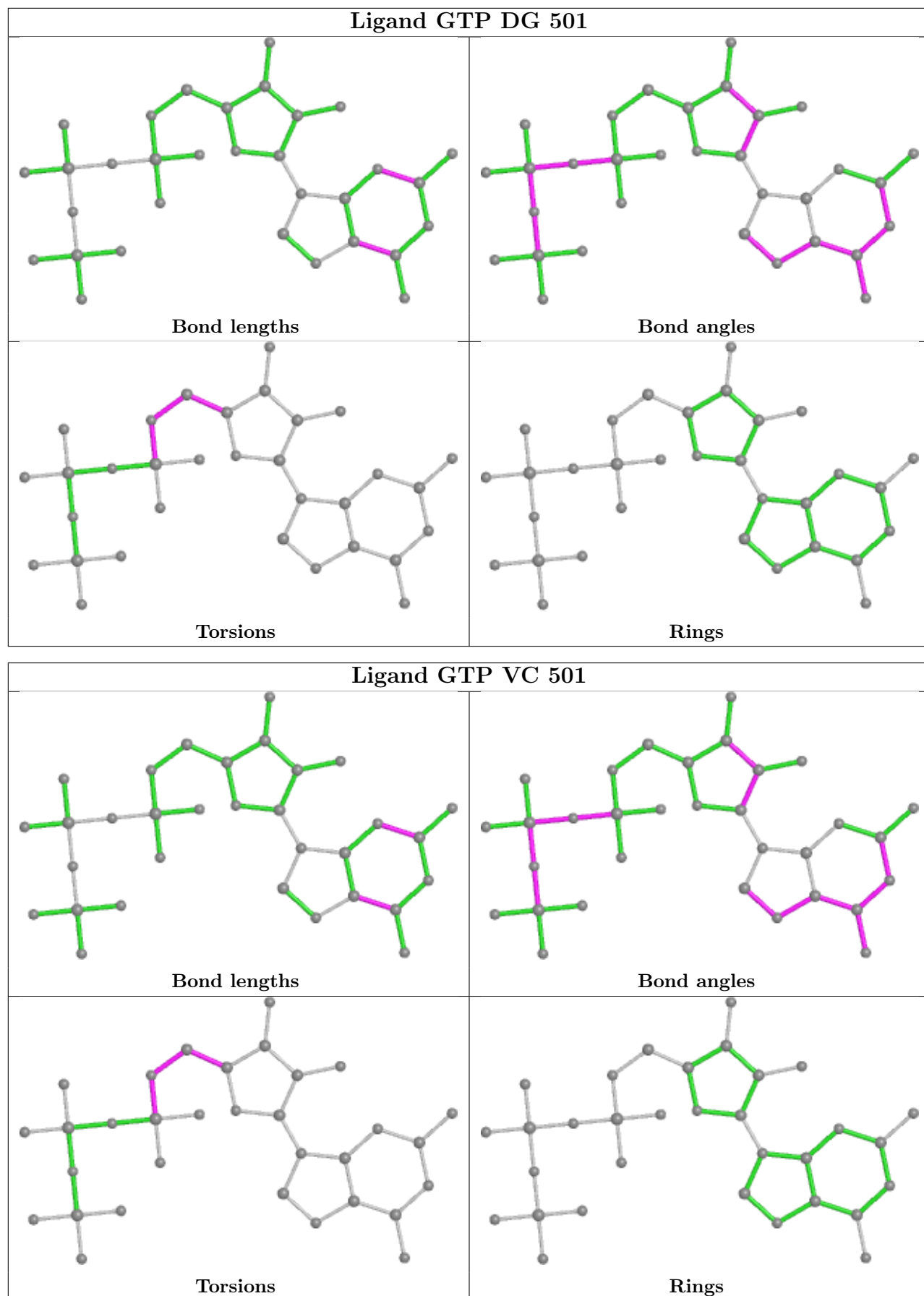


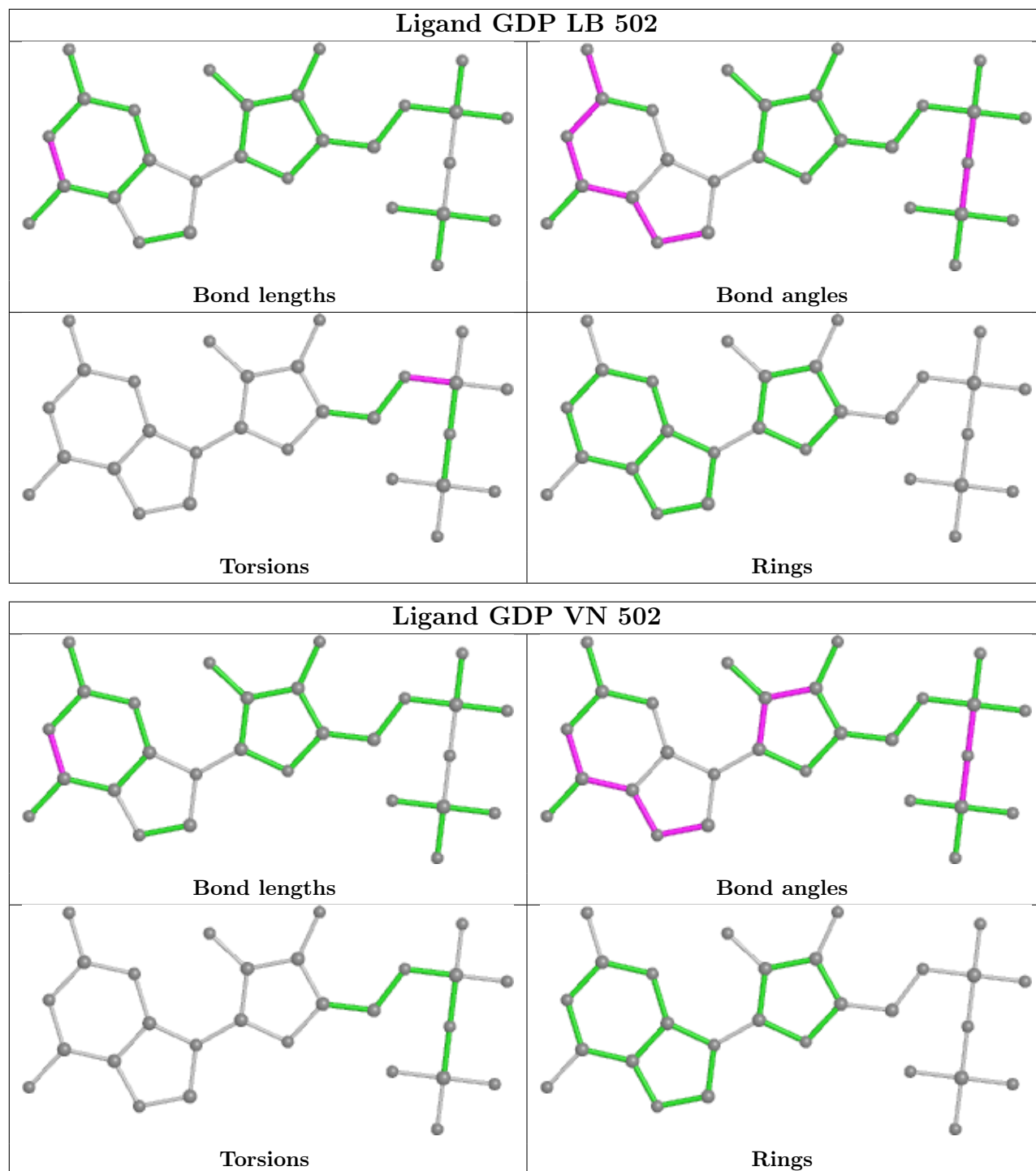


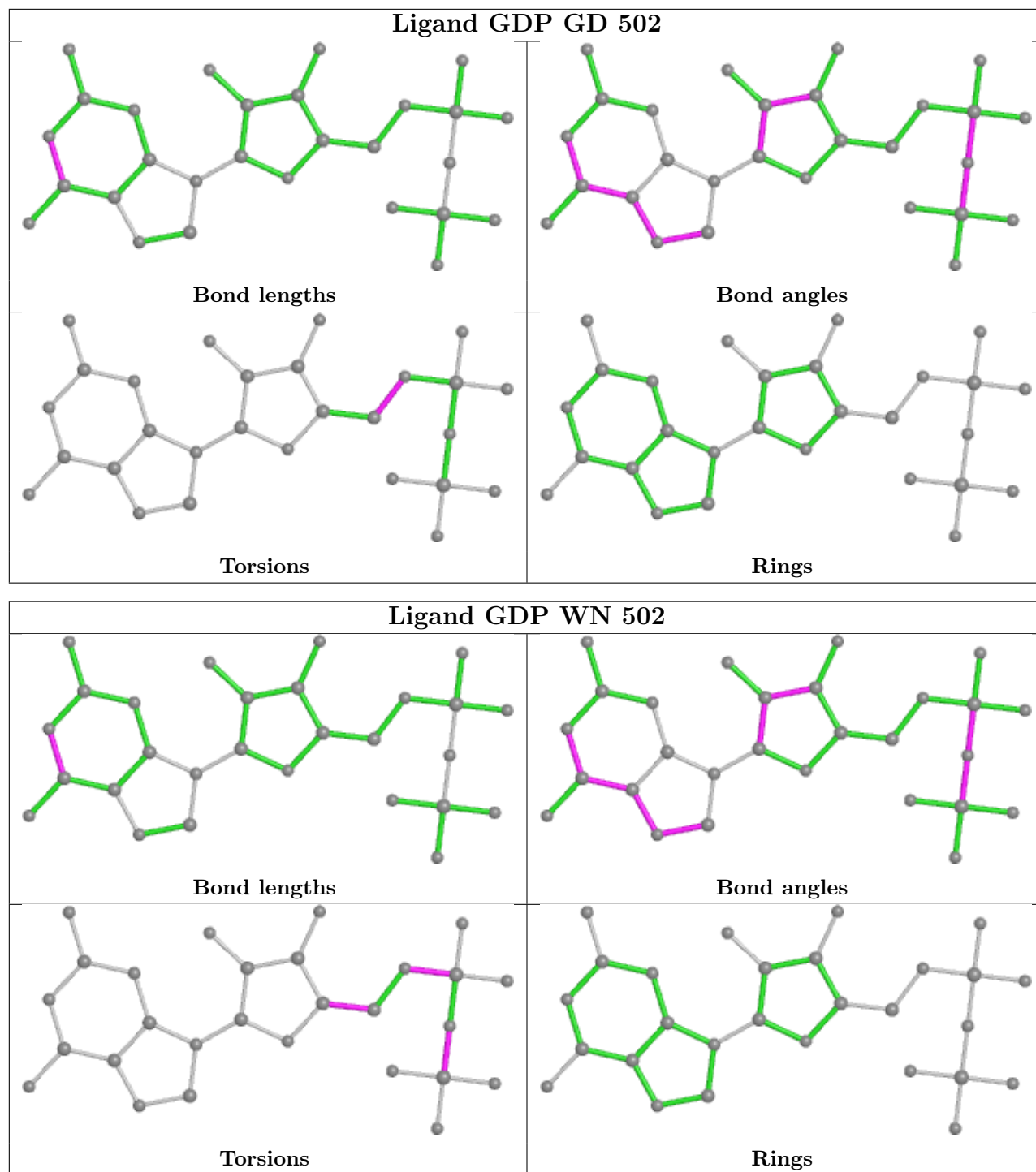


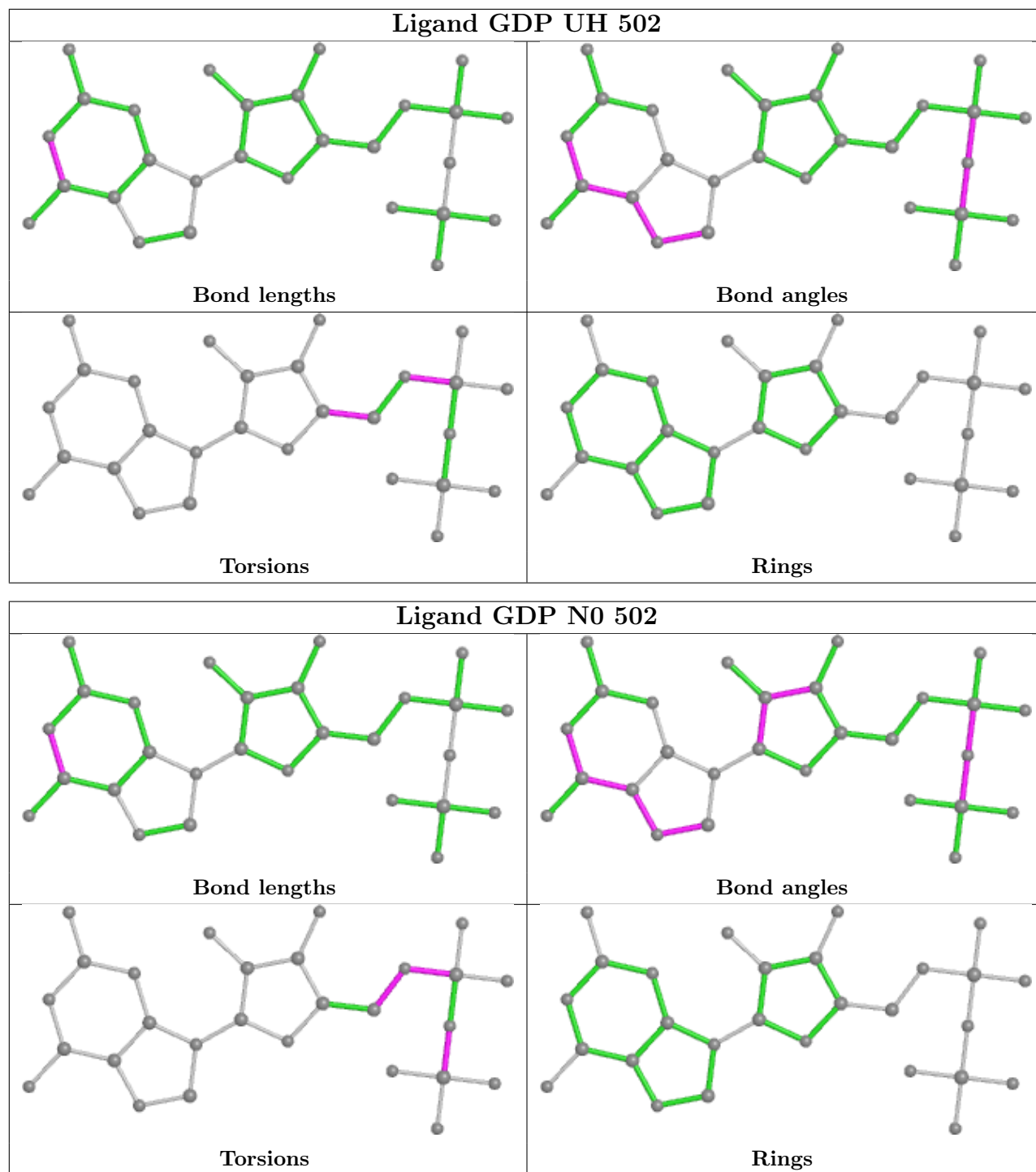


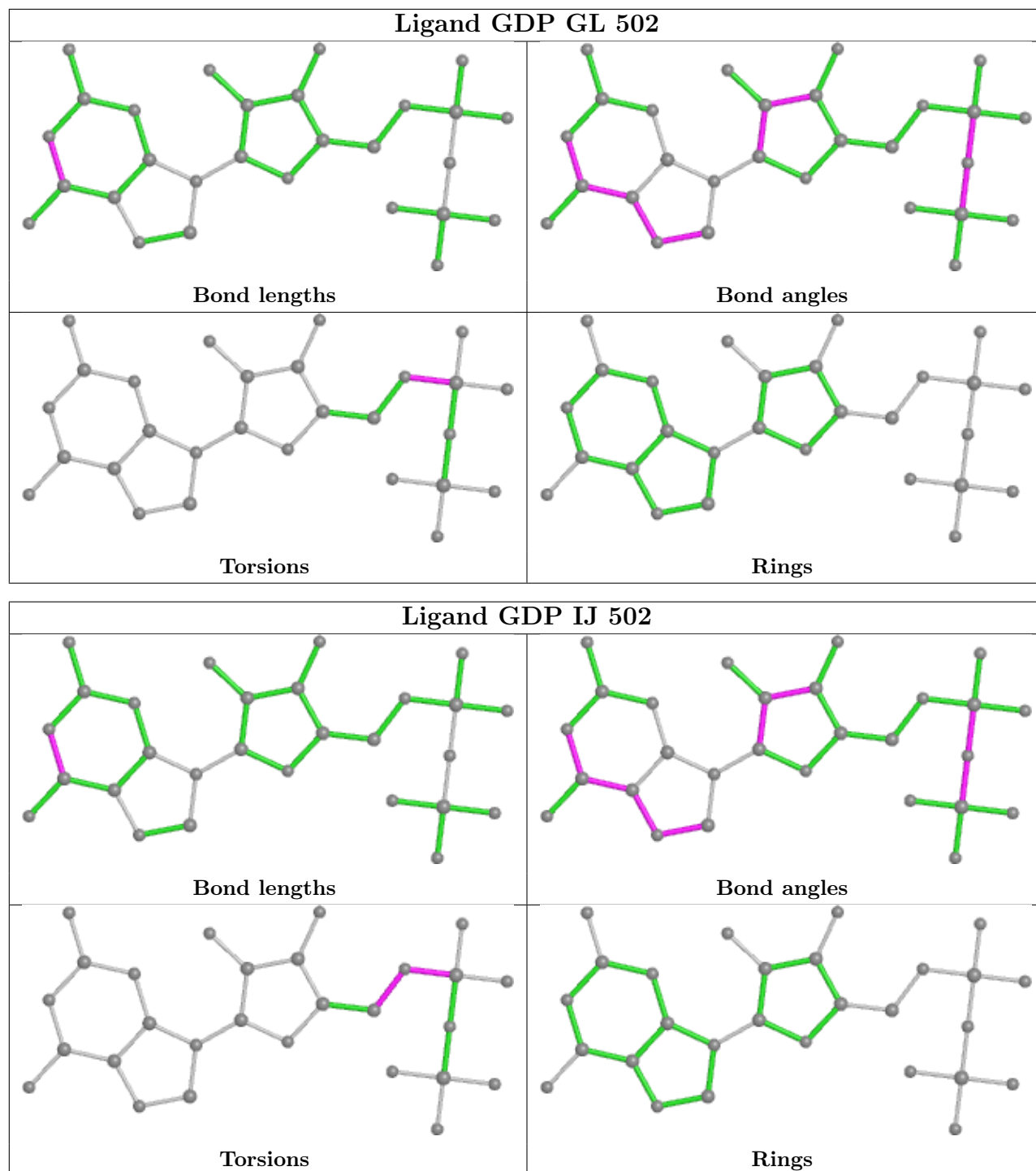


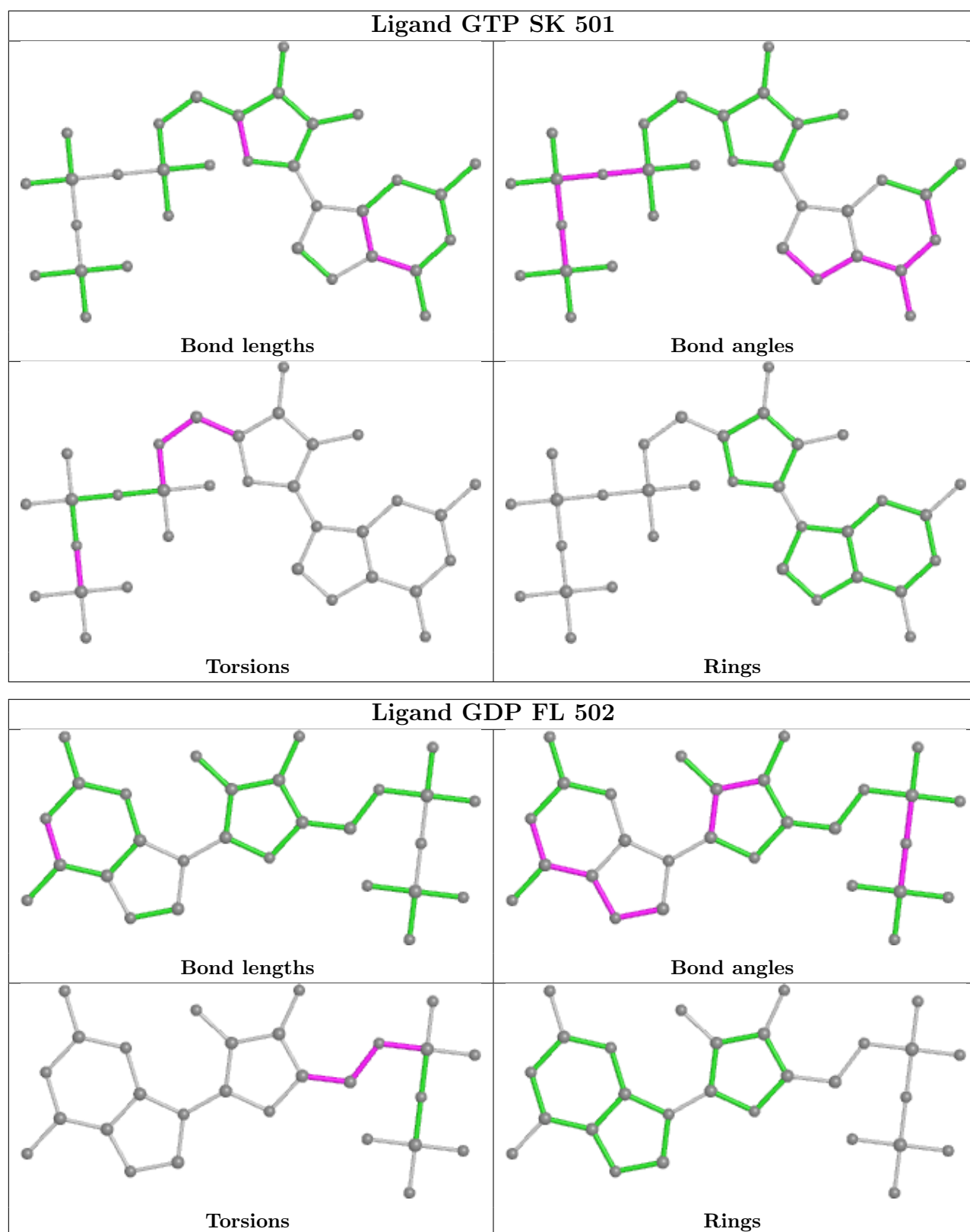




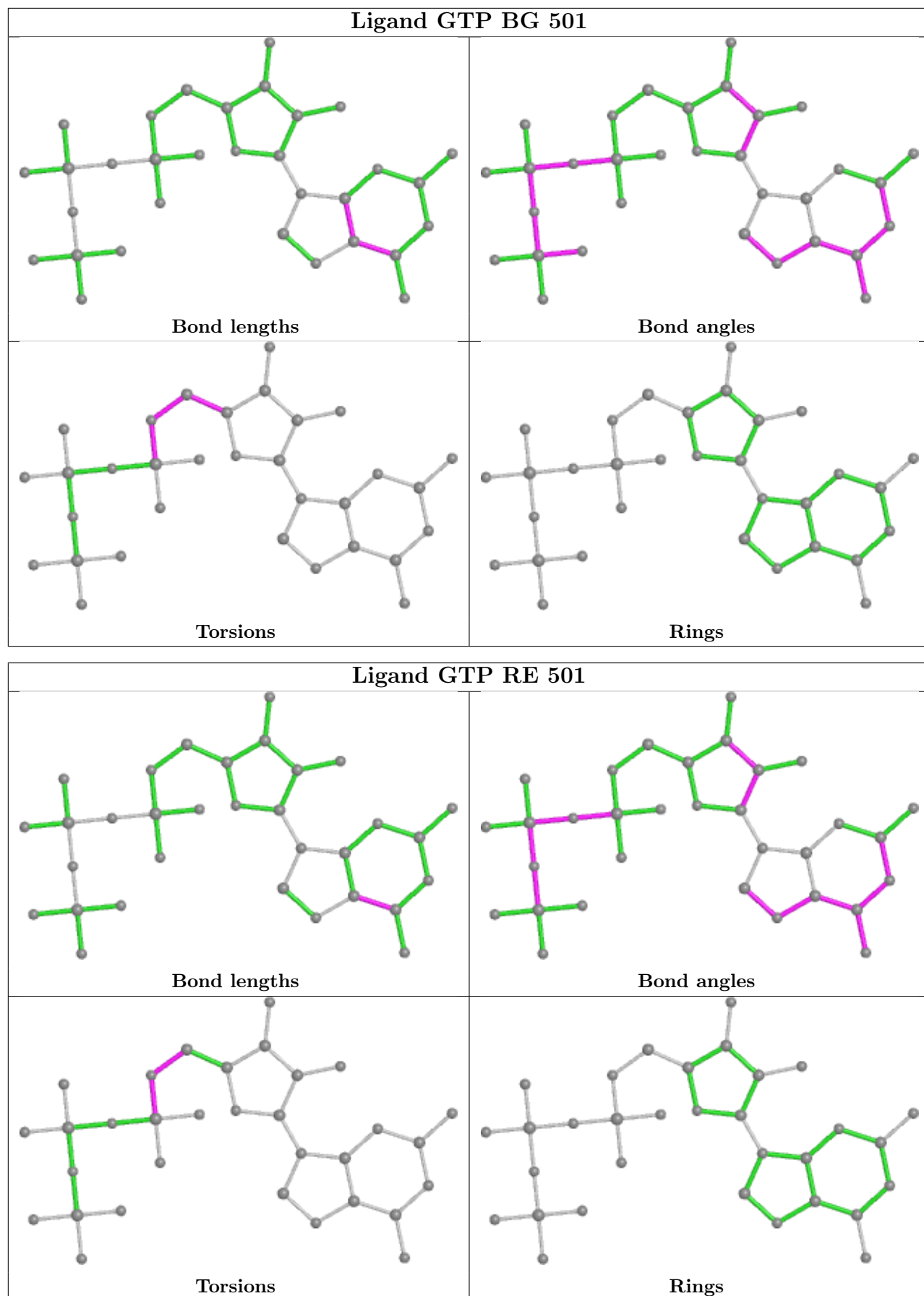


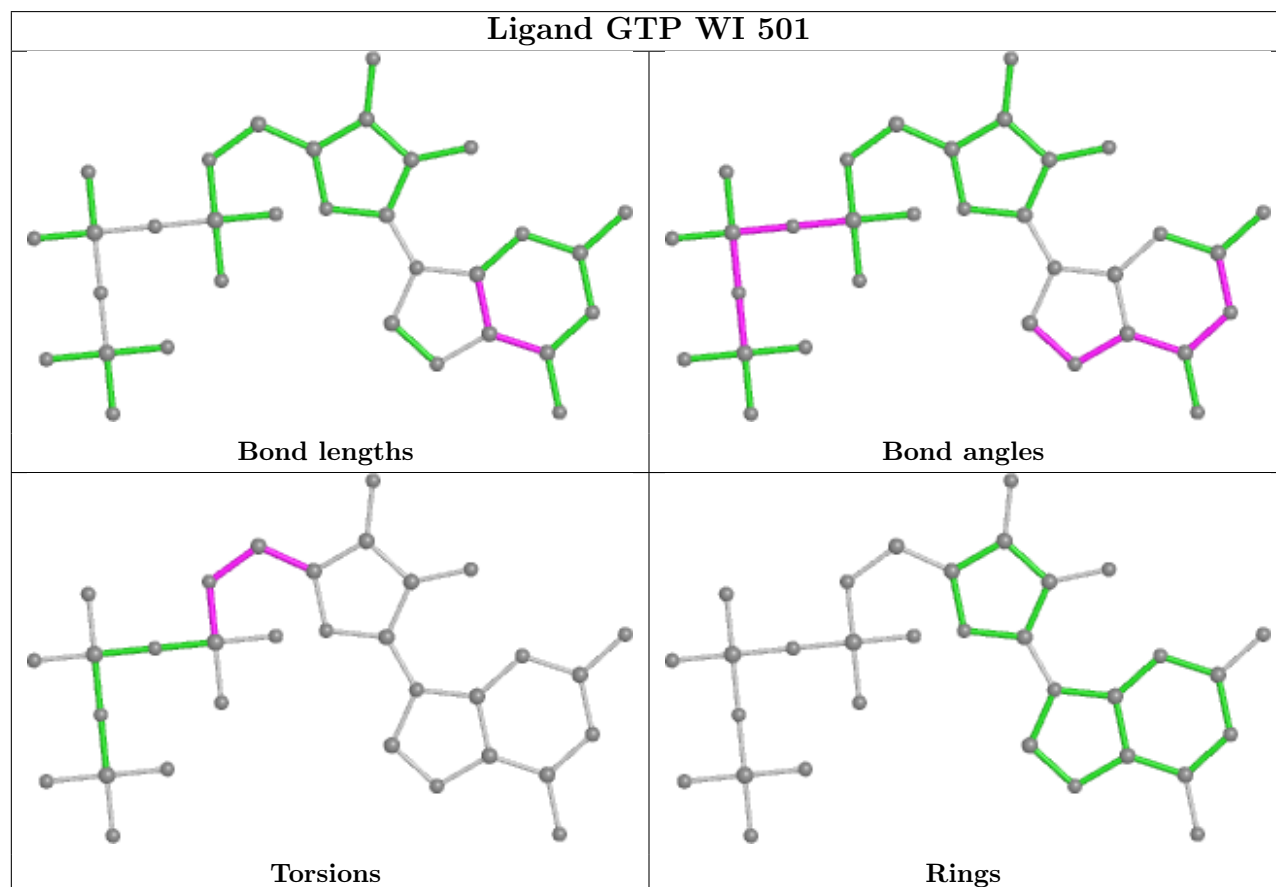
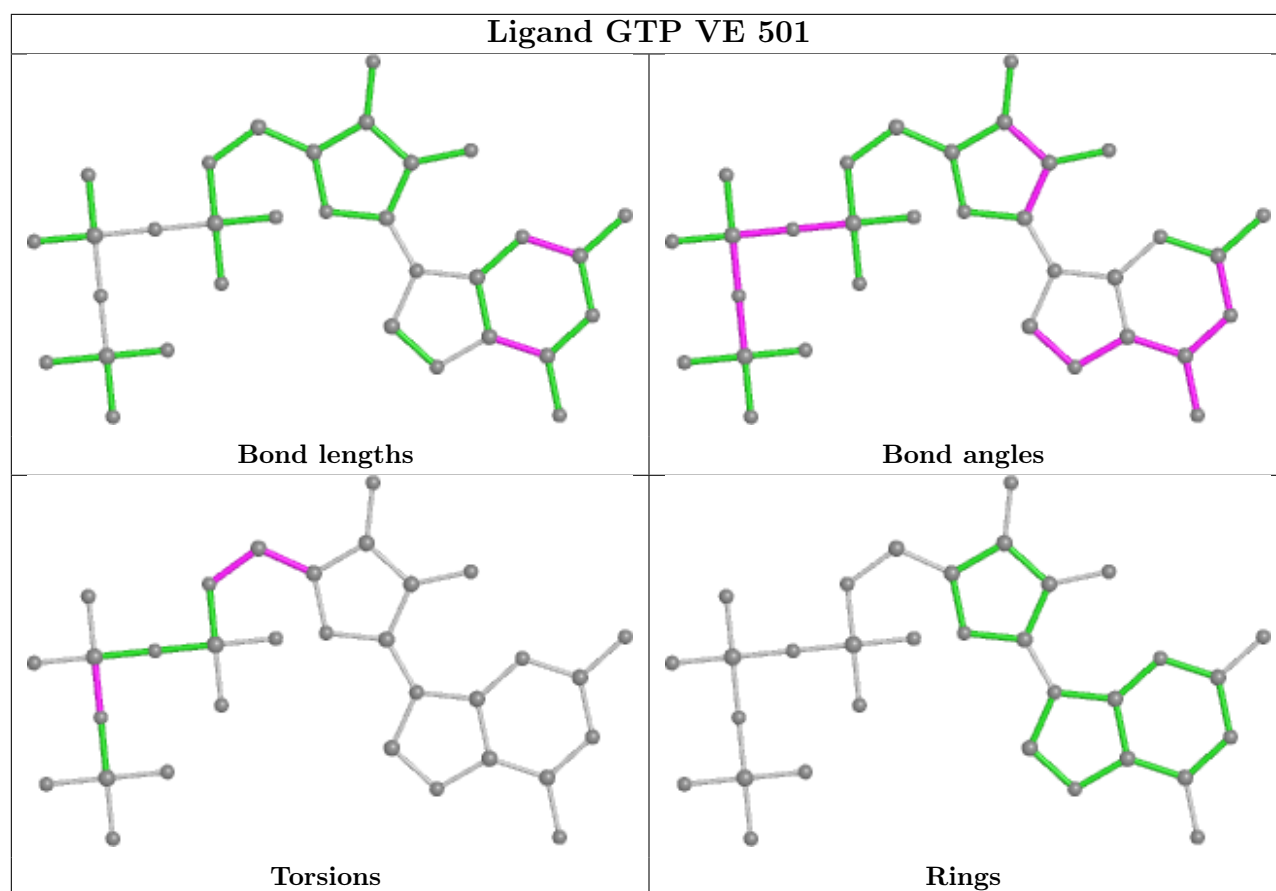


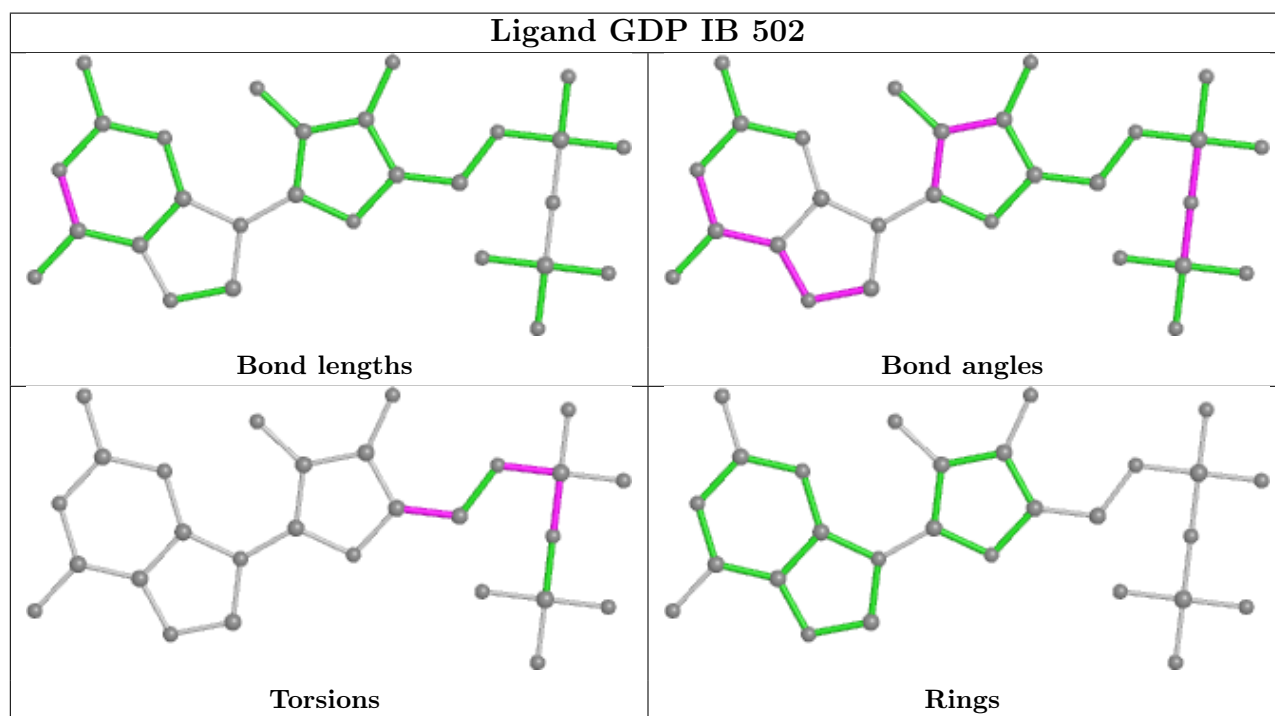
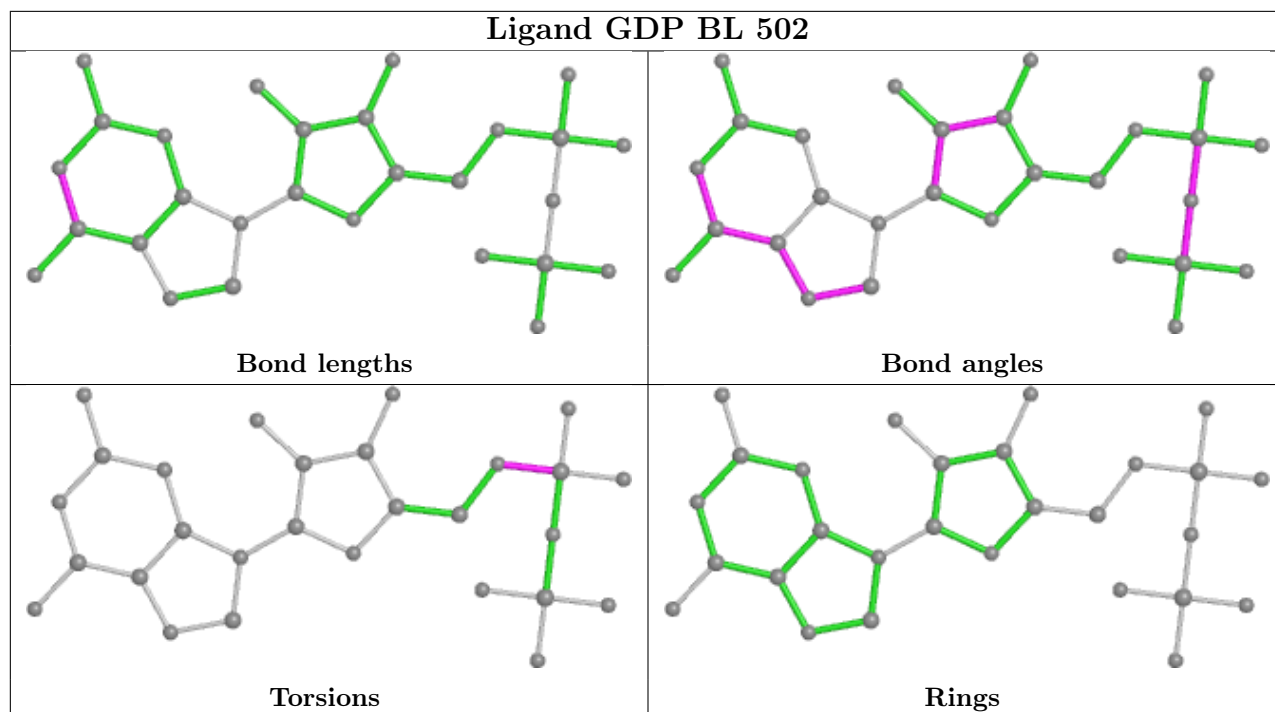


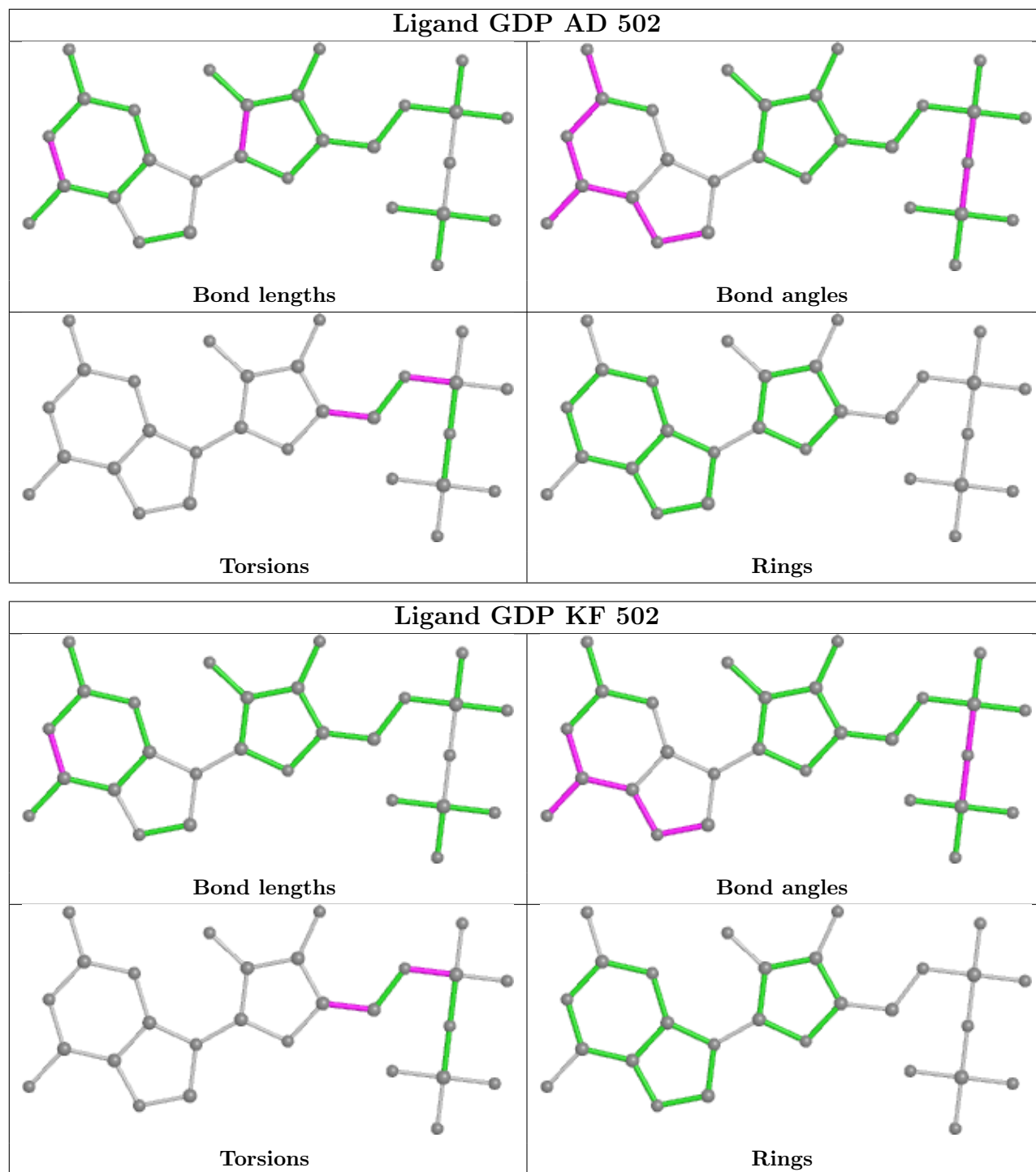


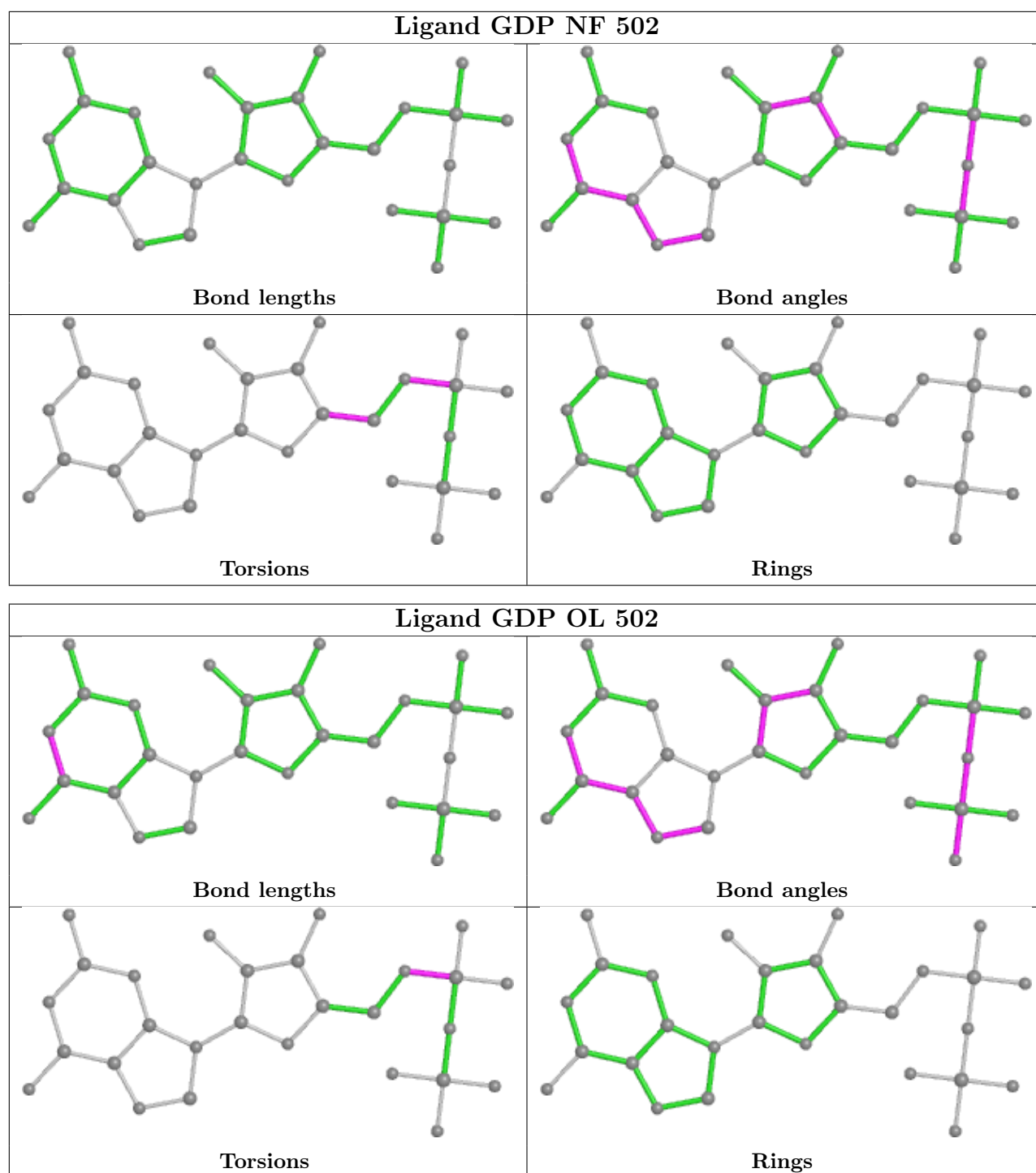


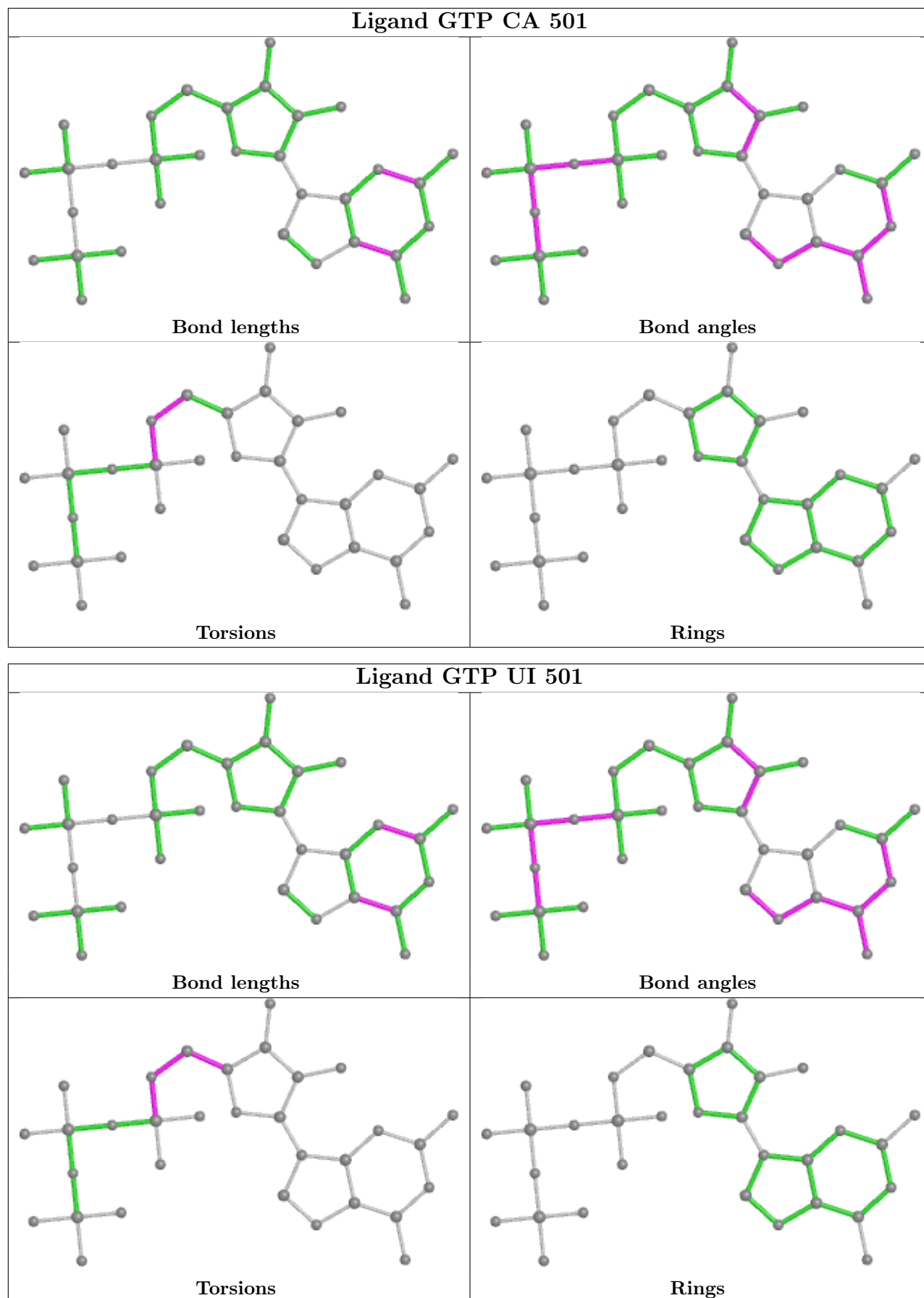


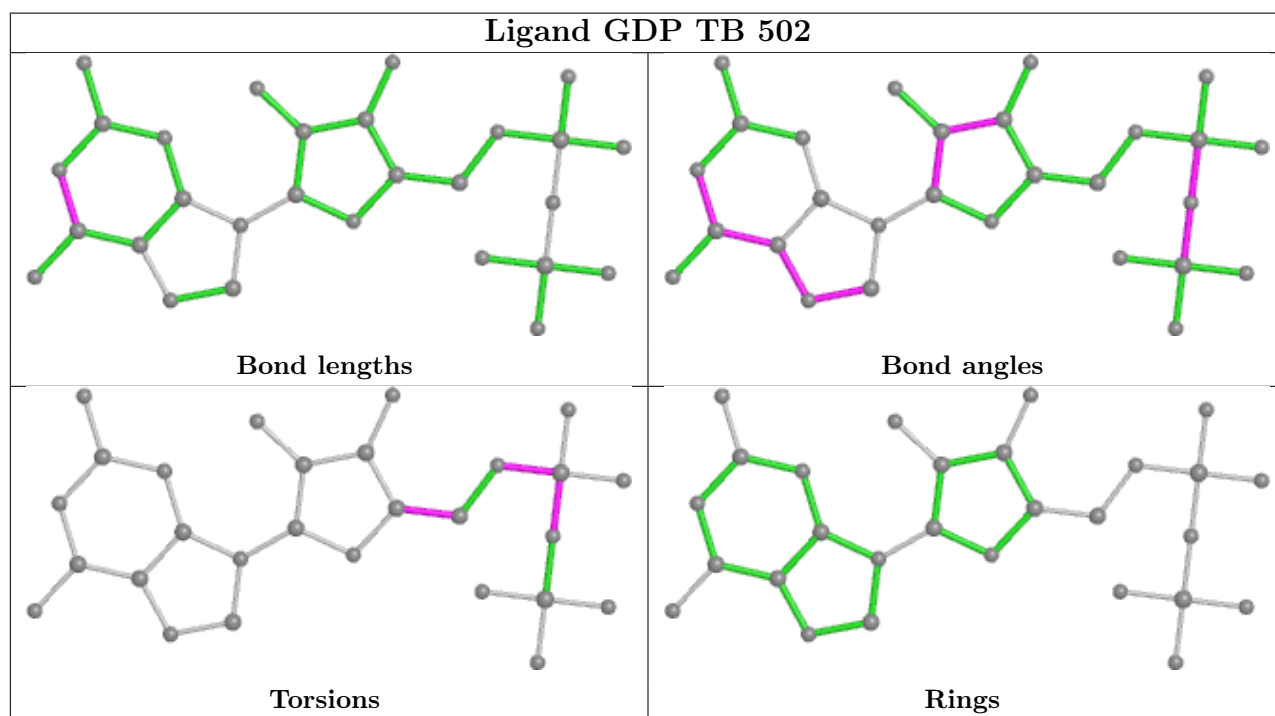
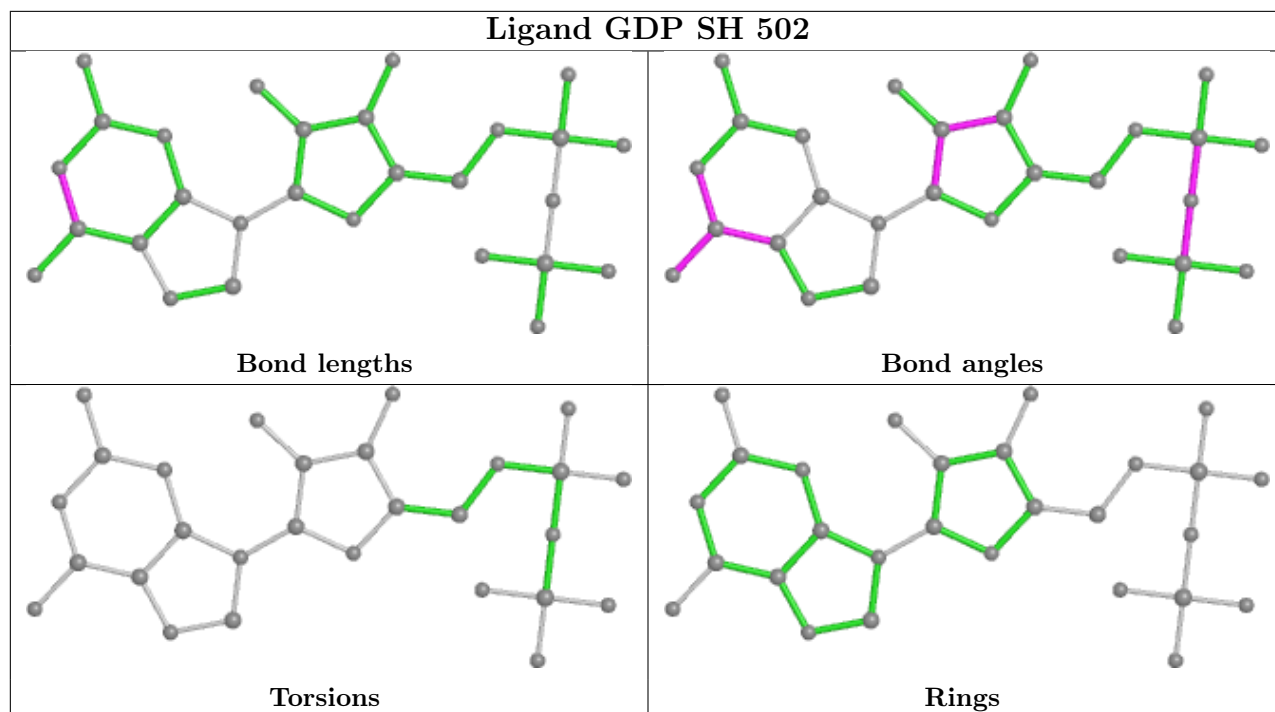


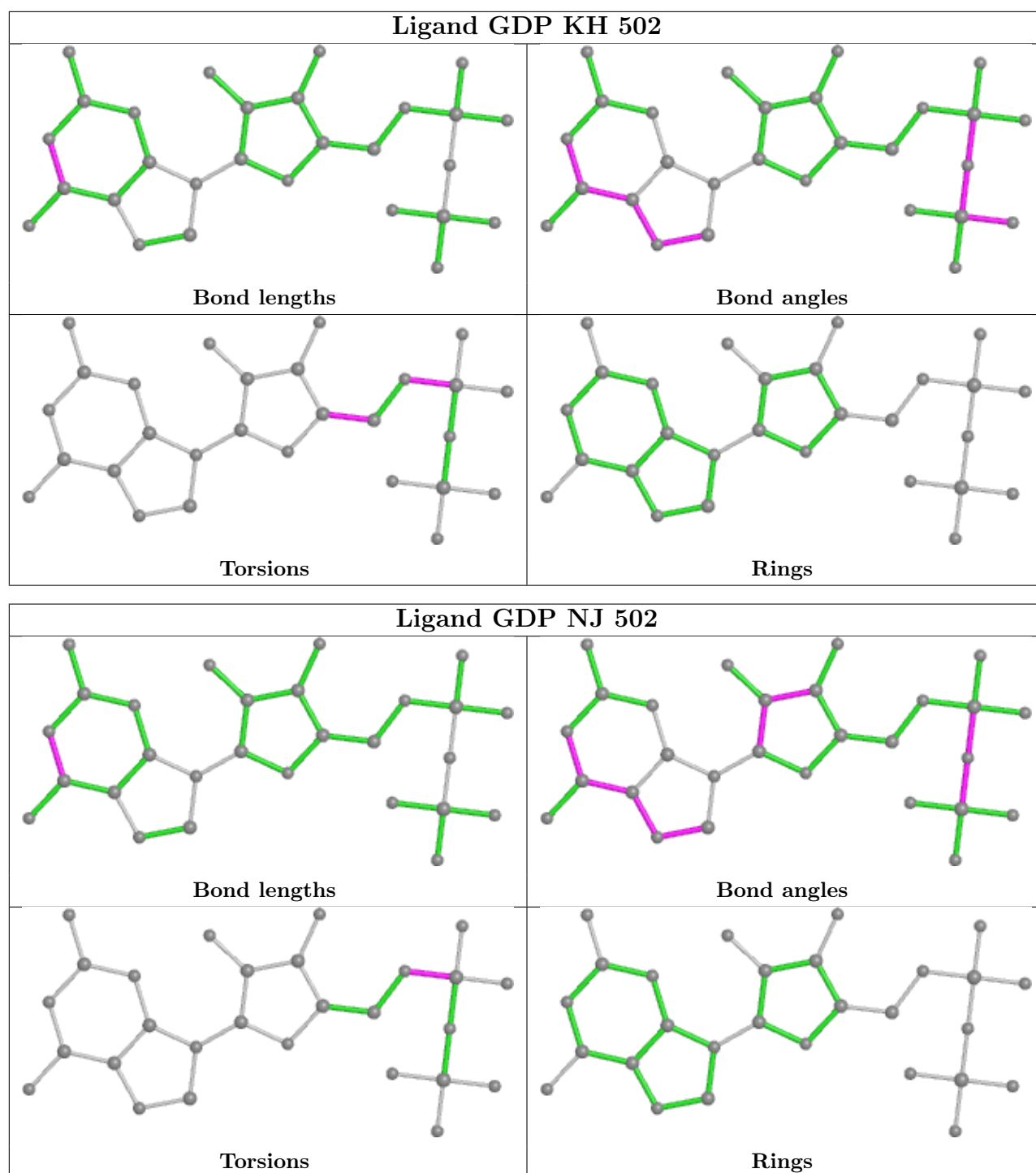




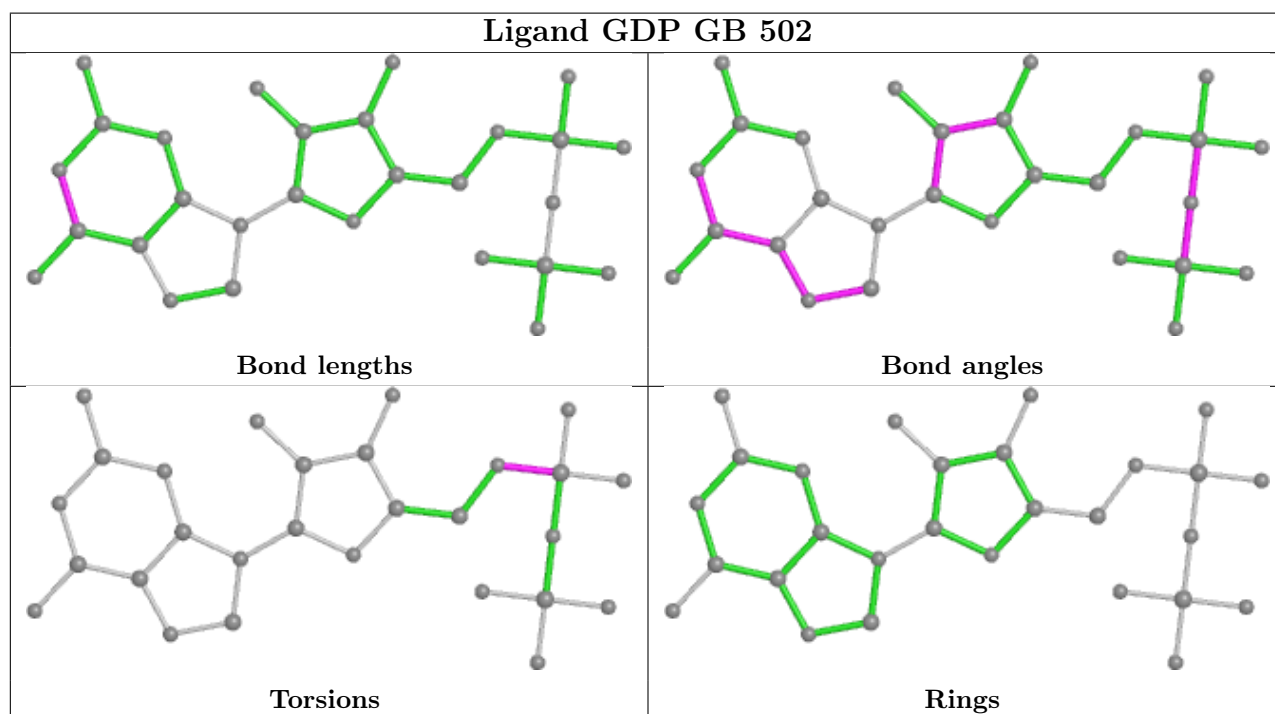
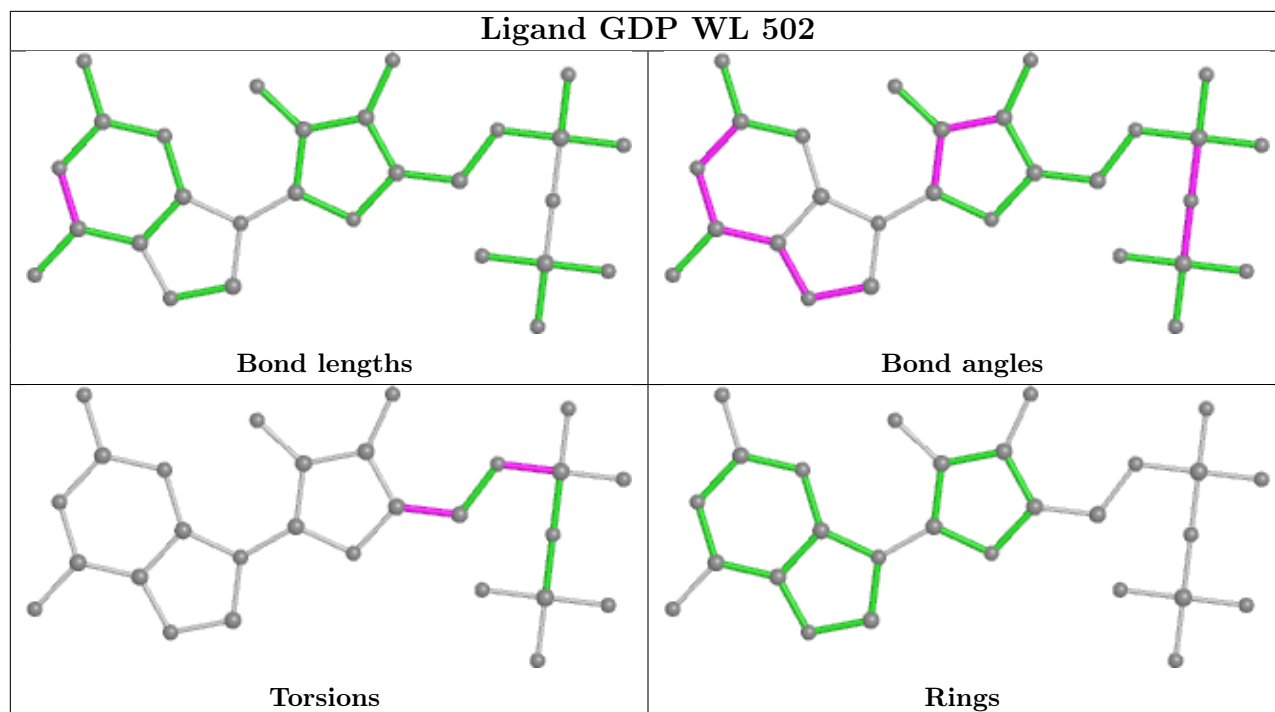


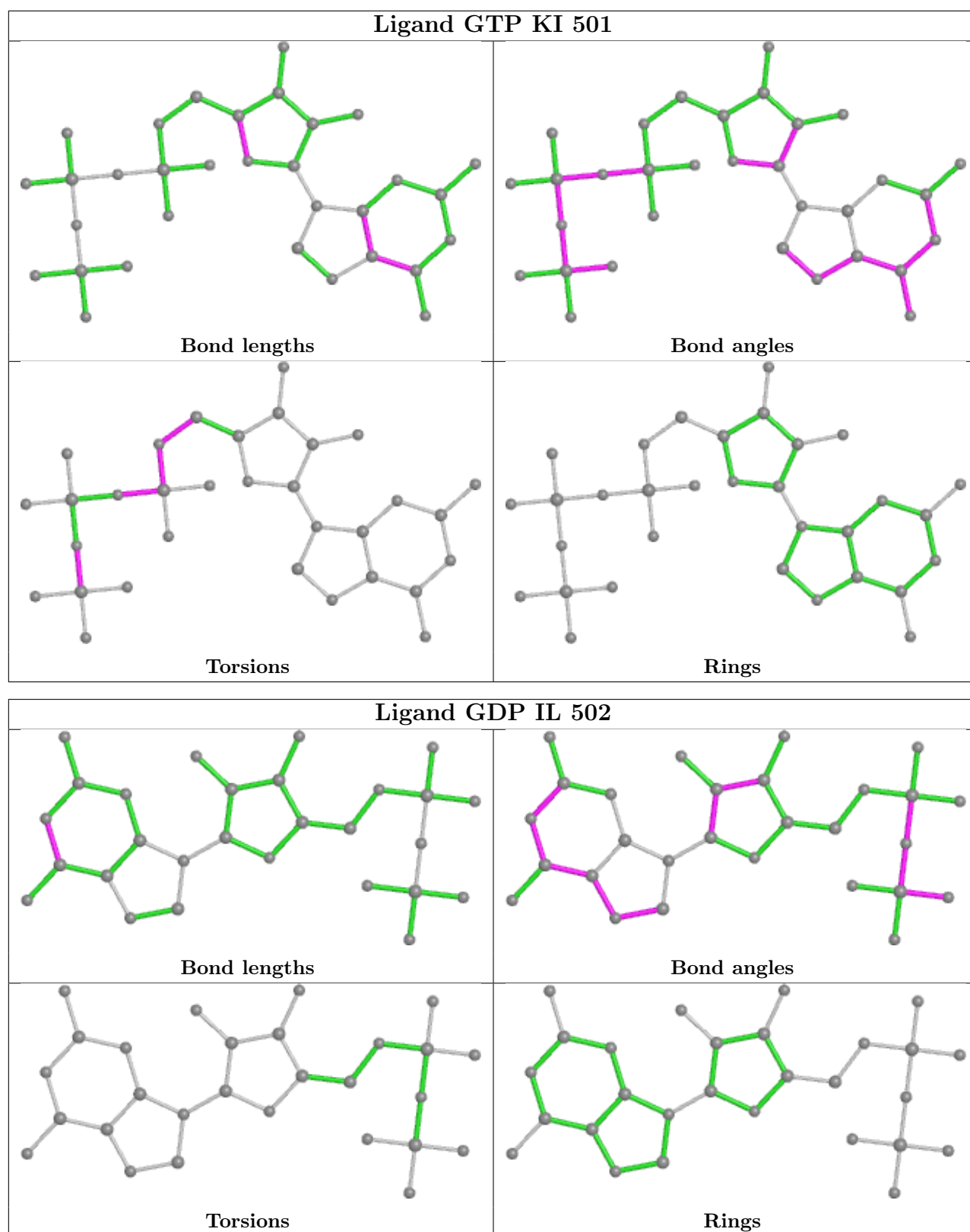


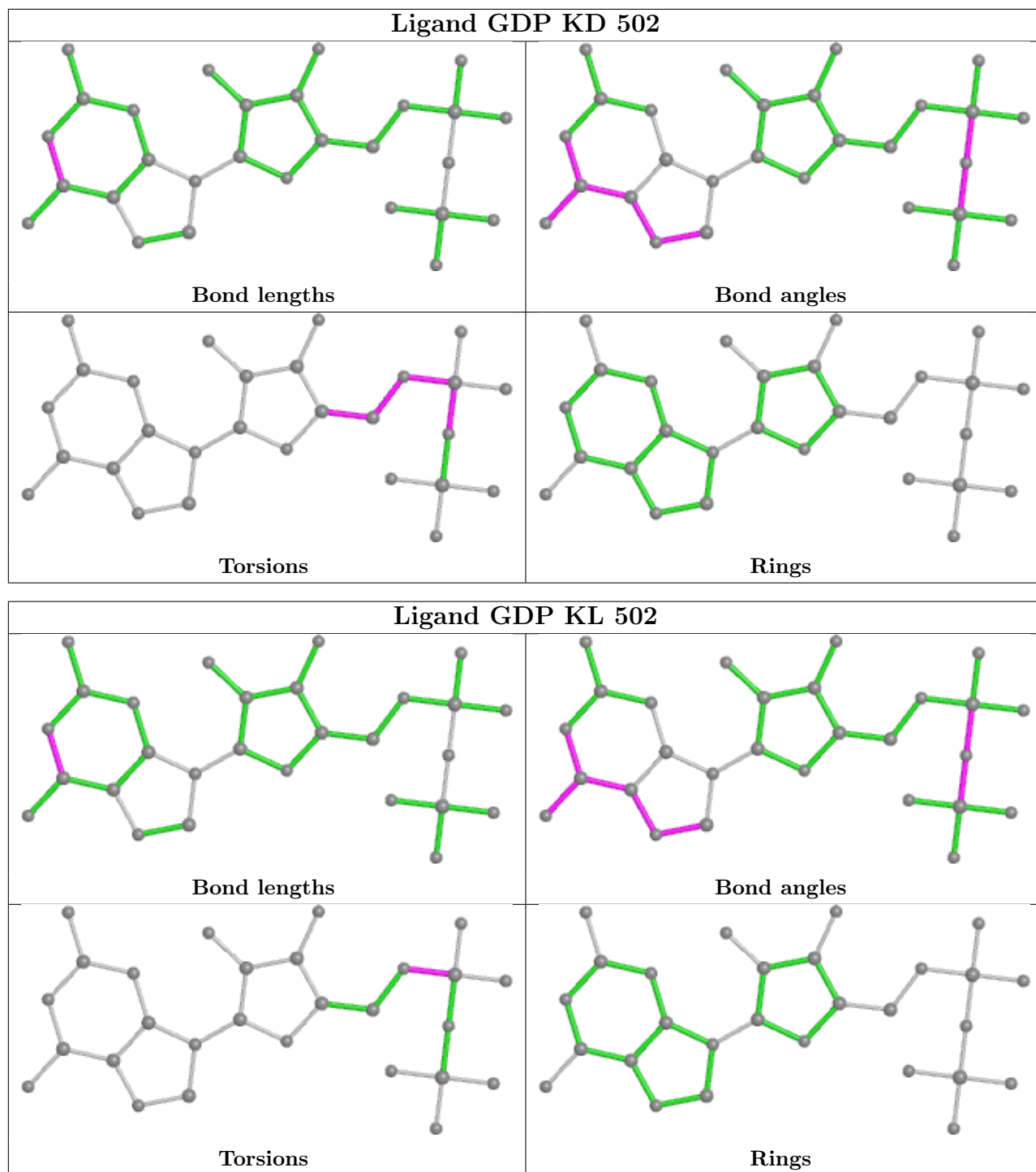


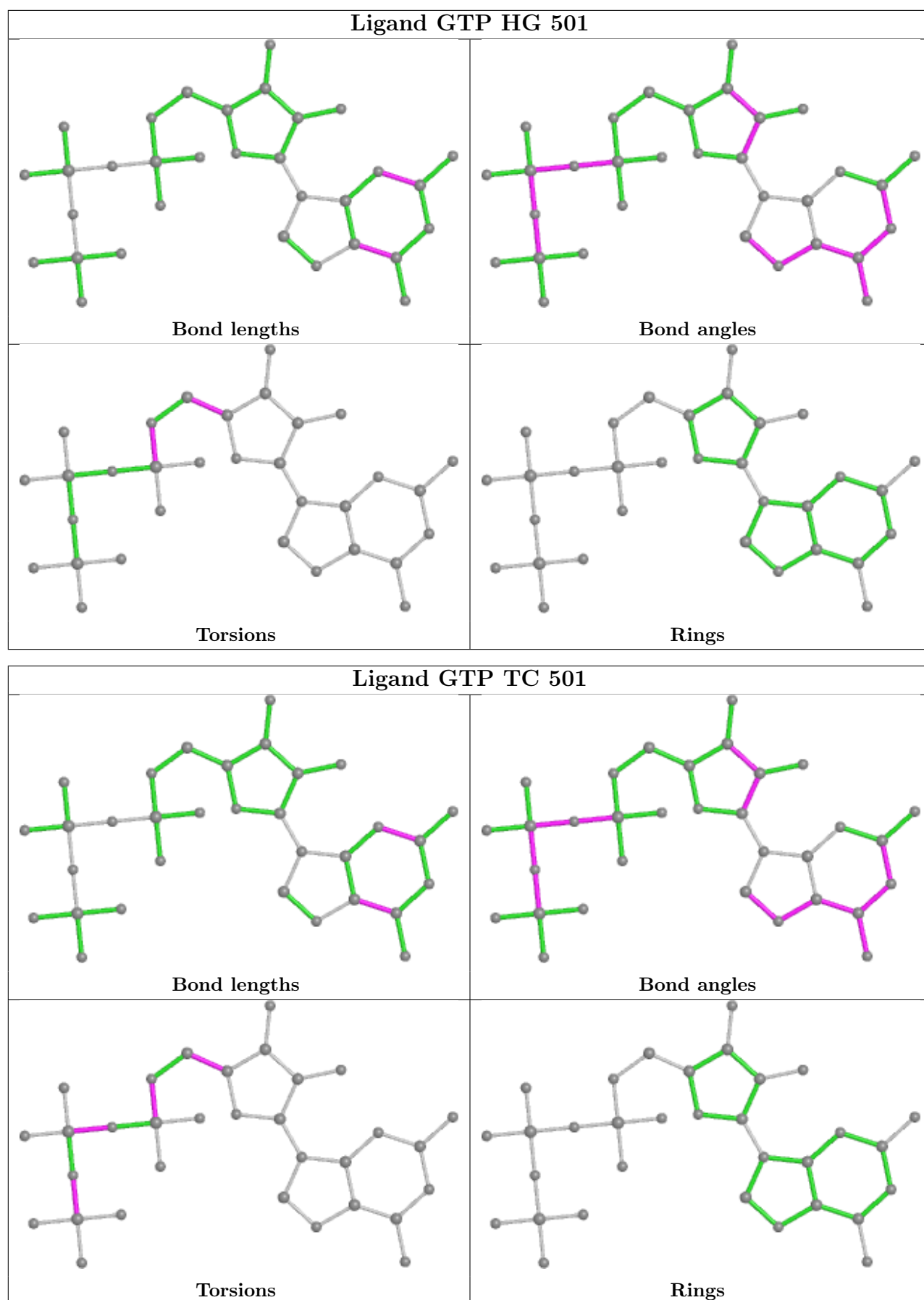


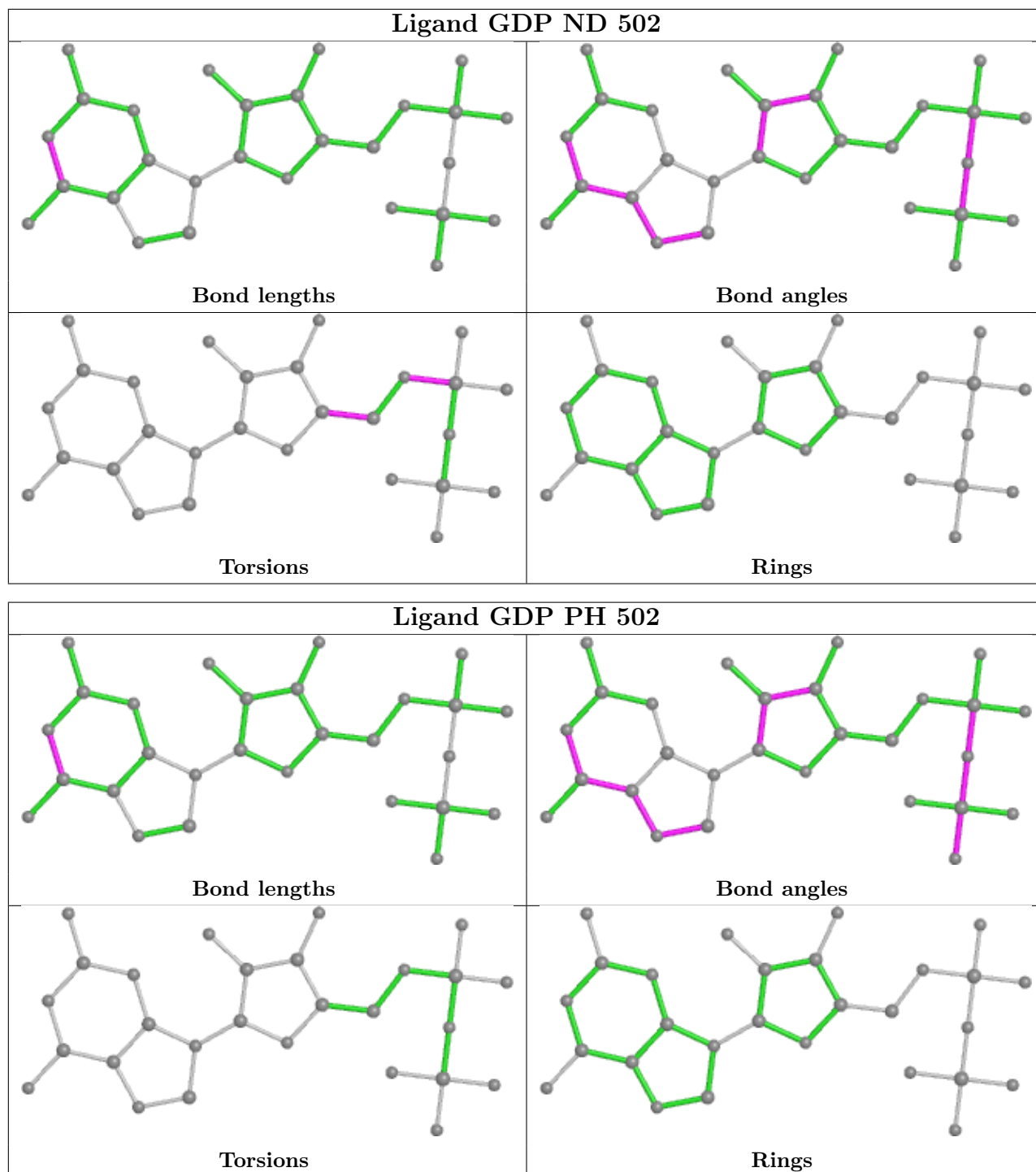


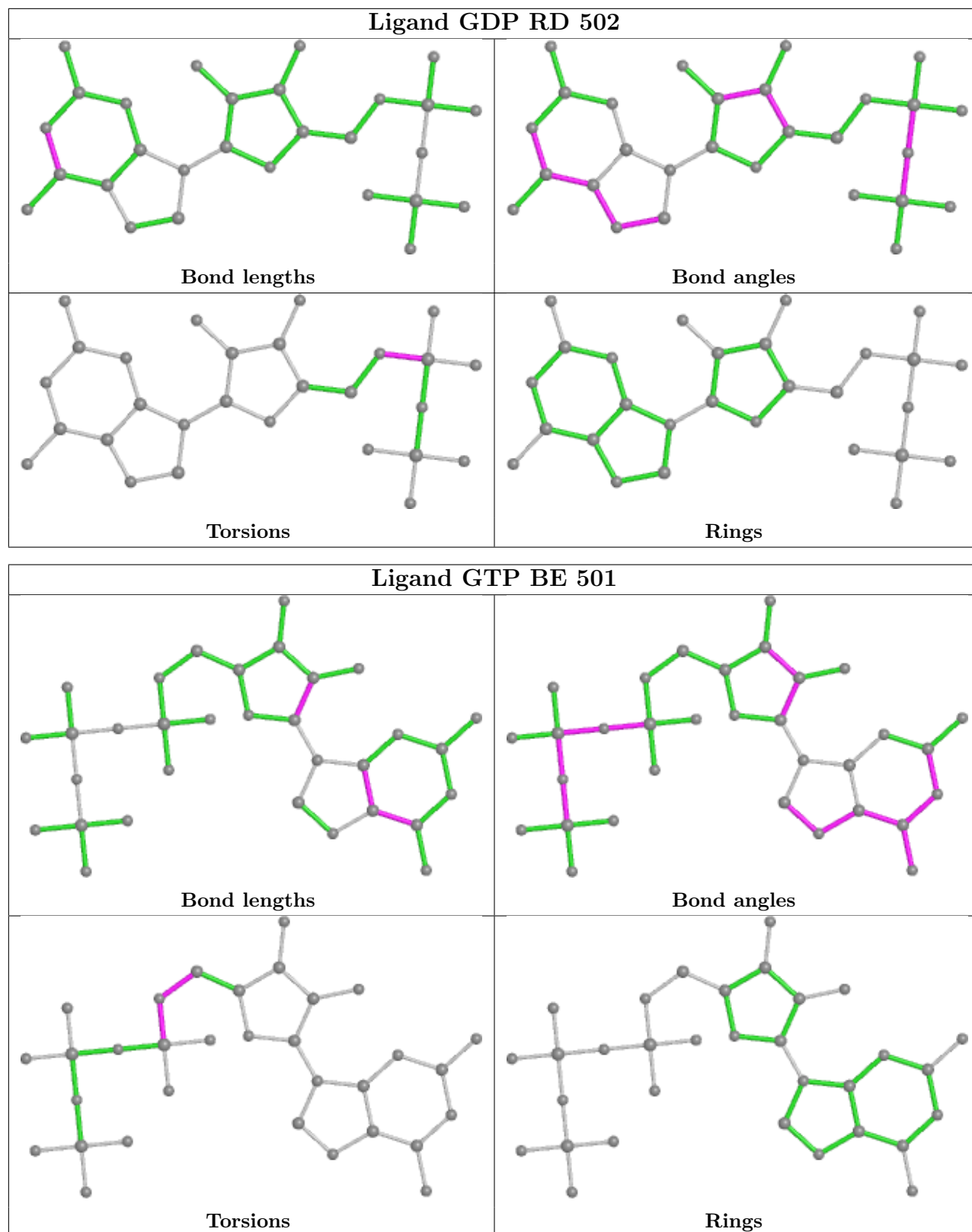


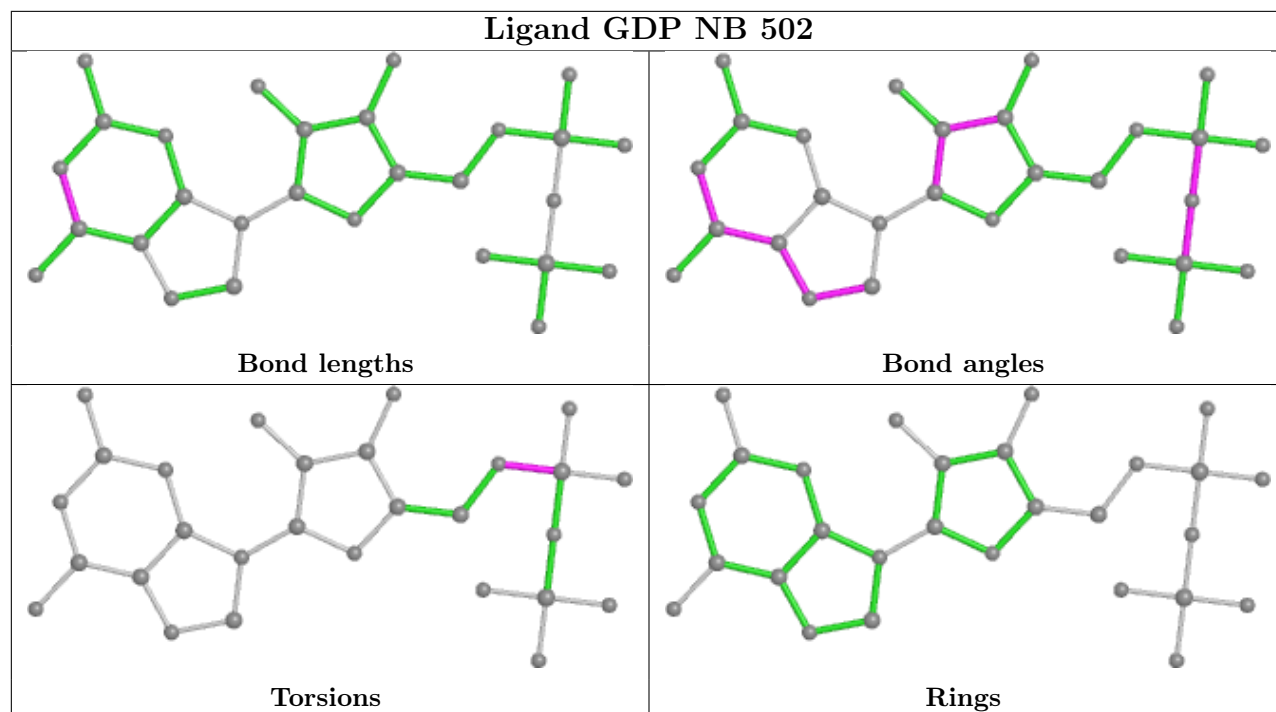












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

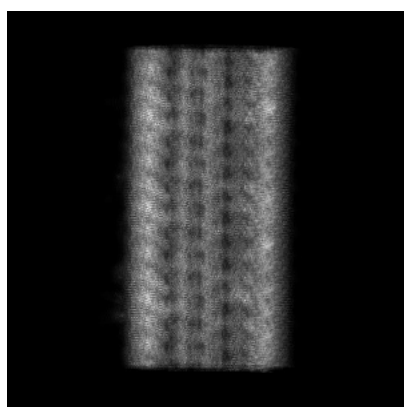
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24664. These allow visual inspection of the internal detail of the map and identification of artifacts.

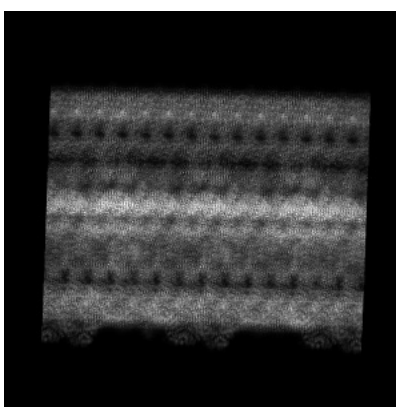
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

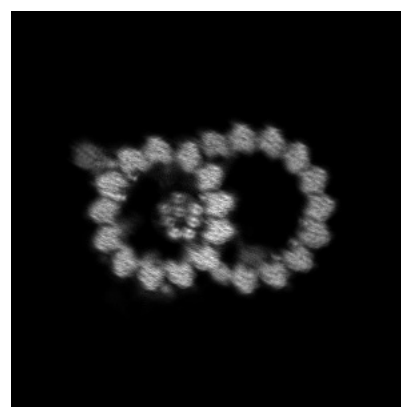
#### 6.1.1 Primary map



X



Y

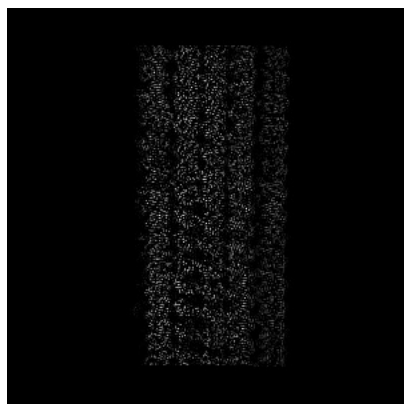


Z

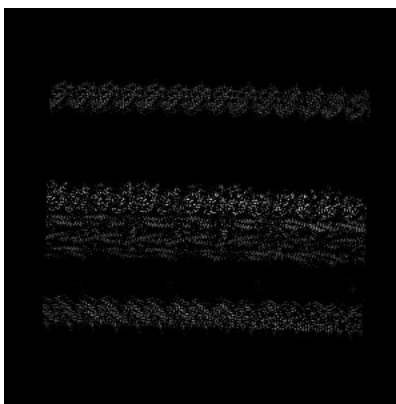
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

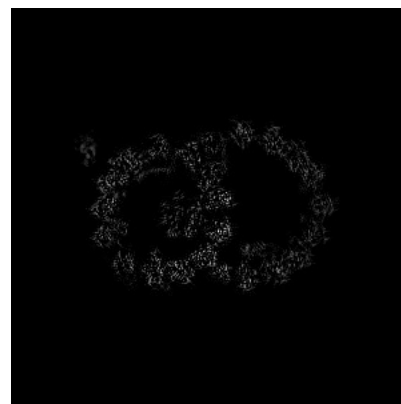
#### 6.2.1 Primary map



X Index: 336



Y Index: 336



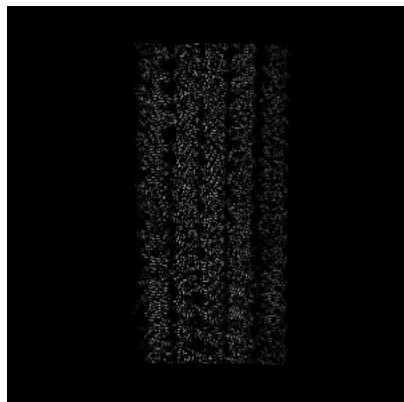
Z Index: 336



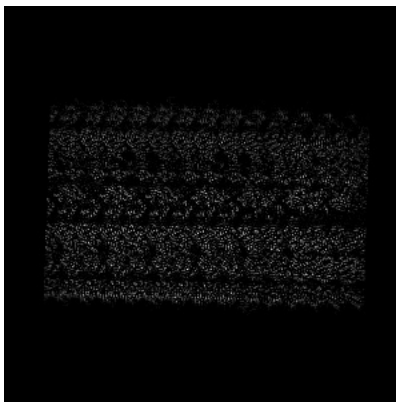
The images above show central slices of the map in three orthogonal directions.

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

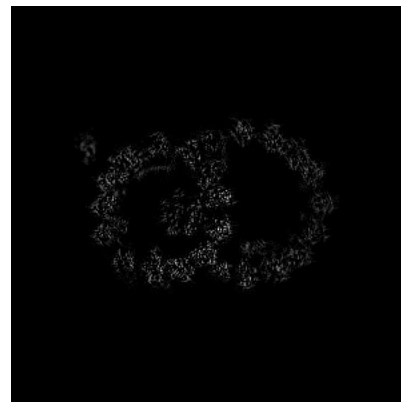
### 6.3.1 Primary map



X Index: 339



Y Index: 236

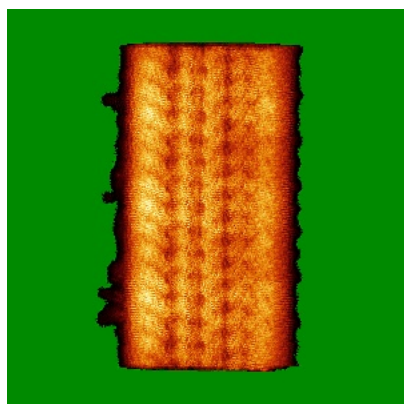


Z Index: 336

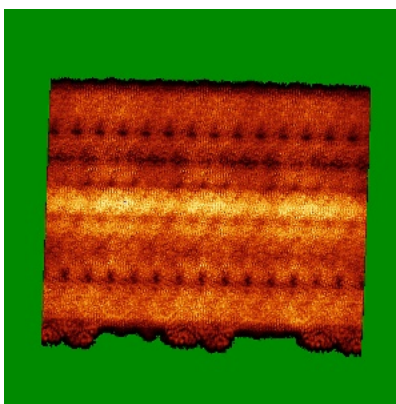
The images above show the largest variance slices of the map in three orthogonal directions.

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

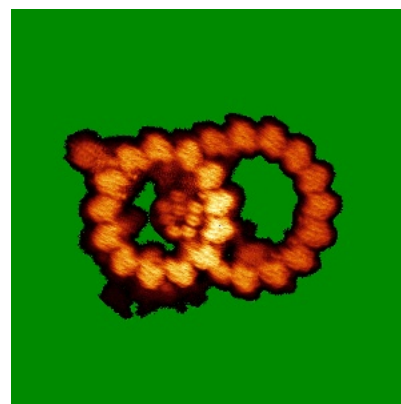
### 6.4.1 Primary map



X



Y

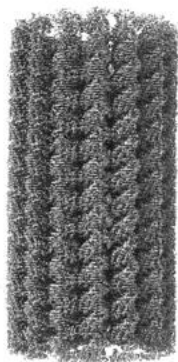


Z

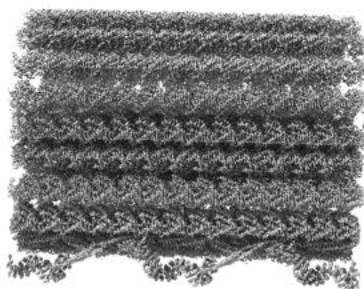
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

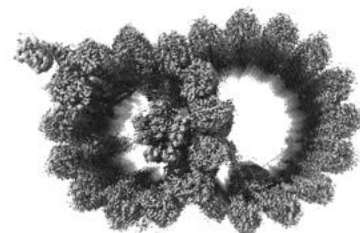
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

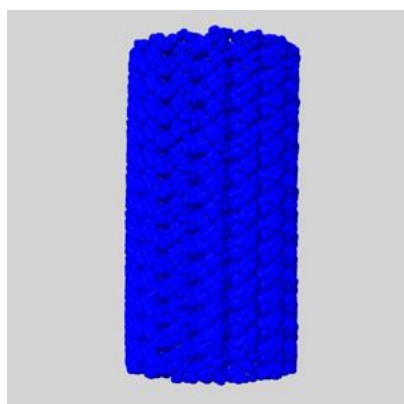
## 6.6 Mask visualisation [i](#)

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

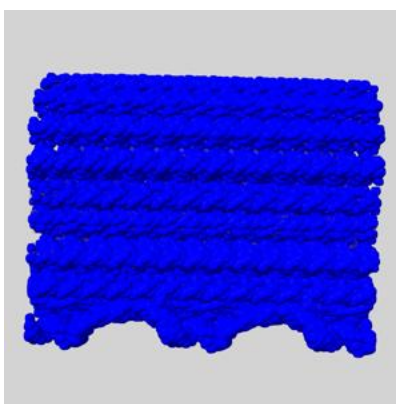
A mask typically either:

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

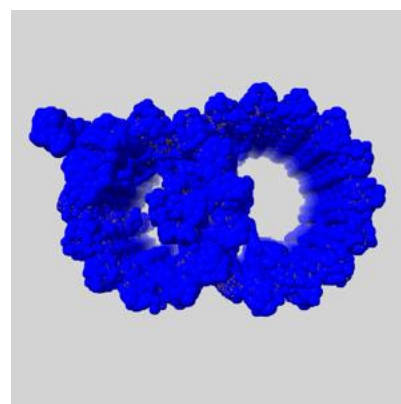
### 6.6.1 emd\_24664\_msk\_1.map [i](#)



X



Y

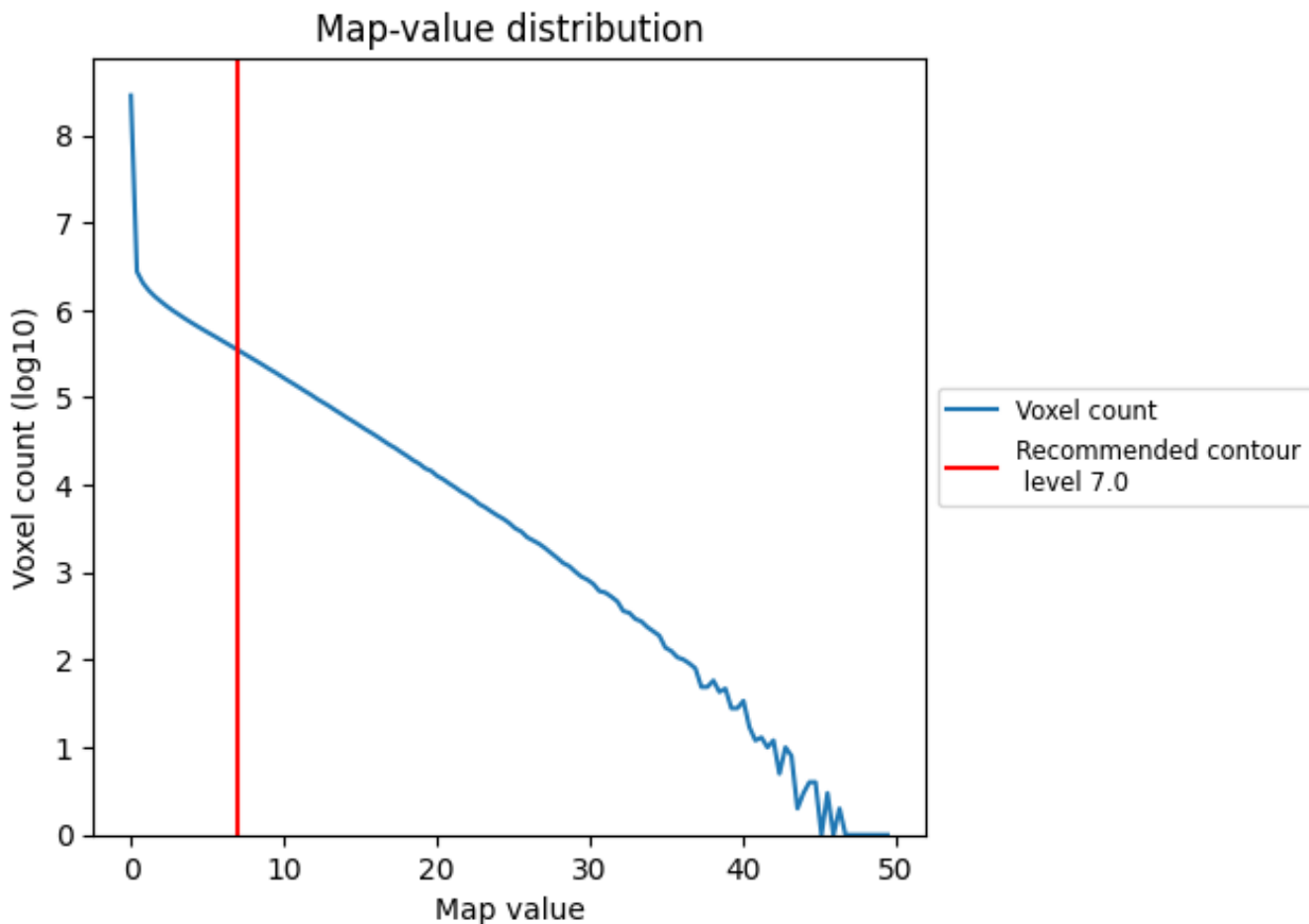


Z

## 7 Map analysis [i](#)

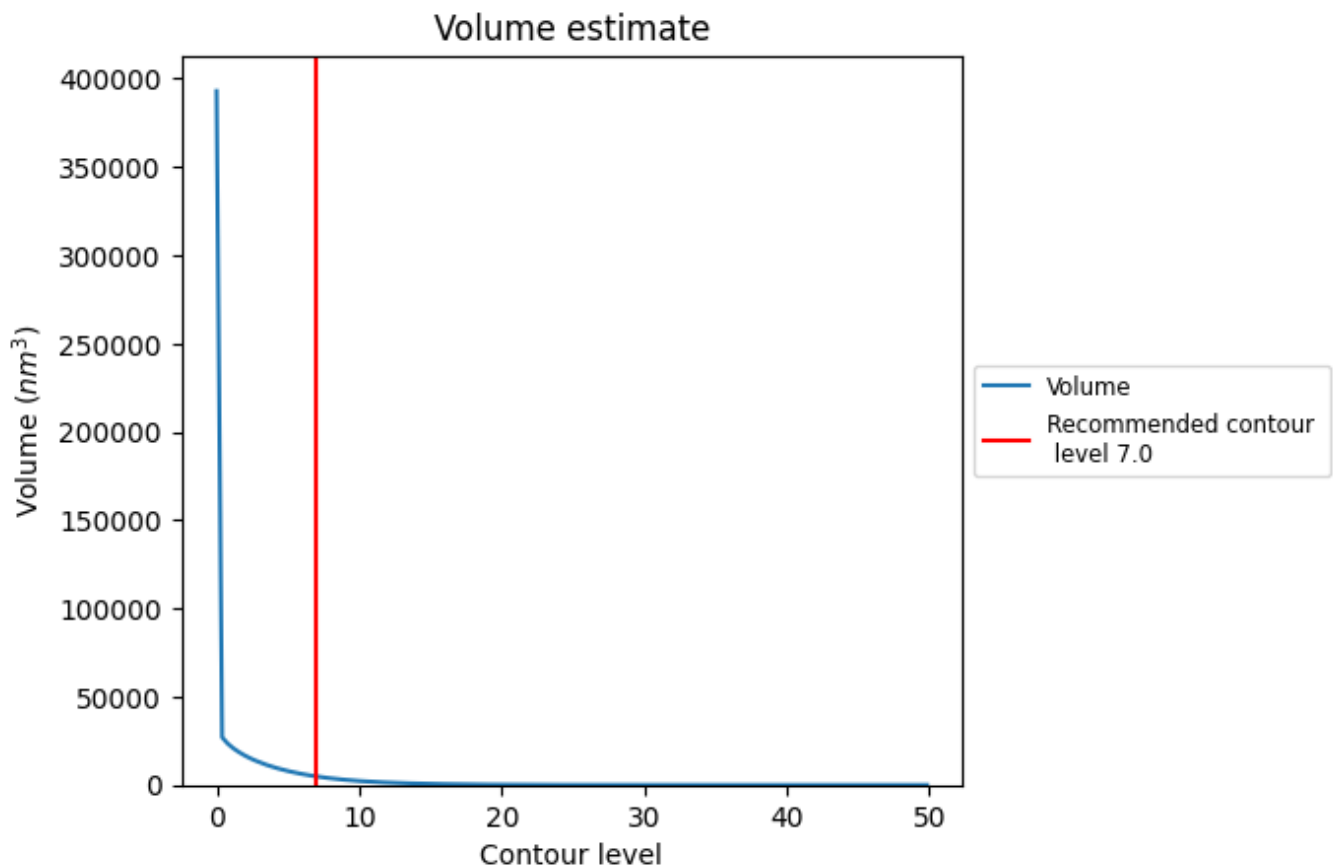
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

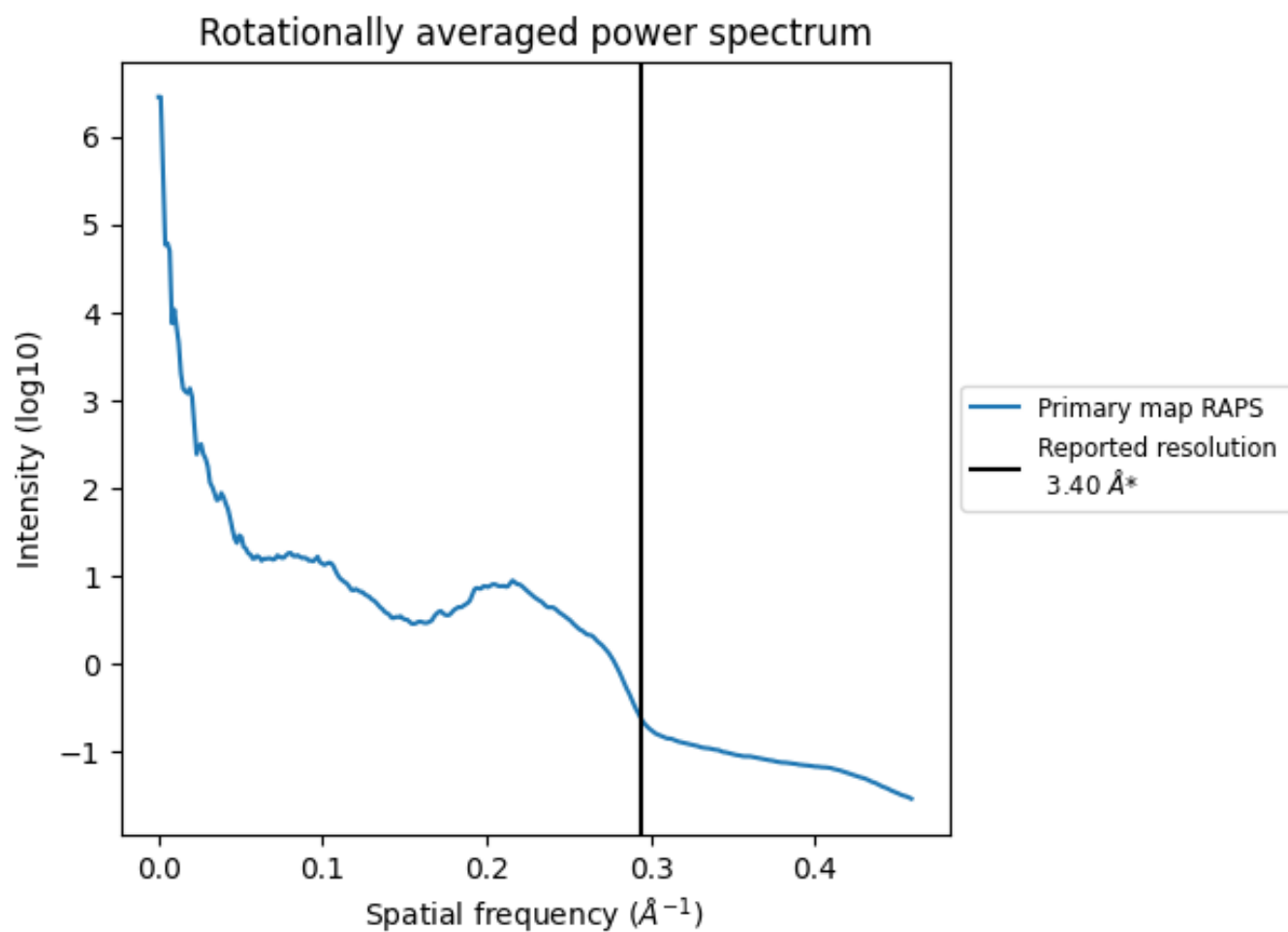
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4833 nm<sup>3</sup>; this corresponds to an approximate mass of 4366 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](#)

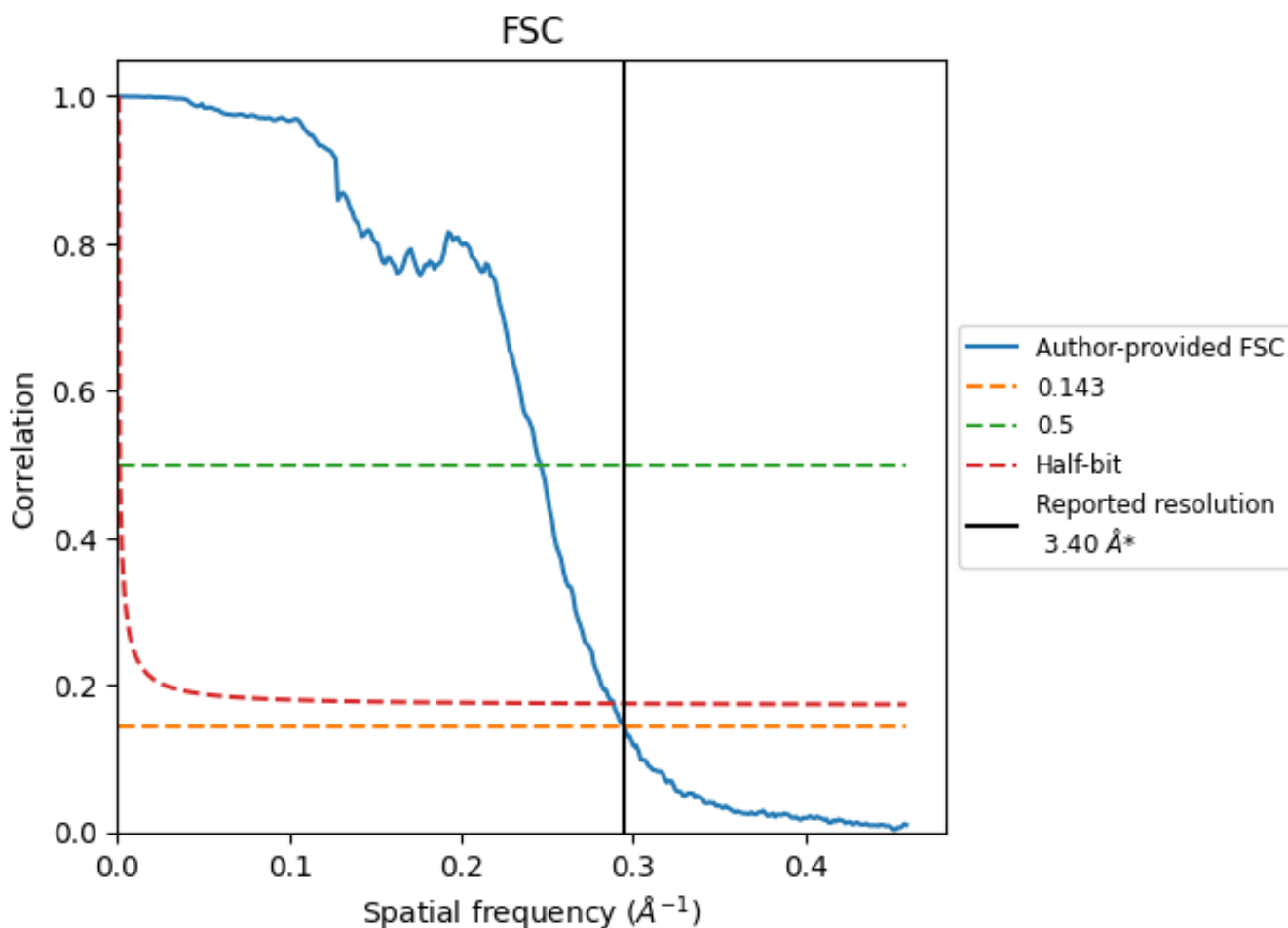


\*Reported resolution corresponds to spatial frequency of  $0.294 \text{\AA}^{-1}$

## 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 0.294 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	3.40	-	-
Author-provided FSC curve	3.39	4.07	3.47
Unmasked-calculated*	-	-	-

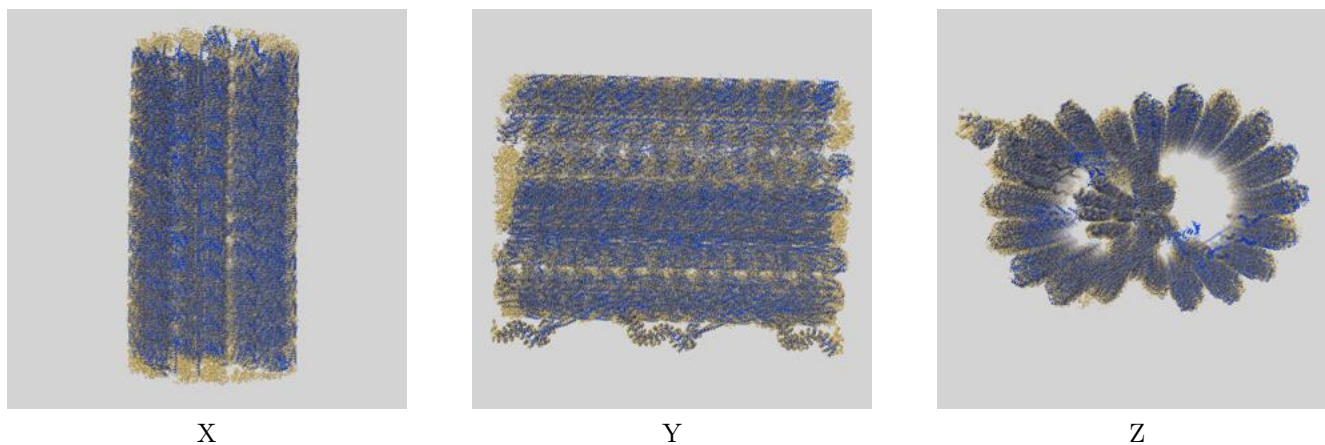
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit [i](#)

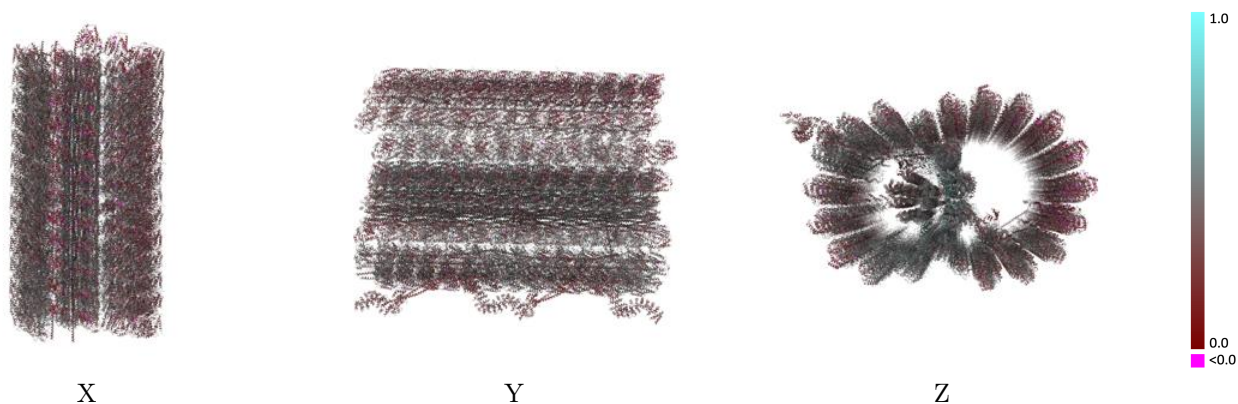
This section contains information regarding the fit between EMDB map EMD-24664 and PDB model 7RRO. Per-residue inclusion information can be found in section [3](#) on page [67](#).

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



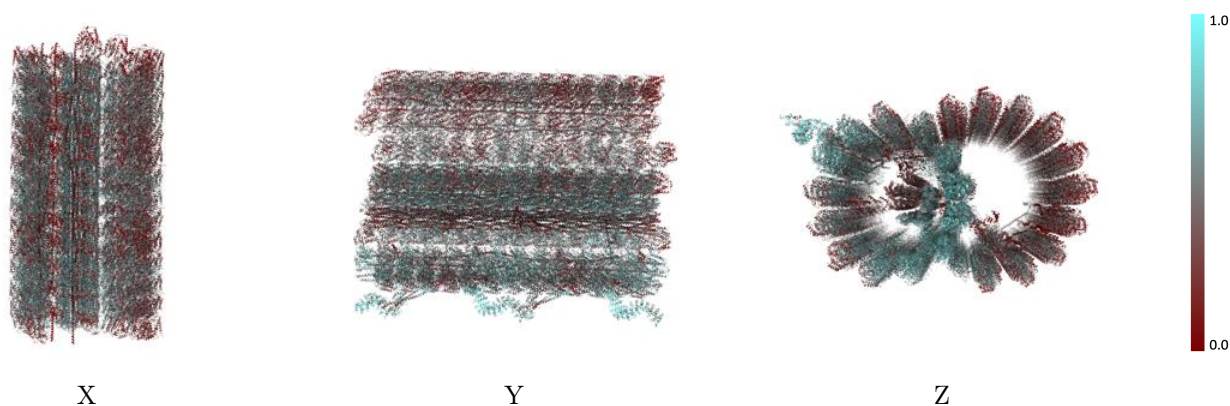
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



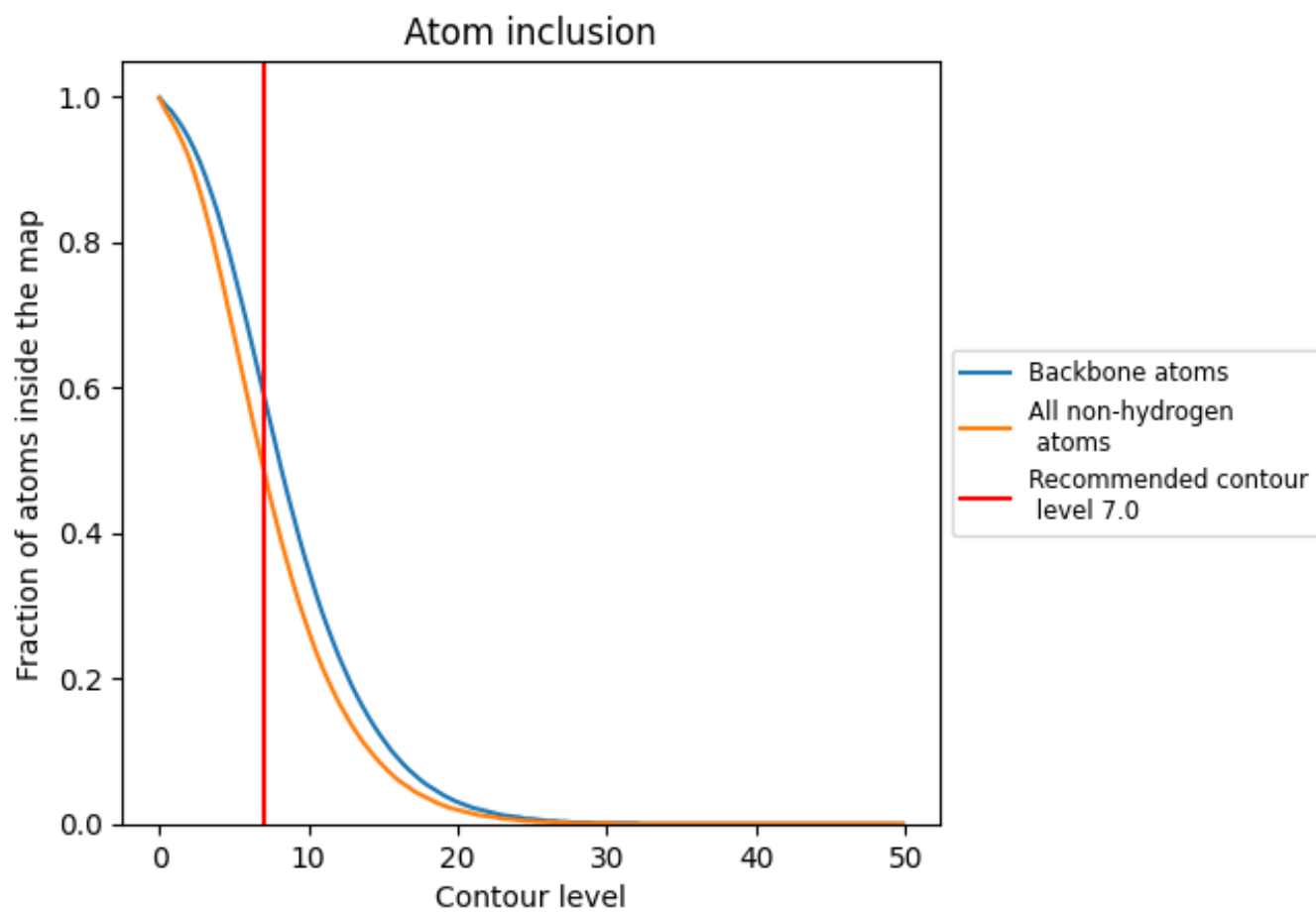
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.0).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 48% 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 (7.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4850	 0.4120
0	 0.4530	 0.4800
1	 0.1420	 0.4210
2	 0.3210	 0.4020
3	 0.4800	 0.3830
4	 0.4820	 0.3920
5	 0.2140	 0.3580
6	 0.3150	 0.3960
7	 0.3950	 0.4240
8	 0.3330	 0.3970
9	 0.2010	 0.3690
A	 0.3940	 0.3750
A0	 0.6410	 0.4760
A1	 0.6340	 0.4830
A2	 0.6190	 0.4770
A3	 0.6000	 0.4740
A4	 0.6010	 0.4770
AA	 0.6780	 0.4680
AB	 0.7330	 0.4910
AC	 0.7440	 0.5040
AD	 0.7110	 0.4870
AE	 0.7070	 0.5050
AF	 0.7420	 0.5060
AG	 0.7570	 0.5230
AH	 0.7160	 0.5000
AI	 0.7280	 0.5170
AJ	 0.7610	 0.5170
AK	 0.7650	 0.5320
AL	 0.7300	 0.5220
AM	 0.6910	 0.5210
B	 0.3790	 0.3710
B0	 0.6250	 0.4730
B1	 0.6210	 0.4730
B2	 0.6110	 0.4720
B3	 0.5790	 0.4590























































































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Chain	Atom inclusion	Q-score
B4	0.5970	0.4510
B5	0.2840	0.3970
B6	0.3090	0.3960
B7	0.2730	0.3840
B8	0.2240	0.3780
B9	0.1920	0.3610
BA	0.6240	0.4680
BB	0.6820	0.4940
BC	0.7130	0.4980
BD	0.6750	0.4890
BE	0.6610	0.4810
BF	0.6900	0.4880
BG	0.7090	0.4950
BH	0.6820	0.4970
BI	0.6590	0.4900
BJ	0.6890	0.5020
BK	0.7180	0.5040
BL	0.6900	0.5070
BM	0.6450	0.5030
C	0.4010	0.3810
C0	0.5360	0.4120
C1	0.5760	0.4370
C2	0.5670	0.4460
C3	0.5180	0.4400
C4	0.5130	0.4290
C5	0.3150	0.4070
C6	0.2990	0.4120
C7	0.3010	0.3990
C8	0.2610	0.3960
C9	0.2110	0.3960
CA	0.5030	0.4270
CB	0.6370	0.4780
CC	0.6880	0.4890
CD	0.6490	0.4800
CE	0.6090	0.4580
CF	0.6300	0.4600
CG	0.6660	0.4720
CH	0.6580	0.4740
CI	0.6060	0.4610
CJ	0.6150	0.4760
CK	0.6630	0.4810
CL	0.6430	0.4890





















































































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Chain	Atom inclusion	Q-score
CM	 0.5720	 0.4760
D	 0.3000	 0.4550
D0	 0.5980	 0.4620
D1	 0.6200	 0.4670
D2	 0.5860	 0.4640
D3	 0.5920	 0.4500
D5	 0.1780	 0.4210
D6	 0.2860	 0.3880
D7	 0.2640	 0.3820
D8	 0.2300	 0.3770
D9	 0.1860	 0.3640
DA	 0.3170	 0.3440
DB	 0.4940	 0.4090
DC	 0.5550	 0.4180
DD	 0.5940	 0.4220
DE	 0.5210	 0.4030
DF	 0.5330	 0.4010
DG	 0.5920	 0.4110
DH	 0.6000	 0.4130
DI	 0.5050	 0.3810
DJ	 0.5310	 0.4090
DK	 0.5450	 0.4040
DL	 0.5560	 0.4210
DM	 0.4910	 0.4120
DN	 0.2660	 0.3230
E	 0.5850	 0.4860
E0	 0.3060	 0.4400
E1	 0.2680	 0.4390
E2	 0.1850	 0.4190
E3	 0.1770	 0.3850
EB	 0.4270	 0.3610
EC	 0.5100	 0.3880
ED	 0.5570	 0.3880
EE	 0.4750	 0.3610
EF	 0.4710	 0.3690
EG	 0.5140	 0.3520
EH	 0.5450	 0.3640
EI	 0.4880	 0.3380
EJ	 0.4360	 0.3260
EK	 0.4620	 0.3430
EL	 0.5020	 0.3580
EM	 0.4380	 0.3590





















































































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Chain	Atom inclusion	Q-score
EN	 0.2380	 0.2790
F	 0.5530	 0.4400
F0	 0.3330	 0.4260
F1	 0.3850	 0.4080
F2	 0.3610	 0.4000
F3	 0.3220	 0.3930
F4	 0.2940	 0.3820
FB	 0.3960	 0.3540
FC	 0.4900	 0.3820
FD	 0.5240	 0.3740
FE	 0.4710	 0.3470
FF	 0.4590	 0.3570
FG	 0.4810	 0.3460
FH	 0.5280	 0.3560
FI	 0.4700	 0.3230
FJ	 0.4170	 0.3180
FK	 0.4090	 0.2970
FL	 0.4930	 0.3580
FM	 0.4140	 0.3030
FN	 0.3040	 0.3230
G	 0.5130	 0.4510
GB	 0.6700	 0.4740
GC	 0.6650	 0.4800
GD	 0.5830	 0.4370
GE	 0.4680	 0.4050
GF	 0.5410	 0.4320
GG	 0.6070	 0.4610
GH	 0.6410	 0.4650
GI	 0.6480	 0.4650
GJ	 0.5810	 0.4370
GK	 0.4890	 0.3890
GL	 0.5480	 0.4270
GM	 0.6260	 0.4630
GN	 0.6880	 0.4760
H	 0.4390	 0.4490
H1	 0.4030	 0.3550
H2	 0.4030	 0.3400
H3	 0.4610	 0.3730
H4	 0.4180	 0.3470
H5	 0.4160	 0.3410
H6	 0.5200	 0.3950
H7	 0.7220	 0.3420

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Chain	Atom inclusion	Q-score
H8	 0.7180	 0.3410
H9	 0.6820	 0.3370
HB	 0.6320	 0.4500
HC	 0.6300	 0.4360
HD	 0.5350	 0.4160
HE	 0.4460	 0.3890
HF	 0.4160	 0.3900
HG	 0.5380	 0.4250
HH	 0.6080	 0.4550
HI	 0.6110	 0.4520
HJ	 0.5390	 0.4160
HK	 0.4570	 0.3810
HL	 0.4340	 0.3890
HM	 0.5660	 0.4150
HN	 0.6270	 0.4500
HO	 0.6290	 0.4350
I	 0.3780	 0.4640
I1	 0.5860	 0.3470
I2	 0.5310	 0.2940
I3	 0.6050	 0.3270
I4	 0.6120	 0.3310
IB	 0.4120	 0.3820
IC	 0.4930	 0.4170
ID	 0.5770	 0.4340
IE	 0.5820	 0.4450
IF	 0.4870	 0.4220
IG	 0.4630	 0.4140
IH	 0.5220	 0.4090
II	 0.5300	 0.4040
IJ	 0.4710	 0.3870
IK	 0.4740	 0.3850
IL	 0.5110	 0.3800
IM	 0.5160	 0.3830
IN	 0.4410	 0.3570
IO	 0.3570	 0.3430
J	 0.5310	 0.4640
JB	 0.5000	 0.4260
JC	 0.5390	 0.4180
JD	 0.5710	 0.4330
JE	 0.5280	 0.4300
JF	 0.4770	 0.4260
JG	 0.5280	 0.4180

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Chain	Atom inclusion	Q-score
JH	0.5250	0.4220
JI	0.4900	0.3790
JJ	0.4810	0.3980
JK	0.5250	0.3970
JL	0.5670	0.4070
JM	0.5120	0.3800
JN	0.4120	0.3690
K	0.3340	0.4470
KB	0.6690	0.4840
KC	0.7420	0.5060
KD	0.7660	0.5190
KE	0.7630	0.5210
KF	0.7400	0.5310
KG	0.7590	0.5270
KH	0.7910	0.5480
KI	0.7930	0.5510
KJ	0.7620	0.5480
KK	0.7750	0.5500
KL	0.7960	0.5450
KM	0.7860	0.5490
KN	0.7670	0.5550
KO	0.7290	0.5380
L	0.5060	0.4620
LB	0.6840	0.4890
LC	0.7370	0.5030
LD	0.7460	0.5180
LE	0.7280	0.5150
LF	0.7130	0.5170
LG	0.7420	0.5250
LH	0.7660	0.5390
LI	0.7550	0.5320
LJ	0.7280	0.5270
LK	0.7430	0.5210
LL	0.7620	0.5270
LM	0.7560	0.5200
LN	0.7220	0.5190
M	0.3880	0.4550
MB	0.5980	0.4460
MC	0.6420	0.4600
MD	0.6520	0.4700
ME	0.6250	0.4630
MF	0.5960	0.4680

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Chain	Atom inclusion	Q-score
MG	 0.6220	 0.4630
MH	 0.6220	 0.4650
MI	 0.6230	 0.4670
MJ	 0.5850	 0.4400
MK	 0.6060	 0.4380
ML	 0.6450	 0.4430
MM	 0.6490	 0.4420
MN	 0.5640	 0.4210
N	 0.4350	 0.4490
NO	 0.2280	 0.3490
NA	 0.3170	 0.3670
NB	 0.3650	 0.3760
NC	 0.3450	 0.3690
ND	 0.2830	 0.3570
NE	 0.3110	 0.3560
NF	 0.3740	 0.3710
NG	 0.3460	 0.3620
NH	 0.2620	 0.3550
NI	 0.2790	 0.3450
NJ	 0.3690	 0.3620
NK	 0.3430	 0.3610
NL	 0.2740	 0.3530
O	 0.4500	 0.4500
OO	 0.2620	 0.3570
OA	 0.3530	 0.3710
OB	 0.4370	 0.3960
OC	 0.4500	 0.4090
OD	 0.3570	 0.3830
OE	 0.3780	 0.3830
OF	 0.4510	 0.3880
OG	 0.4640	 0.4040
OH	 0.3490	 0.3800
OI	 0.3460	 0.3820
OJ	 0.4300	 0.4040
OK	 0.4500	 0.4140
OL	 0.3570	 0.3820
P	 0.5880	 0.4920
PA	 0.2770	 0.3390
PB	 0.3980	 0.3680
PC	 0.4040	 0.3580
PD	 0.3200	 0.3550
PE	 0.3000	 0.3260

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Chain	Atom inclusion	Q-score
PF	0.4290	0.3770
PG	0.4210	0.3720
PH	0.3180	0.3490
PI	0.2980	0.3340
PJ	0.3840	0.3790
PK	0.4070	0.3850
PL	0.3240	0.3580
PM	0.2570	0.3520
Q	0.5710	0.4910
QA	0.2140	0.3030
QB	0.3640	0.3490
QC	0.3860	0.3520
QD	0.3050	0.3480
QE	0.2710	0.3200
QF	0.4050	0.3610
QG	0.4080	0.3470
QH	0.3360	0.3440
QI	0.2620	0.3150
QJ	0.3780	0.3630
QK	0.4100	0.3640
QL	0.3500	0.3560
QM	0.2550	0.3270
R	0.2650	0.4340
RA	0.1960	0.3060
RB	0.3480	0.3580
RC	0.3970	0.3770
RD	0.3180	0.3630
RE	0.2700	0.3210
RF	0.3520	0.3410
RG	0.4030	0.3490
RH	0.3490	0.3420
RI	0.2880	0.3340
RJ	0.3420	0.3610
RK	0.4180	0.3750
RL	0.4020	0.3870
RM	0.3280	0.3610
S	0.2830	0.4370
SA	0.1900	0.2880
SB	0.3350	0.3320
SC	0.3700	0.3300
SD	0.3710	0.3440
SE	0.2840	0.3170

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Chain	Atom inclusion	Q-score
SF	0.3160	0.3280
SG	0.3560	0.3180
SH	0.3650	0.3410
SI	0.3050	0.3220
SJ	0.3190	0.3320
SK	0.4010	0.3500
SL	0.4100	0.3510
SM	0.3530	0.3330
T	0.5870	0.4970
TB	0.2360	0.2890
TC	0.3000	0.3020
TD	0.3080	0.2980
TE	0.2240	0.2730
TF	0.2270	0.2720
TG	0.2930	0.2990
TH	0.3020	0.3060
TI	0.2140	0.2720
TJ	0.2490	0.2830
TK	0.3350	0.3010
TL	0.3660	0.3250
TM	0.3130	0.3070
U	0.5640	0.4890
UB	0.2910	0.3710
UC	0.3730	0.3920
UD	0.4000	0.4120
UE	0.3320	0.3780
UF	0.3160	0.3780
UG	0.4130	0.4030
UH	0.4310	0.4160
UI	0.3680	0.3940
UJ	0.3140	0.3710
UK	0.3870	0.3770
UL	0.4580	0.4170
UM	0.4320	0.4120
UN	0.2900	0.3900
V	0.5420	0.4800
VB	0.3410	0.3790
VC	0.4310	0.3950
VD	0.4700	0.4260
VE	0.4220	0.4000
VF	0.3510	0.3910
VG	0.4170	0.4040



































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Chain	Atom inclusion	Q-score
VH	0.4750	0.4240
VI	0.4490	0.4060
VJ	0.3560	0.3950
VK	0.4060	0.4060
VL	0.5190	0.4350
VM	0.5120	0.4260
VN	0.4320	0.4160
W	0.4100	0.4470
WB	0.4100	0.3750
WC	0.4910	0.4000
WD	0.5610	0.4260
WE	0.5220	0.4300
WF	0.4460	0.4120
WG	0.4600	0.4090
WH	0.5670	0.4300
WI	0.5300	0.4200
WJ	0.4310	0.4140
WK	0.4460	0.4050
WL	0.5770	0.4330
WM	0.5640	0.4380
WN	0.5140	0.4350
X	0.4410	0.4630
XA	0.5270	0.4210
XB	0.6140	0.4450
XC	0.5810	0.4510
XD	0.6550	0.4610
XE	0.5850	0.4660
XF	0.6600	0.4830
XG	0.5490	0.4690
Y	0.4230	0.4520
YB	0.5780	0.4480
YC	0.5010	0.4510
YD	0.6230	0.4760
YE	0.5170	0.4700
YF	0.6190	0.4910
YG	0.2820	0.4460
Z	0.2060	0.4000
a	0.1800	0.3690
b	0.1660	0.3730
c	0.0880	0.3440
d	0.1180	0.3610
e	0.4350	0.4240

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Chain	Atom inclusion	Q-score
f	 0.4290	 0.4260
g	 0.5060	 0.4450
h	 0.3620	 0.3960
i	 0.3760	 0.4470
j	 0.3920	 0.4500
k	 0.4610	 0.4520
l	 0.5750	 0.4620
m	 0.5860	 0.5000
n	 0.5850	 0.5060
o	 0.1940	 0.3240
p	 0.2180	 0.3260
q	 0.5350	 0.4550
r	 0.5340	 0.4590
s	 0.5710	 0.4770
t	 0.0580	 0.3120
y	 0.5830	 0.4800
z	 0.5820	 0.4780