



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 12:35 AM UTC

PDB ID : 8I7O / pdb_00008i7o
EMDB ID : EMD-35229
Title : In situ structure of axonemal doublet microtubules in mouse sperm with 16-nm repeat
Authors : Zhu, Y.; Yin, G.L.; Tai, L.H.; Sun, F.
Deposited on : 2023-02-01
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

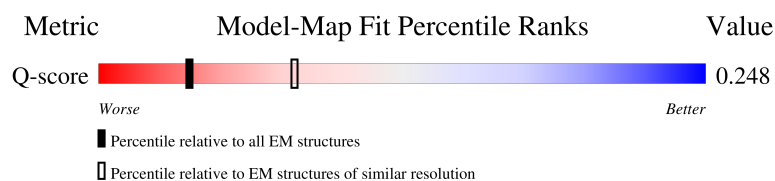
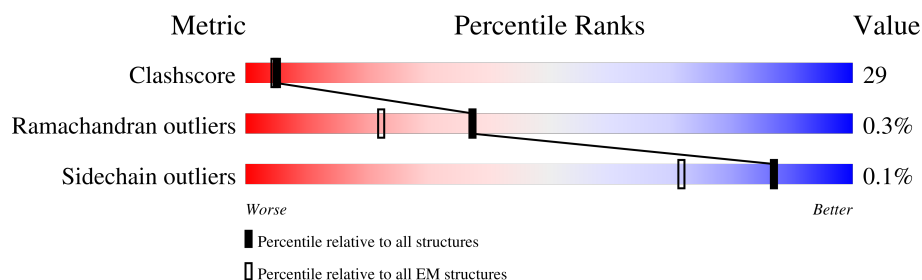
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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

Mol	Chain	Length	Quality of chain
1	A2	418	
1	A3	418	
2	AE	438	
2	AG	438	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	AI	438	
2	BE	438	
2	BG	438	
2	BI	438	
2	CG	438	
2	CI	438	
2	DE	438	
2	DG	438	
2	EE	438	
2	EG	438	
2	FE	438	
2	FG	438	
2	GE	438	
2	GG	438	
2	GI	438	
2	HE	438	
2	HG	438	
2	HI	438	
2	IE	438	
2	IG	438	
2	II	438	
2	JE	438	
2	JG	438	
2	KE	438	
2	KG	438	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
2	KI	438	15%	54% 46%
2	LE	438	7%	53% 47%
2	LG	438	7%	48% 52%
2	LI	438	8%	53% 46%
2	ME	438	8%	49% 51%
2	MG	438	5%	46% 53%
2	MI	438	8%	50% 50%
2	NE	438	53%	40% 60%
2	NG	438	41%	39% 60%
2	NI	438	61%	41% 59%
2	OE	438	49%	42% 58%
2	OG	438	50%	45% 55%
2	OI	438	50%	41% 58%
2	PE	438	46%	43% 57%
2	PG	438	46%	42% 58%
2	PI	438	42%	42% 58%
2	QE	438	44%	40% 60%
2	QG	438	42%	42% 58%
2	QI	438	40%	42% 58%
2	RE	438	43%	42% 58%
2	RG	438	45%	41% 59%
2	RI	438	42%	36% 64%
2	SE	438	37%	46% 54%
2	SG	438	35%	37% 63%
2	SI	438	34%	38% 62%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	TG	438	
2	TI	438	
2	UE	438	
2	UG	438	
2	VE	438	
2	VG	438	
2	WE	438	
2	WG	438	
2	WI	438	
3	AF	427	
3	AH	427	
3	BF	427	
3	BH	427	
3	CF	427	
3	CH	427	
3	CJ	427	
3	DD	427	
3	DF	427	
3	DH	427	
3	ED	427	
3	EF	427	
3	EH	427	
3	FD	427	
3	FF	427	
3	FH	427	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	GD	427	45% 53% 46%
3	GF	427	23% 51% 48%
3	GH	427	29% 52% 48%
3	HD	427	52% 55% 45%
3	HF	427	33% 52% 47%
3	HH	427	27% 52% 48%
3	IF	427	23% 49% 51%
3	IH	427	22% 49% 51%
3	JD	427	17% 52% 48%
3	JF	427	17% 51% 49%
3	JH	427	18% 54% 45%
3	KD	427	9% 54% 46%
3	KF	427	8% 52% 48%
3	KH	427	9% 53% 47%
3	LD	427	8% 51% 48%
3	LF	427	6% 48% 52%
3	LH	427	6% 50% 50%
3	MF	427	7% 52% 48%
3	MH	427	• 44% 55% •
3	ND	427	61% 51% 49%
3	NF	427	37% 45% 55%
3	NH	427	41% 45% 55%
3	OD	427	63% 51% 49%
3	OF	427	45% 50% 49%
3	OH	427	44% 41% 58%

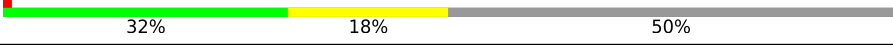
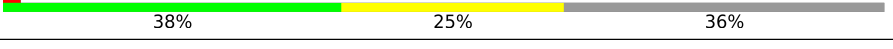
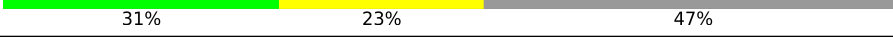
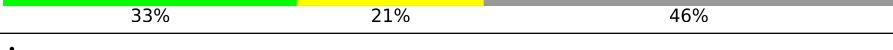
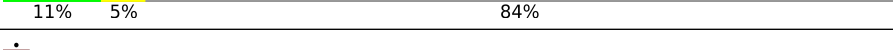
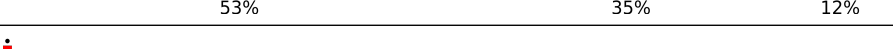
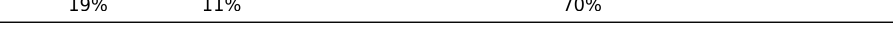
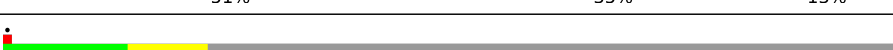
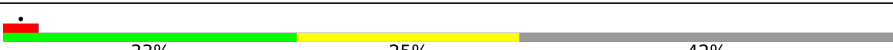
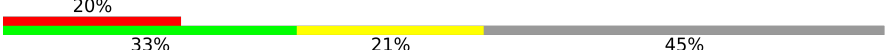
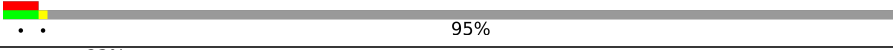
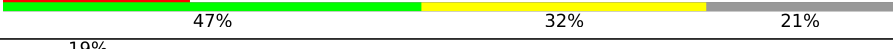
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	PF	427	
3	PH	427	
3	QF	427	
3	QH	427	
3	RF	427	
3	RH	427	
3	RJ	427	
3	SF	427	
3	SH	427	
3	SJ	427	
3	TF	427	
3	TH	427	
3	TJ	427	
3	UD	427	
3	UF	427	
3	UH	427	
3	VD	427	
3	VF	427	
3	VH	427	
3	WF	427	
3	WH	427	
4	B2	430	
4	B3	430	
4	B7	430	
4	B8	430	

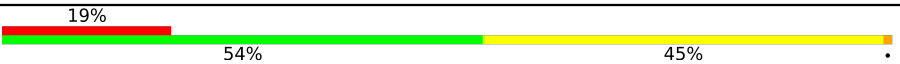
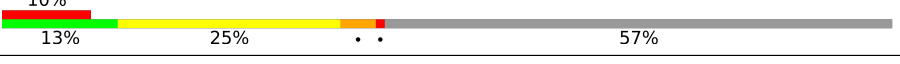
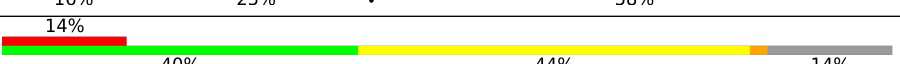
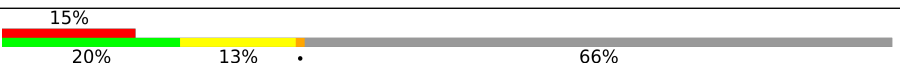
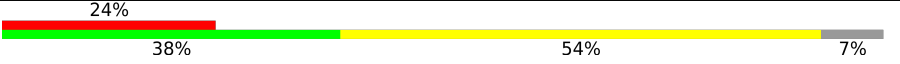
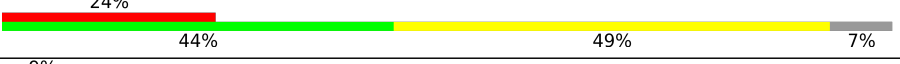
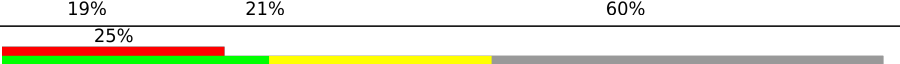
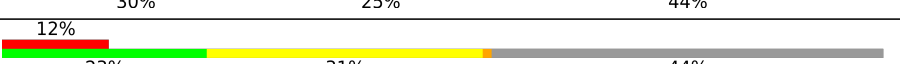
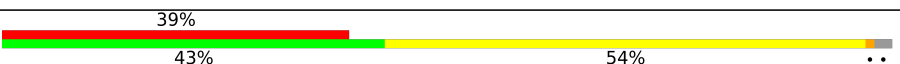
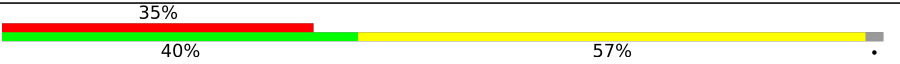
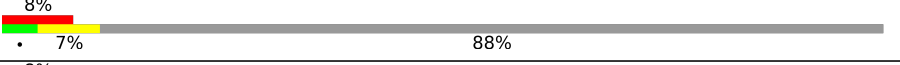
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C2	490	
5	C3	490	
5	C4	490	
5	C7	490	
5	C8	490	
5	Cb	490	
5	Cc	490	
6	D2	447	
6	D3	447	
6	D4	447	
6	D7	447	
6	D8	447	
6	D9	447	
7	E2	206	
7	E3	206	
8	F2	557	
8	F3	557	
8	F6	557	
8	F7	557	
8	Fa	557	
8	Fb	557	
8	Fc	557	
8	F1	557	
9	G1	648	
9	G2	648	

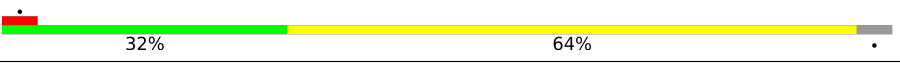
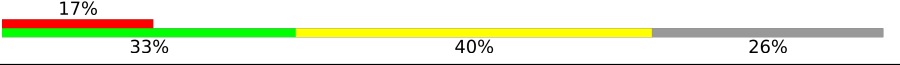
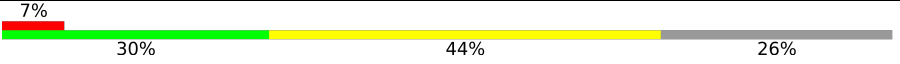
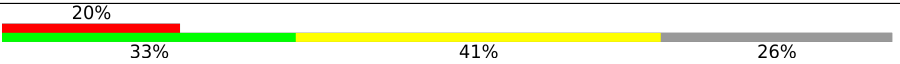
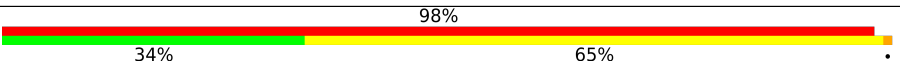
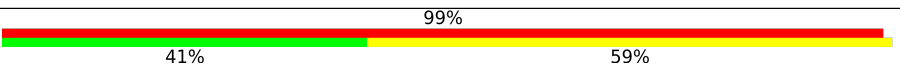
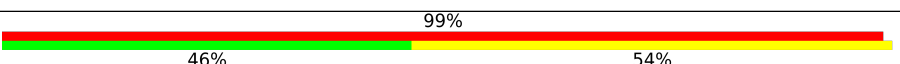
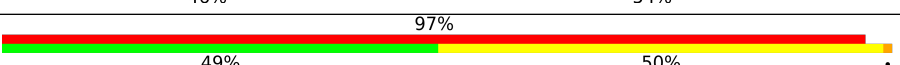
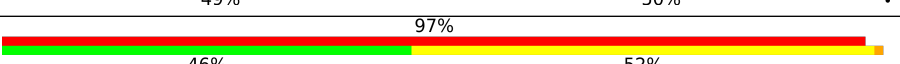
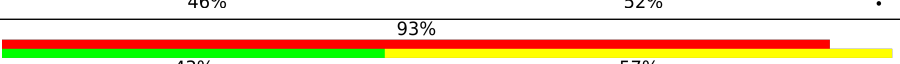
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	G5	750	
11	H3	319	
11	H4	319	
12	I2	200	
12	I3	200	
13	J2	189	
13	J3	189	
14	K2	499	
14	K3	499	
14	K4	499	
15	L2	255	
15	L3	255	
16	M2	141	
16	M3	141	
17	N2	168	
17	N3	168	
18	O1	189	
18	O2	189	
19	P1	620	
19	P2	620	
20	Q1	1516	
20	Q2	1516	
21	R2	283	
22	XC	193	
22	XD	193	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
22	XE	193	
23	XJ	241	
23	XK	241	
23	XL	241	
24	YI	168	
24	YJ	168	
24	YK	168	
24	YL	168	
24	YM	168	
24	YN	168	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	GTP	BF	501	-	-	X	-
25	GTP	BG	501	-	-	X	-
25	GTP	DE	501	-	-	X	-
25	GTP	DG	501	-	-	X	-
25	GTP	EE	501	-	-	X	-
25	GTP	EG	501	-	-	X	-
25	GTP	FD	501	-	-	X	-
25	GTP	FE	501	-	-	X	-
25	GTP	FF	502	-	-	X	-
25	GTP	HD	501	-	-	X	-
25	GTP	IH	501	-	-	X	-
25	GTP	JE	501	-	-	X	-
25	GTP	JF	501	-	-	X	-
25	GTP	KF	501	-	-	X	-
25	GTP	LE	501	-	-	X	-
25	GTP	MF	501	-	-	X	-
25	GTP	MG	501	-	-	X	-
25	GTP	OF	501	-	-	X	-
25	GTP	PE	501	-	-	X	-
25	GTP	PI	501	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	GTP	QE	501	-	-	X	-
25	GTP	QH	501	-	-	X	-
25	GTP	QI	501	-	-	X	-
25	GTP	RF	501	-	-	X	-
25	GTP	RH	501	-	-	X	-
25	GTP	RJ	501	-	-	X	-
25	GTP	SF	501	-	-	X	-
25	GTP	SG	501	-	-	X	-
25	GTP	SH	501	-	-	X	-
25	GTP	UF	501	-	-	X	-
25	GTP	WG	501	-	-	X	-
25	GTP	WH	501	-	-	X	-

2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 540760 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 Tektin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A2	353	Total	C	N	O	S	0	0
			2884	1784	520	570	10		
1	A3	211	Total	C	N	O	S	0	0
			1745	1083	309	351	2		

- Molecule 2 is a protein called Detyrosinated tubulin alpha-3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AE	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	AG	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	AI	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	BE	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	BG	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	BI	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	CG	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	CI	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	DE	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	DG	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	EE	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	EG	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	FE	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	FG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	GE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	GG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	GI	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	HE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	HG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	HI	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	IE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	IG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	II	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	JE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	JG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	KE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	KG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	KI	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	LE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	LG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	LI	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	ME	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	MG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	MI	438	Total 3418	C 2166	N 581	O 649	S 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	NE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	NG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	NI	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	OE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	OG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	OI	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	PE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	PG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	PI	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	QE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	QG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	QI	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	RE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	RG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	RI	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	SE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	SG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	SI	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	TG	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	TI	438	Total 3418	C 2166	N 581	O 649	S 22	0	0
2	UE	438	Total 3418	C 2166	N 581	O 649	S 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	UG	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	VE	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	VG	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	WE	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	WG	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		
2	WI	438	Total	C	N	O	S	0	0
			3418	2166	581	649	22		

- Molecule 3 is a protein called Tubulin beta-4B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	AH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	BF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	BH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	CF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	CH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	CJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	DD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	DF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	DH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	ED	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	EF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	EH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	FD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	FF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	FH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	GD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	GF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	GH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	HD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	HF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	HH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	IF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	IH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	JD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	JF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	JH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	KD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	KF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	KH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	LD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	LF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	LH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	MF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	MH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	ND	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	NF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	NH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	OD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	OF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	OH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	PF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	PH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	QF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	QH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	RF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	RH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	RJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	SF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	SH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	SJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	TF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	TH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	TJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	UD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	UF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	UH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	VD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	VF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	VH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	WF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
3	WH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

- Molecule 4 is a protein called Tektin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B2	250	Total	C	N	O	S	0	0
			2036	1262	369	396	9		
4	B3	343	Total	C	N	O	S	0	0
			2816	1737	516	553	10		
4	B7	376	Total	C	N	O	S	0	0
			3082	1900	566	603	13		
4	B8	177	Total	C	N	O	S	0	0
			1463	905	269	280	9		

- Molecule 5 is a protein called Tektin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C2	142	Total	C	N	O	S	0	0
			1175	716	221	236	2		
5	C3	366	Total	C	N	O	S	0	0
			2978	1825	551	588	14		
5	C4	81	Total	C	N	O	S	0	0
			670	413	122	132	3		
5	C7	243	Total	C	N	O	S	0	0
			1983	1212	368	396	7		
5	C8	312	Total	C	N	O	S	0	0
			2534	1561	461	499	13		
5	Cb	262	Total	C	N	O	S	0	0
			2125	1303	391	418	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Cc	265	Total	C	N	O	S	0	0
			2159	1317	403	431	8		

- Molecule 6 is a protein called Tektin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D2	72	Total	C	N	O	S	0	0
			583	359	110	113	1		
6	D3	394	Total	C	N	O	S	0	0
			3225	1978	592	639	16		
6	D4	132	Total	C	N	O	S	0	0
			1080	662	203	209	6		
6	D7	101	Total	C	N	O	S	0	0
			836	514	159	160	3		
6	D8	388	Total	C	N	O	S	0	0
			3192	1952	596	628	16		
6	D9	102	Total	C	N	O	S	0	0
			849	518	153	175	3		

- Molecule 7 is a protein called Tektin bundle-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E2	187	Total	C	N	O	S	0	0
			1558	992	295	265	6		
7	E3	63	Total	C	N	O	S	0	0
			519	334	97	86	2		

- Molecule 8 is a protein called Tektin-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F2	322	Total	C	N	O	S	0	0
			2640	1638	477	504	21		
8	F3	234	Total	C	N	O	S	0	0
			1927	1182	357	375	13		
8	F6	305	Total	C	N	O	S	0	0
			2503	1535	464	487	17		
8	F7	245	Total	C	N	O	S	0	0
			2003	1244	363	378	18		
8	Fa	214	Total	C	N	O	S	0	0
			1746	1090	311	328	17		
8	Fb	321	Total	C	N	O	S	0	0
			2634	1623	484	509	18		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Fc	26	Total	C	N	O		0	0
			224	136	46	42			
8	F1	332	Total	C	N	O	S	0	0
			2721	1685	493	523	20		

- Molecule 9 is a protein called EF-hand domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G1	510	Total	C	N	O	S	0	0
			4192	2708	704	763	17		
9	G2	495	Total	C	N	O	S	0	0
			4081	2634	687	743	17		

- Molecule 10 is a protein called EF-hand domain-containing family member C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G5	747	Total	C	N	O	S	0	0
			6169	3983	1027	1130	29		

- Molecule 11 is a protein called Protein FAM166A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H3	145	Total	C	N	O	S	0	0
			1185	759	209	211	6		
11	H4	137	Total	C	N	O	S	0	0
			1121	718	198	199	6		

- Molecule 12 is a protein called Protein FAM166C.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I2	38	Total	C	N	O	S	0	0
			298	192	47	58	1		
12	I3	38	Total	C	N	O	S	0	0
			298	192	47	58	1		

- Molecule 13 is a protein called Dual specificity phosphatase 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J2	171	Total	C	N	O	S	0	0
			1378	886	230	253	9		
13	J3	171	Total	C	N	O	S	0	0
			1378	886	230	253	9		

- Molecule 14 is a protein called Coiled-coil domain-containing protein 105.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K2	209	Total	C	N	O	S	0	0
			1722	1070	336	303	13		
14	K3	428	Total	C	N	O	S	0	0
			3465	2147	674	618	26		
14	K4	169	Total	C	N	O	S	0	0
			1327	825	261	232	9		

- Molecule 15 is a protein called Enkurin.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L2	236	Total	C	N	O	S	0	0
			1929	1231	340	349	9		
15	L3	236	Total	C	N	O	S	0	0
			1929	1231	340	349	9		

- Molecule 16 is a protein called Testis-expressed protein 43.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M2	62	Total	C	N	O	S	0	0
			510	327	89	89	5		
16	M3	62	Total	C	N	O	S	0	0
			510	327	89	89	5		

- Molecule 17 is a protein called Cilia- and flagella-associated protein 276.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N2	68	Total	C	N	O	S	0	0
			535	335	95	105			
17	N3	68	Total	C	N	O	S	0	0
			535	335	95	105			

- Molecule 18 is a protein called Protein Flattop.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O1	105	Total	C	N	O	S	0	0
			825	524	148	152	1		
18	O2	105	Total	C	N	O	S	0	0
			825	524	148	152	1		

- Molecule 19 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P1	608	Total	C	N	O	S	0	0
			4696	2970	819	875	32		
19	P2	608	Total	C	N	O	S	0	0
			4696	2970	819	875	32		

- Molecule 20 is a protein called EF-hand calcium-binding domain-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q1	178	Total	C	N	O	S	0	0
			1473	941	254	268	10		
20	Q2	178	Total	C	N	O	S	0	0
			1473	941	254	268	10		

- Molecule 21 is a protein called Cilia and flagella-associated protein 77.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R2	73	Total	C	N	O	S	0	0
			597	367	118	109	3		

- Molecule 22 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	XC	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		
22	XD	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		
22	XE	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		

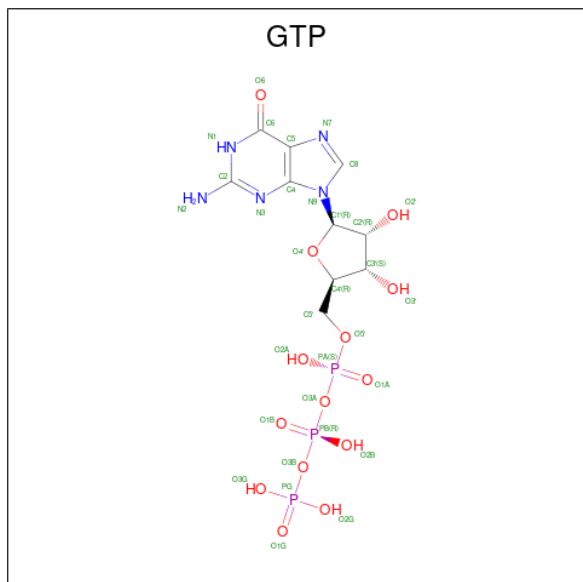
- Molecule 23 is a protein called Parkin coregulated gene protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	XJ	178	Total	C	N	O	S	0	0
			1469	953	247	261	8		
23	XK	178	Total	C	N	O	S	0	0
			1469	953	247	261	8		
23	XL	178	Total	C	N	O	S	0	0
			1469	953	247	261	8		

- Molecule 24 is a protein called Sperm acrosome-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	YI	168	Total	C	N	O	S	0	0
			1365	856	244	254	11		
24	YJ	168	Total	C	N	O	S	0	0
			1365	856	244	254	11		
24	YK	168	Total	C	N	O	S	0	0
			1365	856	244	254	11		
24	YL	168	Total	C	N	O	S	0	0
			1365	856	244	254	11		
24	YM	168	Total	C	N	O	S	0	0
			1365	856	244	254	11		
24	YN	168	Total	C	N	O	S	0	0
			1365	856	244	254	11		

- Molecule 25 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
25	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
25	AF	1	Total	C	N	O	P	0
			32	10	5	14	3	
25	AG	1	Total	C	N	O	P	0
			32	10	5	14	3	
25	AH	1	Total	C	N	O	P	0
			32	10	5	14	3	
25	AI	1	Total	C	N	O	P	0
			32	10	5	14	3	
25	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	BF	1	Total 32	C 10	N 5	O 14	P 3	0
25	BG	1	Total 32	C 10	N 5	O 14	P 3	0
25	BH	1	Total 32	C 10	N 5	O 14	P 3	0
25	BI	1	Total 32	C 10	N 5	O 14	P 3	0
25	CF	1	Total 32	C 10	N 5	O 14	P 3	0
25	CG	1	Total 32	C 10	N 5	O 14	P 3	0
25	CH	1	Total 32	C 10	N 5	O 14	P 3	0
25	CI	1	Total 32	C 10	N 5	O 14	P 3	0
25	CJ	1	Total 32	C 10	N 5	O 14	P 3	0
25	DD	1	Total 32	C 10	N 5	O 14	P 3	0
25	DE	1	Total 32	C 10	N 5	O 14	P 3	0
25	DF	1	Total 32	C 10	N 5	O 14	P 3	0
25	DG	1	Total 32	C 10	N 5	O 14	P 3	0
25	DH	1	Total 32	C 10	N 5	O 14	P 3	0
25	ED	1	Total 32	C 10	N 5	O 14	P 3	0
25	EE	1	Total 32	C 10	N 5	O 14	P 3	0
25	EF	1	Total 32	C 10	N 5	O 14	P 3	0
25	EG	1	Total 32	C 10	N 5	O 14	P 3	0
25	EH	1	Total 32	C 10	N 5	O 14	P 3	0
25	FD	1	Total 32	C 10	N 5	O 14	P 3	0
25	FE	1	Total 32	C 10	N 5	O 14	P 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	FF	1	Total 32	C 10	N 5	O 14	P 3	0
25	FF	1	Total 32	C 10	N 5	O 14	P 3	0
25	FH	1	Total 32	C 10	N 5	O 14	P 3	0
25	GD	1	Total 32	C 10	N 5	O 14	P 3	0
25	GE	1	Total 32	C 10	N 5	O 14	P 3	0
25	GF	1	Total 32	C 10	N 5	O 14	P 3	0
25	GG	1	Total 32	C 10	N 5	O 14	P 3	0
25	GH	1	Total 32	C 10	N 5	O 14	P 3	0
25	GH	1	Total 32	C 10	N 5	O 14	P 3	0
25	HD	1	Total 32	C 10	N 5	O 14	P 3	0
25	HE	1	Total 32	C 10	N 5	O 14	P 3	0
25	HF	1	Total 32	C 10	N 5	O 14	P 3	0
25	HG	1	Total 32	C 10	N 5	O 14	P 3	0
25	HH	1	Total 32	C 10	N 5	O 14	P 3	0
25	HI	1	Total 32	C 10	N 5	O 14	P 3	0
25	IE	1	Total 32	C 10	N 5	O 14	P 3	0
25	IF	1	Total 32	C 10	N 5	O 14	P 3	0
25	IG	1	Total 32	C 10	N 5	O 14	P 3	0
25	IH	1	Total 32	C 10	N 5	O 14	P 3	0
25	II	1	Total 32	C 10	N 5	O 14	P 3	0
25	JD	1	Total 32	C 10	N 5	O 14	P 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	JE	1	Total 32	C 10	N 5	O 14	P 3	0
25	JF	1	Total 32	C 10	N 5	O 14	P 3	0
25	JG	1	Total 32	C 10	N 5	O 14	P 3	0
25	JH	1	Total 32	C 10	N 5	O 14	P 3	0
25	KD	1	Total 32	C 10	N 5	O 14	P 3	0
25	KE	1	Total 32	C 10	N 5	O 14	P 3	0
25	KF	1	Total 32	C 10	N 5	O 14	P 3	0
25	KG	1	Total 32	C 10	N 5	O 14	P 3	0
25	KH	1	Total 32	C 10	N 5	O 14	P 3	0
25	KI	1	Total 32	C 10	N 5	O 14	P 3	0
25	LD	1	Total 32	C 10	N 5	O 14	P 3	0
25	LE	1	Total 32	C 10	N 5	O 14	P 3	0
25	LF	1	Total 32	C 10	N 5	O 14	P 3	0
25	LG	1	Total 32	C 10	N 5	O 14	P 3	0
25	LH	1	Total 32	C 10	N 5	O 14	P 3	0
25	LI	1	Total 32	C 10	N 5	O 14	P 3	0
25	ME	1	Total 32	C 10	N 5	O 14	P 3	0
25	MF	1	Total 32	C 10	N 5	O 14	P 3	0
25	MG	1	Total 32	C 10	N 5	O 14	P 3	0
25	MH	1	Total 32	C 10	N 5	O 14	P 3	0
25	MI	1	Total 32	C 10	N 5	O 14	P 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
25	ND	1	32	10	5	14	3	0
25	NE	1	32	10	5	14	3	0
25	NF	1	32	10	5	14	3	0
25	NG	1	32	10	5	14	3	0
25	NH	1	32	10	5	14	3	0
25	NI	1	32	10	5	14	3	0
25	OD	1	32	10	5	14	3	0
25	OE	1	32	10	5	14	3	0
25	OF	1	32	10	5	14	3	0
25	OG	1	32	10	5	14	3	0
25	OH	1	32	10	5	14	3	0
25	OI	1	32	10	5	14	3	0
25	PE	1	32	10	5	14	3	0
25	PF	1	32	10	5	14	3	0
25	PG	1	32	10	5	14	3	0
25	PH	1	32	10	5	14	3	0
25	PI	1	32	10	5	14	3	0
25	QE	1	32	10	5	14	3	0
25	QF	1	32	10	5	14	3	0
25	QG	1	32	10	5	14	3	0
25	QH	1	32	10	5	14	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	QI	1	Total 32	C 10	N 5	O 14	P 3	0
25	RE	1	Total 32	C 10	N 5	O 14	P 3	0
25	RF	1	Total 32	C 10	N 5	O 14	P 3	0
25	RG	1	Total 32	C 10	N 5	O 14	P 3	0
25	RH	1	Total 32	C 10	N 5	O 14	P 3	0
25	RI	1	Total 32	C 10	N 5	O 14	P 3	0
25	RJ	1	Total 32	C 10	N 5	O 14	P 3	0
25	SE	1	Total 32	C 10	N 5	O 14	P 3	0
25	SF	1	Total 32	C 10	N 5	O 14	P 3	0
25	SG	1	Total 32	C 10	N 5	O 14	P 3	0
25	SH	1	Total 32	C 10	N 5	O 14	P 3	0
25	SI	1	Total 32	C 10	N 5	O 14	P 3	0
25	SJ	1	Total 32	C 10	N 5	O 14	P 3	0
25	TF	1	Total 32	C 10	N 5	O 14	P 3	0
25	TG	1	Total 32	C 10	N 5	O 14	P 3	0
25	TH	1	Total 32	C 10	N 5	O 14	P 3	0
25	TI	1	Total 32	C 10	N 5	O 14	P 3	0
25	TJ	1	Total 32	C 10	N 5	O 14	P 3	0
25	UD	1	Total 32	C 10	N 5	O 14	P 3	0
25	UE	1	Total 32	C 10	N 5	O 14	P 3	0
25	UF	1	Total 32	C 10	N 5	O 14	P 3	0

Continued on next page...

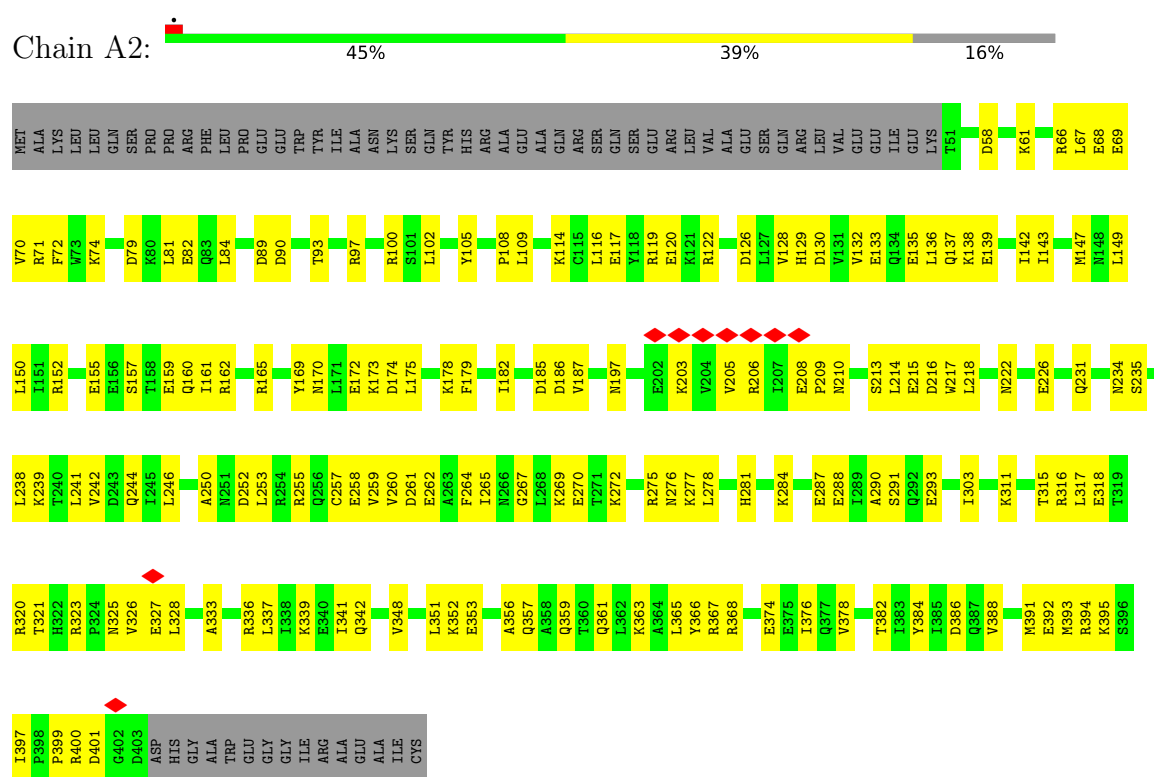
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	UG	1	Total 32	C 10	N 5	O 14	P 3	0
25	UH	1	Total 32	C 10	N 5	O 14	P 3	0
25	VD	1	Total 32	C 10	N 5	O 14	P 3	0
25	VE	1	Total 32	C 10	N 5	O 14	P 3	0
25	VF	1	Total 32	C 10	N 5	O 14	P 3	0
25	VG	1	Total 32	C 10	N 5	O 14	P 3	0
25	VH	1	Total 32	C 10	N 5	O 14	P 3	0
25	WE	1	Total 32	C 10	N 5	O 14	P 3	0
25	WF	1	Total 32	C 10	N 5	O 14	P 3	0
25	WG	1	Total 32	C 10	N 5	O 14	P 3	0
25	WH	1	Total 32	C 10	N 5	O 14	P 3	0
25	WI	1	Total 32	C 10	N 5	O 14	P 3	0

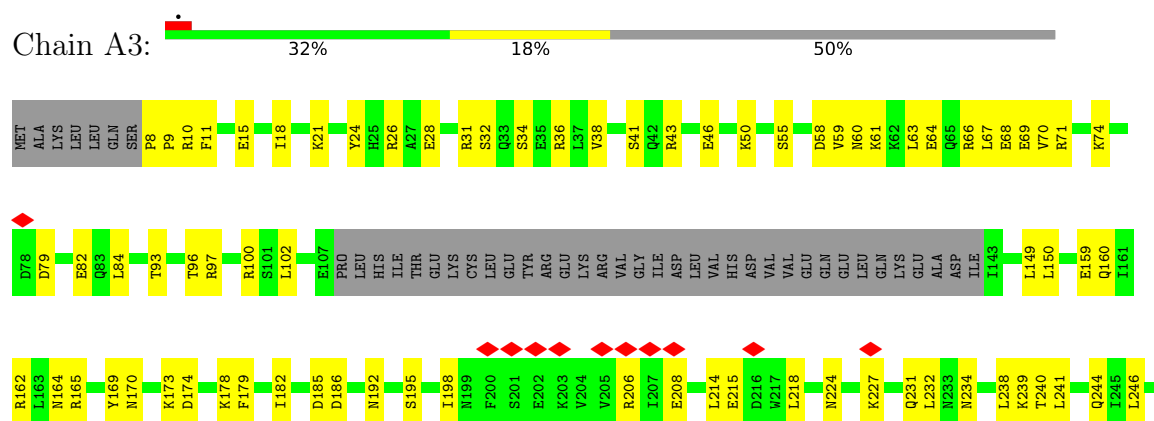
3 Residue-property plots

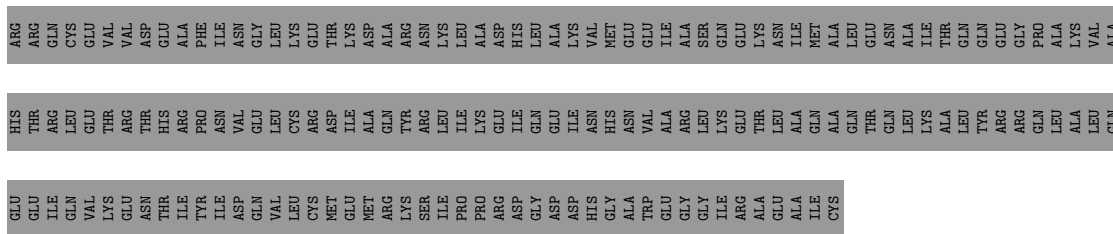
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Tektin-1



• Molecule 1: Tektin-1

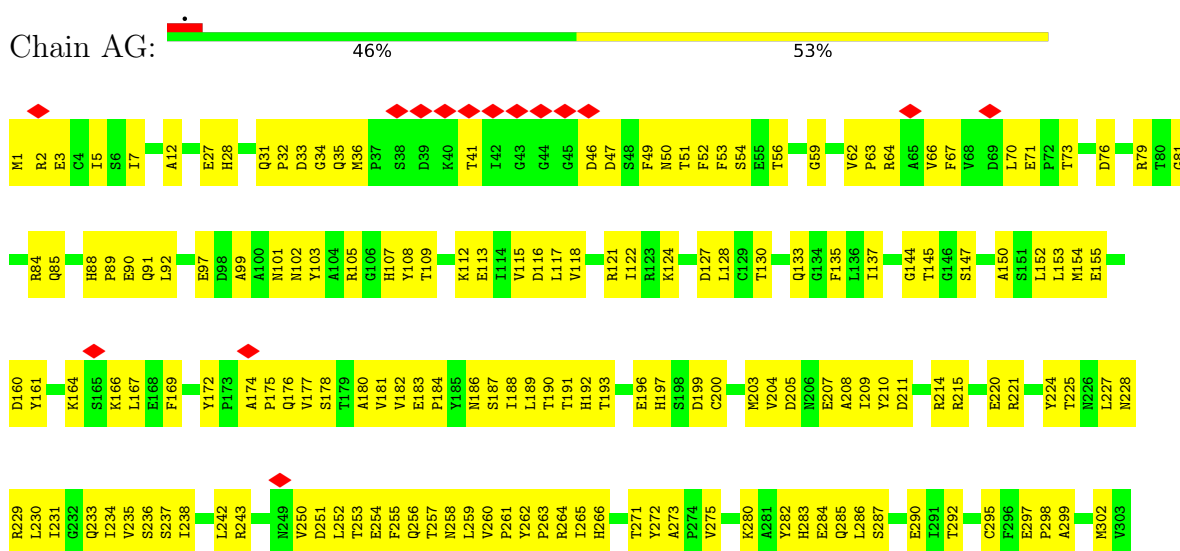


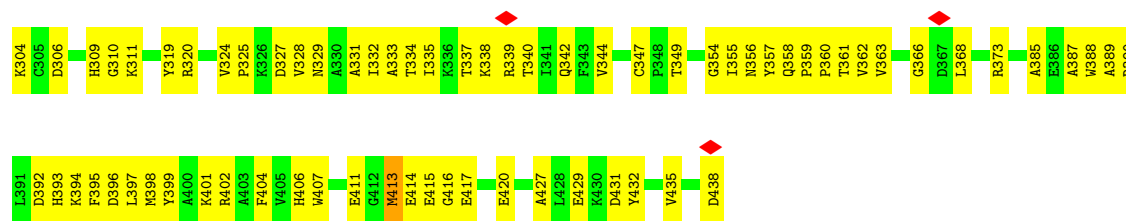


- Molecule 2: Detyrosinated tubulin alpha-3 chain

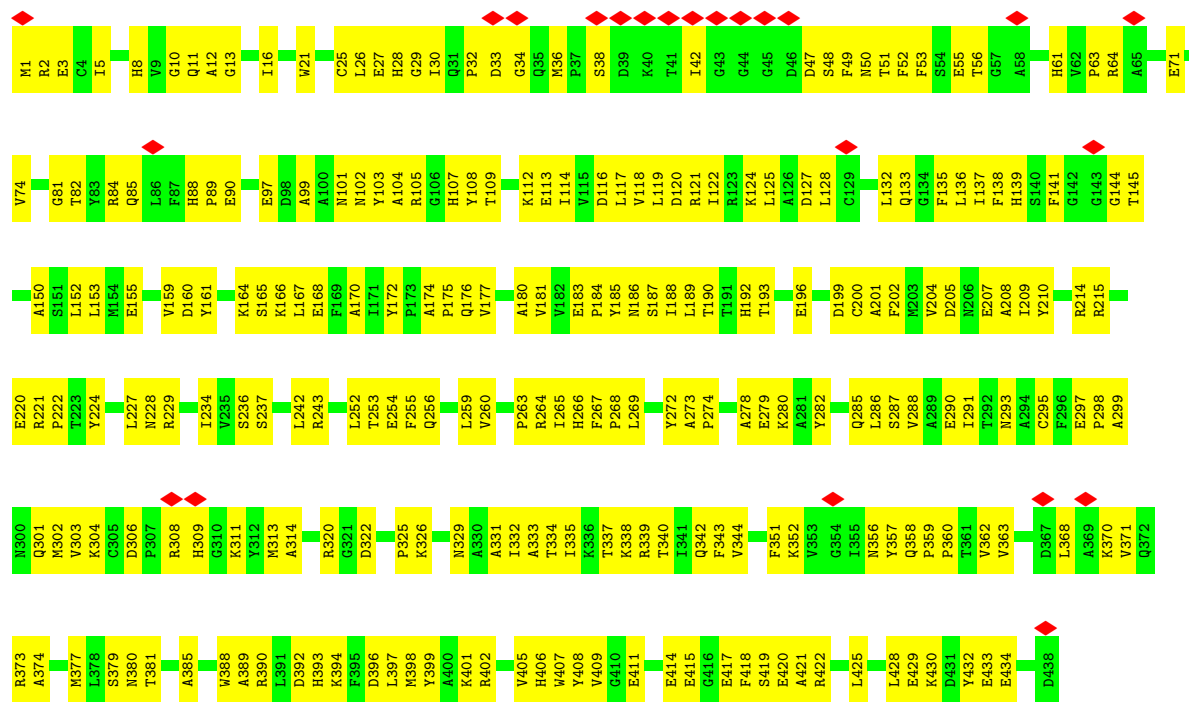
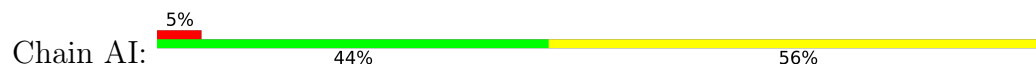


- Molecule 2: Detyrosinated tubulin alpha-3 chain

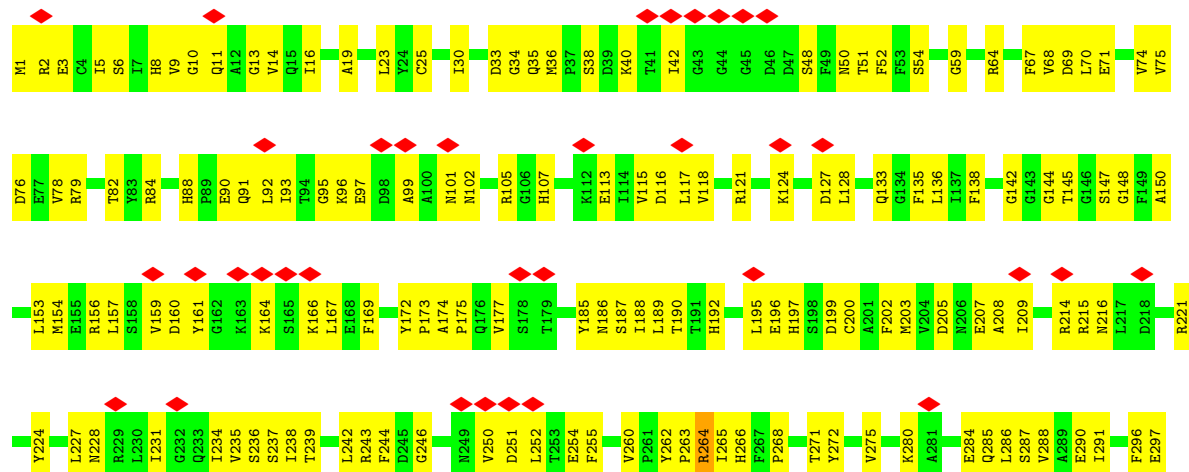


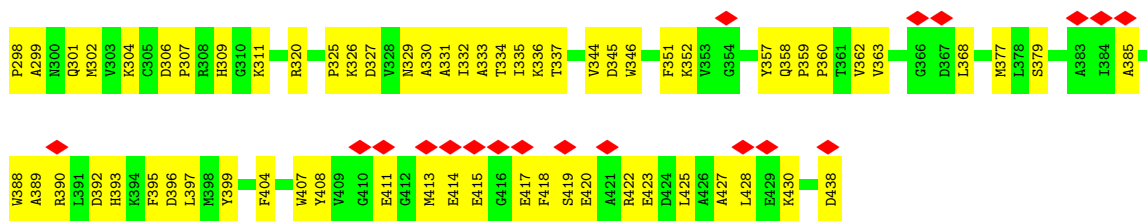


• Molecule 2: Detyrosinated tubulin alpha-3 chain

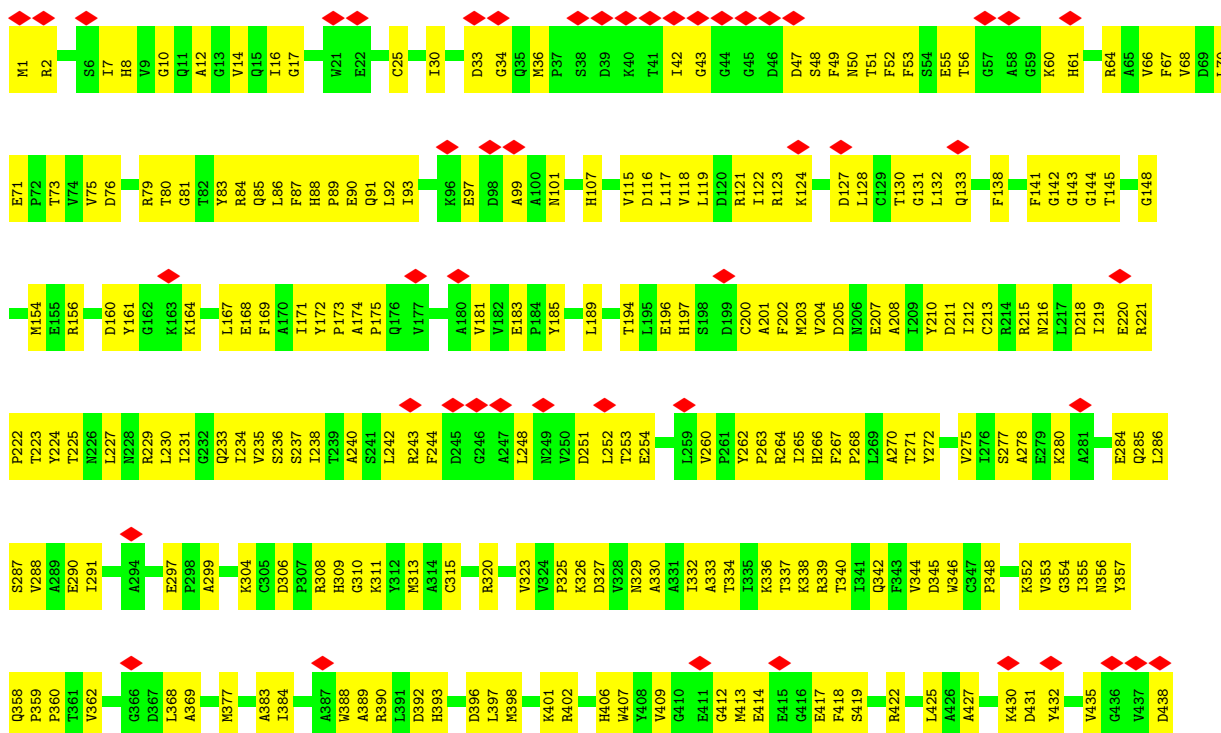


• Molecule 2: Detyrosinated tubulin alpha-3 chain

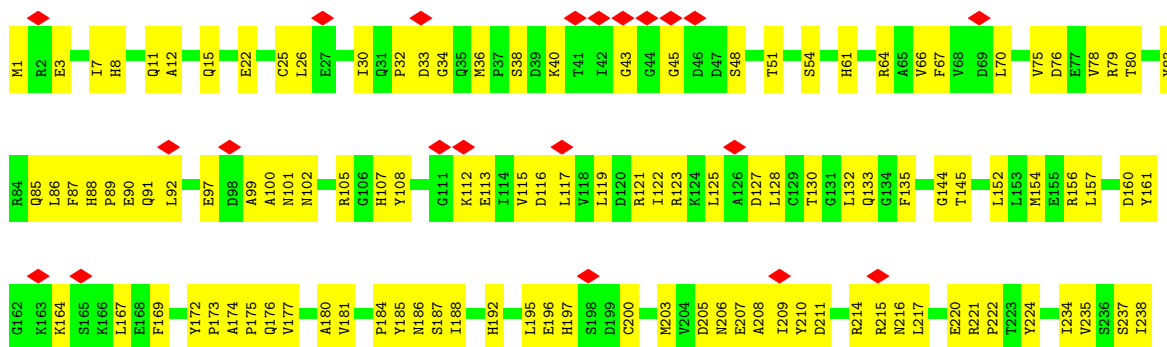


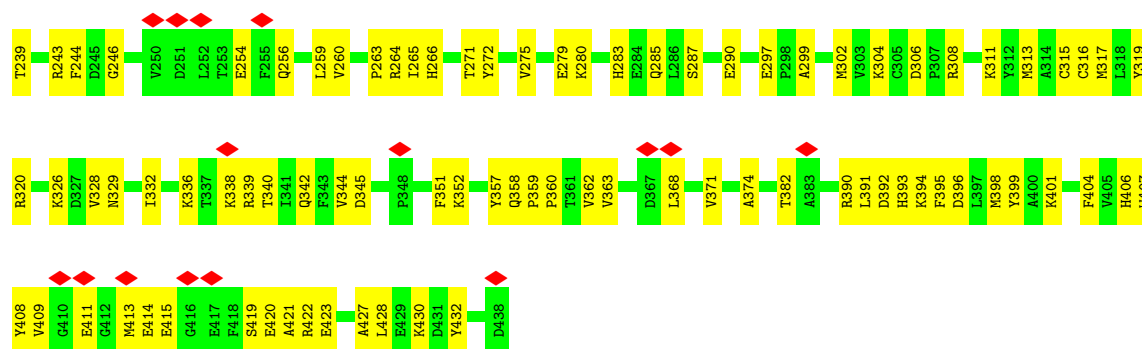


• Molecule 2: Detyrosinated tubulin alpha-3 chain

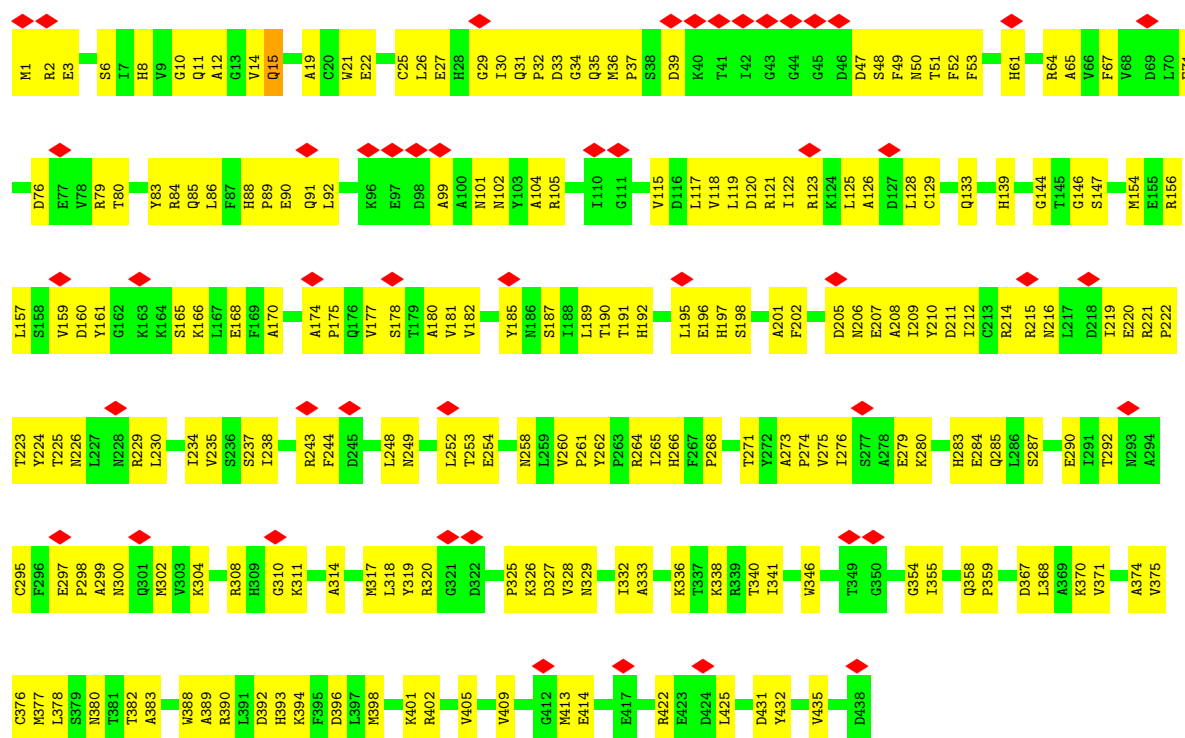


• Molecule 2: Detyrosinated tubulin alpha-3 chain

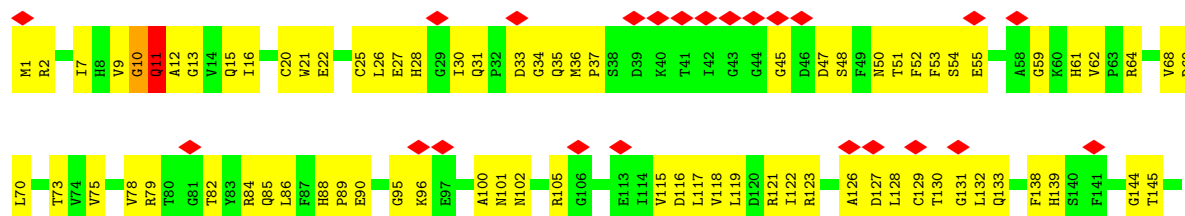


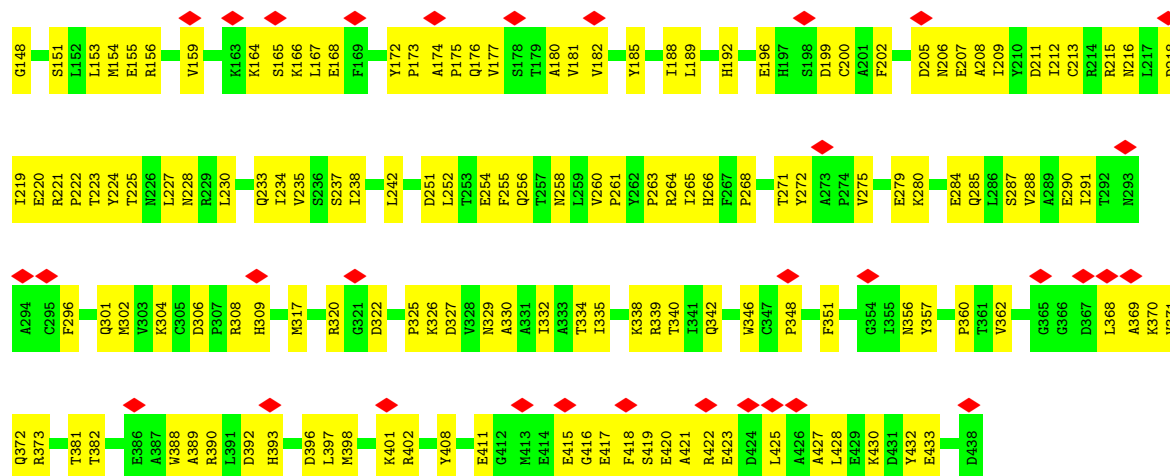


• Molecule 2: Detyrosinated tubulin alpha-3 chain

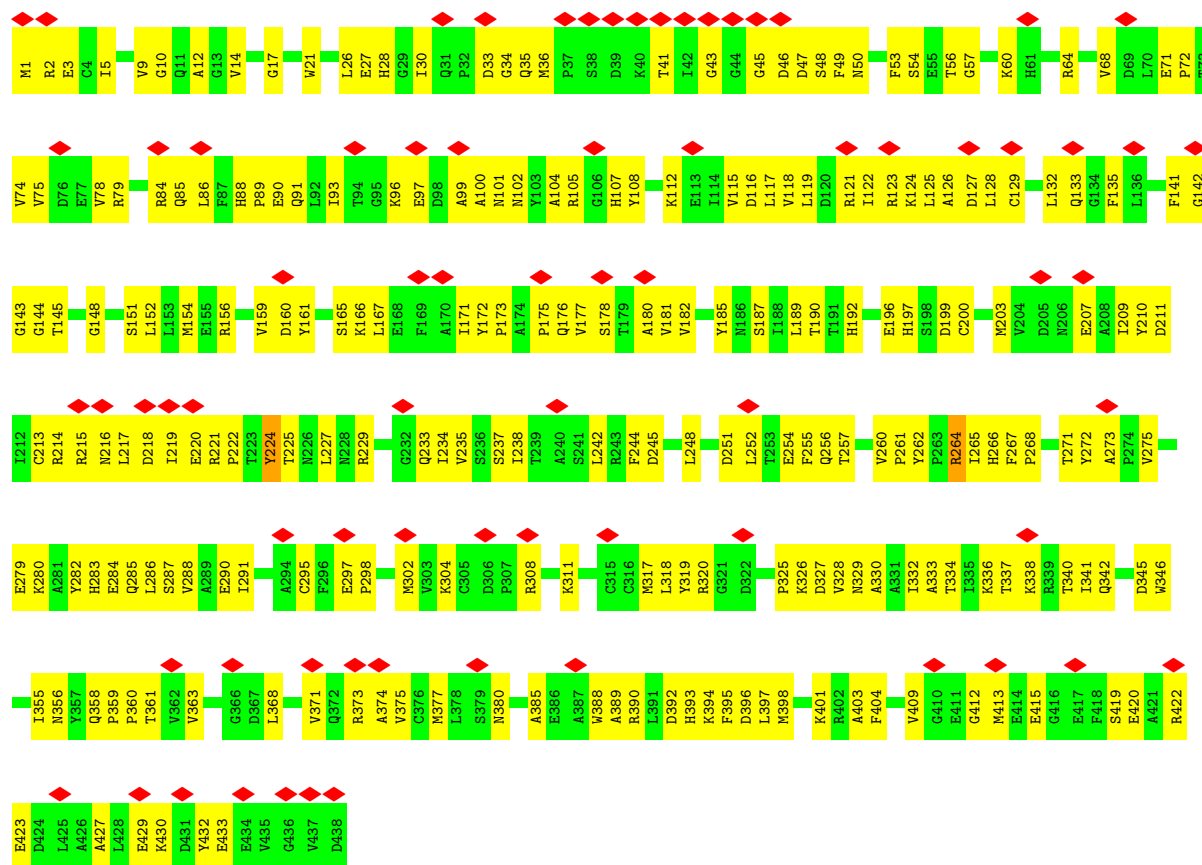


• Molecule 2: Detyrosinated tubulin alpha-3 chain



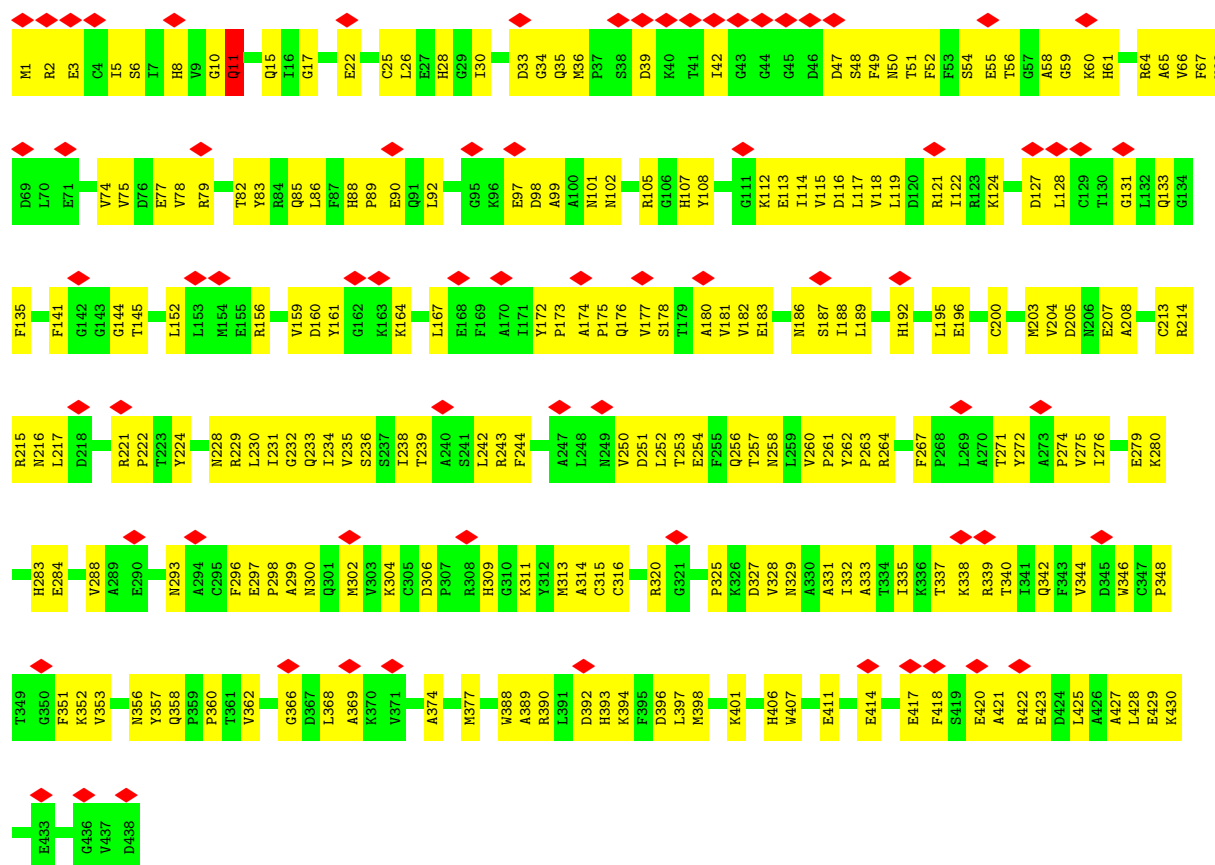


• Molecule 2: Detyrosinated tubulin alpha-3 chain

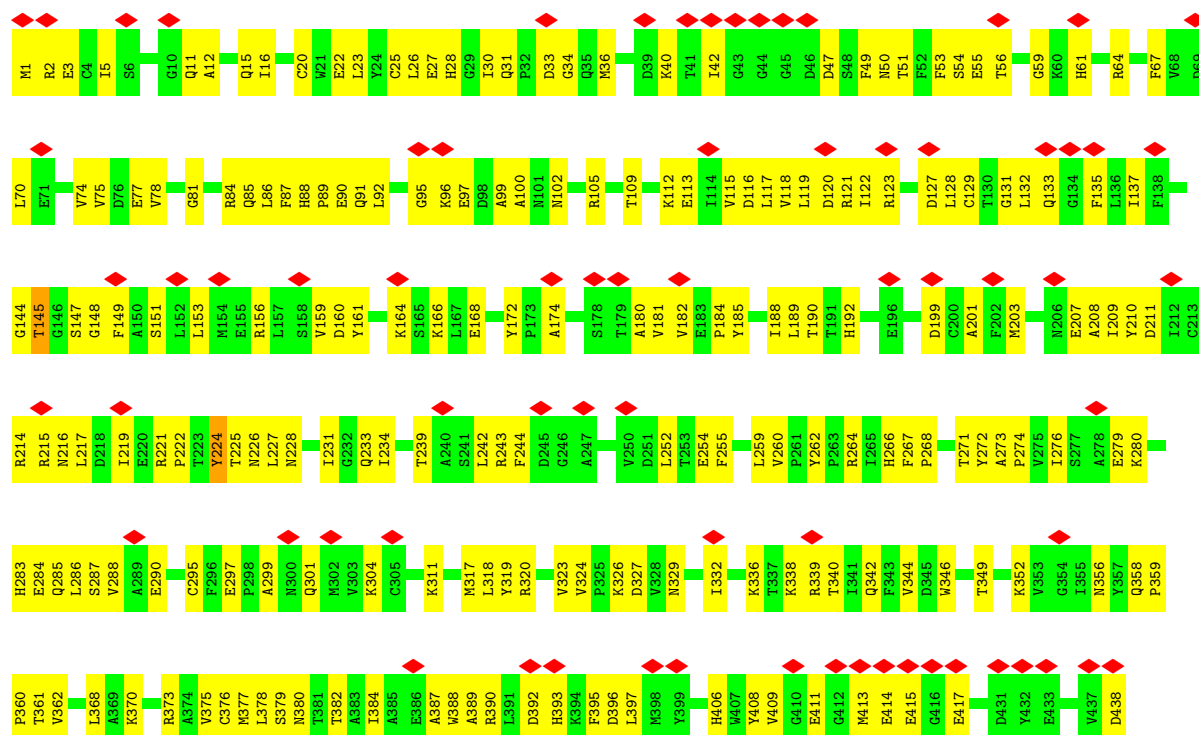


• Molecule 2: Detyrosinated tubulin alpha-3 chain





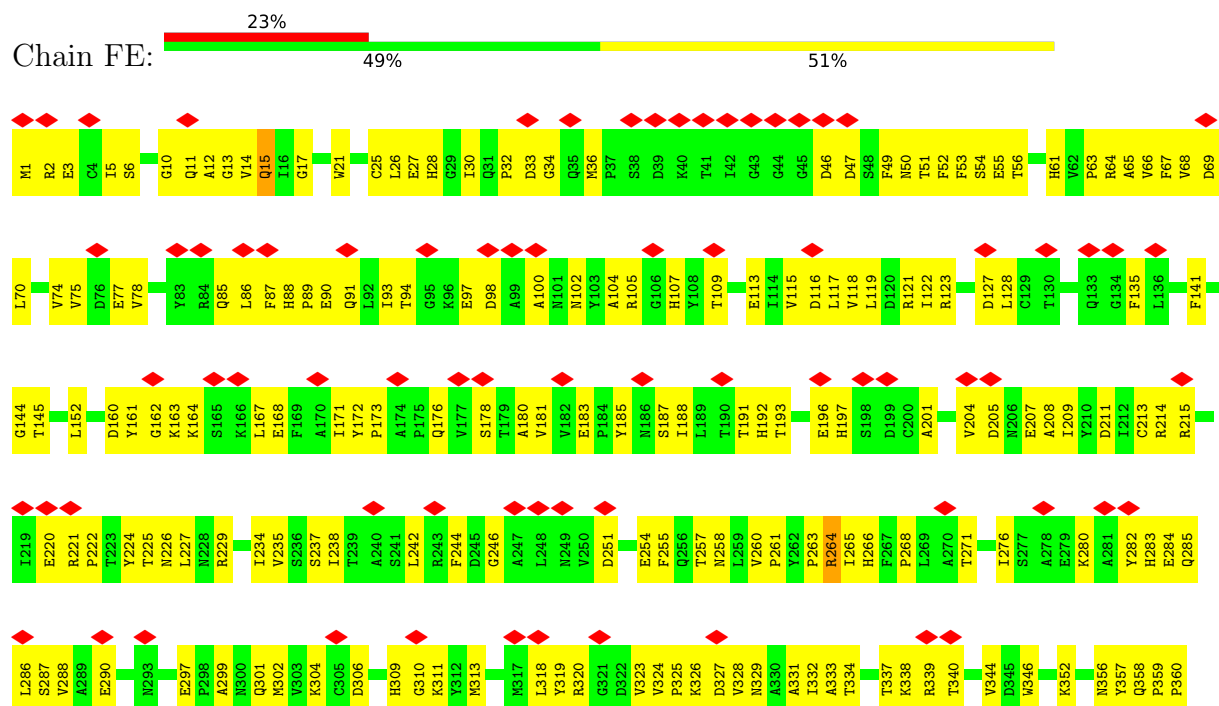
• Molecule 2: Detyrosinated tubulin alpha-3 chain

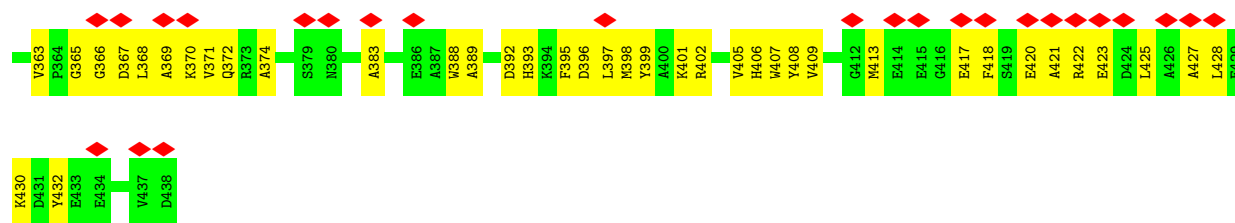


- Molecule 2: Detyrosinated tubulin alpha-3 chain

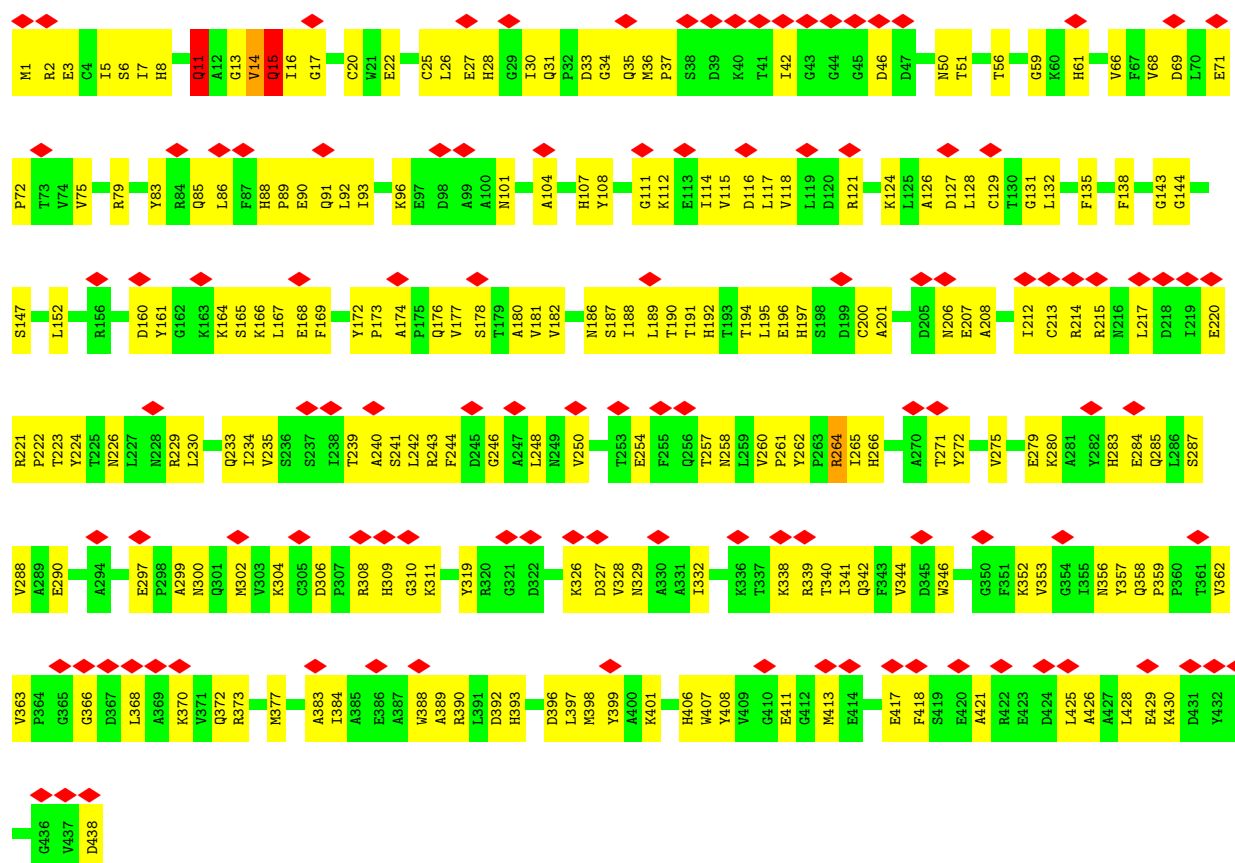


- Molecule 2: Detyrosinated tubulin alpha-3 chain

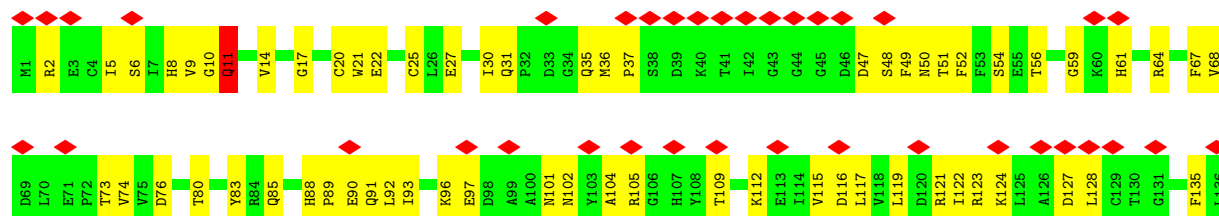


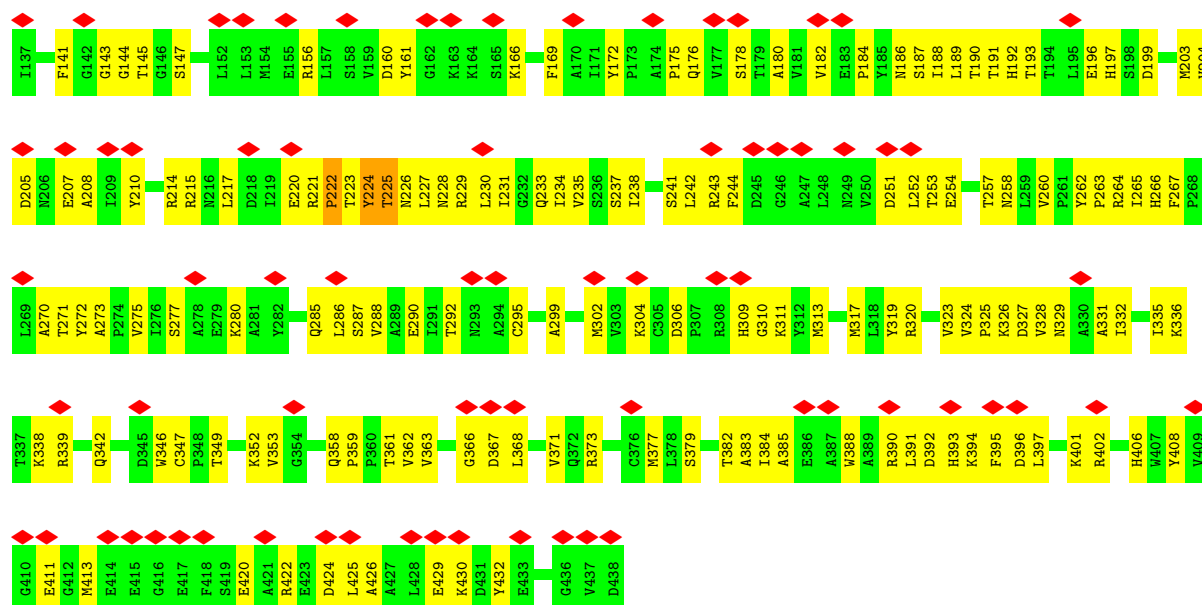


• Molecule 2: Detyrosinated tubulin alpha-3 chain

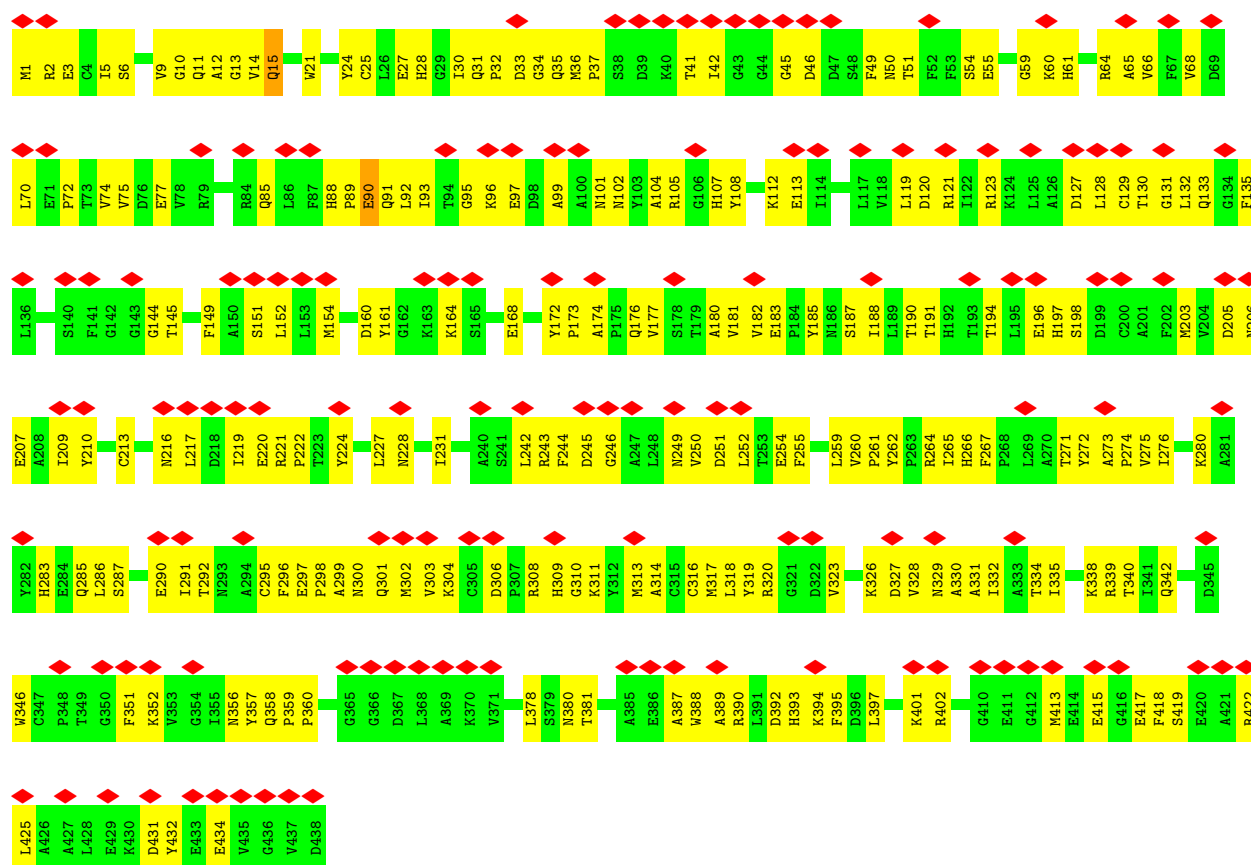


• Molecule 2: Detyrosinated tubulin alpha-3 chain

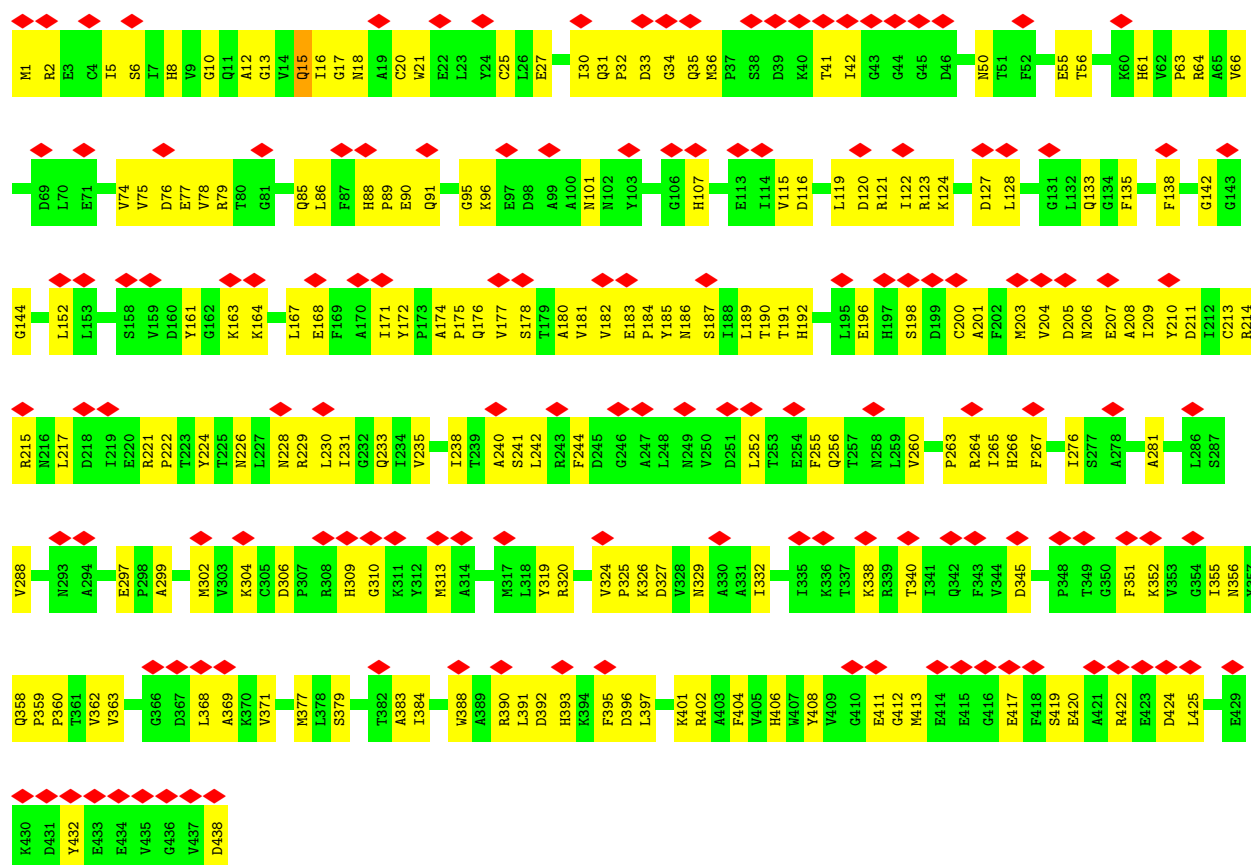




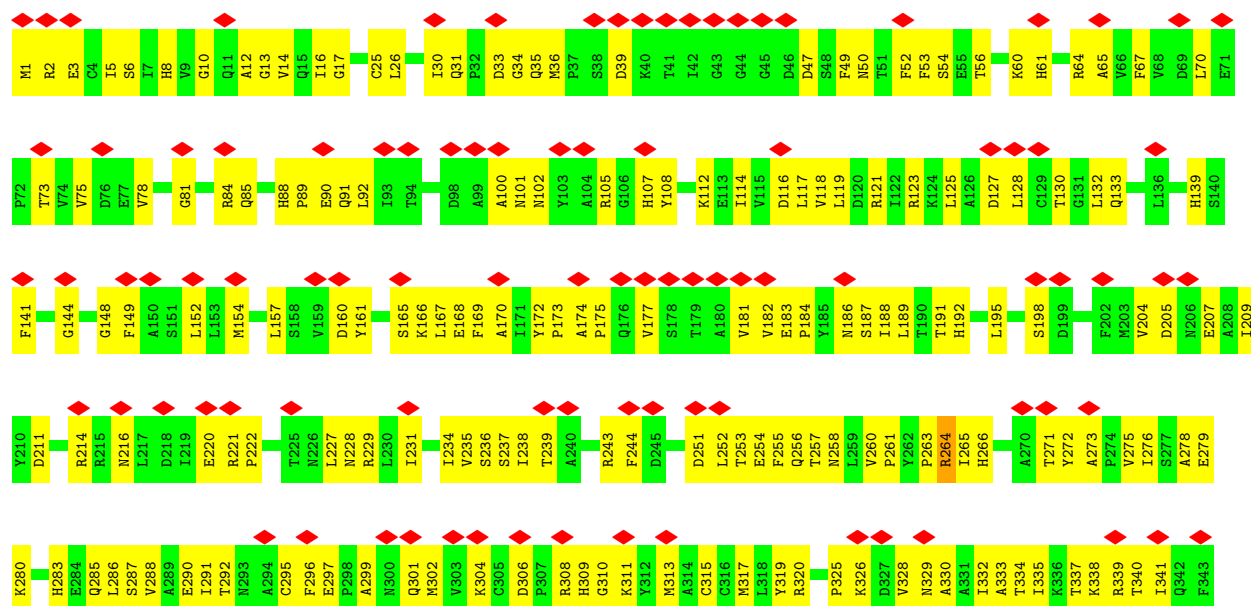
• Molecule 2: Detyrosinated tubulin alpha-3 chain

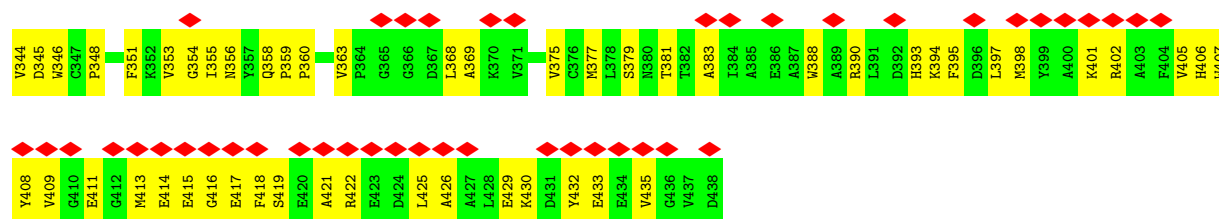


• Molecule 2: Detyrosinated tubulin alpha-3 chain

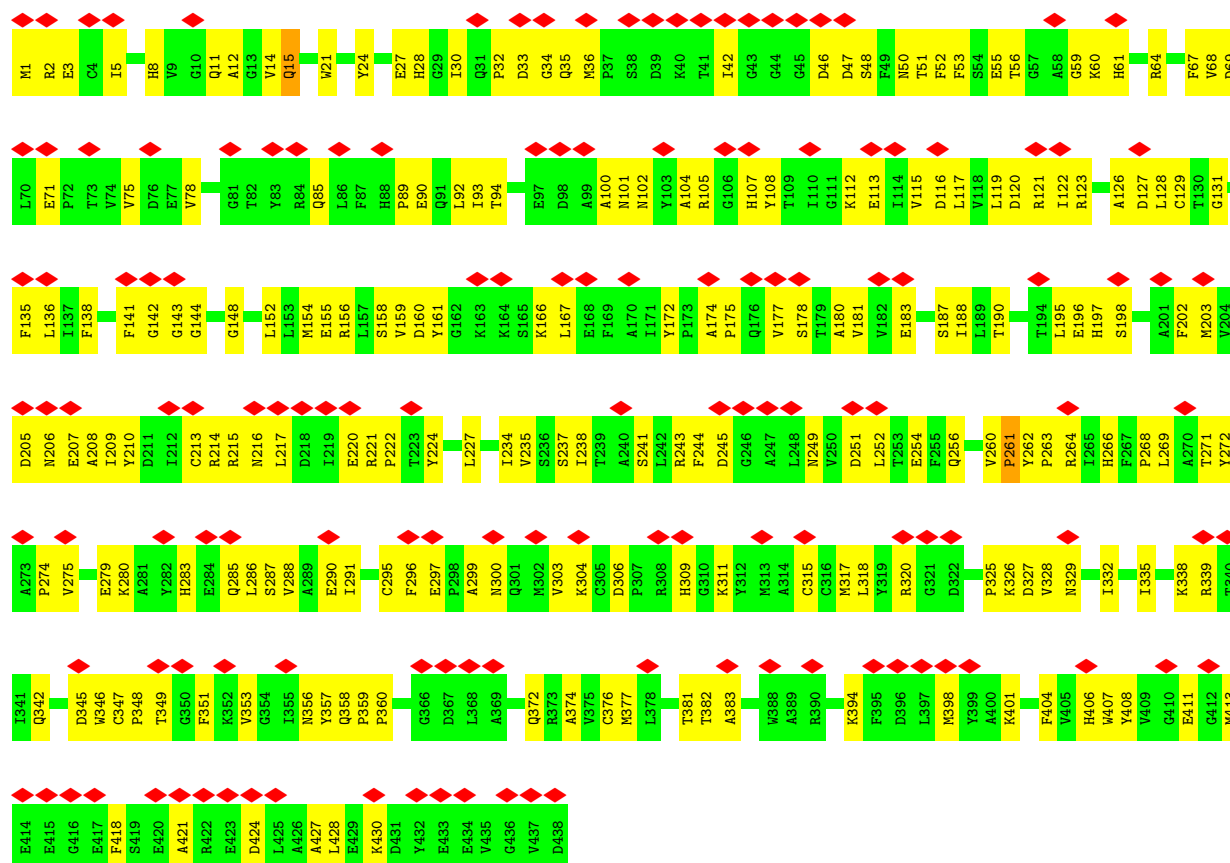


• Molecule 2: Detyrosinated tubulin alpha-3 chain

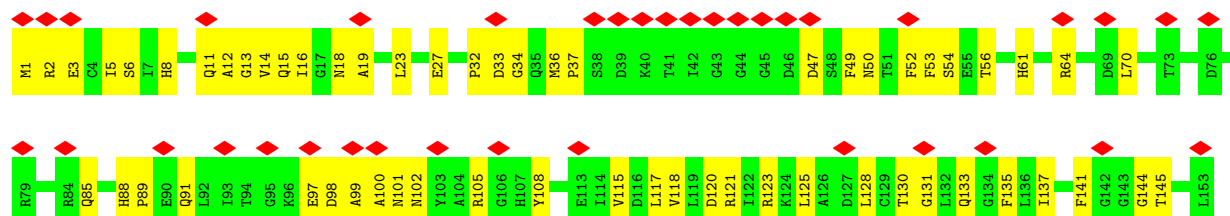


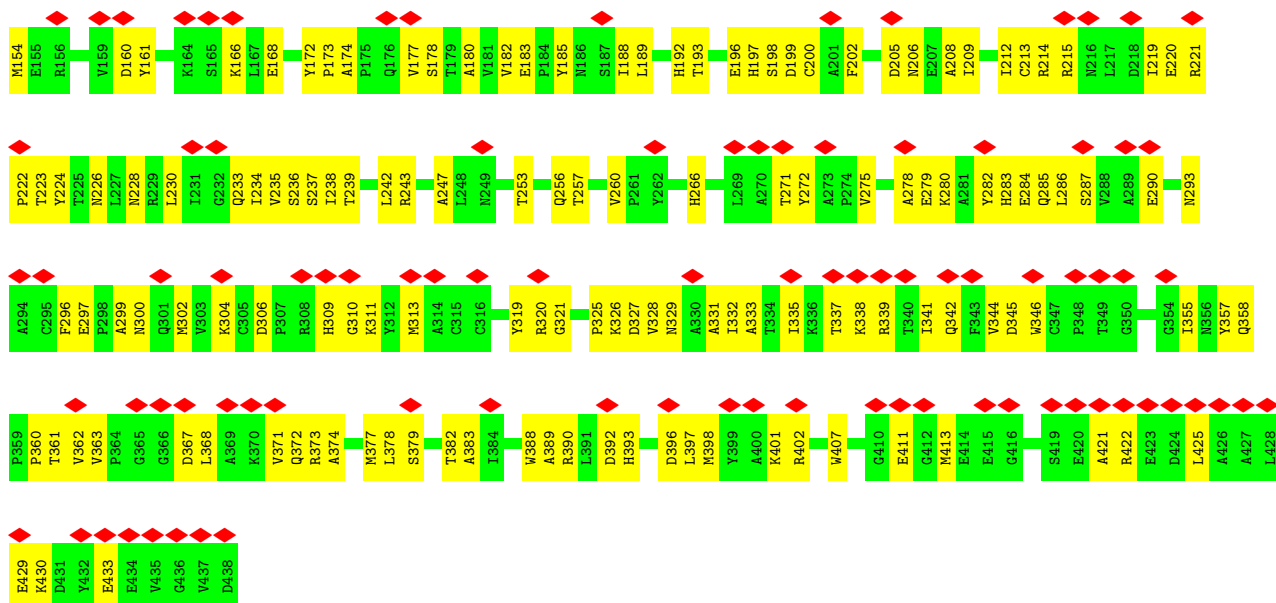


• Molecule 2: Detyrosinated tubulin alpha-3 chain

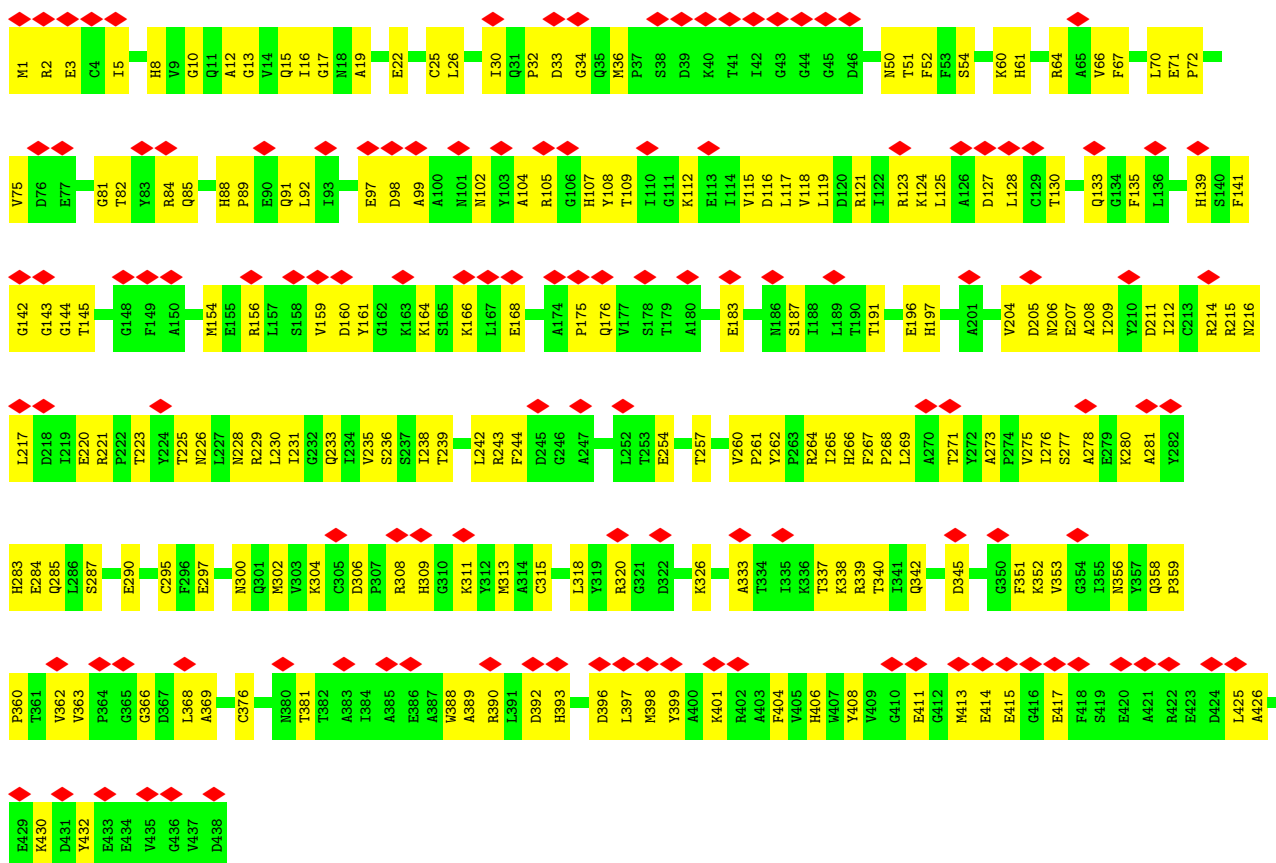


• Molecule 2: Detyrosinated tubulin alpha-3 chain

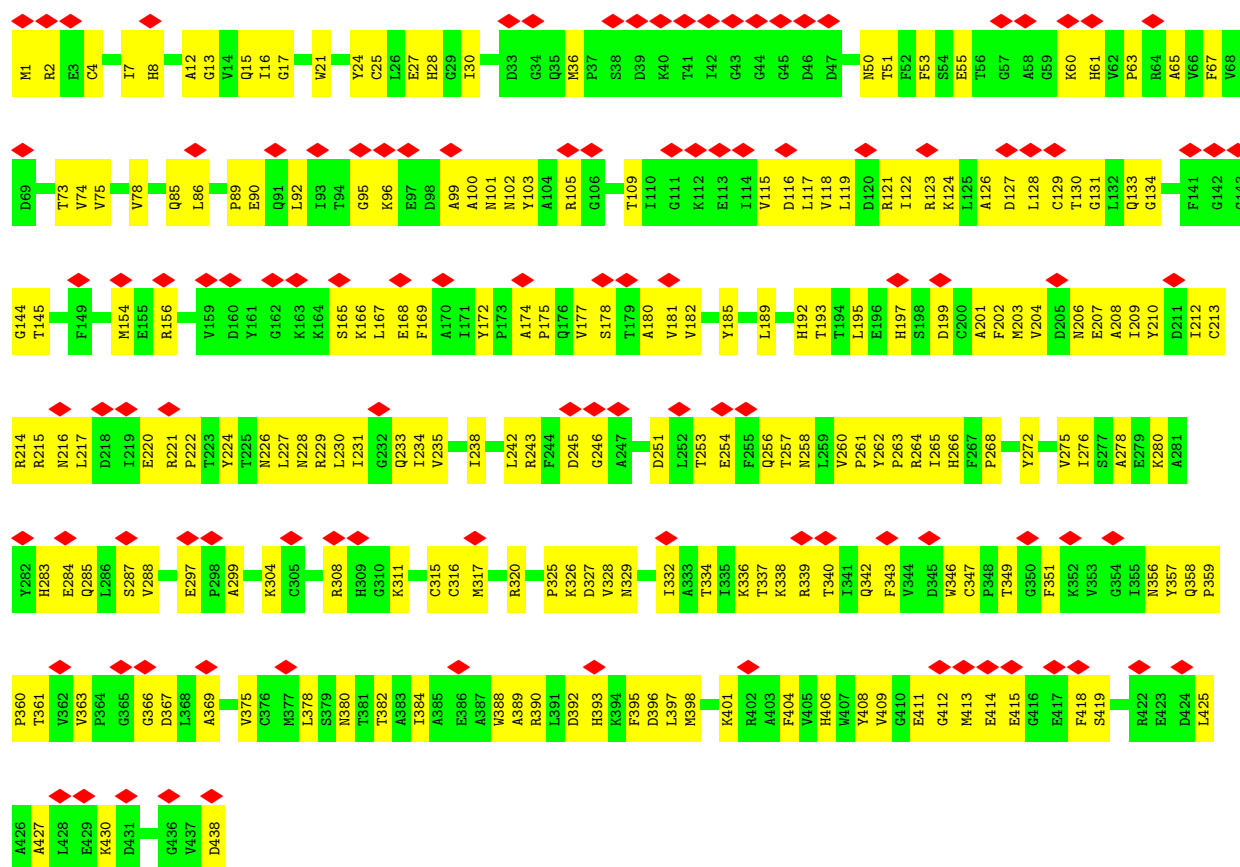




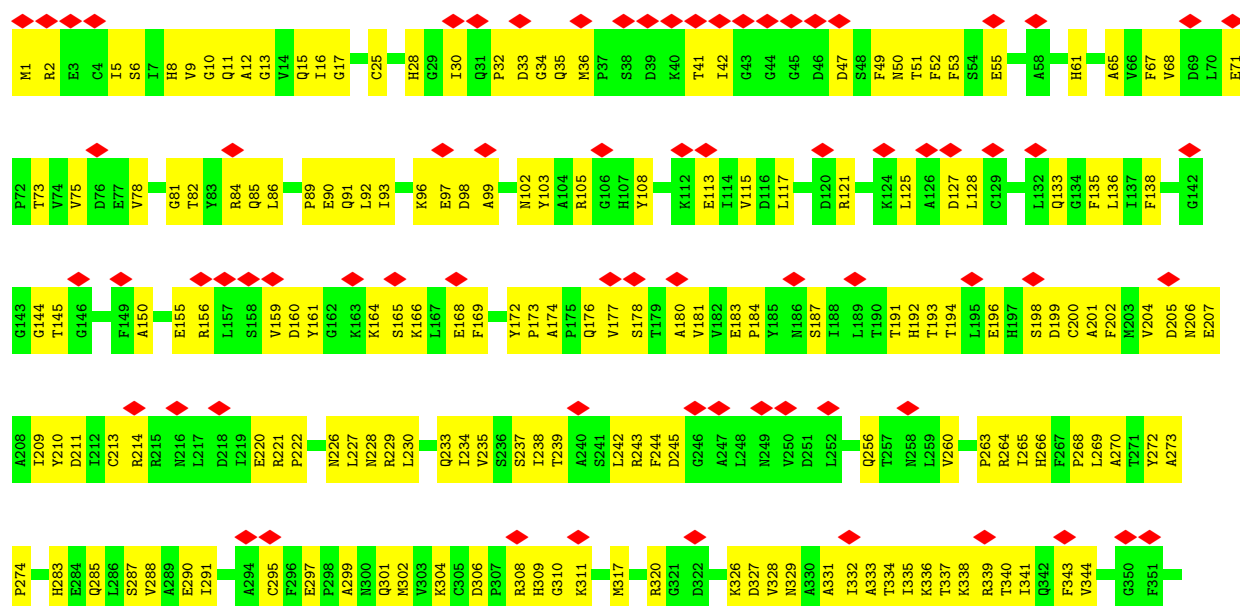
• Molecule 2: Detyrosinated tubulin alpha-3 chain

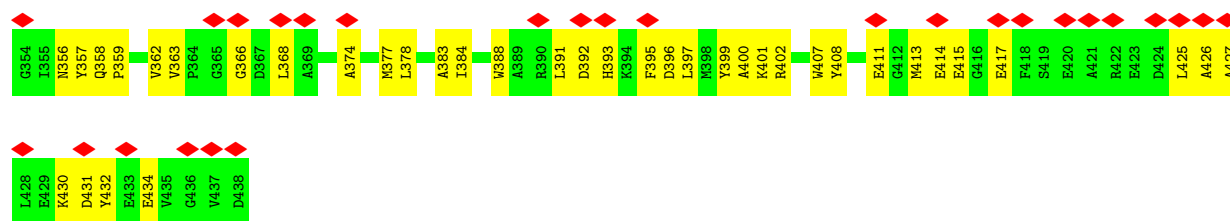


• Molecule 2: Detyrosinated tubulin alpha-3 chain

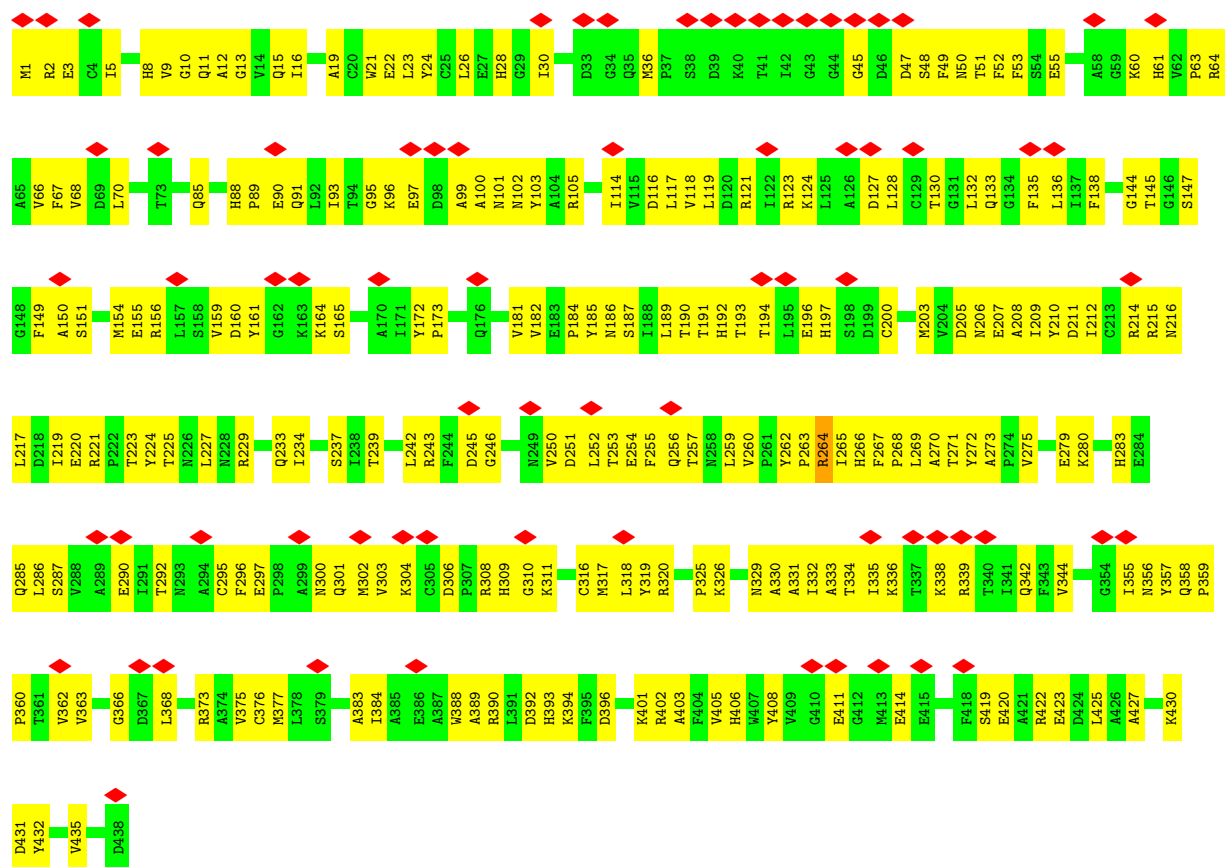


• Molecule 2: Detyrosinated tubulin alpha-3 chain

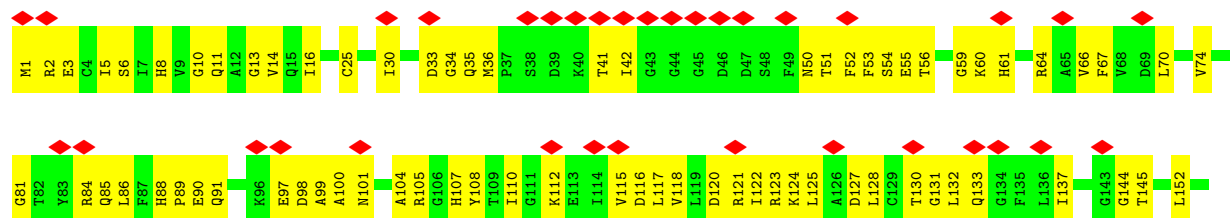


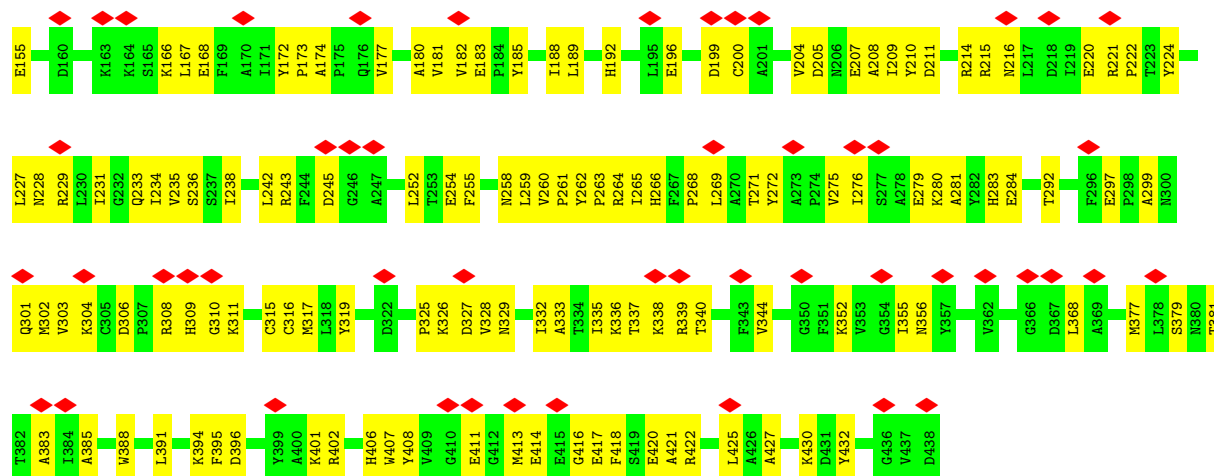


• Molecule 2: Detyrosinated tubulin alpha-3 chain

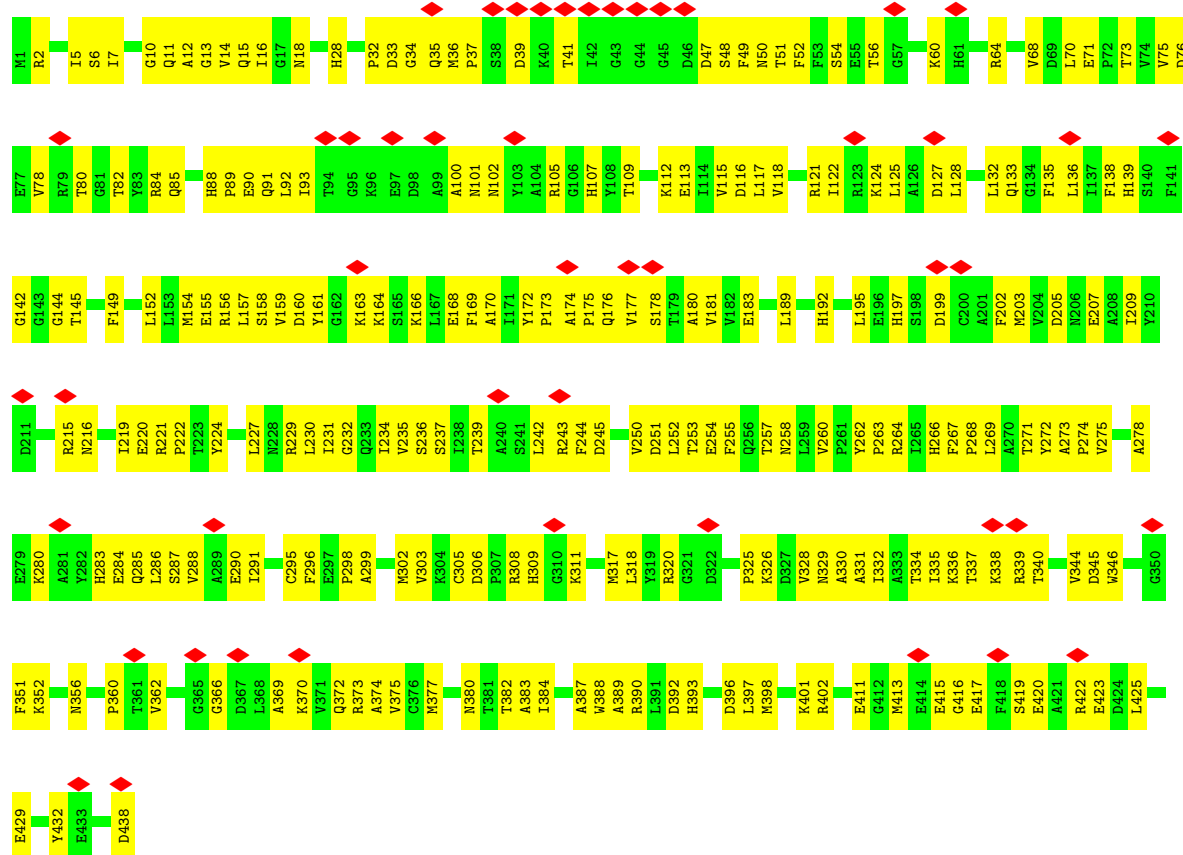


• Molecule 2: Detyrosinated tubulin alpha-3 chain



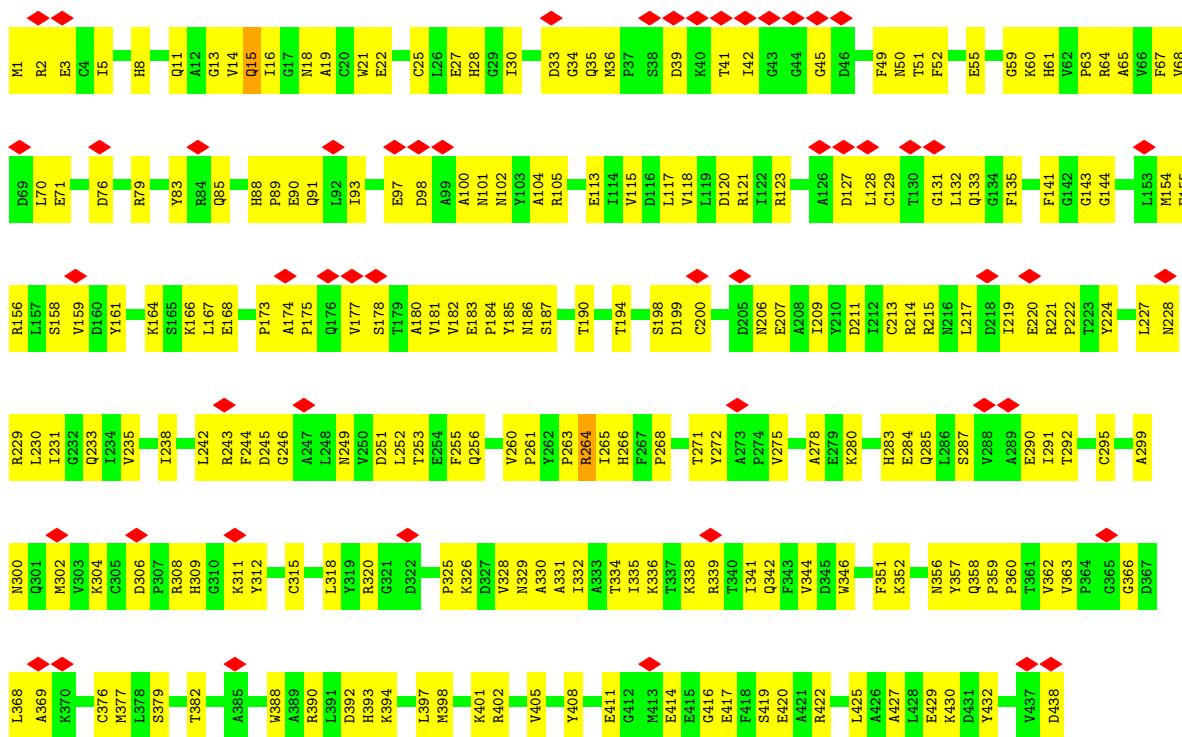


• Molecule 2: Detyrosinated tubulin alpha-3 chain

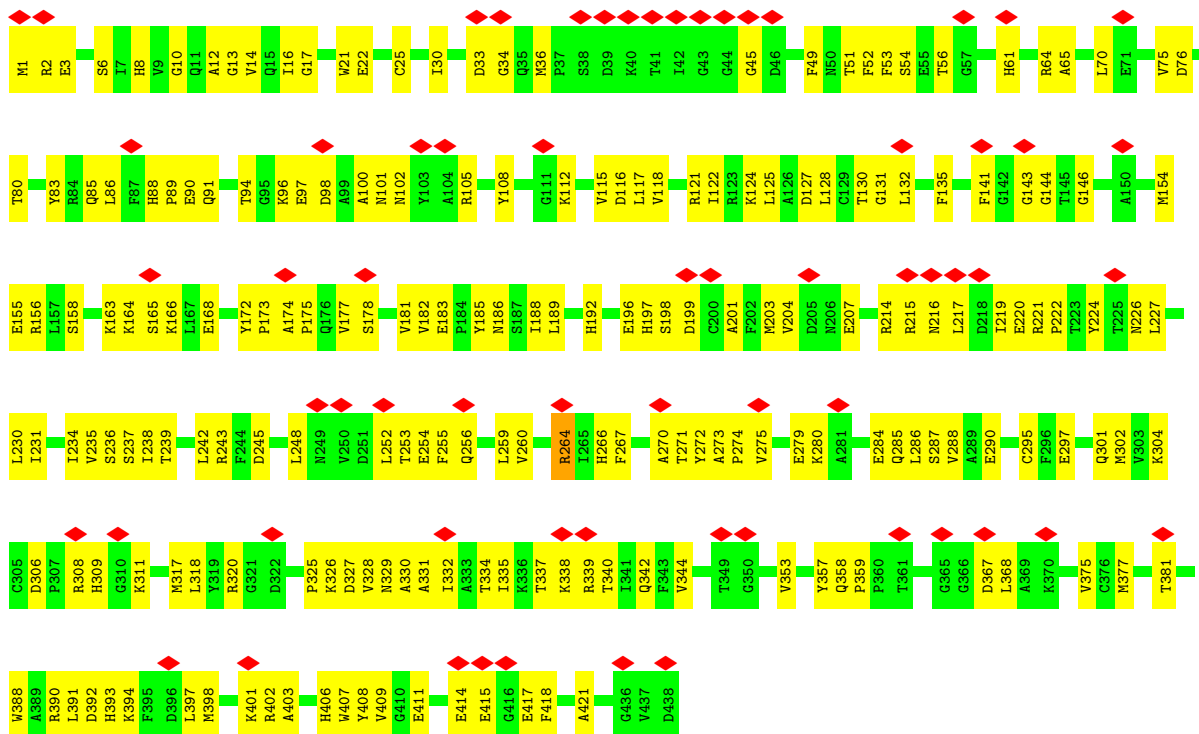


• Molecule 2: Detyrosinated tubulin alpha-3 chain

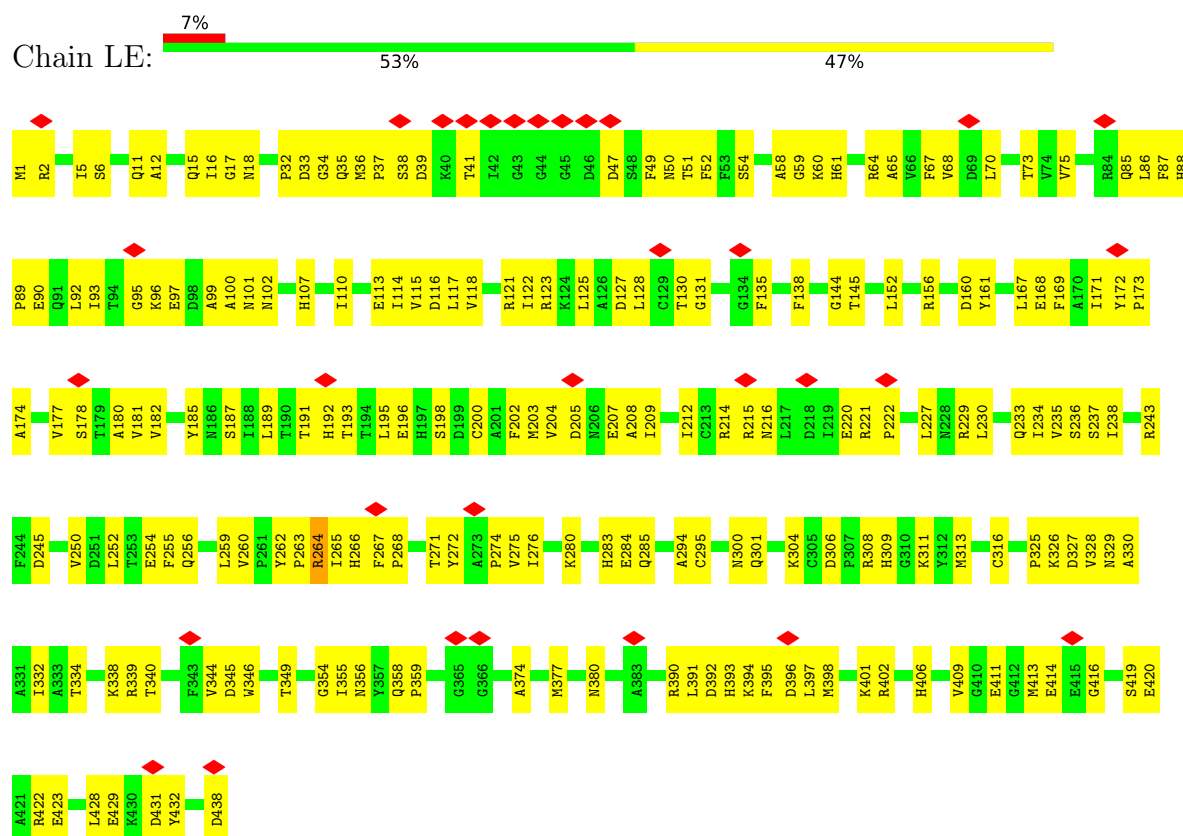




• Molecule 2: Detyrosinated tubulin alpha-3 chain



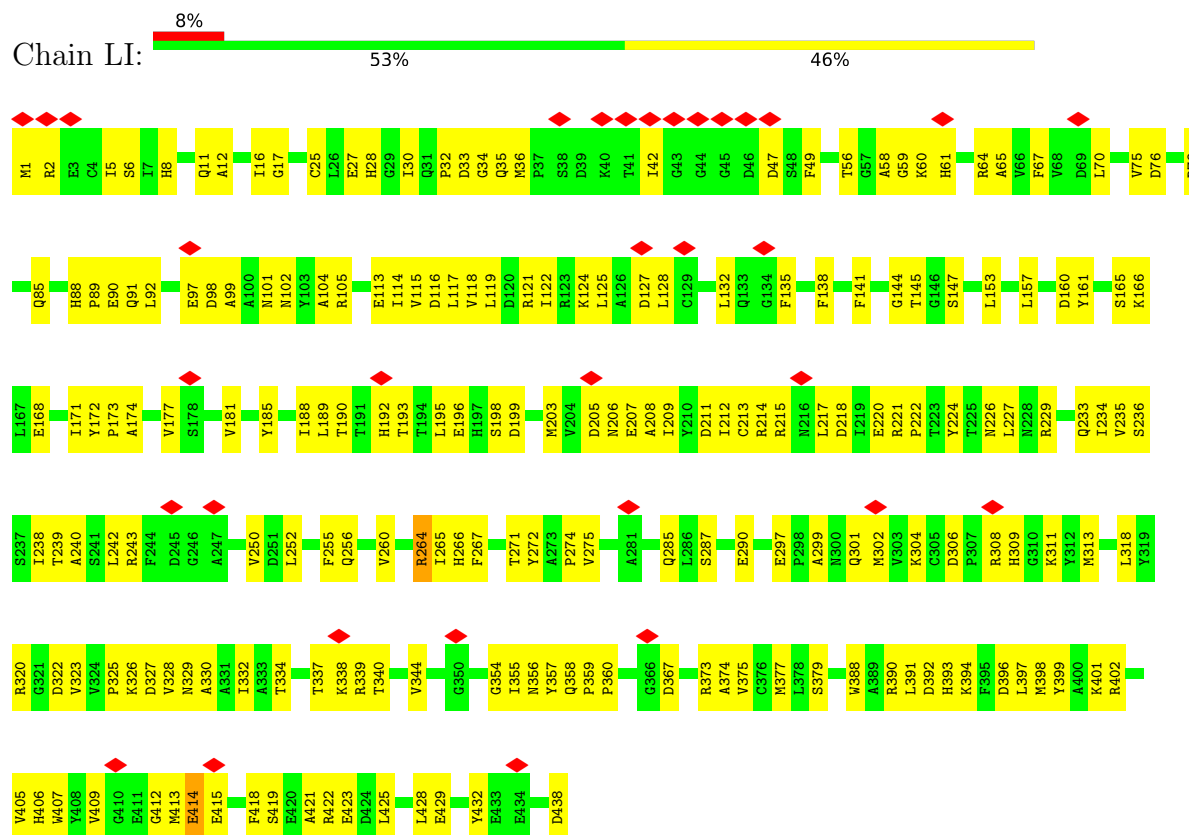
• Molecule 2: Detyrosinated tubulin alpha-3 chain



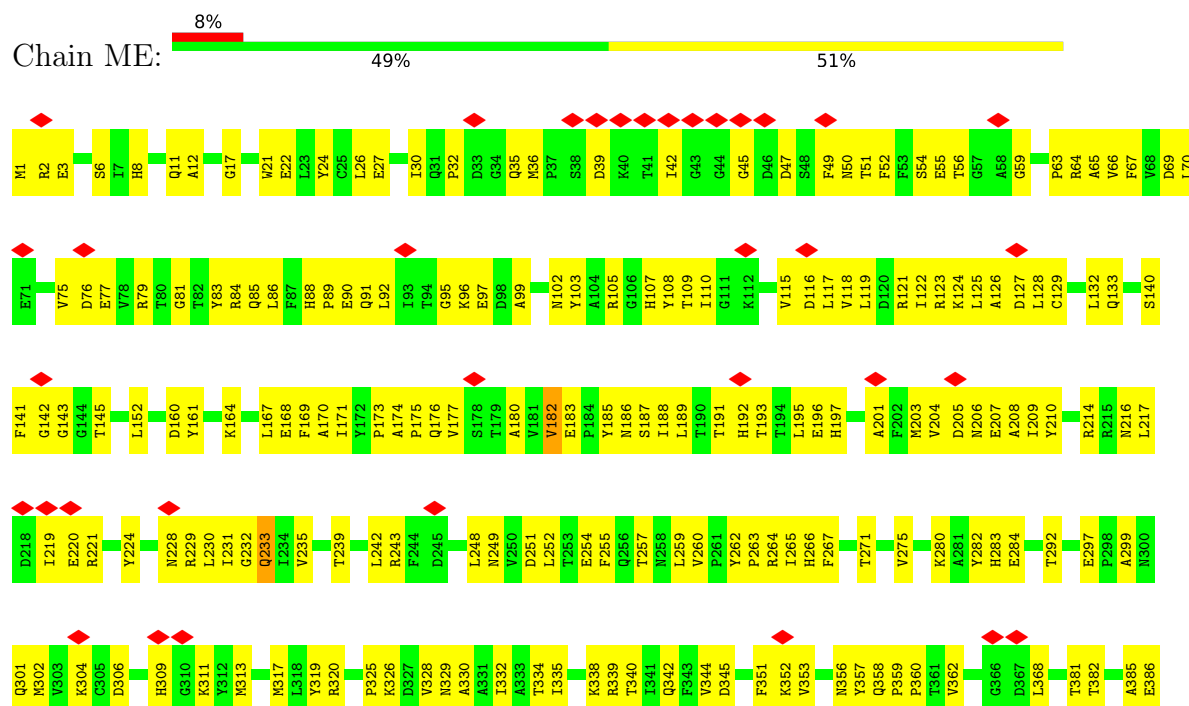
• Molecule 2: Detyrosinated tubulin alpha-3 chain



- Molecule 2: Detyrosinated tubulin alpha-3 chain

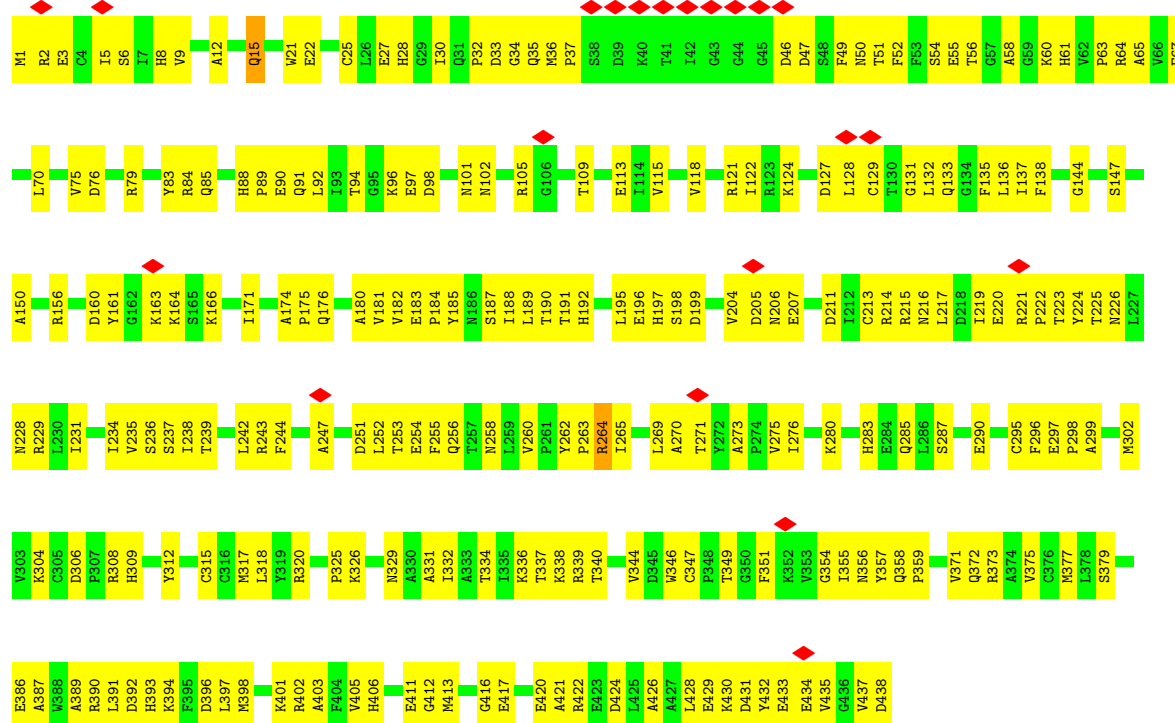


- Molecule 2: Detyrosinated tubulin alpha-3 chain

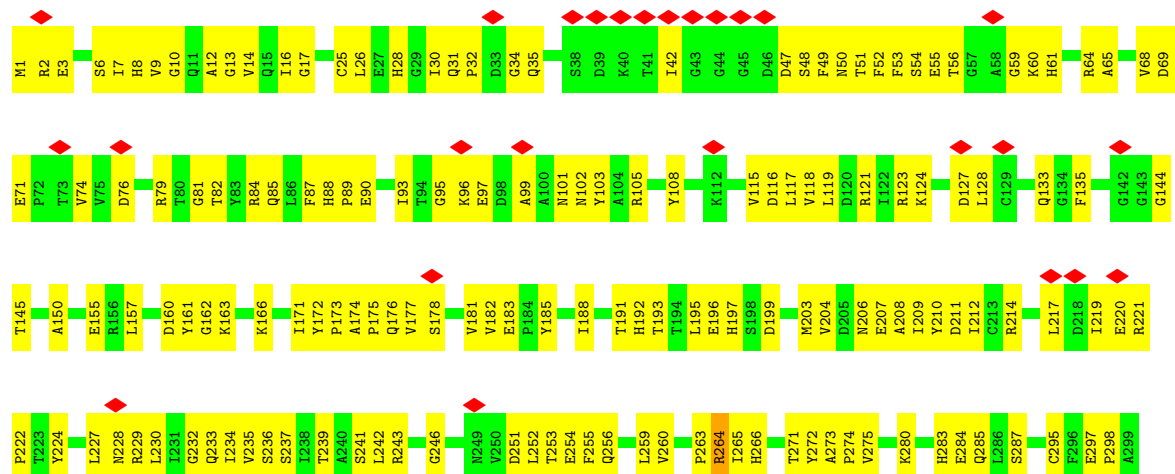


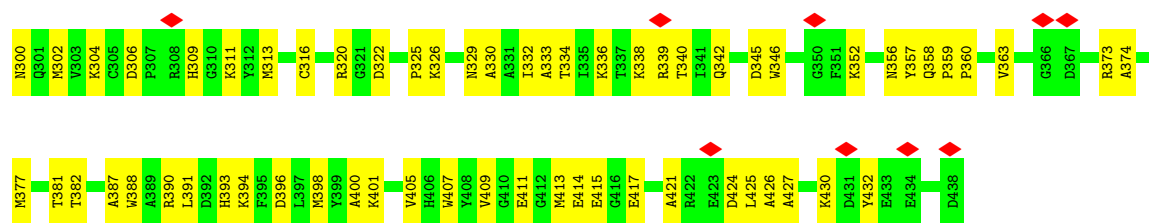


• Molecule 2: Detyrosinated tubulin alpha-3 chain

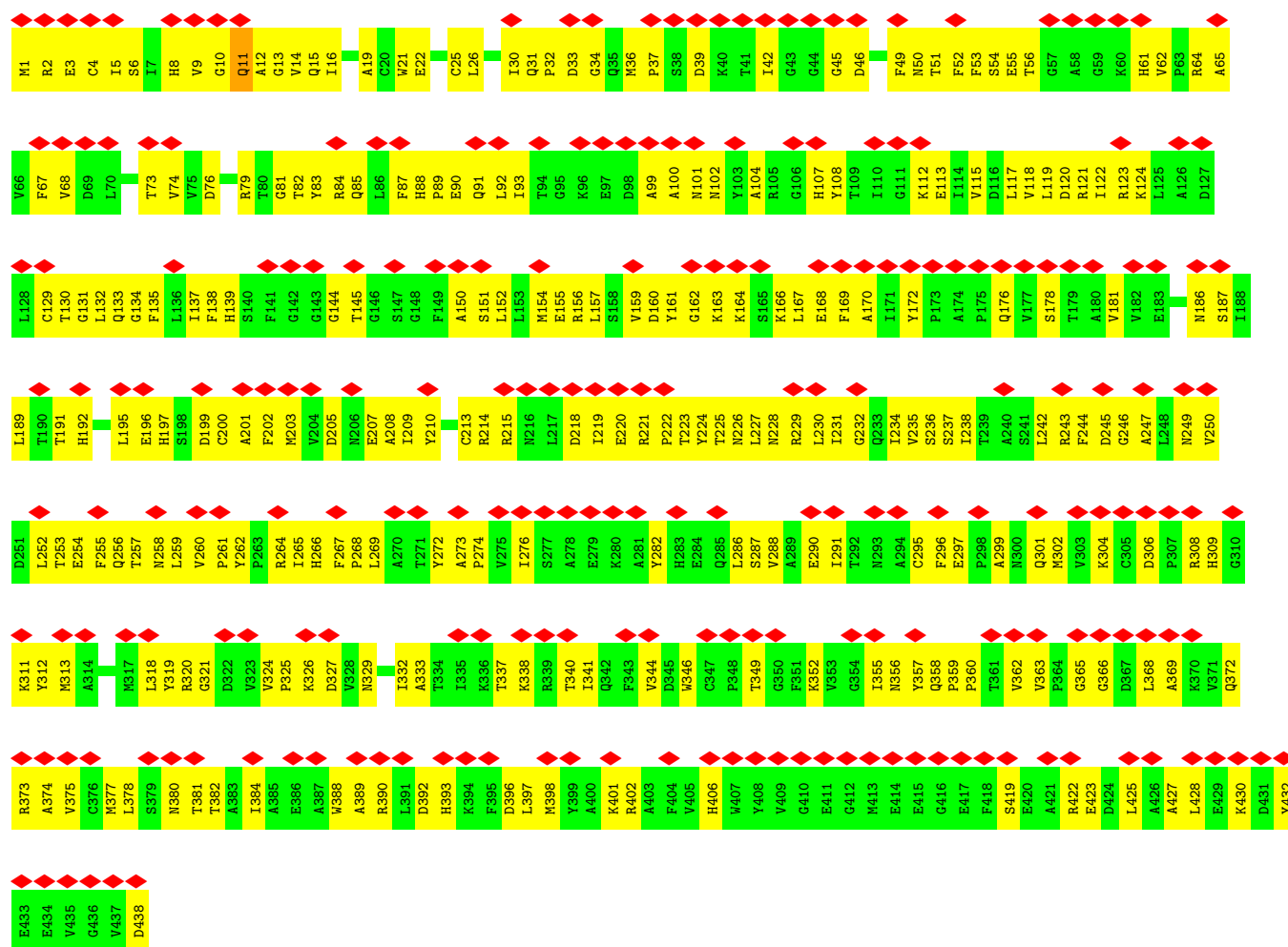
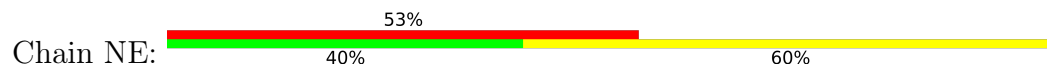


• Molecule 2: Detyrosinated tubulin alpha-3 chain

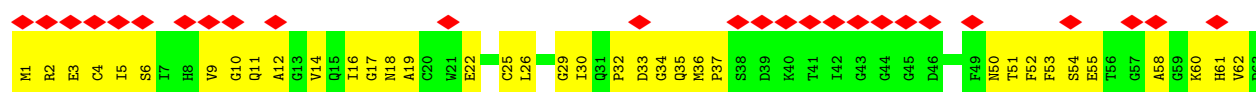


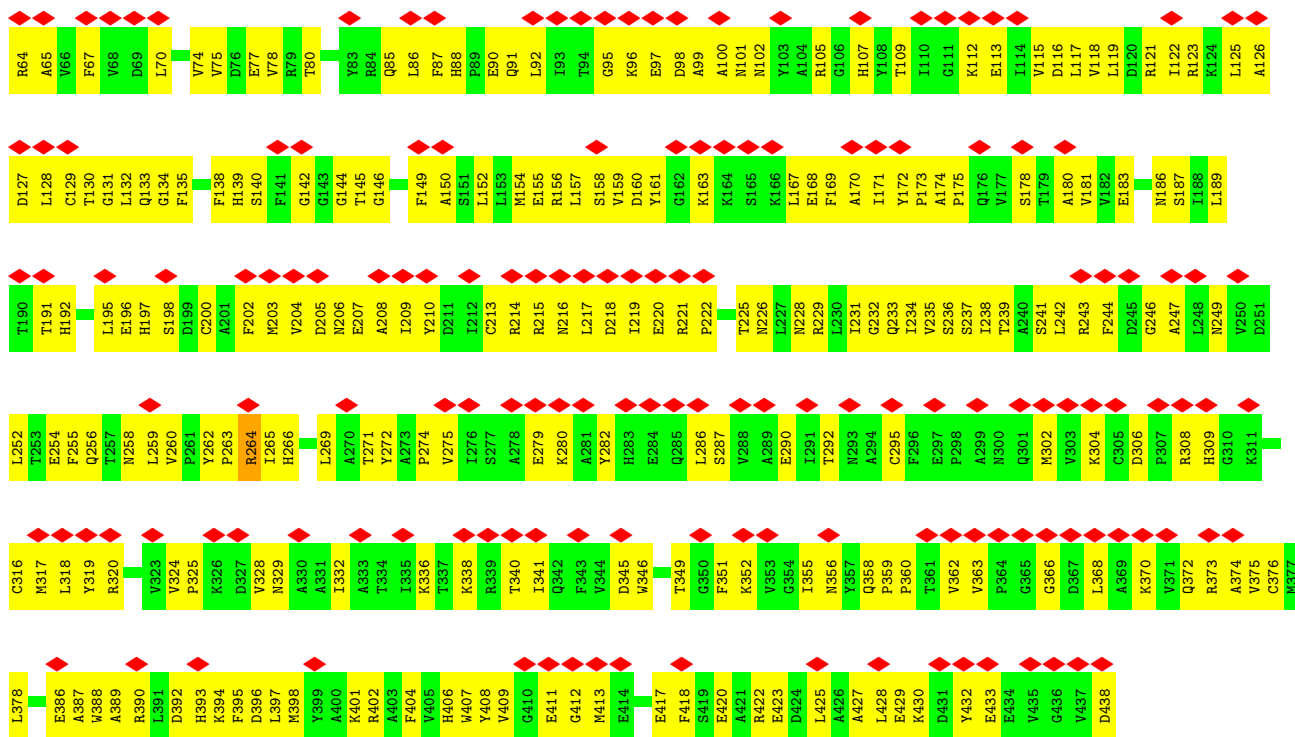


• Molecule 2: Detyrosinated tubulin alpha-3 chain

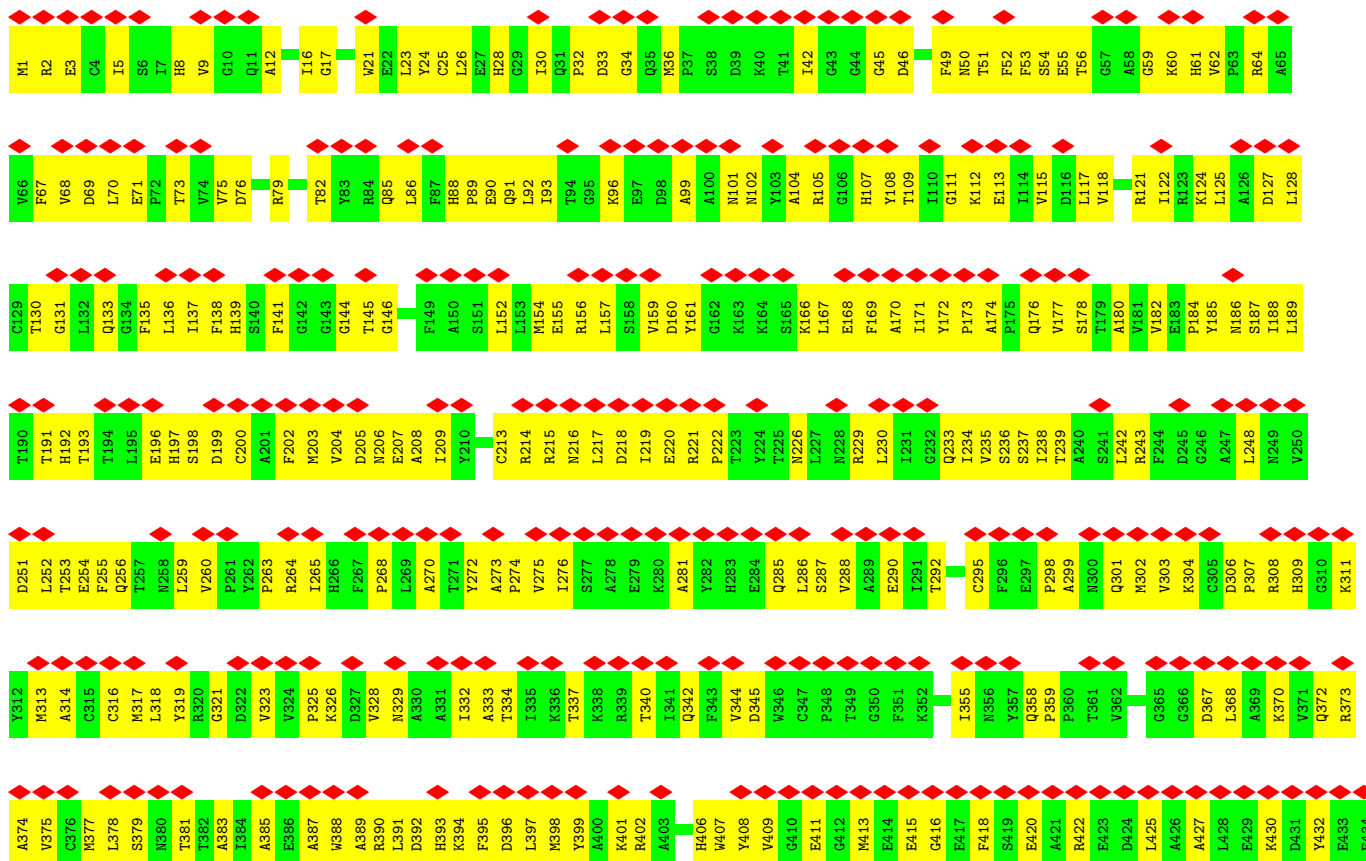
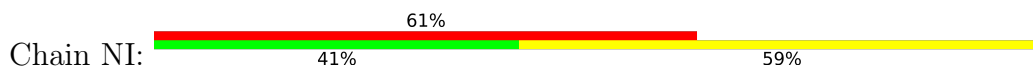


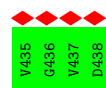
• Molecule 2: Detyrosinated tubulin alpha-3 chain



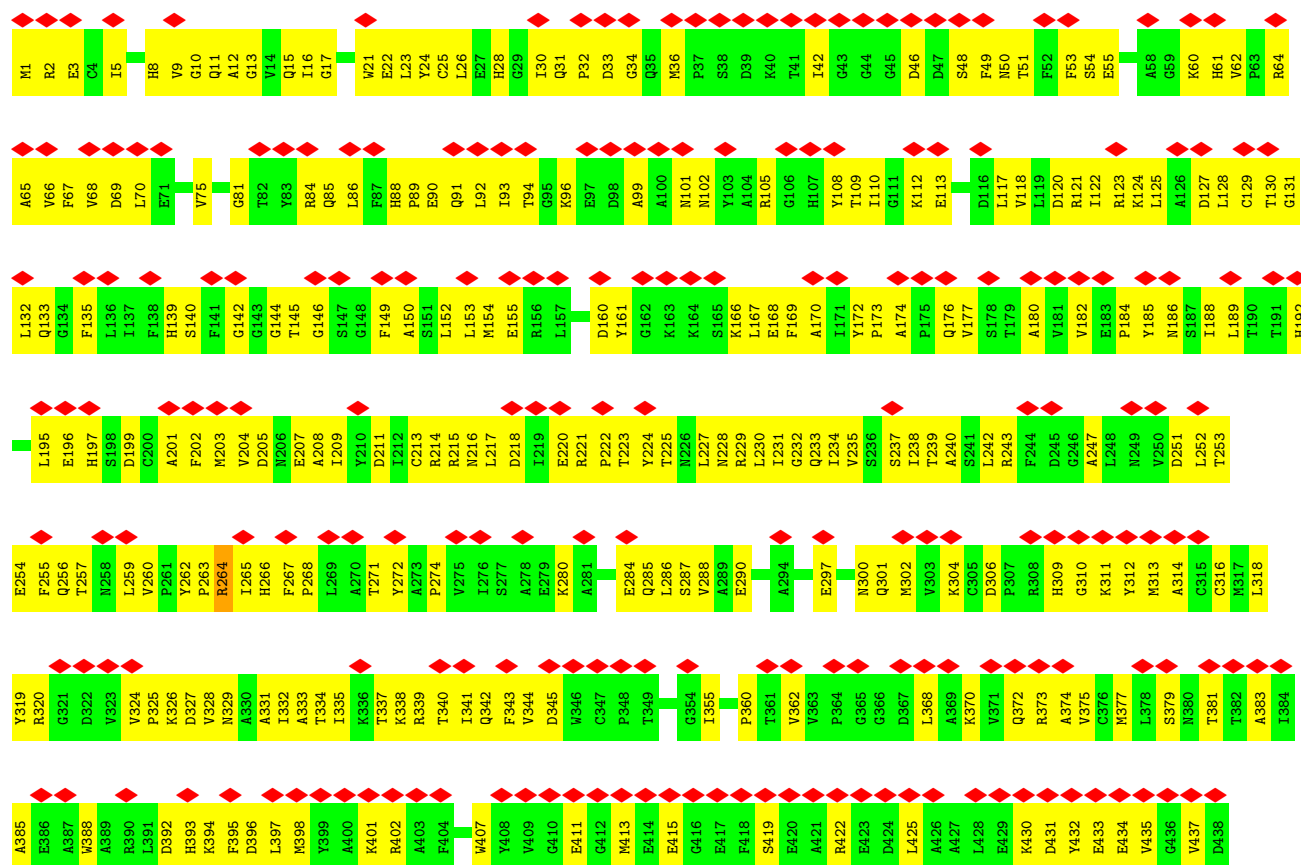


• Molecule 2: Detyrosinated tubulin alpha-3 chain

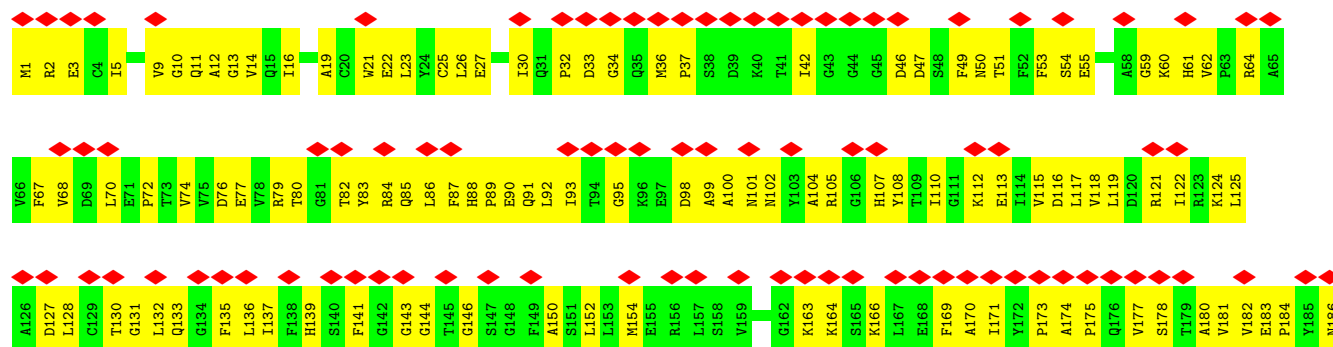


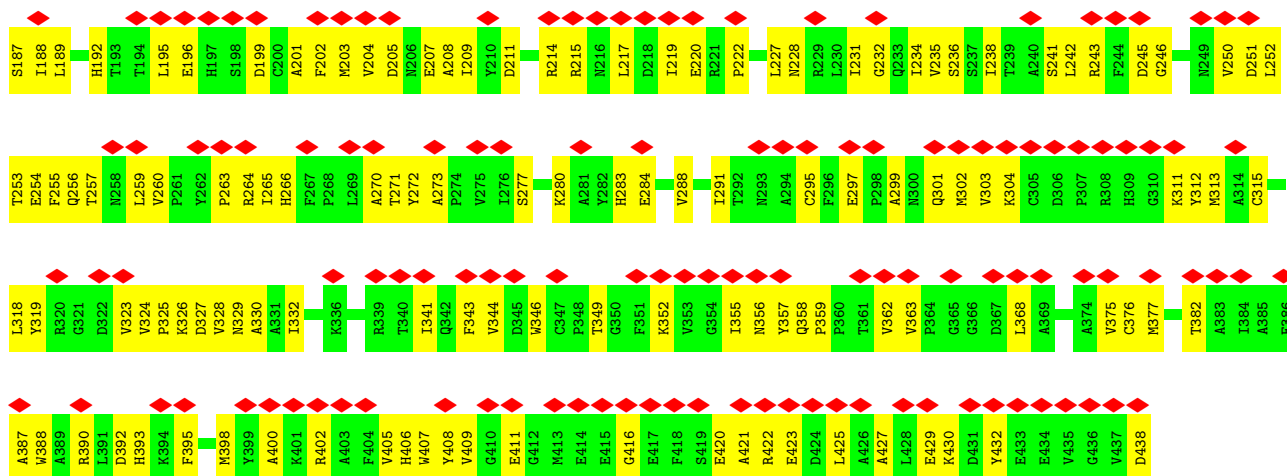


• Molecule 2: Detyrosinated tubulin alpha-3 chain

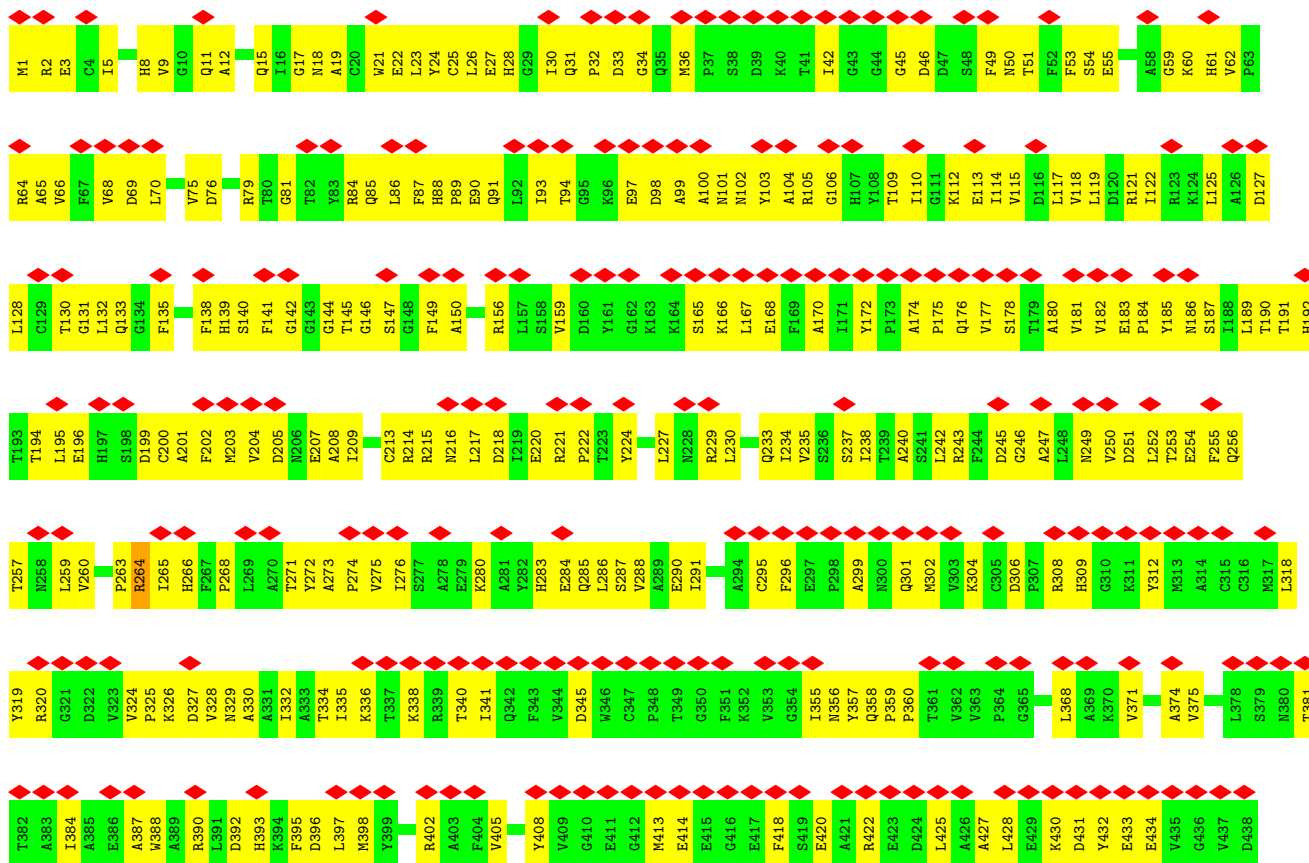


• Molecule 2: Detyrosinated tubulin alpha-3 chain



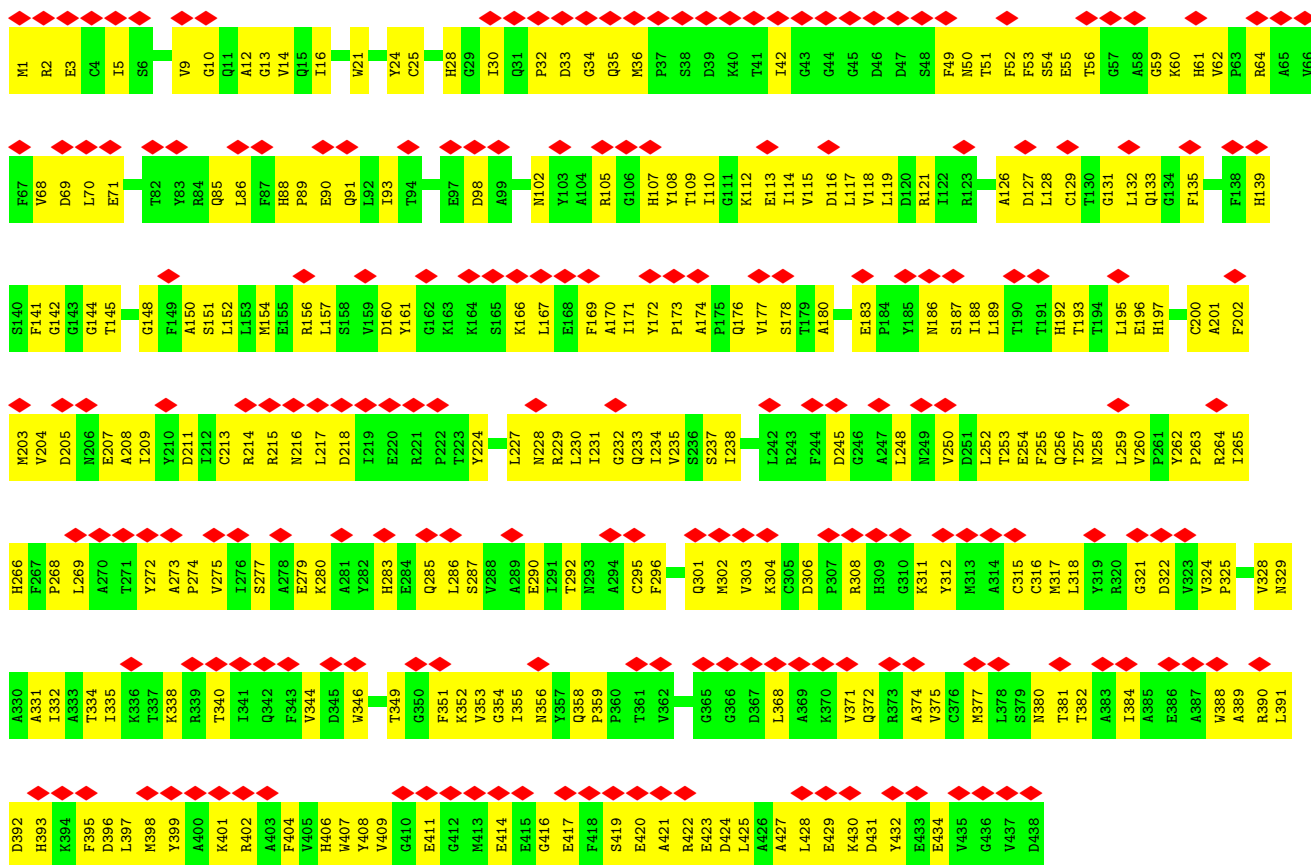


• Molecule 2: Detyrosinated tubulin alpha-3 chain

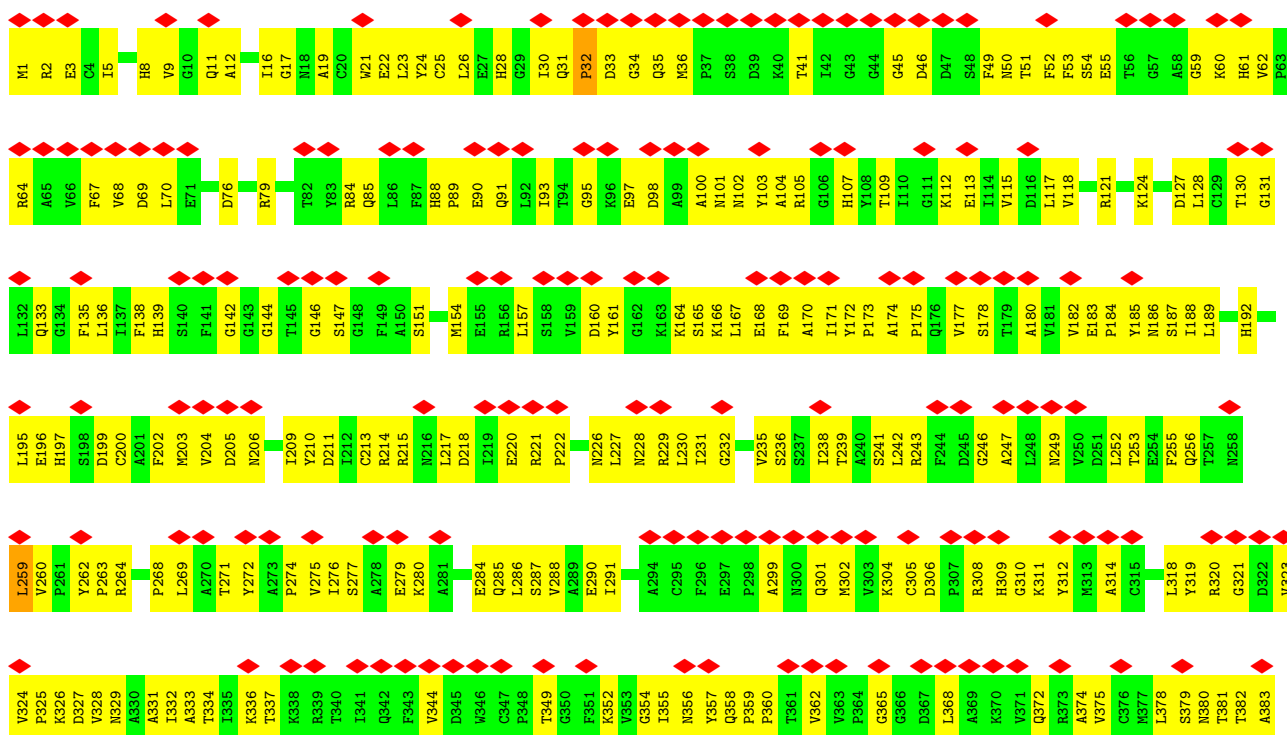
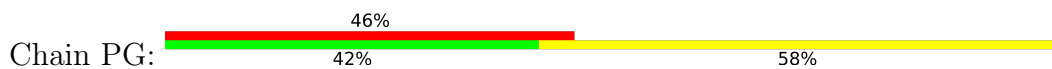


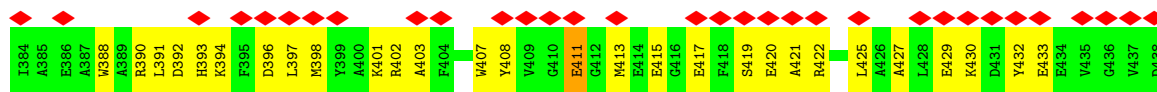
• Molecule 2: Detyrosinated tubulin alpha-3 chain



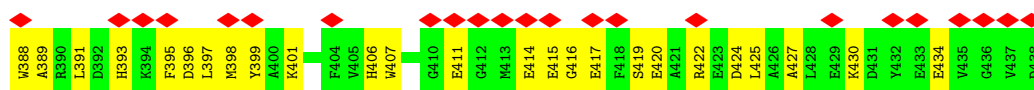
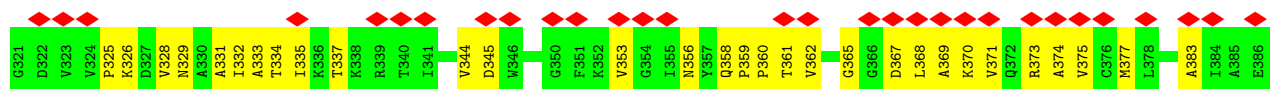
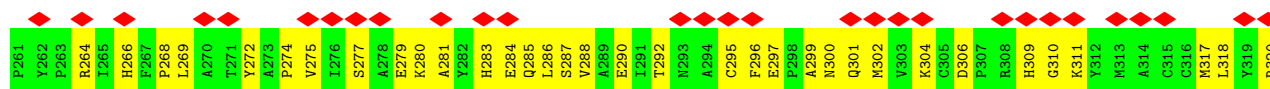
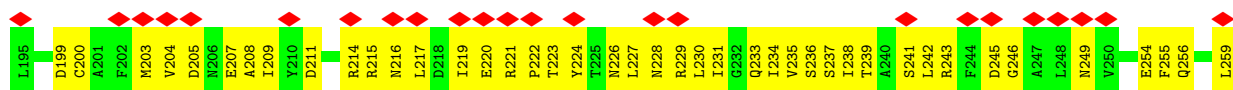
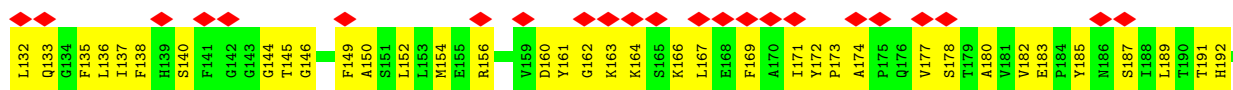
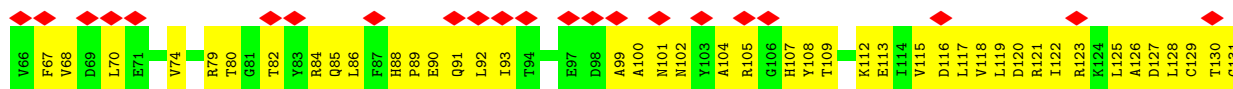
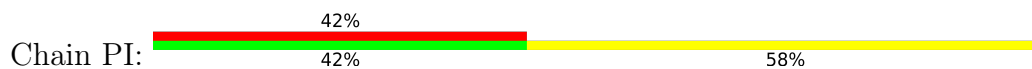


• Molecule 2: Detyrosinated tubulin alpha-3 chain

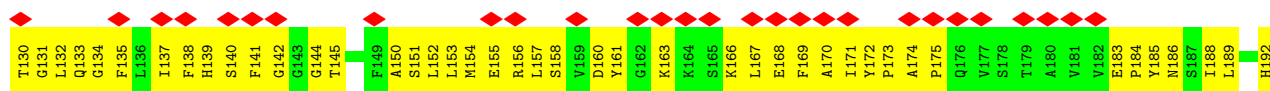
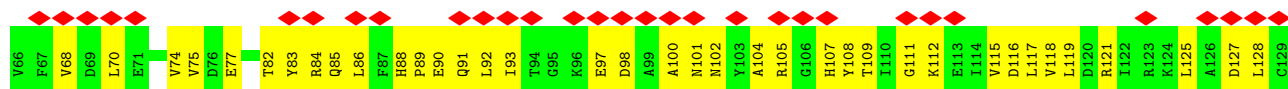
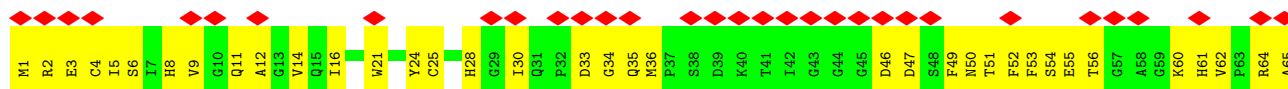
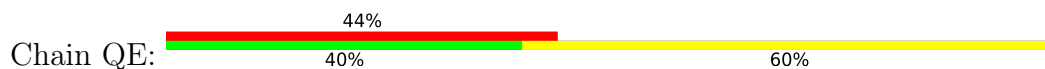


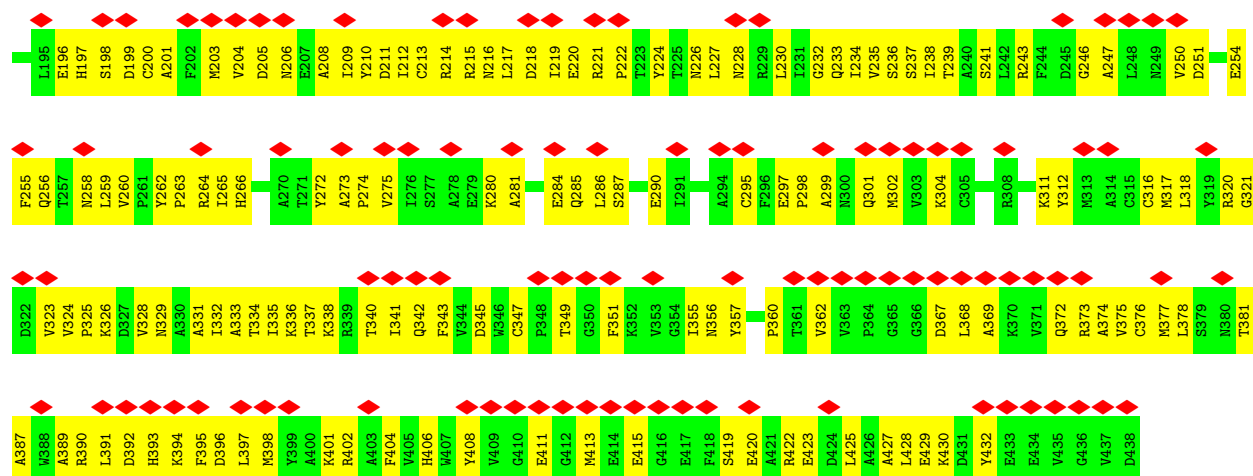


• Molecule 2: Detyrosinated tubulin alpha-3 chain

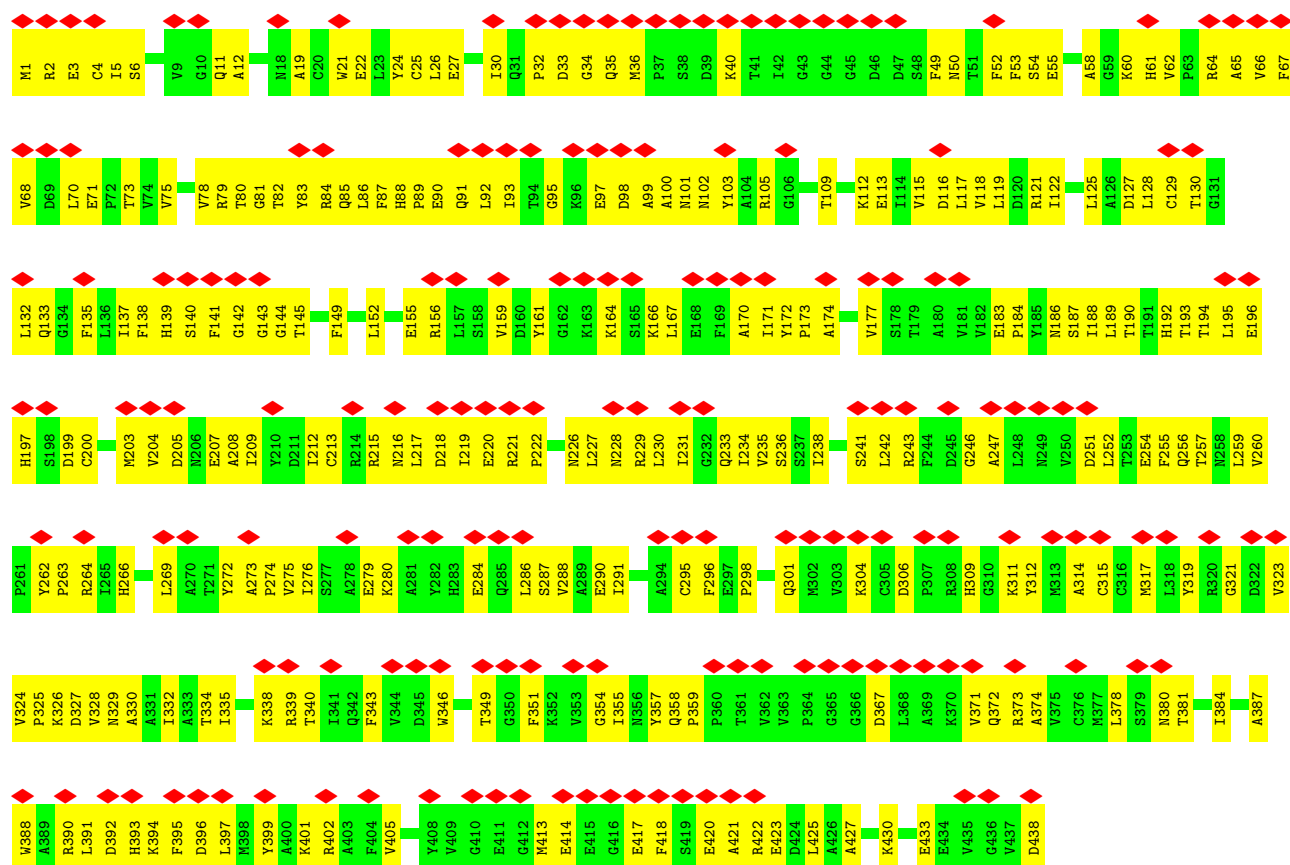


• Molecule 2: Detyrosinated tubulin alpha-3 chain

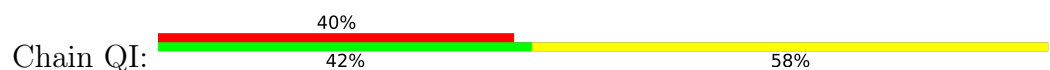


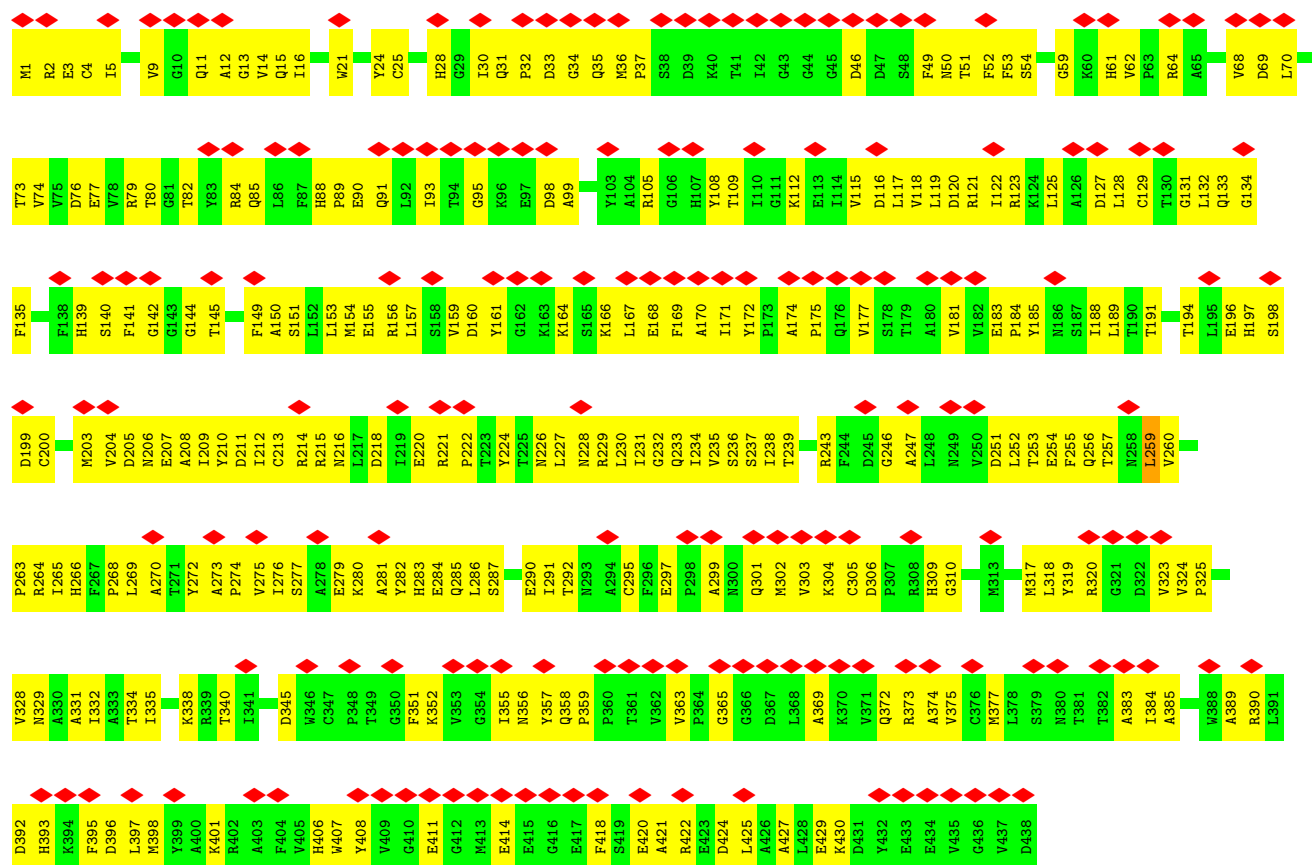


• Molecule 2: Detyrosinated tubulin alpha-3 chain

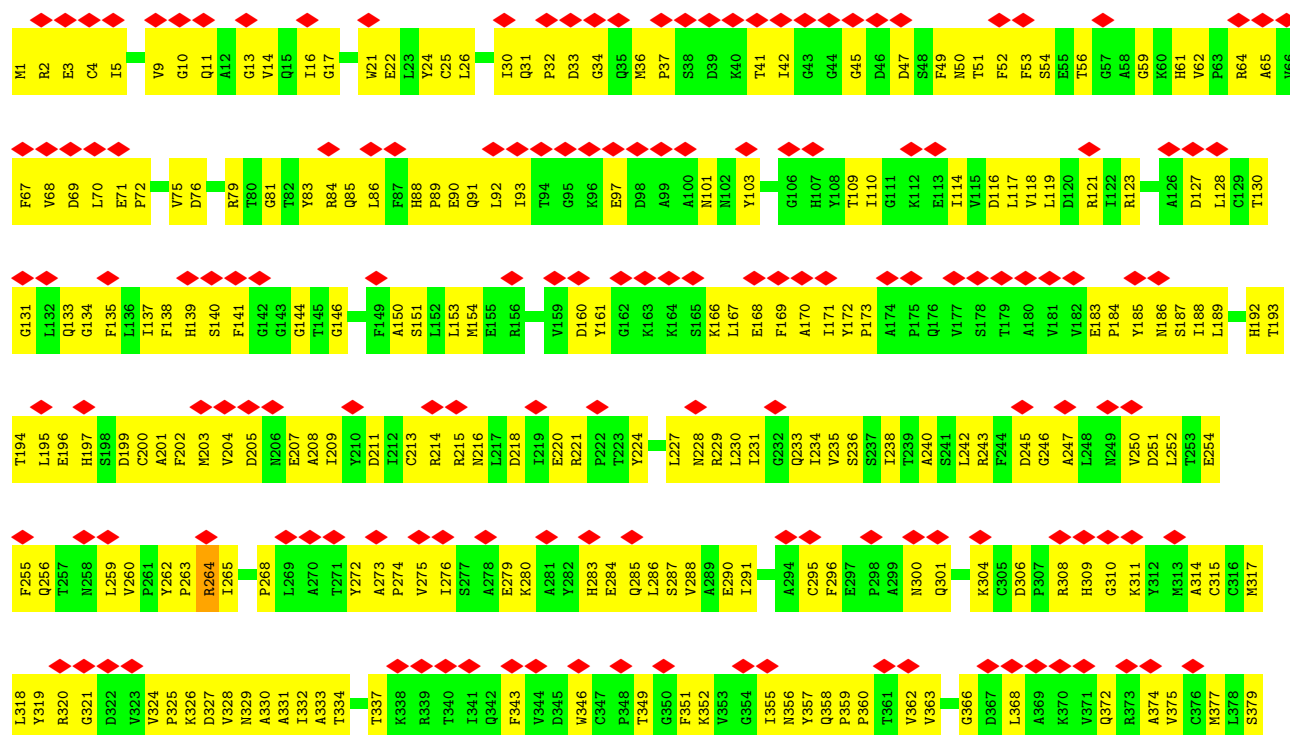
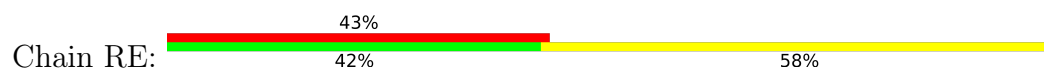


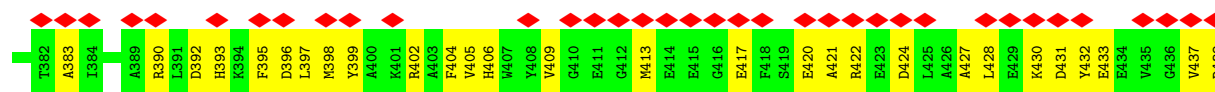
• Molecule 2: Detyrosinated tubulin alpha-3 chain



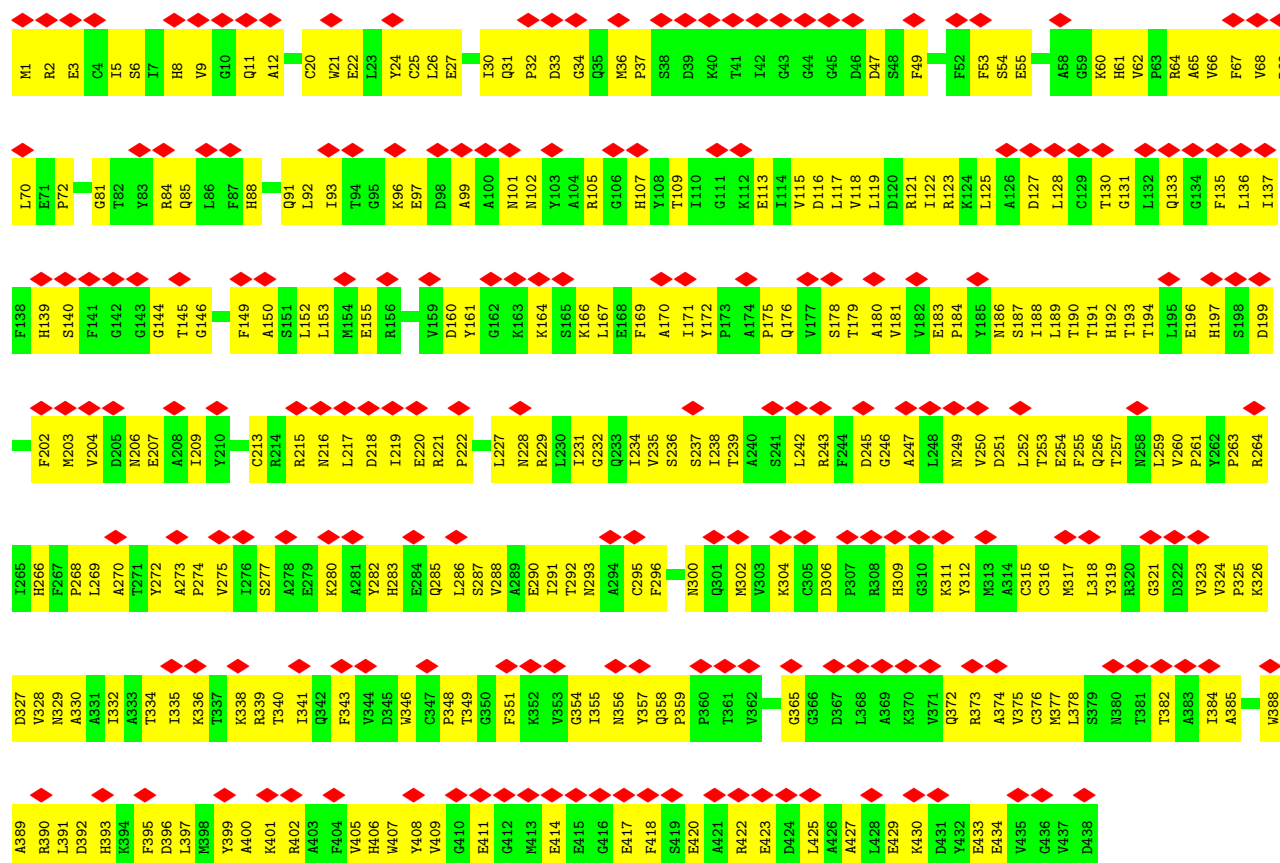
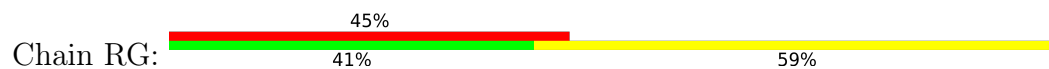


• Molecule 2: Detyrosinated tubulin alpha-3 chain

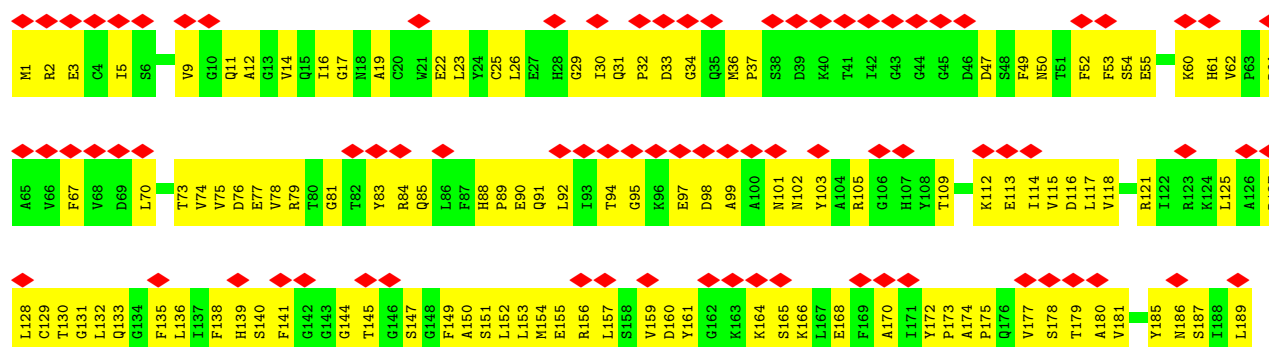


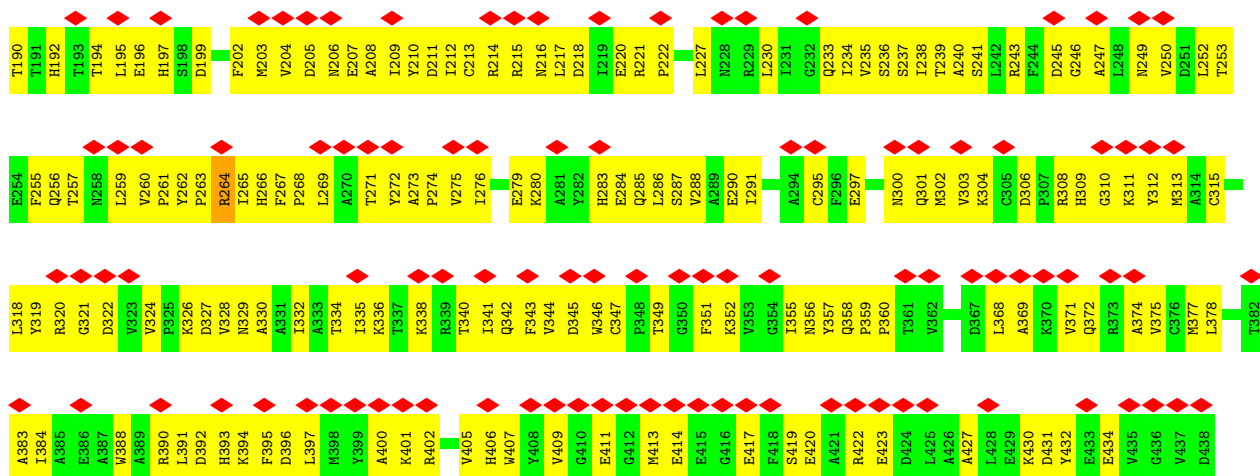


• Molecule 2: Detyrosinated tubulin alpha-3 chain

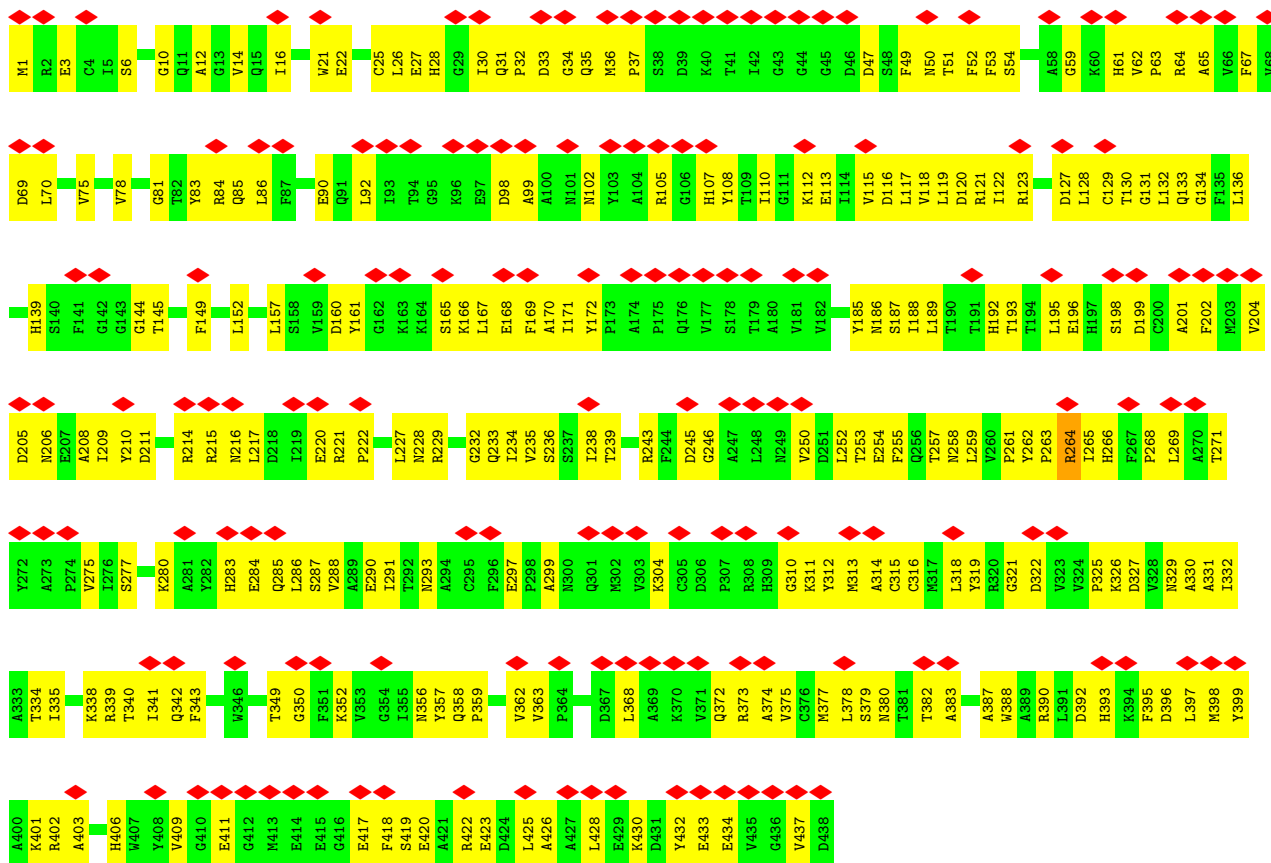
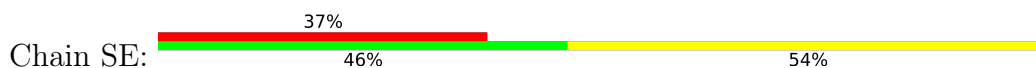


• Molecule 2: Detyrosinated tubulin alpha-3 chain



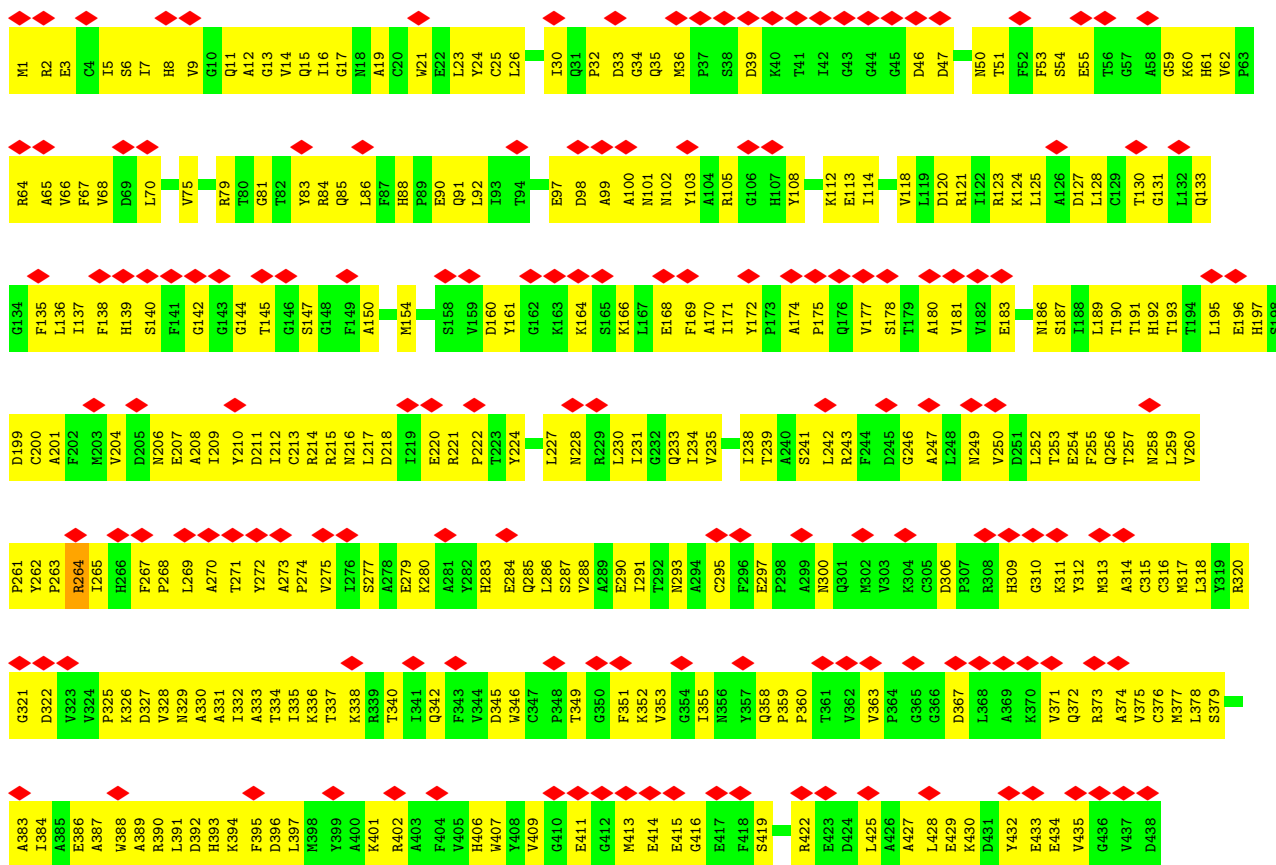


• Molecule 2: Detyrosinated tubulin alpha-3 chain

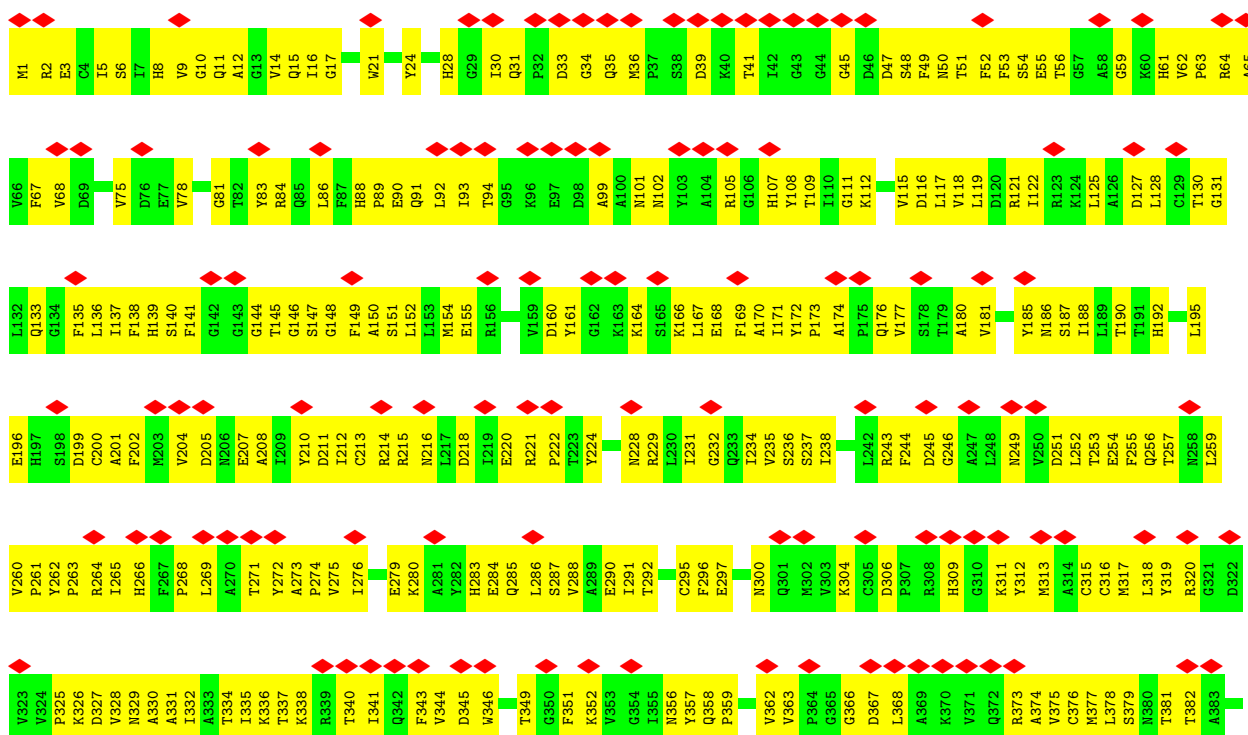


• Molecule 2: Detyrosinated tubulin alpha-3 chain



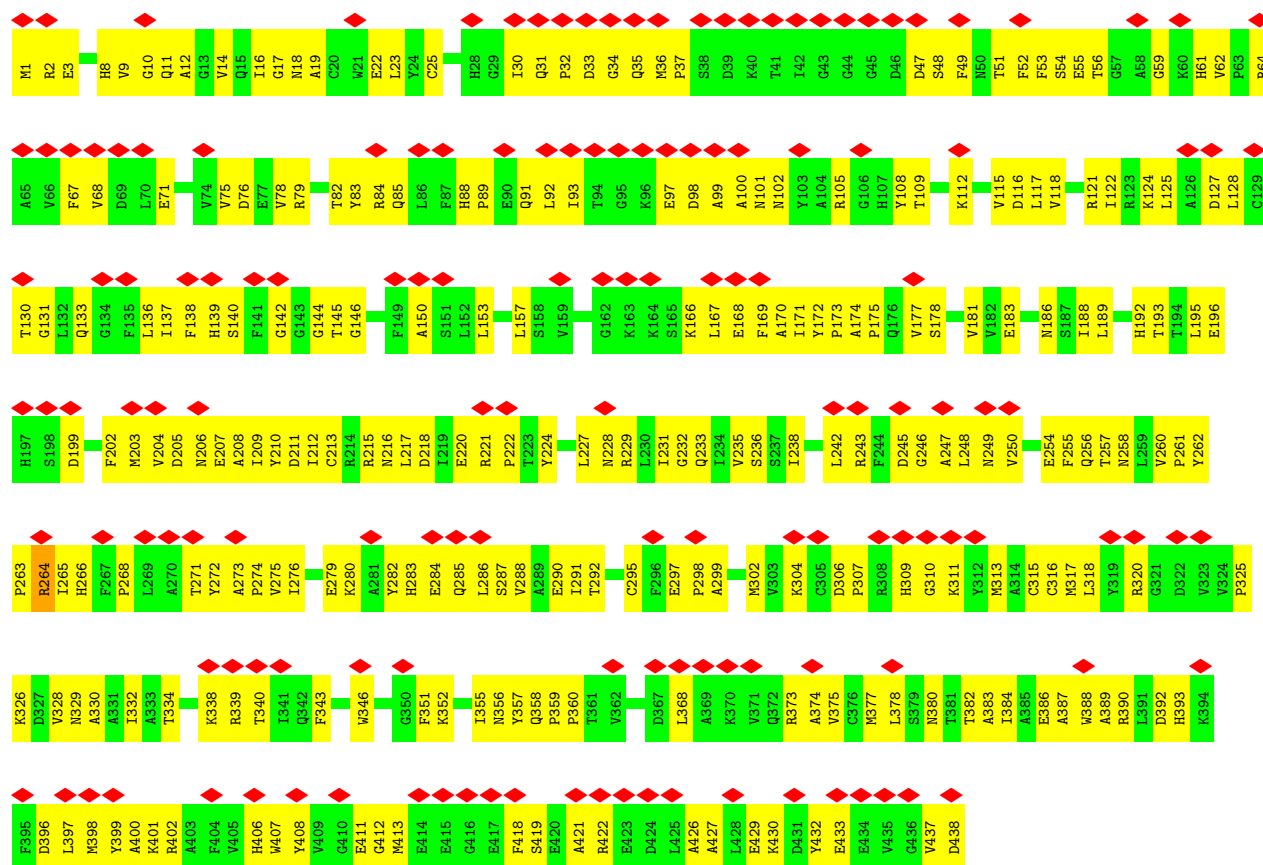
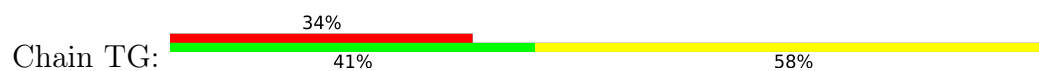


• Molecule 2: Detyrosinated tubulin alpha-3 chain

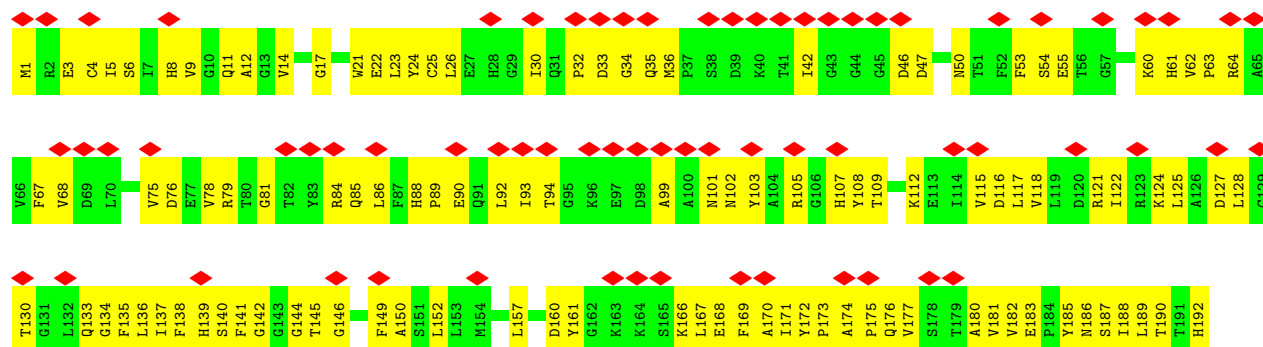
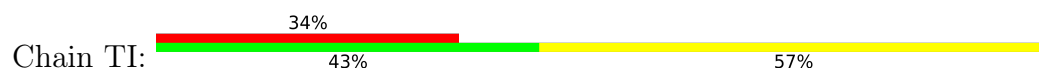


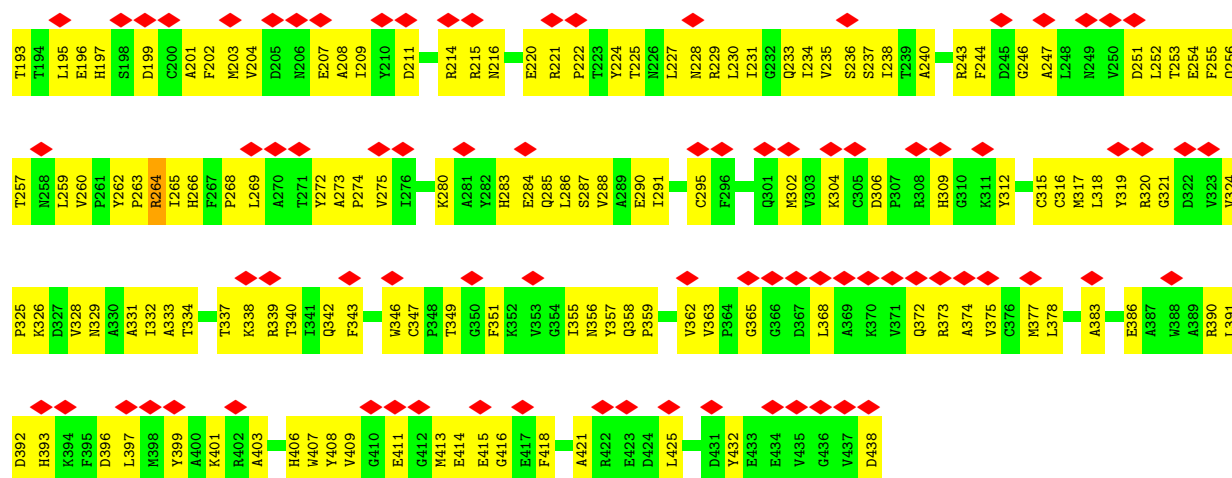


• Molecule 2: Detyrosinated tubulin alpha-3 chain

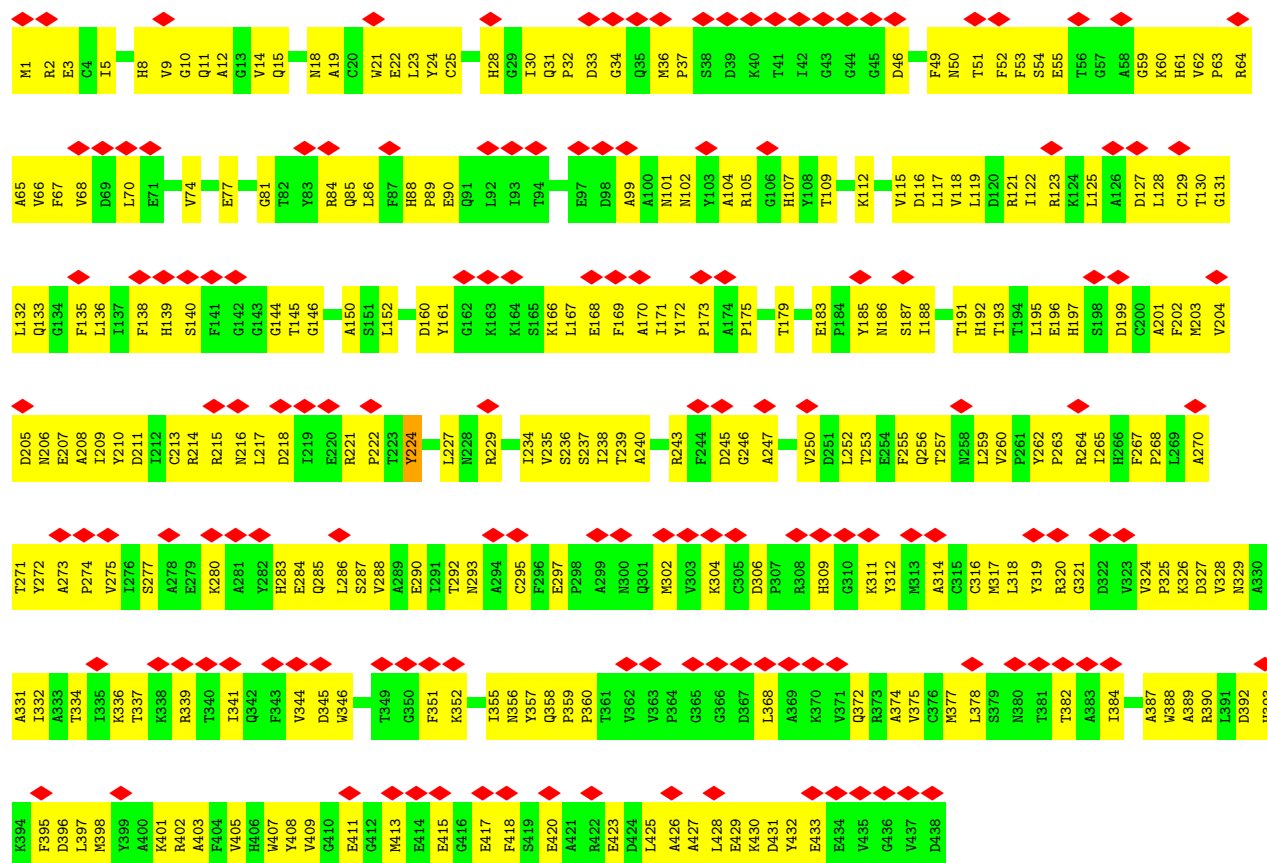
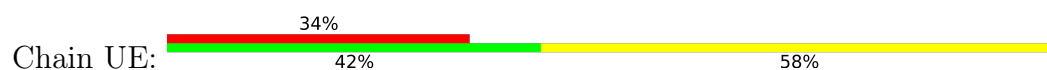


• Molecule 2: Detyrosinated tubulin alpha-3 chain



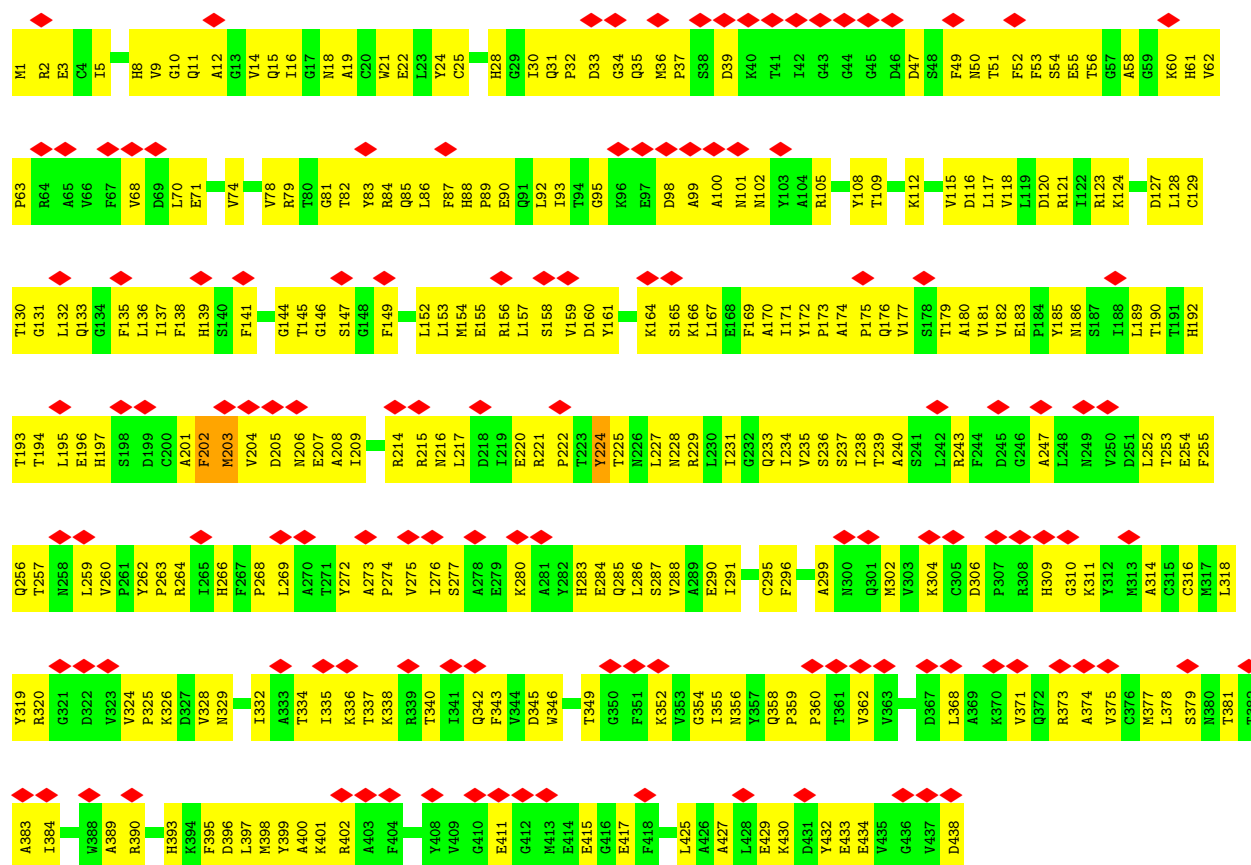


• Molecule 2: Detyrosinated tubulin alpha-3 chain

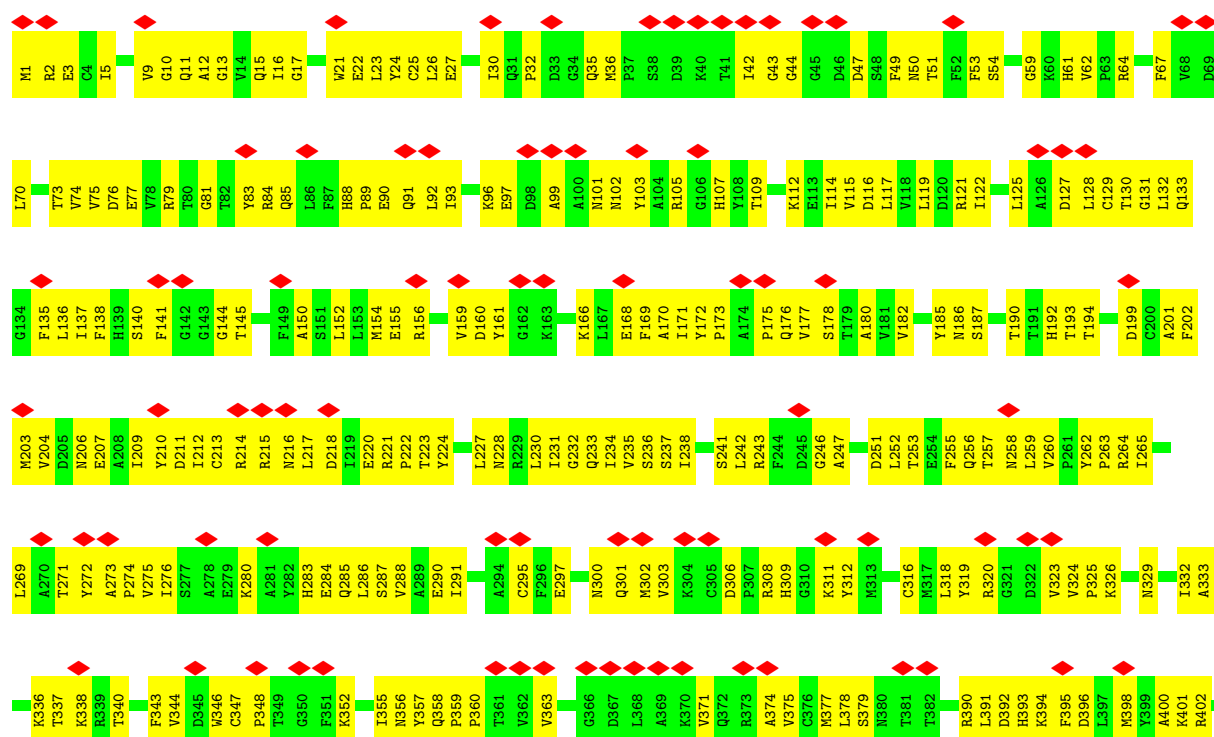
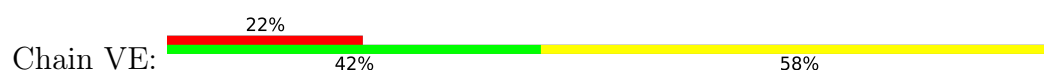


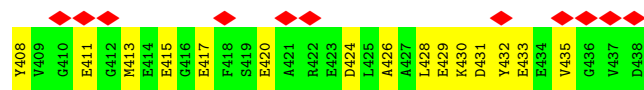
• Molecule 2: Detyrosinated tubulin alpha-3 chain



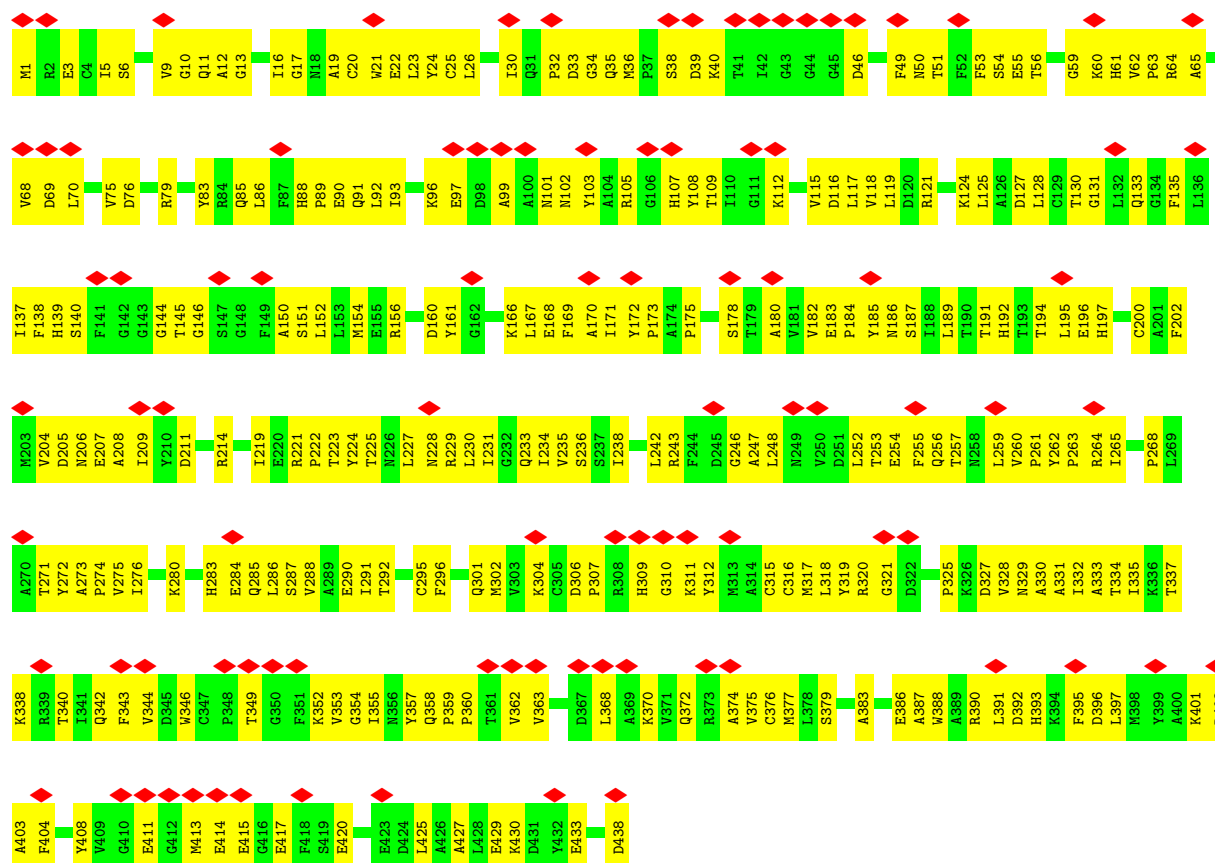
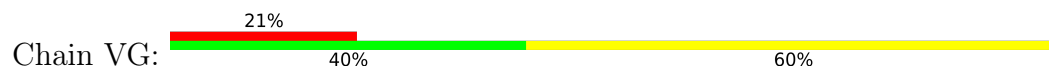


• Molecule 2: Detyrosinated tubulin alpha-3 chain

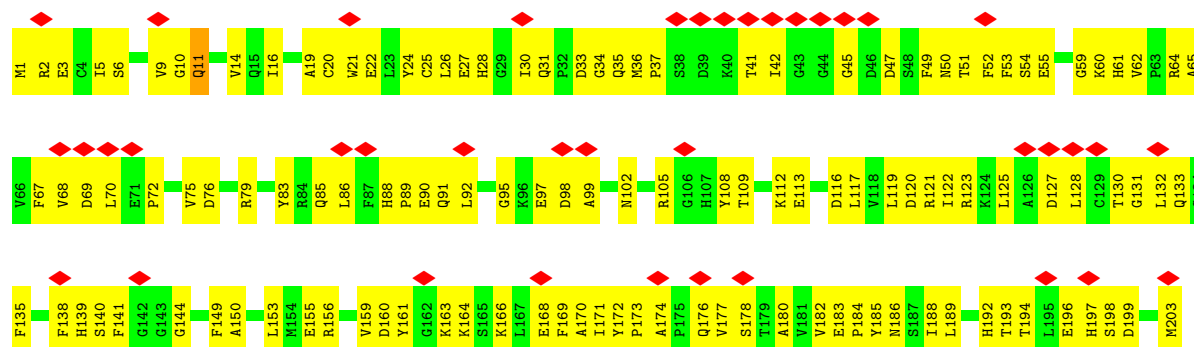


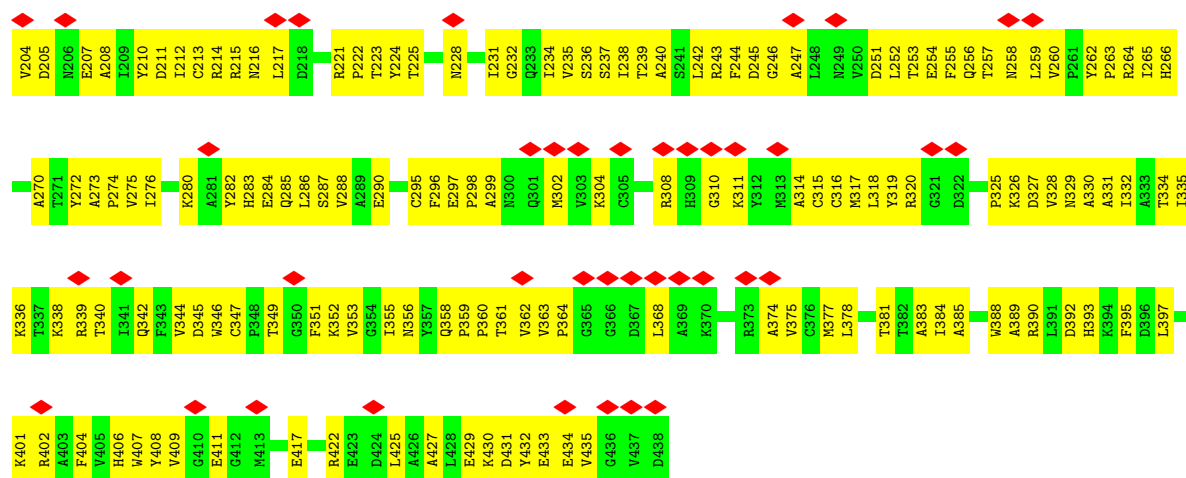


• Molecule 2: Detyrosinated tubulin alpha-3 chain

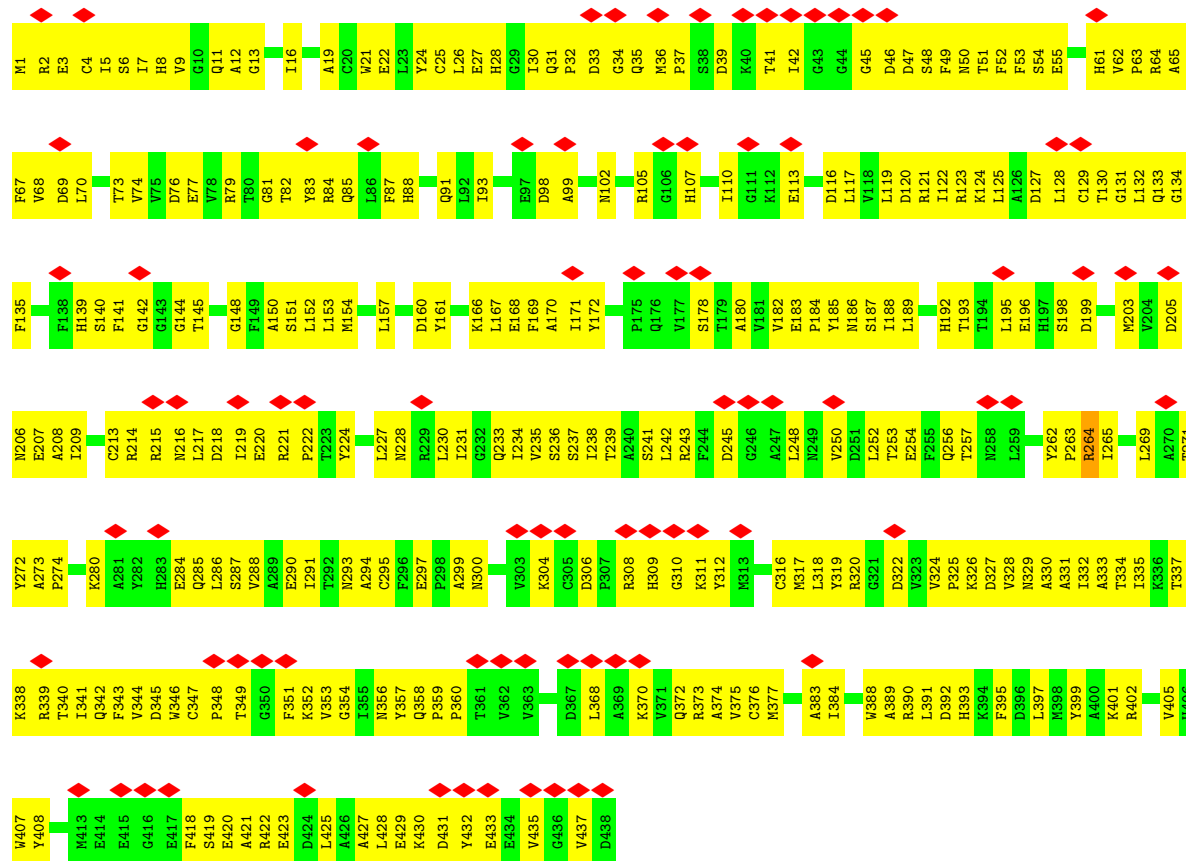


• Molecule 2: Detyrosinated tubulin alpha-3 chain



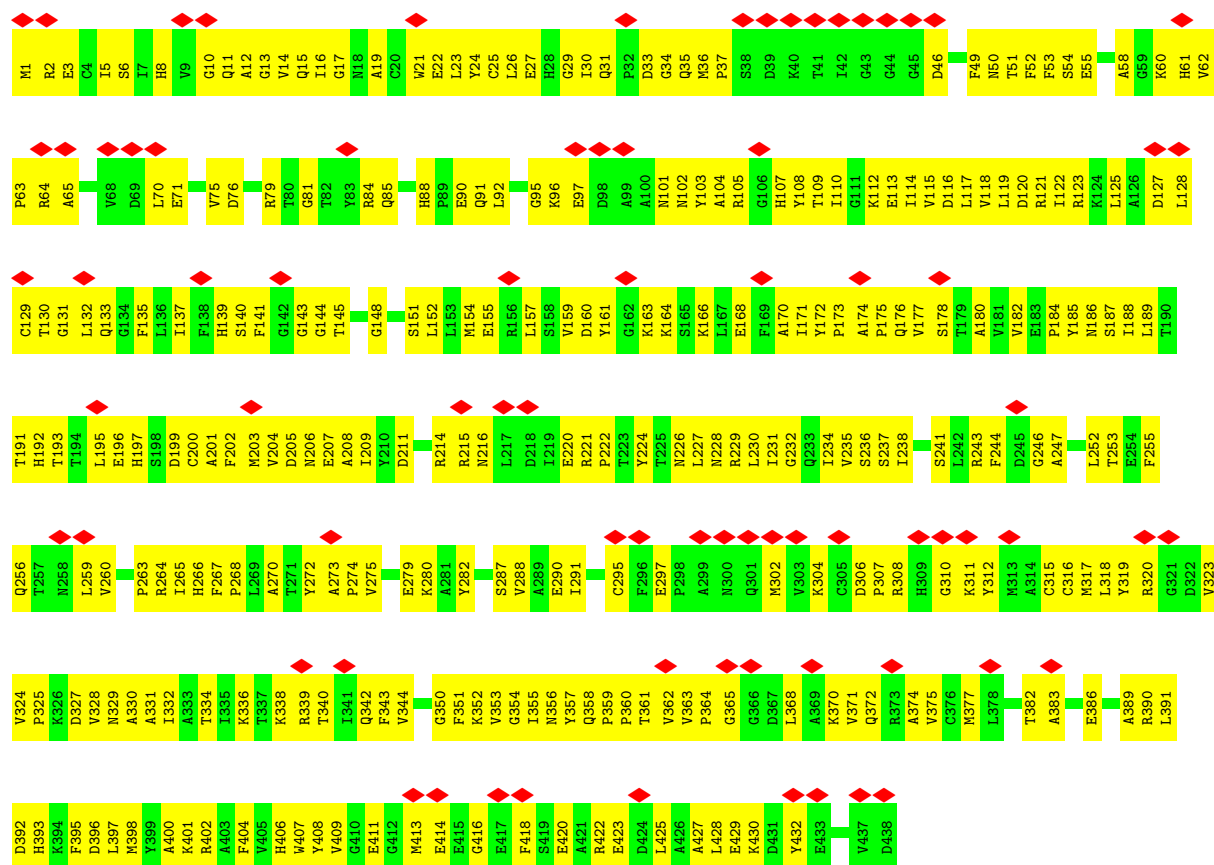


• Molecule 2: Detyrosinated tubulin alpha-3 chain



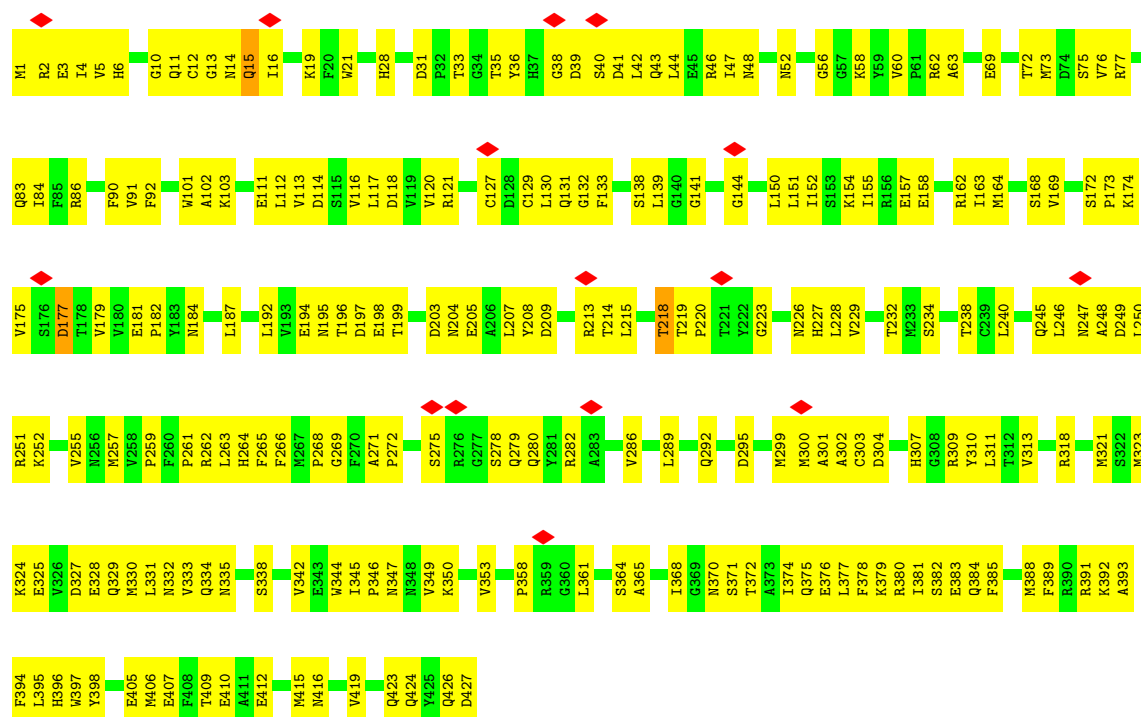
• Molecule 2: Detyrosinated tubulin alpha-3 chain





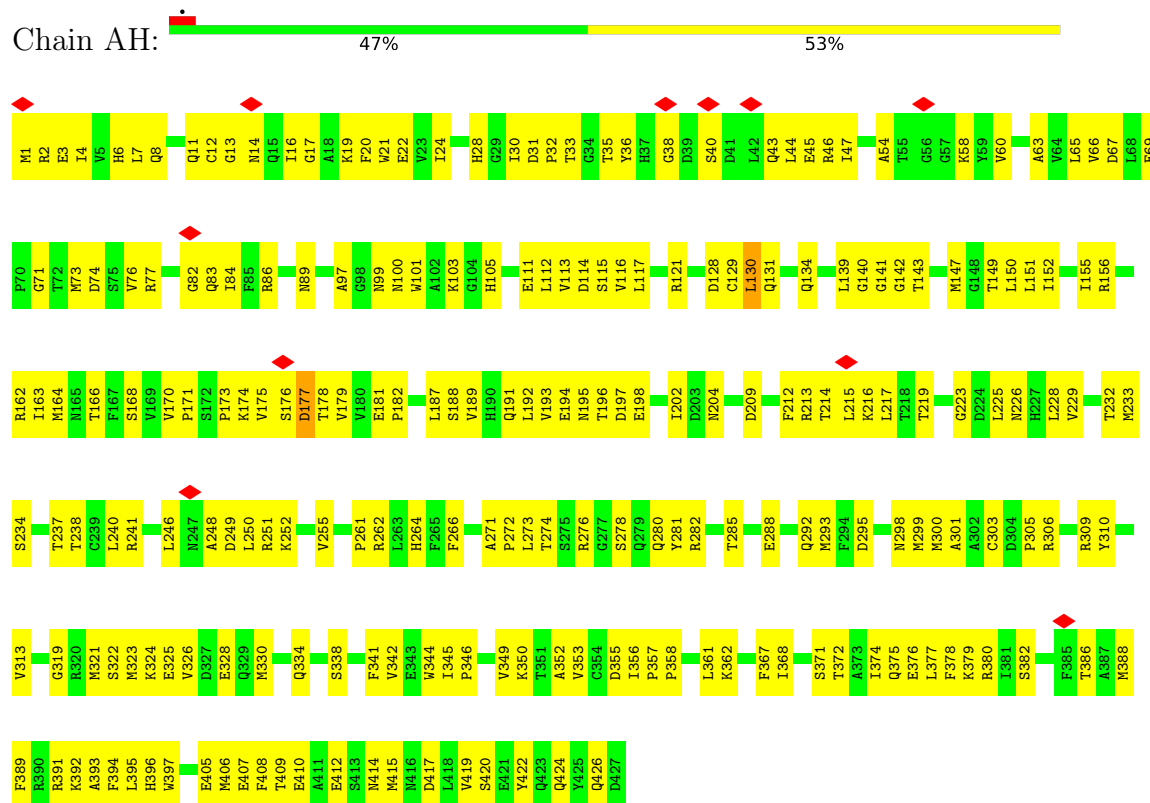
• Molecule 3: Tubulin beta-4B chain

Chain AF: 47% 52% .



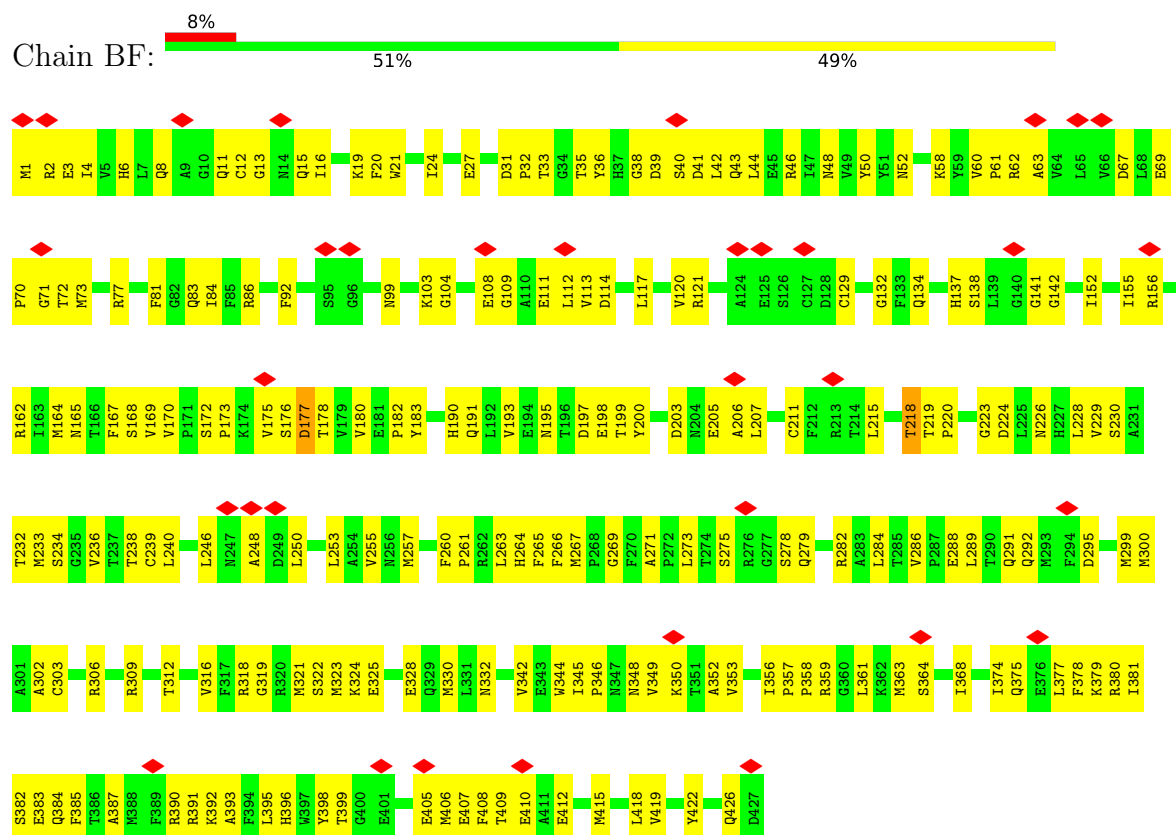
- Molecule 3: Tubulin beta-4B chain

Chain AH:



- Molecule 3: Tubulin beta-4B chain

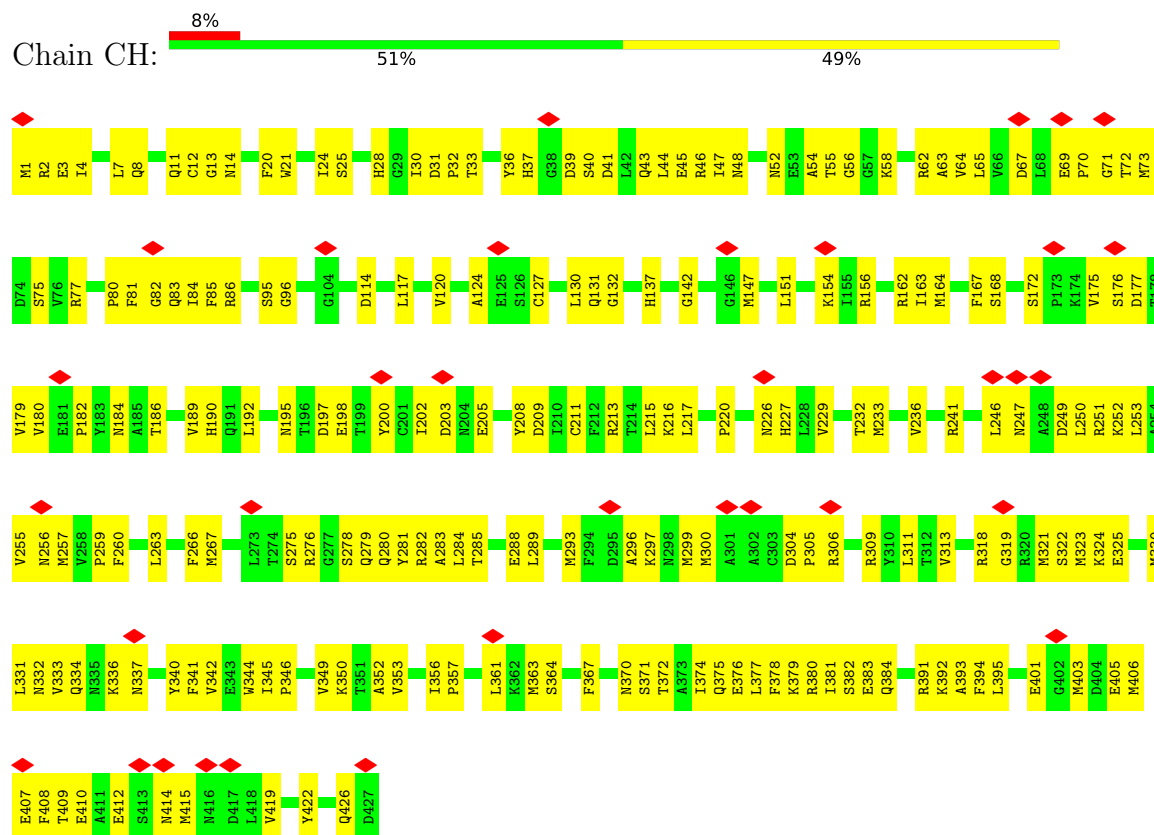
Chain BF:



Chain BH:

Chain CF:

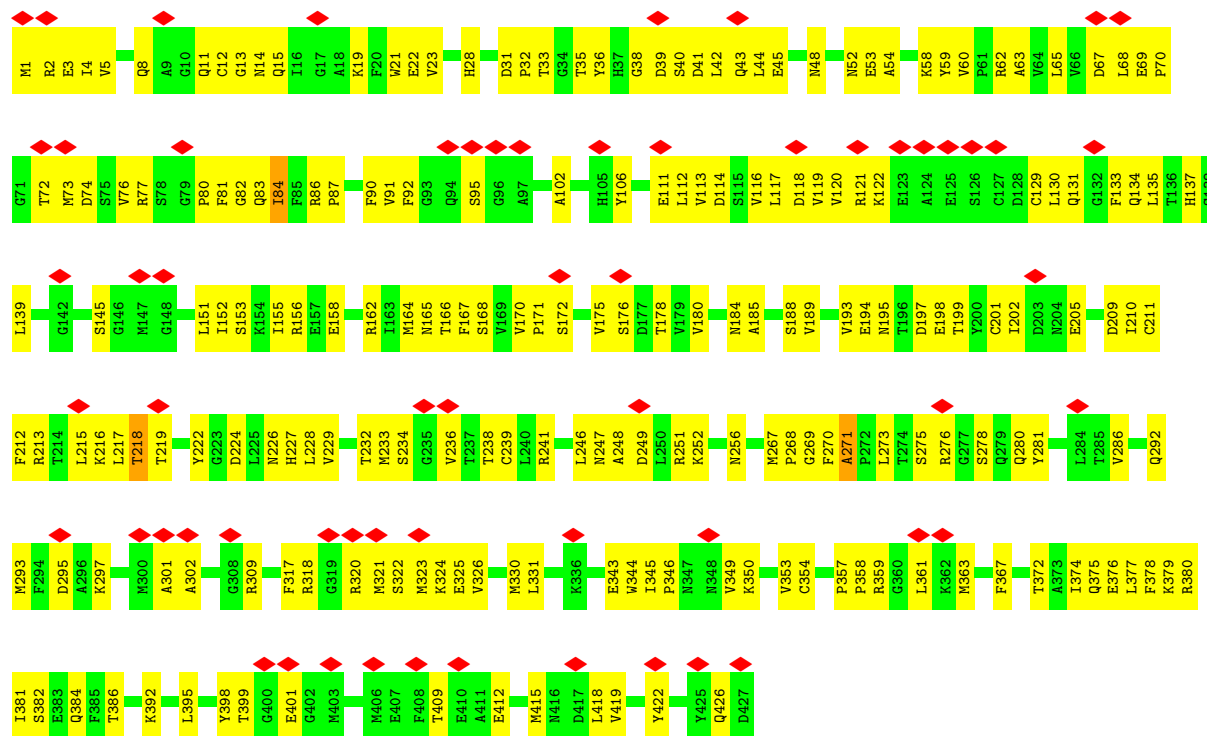
• Molecule 3: Tubulin beta-4B chain



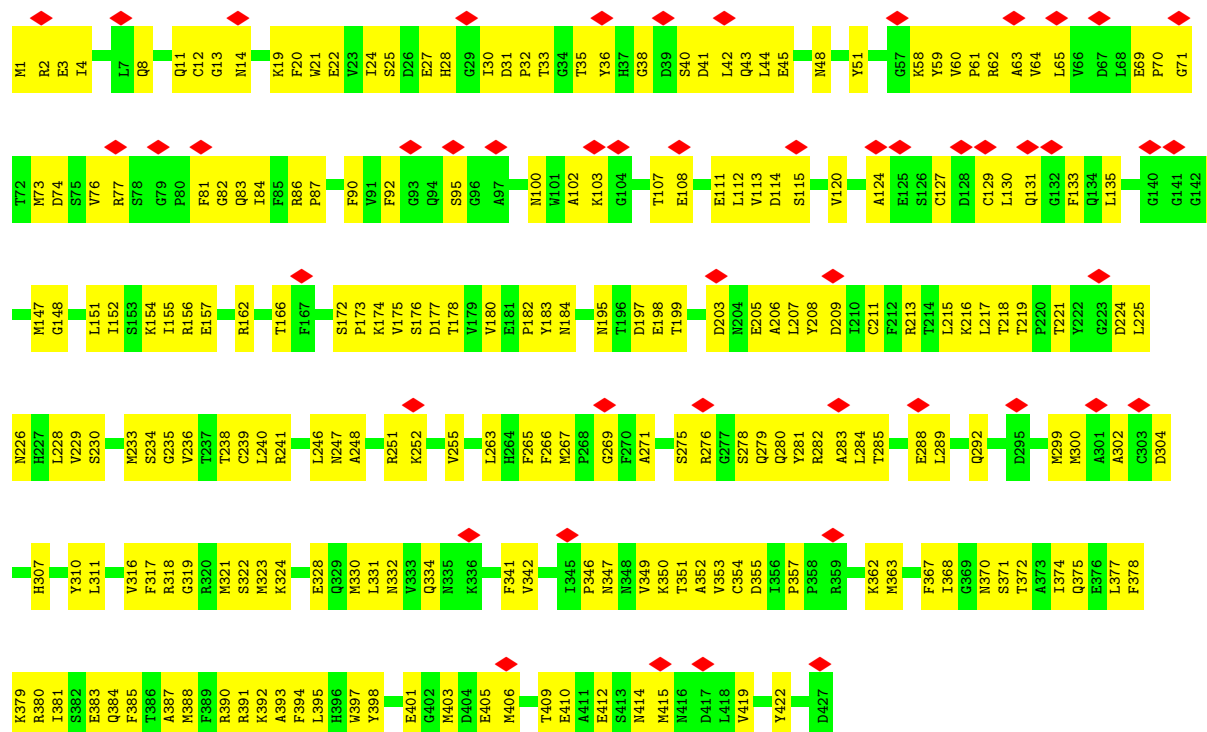
• Molecule 3: Tubulin beta-4B chain



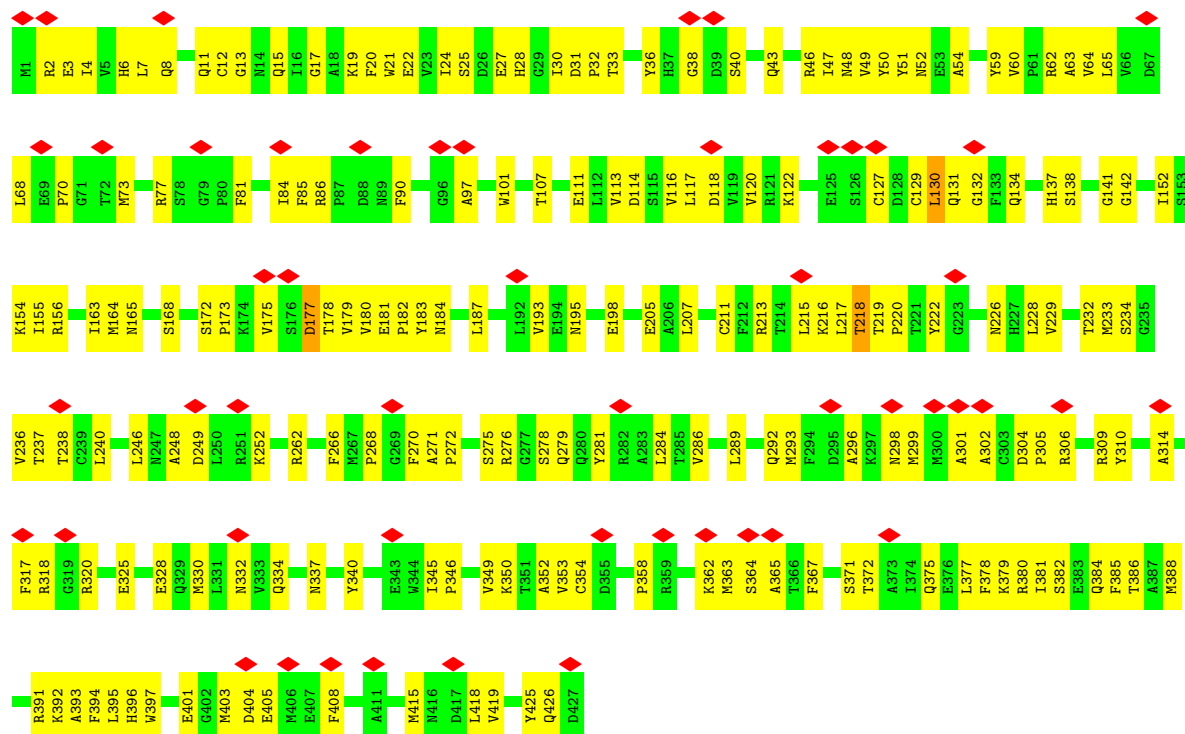
- Molecule 3: Tubulin beta-4B chain



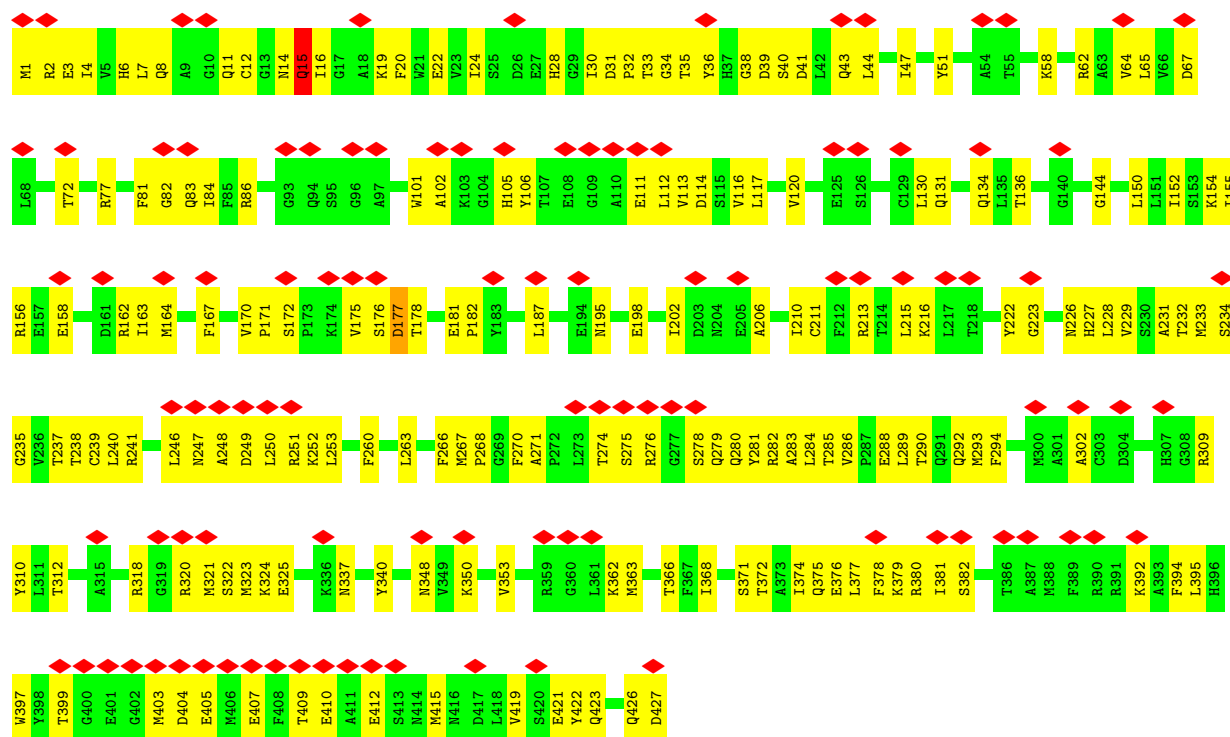
- Molecule 3: Tubulin beta-4B chain



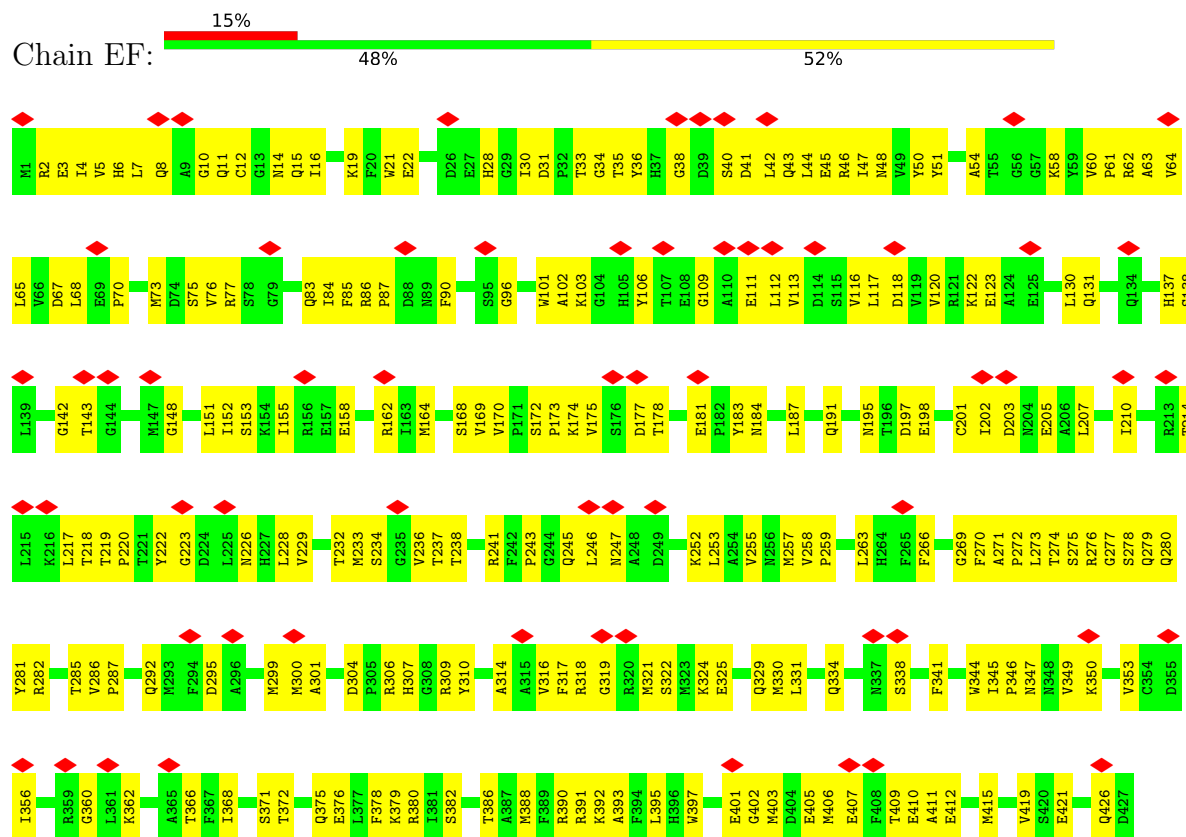
- Molecule 3: Tubulin beta-4B chain



- Molecule 3: Tubulin beta-4B chain



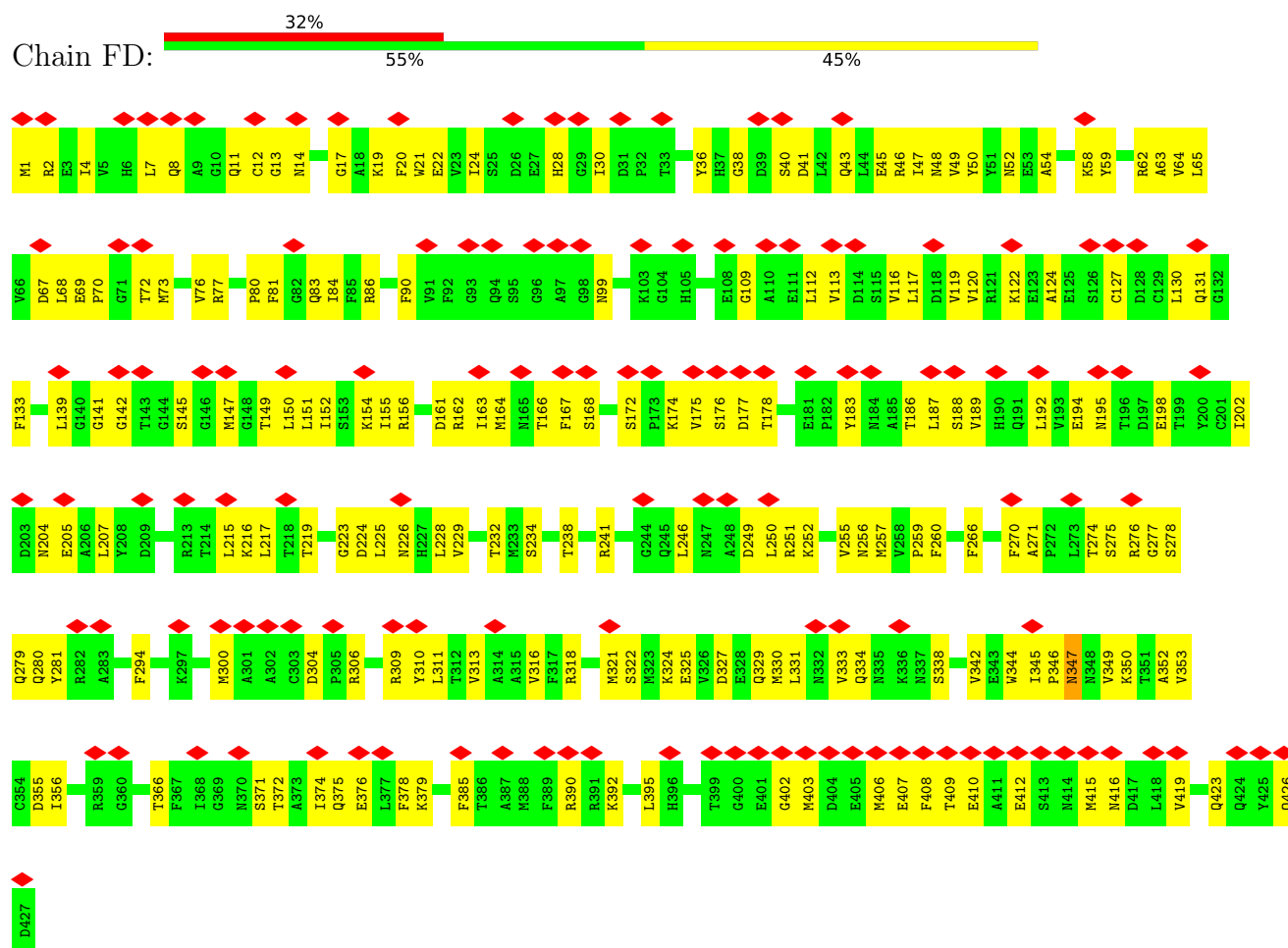
• Molecule 3: Tubulin beta-4B chain



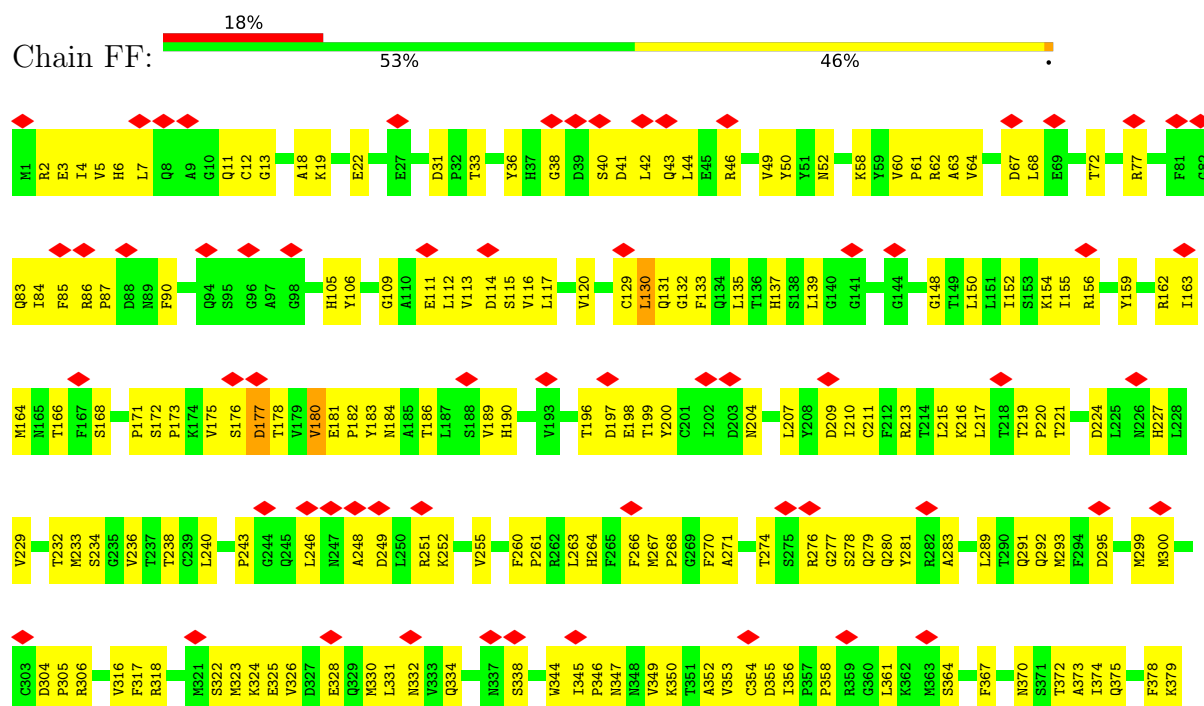
• Molecule 3: Tubulin beta-4B chain

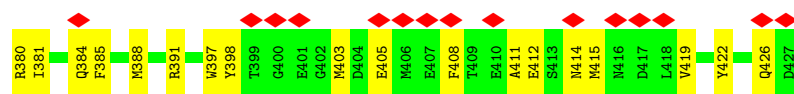


• Molecule 3: Tubulin beta-4B chain

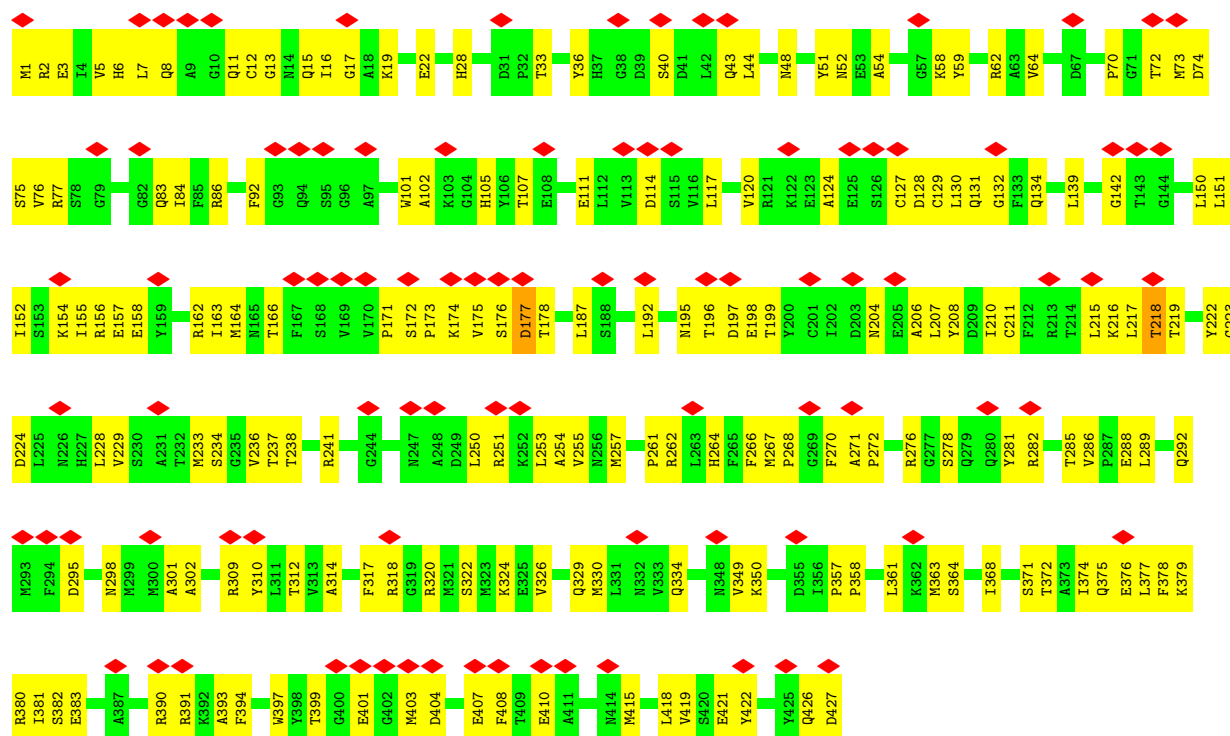


• Molecule 3: Tubulin beta-4B chain

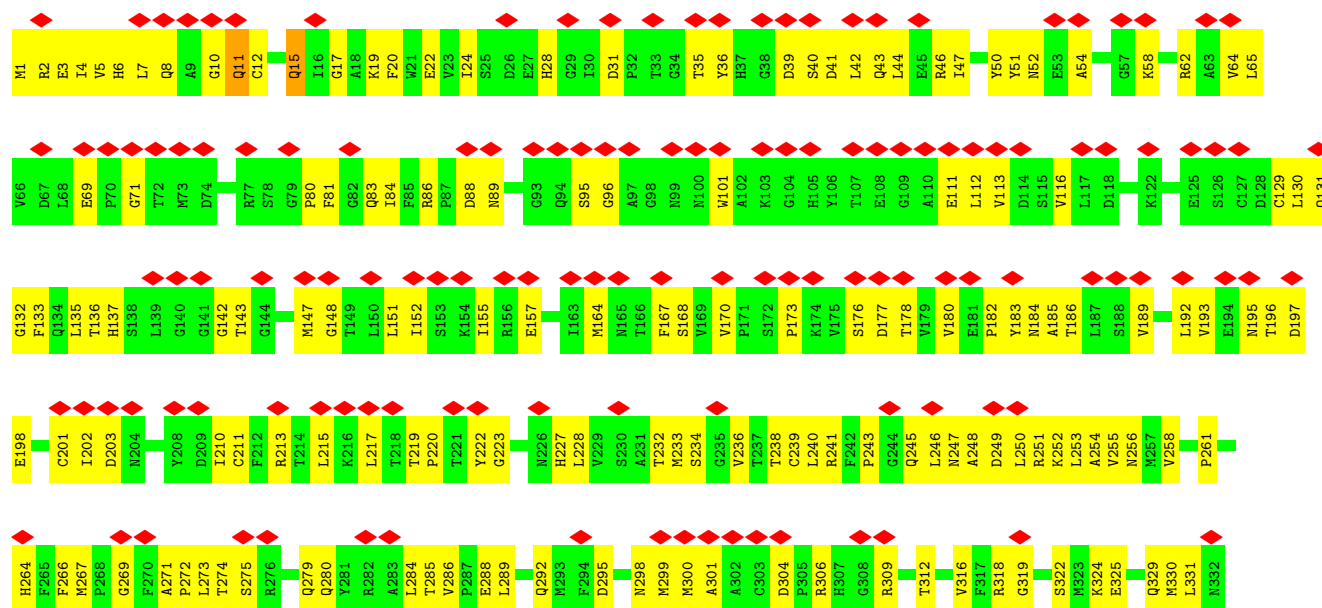


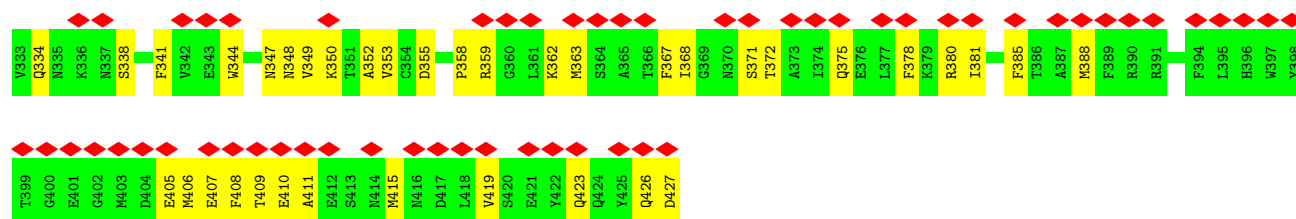


• Molecule 3: Tubulin beta-4B chain

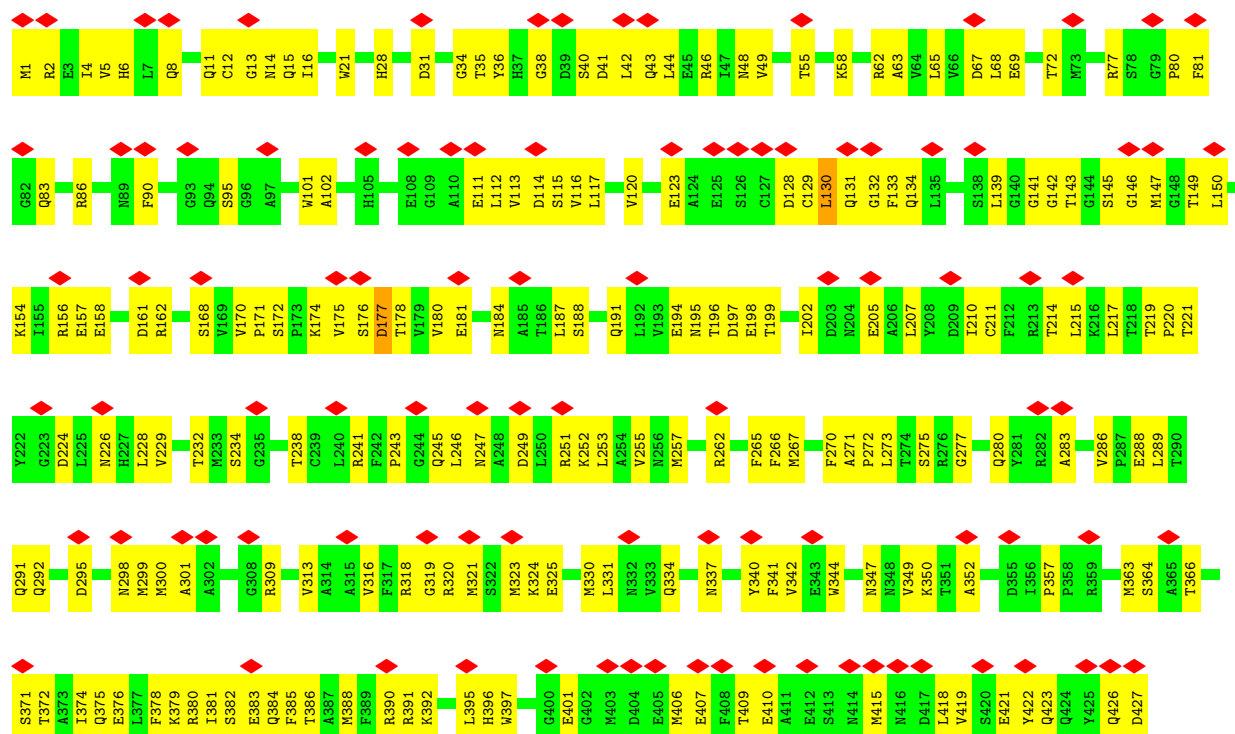


• Molecule 3: Tubulin beta-4B chain

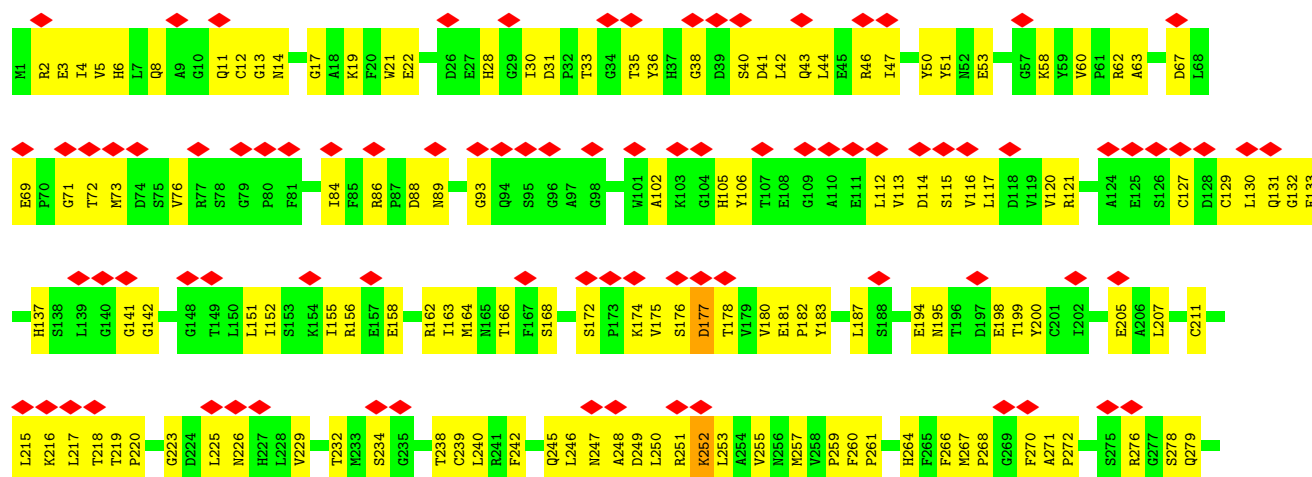


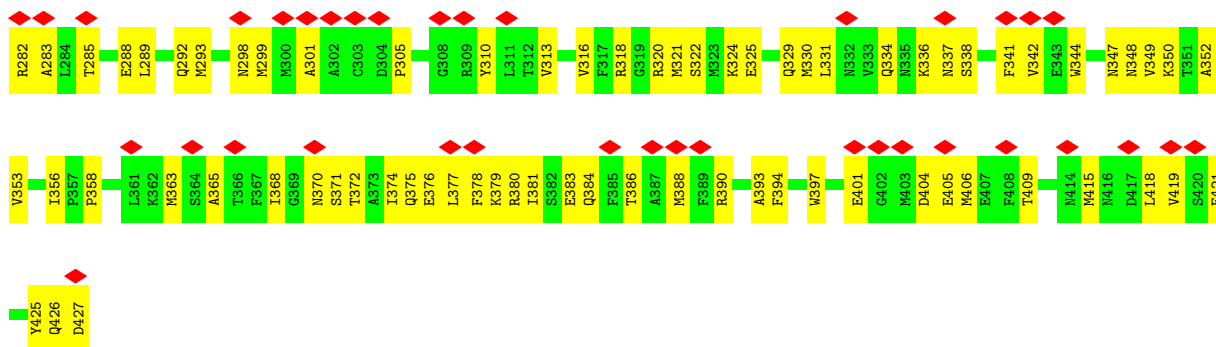


• Molecule 3: Tubulin beta-4B chain

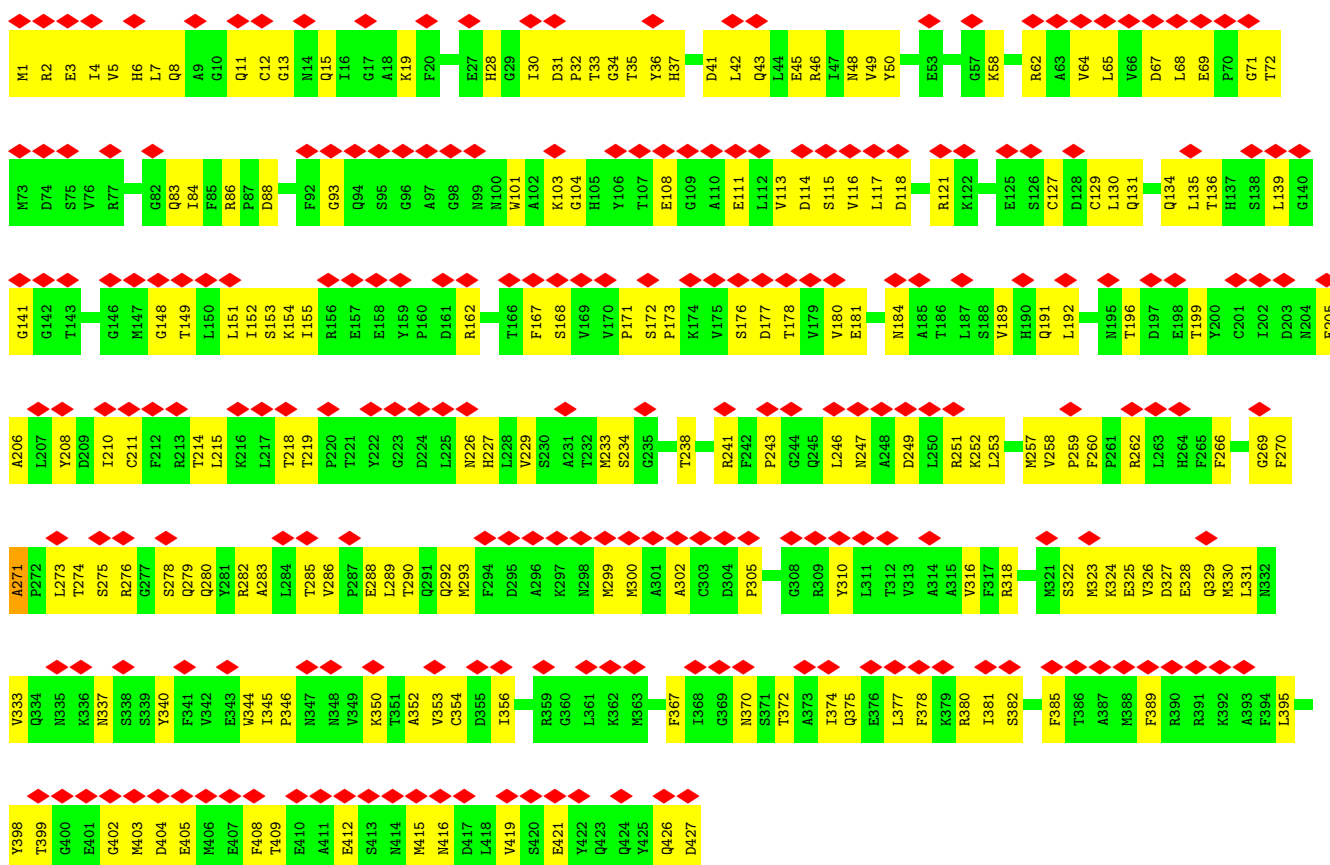


• Molecule 3: Tubulin beta-4B chain

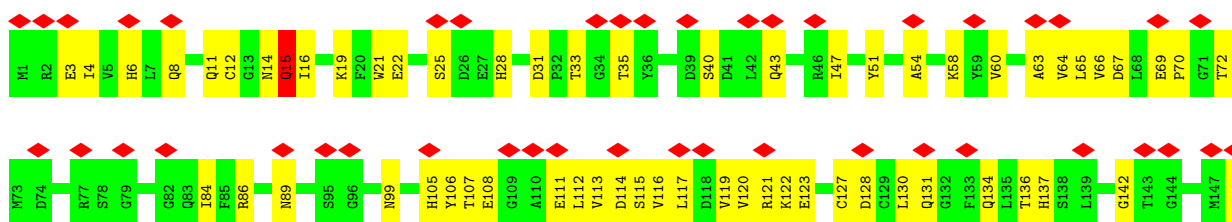


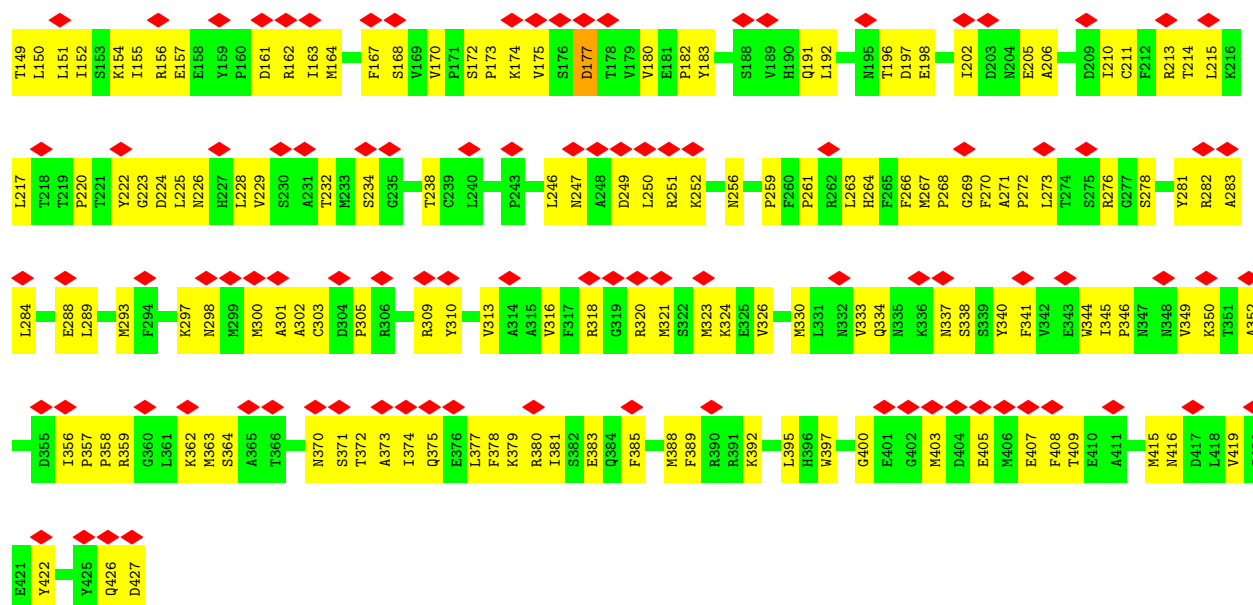


• Molecule 3: Tubulin beta-4B chain

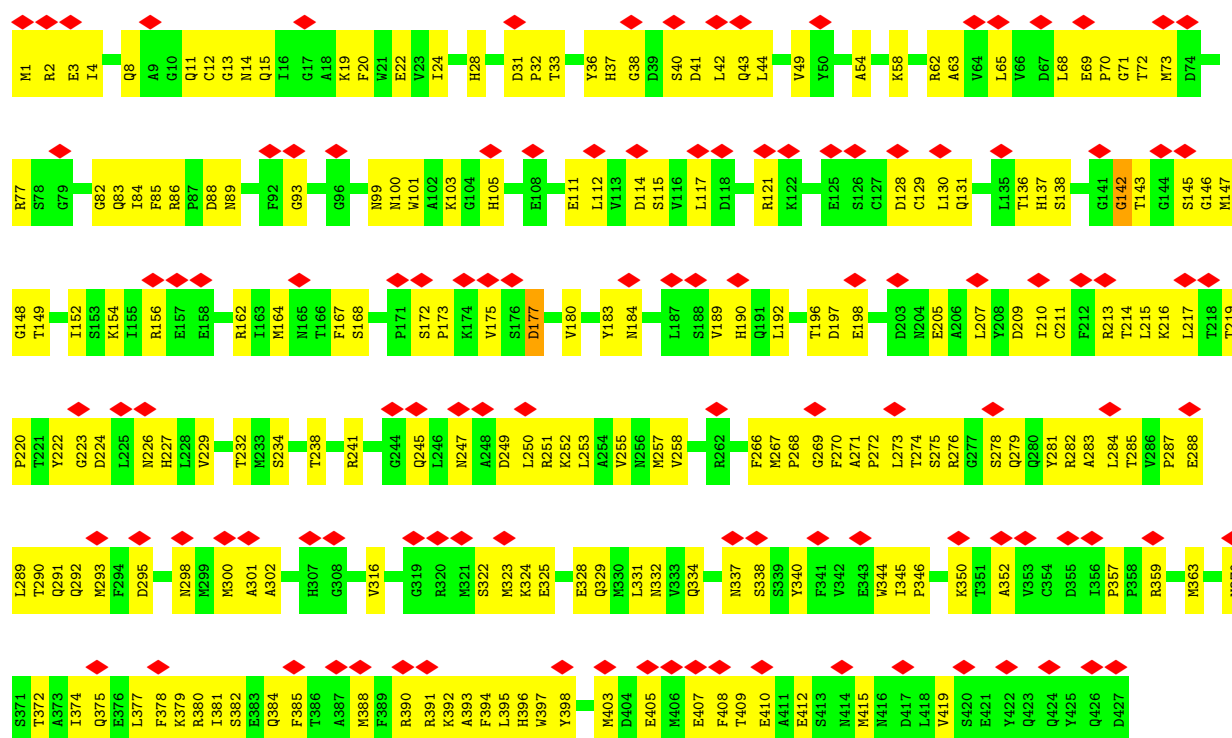


• Molecule 3: Tubulin beta-4B chain



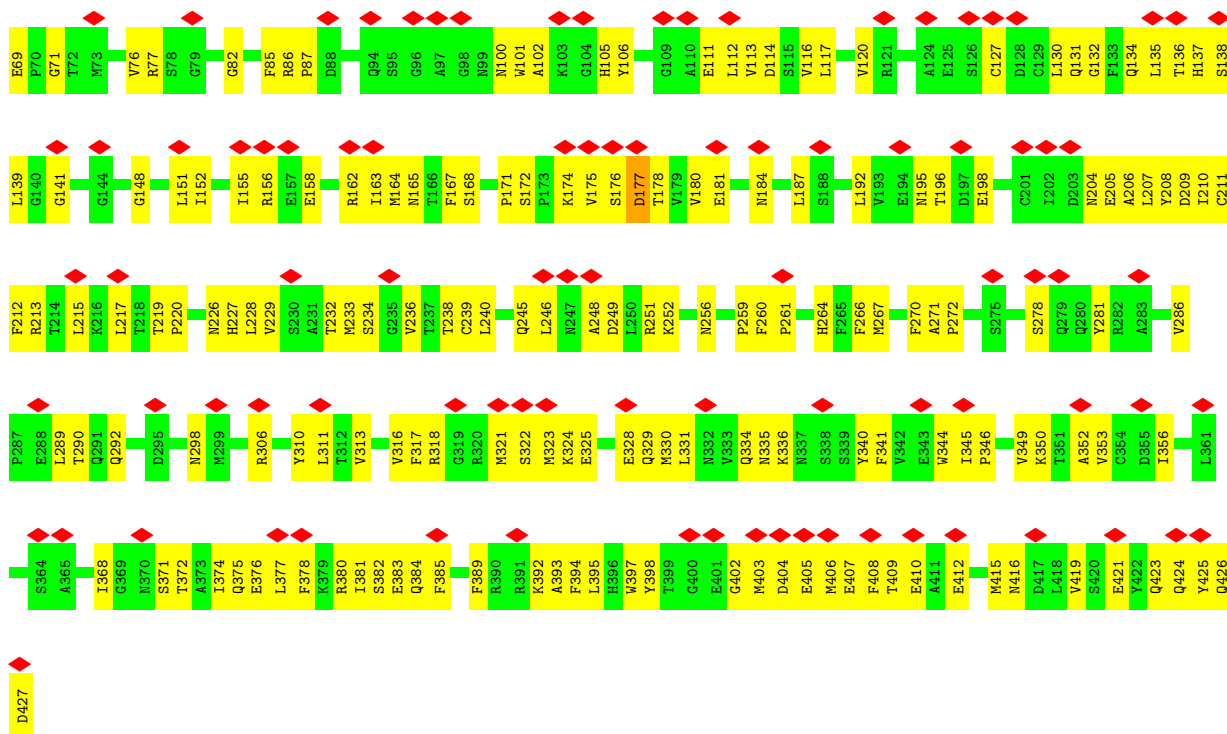


• Molecule 3: Tubulin beta-4B chain

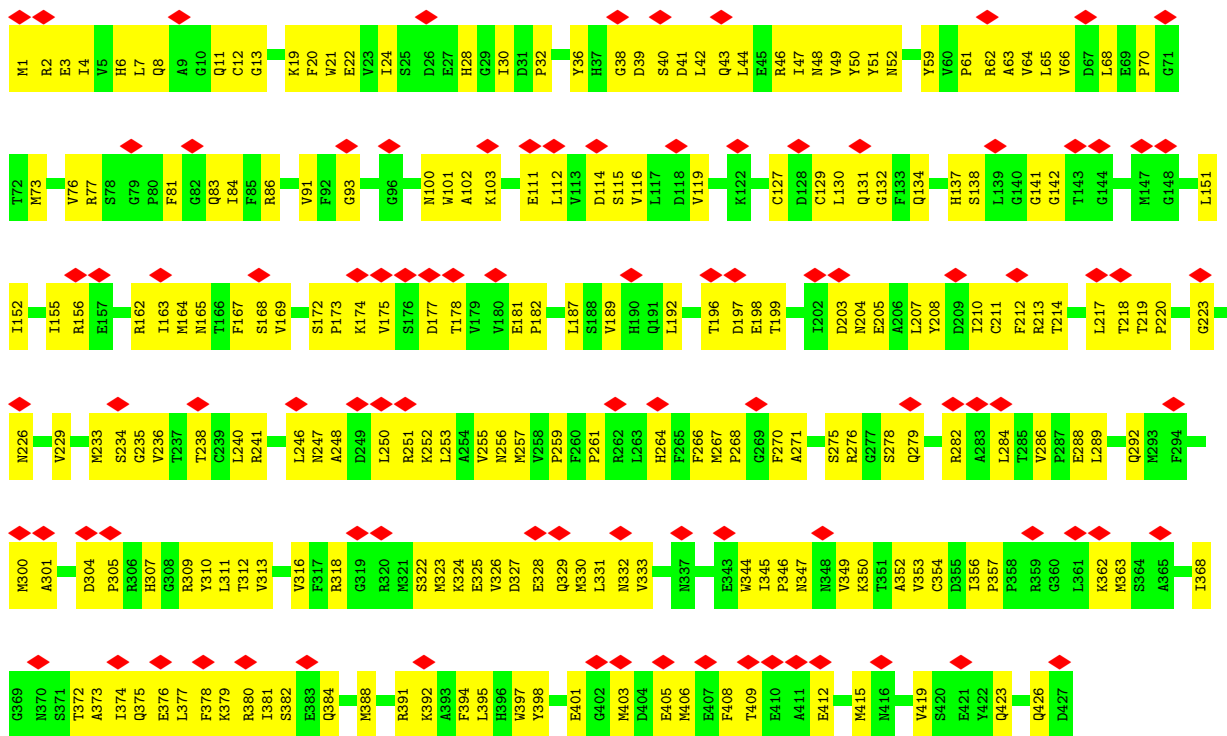


• Molecule 3: Tubulin beta-4B chain



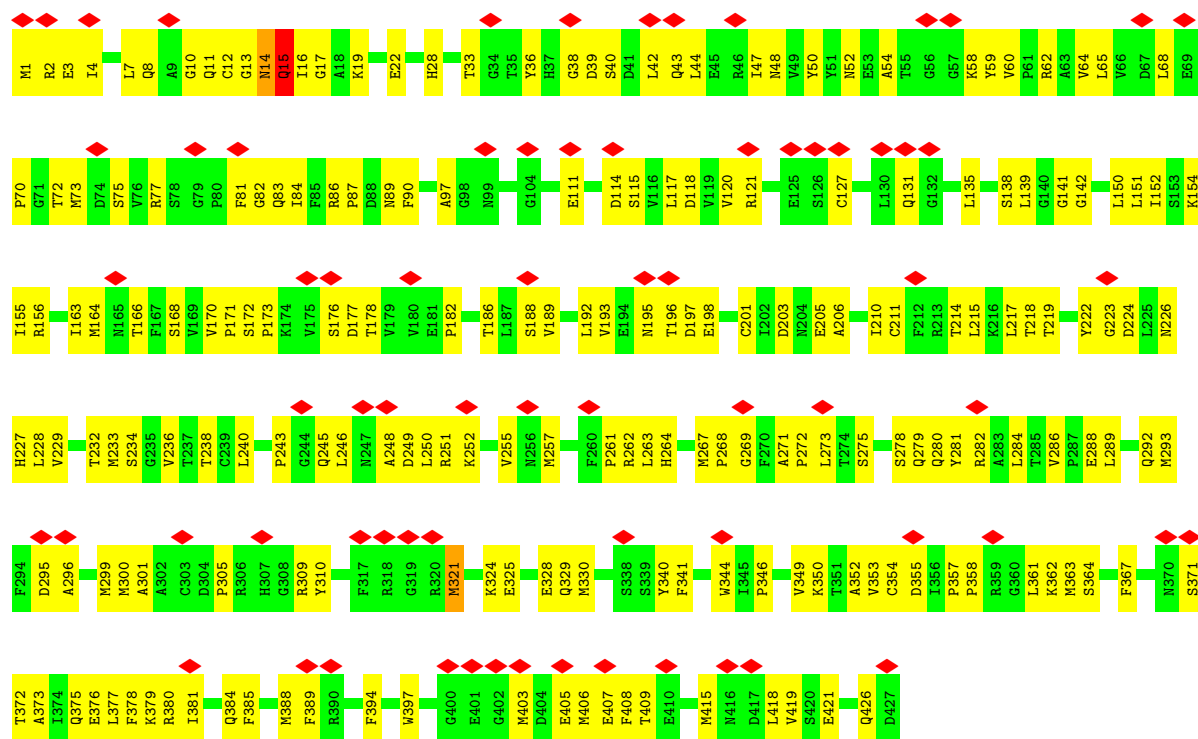


• Molecule 3: Tubulin beta-4B chain

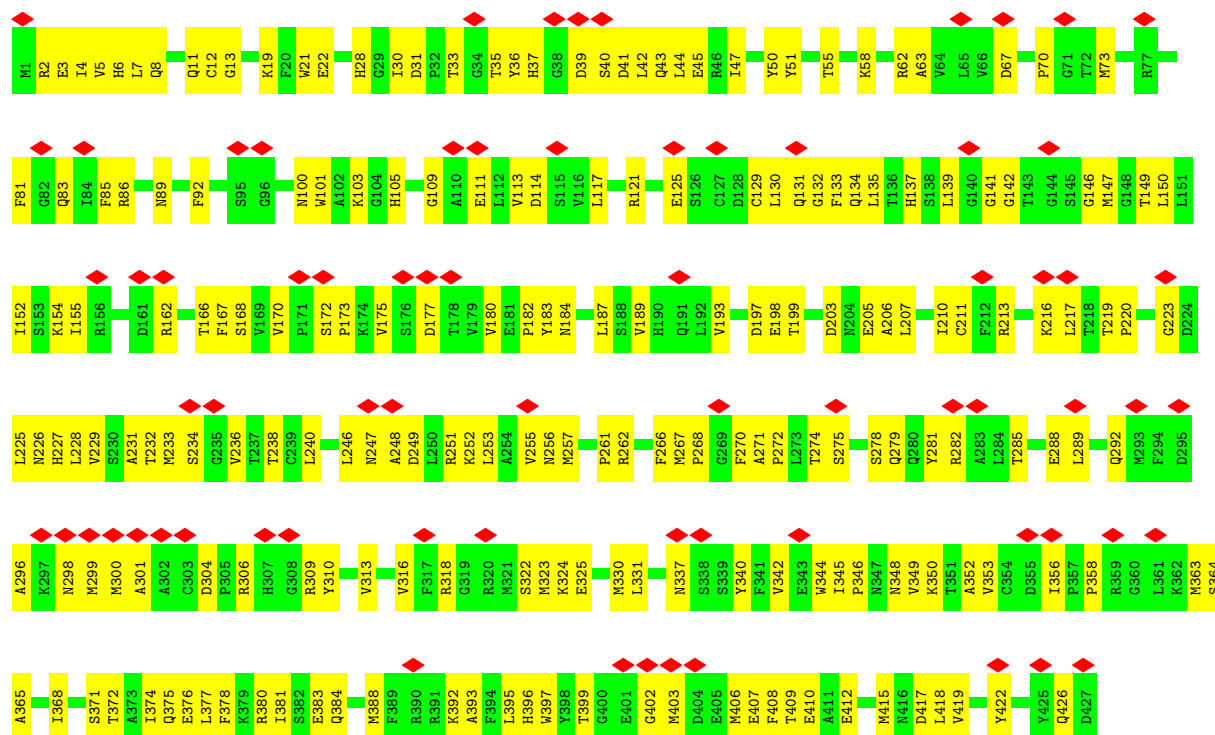


• Molecule 3: Tubulin beta-4B chain



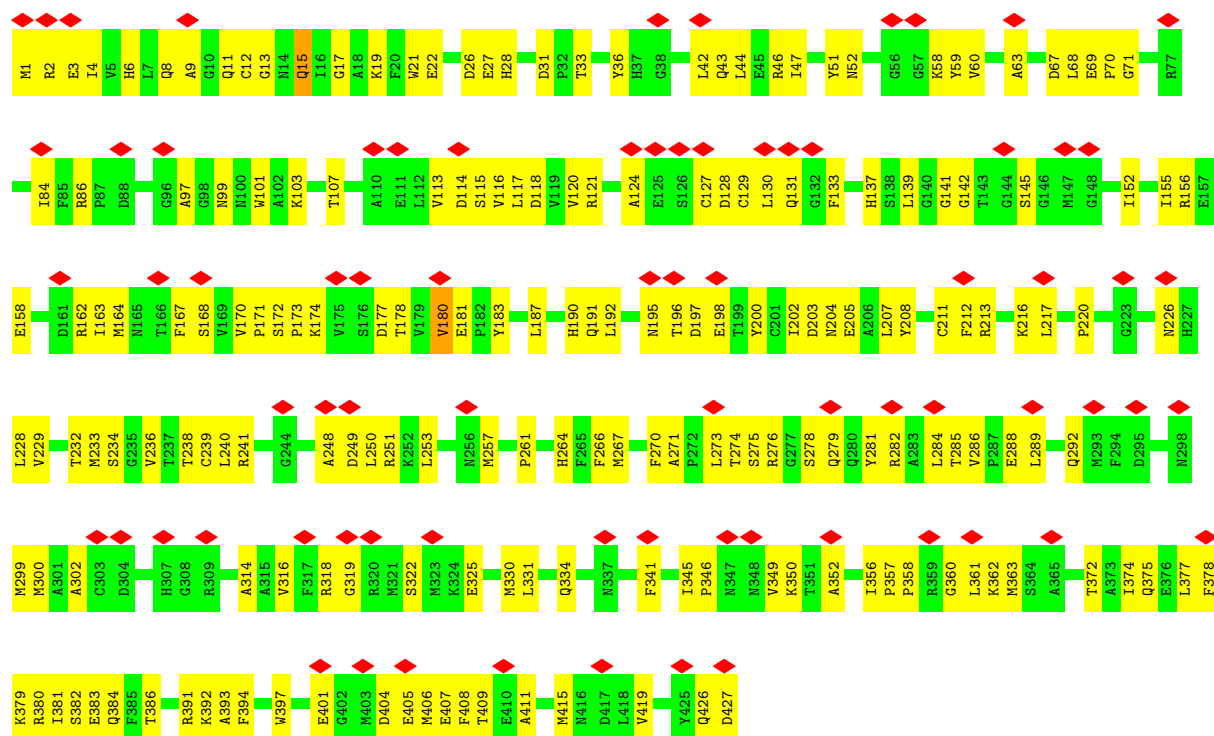


• Molecule 3: Tubulin beta-4B chain

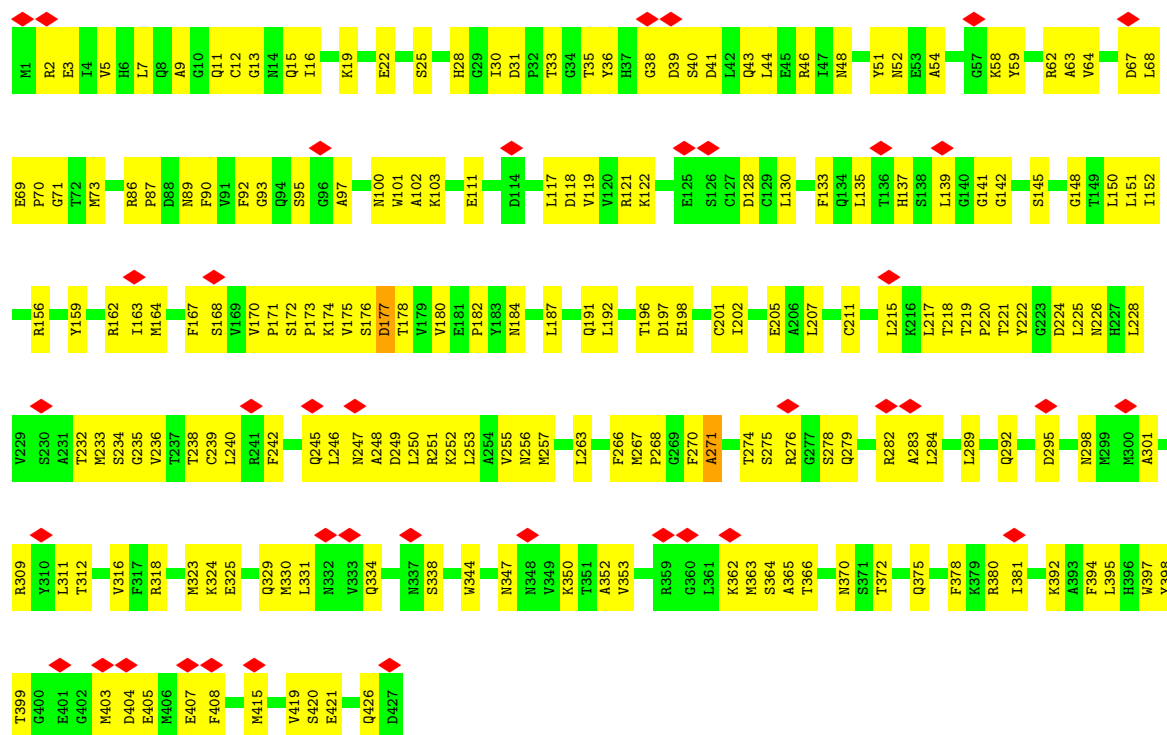


• Molecule 3: Tubulin beta-4B chain



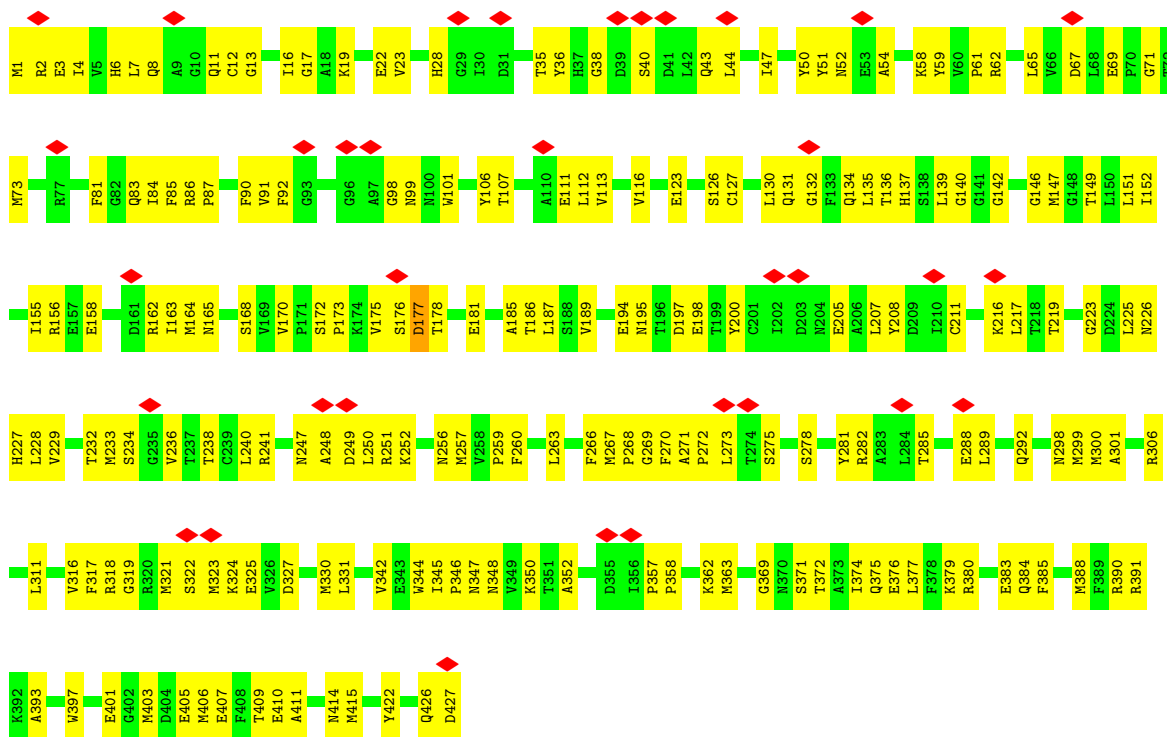


• Molecule 3: Tubulin beta-4B chain

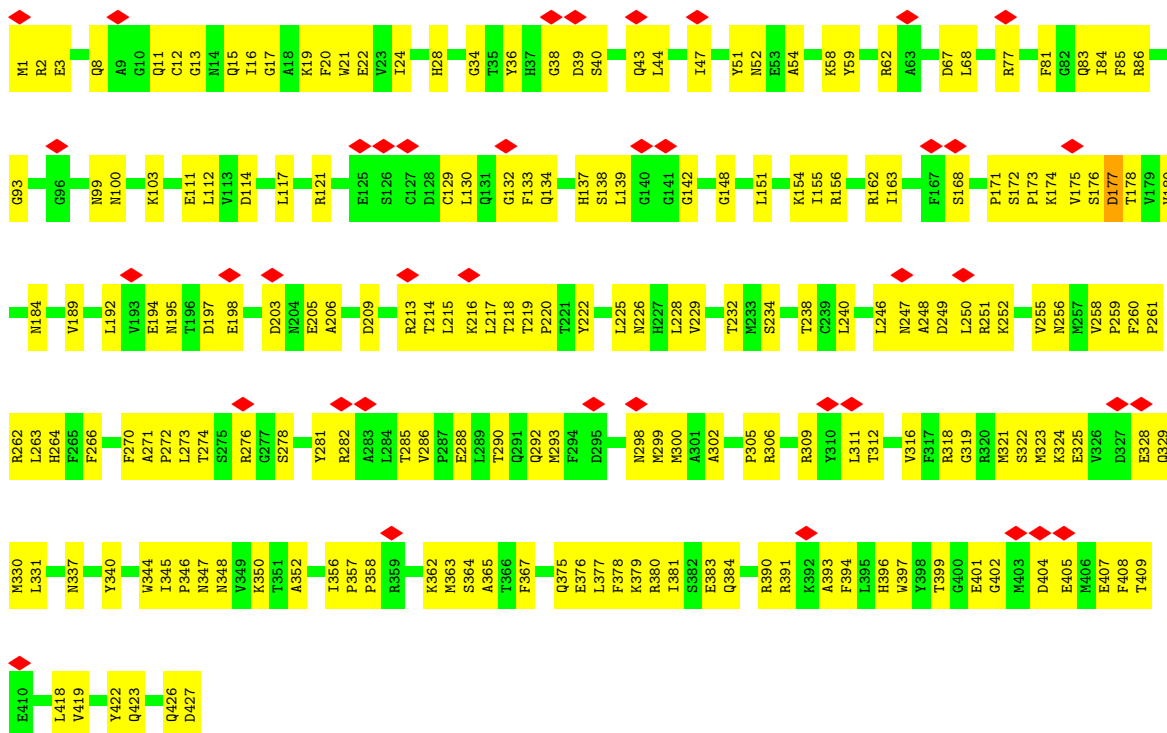


• Molecule 3: Tubulin beta-4B chain



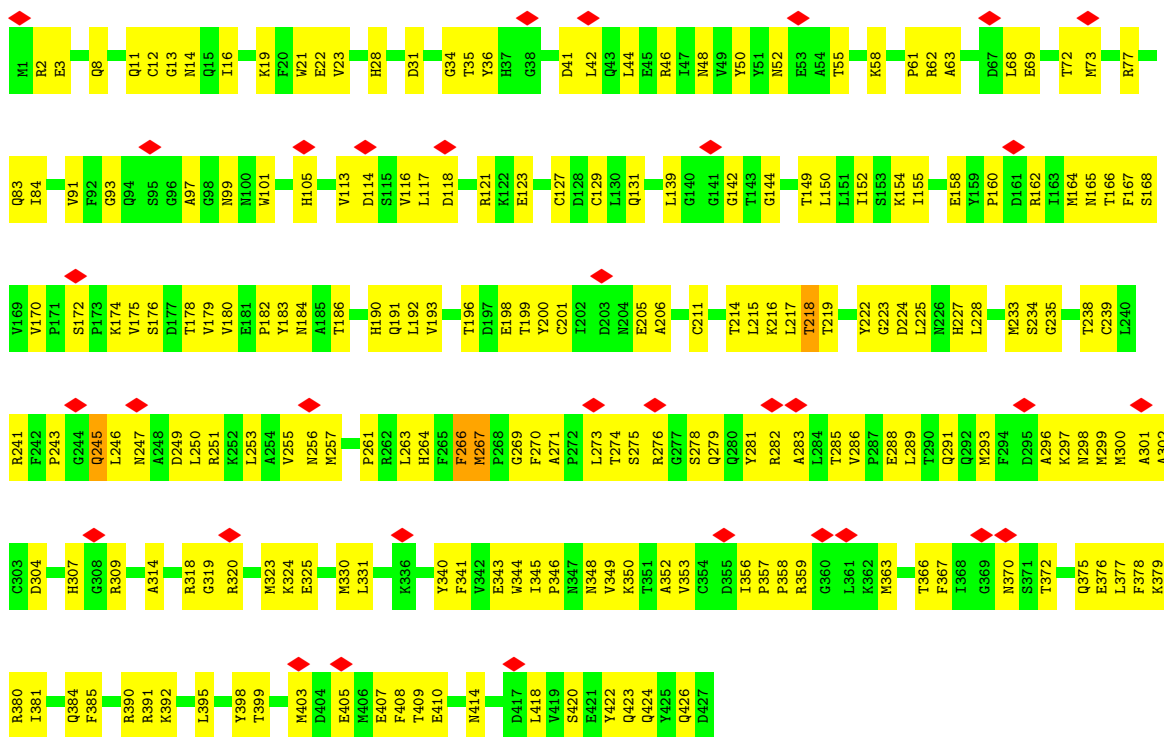


• Molecule 3: Tubulin beta-4B chain

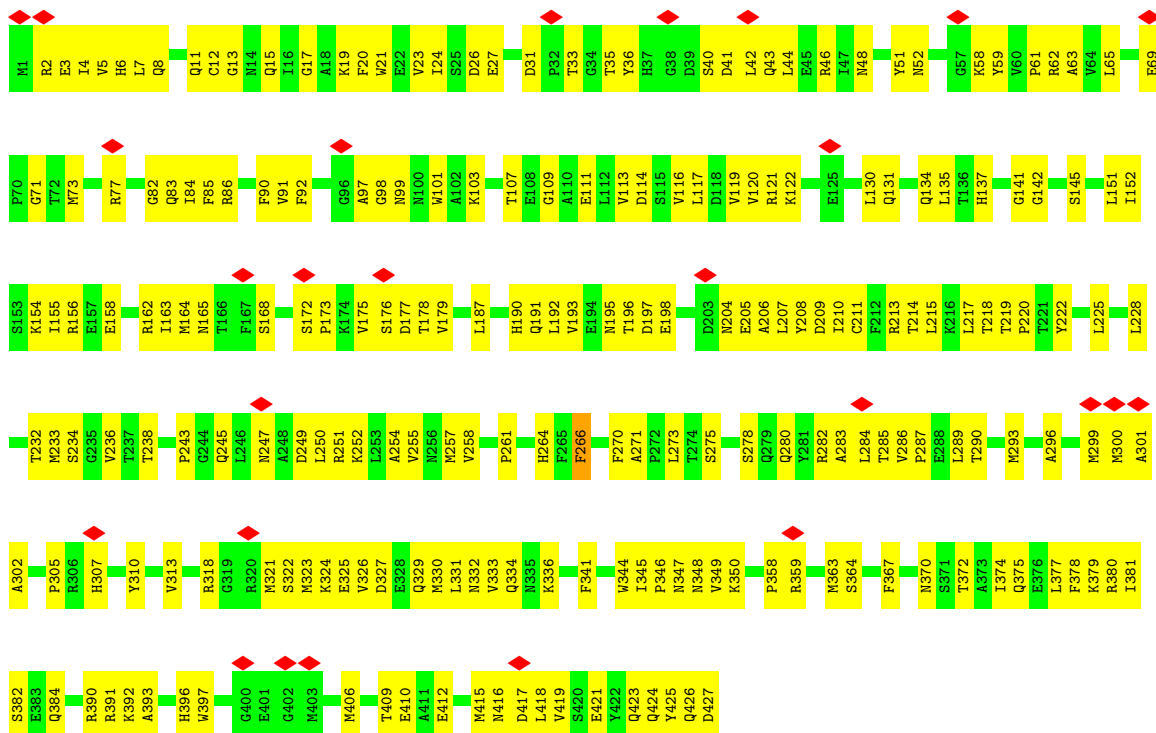


• Molecule 3: Tubulin beta-4B chain



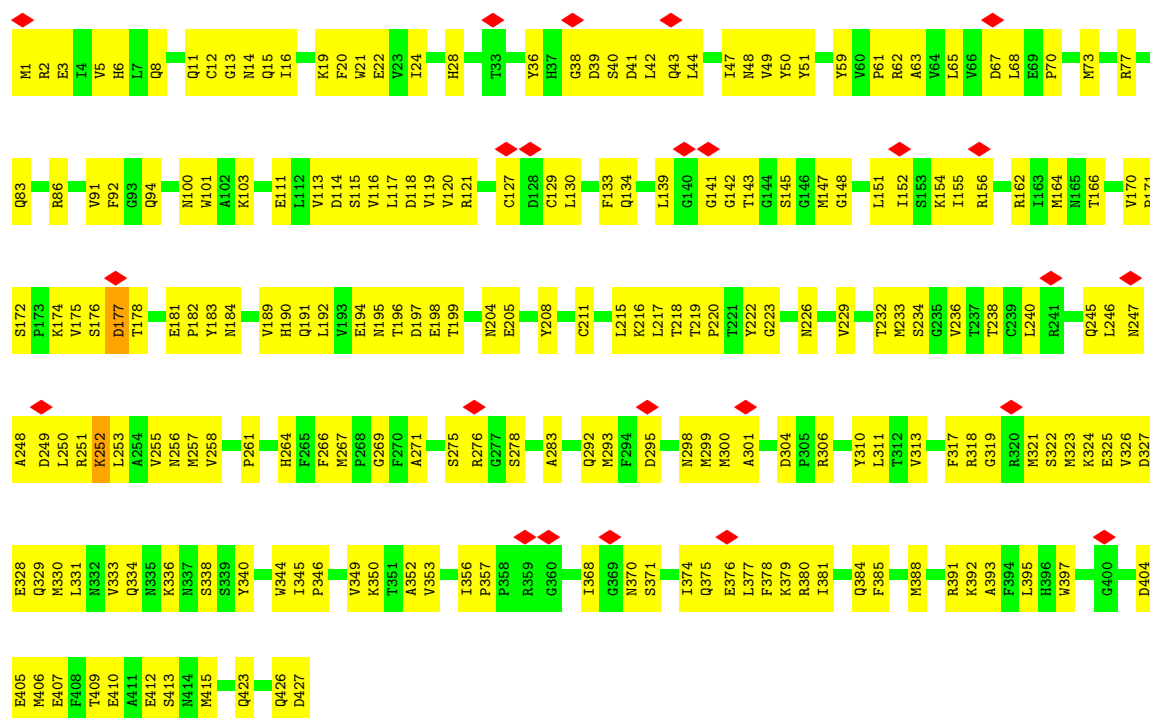


• Molecule 3: Tubulin beta-4B chain

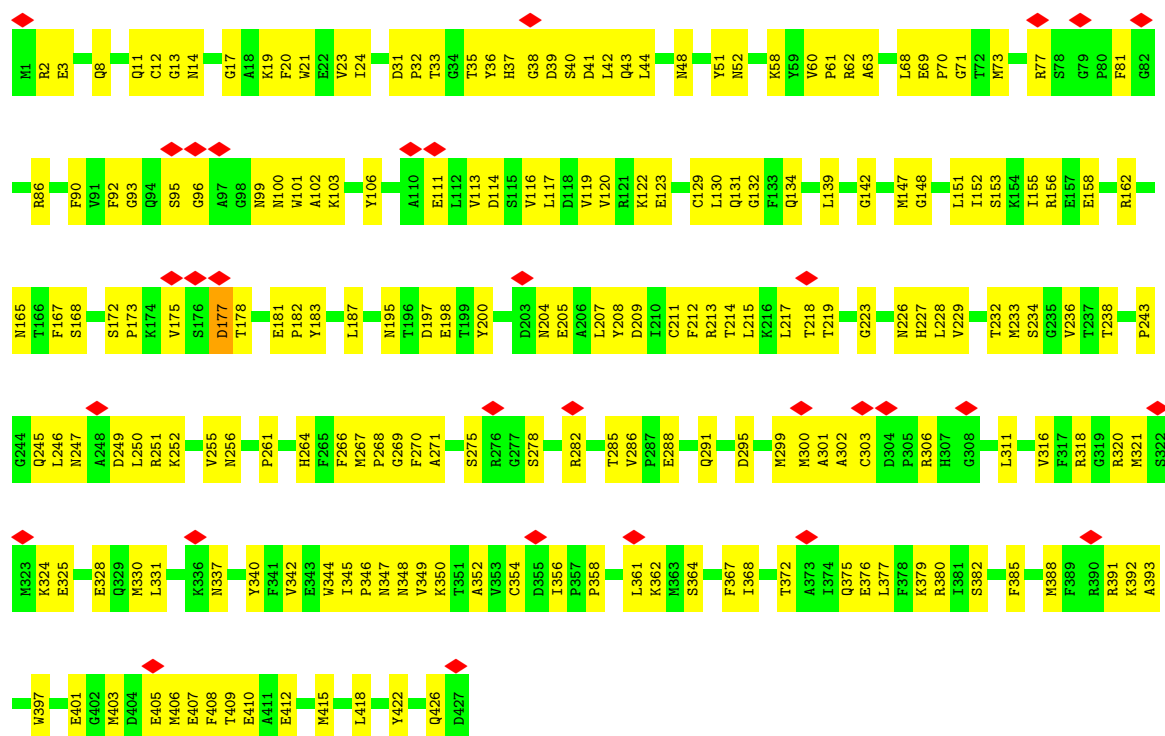


• Molecule 3: Tubulin beta-4B chain



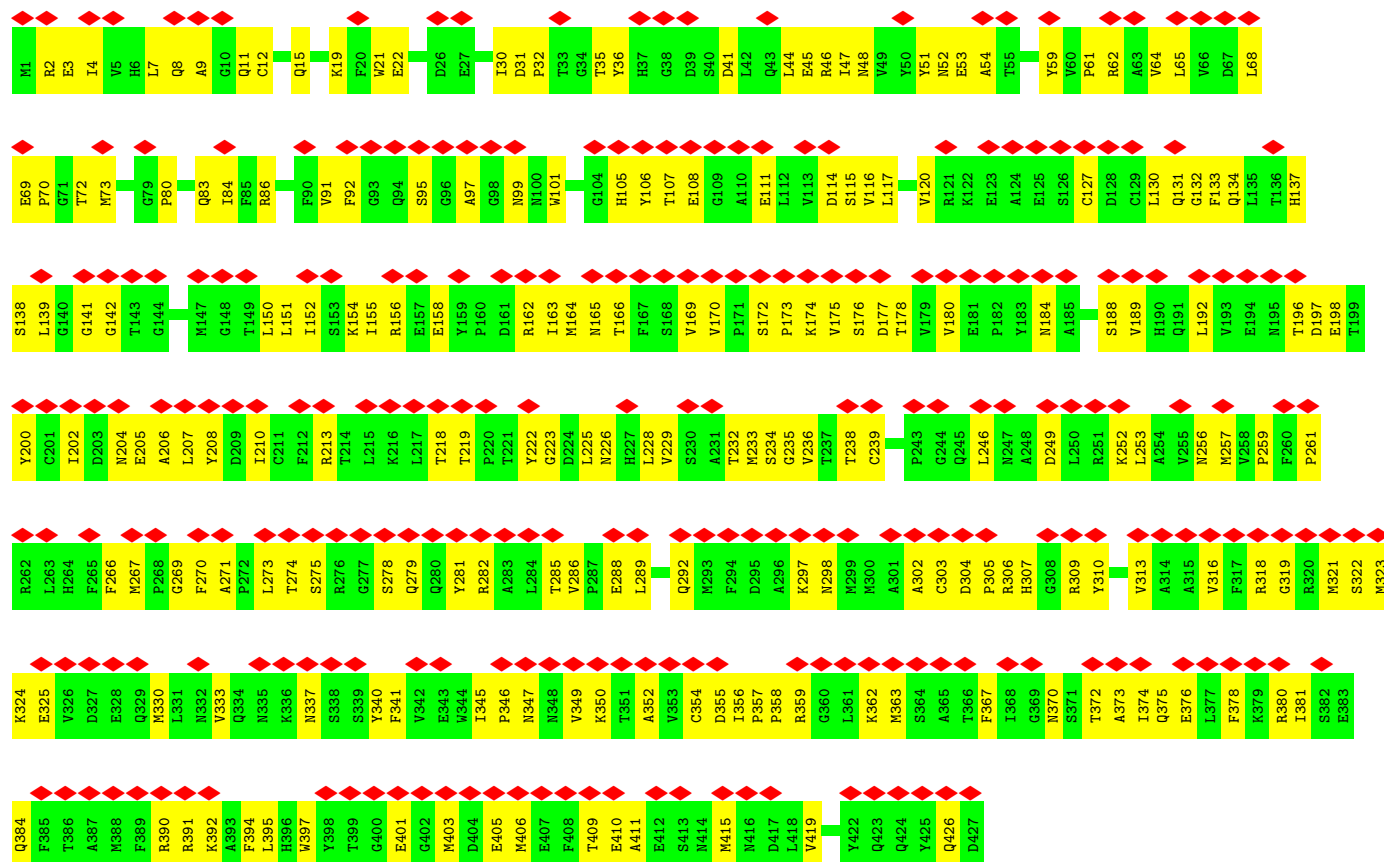


• Molecule 3: Tubulin beta-4B chain

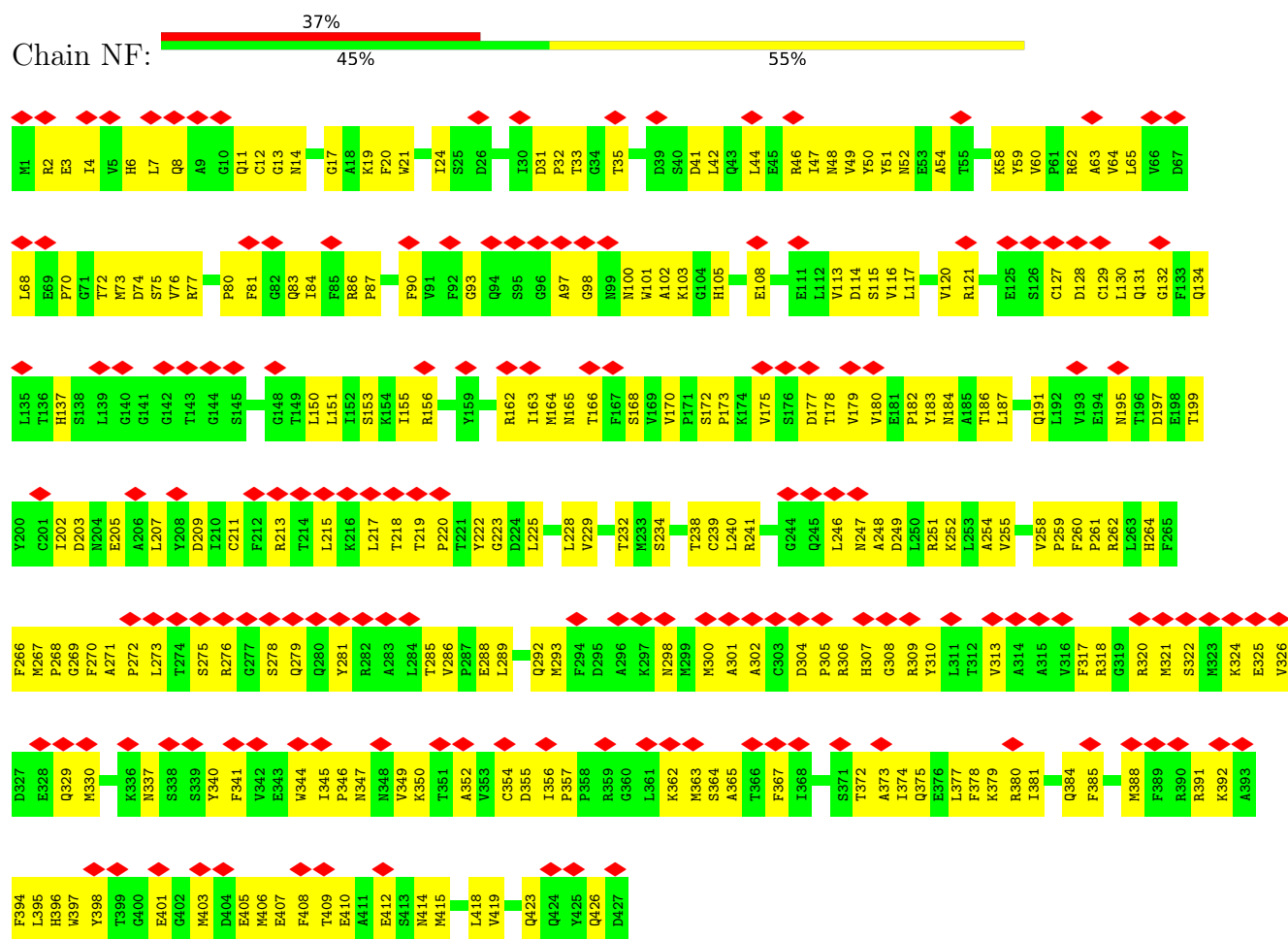


• Molecule 3: Tubulin beta-4B chain

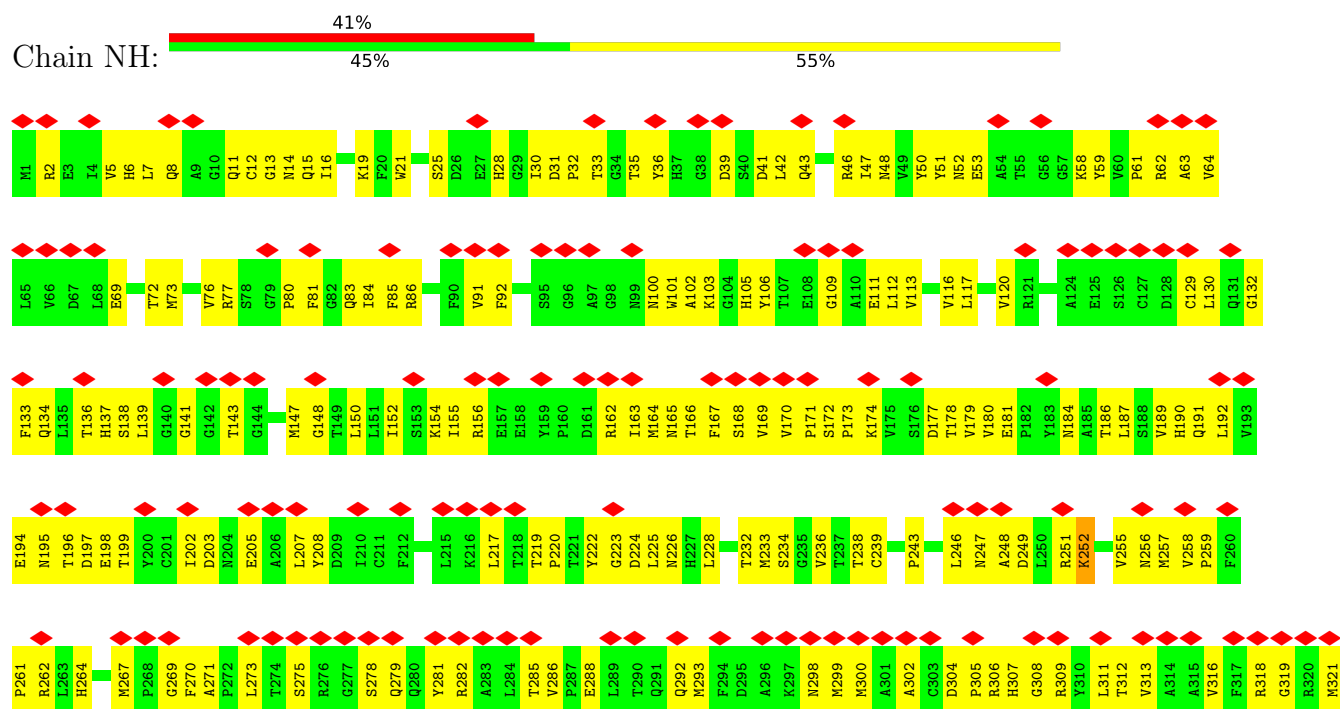


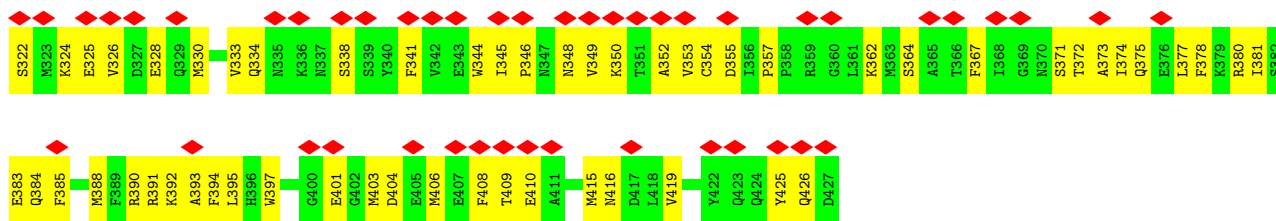


- Molecule 3: Tubulin beta-4B chain

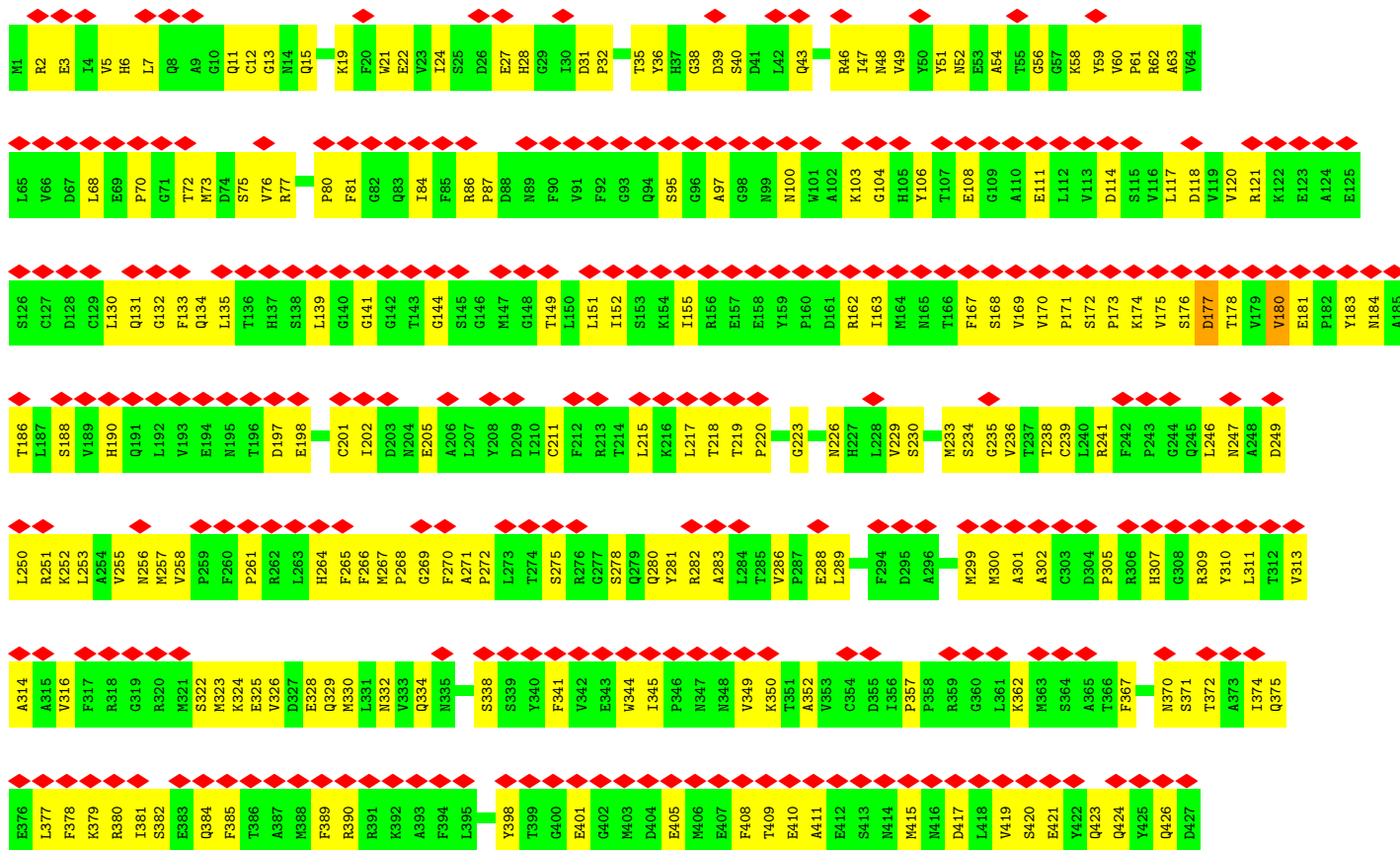


- Molecule 3: Tubulin beta-4B chain

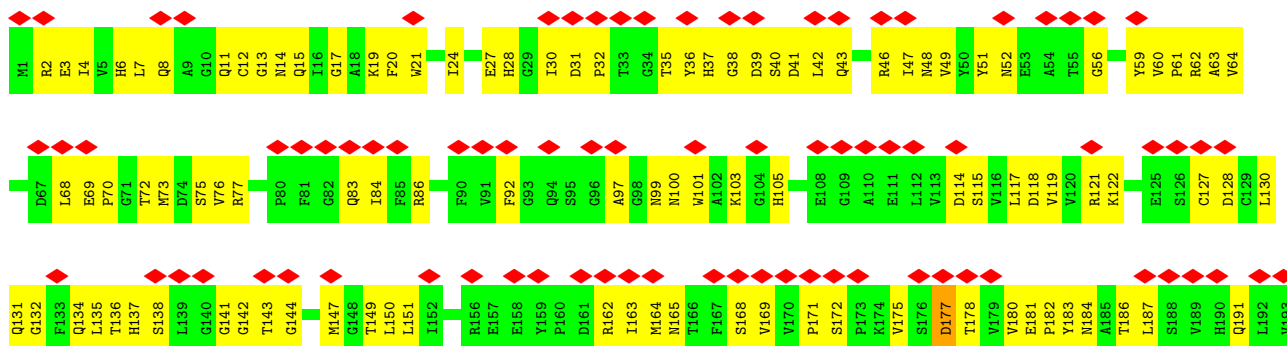


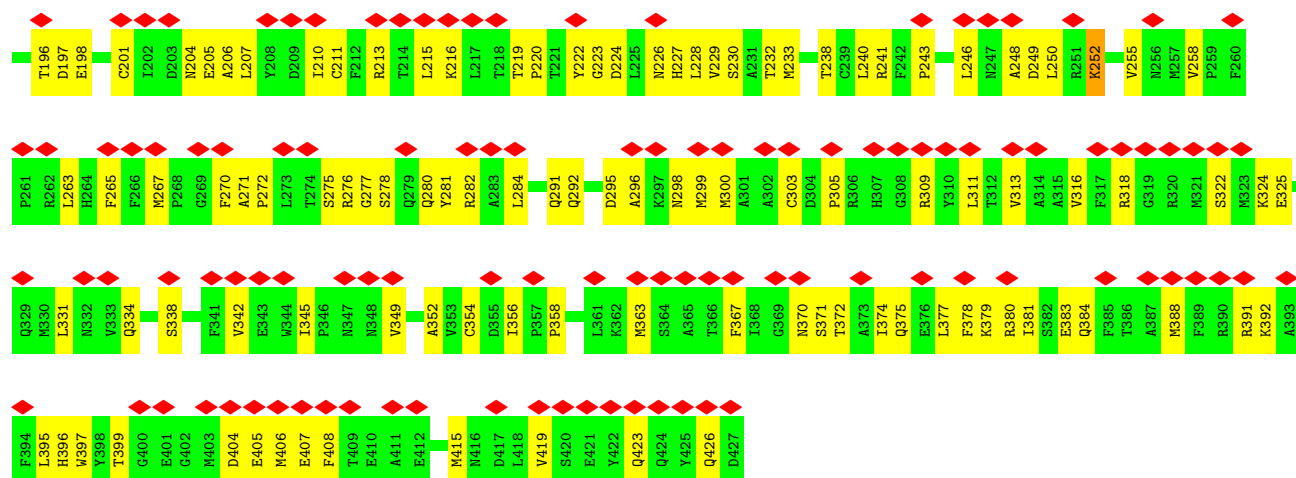


• Molecule 3: Tubulin beta-4B chain

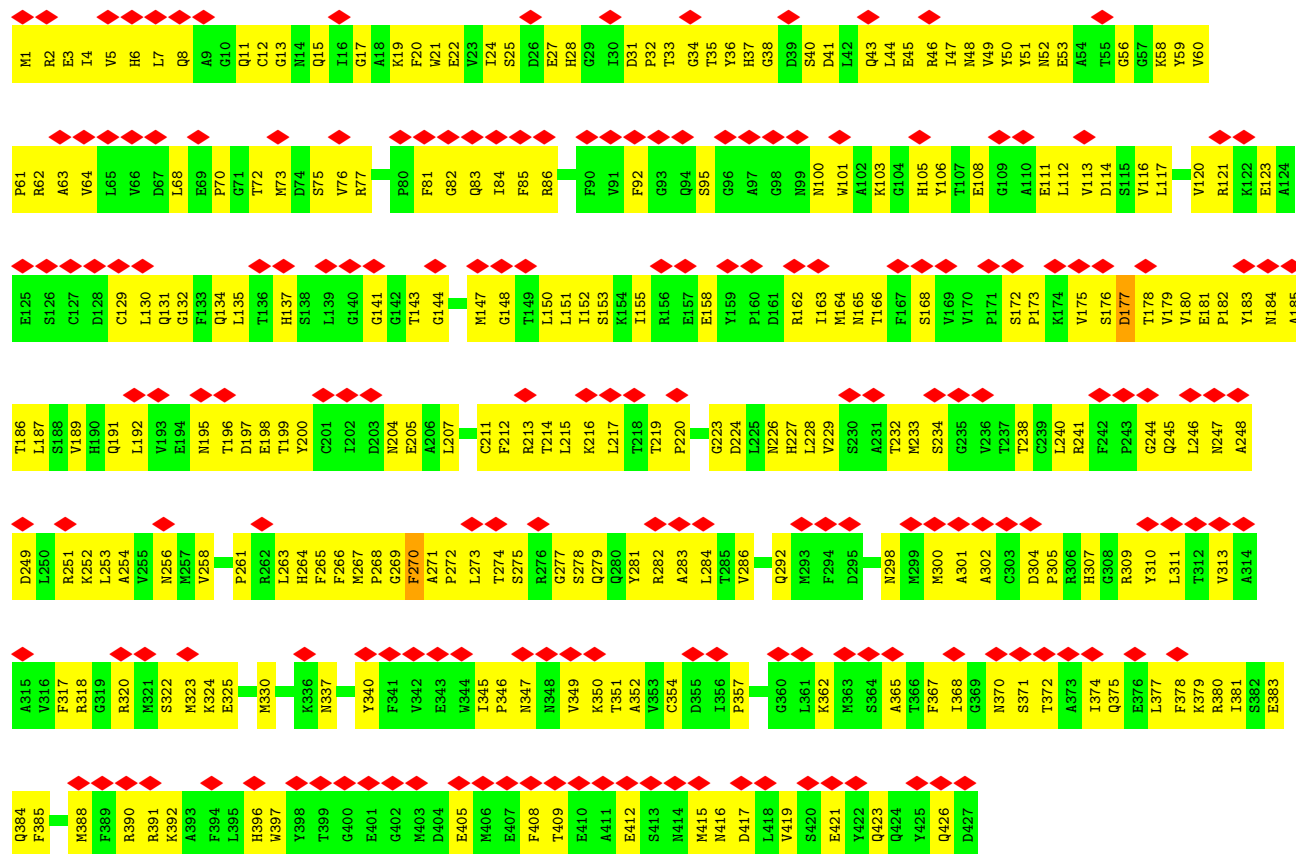
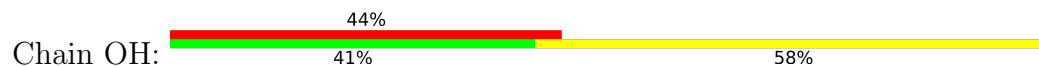


• Molecule 3: Tubulin beta-4B chain

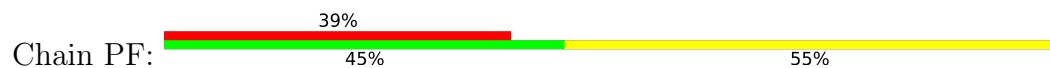


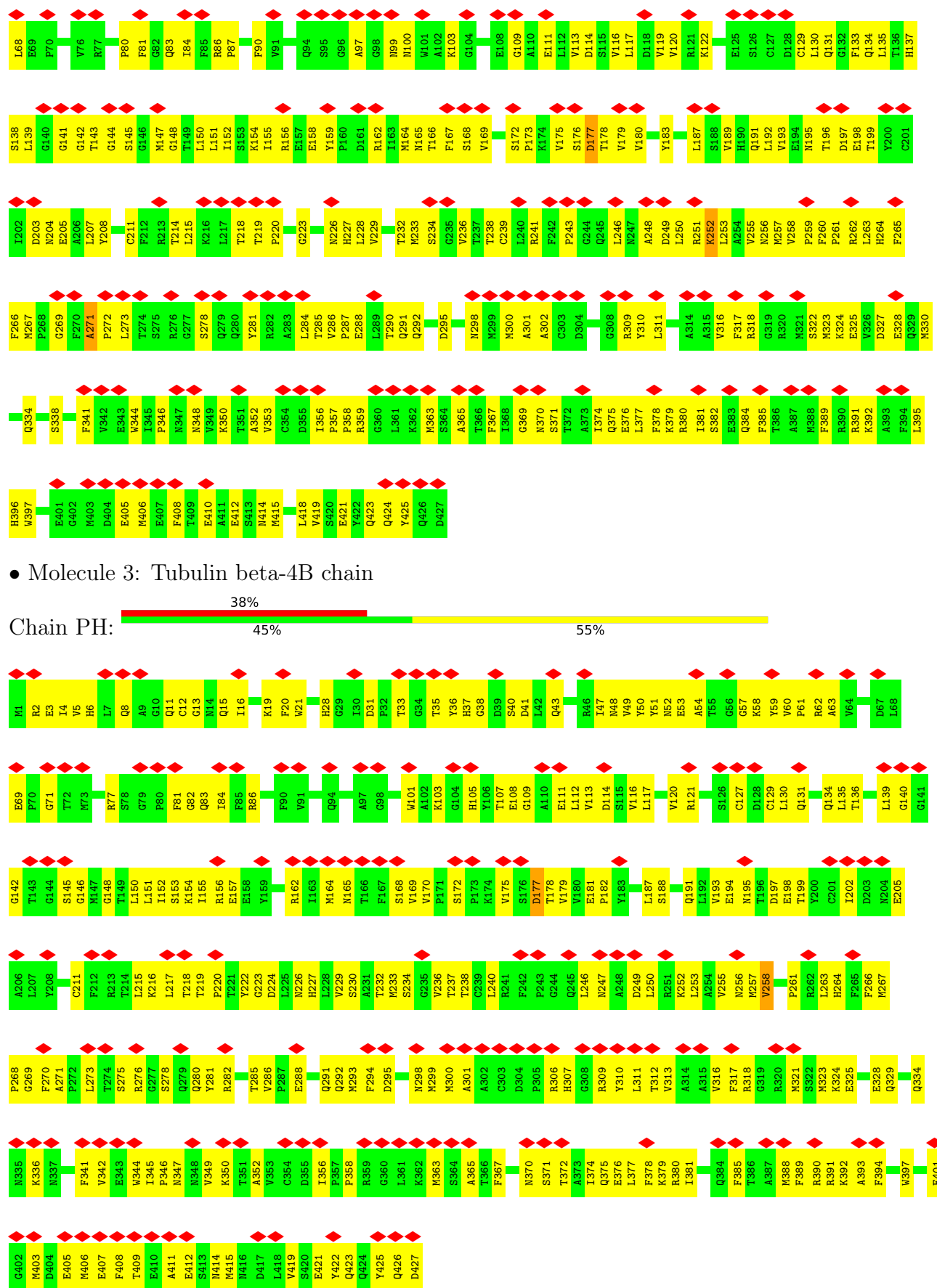


• Molecule 3: Tubulin beta-4B chain

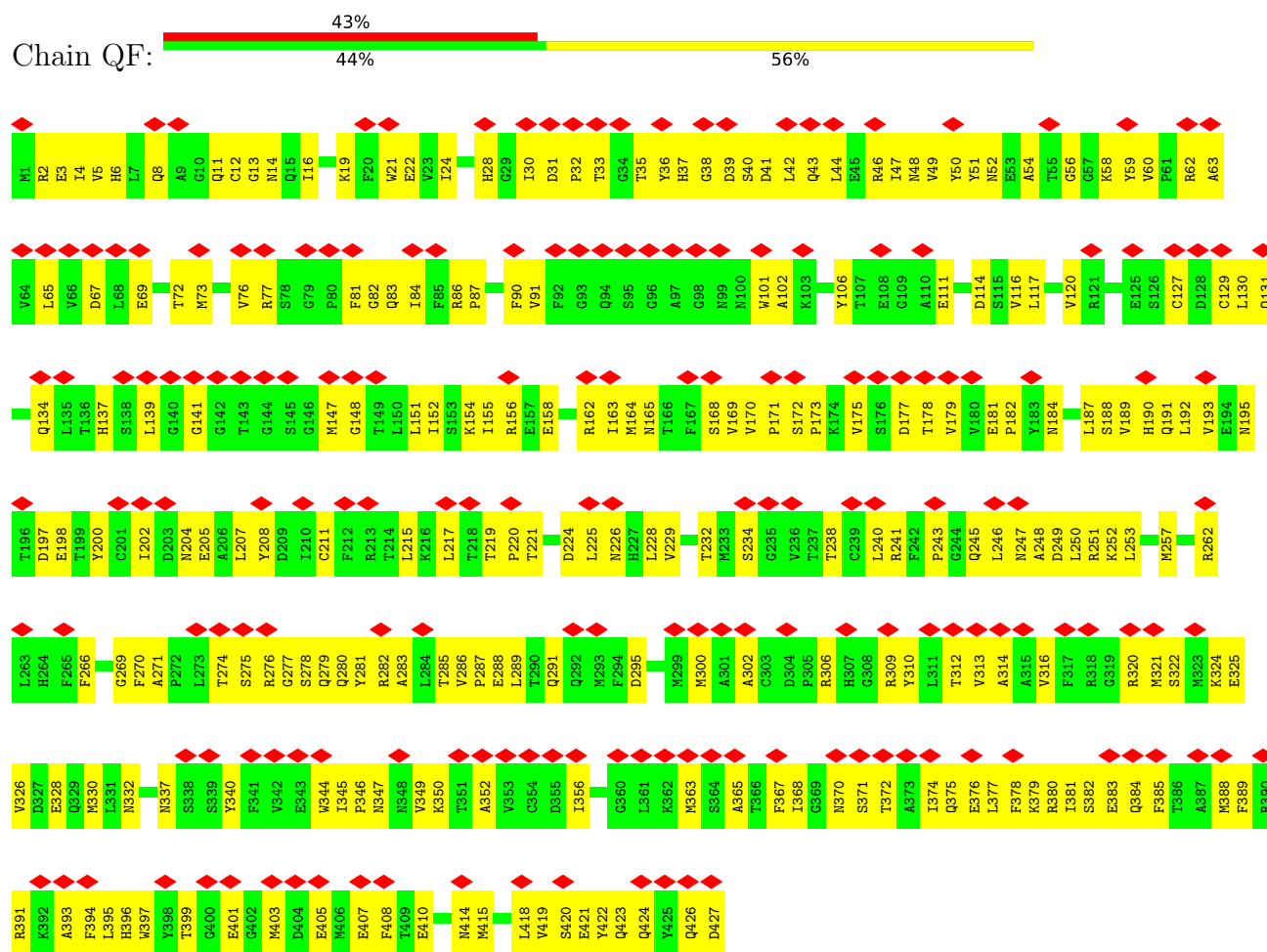


• Molecule 3: Tubulin beta-4B chain

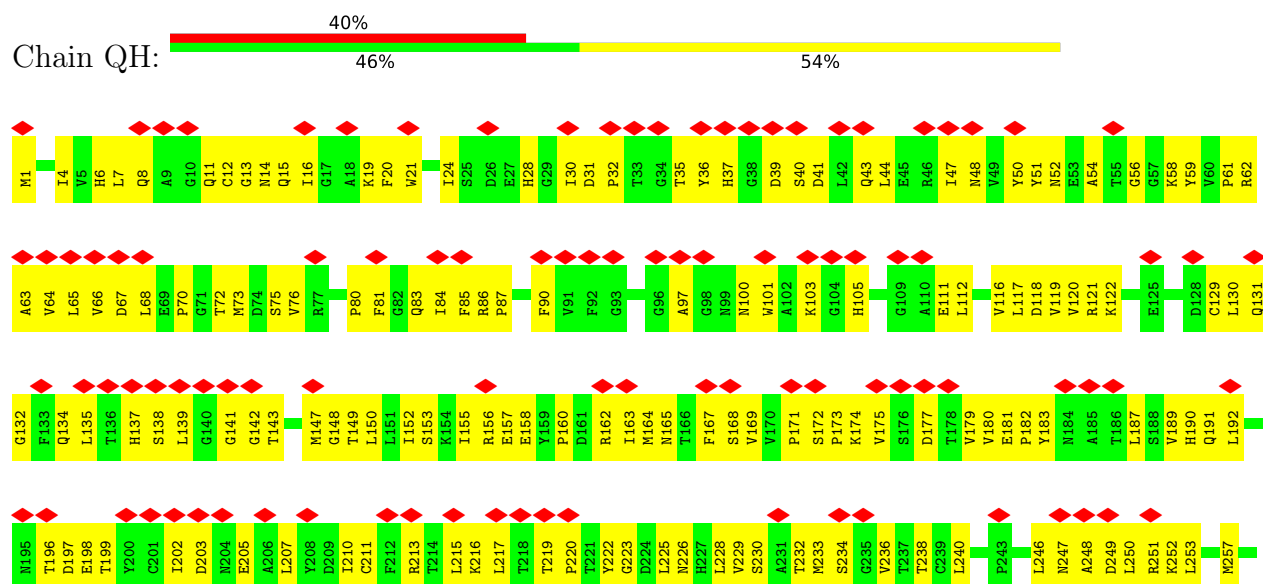


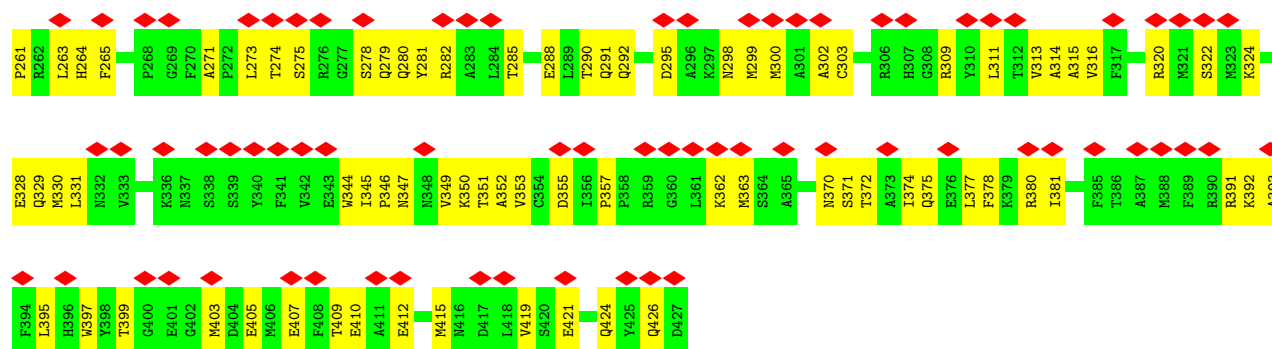


- Molecule 3: Tubulin beta-4B chain

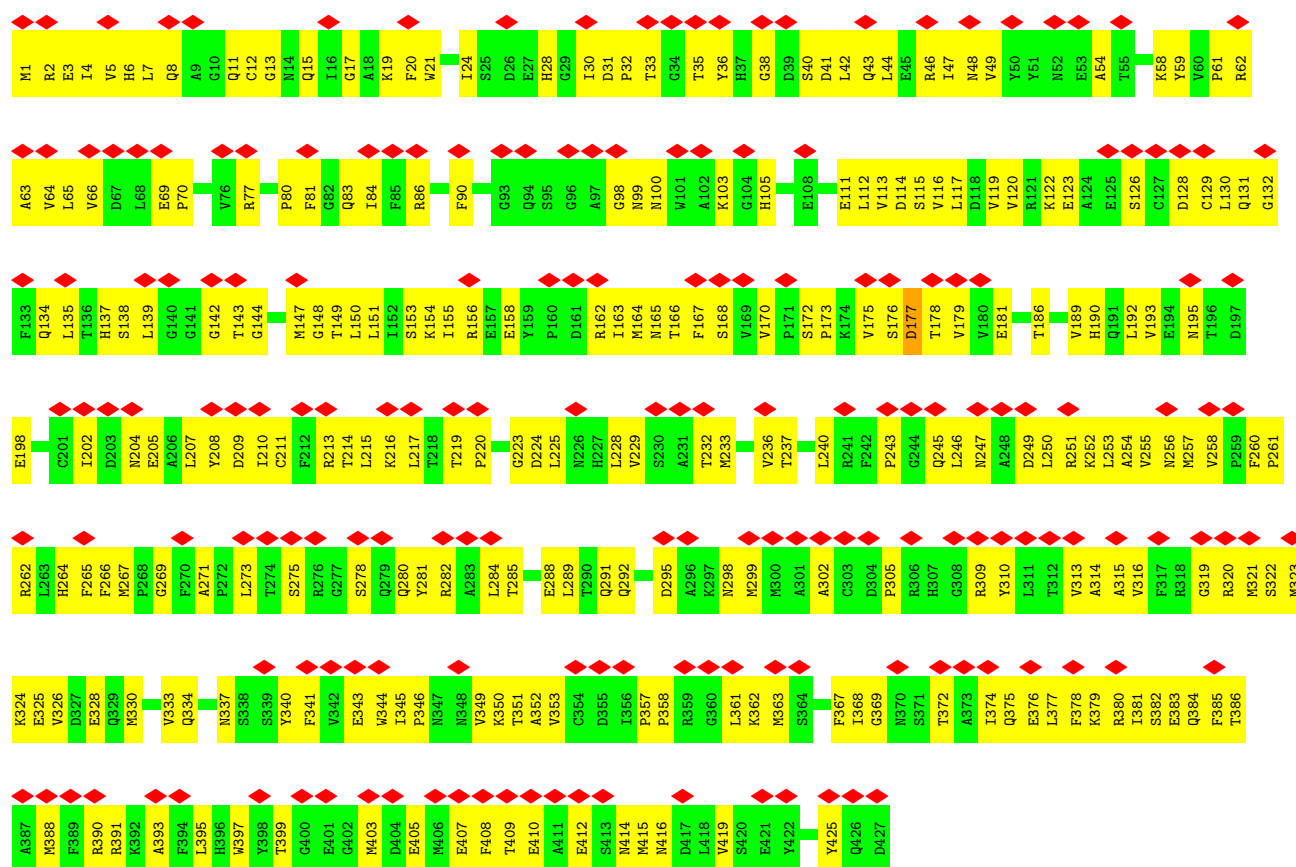


- Molecule 3: Tubulin beta-4B chain



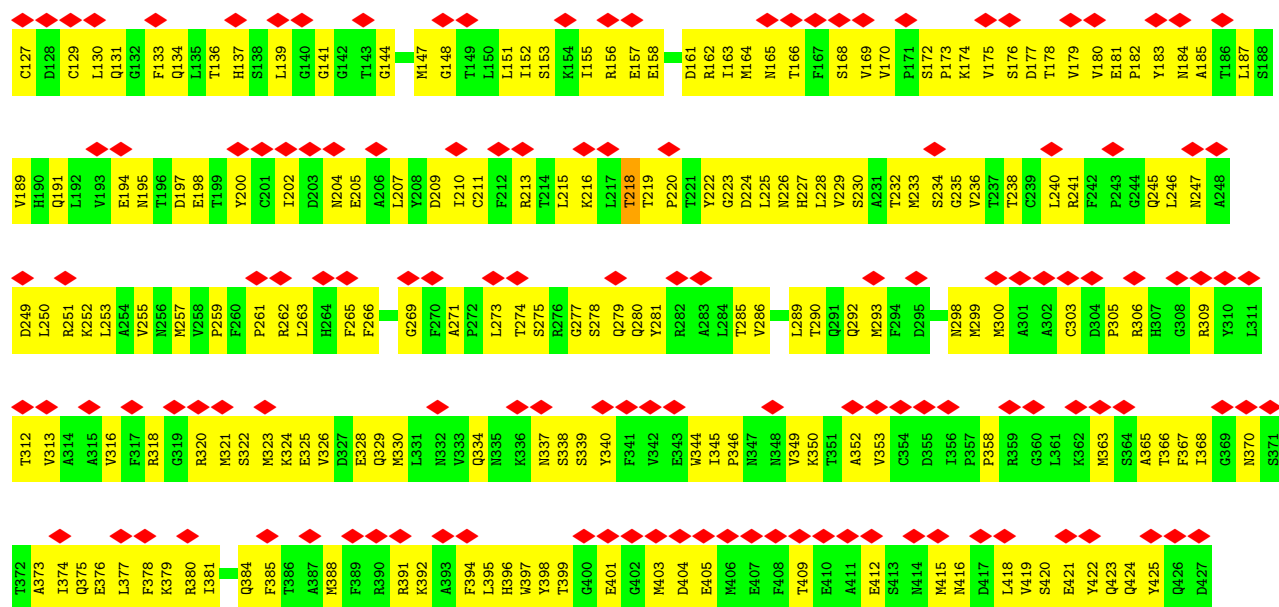


• Molecule 3: Tubulin beta-4B chain

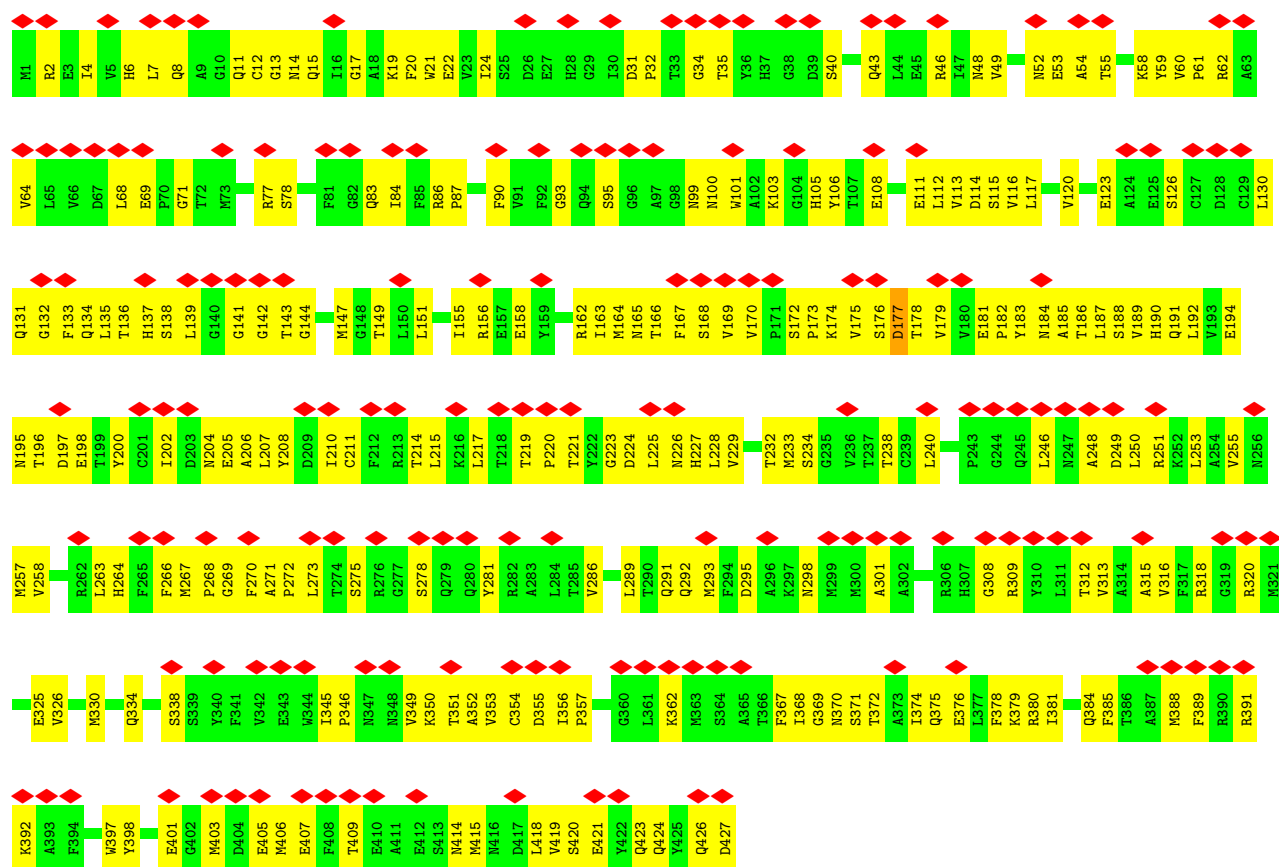
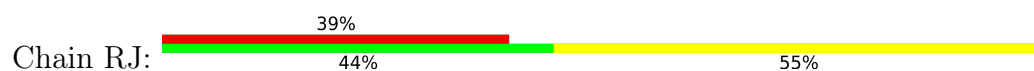


• Molecule 3: Tubulin beta-4B chain

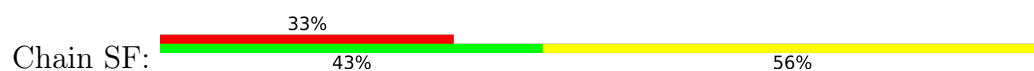


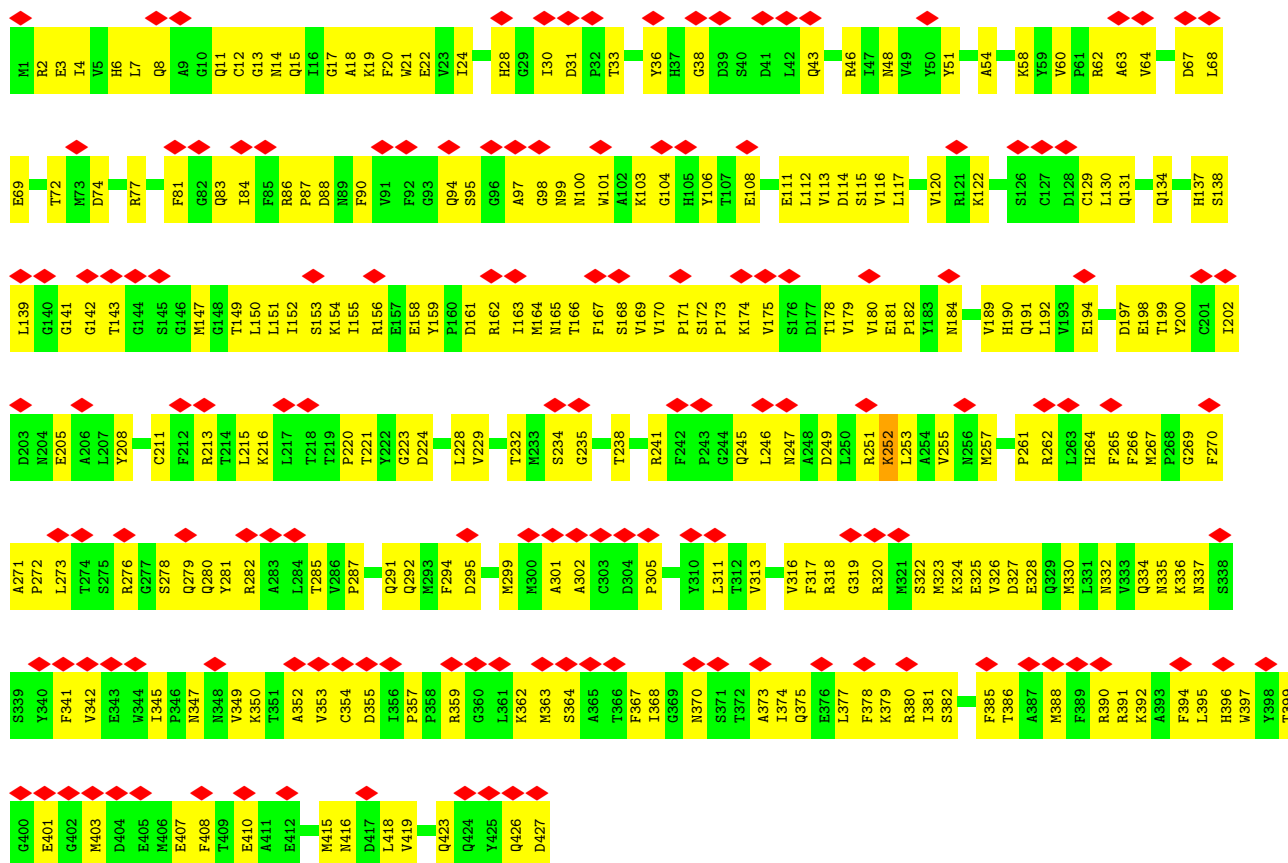


• Molecule 3: Tubulin beta-4B chain

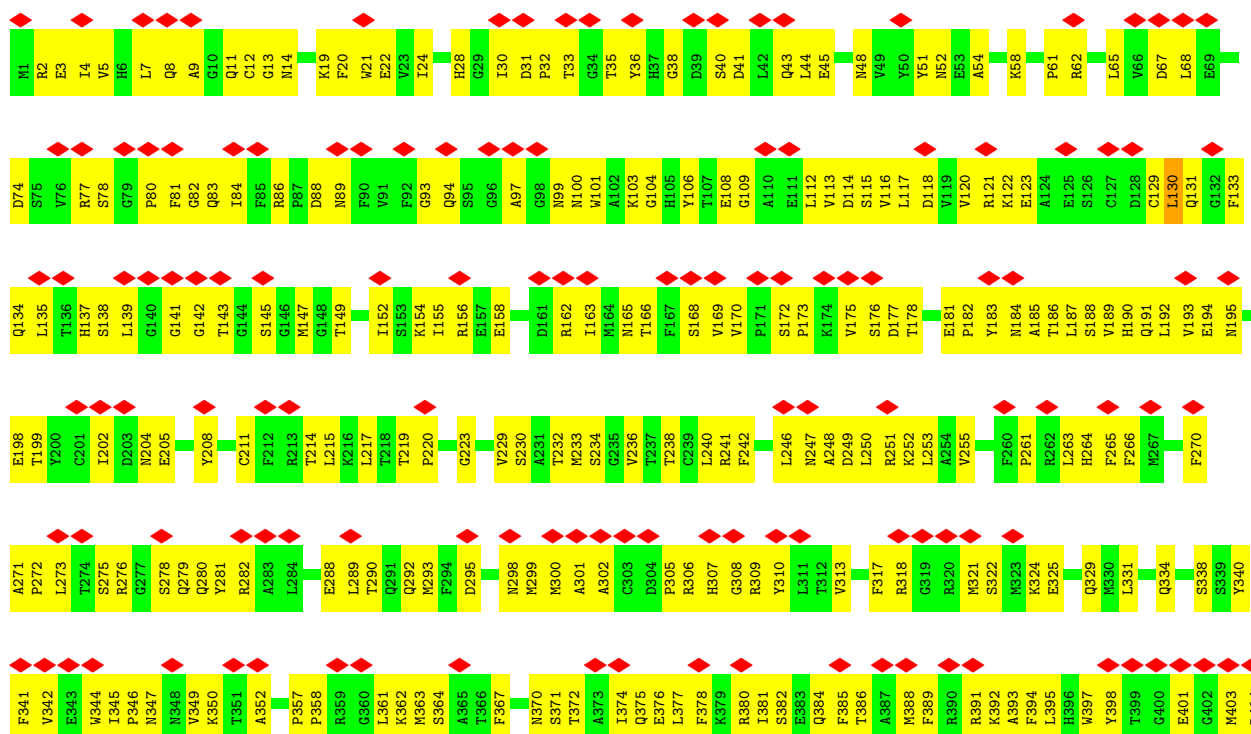


• Molecule 3: Tubulin beta-4B chain

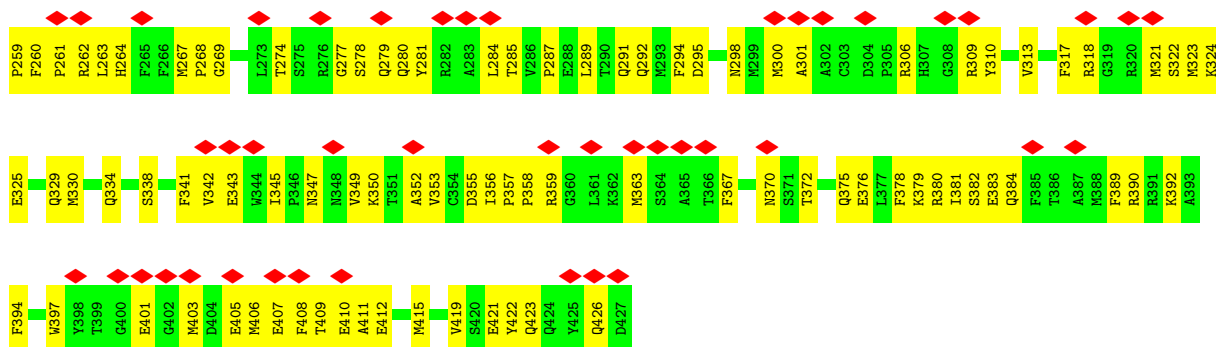




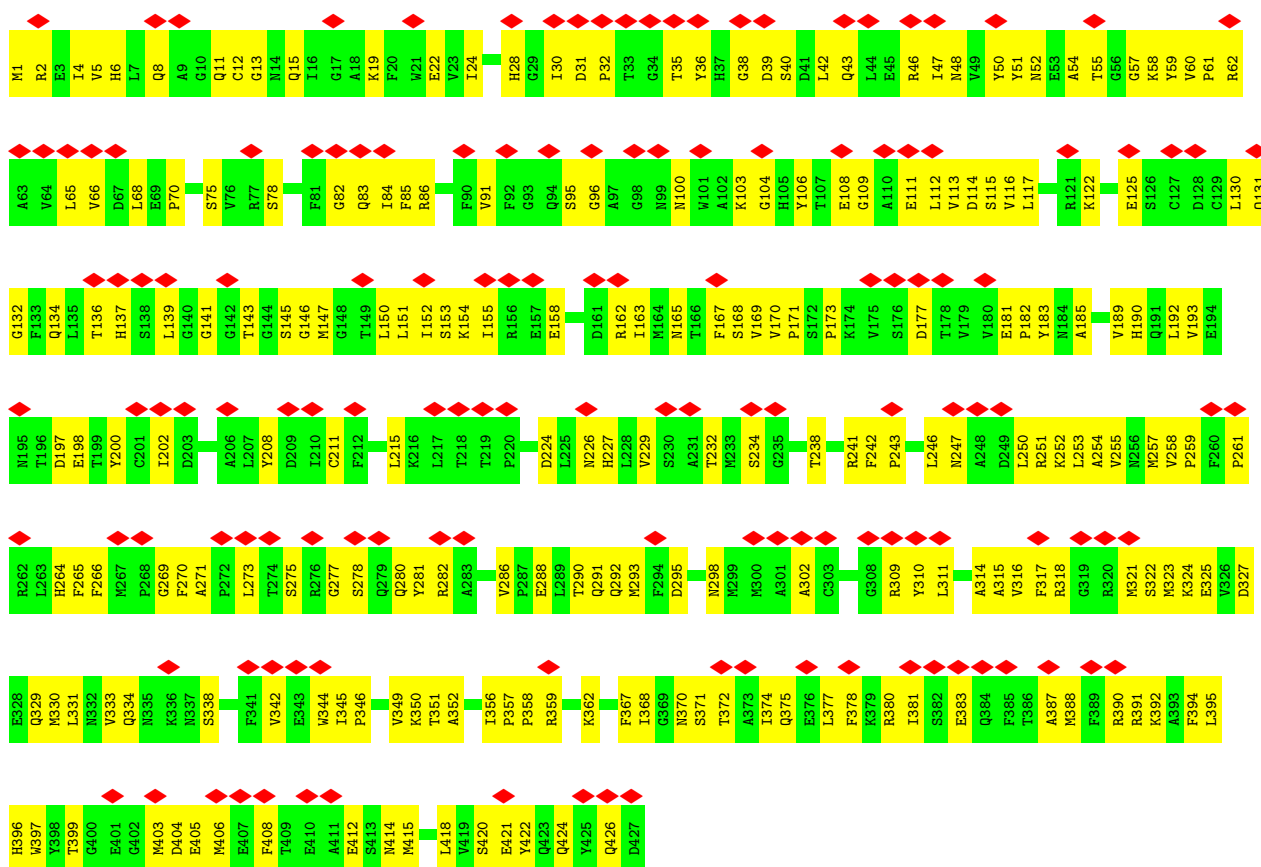
• Molecule 3: Tubulin beta-4B chain



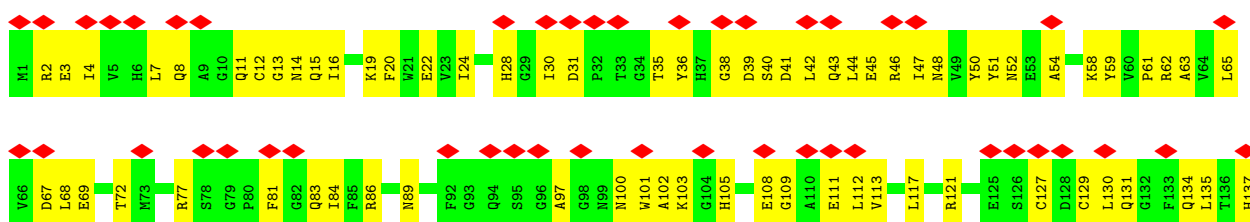


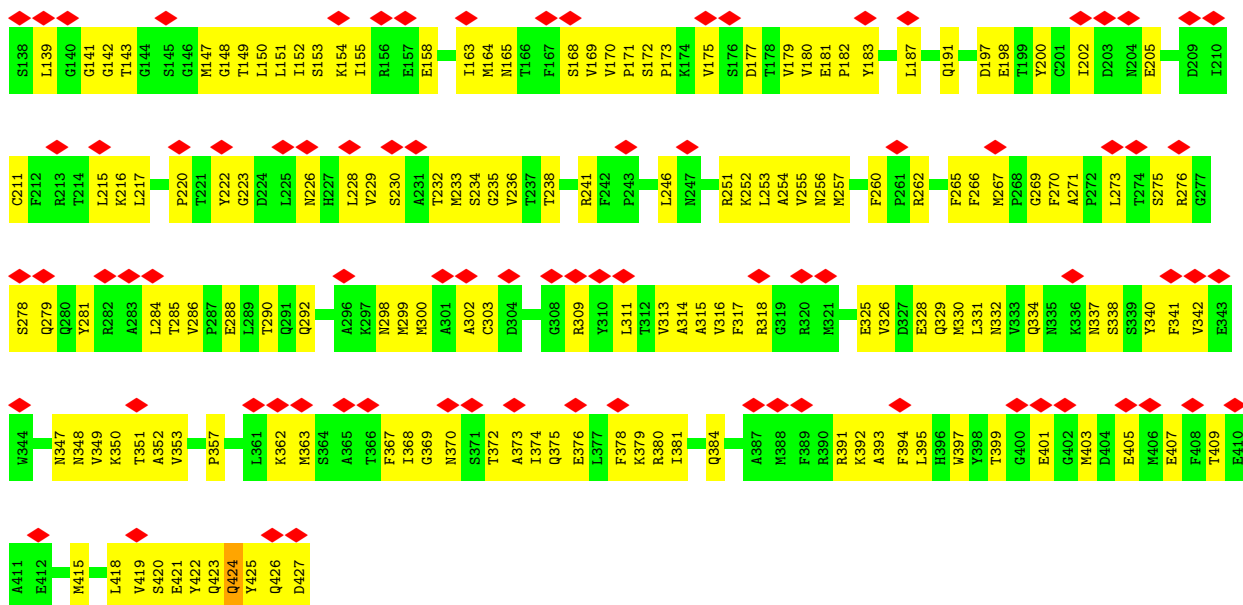


• Molecule 3: Tubulin beta-4B chain

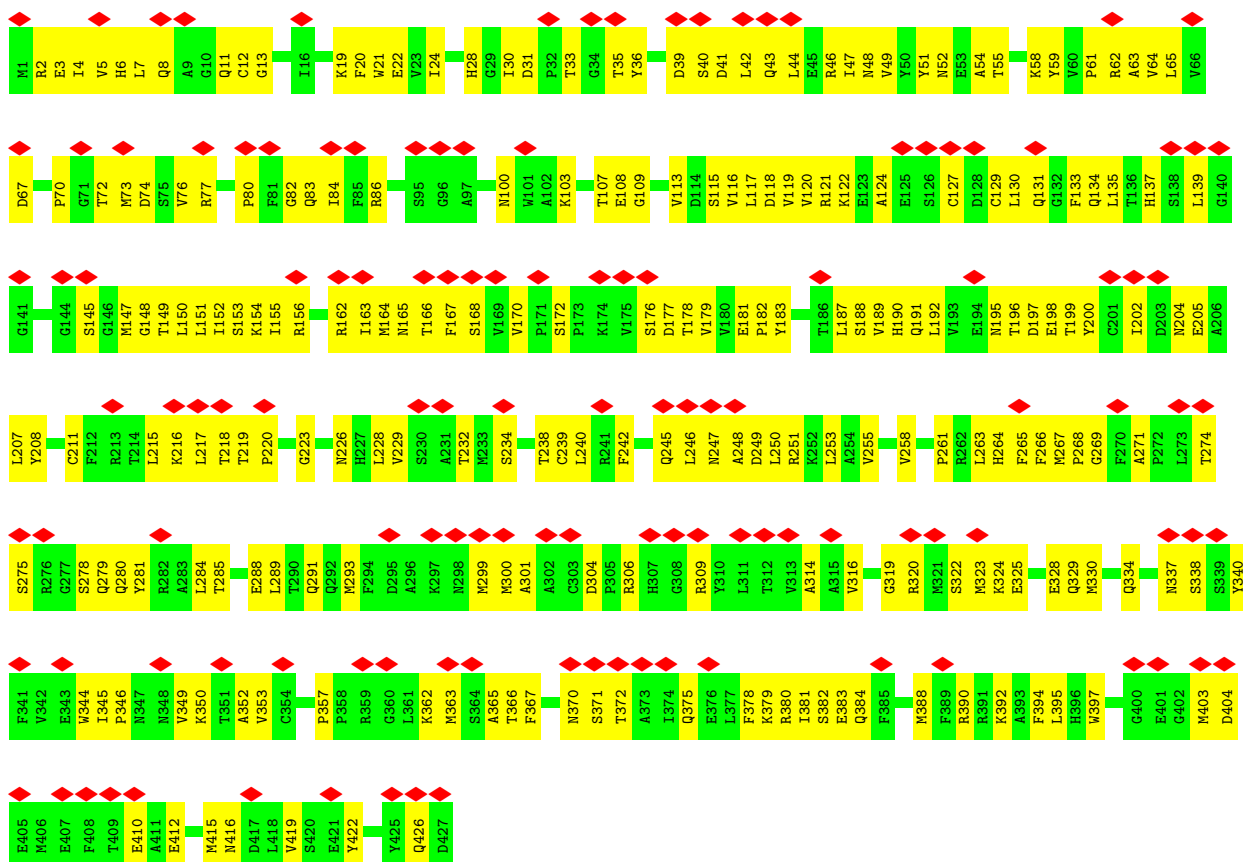


• Molecule 3: Tubulin beta-4B chain

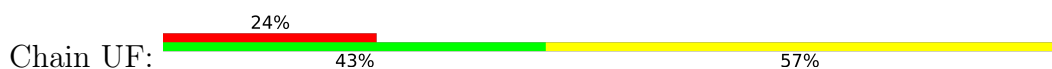


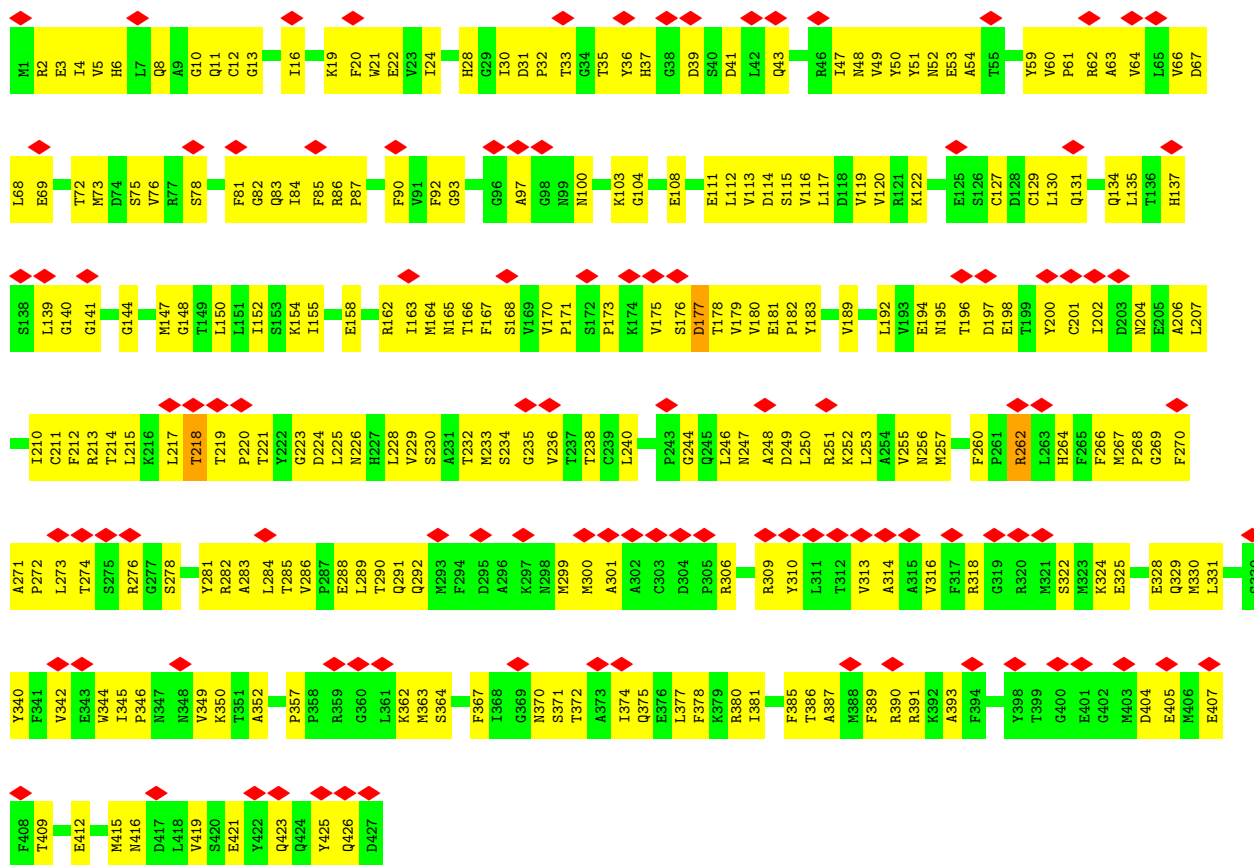


• Molecule 3: Tubulin beta-4B chain

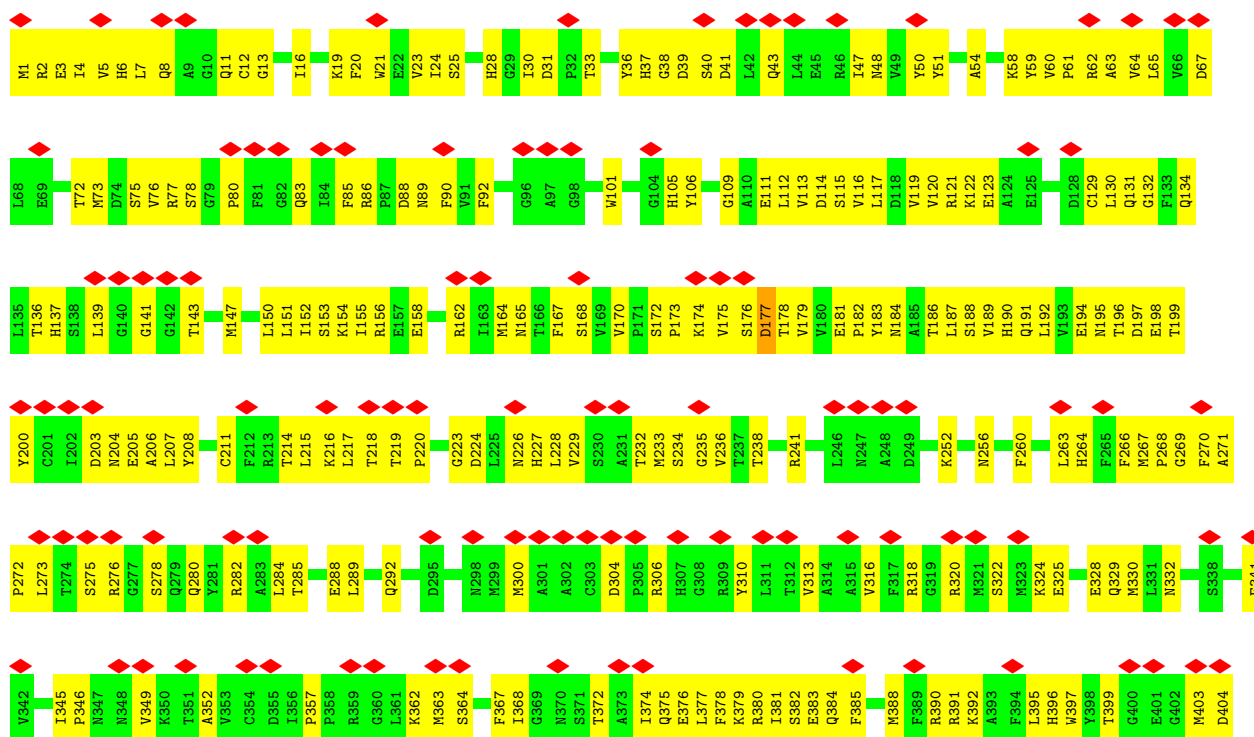


• Molecule 3: Tubulin beta-4B chain



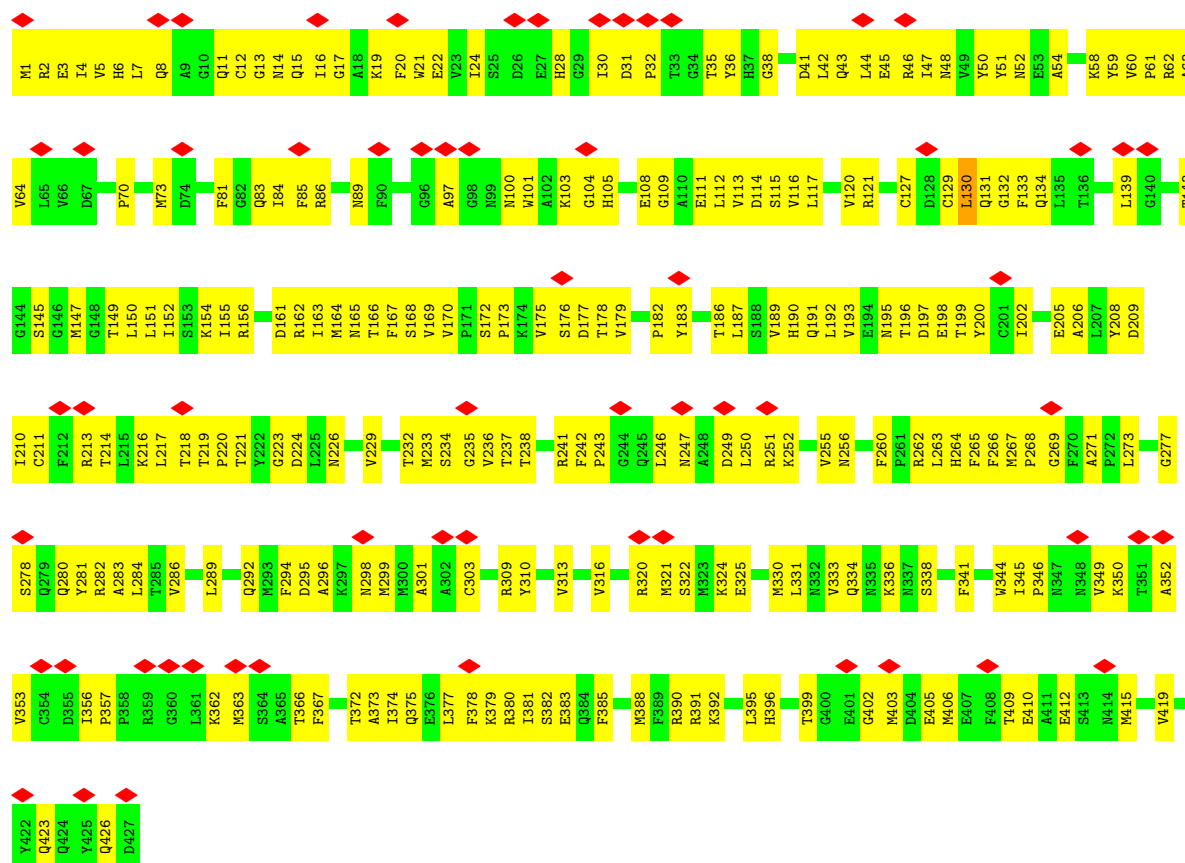
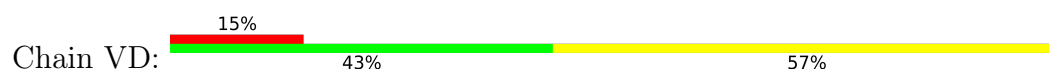


• Molecule 3: Tubulin beta-4B chain

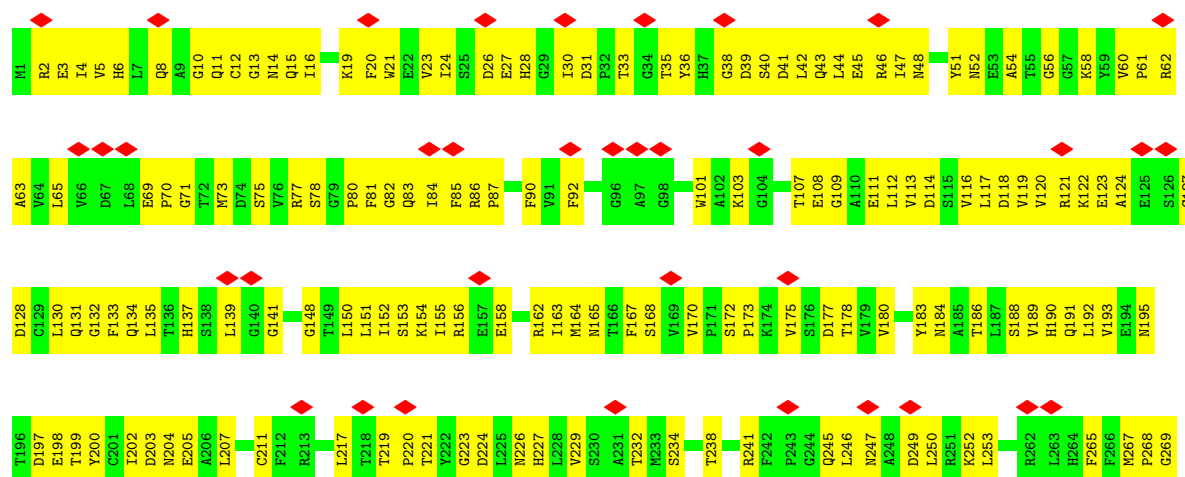


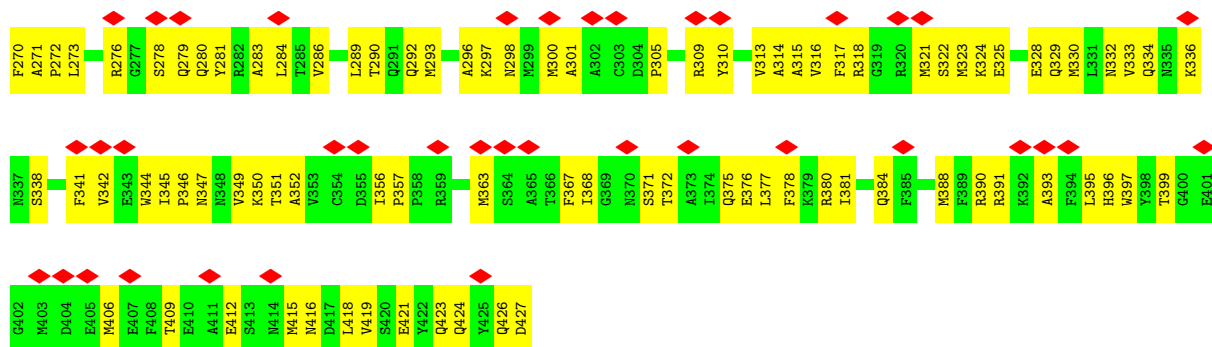


• Molecule 3: Tubulin beta-4B chain

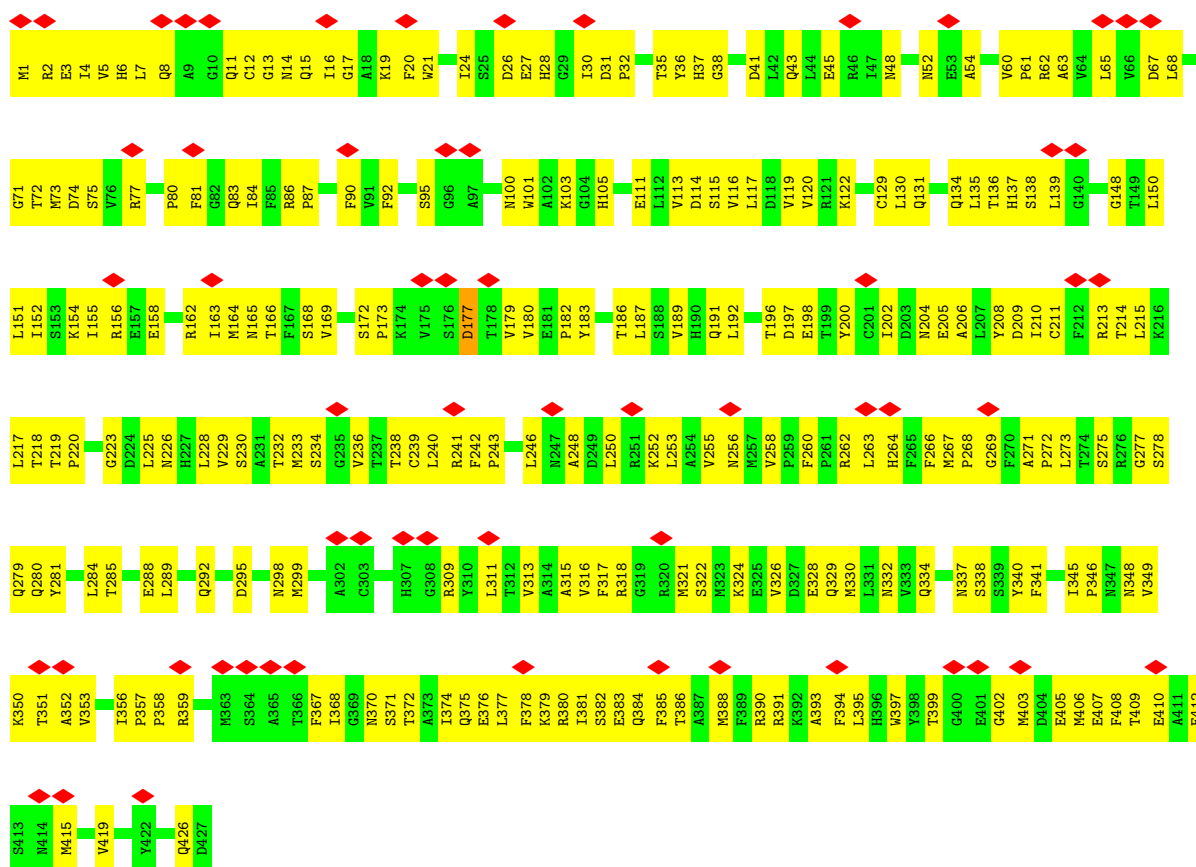
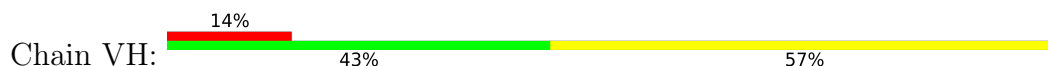


• Molecule 3: Tubulin beta-4B chain

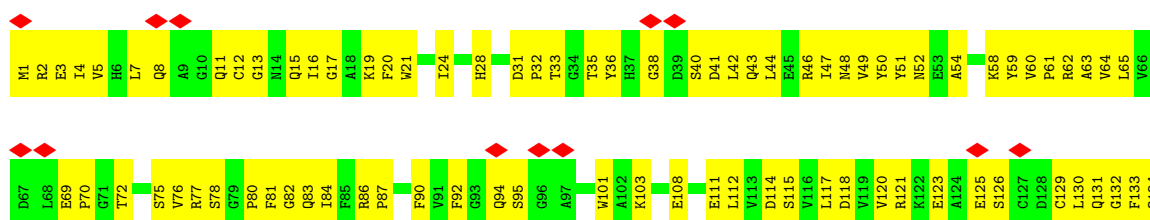
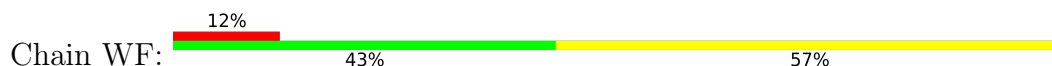


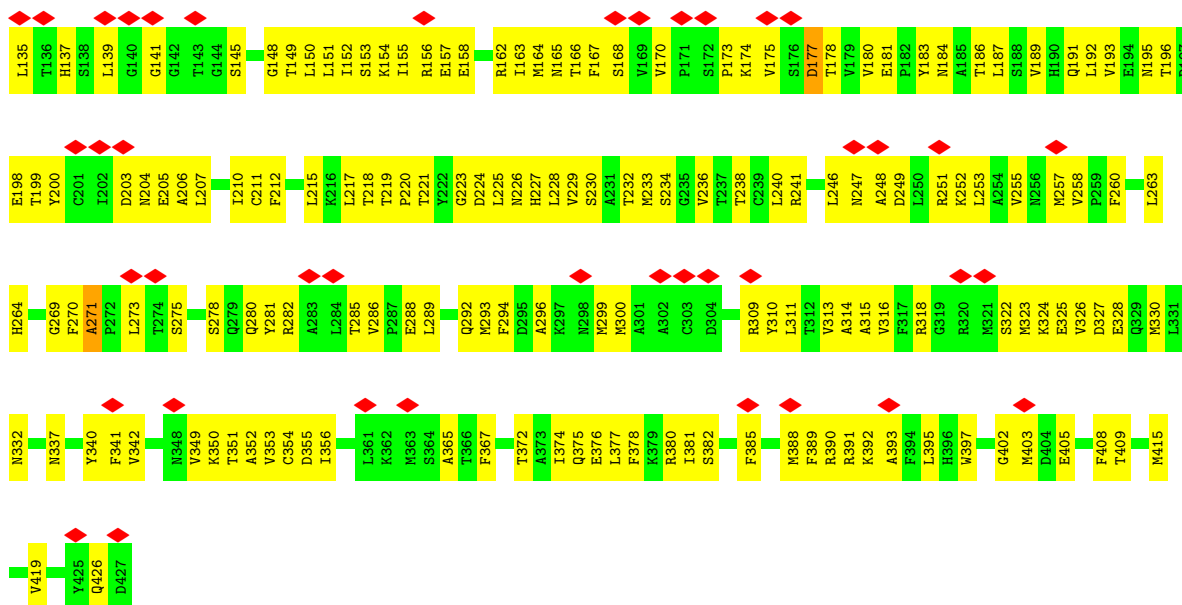


• Molecule 3: Tubulin beta-4B chain

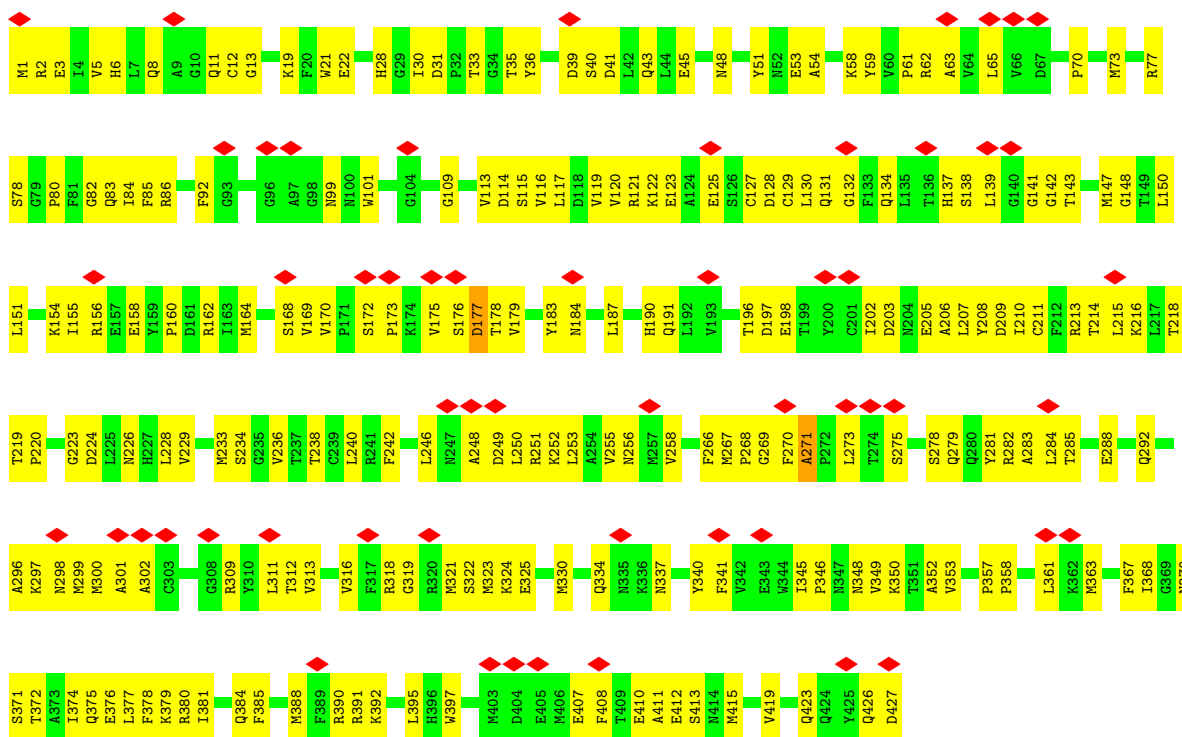


• Molecule 3: Tubulin beta-4B chain





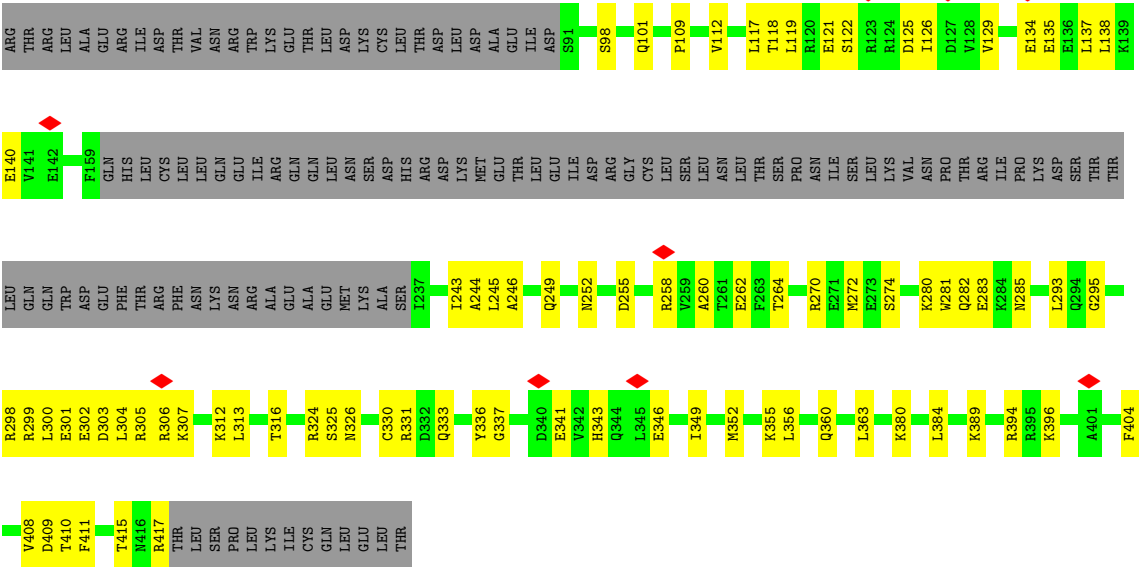
• Molecule 3: Tubulin beta-4B chain



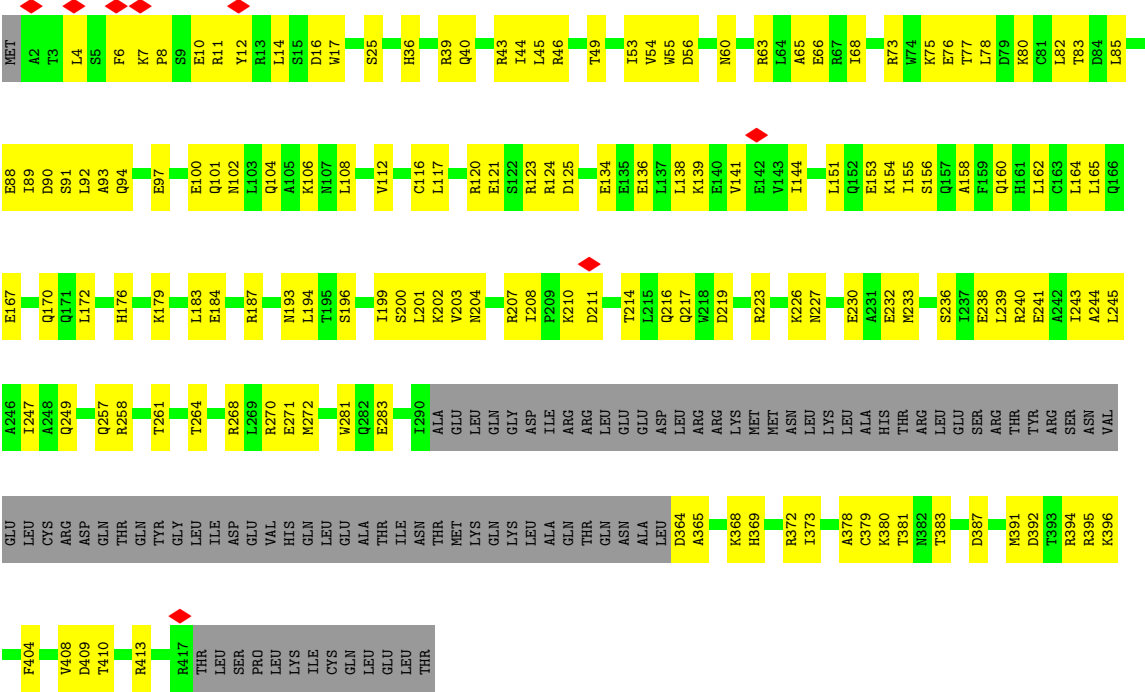
• Molecule 4: Tektin-2



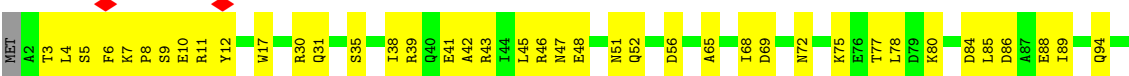
MET	ALA	THR	LEU	SER	PHE	LYS	PRO	SER	GLU	ARG	TYR	ARG	LEU	SER	ASP	TRP	ARG	THR	ASN	SER	LEU	LEU	SER	THR	ASN	ALA	GLU	ARG	GLN	ILE	ARG	GLN	GLU	ALA	ARG	ILE	LEU	ARG	ASN	GLU	THR	ASN	ASN	GLN	ILE	VAL	TRP	ASP	GLU	HIS	ASP	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----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

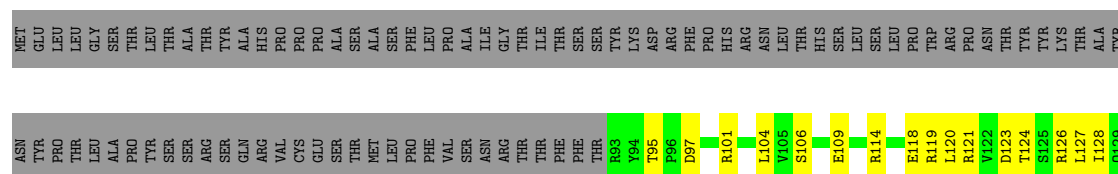


• Molecule 4: Tektin-2



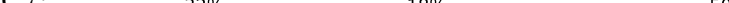
• Molecule 4: Tektin-2

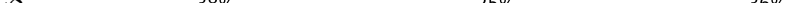




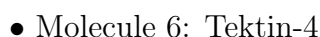
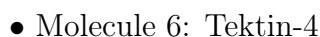


[illegible]

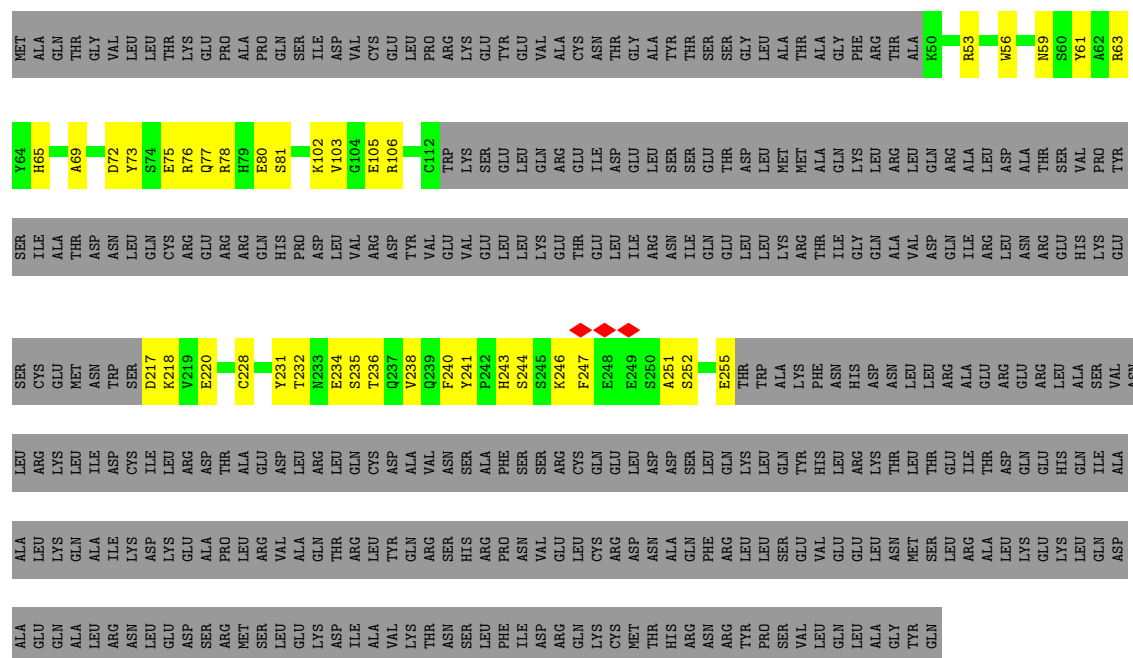
Chain C7: 

Chain C8: 

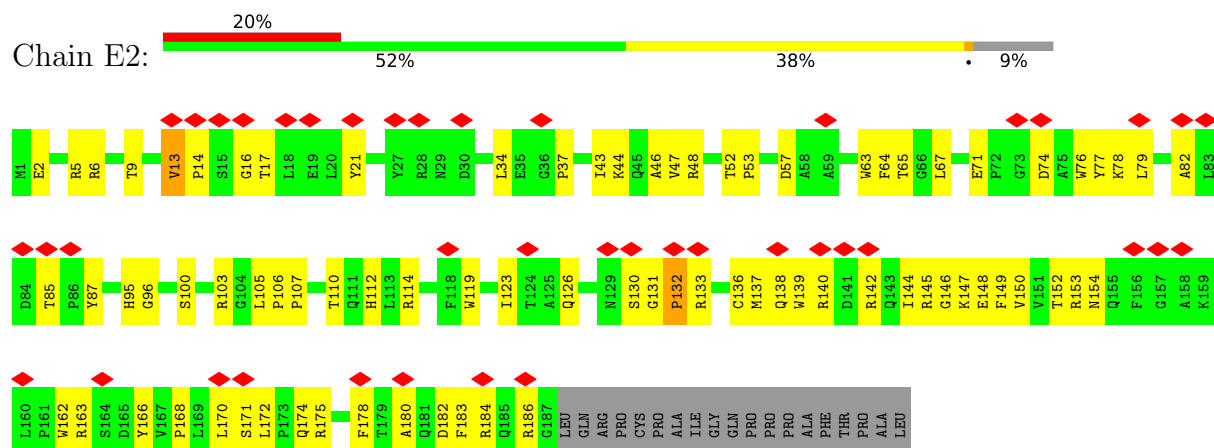




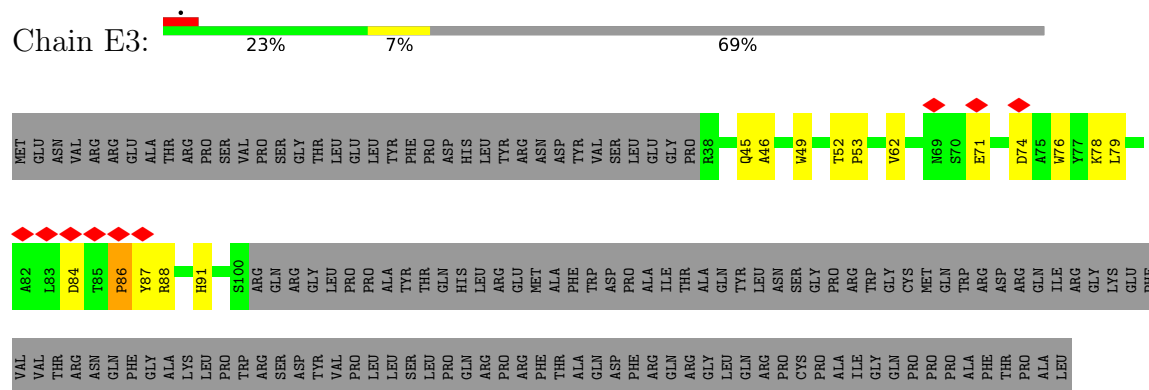




• Molecule 7: Tektin bundle-interacting protein 1



• Molecule 7: Tektin bundle-interacting protein 1



• Molecule 8: Tektin-5



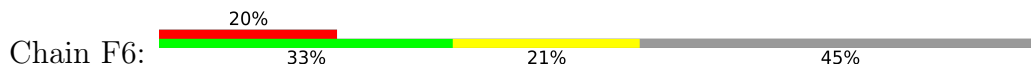
MET	THR	LEU	E199	PHE	T374	T440	CYS
GLU	SER	ARG	K200	PHE	I375	L441	LYS
PHE	GLN	ILE	R201	HIS	M376	L442	GLY
THR	THR	MET	I204	GLY	L377	L443	PRO
GLY	ILE	GLN	I205	VAL	L378	L444	ALA
THR	PRO	ASP	I206	GLU	E379	W445	SER
GLN	GLU	LYS	D207	LYS	R380	M446	CYS
THR	GLU	ASP	H208	F286	A381	T447	GLY
ALA	CYS	GLN	D209	D287	I382	K448	GLY
SER	SER	LEU	N210	G288	V383	S449	GLY
ALA	GLY	ILE	N211		A384	R450	ALA
PHE	ILE	HIS	V211		K385	L451	SER
CYS	ARG	GLN	E212		A386	E452	CYS
GLY	ARG	MET	K213		Y387	H453	GLY
PRO	PRO	GLN	N214		P388	E454	GLY
LYS	THR	GLY	E218		L389	A456	ALA
LYS	ILE	THR	L222		Q393	I457	SER
CYS	LEU	SER	K223		T394	M470	CYS
GLY	PRO	ARG	C224		M395	S471	GLY
LEU	LEU	ILE	C225		L396	M472	ALA
GLN	ARG	G143	Q226		R399	R473	ALA
ALA	SER		D227		R402	P477	PRO
LEU	ALA	L146	R230		P403	THR	GLY
PRO	LEU	F151	K231		M404	PRO	SER
PRO	PHE	W152	L232		V405	THR	ALA
ALA	CYS	K153	A233		E406	GLY	ALA
GLY	ARG	S154	K234		L407	THR	CYS
GLN	TYR	E155	R235		C408	GLY	SER
GLU	THR	L156	L236		R409	TYR	HIS
PRO	PRO	E159	R244		D410	THR	VAL
VAL	ARG	D161	Q247		V411	CYS	SER
GLN	ASP	R162	H248		A412	ALA	ARG
TYR	ARG	L163	S249		Q413	GLY	SER
CYS	SER		L250		P414	ILE	GLY
GLN	ASN	E166	E251		R415	PRO	PRO
PRO	ASP	N167	D252		L416	GLY	ALA
HIS	LEU		I253		E419	TYR	VAL
GLN	ILE	M170	I254		T422	ALA	CYS
PRO	GLY	K174	S258		I423	ASN	VAL
TYR	ARG	R175	Y262		D424	HIS	THR
ARG	ALA	E178	I263		D425	ALA	ALA
ASN	ALA	C179	I266		T426	PRO	GLY
ALA	ARG	A180			L427	ILE	ALA
TRP	LEU	V184	L270		Q428	SER	SER
TRP	TRP	L188	ARG		T429	GLY	GLY
PRO	SER	E193	THR		L430	PRO	CYS
SER	ARG	Y196	SER		R431	VAL	THR
VAL	THR	N197	ASP		L432	PHE	HIS
PHE	THR	I198	ILE		R433	GLY	LYS
HIS	GLY		SER		R435	SER	ILE
LYS	ASP		THR		E436	ALA	ALA
ALA	SER		SER		T437	LEU	LEU
					Q438		
					D439		

• Molecule 8: Tektin-5



MET	THR	GLU	Q129	THR	T374	T440	CYS
GLU	SER	LYS	L130	SER	I375	L441	LYS
PHE	GLN	M214	I131	PHE	M376	L442	GLY
LEU	THR	E218	H132	GLY	L377	L443	PRO
THR	ILE	V219	Q133	VAL	L378	L444	ALA
THR	PRO	D220	M134	GLU	E379	W445	SER
GLN	GLU	Q135	Q135	LYS	R380	M446	CYS
THR	GLU	E136	E136	F286	A381	T447	GLY
ALA	CYS	T138	T138	D287	I382	K448	GLY
THR	SER	Q144	Q144	G288	V383	S449	GLY
ALA	ILE	R145	R145	T289	A384	R450	ALA
LYS	ARG	L146	L146	V290	K385	L451	SER
ILE	ARG	S147	S147	E291	A386	E452	CYS
LEU	PRO	R230	R230	T295	Y387	H453	GLY
LEU	PRO	K231	K231	W296	P388	E454	GLY
GLN	THR	L232	L232	A297	L389	A456	ALA
ASN	ILE	A233	A233	F299	Q393	I457	SER
THR	LEU	T236	T236	N301	T394	M470	CYS
ILE	PRO	D237	D237	T304	M395	S471	GLY
MET	SER	F238	F238	Q308	L396	M472	ALA
LEU	LEU	Q239	Q239	R311	R399	R473	ALA
LEU	SER	D242	D242	ALA	R402	P477	PRO
GLU	ARG	R244	R244	ALA	P403	THR	GLY
ALA	ILE	M170	M170	ALA	M404	PRO	SER
VAL	VAL	K174	K174	ALA	V405	THR	ALA
LYS	LYS	R175	R175	ALA	E406	GLY	ALA
GLU	GLY	E178	E178	ALA	L407	THR	CYS
TYR	TYR	C179	C179	ALA	C408	GLY	SER
PRO	LYS	A180	A180	ALA	R409	TYR	HIS
LEU	ALA	E181	E181	ALA	D410	THR	VAL
GLN	GLY	E182	E182	ALA	V411	CYS	SER
THR	PRO	Q189	Q189	ALA	A412	GLY	SER
MET	HIS	L192	L192	ALA	Q413	ILE	GLY
LEU	LEU	GLU	GLU	ALA	P414	PRO	PRO
ALA	CYS	TYR	TYR	ALA	R415	GLY	ALA
ARG	ARG	ASN	ASN	ALA	L416	TYR	VAL
THR	ASN	LEU	LEU	ALA	E419	ALA	CYS
ARG	ASN	ARG	ARG	ALA	T422	ASN	VAL
PRO	ALA	GLY	GLY	ALA	I423	HIS	THR
VAL	ASN	LYS	LYS	ALA	D424	ALA	ALA
GLU	ASN	ILE	ILE	ALA	D425	PRO	GLY
LEU	ALA	S272	S272	ALA	T426	ILE	ALA
ARG	ARG	T273	T273	ALA	Q428	SER	SER
CYS	ILE	S274	S274	ALA	T429	GLY	GLY
ASP	SER	D275	D275	ALA	L430	PRO	CYS
GLU	GLU	S276	S276	ALA	R431	VAL	THR
VAL	VAL	I277	I277	ALA	L432	PHE	HIS
PRO	PRO	S278	S278	ALA	R433	GLY	LYS
GLN	THR	F279	F279	ALA	R435	SER	ILE
PHE	VAL	V283	V283	ALA	E436	ALA	ALA
ARG	ASN	E284	E284	ALA	T437	LEU	LEU

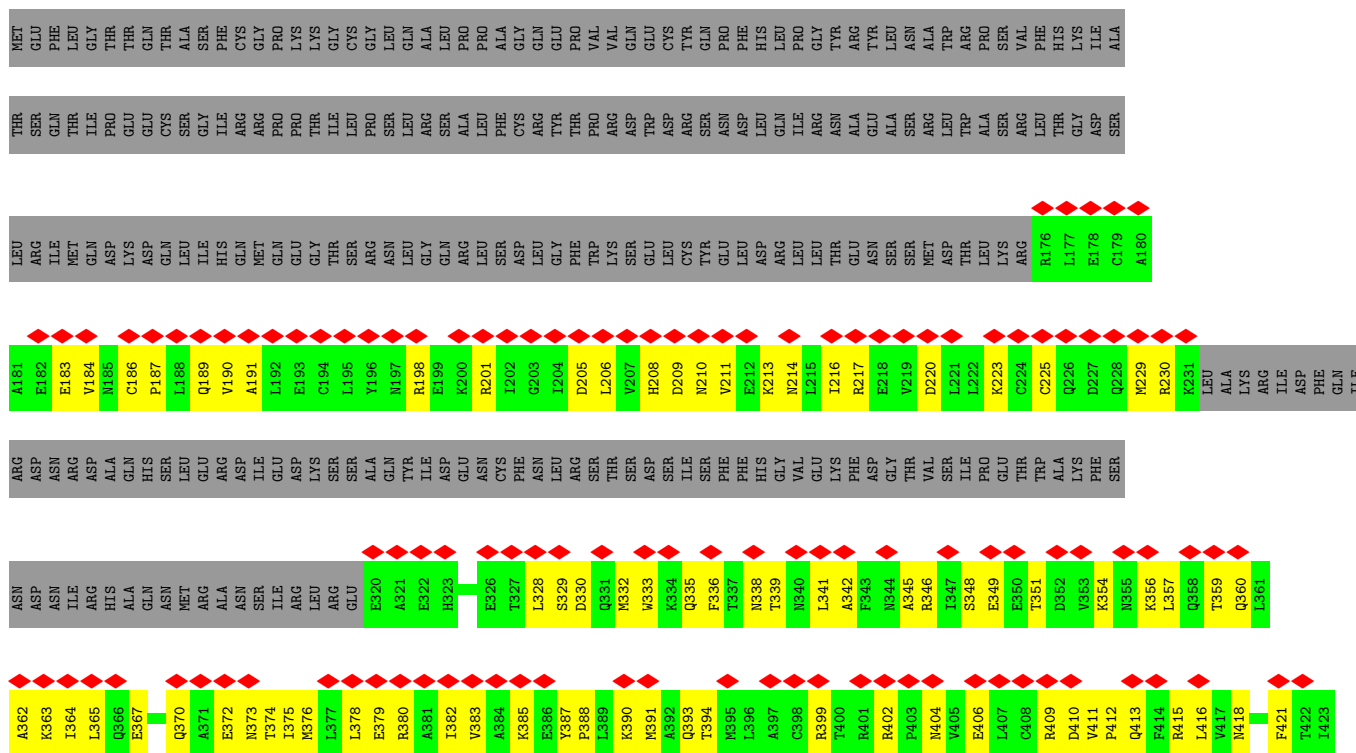
- Molecule 8: Tektin-5

[illegible]

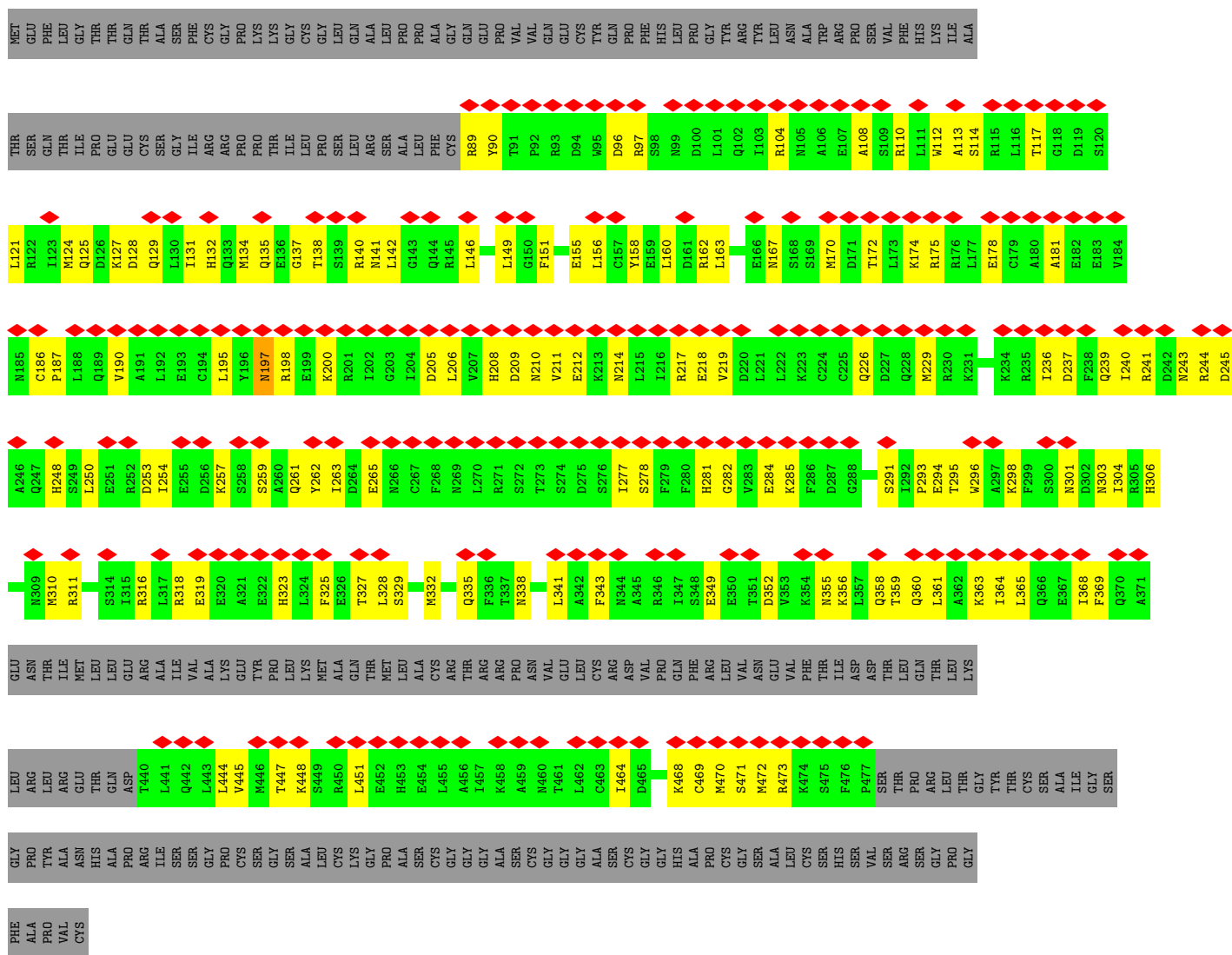
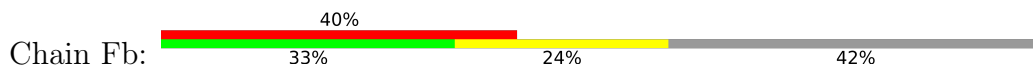
- Molecule 8: Tektin-5

[illegible]

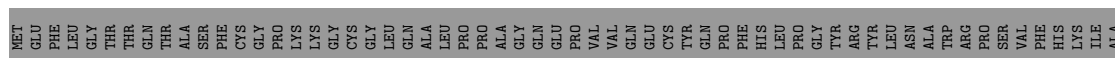
- Molecule 8: Tektin-5



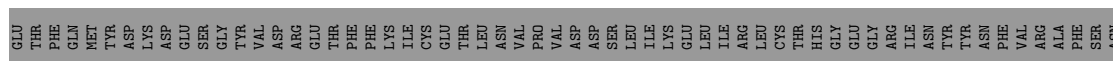
- Molecule 8: Tektin-5



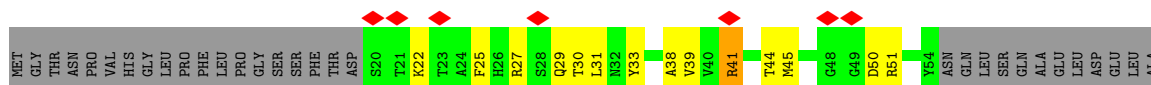
- Molecule 8: Tektin-5

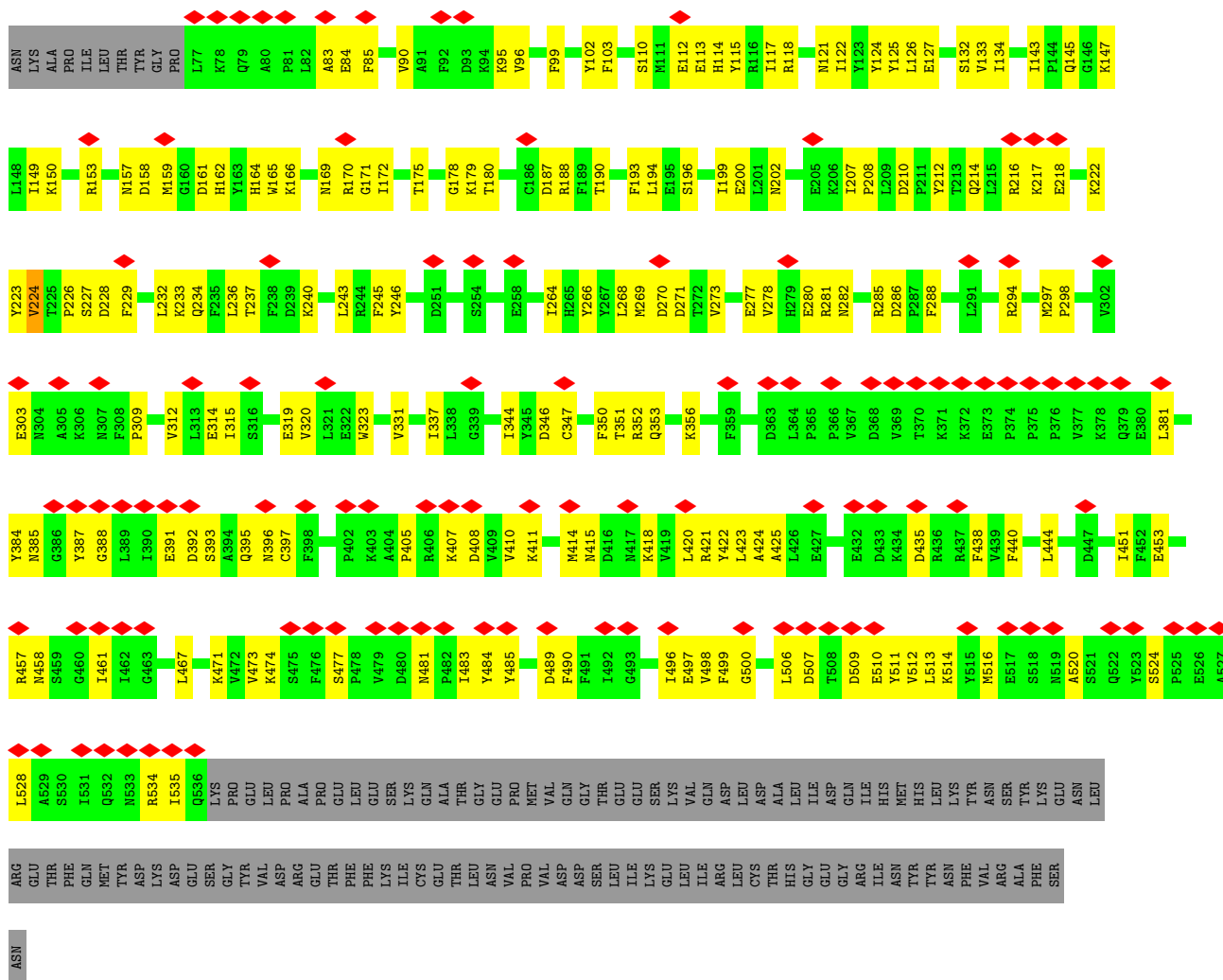


- Molecule 9: EF-hand domain-containing protein 1



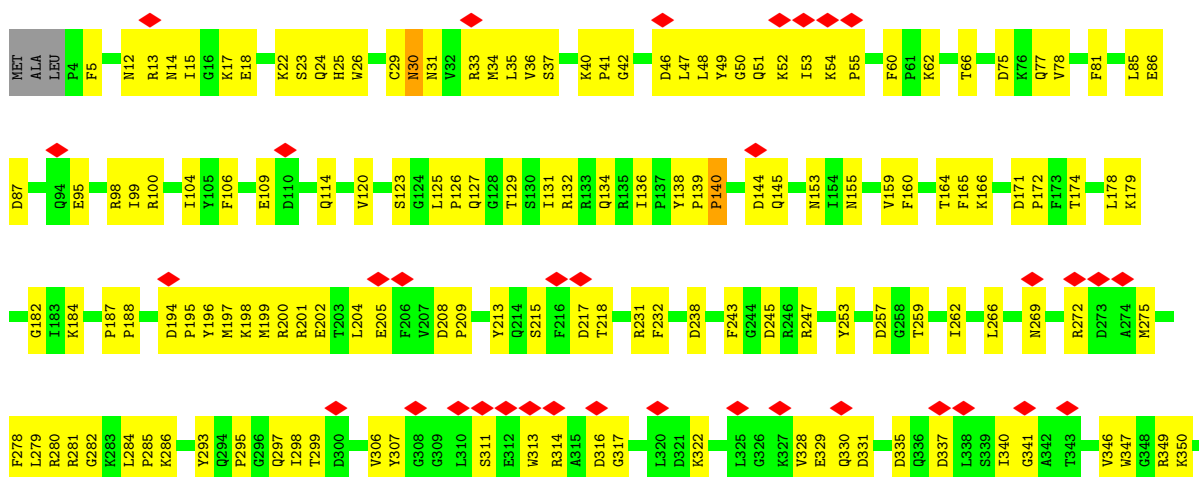
- Molecule 9: EF-hand domain-containing protein 1

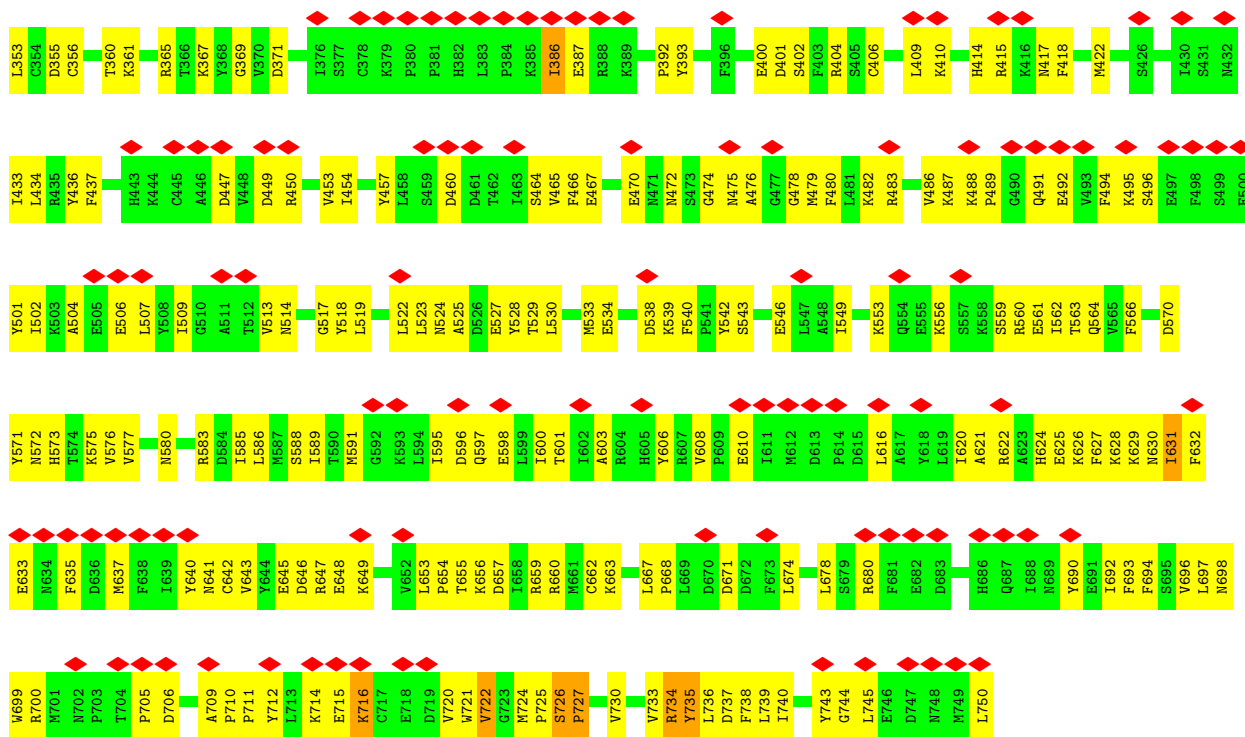




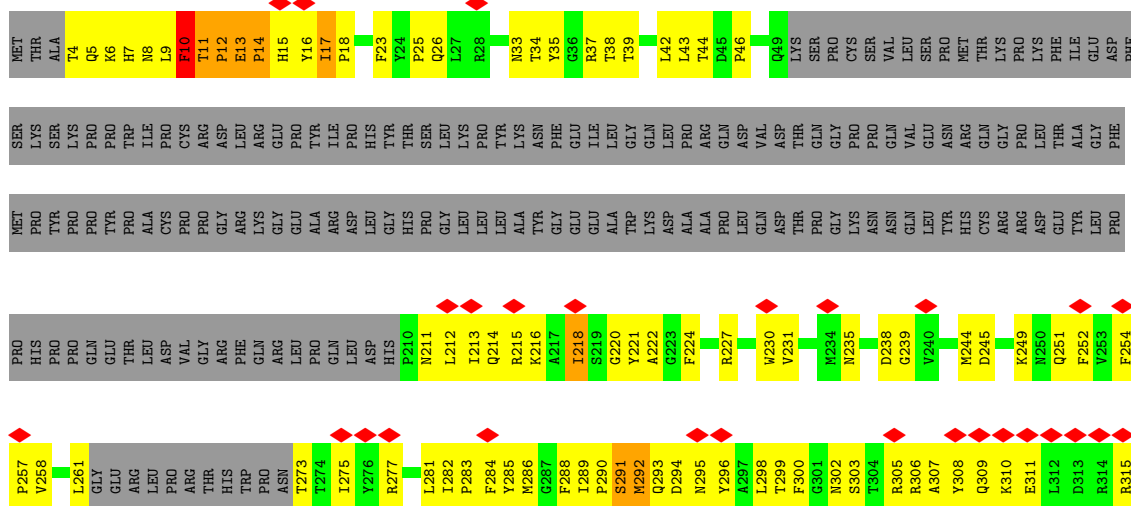
• Molecule 10: EF-hand domain-containing family member C2

Chain G5: 19% 54% 45%

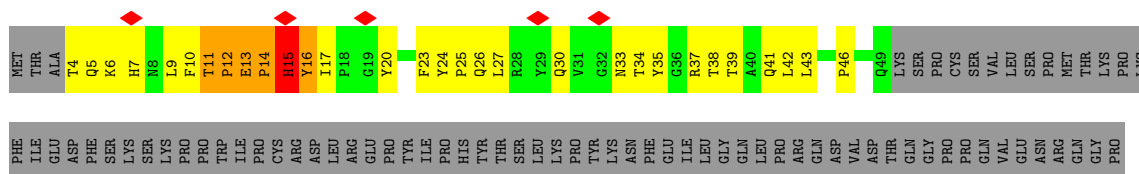


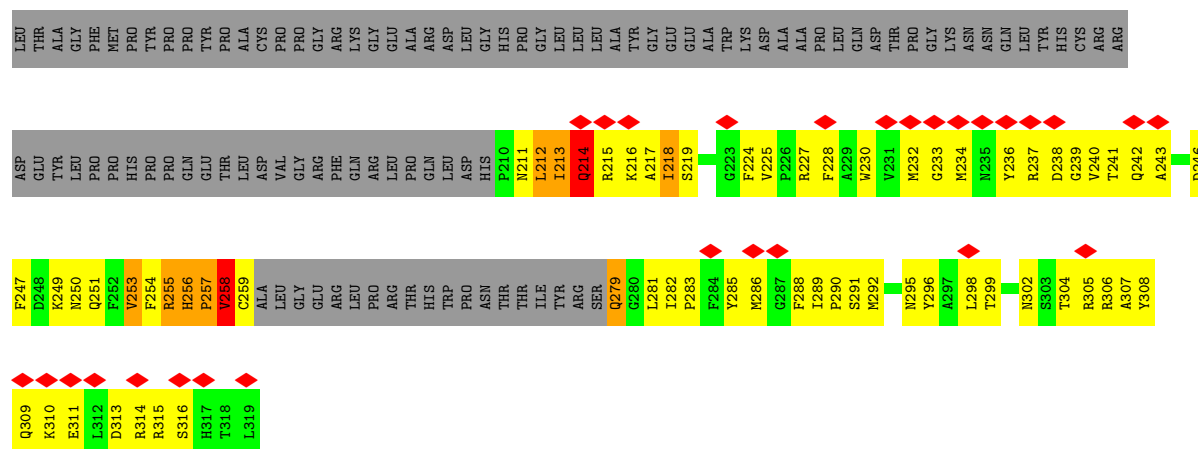


• Molecule 11: Protein FAM166A

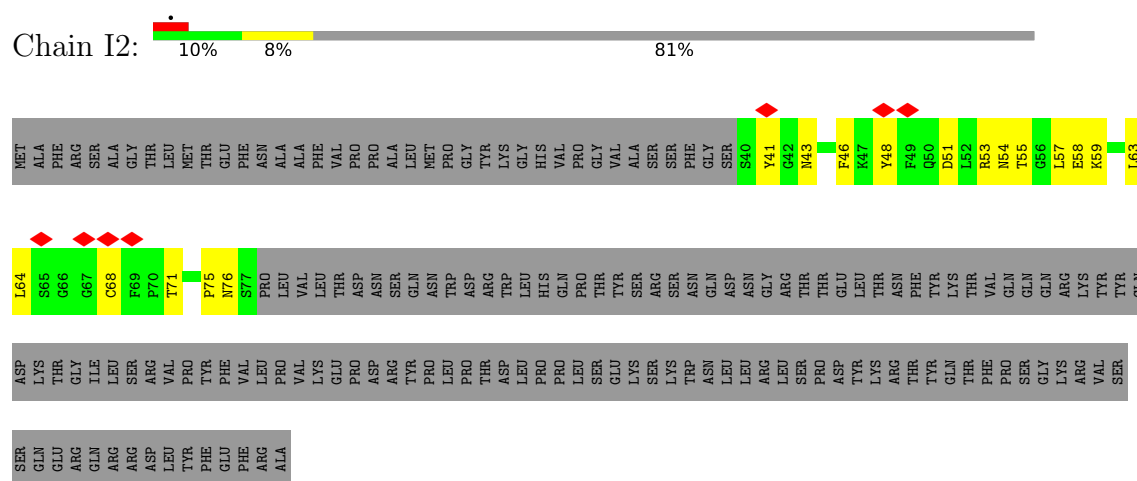


• Molecule 11: Protein FAM166A

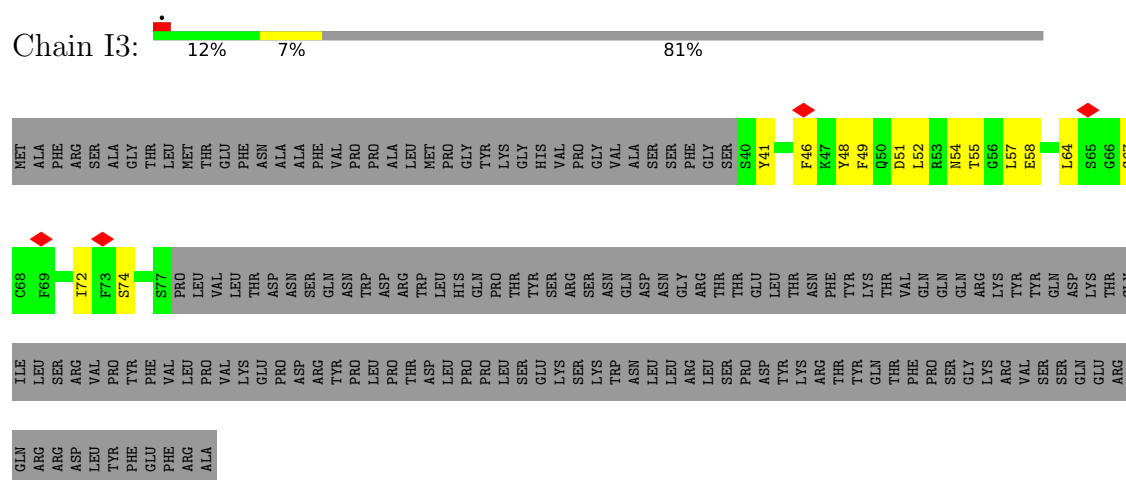




- Molecule 12: Protein FAM166C

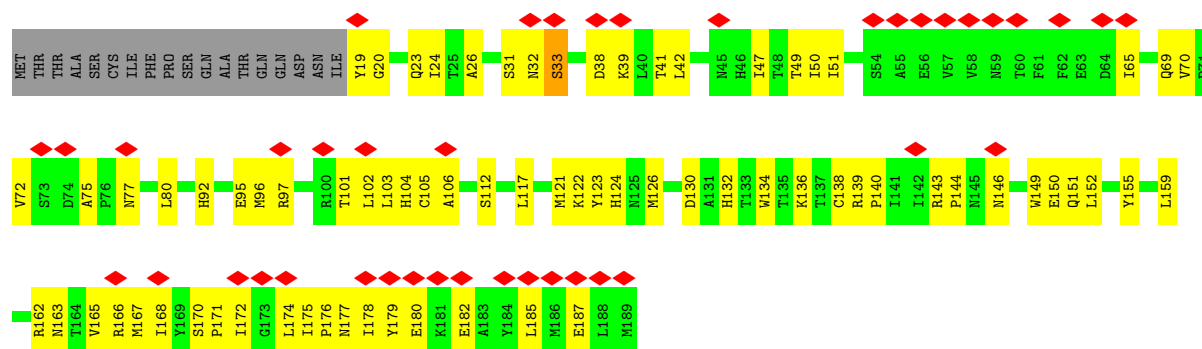


- Molecule 12: Protein FAM166C

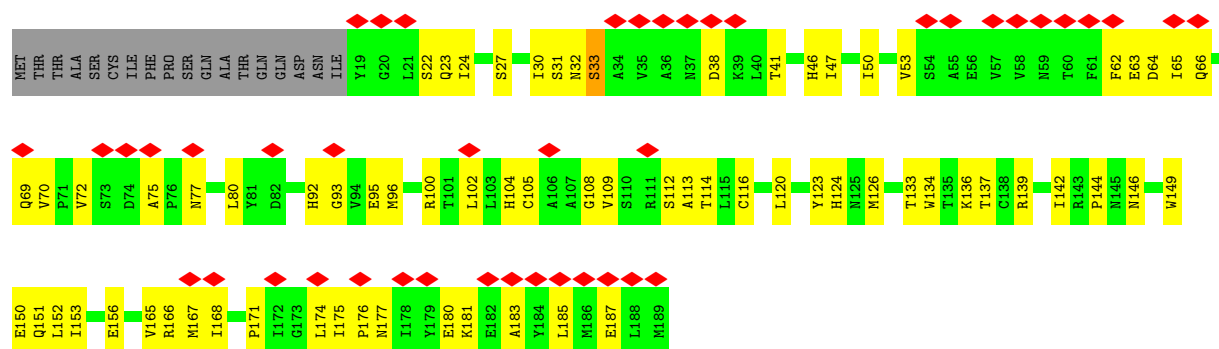


- Molecule 13: Dual specificity phosphatase 21

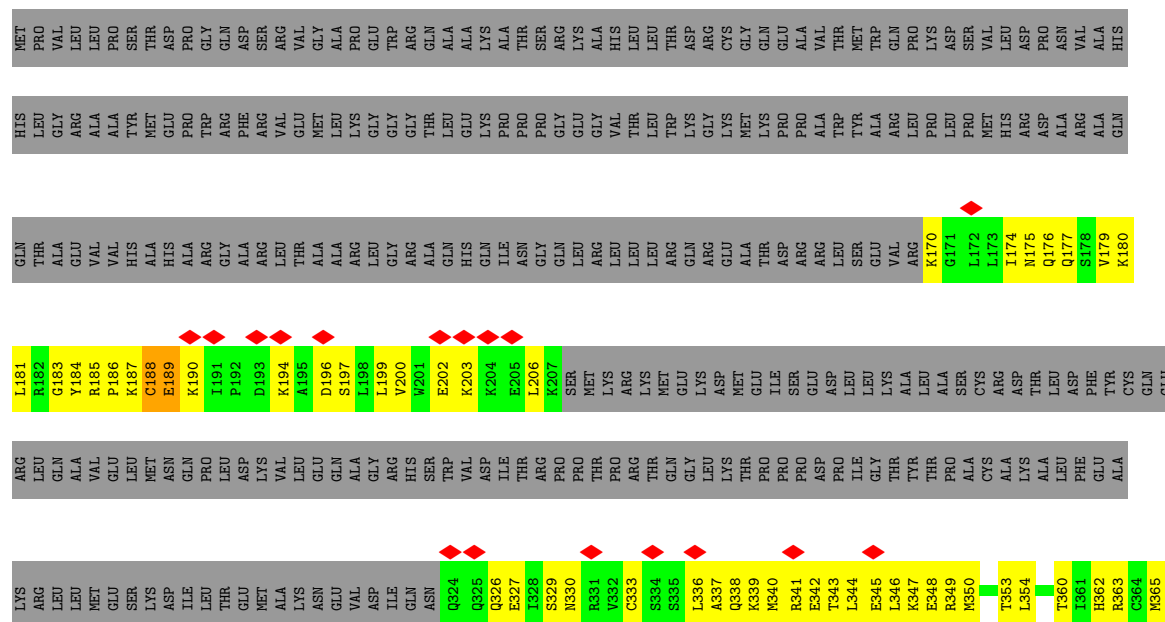


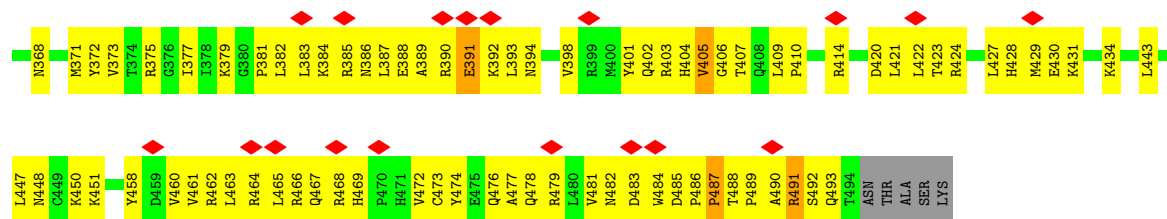


• Molecule 13: Dual specificity phosphatase 21

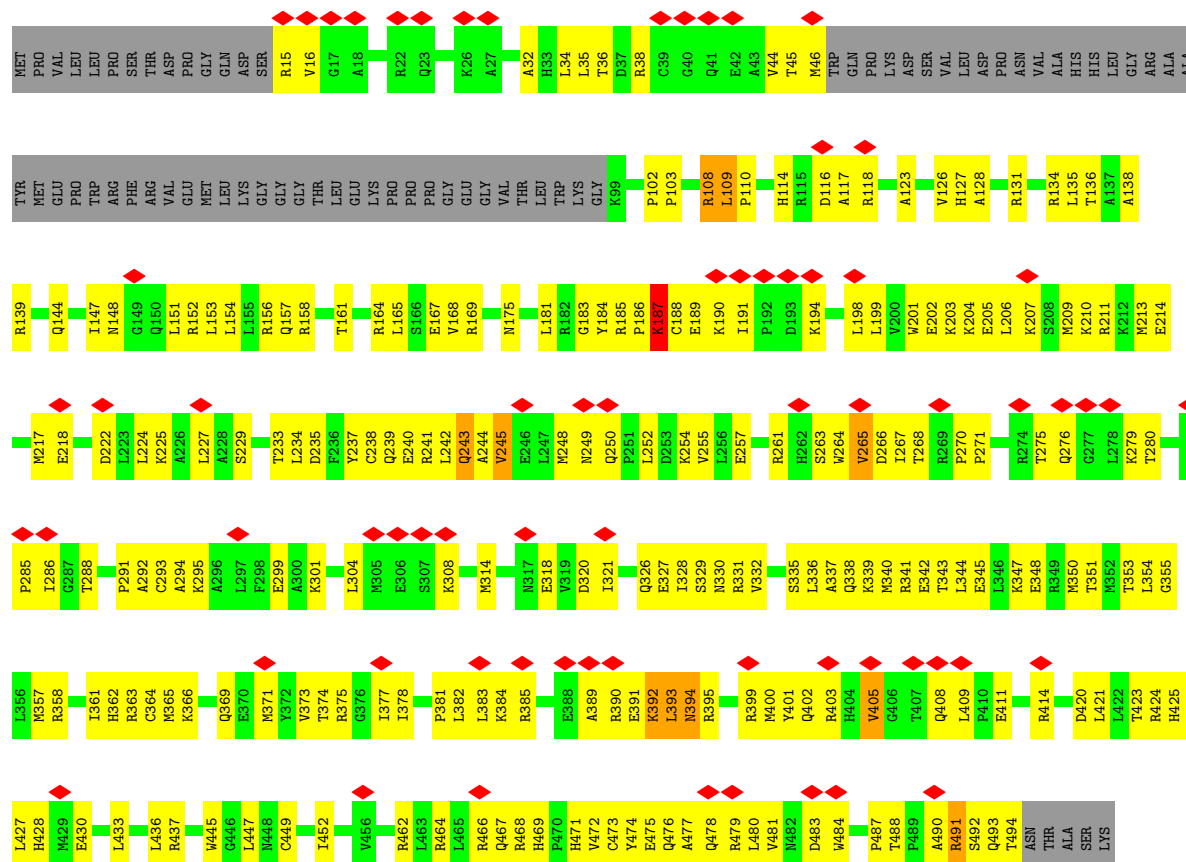


• Molecule 14: Coiled-coil domain-containing protein 105

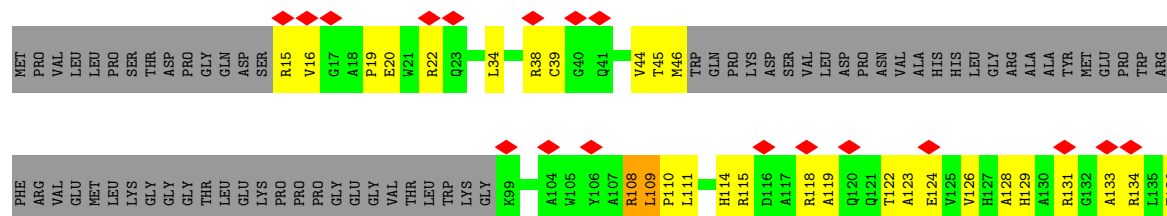


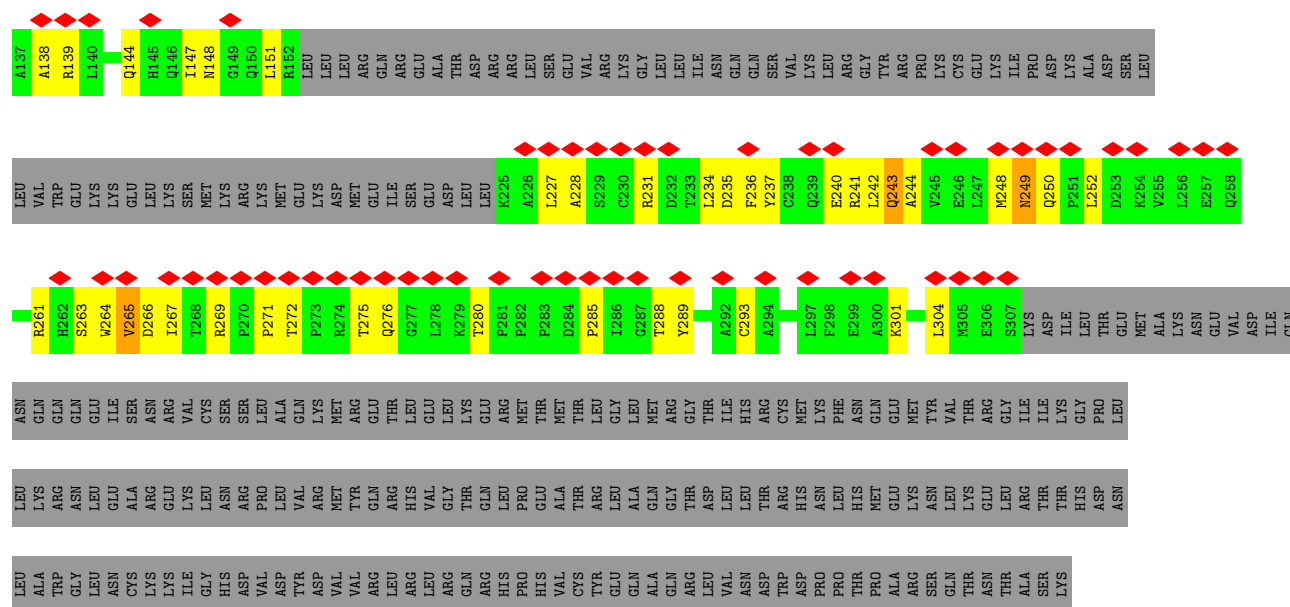


• Molecule 14: Coiled-coil domain-containing protein 105

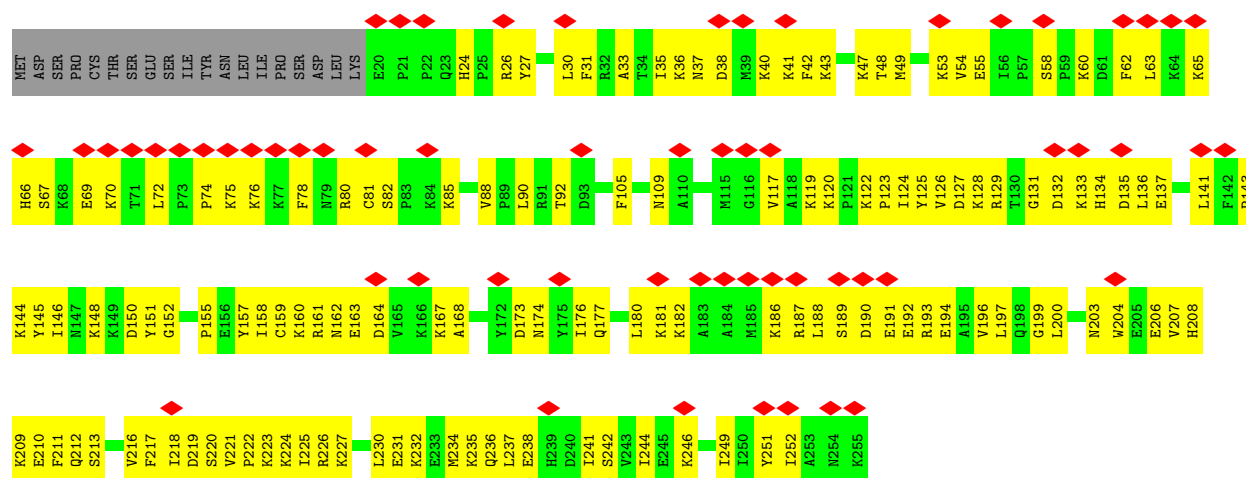


• Molecule 14: Coiled-coil domain-containing protein 105

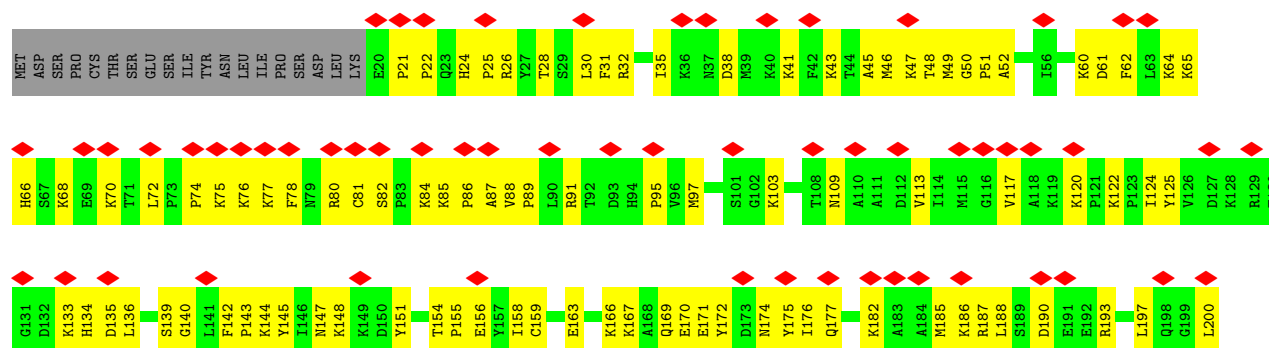


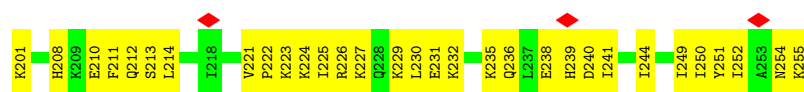


• Molecule 15: Enkurin

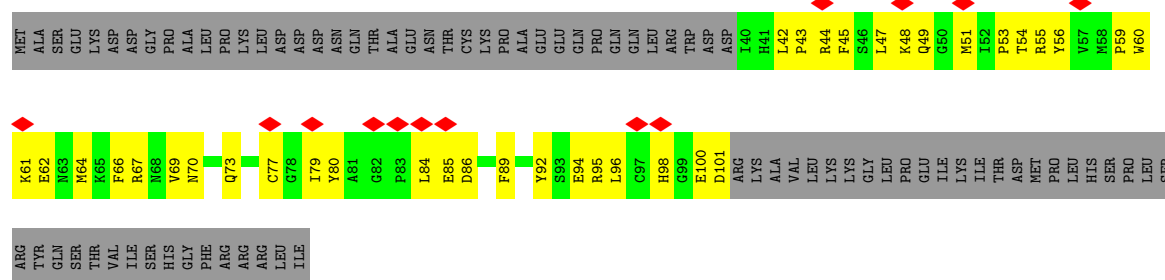


• Molecule 15: Enkurin

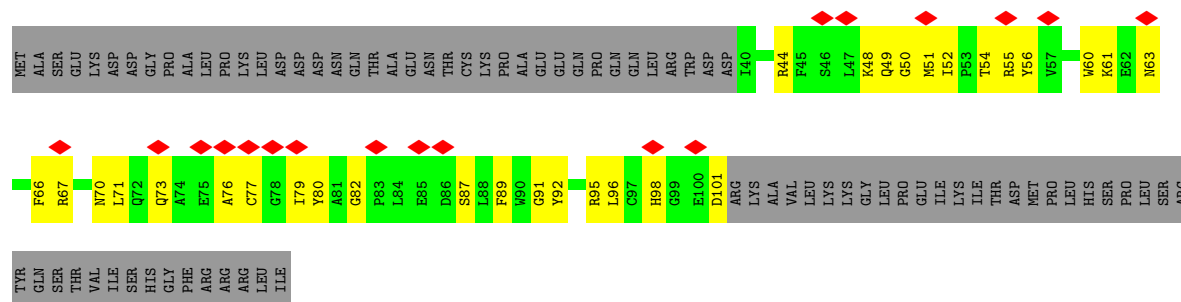




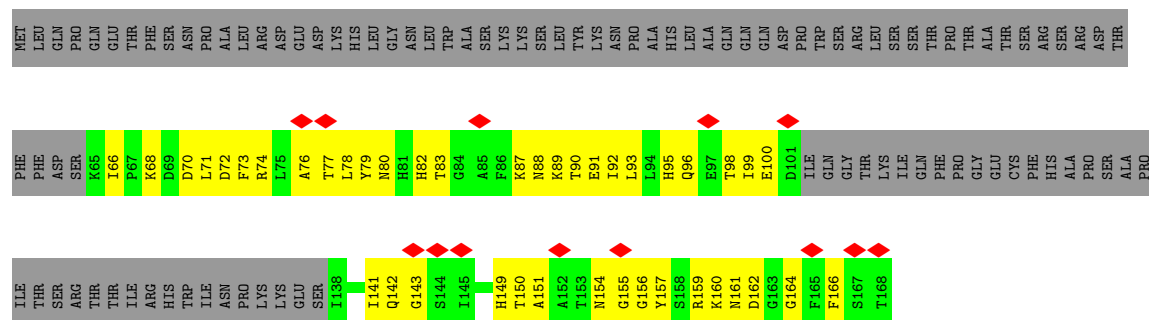
• Molecule 16: Testis-expressed protein 43



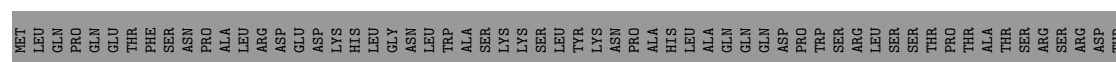
• Molecule 16: Testis-expressed protein 43

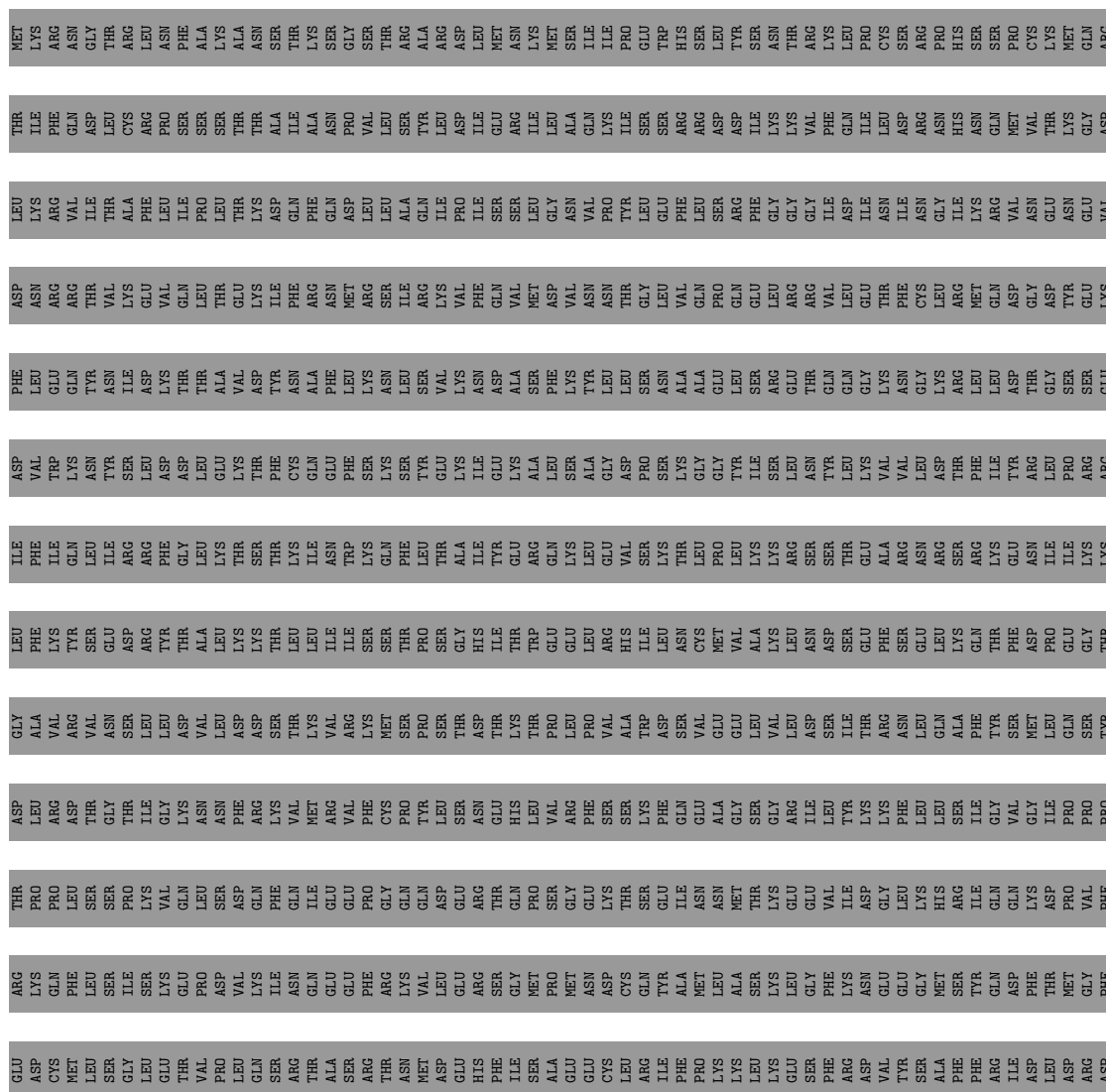


• Molecule 17: Cilia- and flagella-associated protein 276



• Molecule 17: Cilia- and flagella-associated protein 276



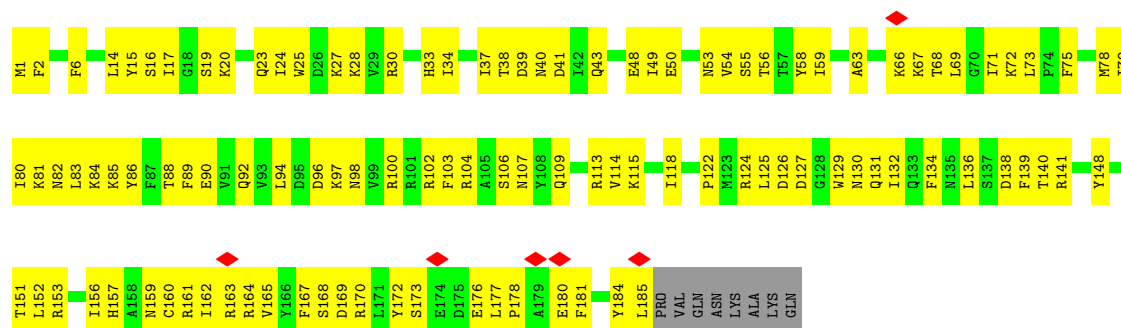


- Molecule 20: EF-hand calcium-binding domain-containing protein 6

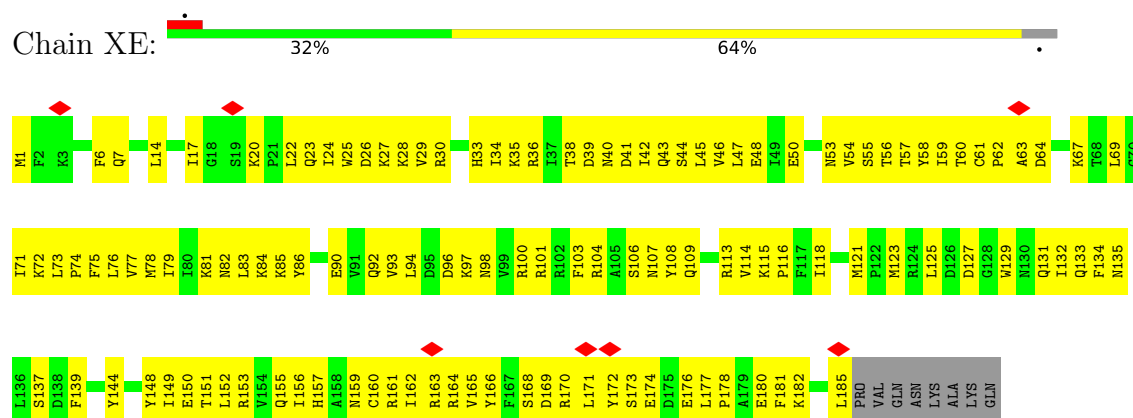
[illegible]



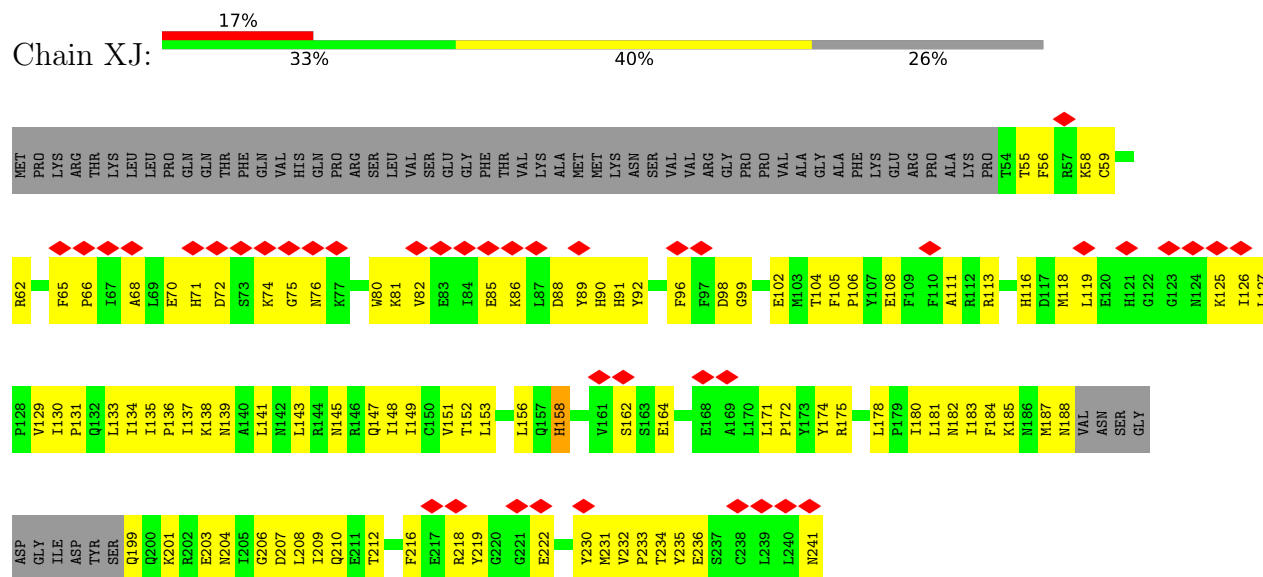




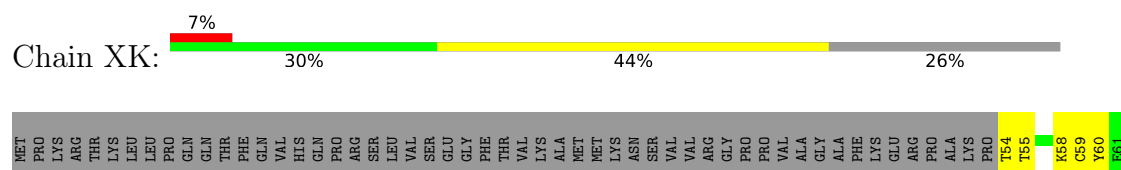
• Molecule 22: Cilia- and flagella-associated protein 20

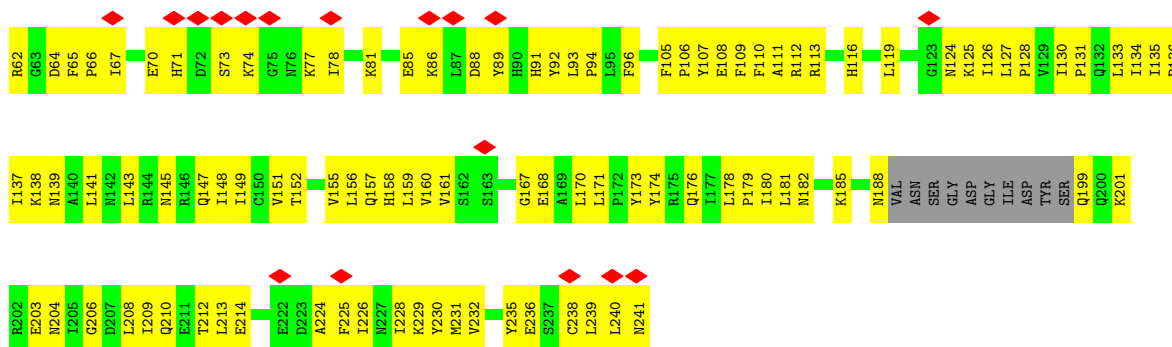


• Molecule 23: Parkin coregulated gene protein homolog

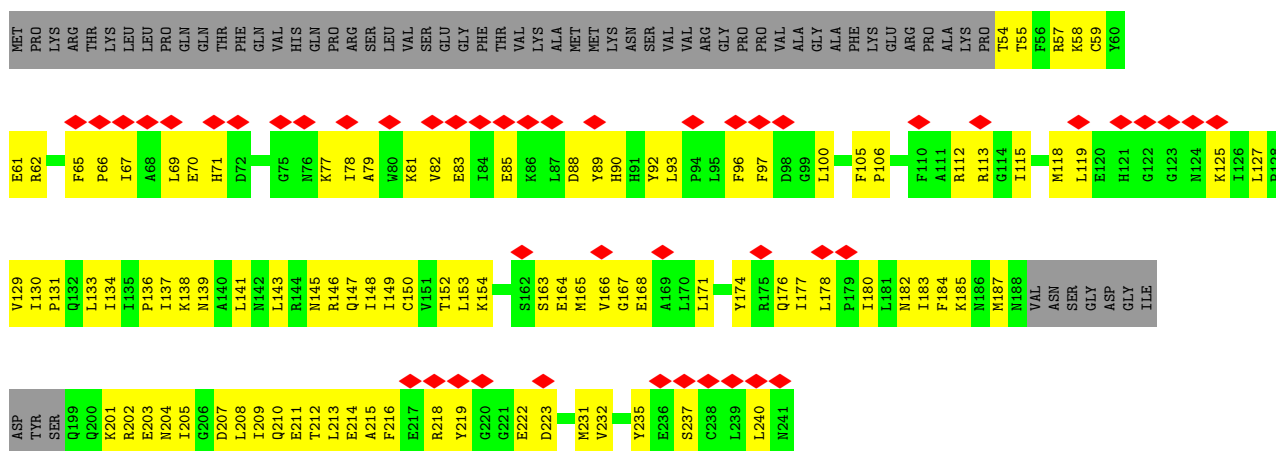


• Molecule 23: Parkin coregulated gene protein homolog

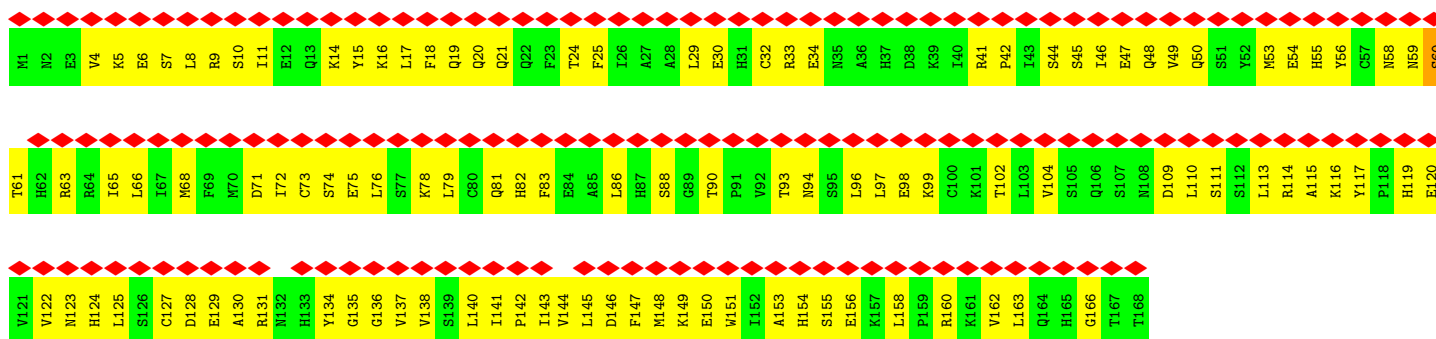




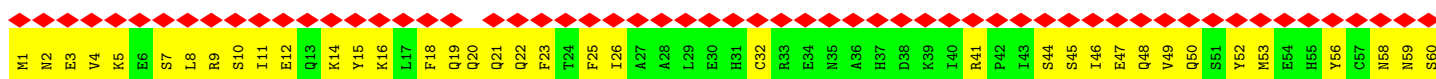
• Molecule 23: Parkin coregulated gene protein homolog

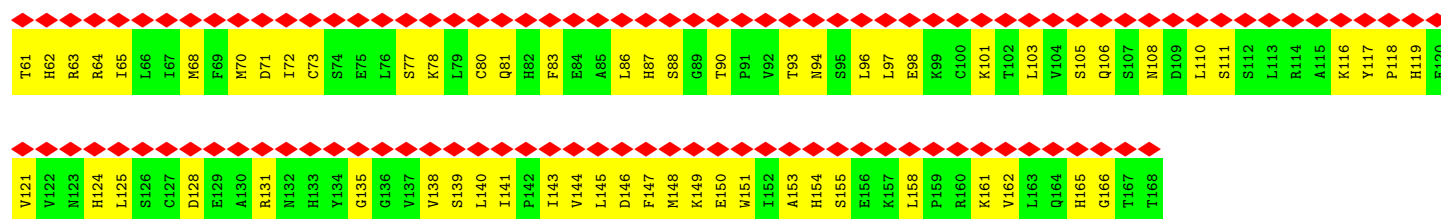


• Molecule 24: Sperm acrosome-associated protein 9

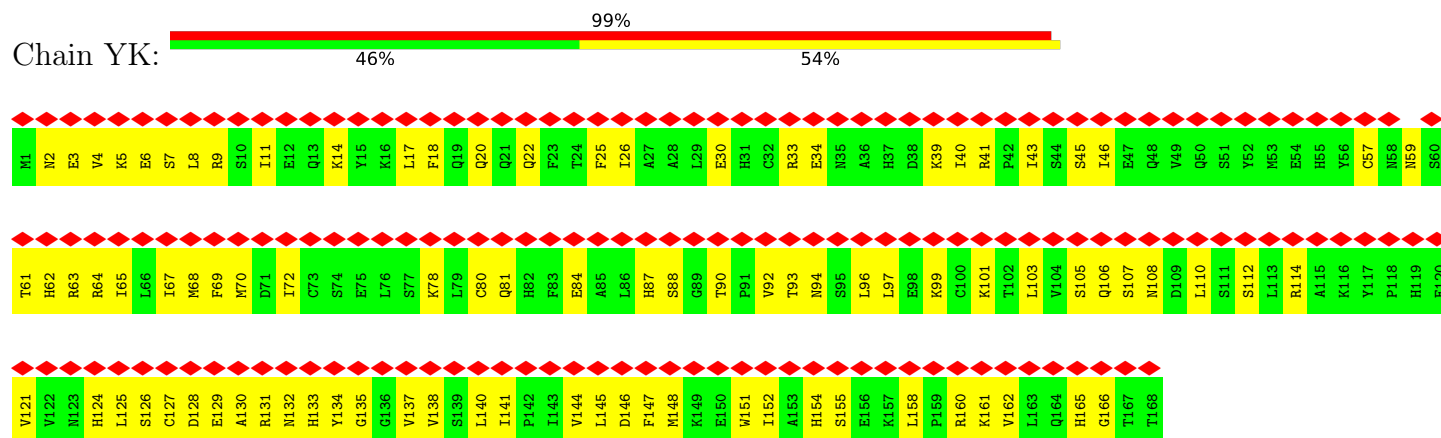


• Molecule 24: Sperm acrosome-associated protein 9

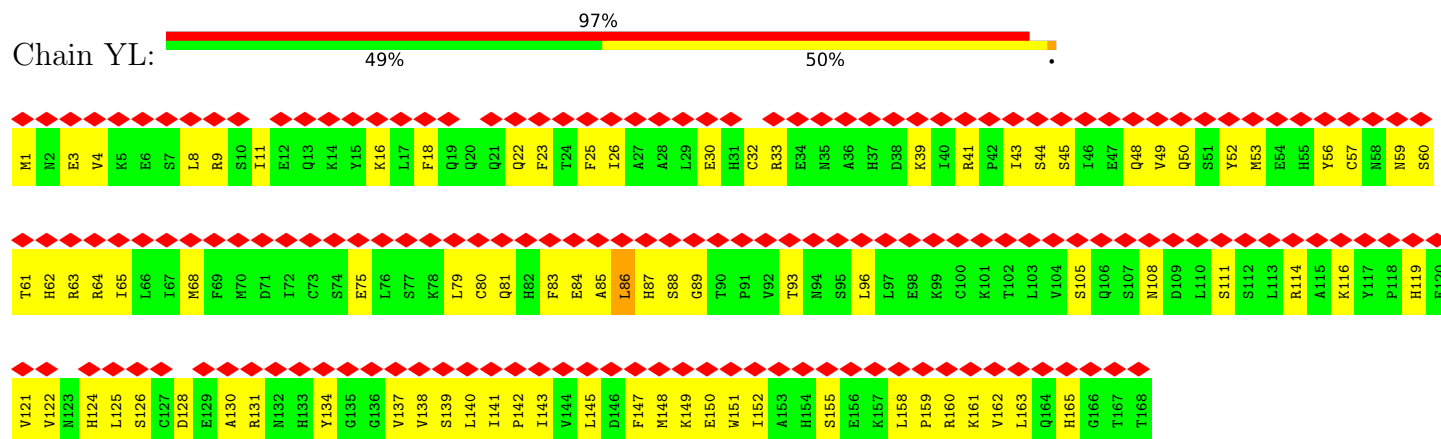




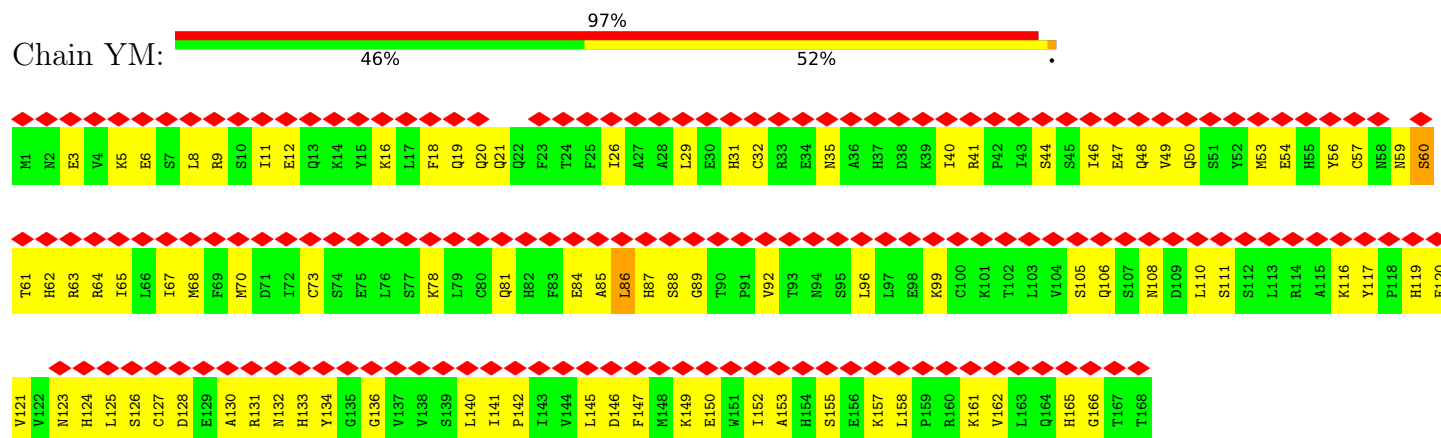
• Molecule 24: Sperm acrosome-associated protein 9



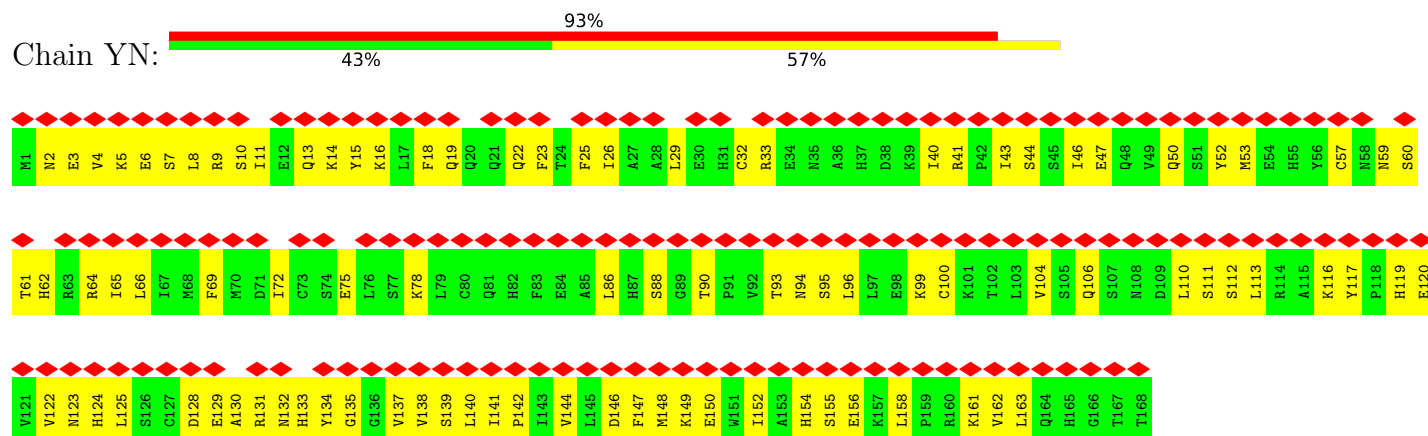
• Molecule 24: Sperm acrosome-associated protein 9



• Molecule 24: Sperm acrosome-associated protein 9



Chain YN:



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	37018	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 ($e^-/\text{\AA}^2$)	117	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.014	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	563.2, 563.2, 563.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.76, 1.76, 1.76	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

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	A2	0.27	0/2914	0.56	0/3926
1	A3	0.30	0/1767	0.57	0/2381
2	AE	0.23	0/3496	0.52	0/4747
2	AG	0.25	0/3496	0.58	1/4747 (0.0%)
2	AI	0.23	0/3496	0.56	0/4747
2	BE	0.20	0/3496	0.54	0/4747
2	BG	0.22	0/3496	0.54	0/4747
2	BI	0.22	0/3496	0.52	0/4747
2	CG	0.22	0/3496	0.55	2/4747 (0.0%)
2	CI	0.24	0/3496	0.58	3/4747 (0.1%)
2	DE	0.23	0/3496	0.60	4/4747 (0.1%)
2	DG	0.22	0/3496	0.54	2/4747 (0.0%)
2	EE	0.23	0/3496	0.58	0/4747
2	EG	0.23	0/3496	0.57	4/4747 (0.1%)
2	FE	0.21	0/3496	0.53	2/4747 (0.0%)
2	FG	0.23	0/3496	0.59	4/4747 (0.1%)
2	GE	0.31	2/3496 (0.1%)	0.61	4/4747 (0.1%)
2	GG	0.22	0/3496	0.55	2/4747 (0.0%)
2	GI	0.23	0/3496	0.59	3/4747 (0.1%)
2	HE	0.20	0/3496	0.51	0/4747
2	HG	0.22	0/3496	0.52	1/4747 (0.0%)
2	HI	0.21	0/3496	0.52	0/4747
2	IE	0.19	0/3496	0.48	0/4747
2	IG	0.20	0/3496	0.52	0/4747
2	II	0.20	0/3496	0.51	0/4747
2	JE	0.21	0/3496	0.51	0/4747
2	JG	0.21	0/3496	0.52	0/4747
2	KE	0.21	0/3496	0.52	0/4747
2	KG	0.24	0/3496	0.56	1/4747 (0.0%)
2	KI	0.22	0/3496	0.54	0/4747
2	LE	0.23	0/3496	0.54	2/4747 (0.0%)
2	LG	0.23	0/3496	0.55	0/4747

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	LI	0.22	0/3496	0.50	0/4747
2	ME	0.21	0/3496	0.53	1/4747 (0.0%)
2	MG	0.26	0/3496	0.57	1/4747 (0.0%)
2	MI	0.22	0/3496	0.56	2/4747 (0.0%)
2	NE	0.19	0/3496	0.48	1/4747 (0.0%)
2	NG	0.18	0/3496	0.48	0/4747
2	NI	0.18	0/3496	0.50	0/4747
2	OE	0.19	0/3496	0.49	0/4747
2	OG	0.18	0/3496	0.50	0/4747
2	OI	0.18	0/3496	0.48	0/4747
2	PE	0.19	0/3496	0.47	0/4747
2	PG	0.29	1/3496 (0.0%)	0.60	5/4747 (0.1%)
2	PI	0.20	0/3496	0.51	0/4747
2	QE	0.19	0/3496	0.48	0/4747
2	QG	0.19	0/3496	0.51	0/4747
2	QI	0.19	0/3496	0.49	2/4747 (0.0%)
2	RE	0.19	0/3496	0.51	0/4747
2	RG	0.19	0/3496	0.47	0/4747
2	RI	0.20	0/3496	0.52	0/4747
2	SE	0.18	0/3496	0.47	0/4747
2	SG	0.20	0/3496	0.50	0/4747
2	SI	0.21	0/3496	0.50	0/4747
2	TG	0.18	0/3496	0.47	0/4747
2	TI	0.19	0/3496	0.47	0/4747
2	UE	0.19	0/3496	0.51	1/4747 (0.0%)
2	UG	0.25	1/3496 (0.0%)	0.55	3/4747 (0.1%)
2	VE	0.19	0/3496	0.48	0/4747
2	VG	0.20	0/3496	0.50	0/4747
2	WE	0.21	0/3496	0.51	1/4747 (0.0%)
2	WG	0.21	0/3496	0.51	0/4747
2	WI	0.20	0/3496	0.52	0/4747
3	AF	0.24	0/3431	0.57	3/4649 (0.1%)
3	AH	0.24	0/3431	0.56	0/4649
3	BF	0.22	0/3431	0.50	0/4649
3	BH	0.22	0/3431	0.55	0/4649
3	CF	0.21	0/3431	0.55	0/4649
3	CH	0.24	0/3431	0.56	0/4649
3	CJ	0.24	0/3431	0.63	7/4649 (0.2%)
3	DD	0.22	0/3431	0.55	1/4649 (0.0%)
3	DF	0.22	0/3431	0.51	0/4649
3	DH	0.20	0/3431	0.51	0/4649
3	ED	0.23	0/3431	0.55	2/4649 (0.0%)
3	EF	0.23	0/3431	0.58	0/4649

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	EH	0.20	0/3431	0.52	0/4649
3	FD	0.21	0/3431	0.56	2/4649 (0.0%)
3	FF	0.22	0/3431	0.55	1/4649 (0.0%)
3	FH	0.21	0/3431	0.55	2/4649 (0.0%)
3	GD	0.24	0/3431	0.54	1/4649 (0.0%)
3	GF	0.22	0/3431	0.56	0/4649
3	GH	0.22	0/3431	0.55	4/4649 (0.1%)
3	HD	0.19	0/3431	0.49	0/4649
3	HF	0.25	0/3431	0.57	1/4649 (0.0%)
3	HH	0.21	0/3431	0.52	1/4649 (0.0%)
3	IF	0.22	0/3431	0.54	0/4649
3	IH	0.21	0/3431	0.52	0/4649
3	JD	0.24	0/3431	0.60	7/4649 (0.2%)
3	JF	0.21	0/3431	0.52	0/4649
3	JH	0.21	0/3431	0.53	2/4649 (0.0%)
3	KD	0.22	0/3431	0.53	0/4649
3	KF	0.22	0/3431	0.53	0/4649
3	KH	0.22	0/3431	0.53	0/4649
3	LD	0.27	0/3431	0.61	4/4649 (0.1%)
3	LF	0.24	0/3431	0.60	2/4649 (0.0%)
3	LH	0.24	0/3431	0.57	2/4649 (0.0%)
3	MF	0.23	0/3431	0.53	0/4649
3	MH	0.27	0/3431	0.58	2/4649 (0.0%)
3	ND	0.19	0/3431	0.50	0/4649
3	NF	0.19	0/3431	0.50	2/4649 (0.0%)
3	NH	0.19	0/3431	0.53	1/4649 (0.0%)
3	OD	0.18	0/3431	0.45	1/4649 (0.0%)
3	OF	0.20	0/3431	0.53	1/4649 (0.0%)
3	OH	0.19	0/3431	0.50	2/4649 (0.0%)
3	PF	0.19	0/3431	0.49	1/4649 (0.0%)
3	PH	0.19	0/3431	0.49	1/4649 (0.0%)
3	QF	0.19	0/3431	0.50	0/4649
3	QH	0.19	0/3431	0.50	0/4649
3	RF	0.21	0/3431	0.52	0/4649
3	RH	0.20	0/3431	0.49	0/4649
3	RJ	0.21	0/3431	0.53	0/4649
3	SF	0.21	0/3431	0.55	1/4649 (0.0%)
3	SH	0.20	0/3431	0.51	0/4649
3	SJ	0.20	0/3431	0.52	0/4649
3	TF	0.19	0/3431	0.48	0/4649
3	TH	0.19	0/3431	0.52	0/4649
3	TJ	0.18	0/3431	0.48	0/4649
3	UD	0.19	0/3431	0.50	0/4649

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	UF	0.20	0/3431	0.50	0/4649
3	UH	0.19	0/3431	0.50	0/4649
3	VD	0.20	0/3431	0.48	0/4649
3	VF	0.21	0/3431	0.52	0/4649
3	VH	0.20	0/3431	0.49	0/4649
3	WF	0.21	0/3431	0.52	0/4649
3	WH	0.20	0/3431	0.50	0/4649
4	B2	0.28	0/2053	0.55	0/2761
4	B3	0.28	0/2850	0.57	0/3845
4	B7	0.27	0/3116	0.54	0/4198
4	B8	0.29	0/1475	0.58	2/1978 (0.1%)
5	C2	0.26	0/1194	0.57	0/1609
5	C3	0.28	0/3011	0.58	0/4052
5	C4	0.32	0/674	0.75	1/904 (0.1%)
5	C7	0.30	0/2010	0.60	2/2708 (0.1%)
5	C8	0.30	0/2561	0.67	2/3447 (0.1%)
5	Cb	0.27	0/2143	0.58	0/2878
5	Cc	0.26	0/2188	0.50	0/2949
6	D2	0.22	0/596	0.50	0/802
6	D3	0.27	0/3270	0.52	0/4400
6	D4	0.26	0/1090	0.51	0/1460
6	D7	0.30	0/843	0.62	0/1129
6	D8	0.29	0/3234	0.55	0/4352
6	D9	0.27	0/866	0.61	0/1166
7	E2	0.23	0/1613	0.57	0/2194
7	E3	0.34	0/540	0.66	2/736 (0.3%)
8	F2	0.27	0/2671	0.58	0/3591
8	F3	0.28	0/1956	0.61	0/2629
8	F6	0.23	0/2537	0.50	0/3406
8	F7	0.26	0/2021	0.60	0/2714
8	Fa	0.23	0/1763	0.54	0/2370
8	Fb	0.22	0/2669	0.51	0/3584
8	Fc	0.16	0/229	0.34	0/310
8	Fl	0.23	0/2751	0.56	0/3693
9	G1	0.20	0/4309	0.50	2/5839 (0.0%)
9	G2	0.20	0/4192	0.48	2/5678 (0.0%)
10	G5	0.22	0/6339	0.51	0/8570
11	H3	0.27	0/1219	0.75	0/1649
11	H4	0.35	0/1154	0.78	2/1560 (0.1%)
12	I2	0.33	0/306	0.63	0/413
12	I3	0.27	0/306	0.55	0/413
13	J2	0.22	0/1413	0.55	0/1923
13	J3	0.22	0/1413	0.57	1/1923 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	K2	0.23	0/1749	0.57	0/2347
14	K3	0.23	0/3523	0.58	2/4741 (0.0%)
14	K4	0.21	0/1355	0.60	0/1833
15	L2	0.22	0/1970	0.58	0/2636
15	L3	0.23	0/1970	0.61	1/2636 (0.0%)
16	M2	0.24	0/525	0.63	0/708
16	M3	0.17	0/525	0.49	0/708
17	N2	0.23	0/546	0.63	0/734
17	N3	0.22	0/546	0.53	0/734
18	O1	0.19	0/849	0.52	0/1160
18	O2	0.23	0/849	0.67	2/1160 (0.2%)
19	P1	0.20	0/4793	0.51	1/6480 (0.0%)
19	P2	0.22	1/4793 (0.0%)	0.54	1/6480 (0.0%)
20	Q1	0.19	0/1500	0.57	0/2007
20	Q2	0.22	0/1500	0.62	2/2007 (0.1%)
21	R2	0.19	0/605	0.60	0/810
22	XC	0.20	0/1573	0.50	0/2122
22	XD	0.21	0/1573	0.49	0/2122
22	XE	0.22	0/1573	0.52	0/2122
23	XJ	0.22	0/1503	0.56	0/2028
23	XK	0.21	0/1503	0.54	0/2028
23	XL	0.20	0/1503	0.53	0/2028
24	YI	0.22	0/1393	0.61	0/1876
24	YJ	0.20	0/1393	0.55	0/1876
24	YK	0.21	0/1393	0.59	0/1876
24	YL	0.19	0/1393	0.48	0/1876
24	YM	0.18	0/1393	0.54	0/1876
24	YN	0.20	0/1393	0.56	0/1876
All	All	0.22	5/548418 (0.0%)	0.54	131/742832 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	CI	0	1
2	DG	0	2
2	EE	0	2
2	EG	0	2
2	FG	0	3
2	GE	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	GG	0	1
2	LI	0	2
2	PG	0	1
2	UG	0	1
3	AH	0	2
3	BF	0	1
3	BH	0	1
3	CF	0	2
3	CJ	0	2
3	DD	0	1
3	DF	0	1
3	DH	0	1
3	ED	0	2
3	FD	0	2
3	FF	0	2
3	FH	0	2
3	GF	0	2
3	HD	0	1
3	IH	0	1
3	JD	0	1
3	JH	0	1
3	KD	0	1
3	KF	0	1
3	KH	0	1
3	LD	0	2
3	LF	0	1
3	LH	0	1
3	MF	0	1
3	MH	0	1
3	ND	0	1
3	NH	0	1
3	OF	0	1
3	PF	0	1
3	PH	0	1
3	QF	0	1
3	QH	0	1
3	RF	0	1
3	SH	0	2
3	SJ	0	1
3	UD	0	1
3	UF	0	1
3	VD	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	VH	0	1
3	WF	0	1
3	WH	0	1
5	C4	0	1
7	E2	0	1
8	F3	0	1
10	G5	0	5
13	J3	0	1
14	K3	0	2
19	P1	0	1
All	All	0	81

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	PG	32	PRO	CG-CD	-12.74	1.07	1.50
2	UG	171	ILE	C-N	8.25	1.47	1.33
2	GE	224	TYR	CB-CG	-7.39	1.35	1.51
2	GE	224	TYR	CE1-CZ	-5.42	1.25	1.38
19	P2	277	LYS	CA-C	-5.05	1.50	1.53

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	PG	32	PRO	N-CD-CG	-17.36	77.15	103.20
3	CJ	15	GLN	CA-CB-CG	16.14	146.38	114.10
2	MI	87	PHE	CA-C-N	11.95	138.22	121.61
2	MI	87	PHE	C-N-CA	11.95	138.22	121.61
2	PG	32	PRO	CA-CB-CG	-11.48	82.69	104.50

There are no chirality outliers.

5 of 81 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AH	130	LEU	Peptide
3	AH	271	ALA	Peptide
3	BF	271	ALA	Peptide
3	BH	271	ALA	Peptide
5	C4	419	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A2	2884	0	2918	149	0
1	A3	1745	0	1736	89	0
2	AE	3418	0	3327	228	0
2	AG	3418	0	3328	239	0
2	AI	3418	0	3329	259	0
2	BE	3418	0	3327	181	0
2	BG	3418	0	3328	216	0
2	BI	3418	0	3328	195	0
2	CG	3418	0	3329	203	0
2	CI	3418	0	3329	211	0
2	DE	3418	0	3328	225	0
2	DG	3418	0	3329	210	0
2	EE	3418	0	3329	203	0
2	EG	3418	0	3329	205	0
2	FE	3418	0	3328	202	0
2	FG	3418	0	3329	194	0
2	GE	3418	0	3328	209	0
2	GG	3418	0	3328	209	0
2	GI	3418	0	3328	173	0
2	HE	3418	0	3327	206	0
2	HG	3418	0	3329	199	0
2	HI	3418	0	3329	169	0
2	IE	3418	0	3328	165	0
2	IG	3418	0	3328	187	0
2	II	3418	0	3328	167	0
2	JE	3418	0	3329	217	0
2	JG	3418	0	3327	186	0
2	KE	3418	0	3327	218	0
2	KG	3418	0	3328	199	0
2	KI	3418	0	3329	191	0
2	LE	3418	0	3331	201	0
2	LG	3418	0	3329	232	0
2	LI	3418	0	3328	201	0
2	ME	3418	0	3328	197	0
2	MG	3418	0	3328	256	0
2	MI	3418	0	3328	187	0
2	NE	3418	0	3328	249	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	NG	3418	0	3329	243	0
2	NI	3418	0	3328	216	0
2	OE	3418	0	3327	224	0
2	OG	3418	0	3327	237	0
2	OI	3418	0	3328	251	0
2	PE	3418	0	3327	222	0
2	PG	3418	0	3329	234	0
2	PI	3418	0	3328	244	0
2	QE	3418	0	3328	240	0
2	QG	3418	0	3329	235	0
2	QI	3418	0	3328	235	0
2	RE	3418	0	3329	232	0
2	RG	3418	0	3328	239	0
2	RI	3418	0	3327	271	0
2	SE	3418	0	3327	196	0
2	SG	3418	0	3328	272	0
2	SI	3418	0	3328	256	0
2	TG	3418	0	3328	230	0
2	TI	3418	0	3329	236	0
2	UE	3418	0	3327	242	0
2	UG	3418	0	3329	253	0
2	VE	3418	0	3327	237	0
2	VG	3418	0	3328	264	0
2	WE	3418	0	3329	270	0
2	WG	3418	0	3328	283	0
2	WI	3418	0	3329	272	0
3	AF	3356	0	3236	210	0
3	AH	3356	0	3235	223	0
3	BF	3356	0	3235	191	0
3	BH	3356	0	3235	210	0
3	CF	3356	0	3236	182	0
3	CH	3356	0	3237	206	0
3	CJ	3356	0	3237	173	0
3	DD	3356	0	3236	193	0
3	DF	3356	0	3236	202	0
3	DH	3356	0	3238	159	0
3	ED	3356	0	3237	185	0
3	EF	3356	0	3235	211	0
3	EH	3356	0	3237	179	0
3	FD	3356	0	3237	175	0
3	FF	3356	0	3235	181	0
3	FH	3356	0	3237	150	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	GD	3356	0	3237	184	0
3	GF	3356	0	3235	196	0
3	GH	3356	0	3235	185	0
3	HD	3356	0	3235	176	0
3	HF	3356	0	3235	188	0
3	HH	3356	0	3235	185	0
3	IF	3356	0	3237	205	0
3	IH	3356	0	3235	191	0
3	JD	3356	0	3235	183	0
3	JF	3356	0	3235	197	0
3	JH	3356	0	3237	167	0
3	KD	3356	0	3235	178	0
3	KF	3356	0	3236	180	0
3	KH	3356	0	3236	184	0
3	LD	3356	0	3233	189	0
3	LF	3356	0	3236	213	0
3	LH	3356	0	3235	204	0
3	MF	3356	0	3235	180	0
3	MH	3356	0	3235	253	0
3	ND	3356	0	3235	186	0
3	NF	3356	0	3236	218	0
3	NH	3356	0	3235	235	0
3	OD	3356	0	3235	183	0
3	OF	3356	0	3236	202	0
3	OH	3356	0	3234	251	0
3	PF	3356	0	3234	214	0
3	PH	3356	0	3236	226	0
3	QF	3356	0	3235	220	0
3	QH	3356	0	3235	220	0
3	RF	3356	0	3235	242	0
3	RH	3356	0	3235	254	0
3	RJ	3356	0	3237	213	0
3	SF	3356	0	3235	226	0
3	SH	3356	0	3235	244	0
3	SJ	3356	0	3237	216	0
3	TF	3356	0	3236	212	0
3	TH	3356	0	3236	203	0
3	TJ	3356	0	3238	189	0
3	UD	3356	0	3235	208	0
3	UF	3356	0	3235	221	0
3	UH	3356	0	3238	210	0
3	VD	3356	0	3234	229	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	VF	3356	0	3235	246	0
3	VH	3356	0	3236	215	0
3	WF	3356	0	3235	234	0
3	WH	3356	0	3235	216	0
4	B2	2036	0	2084	74	0
4	B3	2816	0	2822	138	0
4	B7	3082	0	3105	129	0
4	B8	1463	0	1499	94	0
5	C2	1175	0	1120	61	0
5	C3	2978	0	2969	175	0
5	C4	670	0	685	62	0
5	C7	1983	0	1923	86	0
5	C8	2534	0	2543	116	0
5	Cb	2125	0	2142	101	0
5	Cc	2159	0	2100	101	0
6	D2	583	0	539	21	0
6	D3	3225	0	3158	148	0
6	D4	1080	0	1095	51	0
6	D7	836	0	857	80	0
6	D8	3192	0	3146	150	0
6	D9	849	0	771	40	0
7	E2	1558	0	1502	95	0
7	E3	519	0	490	16	0
8	F2	2640	0	2658	131	0
8	F3	1927	0	1862	102	0
8	F6	2503	0	2456	112	0
8	F7	2003	0	2062	106	0
8	Fa	1746	0	1798	91	0
8	Fb	2634	0	2604	125	0
8	Fc	224	0	208	5	0
8	F1	2721	0	2733	168	0
9	G1	4192	0	4130	188	0
9	G2	4081	0	4025	180	0
10	G5	6169	0	6044	346	0
11	H3	1185	0	1141	132	0
11	H4	1121	0	1073	160	0
12	I2	298	0	281	18	0
12	I3	298	0	281	15	0
13	J2	1378	0	1354	70	0
13	J3	1378	0	1354	57	0
14	K2	1722	0	1785	136	0
14	K3	3465	0	3572	232	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	K4	1327	0	1348	67	0
15	L2	1929	0	2013	158	0
15	L3	1929	0	2013	131	0
16	M2	510	0	492	43	0
16	M3	510	0	492	29	0
17	N2	535	0	512	41	0
17	N3	535	0	512	41	0
18	O1	825	0	817	40	0
18	O2	825	0	817	78	0
19	P1	4696	0	4674	285	0
19	P2	4696	0	4674	301	0
20	Q1	1473	0	1492	120	0
20	Q2	1473	0	1492	129	0
21	R2	597	0	589	48	0
22	XC	1540	0	1570	122	0
22	XD	1540	0	1570	112	0
22	XE	1540	0	1570	126	0
23	XJ	1469	0	1477	101	0
23	XK	1469	0	1477	105	0
23	XL	1469	0	1477	95	0
24	YI	1365	0	1356	110	0
24	YJ	1365	0	1356	81	0
24	YK	1365	0	1356	88	0
24	YL	1365	0	1356	76	0
24	YM	1365	0	1356	81	0
24	YN	1365	0	1356	90	0
25	AE	32	0	12	3	0
25	AF	32	0	11	5	0
25	AG	32	0	12	4	0
25	AH	32	0	10	8	0
25	AI	32	0	12	6	0
25	BE	32	0	12	4	0
25	BF	32	0	10	9	0
25	BG	32	0	12	10	0
25	BH	32	0	11	8	0
25	BI	32	0	12	8	0
25	CF	32	0	10	6	0
25	CG	32	0	12	6	0
25	CH	32	0	11	4	0
25	CI	32	0	12	5	0
25	CJ	32	0	10	4	0
25	DD	32	0	10	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DE	32	0	12	11	0
25	DF	32	0	10	8	0
25	DG	32	0	12	9	0
25	DH	32	0	10	6	0
25	ED	32	0	10	5	0
25	EE	32	0	12	11	0
25	EF	32	0	11	7	0
25	EG	32	0	11	13	0
25	EH	32	0	11	6	0
25	FD	32	0	11	9	0
25	FE	32	0	12	9	0
25	FF	64	0	22	13	0
25	FH	32	0	10	4	0
25	GD	32	0	10	5	0
25	GE	32	0	9	7	0
25	GF	32	0	10	6	0
25	GG	32	0	12	6	0
25	GH	64	0	22	12	0
25	HD	32	0	11	10	0
25	HE	32	0	11	4	0
25	HF	32	0	10	3	0
25	HG	32	0	12	5	0
25	HH	32	0	10	4	0
25	HI	32	0	12	8	0
25	IE	32	0	12	3	0
25	IF	32	0	10	8	0
25	IG	32	0	12	3	0
25	IH	32	0	10	9	0
25	II	32	0	12	8	0
25	JD	32	0	10	4	0
25	JE	32	0	12	12	0
25	JF	32	0	10	9	0
25	JG	32	0	12	4	0
25	JH	32	0	11	5	0
25	KD	32	0	10	5	0
25	KE	32	0	12	6	0
25	KF	32	0	11	9	0
25	KG	32	0	11	5	0
25	KH	32	0	11	5	0
25	KI	32	0	11	5	0
25	LD	32	0	11	6	0
25	LE	32	0	12	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	LF	32	0	10	3	0
25	LG	32	0	12	5	0
25	LH	32	0	10	6	0
25	LI	32	0	12	7	0
25	ME	32	0	12	5	0
25	MF	32	0	11	10	0
25	MG	32	0	11	11	0
25	MH	32	0	11	3	0
25	MI	32	0	12	4	0
25	ND	32	0	10	6	0
25	NE	32	0	12	5	0
25	NF	32	0	11	4	0
25	NG	32	0	12	5	0
25	NH	32	0	11	7	0
25	NI	32	0	12	5	0
25	OD	32	0	11	7	0
25	OE	32	0	12	7	0
25	OF	32	0	10	10	0
25	OG	32	0	12	7	0
25	OH	32	0	11	7	0
25	OI	32	0	12	5	0
25	PE	32	0	12	10	0
25	PF	32	0	10	7	0
25	PG	32	0	12	4	0
25	PH	32	0	11	7	0
25	PI	32	0	12	11	0
25	QE	32	0	12	9	0
25	QF	32	0	10	6	0
25	QG	32	0	12	4	0
25	QH	32	0	11	11	0
25	QI	32	0	12	9	0
25	RE	32	0	12	2	0
25	RF	32	0	10	11	0
25	RG	32	0	12	5	0
25	RH	32	0	11	9	0
25	RI	32	0	12	6	0
25	RJ	32	0	10	10	0
25	SE	32	0	12	4	0
25	SF	32	0	11	9	0
25	SG	32	0	12	9	0
25	SH	32	0	10	9	0
25	SI	32	0	12	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	SJ	32	0	11	8	0
25	TF	32	0	11	7	0
25	TG	32	0	12	7	0
25	TH	32	0	11	7	0
25	TI	32	0	12	8	0
25	TJ	32	0	11	6	0
25	UD	32	0	10	6	0
25	UE	32	0	12	5	0
25	UF	32	0	10	9	0
25	UG	32	0	12	5	0
25	UH	32	0	10	8	0
25	VD	32	0	10	5	0
25	VE	32	0	12	4	0
25	VF	32	0	11	8	0
25	VG	32	0	12	2	0
25	VH	32	0	10	7	0
25	WE	32	0	12	7	0
25	WF	32	0	10	6	0
25	WG	32	0	12	9	0
25	WH	32	0	10	9	0
25	WI	32	0	12	5	0
All	All	540760	0	524837	30691	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

The worst 5 of 30691 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D7:316:GLN:HE21	6:D7:316:GLN:N	1.37	1.21
2:KI:402:ARG:HH22	21:R2:129:LYS:HG2	1.09	1.09
11:H4:212:LEU:HD13	11:H4:214:GLN:HE22	1.04	1.07
2:EE:326:LYS:HE3	3:EF:219:THR:HA	1.34	1.06
5:C3:141:HIS:HB3	5:C4:419:ARG:HH22	1.22	1.04

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A2	351/418 (84%)	332 (95%)	18 (5%)	1 (0%)	36	71
1	A3	207/418 (50%)	198 (96%)	9 (4%)	0	100	100
2	AE	436/438 (100%)	404 (93%)	31 (7%)	1 (0%)	43	77
2	AG	436/438 (100%)	407 (93%)	29 (7%)	0	100	100
2	AI	436/438 (100%)	402 (92%)	34 (8%)	0	100	100
2	BE	436/438 (100%)	397 (91%)	38 (9%)	1 (0%)	43	77
2	BG	436/438 (100%)	398 (91%)	38 (9%)	0	100	100
2	BI	436/438 (100%)	409 (94%)	27 (6%)	0	100	100
2	CG	436/438 (100%)	406 (93%)	30 (7%)	0	100	100
2	CI	436/438 (100%)	397 (91%)	38 (9%)	1 (0%)	43	77
2	DE	436/438 (100%)	403 (92%)	32 (7%)	1 (0%)	43	77
2	DG	436/438 (100%)	407 (93%)	29 (7%)	0	100	100
2	EE	436/438 (100%)	406 (93%)	30 (7%)	0	100	100
2	EG	436/438 (100%)	400 (92%)	35 (8%)	1 (0%)	43	77
2	FE	436/438 (100%)	403 (92%)	32 (7%)	1 (0%)	43	77
2	FG	436/438 (100%)	399 (92%)	35 (8%)	2 (0%)	24	63
2	GE	436/438 (100%)	398 (91%)	38 (9%)	0	100	100
2	GG	436/438 (100%)	399 (92%)	37 (8%)	0	100	100
2	GI	436/438 (100%)	406 (93%)	30 (7%)	0	100	100
2	HE	436/438 (100%)	401 (92%)	34 (8%)	1 (0%)	43	77
2	HG	436/438 (100%)	404 (93%)	31 (7%)	1 (0%)	43	77
2	HI	436/438 (100%)	414 (95%)	22 (5%)	0	100	100
2	IE	436/438 (100%)	404 (93%)	32 (7%)	0	100	100
2	IG	436/438 (100%)	409 (94%)	27 (6%)	0	100	100
2	II	436/438 (100%)	407 (93%)	29 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	JE	436/438 (100%)	398 (91%)	37 (8%)	1 (0%)	43	77
2	JG	436/438 (100%)	403 (92%)	33 (8%)	0	100	100
2	KE	436/438 (100%)	401 (92%)	35 (8%)	0	100	100
2	KG	436/438 (100%)	407 (93%)	28 (6%)	1 (0%)	43	77
2	KI	436/438 (100%)	400 (92%)	35 (8%)	1 (0%)	43	77
2	LE	436/438 (100%)	398 (91%)	37 (8%)	1 (0%)	43	77
2	LG	436/438 (100%)	396 (91%)	38 (9%)	2 (0%)	24	63
2	LI	436/438 (100%)	404 (93%)	31 (7%)	1 (0%)	43	77
2	ME	436/438 (100%)	404 (93%)	32 (7%)	0	100	100
2	MG	436/438 (100%)	395 (91%)	40 (9%)	1 (0%)	43	77
2	MI	436/438 (100%)	408 (94%)	27 (6%)	1 (0%)	43	77
2	NE	436/438 (100%)	400 (92%)	36 (8%)	0	100	100
2	NG	436/438 (100%)	412 (94%)	23 (5%)	1 (0%)	43	77
2	NI	436/438 (100%)	409 (94%)	27 (6%)	0	100	100
2	OE	436/438 (100%)	403 (92%)	32 (7%)	1 (0%)	43	77
2	OG	436/438 (100%)	405 (93%)	31 (7%)	0	100	100
2	OI	436/438 (100%)	407 (93%)	28 (6%)	1 (0%)	43	77
2	PE	436/438 (100%)	409 (94%)	27 (6%)	0	100	100
2	PG	436/438 (100%)	406 (93%)	30 (7%)	0	100	100
2	PI	436/438 (100%)	413 (95%)	23 (5%)	0	100	100
2	QE	436/438 (100%)	402 (92%)	34 (8%)	0	100	100
2	QG	436/438 (100%)	405 (93%)	31 (7%)	0	100	100
2	QI	436/438 (100%)	405 (93%)	31 (7%)	0	100	100
2	RE	436/438 (100%)	406 (93%)	29 (7%)	1 (0%)	43	77
2	RG	436/438 (100%)	405 (93%)	31 (7%)	0	100	100
2	RI	436/438 (100%)	405 (93%)	30 (7%)	1 (0%)	43	77
2	SE	436/438 (100%)	409 (94%)	26 (6%)	1 (0%)	43	77
2	SG	436/438 (100%)	405 (93%)	30 (7%)	1 (0%)	43	77
2	SI	436/438 (100%)	405 (93%)	31 (7%)	0	100	100
2	TG	436/438 (100%)	411 (94%)	24 (6%)	1 (0%)	43	77
2	TI	436/438 (100%)	398 (91%)	37 (8%)	1 (0%)	43	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	UE	436/438 (100%)	406 (93%)	30 (7%)	0	100	100
2	UG	436/438 (100%)	399 (92%)	37 (8%)	0	100	100
2	VE	436/438 (100%)	405 (93%)	31 (7%)	0	100	100
2	VG	436/438 (100%)	402 (92%)	34 (8%)	0	100	100
2	WE	436/438 (100%)	401 (92%)	35 (8%)	0	100	100
2	WG	436/438 (100%)	408 (94%)	27 (6%)	1 (0%)	43	77
2	WI	436/438 (100%)	405 (93%)	31 (7%)	0	100	100
3	AF	425/427 (100%)	397 (93%)	26 (6%)	2 (0%)	24	63
3	AH	425/427 (100%)	394 (93%)	30 (7%)	1 (0%)	43	77
3	BF	425/427 (100%)	394 (93%)	29 (7%)	2 (0%)	24	63
3	BH	425/427 (100%)	392 (92%)	32 (8%)	1 (0%)	43	77
3	CF	425/427 (100%)	403 (95%)	21 (5%)	1 (0%)	43	77
3	CH	425/427 (100%)	400 (94%)	24 (6%)	1 (0%)	43	77
3	CJ	425/427 (100%)	402 (95%)	22 (5%)	1 (0%)	43	77
3	DD	425/427 (100%)	387 (91%)	37 (9%)	1 (0%)	43	77
3	DF	425/427 (100%)	389 (92%)	35 (8%)	1 (0%)	43	77
3	DH	425/427 (100%)	398 (94%)	25 (6%)	2 (0%)	24	63
3	ED	425/427 (100%)	389 (92%)	35 (8%)	1 (0%)	43	77
3	EF	425/427 (100%)	402 (95%)	22 (5%)	1 (0%)	43	77
3	EH	425/427 (100%)	402 (95%)	22 (5%)	1 (0%)	43	77
3	FD	425/427 (100%)	398 (94%)	26 (6%)	1 (0%)	43	77
3	FF	425/427 (100%)	394 (93%)	30 (7%)	1 (0%)	43	77
3	FH	425/427 (100%)	398 (94%)	25 (6%)	2 (0%)	24	63
3	GD	425/427 (100%)	402 (95%)	22 (5%)	1 (0%)	43	77
3	GF	425/427 (100%)	395 (93%)	29 (7%)	1 (0%)	43	77
3	GH	425/427 (100%)	400 (94%)	24 (6%)	1 (0%)	43	77
3	HD	425/427 (100%)	392 (92%)	32 (8%)	1 (0%)	43	77
3	HF	425/427 (100%)	389 (92%)	34 (8%)	2 (0%)	24	63
3	HH	425/427 (100%)	399 (94%)	25 (6%)	1 (0%)	43	77
3	IF	425/427 (100%)	401 (94%)	23 (5%)	1 (0%)	43	77
3	IH	425/427 (100%)	406 (96%)	18 (4%)	1 (0%)	43	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	JD	425/427 (100%)	404 (95%)	20 (5%)	1 (0%)	43	77
3	JF	425/427 (100%)	394 (93%)	30 (7%)	1 (0%)	43	77
3	JH	425/427 (100%)	399 (94%)	25 (6%)	1 (0%)	43	77
3	KD	425/427 (100%)	395 (93%)	29 (7%)	1 (0%)	43	77
3	KF	425/427 (100%)	405 (95%)	19 (4%)	1 (0%)	43	77
3	KH	425/427 (100%)	396 (93%)	28 (7%)	1 (0%)	43	77
3	LD	425/427 (100%)	401 (94%)	23 (5%)	1 (0%)	43	77
3	LF	425/427 (100%)	393 (92%)	31 (7%)	1 (0%)	43	77
3	LH	425/427 (100%)	400 (94%)	24 (6%)	1 (0%)	43	77
3	MF	425/427 (100%)	398 (94%)	26 (6%)	1 (0%)	43	77
3	MH	425/427 (100%)	391 (92%)	34 (8%)	0	100	100
3	ND	425/427 (100%)	400 (94%)	24 (6%)	1 (0%)	43	77
3	NF	425/427 (100%)	397 (93%)	28 (7%)	0	100	100
3	NH	425/427 (100%)	397 (93%)	28 (7%)	0	100	100
3	OD	425/427 (100%)	405 (95%)	19 (4%)	1 (0%)	43	77
3	OF	425/427 (100%)	396 (93%)	28 (7%)	1 (0%)	43	77
3	OH	425/427 (100%)	399 (94%)	25 (6%)	1 (0%)	43	77
3	PF	425/427 (100%)	400 (94%)	24 (6%)	1 (0%)	43	77
3	PH	425/427 (100%)	389 (92%)	35 (8%)	1 (0%)	43	77
3	QF	425/427 (100%)	394 (93%)	30 (7%)	1 (0%)	43	77
3	QH	425/427 (100%)	399 (94%)	25 (6%)	1 (0%)	43	77
3	RF	425/427 (100%)	399 (94%)	25 (6%)	1 (0%)	43	77
3	RH	425/427 (100%)	397 (93%)	26 (6%)	2 (0%)	24	63
3	RJ	425/427 (100%)	394 (93%)	30 (7%)	1 (0%)	43	77
3	SF	425/427 (100%)	405 (95%)	20 (5%)	0	100	100
3	SH	425/427 (100%)	395 (93%)	30 (7%)	0	100	100
3	SJ	425/427 (100%)	393 (92%)	31 (7%)	1 (0%)	43	77
3	TF	425/427 (100%)	402 (95%)	23 (5%)	0	100	100
3	TH	425/427 (100%)	405 (95%)	19 (4%)	1 (0%)	43	77
3	TJ	425/427 (100%)	393 (92%)	31 (7%)	1 (0%)	43	77
3	UD	425/427 (100%)	398 (94%)	26 (6%)	1 (0%)	43	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	UF	425/427 (100%)	401 (94%)	22 (5%)	2 (0%)	24	63
3	UH	425/427 (100%)	395 (93%)	29 (7%)	1 (0%)	43	77
3	VD	425/427 (100%)	397 (93%)	27 (6%)	1 (0%)	43	77
3	VF	425/427 (100%)	405 (95%)	19 (4%)	1 (0%)	43	77
3	VH	425/427 (100%)	398 (94%)	26 (6%)	1 (0%)	43	77
3	WF	425/427 (100%)	397 (93%)	27 (6%)	1 (0%)	43	77
3	WH	425/427 (100%)	400 (94%)	24 (6%)	1 (0%)	43	77
4	B2	246/430 (57%)	233 (95%)	13 (5%)	0	100	100
4	B3	339/430 (79%)	317 (94%)	21 (6%)	1 (0%)	36	71
4	B7	372/430 (86%)	355 (95%)	14 (4%)	3 (1%)	16	53
4	B8	173/430 (40%)	165 (95%)	8 (5%)	0	100	100
5	C2	138/490 (28%)	127 (92%)	11 (8%)	0	100	100
5	C3	364/490 (74%)	348 (96%)	16 (4%)	0	100	100
5	C4	79/490 (16%)	75 (95%)	4 (5%)	0	100	100
5	C7	239/490 (49%)	228 (95%)	11 (5%)	0	100	100
5	C8	308/490 (63%)	296 (96%)	12 (4%)	0	100	100
5	Cb	258/490 (53%)	248 (96%)	10 (4%)	0	100	100
5	Cc	263/490 (54%)	246 (94%)	17 (6%)	0	100	100
6	D2	70/447 (16%)	65 (93%)	5 (7%)	0	100	100
6	D3	390/447 (87%)	373 (96%)	17 (4%)	0	100	100
6	D4	130/447 (29%)	124 (95%)	6 (5%)	0	100	100
6	D7	99/447 (22%)	93 (94%)	6 (6%)	0	100	100
6	D8	386/447 (86%)	366 (95%)	19 (5%)	1 (0%)	36	71
6	D9	98/447 (22%)	89 (91%)	9 (9%)	0	100	100
7	E2	185/206 (90%)	140 (76%)	44 (24%)	1 (0%)	24	63
7	E3	61/206 (30%)	49 (80%)	12 (20%)	0	100	100
8	F2	318/557 (57%)	300 (94%)	18 (6%)	0	100	100
8	F3	230/557 (41%)	220 (96%)	10 (4%)	0	100	100
8	F6	301/557 (54%)	283 (94%)	18 (6%)	0	100	100
8	F7	241/557 (43%)	227 (94%)	14 (6%)	0	100	100
8	Fa	210/557 (38%)	200 (95%)	9 (4%)	1 (0%)	24	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Fb	317/557 (57%)	307 (97%)	9 (3%)	1 (0%)	36	71
8	Fc	24/557 (4%)	24 (100%)	0	0	100	100
8	F1	326/557 (58%)	312 (96%)	13 (4%)	1 (0%)	36	71
9	G1	506/648 (78%)	448 (88%)	56 (11%)	2 (0%)	30	67
9	G2	491/648 (76%)	428 (87%)	61 (12%)	2 (0%)	30	67
10	G5	745/750 (99%)	631 (85%)	107 (14%)	7 (1%)	14	49
11	H3	139/319 (44%)	99 (71%)	32 (23%)	8 (6%)	1	14
11	H4	131/319 (41%)	95 (72%)	26 (20%)	10 (8%)	1	10
12	I2	36/200 (18%)	31 (86%)	5 (14%)	0	100	100
12	I3	36/200 (18%)	33 (92%)	3 (8%)	0	100	100
13	J2	169/189 (89%)	131 (78%)	37 (22%)	1 (1%)	21	58
13	J3	169/189 (89%)	132 (78%)	36 (21%)	1 (1%)	21	58
14	K2	205/499 (41%)	177 (86%)	21 (10%)	7 (3%)	3	21
14	K3	424/499 (85%)	358 (84%)	53 (12%)	13 (3%)	3	22
14	K4	163/499 (33%)	130 (80%)	28 (17%)	5 (3%)	3	22
15	L2	234/255 (92%)	193 (82%)	39 (17%)	2 (1%)	14	49
15	L3	234/255 (92%)	189 (81%)	44 (19%)	1 (0%)	30	67
16	M2	60/141 (43%)	46 (77%)	14 (23%)	0	100	100
16	M3	60/141 (43%)	51 (85%)	9 (15%)	0	100	100
17	N2	64/168 (38%)	40 (62%)	24 (38%)	0	100	100
17	N3	64/168 (38%)	51 (80%)	13 (20%)	0	100	100
18	O1	101/189 (53%)	81 (80%)	20 (20%)	0	100	100
18	O2	101/189 (53%)	78 (77%)	22 (22%)	1 (1%)	12	47
19	P1	606/620 (98%)	563 (93%)	40 (7%)	3 (0%)	24	63
19	P2	606/620 (98%)	564 (93%)	39 (6%)	3 (0%)	24	63
20	Q1	176/1516 (12%)	143 (81%)	32 (18%)	1 (1%)	21	58
20	Q2	176/1516 (12%)	140 (80%)	34 (19%)	2 (1%)	11	45
21	R2	67/283 (24%)	58 (87%)	8 (12%)	1 (2%)	8	38
22	XC	183/193 (95%)	169 (92%)	14 (8%)	0	100	100
22	XD	183/193 (95%)	174 (95%)	9 (5%)	0	100	100
22	XE	183/193 (95%)	168 (92%)	15 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	XJ	174/241 (72%)	150 (86%)	24 (14%)	0	100	100
23	XK	174/241 (72%)	154 (88%)	20 (12%)	0	100	100
23	XL	174/241 (72%)	150 (86%)	24 (14%)	0	100	100
24	YI	166/168 (99%)	147 (89%)	18 (11%)	1 (1%)	21	58
24	YJ	166/168 (99%)	152 (92%)	13 (8%)	1 (1%)	21	58
24	YK	166/168 (99%)	148 (89%)	18 (11%)	0	100	100
24	YL	166/168 (99%)	148 (89%)	16 (10%)	2 (1%)	10	43
24	YM	166/168 (99%)	150 (90%)	14 (8%)	2 (1%)	10	43
24	YN	166/168 (99%)	144 (87%)	20 (12%)	2 (1%)	10	43
All	All	67499/80058 (84%)	62373 (92%)	4946 (7%)	180 (0%)	37	71

5 of 180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A2	209	PRO
2	BE	264	ARG
2	FE	264	ARG
2	FG	15	GLN
9	G2	226	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A2	326/380 (86%)	326 (100%)	0	100	100
1	A3	200/380 (53%)	200 (100%)	0	100	100
2	AE	366/366 (100%)	366 (100%)	0	100	100
2	AG	366/366 (100%)	366 (100%)	0	100	100
2	AI	366/366 (100%)	366 (100%)	0	100	100
2	BE	366/366 (100%)	366 (100%)	0	100	100
2	BG	366/366 (100%)	366 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BI	366/366 (100%)	366 (100%)	0	100	100
2	CG	366/366 (100%)	366 (100%)	0	100	100
2	CI	366/366 (100%)	366 (100%)	0	100	100
2	DE	366/366 (100%)	366 (100%)	0	100	100
2	DG	366/366 (100%)	366 (100%)	0	100	100
2	EE	366/366 (100%)	365 (100%)	1 (0%)	86	84
2	EG	366/366 (100%)	366 (100%)	0	100	100
2	FE	366/366 (100%)	366 (100%)	0	100	100
2	FG	366/366 (100%)	366 (100%)	0	100	100
2	GE	366/366 (100%)	366 (100%)	0	100	100
2	GG	366/366 (100%)	366 (100%)	0	100	100
2	GI	366/366 (100%)	366 (100%)	0	100	100
2	HE	366/366 (100%)	366 (100%)	0	100	100
2	HG	366/366 (100%)	366 (100%)	0	100	100
2	HI	366/366 (100%)	366 (100%)	0	100	100
2	IE	366/366 (100%)	366 (100%)	0	100	100
2	IG	366/366 (100%)	366 (100%)	0	100	100
2	II	366/366 (100%)	366 (100%)	0	100	100
2	JE	366/366 (100%)	366 (100%)	0	100	100
2	JG	366/366 (100%)	366 (100%)	0	100	100
2	KE	366/366 (100%)	366 (100%)	0	100	100
2	KG	366/366 (100%)	366 (100%)	0	100	100
2	KI	366/366 (100%)	366 (100%)	0	100	100
2	LE	366/366 (100%)	366 (100%)	0	100	100
2	LG	366/366 (100%)	366 (100%)	0	100	100
2	LI	366/366 (100%)	366 (100%)	0	100	100
2	ME	366/366 (100%)	365 (100%)	1 (0%)	86	84
2	MG	366/366 (100%)	366 (100%)	0	100	100
2	MI	366/366 (100%)	366 (100%)	0	100	100
2	NE	366/366 (100%)	365 (100%)	1 (0%)	86	84
2	NG	366/366 (100%)	366 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	NI	366/366 (100%)	366 (100%)	0	100	100
2	OE	366/366 (100%)	366 (100%)	0	100	100
2	OG	366/366 (100%)	366 (100%)	0	100	100
2	OI	366/366 (100%)	366 (100%)	0	100	100
2	PE	366/366 (100%)	366 (100%)	0	100	100
2	PG	366/366 (100%)	366 (100%)	0	100	100
2	PI	366/366 (100%)	366 (100%)	0	100	100
2	QE	366/366 (100%)	366 (100%)	0	100	100
2	QG	366/366 (100%)	366 (100%)	0	100	100
2	QI	366/366 (100%)	366 (100%)	0	100	100
2	RE	366/366 (100%)	366 (100%)	0	100	100
2	RG	366/366 (100%)	366 (100%)	0	100	100
2	RI	366/366 (100%)	366 (100%)	0	100	100
2	SE	366/366 (100%)	366 (100%)	0	100	100
2	SG	366/366 (100%)	366 (100%)	0	100	100
2	SI	366/366 (100%)	366 (100%)	0	100	100
2	TG	366/366 (100%)	366 (100%)	0	100	100
2	TI	366/366 (100%)	366 (100%)	0	100	100
2	UE	366/366 (100%)	366 (100%)	0	100	100
2	UG	366/366 (100%)	365 (100%)	1 (0%)	86	84
2	VE	366/366 (100%)	366 (100%)	0	100	100
2	VG	366/366 (100%)	366 (100%)	0	100	100
2	WE	366/366 (100%)	366 (100%)	0	100	100
2	WG	366/366 (100%)	366 (100%)	0	100	100
2	WI	366/366 (100%)	366 (100%)	0	100	100
3	AF	367/367 (100%)	367 (100%)	0	100	100
3	AH	367/367 (100%)	367 (100%)	0	100	100
3	BF	367/367 (100%)	367 (100%)	0	100	100
3	BH	367/367 (100%)	367 (100%)	0	100	100
3	CF	367/367 (100%)	366 (100%)	1 (0%)	86	84
3	CH	367/367 (100%)	367 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CJ	367/367 (100%)	367 (100%)	0	100	100
3	DD	367/367 (100%)	367 (100%)	0	100	100
3	DF	367/367 (100%)	367 (100%)	0	100	100
3	DH	367/367 (100%)	367 (100%)	0	100	100
3	ED	367/367 (100%)	367 (100%)	0	100	100
3	EF	367/367 (100%)	367 (100%)	0	100	100
3	EH	367/367 (100%)	366 (100%)	1 (0%)	86	84
3	FD	367/367 (100%)	367 (100%)	0	100	100
3	FF	367/367 (100%)	367 (100%)	0	100	100
3	FH	367/367 (100%)	367 (100%)	0	100	100
3	GD	367/367 (100%)	365 (100%)	2 (0%)	81	81
3	GF	367/367 (100%)	367 (100%)	0	100	100
3	GH	367/367 (100%)	367 (100%)	0	100	100
3	HD	367/367 (100%)	367 (100%)	0	100	100
3	HF	367/367 (100%)	367 (100%)	0	100	100
3	HH	367/367 (100%)	367 (100%)	0	100	100
3	IF	367/367 (100%)	367 (100%)	0	100	100
3	IH	367/367 (100%)	367 (100%)	0	100	100
3	JD	367/367 (100%)	366 (100%)	1 (0%)	86	84
3	JF	367/367 (100%)	367 (100%)	0	100	100
3	JH	367/367 (100%)	367 (100%)	0	100	100
3	KD	367/367 (100%)	367 (100%)	0	100	100
3	KF	367/367 (100%)	367 (100%)	0	100	100
3	KH	367/367 (100%)	367 (100%)	0	100	100
3	LD	367/367 (100%)	367 (100%)	0	100	100
3	LF	367/367 (100%)	365 (100%)	2 (0%)	81	81
3	LH	367/367 (100%)	367 (100%)	0	100	100
3	MF	367/367 (100%)	367 (100%)	0	100	100
3	MH	367/367 (100%)	366 (100%)	1 (0%)	86	84
3	ND	367/367 (100%)	367 (100%)	0	100	100
3	NF	367/367 (100%)	367 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	NH	367/367 (100%)	367 (100%)	0	100	100
3	OD	367/367 (100%)	367 (100%)	0	100	100
3	OF	367/367 (100%)	367 (100%)	0	100	100
3	OH	367/367 (100%)	367 (100%)	0	100	100
3	PF	367/367 (100%)	367 (100%)	0	100	100
3	PH	367/367 (100%)	366 (100%)	1 (0%)	86	84
3	QF	367/367 (100%)	367 (100%)	0	100	100
3	QH	367/367 (100%)	366 (100%)	1 (0%)	86	84
3	RF	367/367 (100%)	367 (100%)	0	100	100
3	RH	367/367 (100%)	367 (100%)	0	100	100
3	RJ	367/367 (100%)	367 (100%)	0	100	100
3	SF	367/367 (100%)	367 (100%)	0	100	100
3	SH	367/367 (100%)	367 (100%)	0	100	100
3	SJ	367/367 (100%)	367 (100%)	0	100	100
3	TF	367/367 (100%)	367 (100%)	0	100	100
3	TH	367/367 (100%)	367 (100%)	0	100	100
3	TJ	367/367 (100%)	365 (100%)	2 (0%)	81	81
3	UD	367/367 (100%)	367 (100%)	0	100	100
3	UF	367/367 (100%)	367 (100%)	0	100	100
3	UH	367/367 (100%)	367 (100%)	0	100	100
3	VD	367/367 (100%)	367 (100%)	0	100	100
3	VF	367/367 (100%)	367 (100%)	0	100	100
3	VH	367/367 (100%)	367 (100%)	0	100	100
3	WF	367/367 (100%)	366 (100%)	1 (0%)	86	84
3	WH	367/367 (100%)	367 (100%)	0	100	100
4	B2	225/395 (57%)	225 (100%)	0	100	100
4	B3	315/395 (80%)	315 (100%)	0	100	100
4	B7	343/395 (87%)	343 (100%)	0	100	100
4	B8	163/395 (41%)	163 (100%)	0	100	100
5	C2	132/445 (30%)	131 (99%)	1 (1%)	73	77
5	C3	331/445 (74%)	331 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C4	76/445 (17%)	76 (100%)	0	100	100
5	C7	219/445 (49%)	219 (100%)	0	100	100
5	C8	282/445 (63%)	282 (100%)	0	100	100
5	Cb	236/445 (53%)	236 (100%)	0	100	100
5	Cc	238/445 (54%)	238 (100%)	0	100	100
6	D2	56/402 (14%)	56 (100%)	0	100	100
6	D3	354/402 (88%)	353 (100%)	1 (0%)	86	84
6	D4	121/402 (30%)	121 (100%)	0	100	100
6	D7	92/402 (23%)	91 (99%)	1 (1%)	65	74
6	D8	354/402 (88%)	354 (100%)	0	100	100
6	D9	92/402 (23%)	92 (100%)	0	100	100
7	E2	159/174 (91%)	159 (100%)	0	100	100
7	E3	50/174 (29%)	50 (100%)	0	100	100
8	F2	298/487 (61%)	298 (100%)	0	100	100
8	F3	214/487 (44%)	214 (100%)	0	100	100
8	F6	280/487 (58%)	280 (100%)	0	100	100
8	F7	228/487 (47%)	228 (100%)	0	100	100
8	Fa	199/487 (41%)	199 (100%)	0	100	100
8	Fb	295/487 (61%)	295 (100%)	0	100	100
8	Fc	23/487 (5%)	23 (100%)	0	100	100
8	F1	305/487 (63%)	304 (100%)	1 (0%)	86	84
9	G1	465/589 (79%)	465 (100%)	0	100	100
9	G2	452/589 (77%)	452 (100%)	0	100	100
10	G5	681/683 (100%)	681 (100%)	0	100	100
11	H3	125/279 (45%)	122 (98%)	3 (2%)	43	63
11	H4	118/279 (42%)	108 (92%)	10 (8%)	10	30
12	I2	33/180 (18%)	33 (100%)	0	100	100
12	I3	33/180 (18%)	33 (100%)	0	100	100
13	J2	153/169 (90%)	153 (100%)	0	100	100
13	J3	153/169 (90%)	153 (100%)	0	100	100
14	K2	191/434 (44%)	191 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	K3	375/434 (86%)	375 (100%)	0	100	100
14	K4	136/434 (31%)	136 (100%)	0	100	100
15	L2	216/235 (92%)	216 (100%)	0	100	100
15	L3	216/235 (92%)	216 (100%)	0	100	100
16	M2	54/125 (43%)	54 (100%)	0	100	100
16	M3	54/125 (43%)	54 (100%)	0	100	100
17	N2	58/148 (39%)	58 (100%)	0	100	100
17	N3	58/148 (39%)	58 (100%)	0	100	100
18	O1	88/165 (53%)	88 (100%)	0	100	100
18	O2	88/165 (53%)	88 (100%)	0	100	100
19	P1	511/522 (98%)	508 (99%)	3 (1%)	78	80
19	P2	511/522 (98%)	510 (100%)	1 (0%)	87	85
20	Q1	162/1391 (12%)	162 (100%)	0	100	100
20	Q2	162/1391 (12%)	162 (100%)	0	100	100
21	R2	61/250 (24%)	60 (98%)	1 (2%)	55	69
22	XC	173/180 (96%)	173 (100%)	0	100	100
22	XD	173/180 (96%)	173 (100%)	0	100	100
22	XE	173/180 (96%)	173 (100%)	0	100	100
23	XJ	161/215 (75%)	160 (99%)	1 (1%)	78	80
23	XK	161/215 (75%)	161 (100%)	0	100	100
23	XL	161/215 (75%)	161 (100%)	0	100	100
24	YI	157/157 (100%)	157 (100%)	0	100	100
24	YJ	157/157 (100%)	157 (100%)	0	100	100
24	YK	157/157 (100%)	157 (100%)	0	100	100
24	YL	157/157 (100%)	157 (100%)	0	100	100
24	YM	157/157 (100%)	157 (100%)	0	100	100
24	YN	157/157 (100%)	157 (100%)	0	100	100
All	All	58384/69159 (84%)	58344 (100%)	40 (0%)	87	88

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	P1	242	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	TJ	348	ASN
19	P1	277	LYS
3	PH	280	GLN
2	UG	224	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 790 such sidechains are listed below:

Mol	Chain	Res	Type
2	MI	88	HIS
3	QF	190	HIS
2	NG	91	GLN
2	MI	35	GLN
2	OI	88	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

123 ligands are modelled in this entry.

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
25	GTP	DG	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.43	5 (10%)
25	GTP	TJ	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.75	10 (20%)
25	GTP	QF	501	-	33,34,34	1.04	4 (12%)	50,54,54	1.88	9 (18%)
25	GTP	BI	501	-	33,34,34	1.08	3 (9%)	50,54,54	1.57	11 (22%)
25	GTP	GD	501	-	33,34,34	1.18	4 (12%)	50,54,54	2.16	11 (22%)
25	GTP	NF	501	-	33,34,34	1.08	1 (3%)	50,54,54	2.02	11 (22%)
25	GTP	EE	501	-	33,34,34	1.37	4 (12%)	50,54,54	1.61	11 (22%)
25	GTP	KE	501	-	33,34,34	1.02	2 (6%)	50,54,54	1.67	14 (28%)
25	GTP	GH	501	-	33,34,34	1.10	3 (9%)	50,54,54	1.81	10 (20%)
25	GTP	HI	501	-	33,34,34	1.10	3 (9%)	50,54,54	2.91	16 (32%)
25	GTP	CH	501	-	33,34,34	1.14	4 (12%)	50,54,54	1.85	10 (20%)
25	GTP	KD	501	-	33,34,34	1.03	3 (9%)	50,54,54	2.05	15 (30%)
25	GTP	PE	501	-	33,34,34	1.07	3 (9%)	50,54,54	1.77	14 (28%)
25	GTP	PI	501	-	33,34,34	0.96	2 (6%)	50,54,54	1.79	14 (28%)
25	GTP	RE	501	-	33,34,34	1.05	4 (12%)	50,54,54	1.77	10 (20%)
25	GTP	VE	501	-	33,34,34	1.01	3 (9%)	50,54,54	1.62	12 (24%)
25	GTP	PH	501	-	33,34,34	0.94	2 (6%)	50,54,54	1.79	10 (20%)
25	GTP	SG	501	-	33,34,34	0.97	2 (6%)	50,54,54	1.85	13 (26%)
25	GTP	GF	501	-	33,34,34	1.20	5 (15%)	50,54,54	1.99	14 (28%)
25	GTP	OI	501	-	33,34,34	1.00	3 (9%)	50,54,54	1.60	11 (22%)
25	GTP	ED	501	-	33,34,34	1.73	6 (18%)	50,54,54	2.83	19 (38%)
25	GTP	QI	501	-	33,34,34	1.00	2 (6%)	50,54,54	1.67	13 (26%)
25	GTP	IH	501	-	33,34,34	1.11	5 (15%)	50,54,54	1.83	9 (18%)
25	GTP	TG	501	-	33,34,34	1.01	3 (9%)	50,54,54	1.59	10 (20%)
25	GTP	EF	501	-	33,34,34	1.12	4 (12%)	50,54,54	2.00	11 (22%)
25	GTP	CI	501	-	33,34,34	1.09	3 (9%)	50,54,54	1.92	15 (30%)
25	GTP	NH	501	-	33,34,34	1.23	5 (15%)	50,54,54	2.00	12 (24%)
25	GTP	HG	501	-	33,34,34	1.10	3 (9%)	50,54,54	2.05	14 (28%)
25	GTP	JG	501	-	33,34,34	1.01	2 (6%)	50,54,54	1.64	12 (24%)
25	GTP	OD	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.74	10 (20%)
25	GTP	BF	501	-	33,34,34	1.08	4 (12%)	50,54,54	1.80	10 (20%)
25	GTP	WF	501	-	33,34,34	1.17	3 (9%)	50,54,54	2.19	13 (26%)
25	GTP	DD	501	-	33,34,34	1.31	6 (18%)	50,54,54	2.22	15 (30%)
25	GTP	KF	501	-	33,34,34	1.20	5 (15%)	50,54,54	1.80	11 (22%)
25	GTP	LG	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.56	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	GTP	ND	501	-	33,34,34	1.48	3 (9%)	50,54,54	2.69	16 (32%)
25	GTP	WG	501	-	33,34,34	0.94	2 (6%)	50,54,54	1.60	9 (18%)
25	GTP	LE	501	-	33,34,34	1.33	4 (12%)	50,54,54	2.33	19 (38%)
25	GTP	AI	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.75	13 (26%)
25	GTP	HH	501	-	33,34,34	1.19	4 (12%)	50,54,54	2.06	15 (30%)
25	GTP	GH	502	-	33,34,34	1.14	3 (9%)	50,54,54	1.70	15 (30%)
25	GTP	FF	502	-	33,34,34	1.26	3 (9%)	50,54,54	1.97	11 (22%)
25	GTP	MH	501	-	33,34,34	1.34	2 (6%)	50,54,54	2.78	17 (34%)
25	GTP	JH	501	-	33,34,34	1.17	4 (12%)	50,54,54	2.15	12 (24%)
25	GTP	MI	501	-	33,34,34	0.85	0	50,54,54	1.64	12 (24%)
25	GTP	LD	501	-	33,34,34	1.16	4 (12%)	50,54,54	1.81	12 (24%)
25	GTP	QH	501	-	33,34,34	1.03	3 (9%)	50,54,54	1.81	10 (20%)
25	GTP	WE	501	-	33,34,34	1.08	4 (12%)	50,54,54	1.65	11 (22%)
25	GTP	OG	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.65	9 (18%)
25	GTP	RH	501	-	33,34,34	0.98	1 (3%)	50,54,54	1.74	10 (20%)
25	GTP	RF	501	-	33,34,34	1.04	2 (6%)	50,54,54	1.66	9 (18%)
25	GTP	LH	501	-	33,34,34	1.10	4 (12%)	50,54,54	1.94	13 (26%)
25	GTP	SF	501	-	33,34,34	1.14	3 (9%)	50,54,54	1.87	11 (22%)
25	GTP	HE	501	-	33,34,34	1.10	3 (9%)	50,54,54	1.80	13 (26%)
25	GTP	TF	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.66	10 (20%)
25	GTP	IE	501	-	33,34,34	0.97	2 (6%)	50,54,54	1.66	13 (26%)
25	GTP	SI	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.66	10 (20%)
25	GTP	SE	501	-	33,34,34	0.90	2 (6%)	50,54,54	1.57	10 (20%)
25	GTP	BG	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.75	15 (30%)
25	GTP	UD	501	-	33,34,34	1.05	5 (15%)	50,54,54	1.69	7 (14%)
25	GTP	VD	501	-	33,34,34	1.02	3 (9%)	50,54,54	1.72	10 (20%)
25	GTP	DE	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.97	16 (32%)
25	GTP	WI	501	-	33,34,34	1.05	2 (6%)	50,54,54	1.65	11 (22%)
25	GTP	NG	501	-	33,34,34	1.11	4 (12%)	50,54,54	1.79	14 (28%)
25	GTP	EG	501	-	33,34,34	1.33	3 (9%)	50,54,54	1.86	16 (32%)
25	GTP	EH	501	-	33,34,34	1.23	3 (9%)	50,54,54	1.95	13 (26%)
25	GTP	OE	501	-	33,34,34	0.91	2 (6%)	50,54,54	1.57	9 (18%)
25	GTP	PG	501	-	33,34,34	1.08	4 (12%)	50,54,54	1.66	12 (24%)
25	GTP	BE	501	-	33,34,34	1.04	1 (3%)	50,54,54	1.66	13 (26%)
25	GTP	QG	501	-	33,34,34	1.07	4 (12%)	50,54,54	1.74	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	GTP	MG	501	-	33,34,34	1.03	2 (6%)	50,54,54	1.59	11 (22%)
25	GTP	RG	501	-	33,34,34	0.91	2 (6%)	50,54,54	1.68	12 (24%)
25	GTP	WH	501	-	33,34,34	1.11	5 (15%)	50,54,54	1.81	10 (20%)
25	GTP	GE	501	-	33,34,34	1.47	5 (15%)	50,54,54	2.14	14 (28%)
25	GTP	LF	501	-	33,34,34	1.07	4 (12%)	50,54,54	1.95	14 (28%)
25	GTP	FD	501	-	33,34,34	1.03	2 (6%)	50,54,54	1.81	11 (22%)
25	GTP	BH	501	-	33,34,34	1.16	4 (12%)	50,54,54	1.77	13 (26%)
25	GTP	TH	501	-	33,34,34	1.06	4 (12%)	50,54,54	1.79	10 (20%)
25	GTP	CF	501	-	33,34,34	1.09	3 (9%)	50,54,54	1.73	11 (22%)
25	GTP	UG	501	-	33,34,34	1.17	3 (9%)	50,54,54	1.65	12 (24%)
25	GTP	OH	501	-	33,34,34	1.02	2 (6%)	50,54,54	1.68	9 (18%)
25	GTP	HF	501	-	33,34,34	1.33	4 (12%)	50,54,54	2.76	16 (32%)
25	GTP	VH	501	-	33,34,34	1.00	2 (6%)	50,54,54	1.73	9 (18%)
25	GTP	KG	501	-	33,34,34	1.00	2 (6%)	50,54,54	2.09	15 (30%)
25	GTP	GG	501	-	33,34,34	1.00	2 (6%)	50,54,54	1.74	14 (28%)
25	GTP	KH	501	-	33,34,34	1.15	4 (12%)	50,54,54	1.94	15 (30%)
25	GTP	TI	501	-	33,34,34	0.96	3 (9%)	50,54,54	1.60	10 (20%)
25	GTP	AG	501	-	33,34,34	0.99	3 (9%)	50,54,54	1.69	14 (28%)
25	GTP	NE	501	-	33,34,34	1.09	2 (6%)	50,54,54	1.67	11 (22%)
25	GTP	HD	501	-	33,34,34	1.08	4 (12%)	50,54,54	1.76	10 (20%)
25	GTP	KI	501	-	33,34,34	0.88	1 (3%)	50,54,54	1.78	11 (22%)
25	GTP	IG	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.58	7 (14%)
25	GTP	SJ	501	-	33,34,34	0.98	1 (3%)	50,54,54	1.72	9 (18%)
25	GTP	ME	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.51	9 (18%)
25	GTP	AF	501	-	33,34,34	1.14	4 (12%)	50,54,54	1.94	11 (22%)
25	GTP	AE	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.70	11 (22%)
25	GTP	CG	501	-	33,34,34	0.94	0	50,54,54	1.81	14 (28%)
25	GTP	RI	501	-	33,34,34	1.00	3 (9%)	50,54,54	1.62	9 (18%)
25	GTP	VF	501	-	33,34,34	1.20	4 (12%)	50,54,54	1.86	12 (24%)
25	GTP	UH	501	-	33,34,34	1.08	4 (12%)	50,54,54	1.84	10 (20%)
25	GTP	IF	501	-	33,34,34	1.13	4 (12%)	50,54,54	1.93	15 (30%)
25	GTP	FH	501	-	33,34,34	1.27	4 (12%)	50,54,54	2.08	15 (30%)
25	GTP	II	501	-	33,34,34	1.08	3 (9%)	50,54,54	1.77	16 (32%)
25	GTP	RJ	501	-	33,34,34	1.03	3 (9%)	50,54,54	1.96	13 (26%)
25	GTP	VG	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.58	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	GTP	DH	501	-	33,34,34	1.05	2 (6%)	50,54,54	2.05	13 (26%)
25	GTP	LI	501	-	33,34,34	0.99	3 (9%)	50,54,54	1.77	14 (28%)
25	GTP	JF	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.81	11 (22%)
25	GTP	AH	501	-	33,34,34	1.19	5 (15%)	50,54,54	1.84	8 (16%)
25	GTP	UE	501	-	33,34,34	0.98	3 (9%)	50,54,54	1.65	10 (20%)
25	GTP	FE	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.96	16 (32%)
25	GTP	PF	501	-	33,34,34	1.10	3 (9%)	50,54,54	1.93	14 (28%)
25	GTP	OF	501	-	33,34,34	1.26	4 (12%)	50,54,54	2.11	12 (24%)
25	GTP	FF	501	-	33,34,34	1.08	3 (9%)	50,54,54	2.15	14 (28%)
25	GTP	QE	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.77	14 (28%)
25	GTP	MF	501	-	33,34,34	1.09	4 (12%)	50,54,54	1.99	13 (26%)
25	GTP	JD	501	-	33,34,34	1.93	7 (21%)	50,54,54	3.04	16 (32%)
25	GTP	DF	501	-	33,34,34	1.29	4 (12%)	50,54,54	1.89	12 (24%)
25	GTP	NI	501	-	33,34,34	1.02	1 (3%)	50,54,54	1.67	12 (24%)
25	GTP	CJ	501	-	33,34,34	1.60	5 (15%)	50,54,54	2.72	15 (30%)
25	GTP	JE	501	-	33,34,34	1.07	2 (6%)	50,54,54	1.64	12 (24%)
25	GTP	UF	501	-	33,34,34	1.12	4 (12%)	50,54,54	1.80	11 (22%)
25	GTP	SH	501	-	33,34,34	1.06	3 (9%)	50,54,54	1.78	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GTP	DG	501	-	-	4/22/38/38	0/3/3/3
25	GTP	TJ	501	-	-	4/22/38/38	0/3/3/3
25	GTP	QF	501	-	-	6/22/38/38	0/3/3/3
25	GTP	BI	501	-	-	7/22/38/38	0/3/3/3
25	GTP	GD	501	-	-	7/22/38/38	0/3/3/3
25	GTP	NF	501	-	-	7/22/38/38	0/3/3/3
25	GTP	EE	501	-	-	9/22/38/38	0/3/3/3
25	GTP	KE	501	-	-	6/22/38/38	0/3/3/3
25	GTP	GH	501	-	-	7/22/38/38	0/3/3/3
25	GTP	HI	501	-	-	6/22/38/38	0/3/3/3
25	GTP	CH	501	-	-	8/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GTP	KD	501	-	-	2/22/38/38	0/3/3/3
25	GTP	PE	501	-	-	9/22/38/38	0/3/3/3
25	GTP	PI	501	-	-	9/22/38/38	0/3/3/3
25	GTP	RE	501	-	-	9/22/38/38	0/3/3/3
25	GTP	VE	501	-	-	7/22/38/38	0/3/3/3
25	GTP	PH	501	-	-	4/22/38/38	0/3/3/3
25	GTP	SG	501	-	-	8/22/38/38	0/3/3/3
25	GTP	GF	501	-	-	10/22/38/38	0/3/3/3
25	GTP	OI	501	-	-	8/22/38/38	0/3/3/3
25	GTP	ED	501	-	-	5/22/38/38	0/3/3/3
25	GTP	QI	501	-	-	7/22/38/38	0/3/3/3
25	GTP	IH	501	-	-	8/22/38/38	0/3/3/3
25	GTP	TG	501	-	-	9/22/38/38	0/3/3/3
25	GTP	EF	501	-	-	8/22/38/38	0/3/3/3
25	GTP	CI	501	-	-	7/22/38/38	0/3/3/3
25	GTP	NH	501	-	-	7/22/38/38	0/3/3/3
25	GTP	HG	501	-	-	7/22/38/38	0/3/3/3
25	GTP	JG	501	-	-	12/22/38/38	0/3/3/3
25	GTP	OD	501	-	-	8/22/38/38	0/3/3/3
25	GTP	BF	501	-	-	12/22/38/38	0/3/3/3
25	GTP	WF	501	-	-	2/22/38/38	0/3/3/3
25	GTP	DD	501	-	-	8/22/38/38	0/3/3/3
25	GTP	KF	501	-	-	11/22/38/38	0/3/3/3
25	GTP	LG	501	-	-	6/22/38/38	0/3/3/3
25	GTP	ND	501	-	-	9/22/38/38	0/3/3/3
25	GTP	WG	501	-	-	9/22/38/38	0/3/3/3
25	GTP	LE	501	-	-	8/22/38/38	0/3/3/3
25	GTP	AI	501	-	-	7/22/38/38	0/3/3/3
25	GTP	HH	501	-	-	9/22/38/38	0/3/3/3
25	GTP	GH	502	-	-	12/22/38/38	0/3/3/3
25	GTP	FF	502	-	-	10/22/38/38	0/3/3/3
25	GTP	MH	501	-	-	5/22/38/38	0/3/3/3
25	GTP	JH	501	-	-	2/22/38/38	0/3/3/3
25	GTP	MI	501	-	-	7/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GTP	LD	501	-	-	4/22/38/38	0/3/3/3
25	GTP	QH	501	-	-	10/22/38/38	0/3/3/3
25	GTP	WE	501	-	-	8/22/38/38	0/3/3/3
25	GTP	OG	501	-	-	8/22/38/38	0/3/3/3
25	GTP	RH	501	-	-	4/22/38/38	0/3/3/3
25	GTP	RF	501	-	-	6/22/38/38	0/3/3/3
25	GTP	LH	501	-	-	5/22/38/38	0/3/3/3
25	GTP	SF	501	-	-	4/22/38/38	0/3/3/3
25	GTP	HE	501	-	-	7/22/38/38	0/3/3/3
25	GTP	TF	501	-	-	6/22/38/38	0/3/3/3
25	GTP	IE	501	-	-	9/22/38/38	0/3/3/3
25	GTP	SI	501	-	-	8/22/38/38	0/3/3/3
25	GTP	SE	501	-	-	7/22/38/38	0/3/3/3
25	GTP	BG	501	-	-	6/22/38/38	0/3/3/3
25	GTP	UD	501	-	-	8/22/38/38	0/3/3/3
25	GTP	VD	501	-	-	7/22/38/38	0/3/3/3
25	GTP	DE	501	-	-	5/22/38/38	0/3/3/3
25	GTP	WI	501	-	-	9/22/38/38	0/3/3/3
25	GTP	NG	501	-	-	9/22/38/38	0/3/3/3
25	GTP	EG	501	-	-	10/22/38/38	0/3/3/3
25	GTP	EH	501	-	-	12/22/38/38	0/3/3/3
25	GTP	OE	501	-	-	6/22/38/38	0/3/3/3
25	GTP	PG	501	-	-	9/22/38/38	0/3/3/3
25	GTP	BE	501	-	-	4/22/38/38	0/3/3/3
25	GTP	QG	501	-	-	9/22/38/38	0/3/3/3
25	GTP	MG	501	-	-	10/22/38/38	0/3/3/3
25	GTP	RG	501	-	-	7/22/38/38	0/3/3/3
25	GTP	WH	501	-	-	8/22/38/38	0/3/3/3
25	GTP	GE	501	-	-	8/22/38/38	0/3/3/3
25	GTP	LF	501	-	-	6/22/38/38	0/3/3/3
25	GTP	FD	501	-	-	6/22/38/38	0/3/3/3
25	GTP	BH	501	-	-	10/22/38/38	0/3/3/3
25	GTP	TH	501	-	-	8/22/38/38	0/3/3/3
25	GTP	CF	501	-	-	5/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GTP	UG	501	-	-	9/22/38/38	0/3/3/3
25	GTP	OH	501	-	-	6/22/38/38	0/3/3/3
25	GTP	HF	501	-	-	4/22/38/38	0/3/3/3
25	GTP	VH	501	-	-	4/22/38/38	0/3/3/3
25	GTP	KG	501	-	-	8/22/38/38	0/3/3/3
25	GTP	GG	501	-	-	9/22/38/38	0/3/3/3
25	GTP	KH	501	-	-	9/22/38/38	0/3/3/3
25	GTP	TI	501	-	-	8/22/38/38	0/3/3/3
25	GTP	AG	501	-	-	6/22/38/38	0/3/3/3
25	GTP	NE	501	-	-	8/22/38/38	0/3/3/3
25	GTP	HD	501	-	-	5/22/38/38	0/3/3/3
25	GTP	KI	501	-	-	6/22/38/38	0/3/3/3
25	GTP	IG	501	-	-	6/22/38/38	0/3/3/3
25	GTP	SJ	501	-	-	3/22/38/38	0/3/3/3
25	GTP	ME	501	-	-	11/22/38/38	0/3/3/3
25	GTP	AF	501	-	-	8/22/38/38	0/3/3/3
25	GTP	AE	501	-	-	8/22/38/38	0/3/3/3
25	GTP	CG	501	-	-	10/22/38/38	0/3/3/3
25	GTP	RI	501	-	-	9/22/38/38	0/3/3/3
25	GTP	VF	501	-	-	10/22/38/38	0/3/3/3
25	GTP	UH	501	-	-	8/22/38/38	0/3/3/3
25	GTP	IF	501	-	-	4/22/38/38	0/3/3/3
25	GTP	FH	501	-	-	10/22/38/38	0/3/3/3
25	GTP	II	501	-	-	12/22/38/38	0/3/3/3
25	GTP	RJ	501	-	-	5/22/38/38	0/3/3/3
25	GTP	VG	501	-	-	7/22/38/38	0/3/3/3
25	GTP	DH	501	-	-	2/22/38/38	0/3/3/3
25	GTP	LI	501	-	-	8/22/38/38	0/3/3/3
25	GTP	JF	501	-	-	12/22/38/38	0/3/3/3
25	GTP	AH	501	-	-	10/22/38/38	0/3/3/3
25	GTP	UE	501	-	-	7/22/38/38	0/3/3/3
25	GTP	FE	501	-	-	8/22/38/38	0/3/3/3
25	GTP	PF	501	-	-	2/22/38/38	0/3/3/3
25	GTP	OF	501	-	-	10/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GTP	FF	501	-	-	4/22/38/38	0/3/3/3
25	GTP	QE	501	-	-	8/22/38/38	0/3/3/3
25	GTP	MF	501	-	-	9/22/38/38	0/3/3/3
25	GTP	JD	501	-	-	9/22/38/38	0/3/3/3
25	GTP	DF	501	-	-	8/22/38/38	0/3/3/3
25	GTP	NI	501	-	-	7/22/38/38	0/3/3/3
25	GTP	CJ	501	-	-	6/22/38/38	0/3/3/3
25	GTP	JE	501	-	-	8/22/38/38	0/3/3/3
25	GTP	UF	501	-	-	7/22/38/38	0/3/3/3
25	GTP	SH	501	-	-	10/22/38/38	0/3/3/3

The worst 5 of 357 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	JD	501	GTP	C2-N2	7.16	1.50	1.34
25	ED	501	GTP	C2-N3	5.76	1.47	1.33
25	ND	501	GTP	C2-N3	5.22	1.45	1.33
25	MH	501	GTP	C2-N3	4.84	1.44	1.33
25	CJ	501	GTP	C2-N2	4.78	1.45	1.34

The worst 5 of 1481 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	JD	501	GTP	N9-C4-N3	9.16	144.27	125.95
25	HF	501	GTP	O4'-C1'-N9	8.80	128.29	108.36
25	ED	501	GTP	N9-C4-N3	8.55	143.05	125.95
25	JD	501	GTP	C5-C4-N3	-8.28	115.22	128.39
25	HI	501	GTP	O3G-PG-O3B	-7.88	78.20	104.64

There are no chirality outliers.

5 of 908 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	AF	501	GTP	C5'-O5'-PA-O2A
25	AI	501	GTP	O4'-C4'-C5'-O5'
25	AI	501	GTP	C3'-C4'-C5'-O5'
25	BF	501	GTP	C5'-O5'-PA-O3A
25	BF	501	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

123 monomers are involved in 812 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	DG	501	GTP	9	0
25	TJ	501	GTP	6	0
25	QF	501	GTP	6	0
25	BI	501	GTP	8	0
25	GD	501	GTP	5	0
25	NF	501	GTP	4	0
25	EE	501	GTP	11	0
25	KE	501	GTP	6	0
25	GH	501	GTP	7	0
25	HI	501	GTP	8	0
25	CH	501	GTP	4	0
25	KD	501	GTP	5	0
25	PE	501	GTP	10	0
25	PI	501	GTP	11	0
25	RE	501	GTP	2	0
25	VE	501	GTP	4	0
25	PH	501	GTP	7	0
25	SG	501	GTP	9	0
25	GF	501	GTP	6	0
25	OI	501	GTP	5	0
25	ED	501	GTP	5	0
25	QI	501	GTP	9	0
25	IH	501	GTP	9	0
25	TG	501	GTP	7	0
25	EF	501	GTP	7	0
25	CI	501	GTP	5	0
25	NH	501	GTP	7	0
25	HG	501	GTP	5	0
25	JG	501	GTP	4	0
25	OD	501	GTP	7	0
25	BF	501	GTP	9	0
25	WF	501	GTP	6	0
25	DD	501	GTP	2	0
25	KF	501	GTP	9	0
25	LG	501	GTP	5	0
25	ND	501	GTP	6	0
25	WG	501	GTP	9	0
25	LE	501	GTP	9	0
25	AI	501	GTP	6	0
25	HH	501	GTP	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	GH	502	GTP	5	0
25	FF	502	GTP	10	0
25	MH	501	GTP	3	0
25	JH	501	GTP	5	0
25	MI	501	GTP	4	0
25	LD	501	GTP	6	0
25	QH	501	GTP	11	0
25	WE	501	GTP	7	0
25	OG	501	GTP	7	0
25	RH	501	GTP	9	0
25	RF	501	GTP	11	0
25	LH	501	GTP	6	0
25	SF	501	GTP	9	0
25	HE	501	GTP	4	0
25	TF	501	GTP	7	0
25	IE	501	GTP	3	0
25	SI	501	GTP	5	0
25	SE	501	GTP	4	0
25	BG	501	GTP	10	0
25	UD	501	GTP	6	0
25	VD	501	GTP	5	0
25	DE	501	GTP	11	0
25	WI	501	GTP	5	0
25	NG	501	GTP	5	0
25	EG	501	GTP	13	0
25	EH	501	GTP	6	0
25	OE	501	GTP	7	0
25	PG	501	GTP	4	0
25	BE	501	GTP	4	0
25	QG	501	GTP	4	0
25	MG	501	GTP	11	0
25	RG	501	GTP	5	0
25	WH	501	GTP	9	0
25	GE	501	GTP	7	0
25	LF	501	GTP	3	0
25	FD	501	GTP	9	0
25	BH	501	GTP	8	0
25	TH	501	GTP	7	0
25	CF	501	GTP	6	0
25	UG	501	GTP	5	0
25	OH	501	GTP	7	0
25	HF	501	GTP	3	0

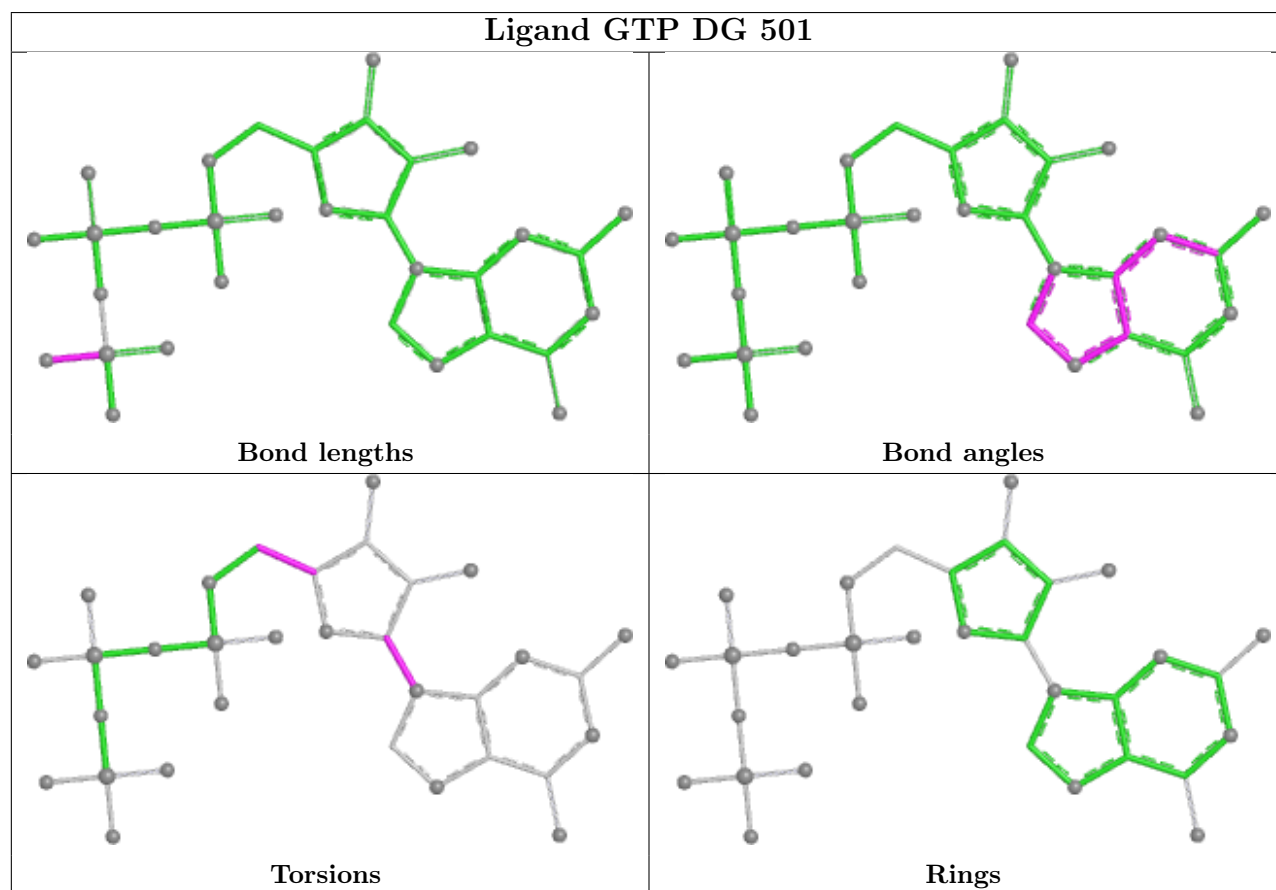
Continued on next page...

Continued from previous page...

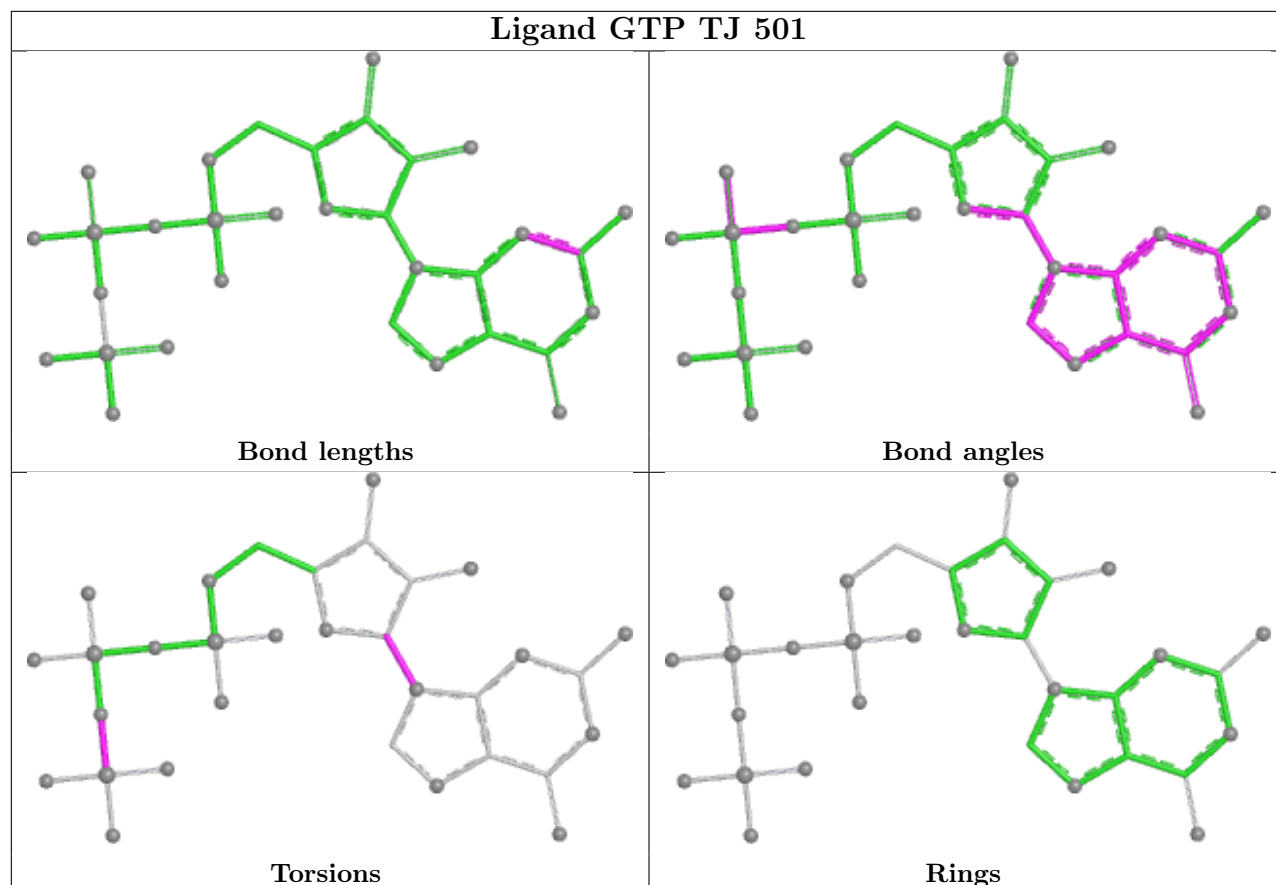
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	VH	501	GTP	7	0
25	KG	501	GTP	5	0
25	GG	501	GTP	6	0
25	KH	501	GTP	5	0
25	TI	501	GTP	8	0
25	AG	501	GTP	4	0
25	NE	501	GTP	5	0
25	HD	501	GTP	10	0
25	KI	501	GTP	5	0
25	IG	501	GTP	3	0
25	SJ	501	GTP	8	0
25	ME	501	GTP	5	0
25	AF	501	GTP	5	0
25	AE	501	GTP	3	0
25	CG	501	GTP	6	0
25	RI	501	GTP	6	0
25	VF	501	GTP	8	0
25	UH	501	GTP	8	0
25	IF	501	GTP	8	0
25	FH	501	GTP	4	0
25	II	501	GTP	8	0
25	RJ	501	GTP	10	0
25	VG	501	GTP	2	0
25	DH	501	GTP	6	0
25	LI	501	GTP	7	0
25	JF	501	GTP	9	0
25	AH	501	GTP	8	0
25	UE	501	GTP	5	0
25	FE	501	GTP	9	0
25	PF	501	GTP	7	0
25	OF	501	GTP	10	0
25	FF	501	GTP	3	0
25	QE	501	GTP	9	0
25	MF	501	GTP	10	0
25	JD	501	GTP	4	0
25	DF	501	GTP	8	0
25	NI	501	GTP	5	0
25	CJ	501	GTP	4	0
25	JE	501	GTP	12	0
25	UF	501	GTP	9	0
25	SH	501	GTP	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

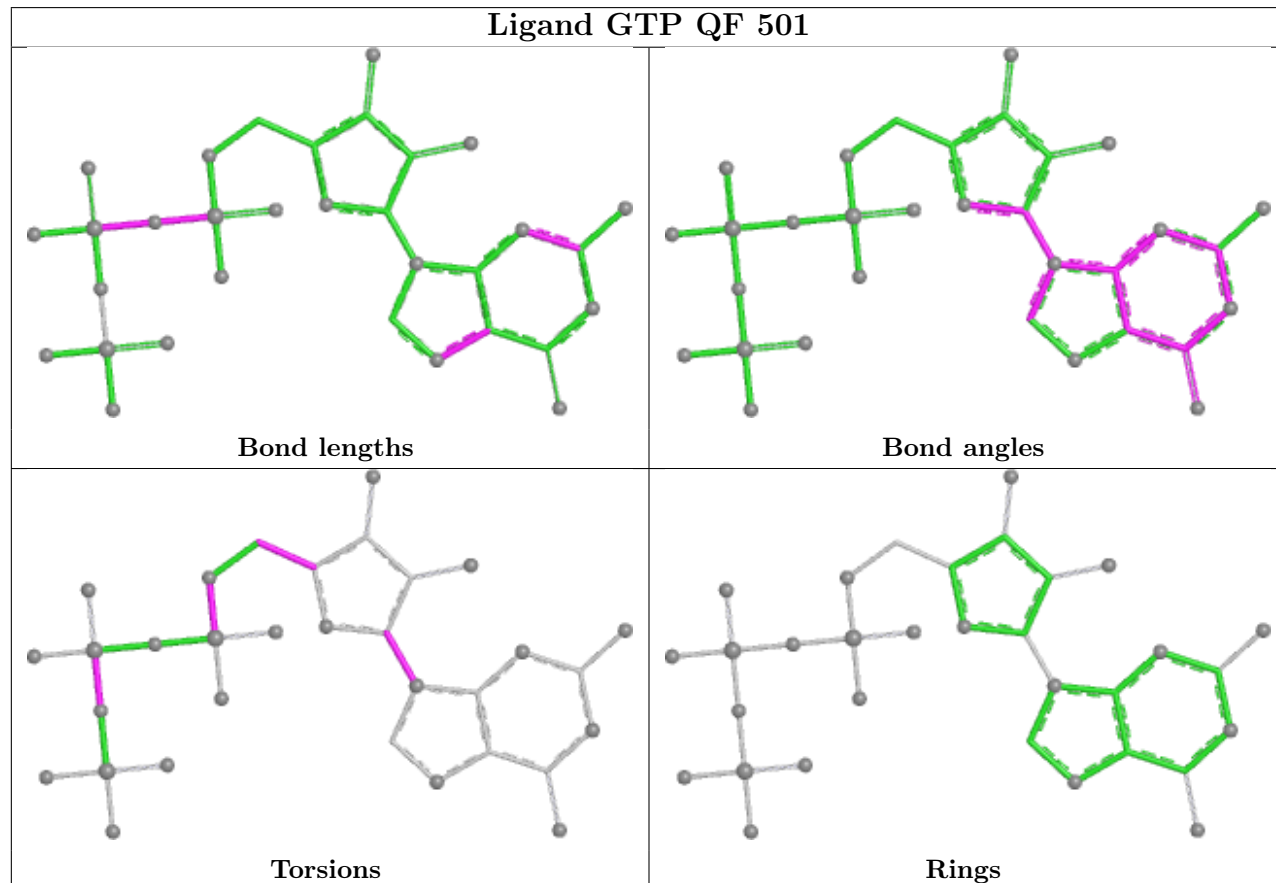
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

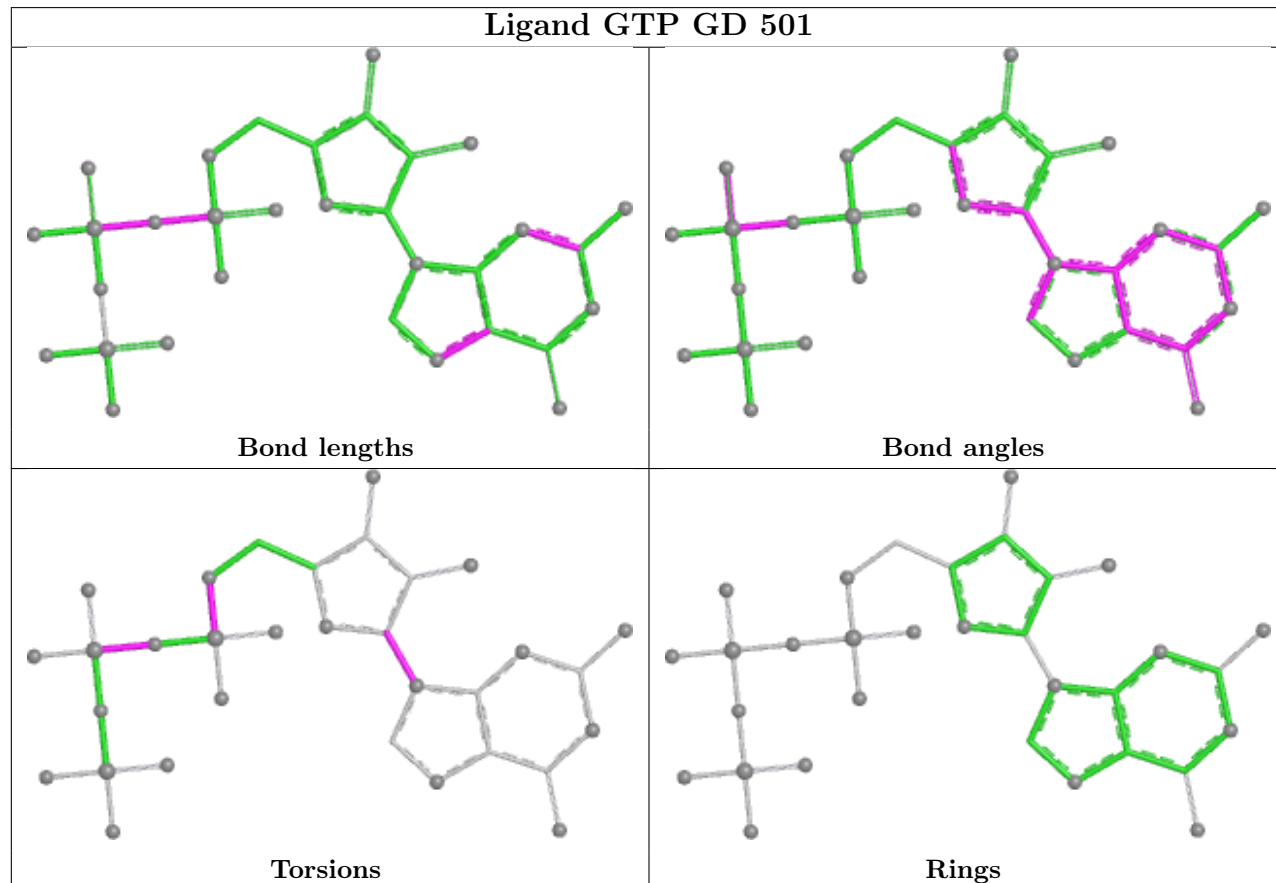
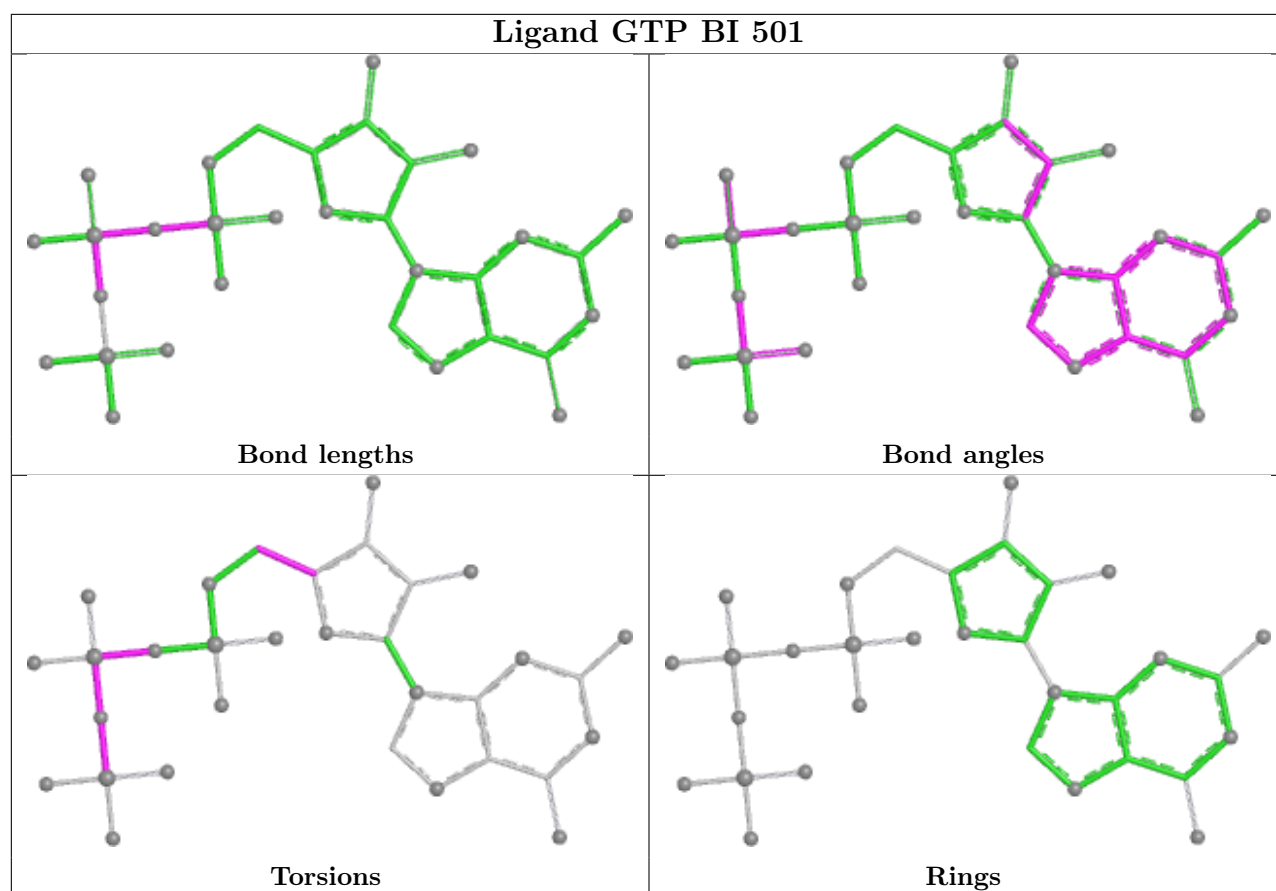


Ligand GTP TJ 501

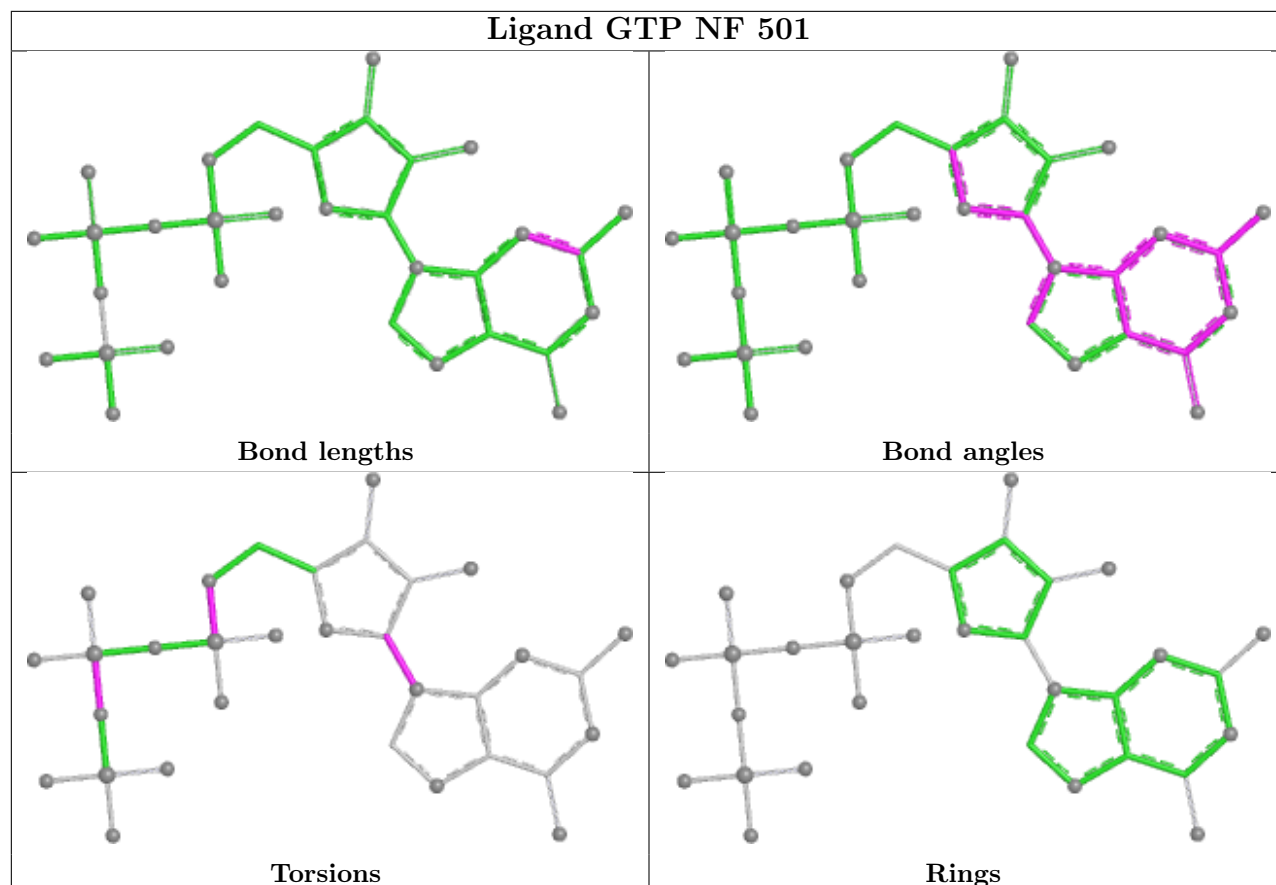


Ligand GTP QF 501

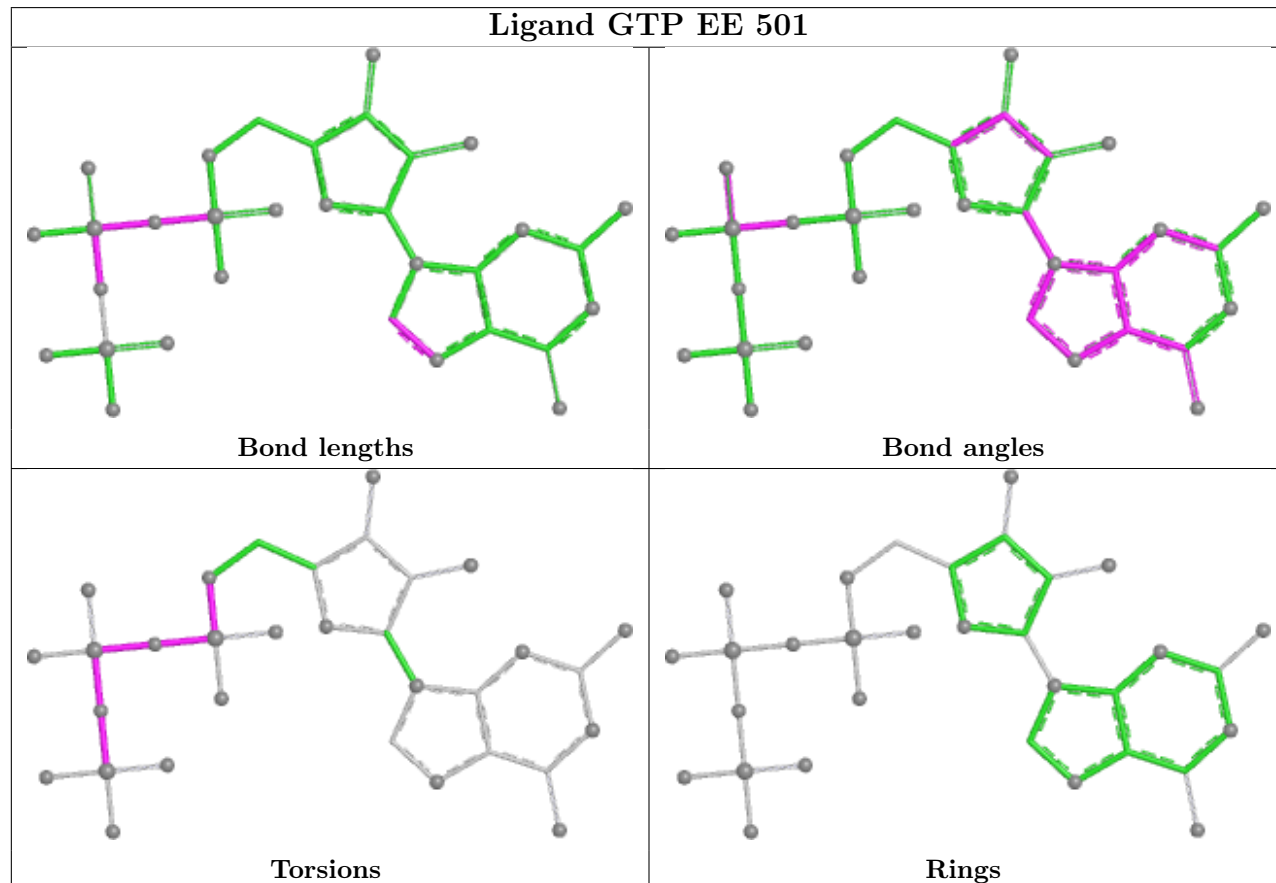




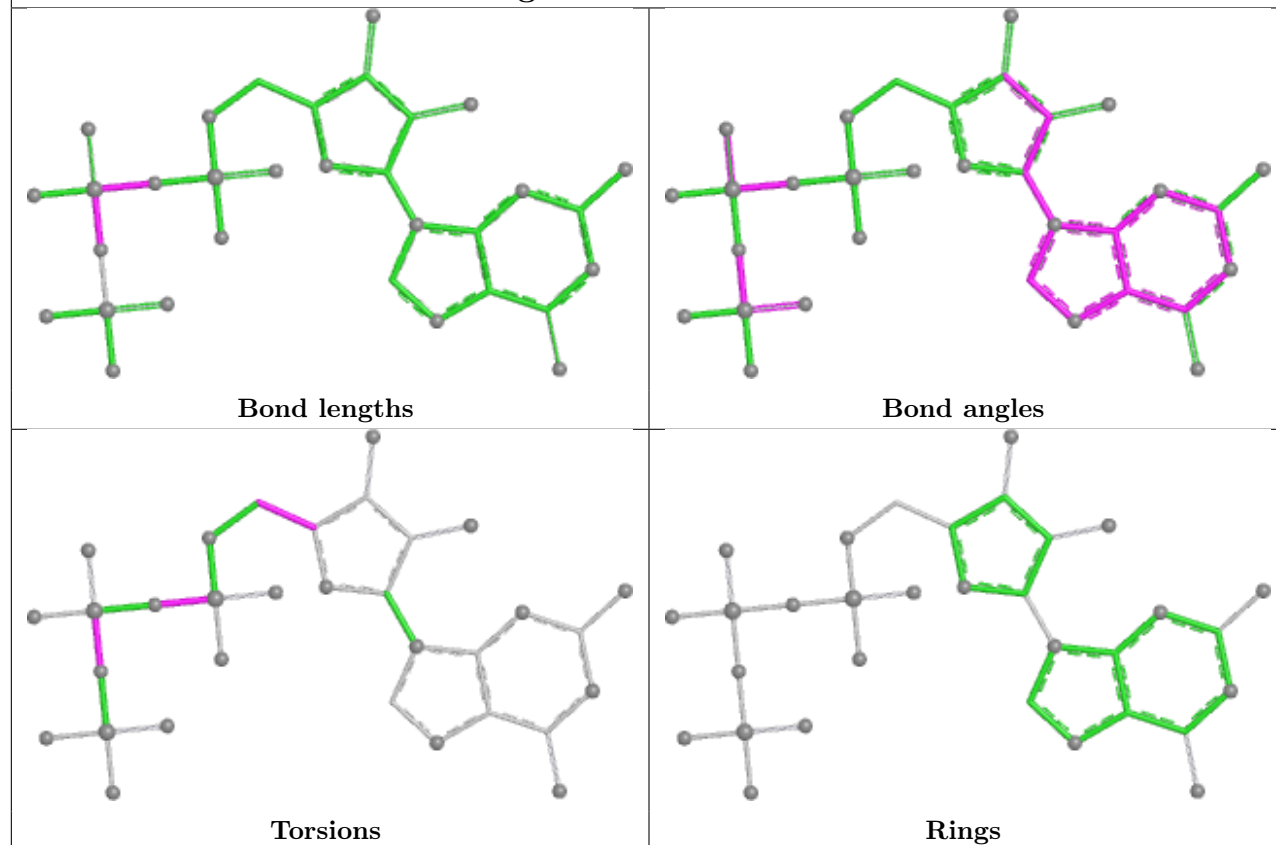
Ligand GTP NF 501



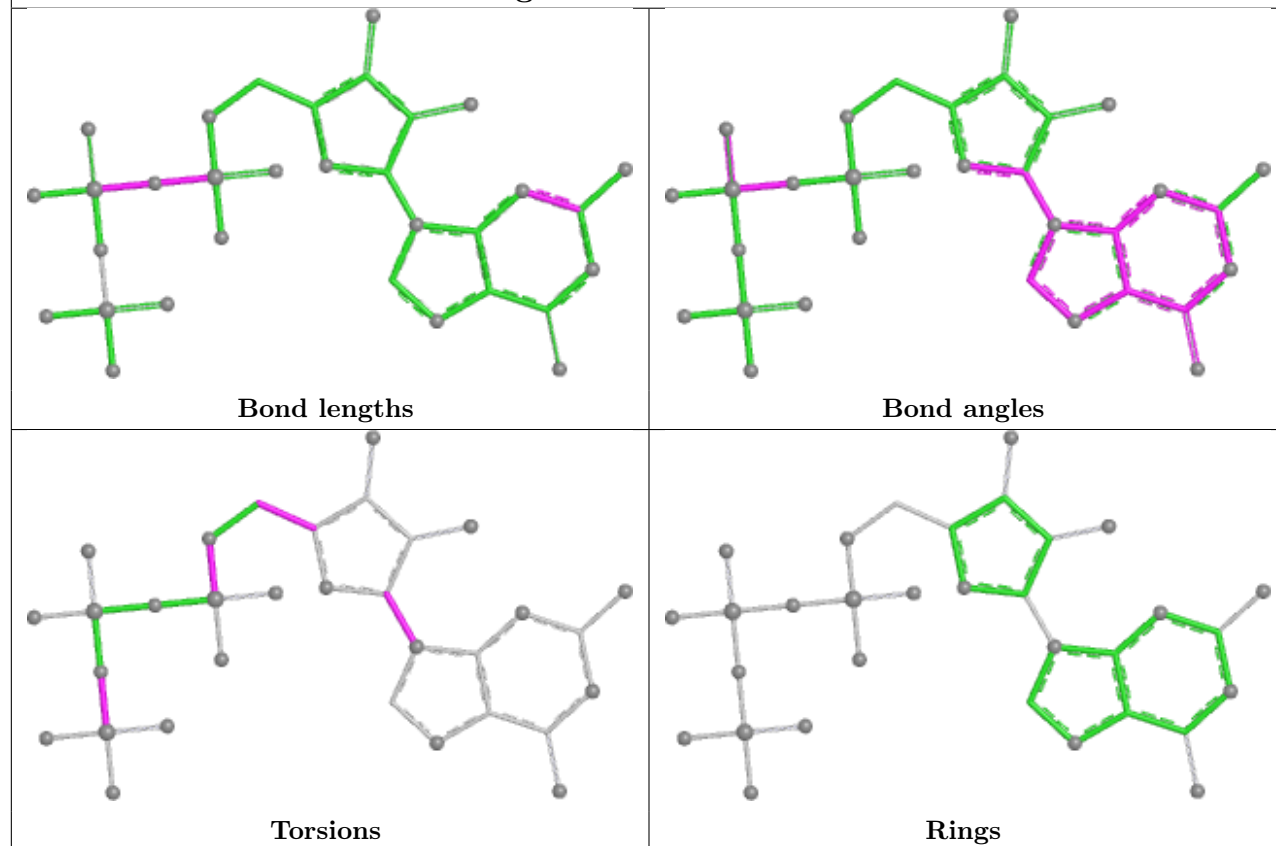
Ligand GTP EE 501

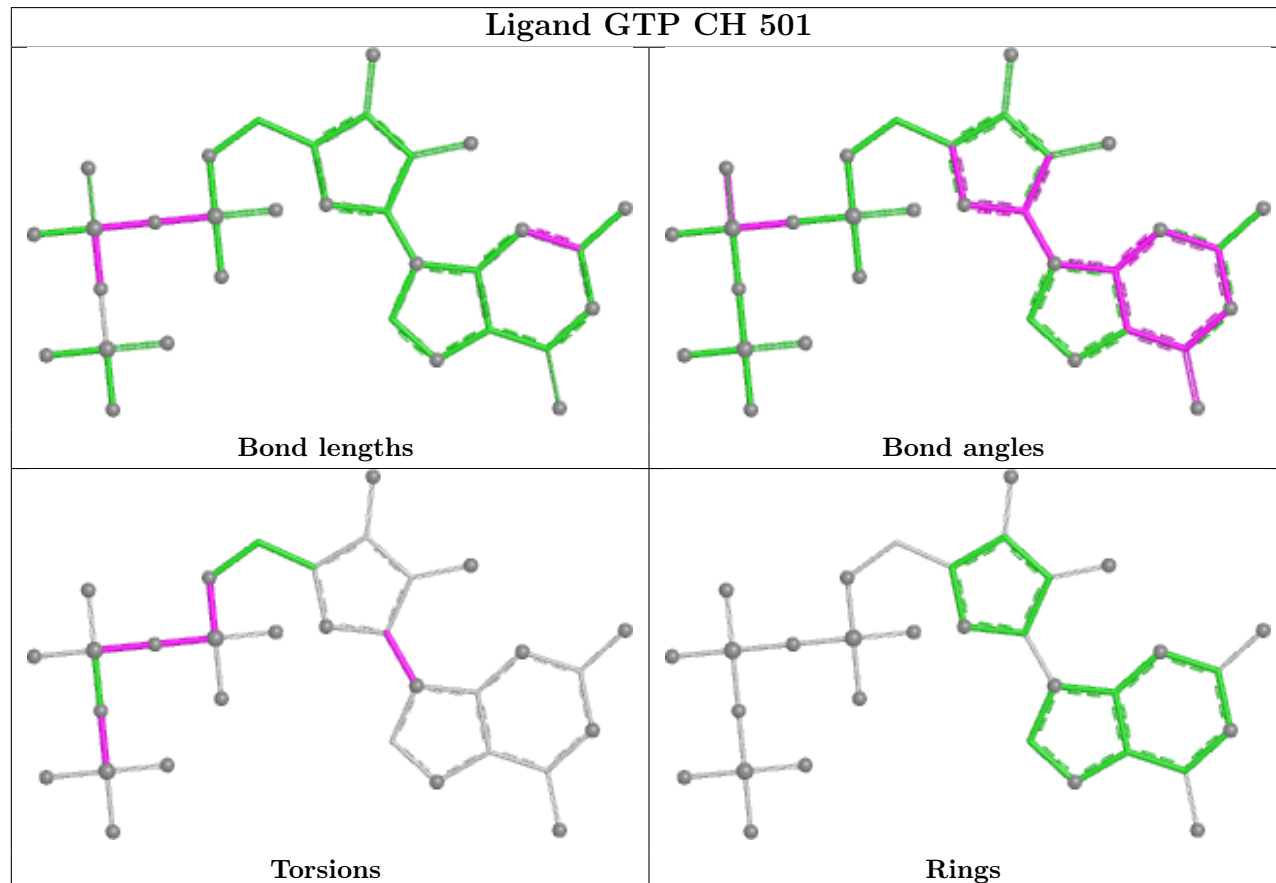
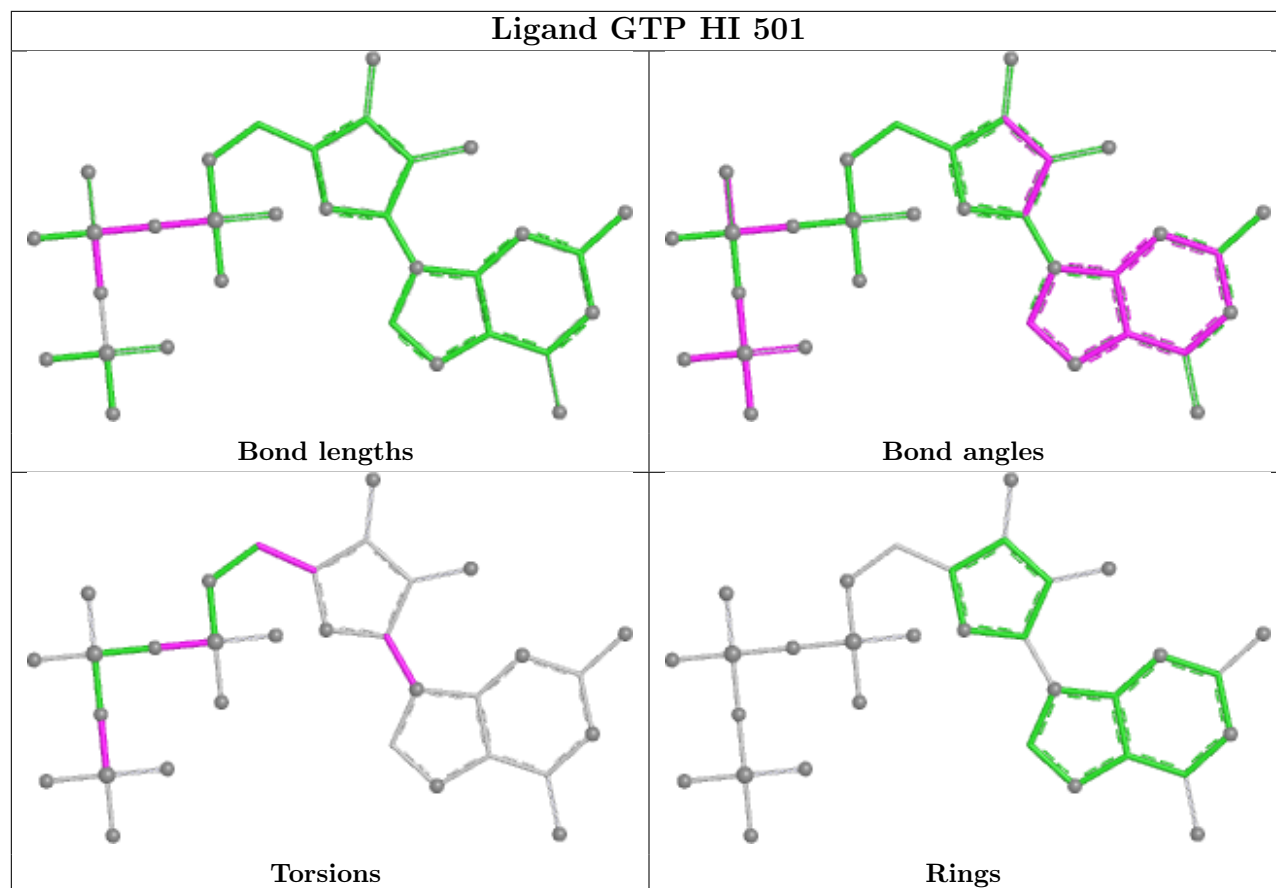


Ligand GTP KE 501

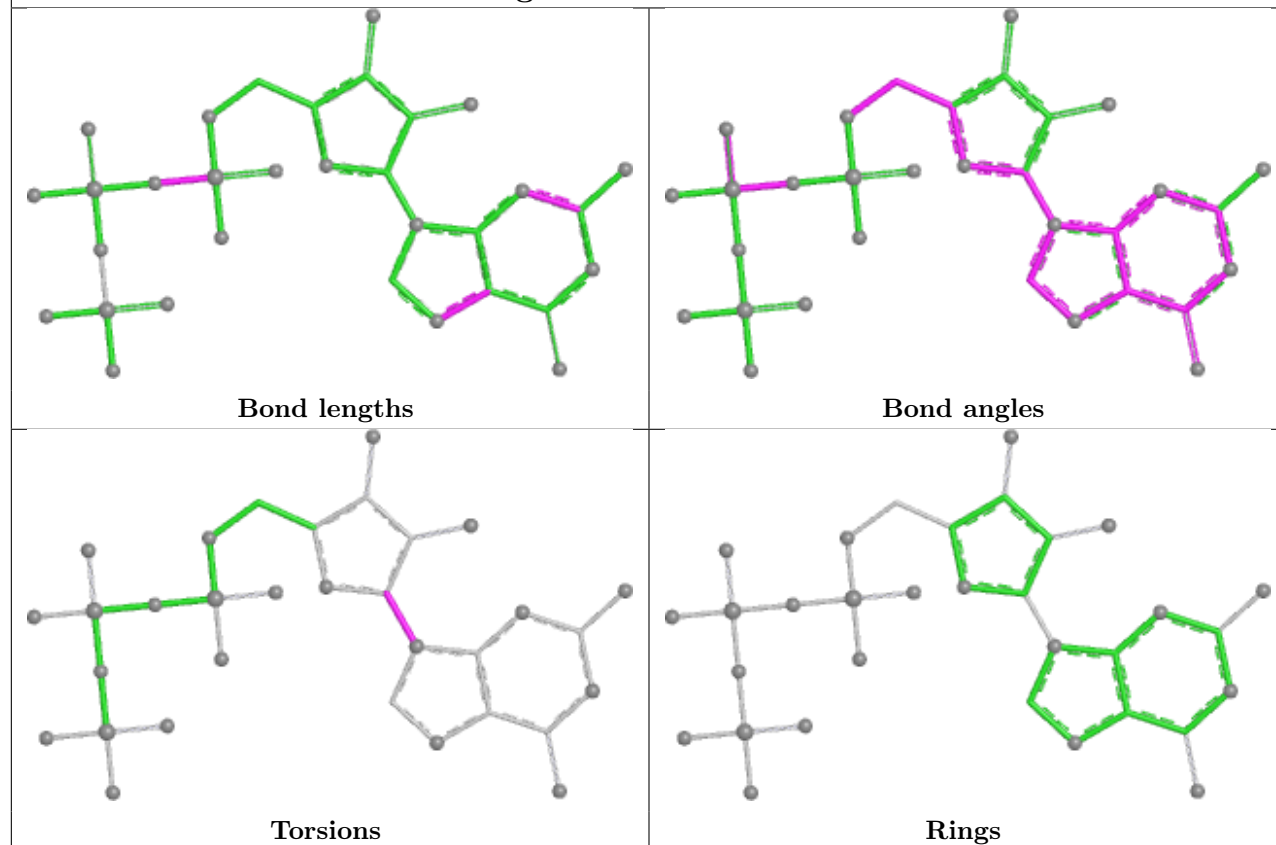


Ligand GTP GH 501

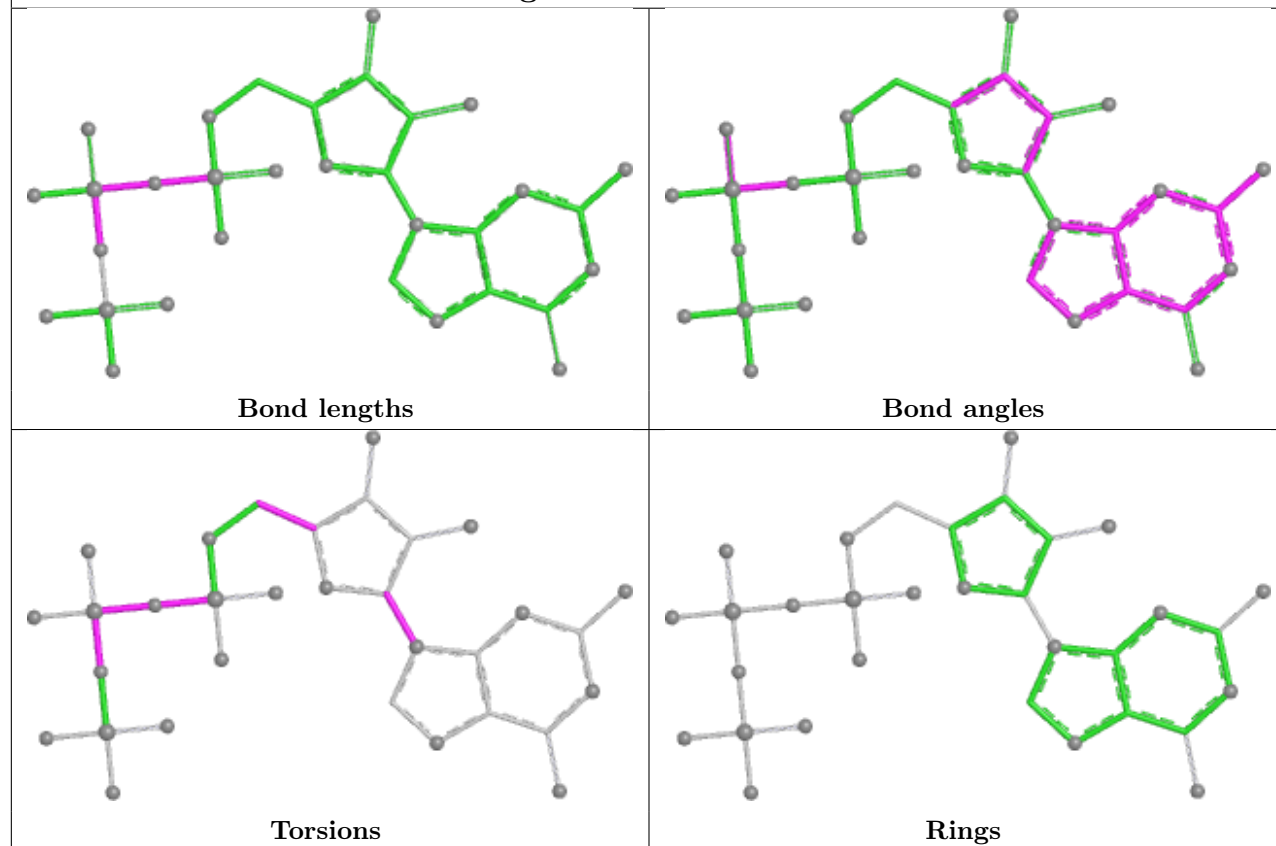


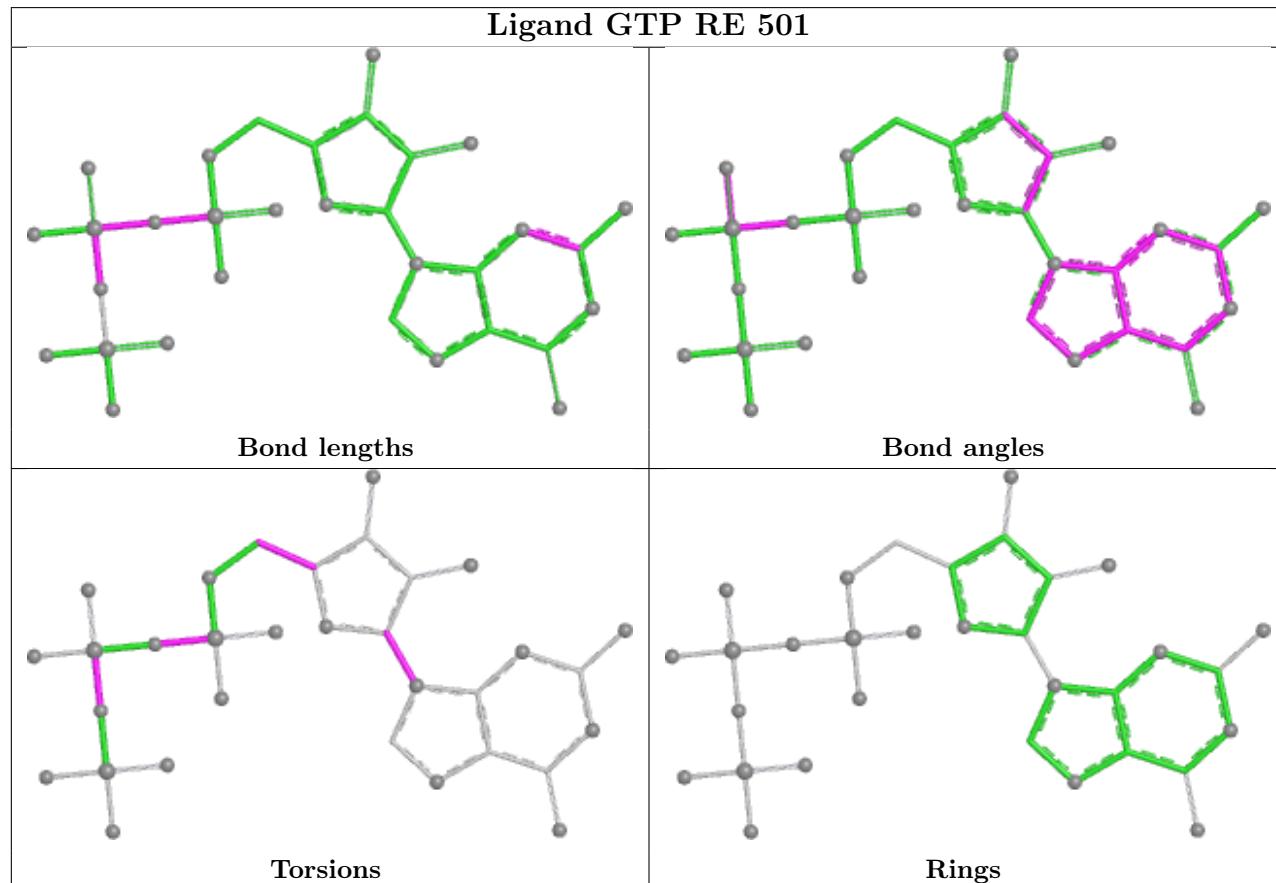
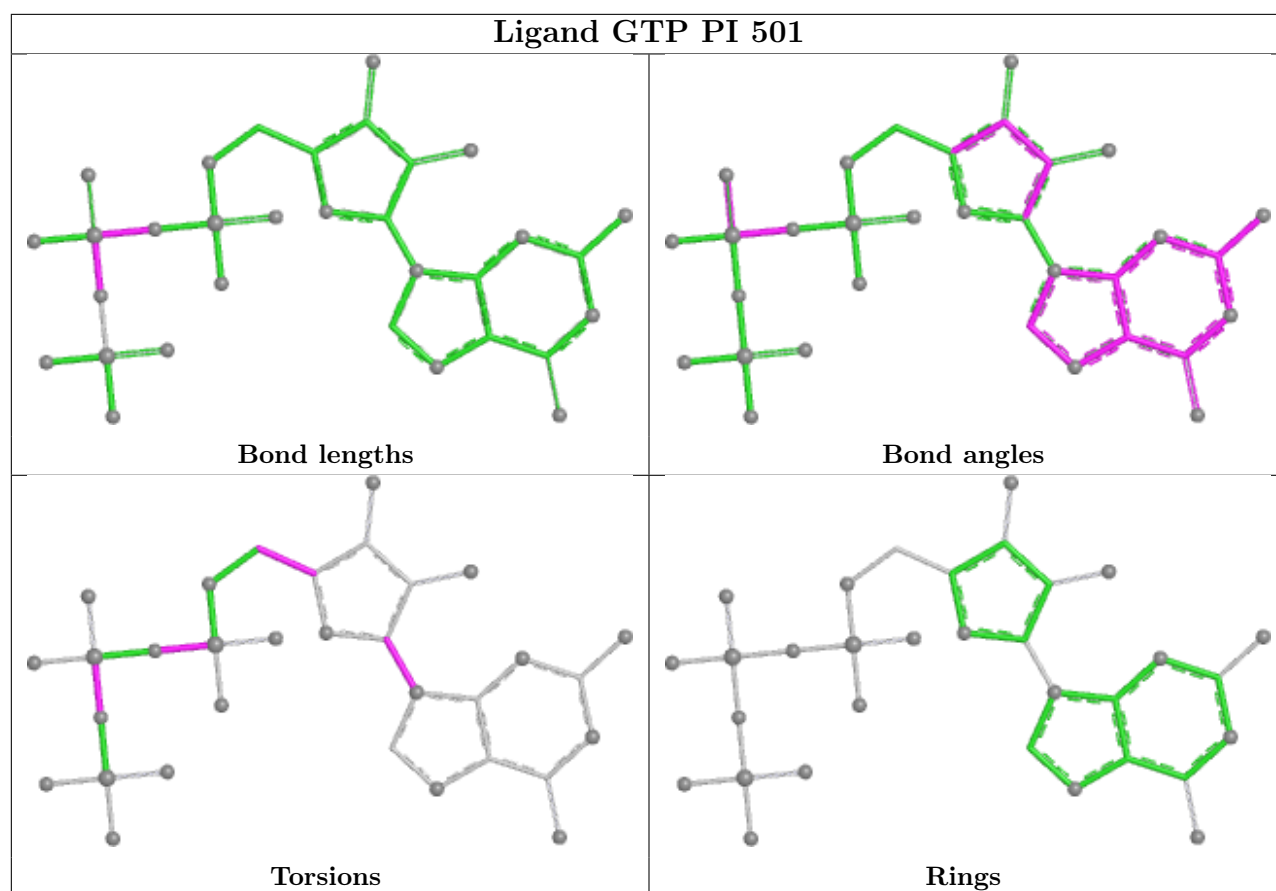


Ligand GTP KD 501

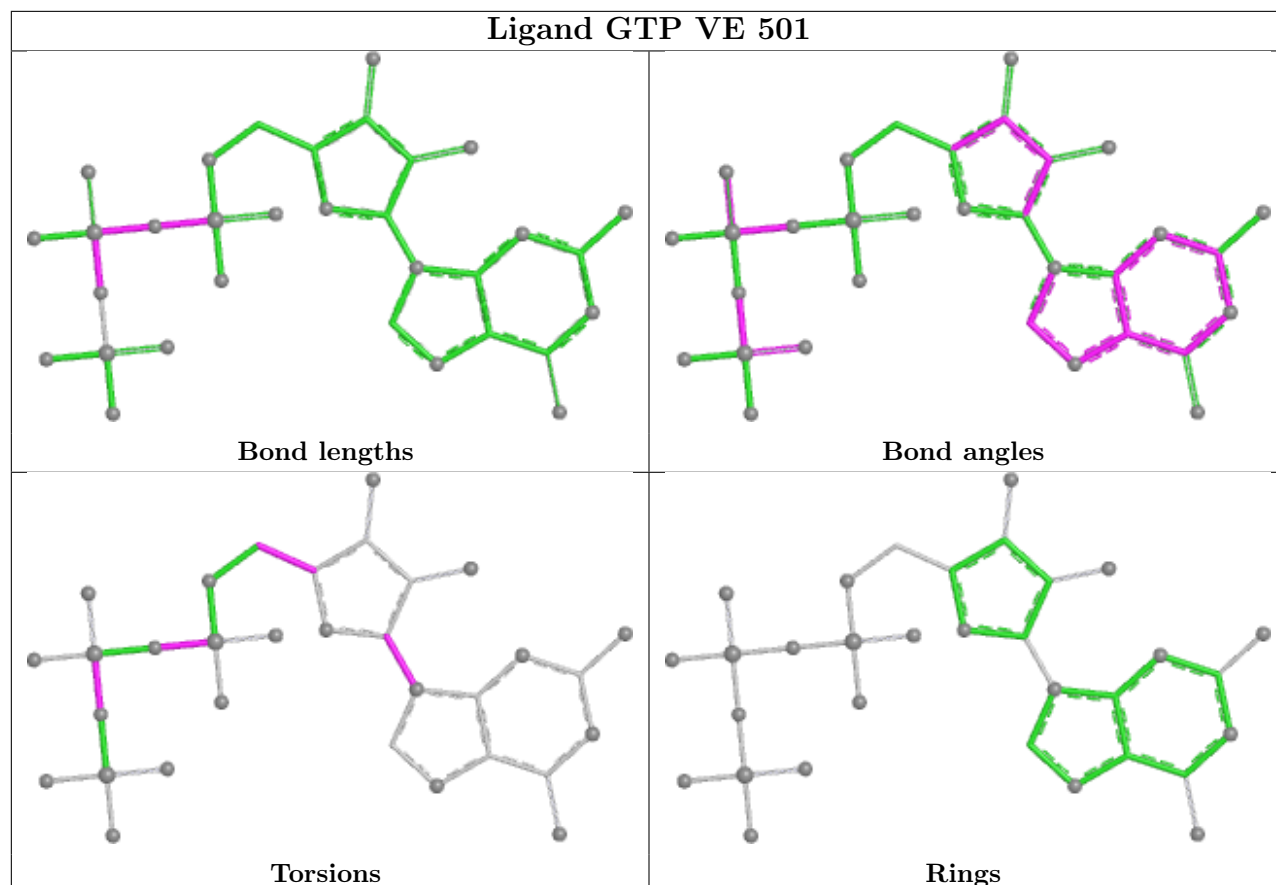


Ligand GTP PE 501

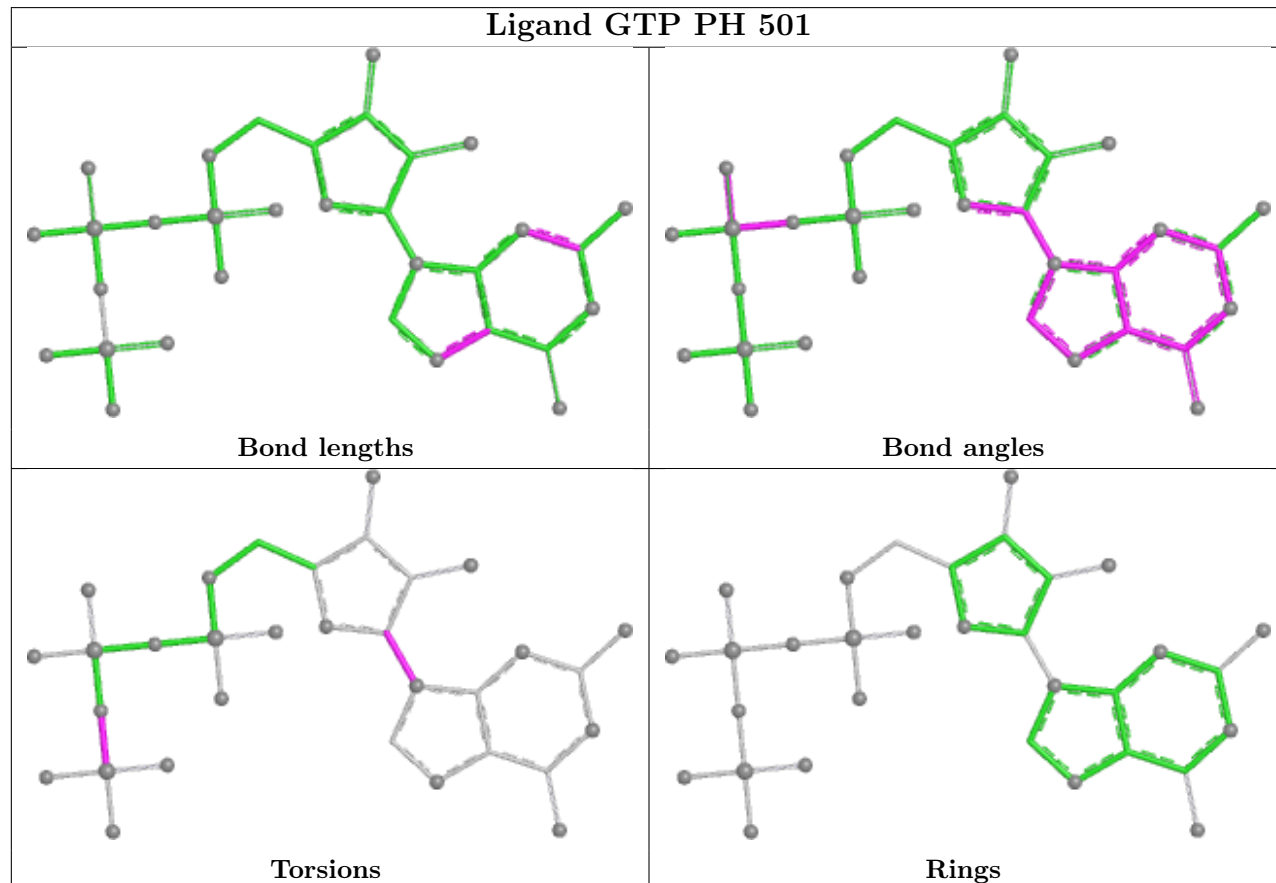




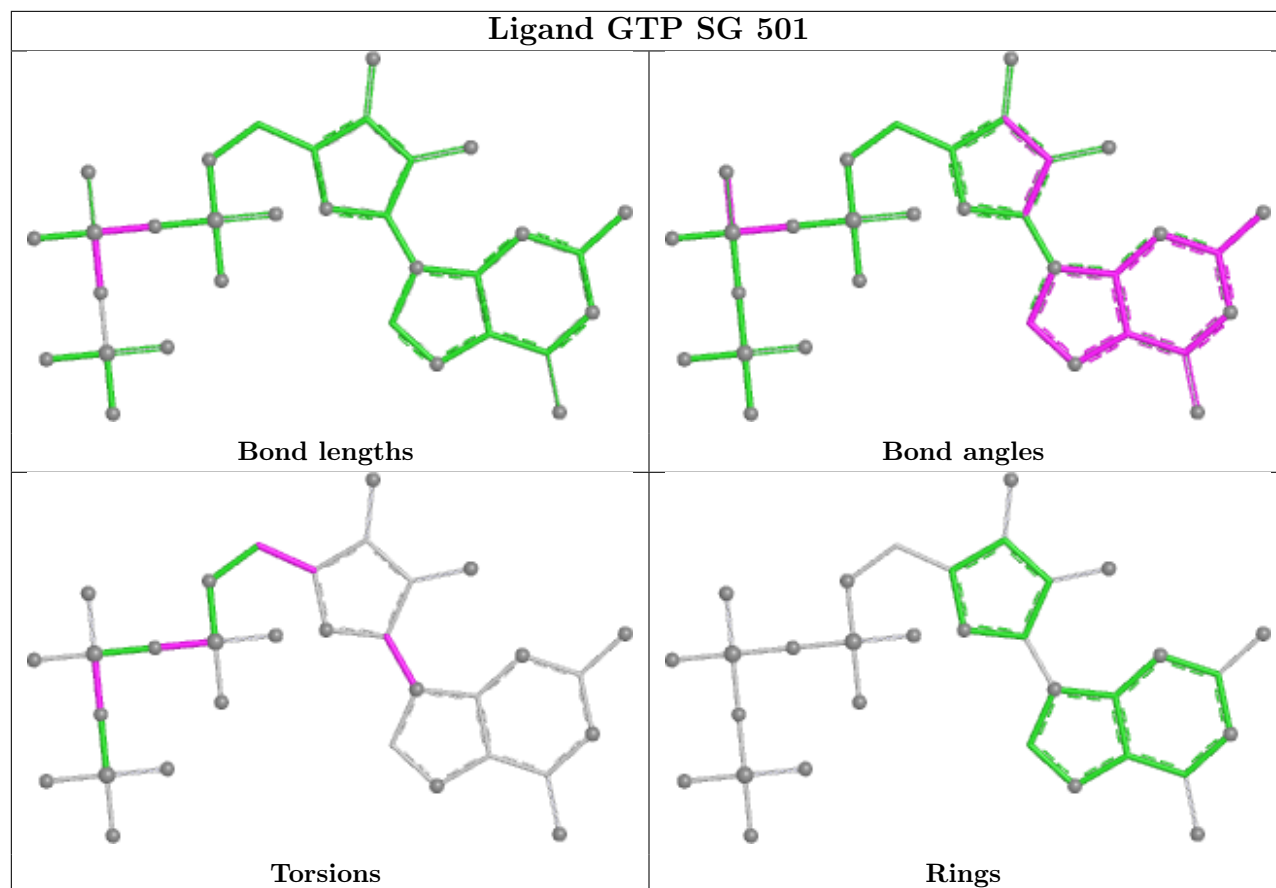
Ligand GTP VE 501



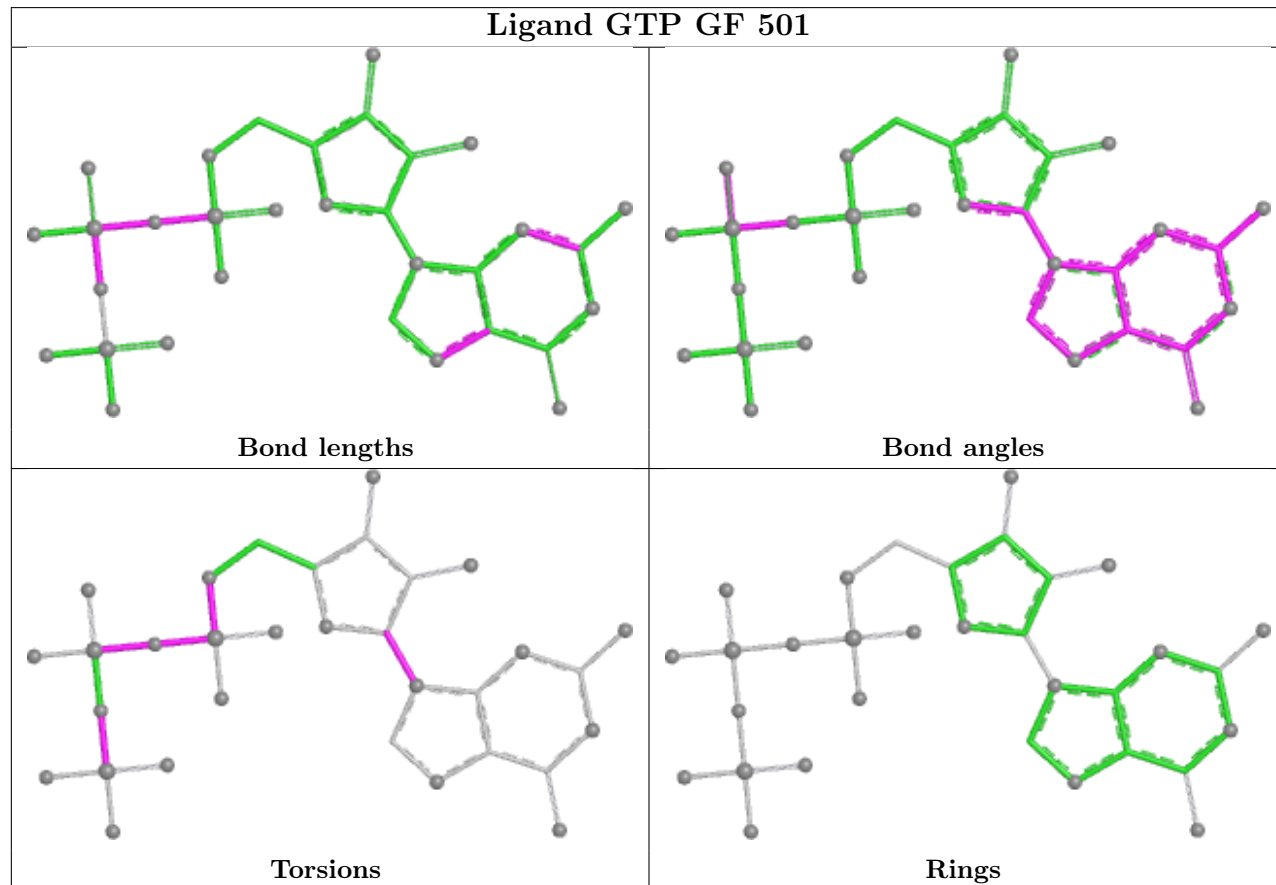
Ligand GTP PH 501



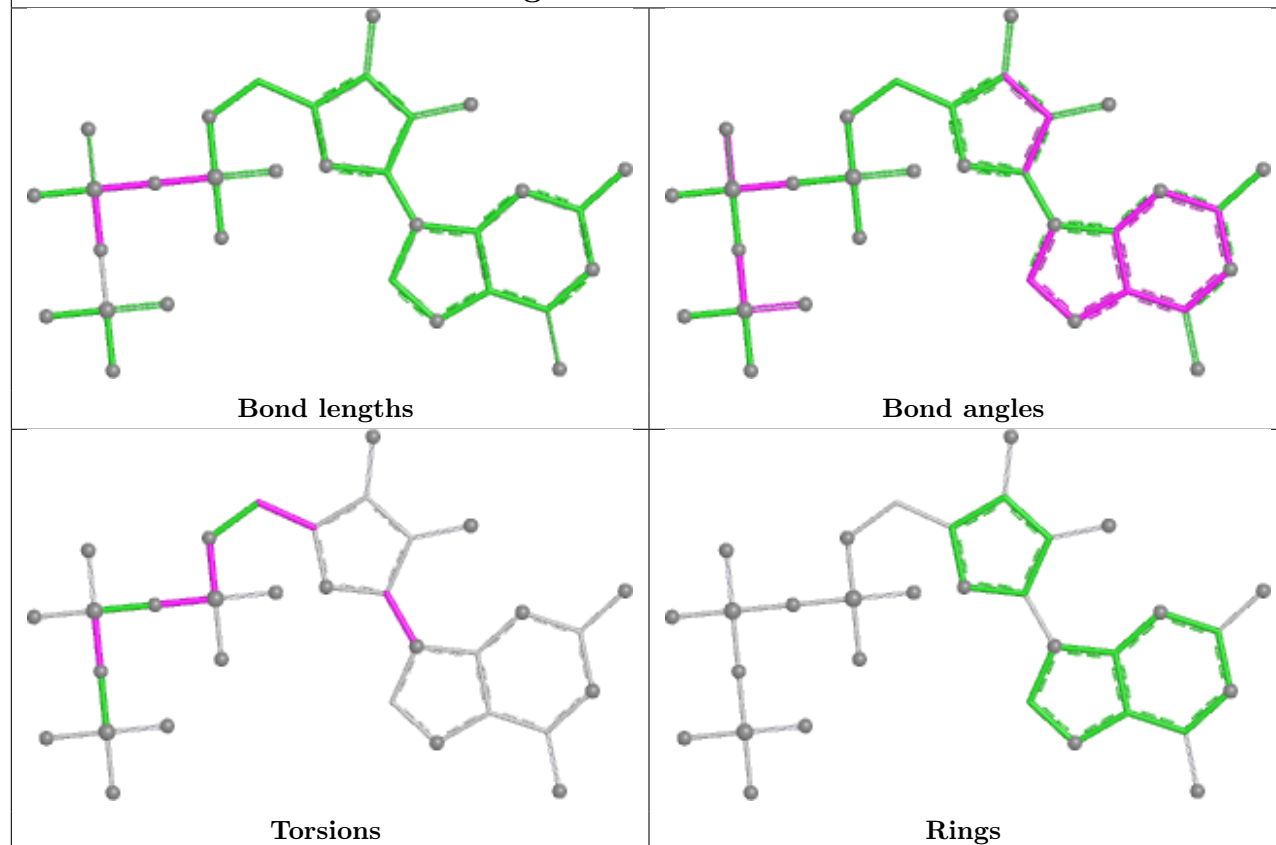
Ligand GTP SG 501



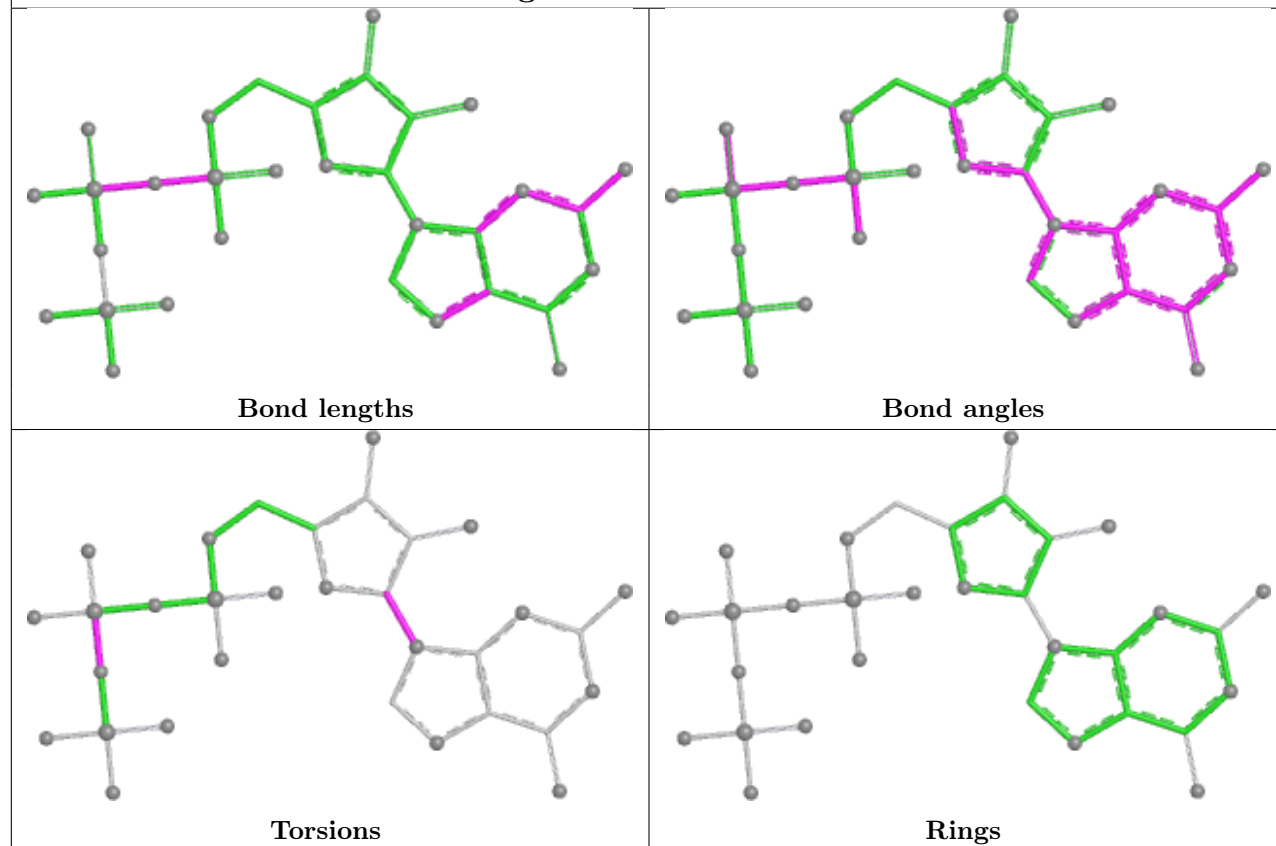
Ligand GTP GF 501

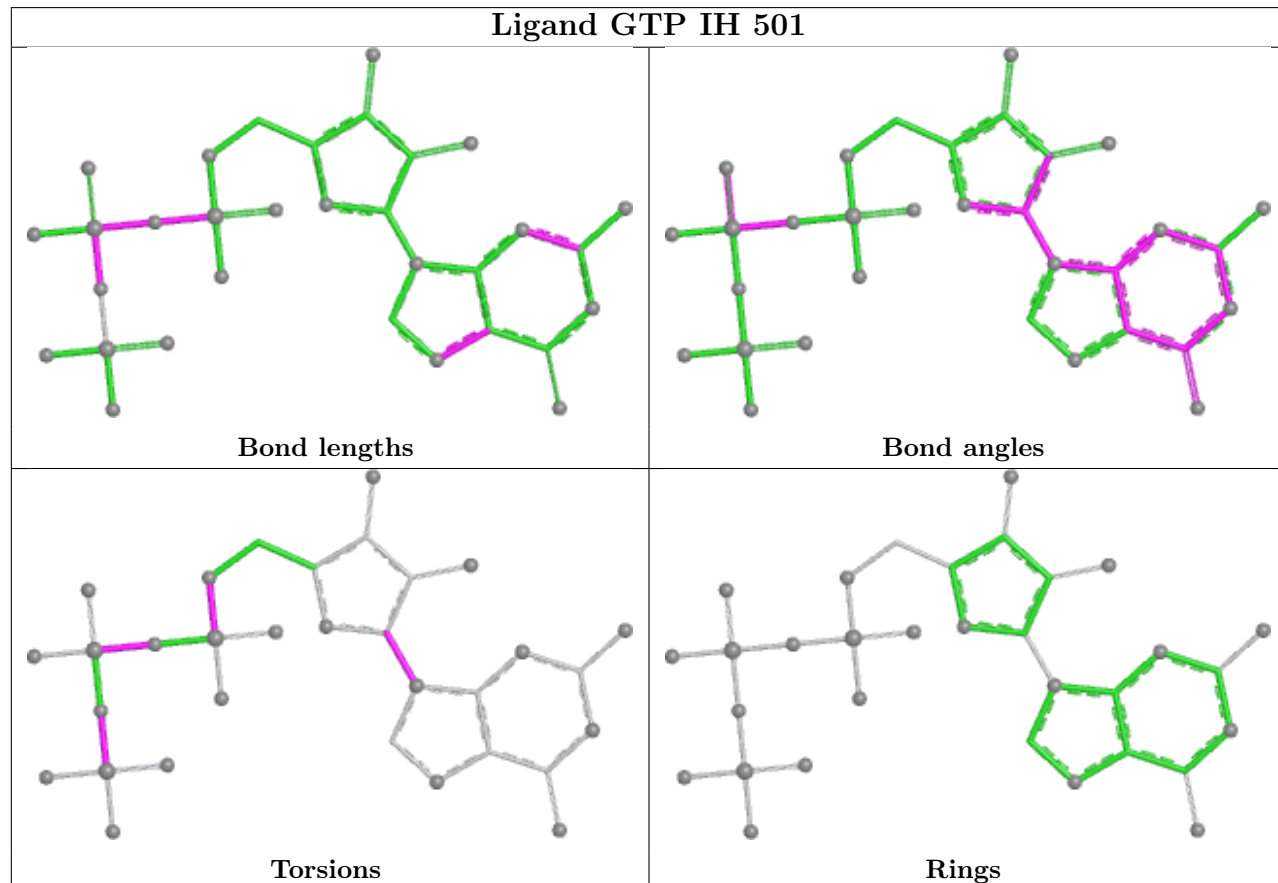
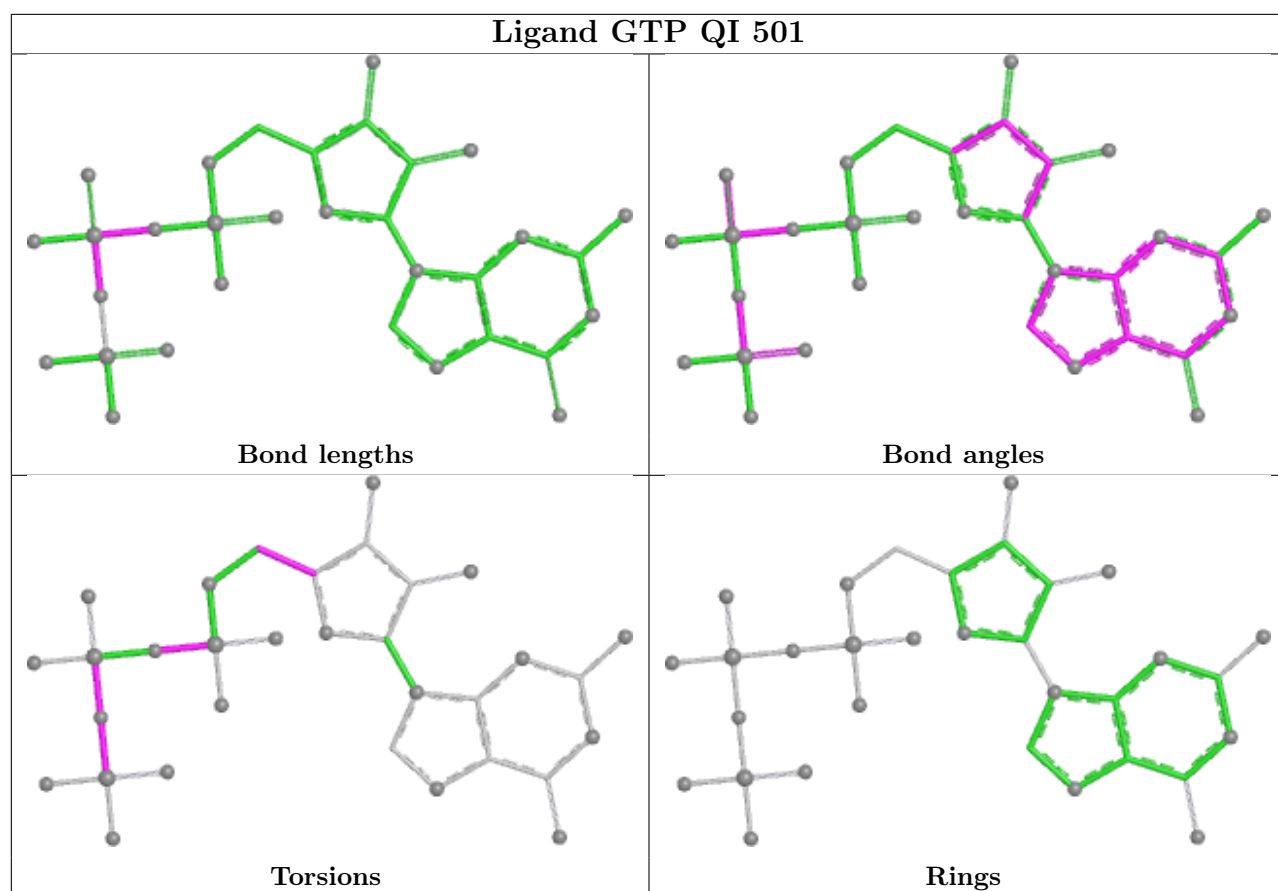


Ligand GTP OI 501

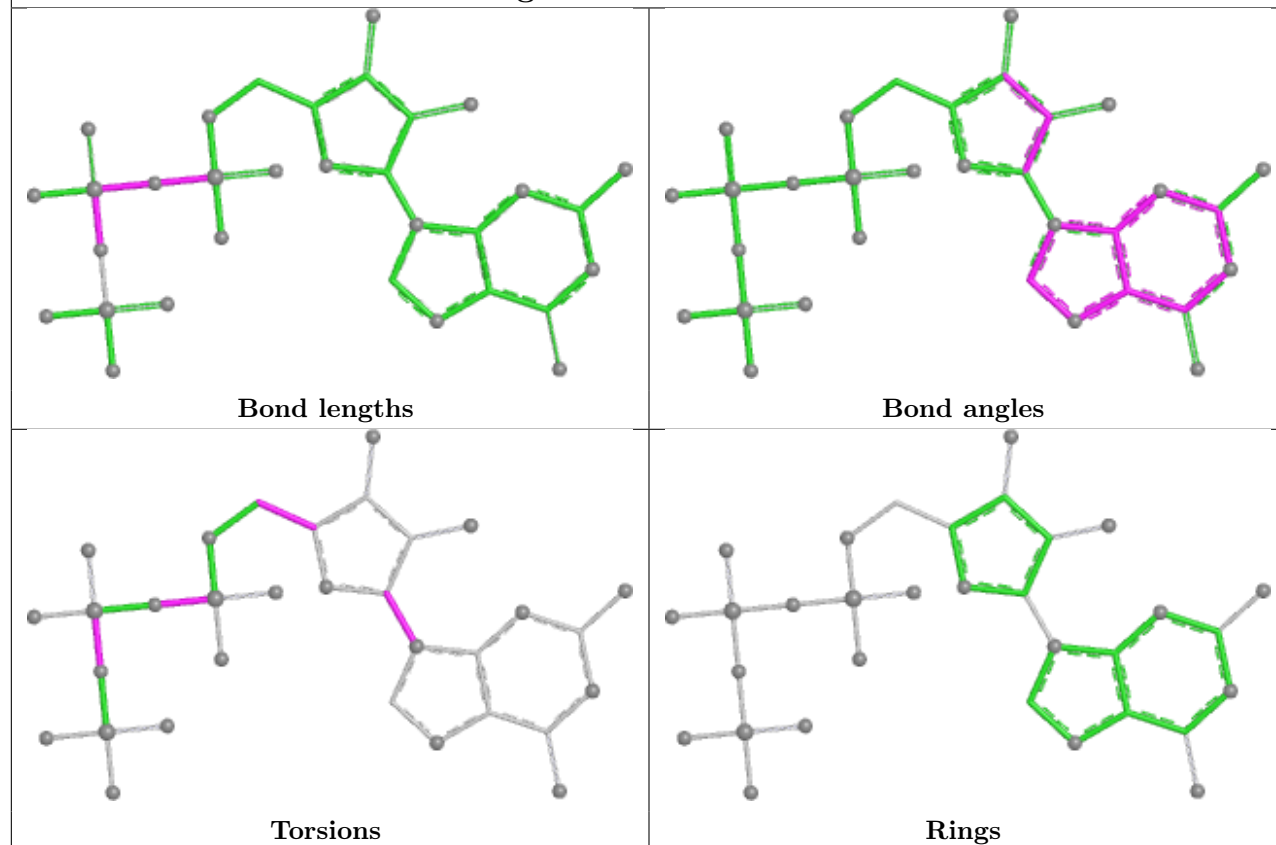


Ligand GTP ED 501

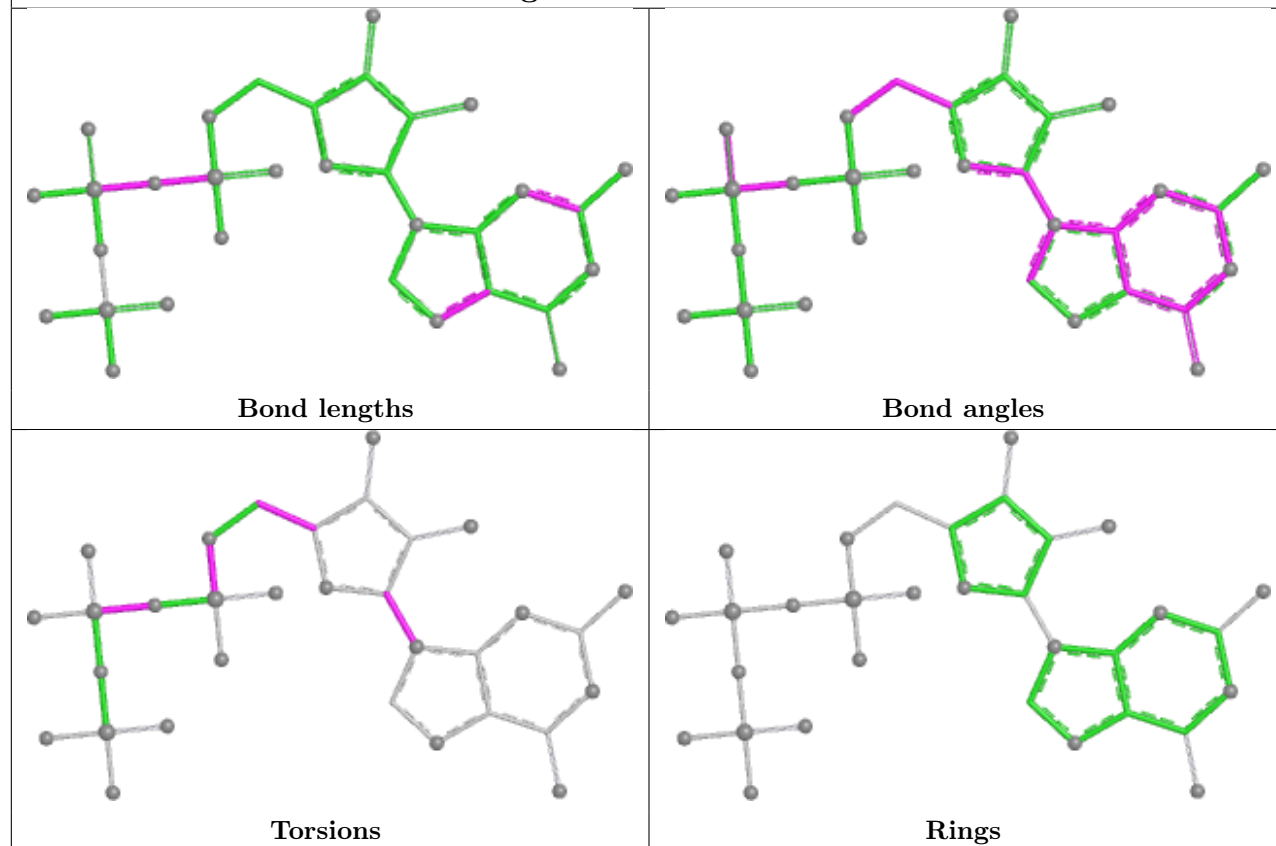




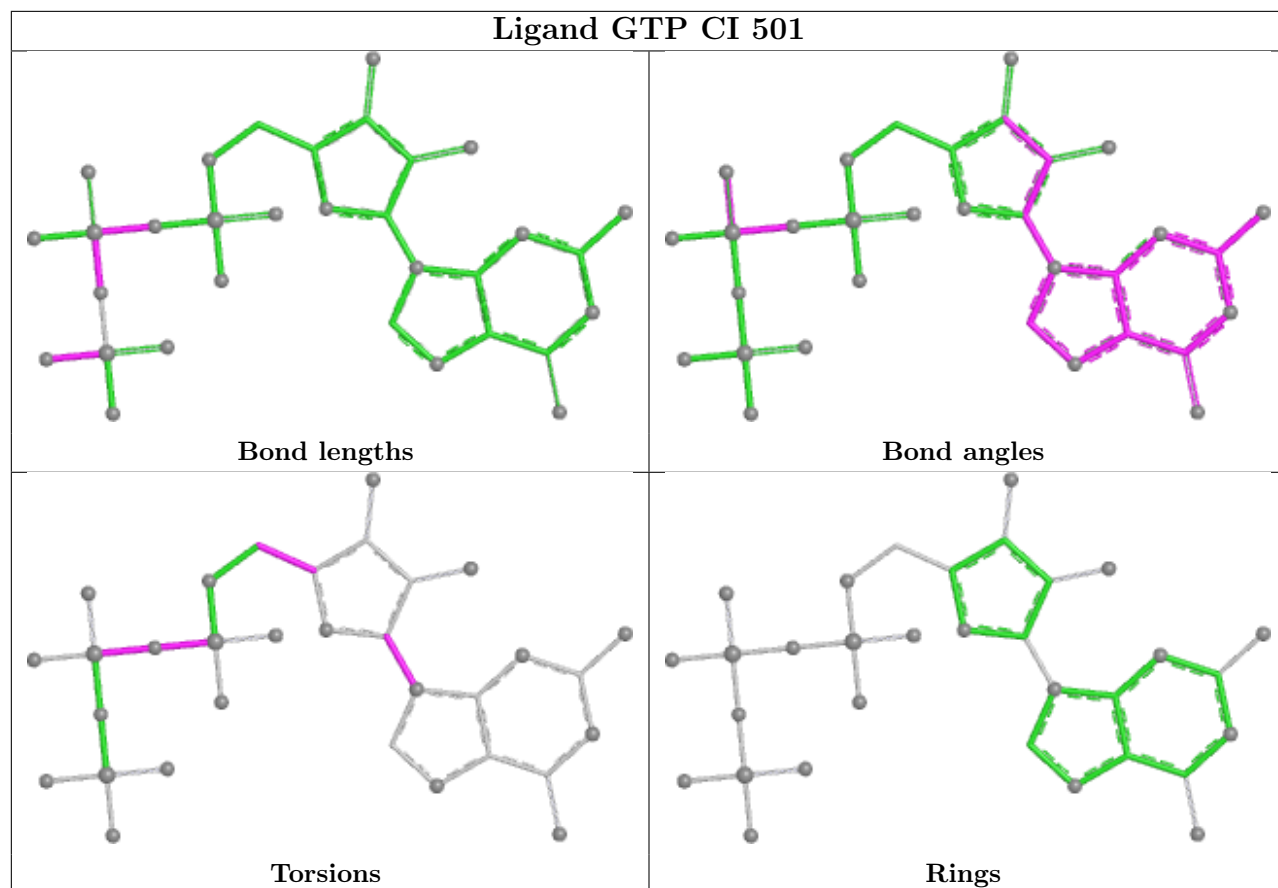
Ligand GTP TG 501



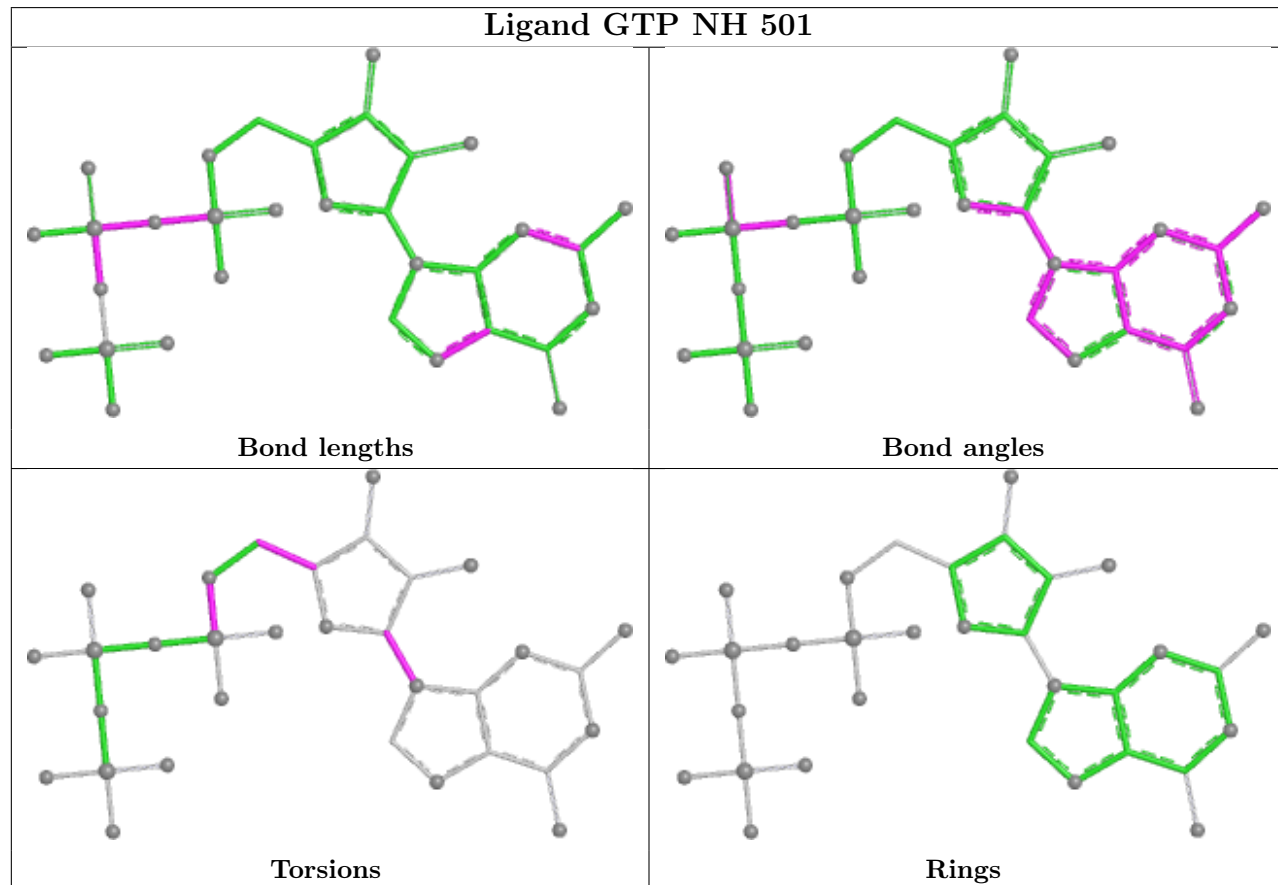
Ligand GTP EF 501



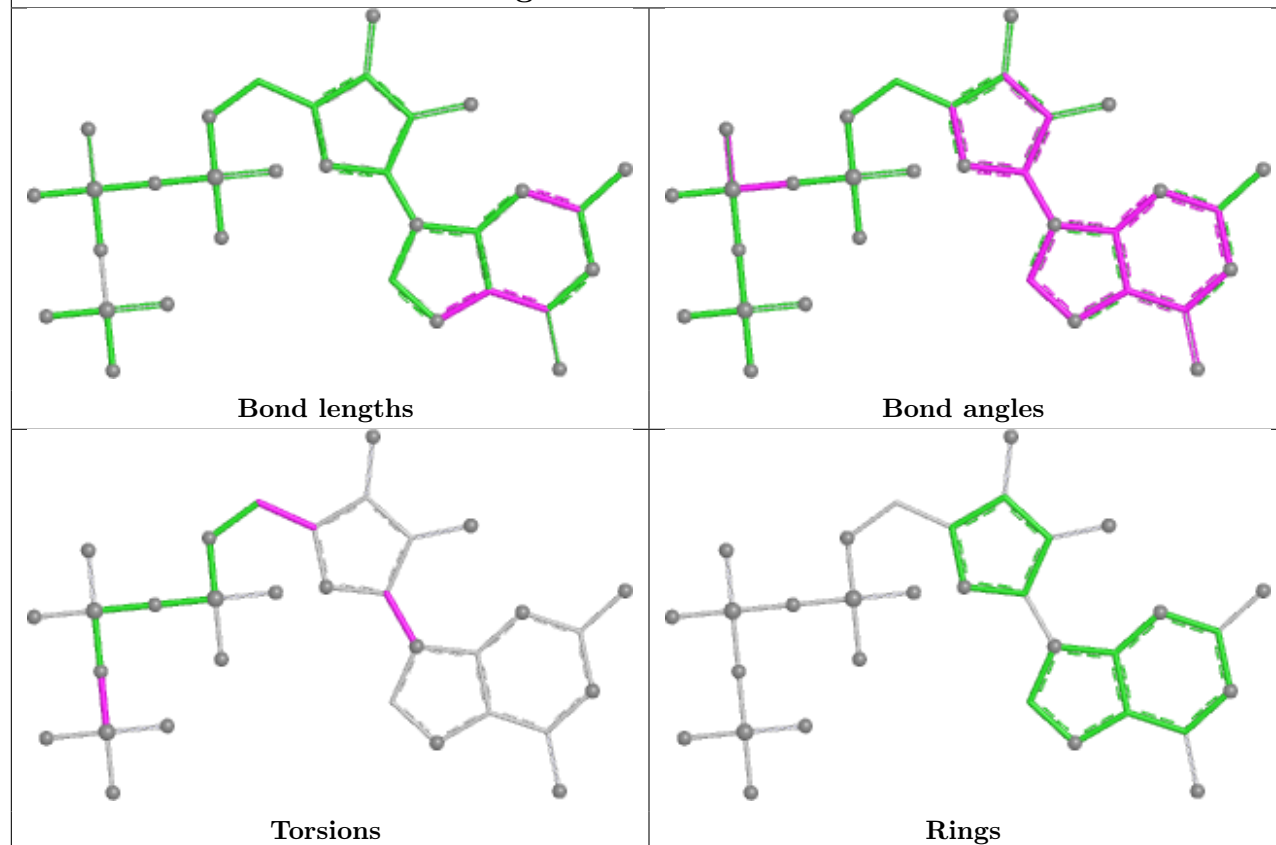
Ligand GTP CI 501



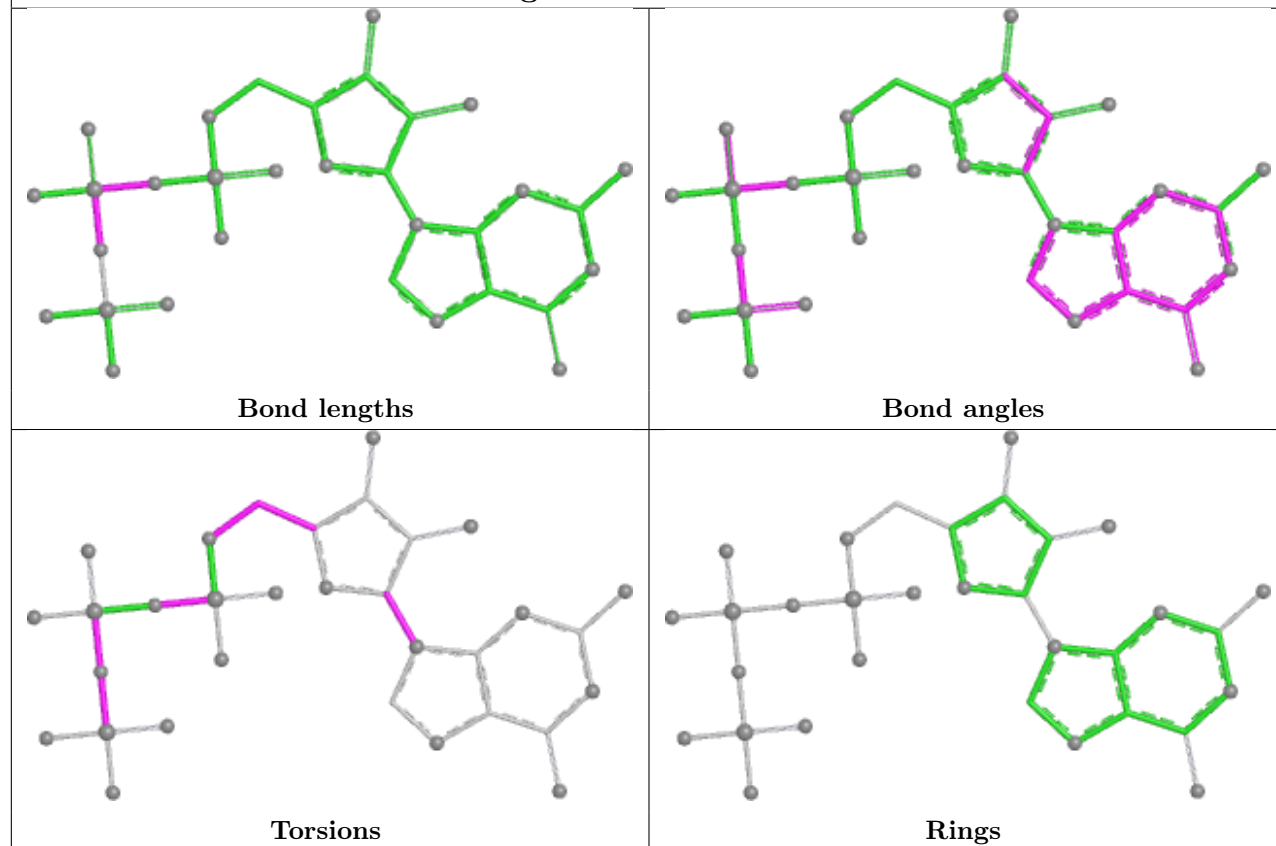
Ligand GTP NH 501



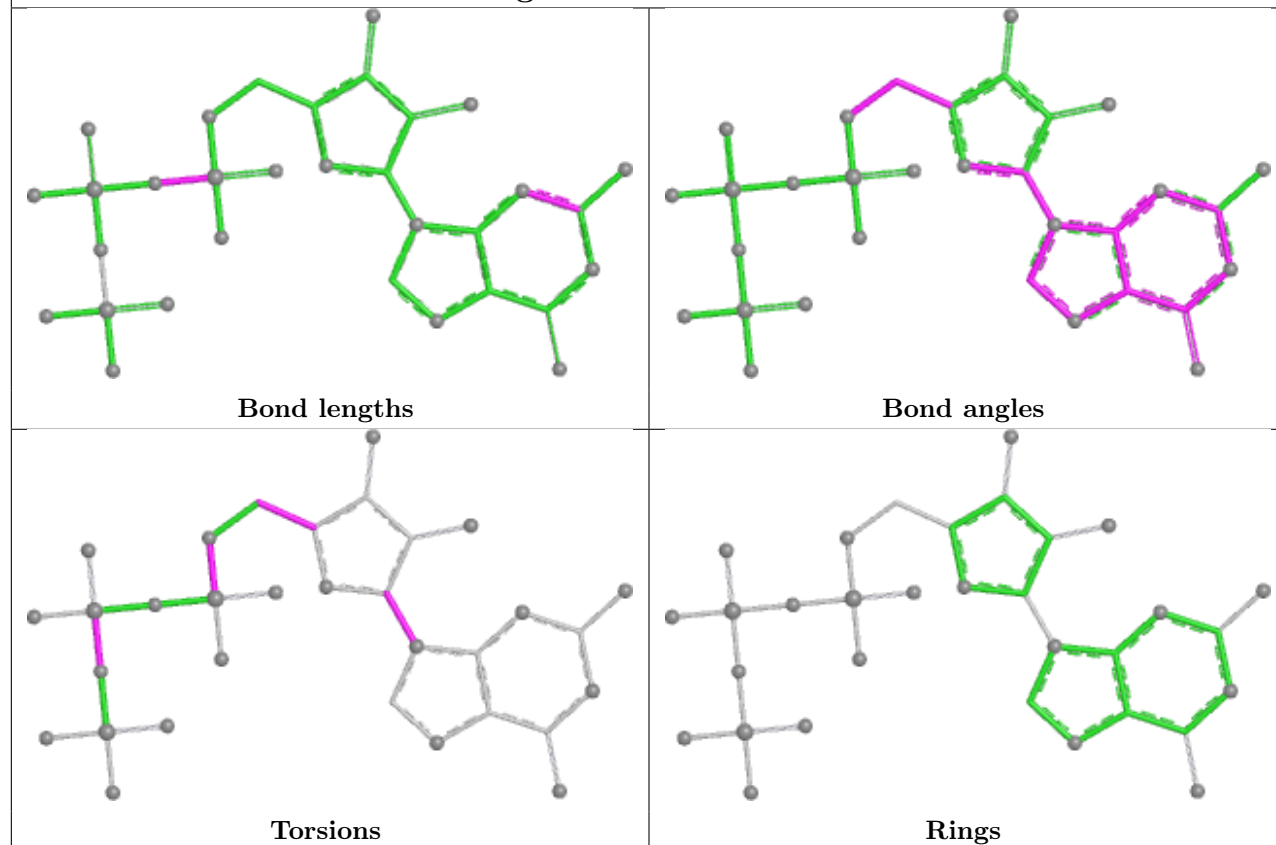
Ligand GTP HG 501



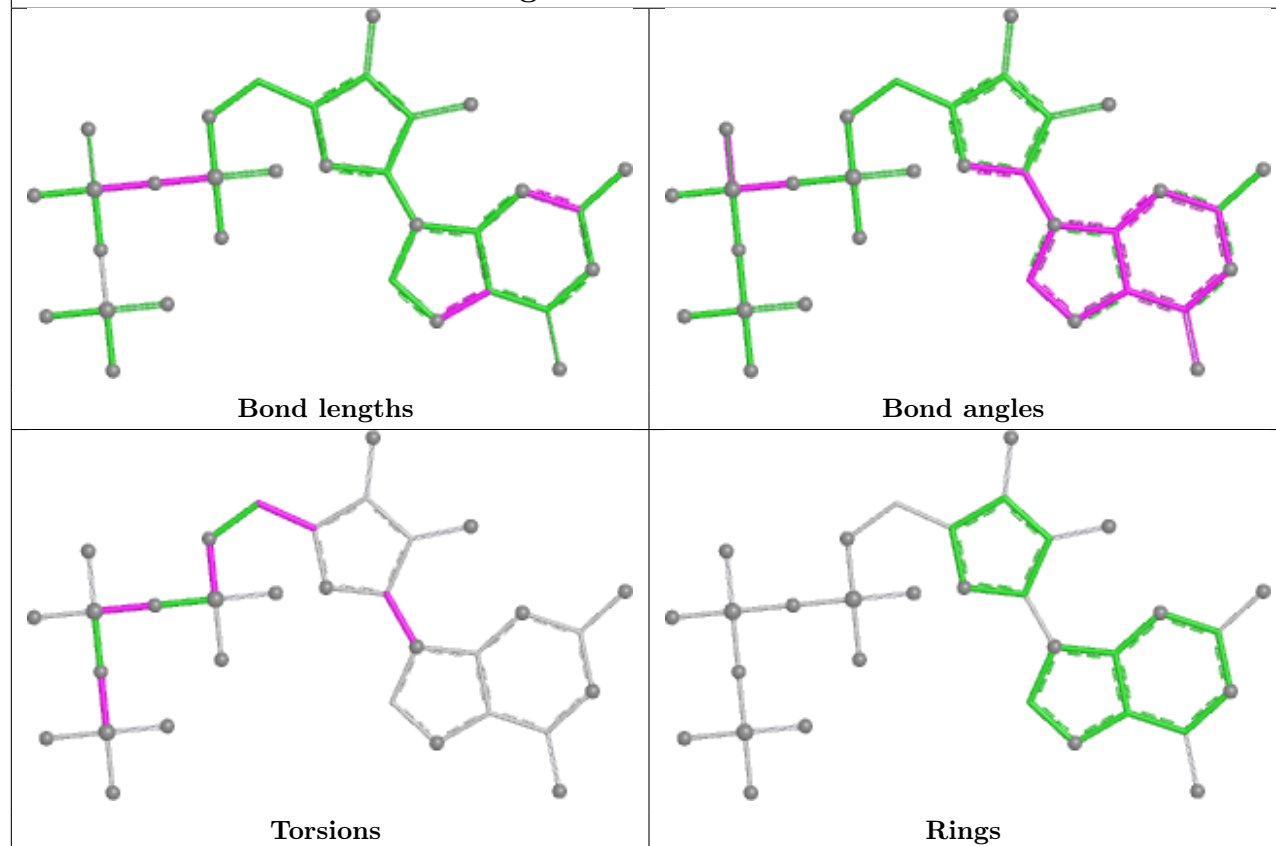
Ligand GTP JG 501



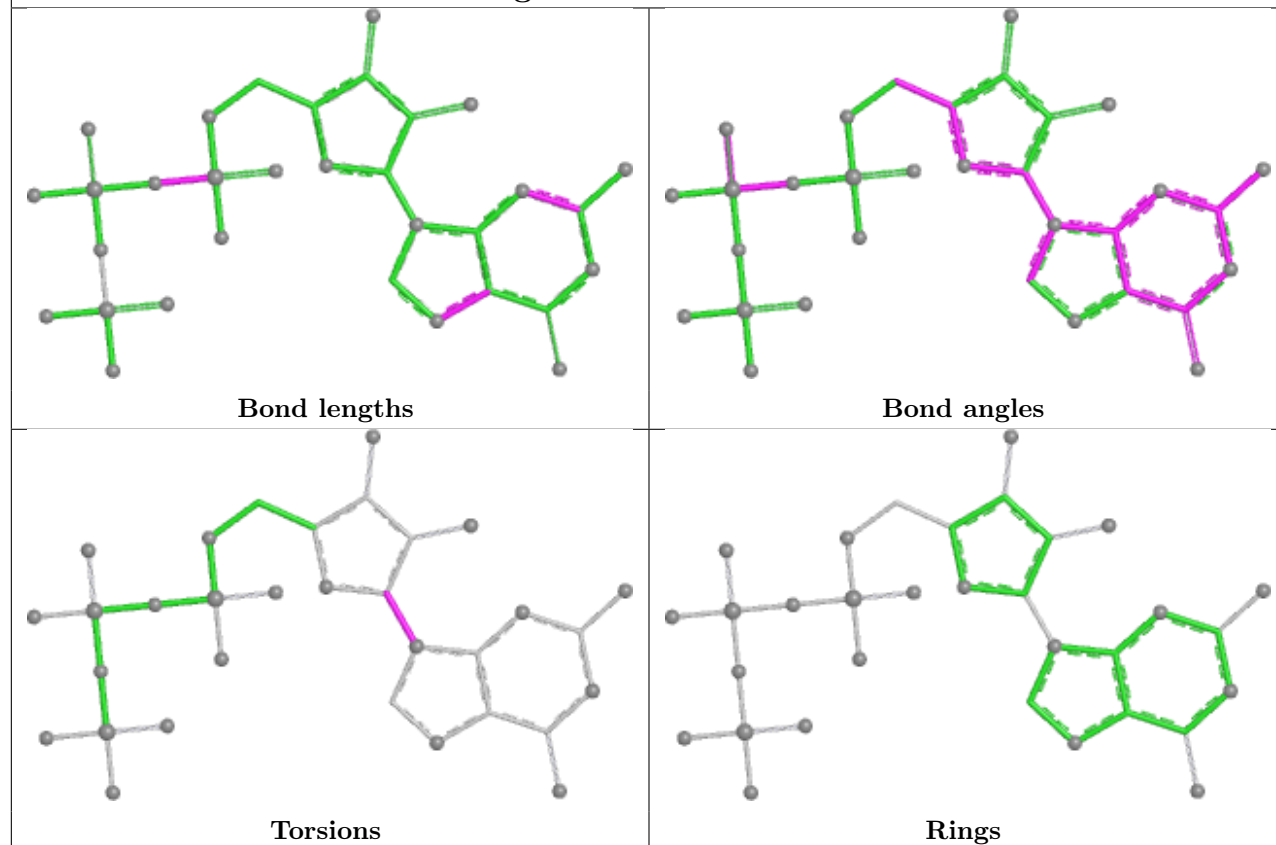
Ligand GTP OD 501



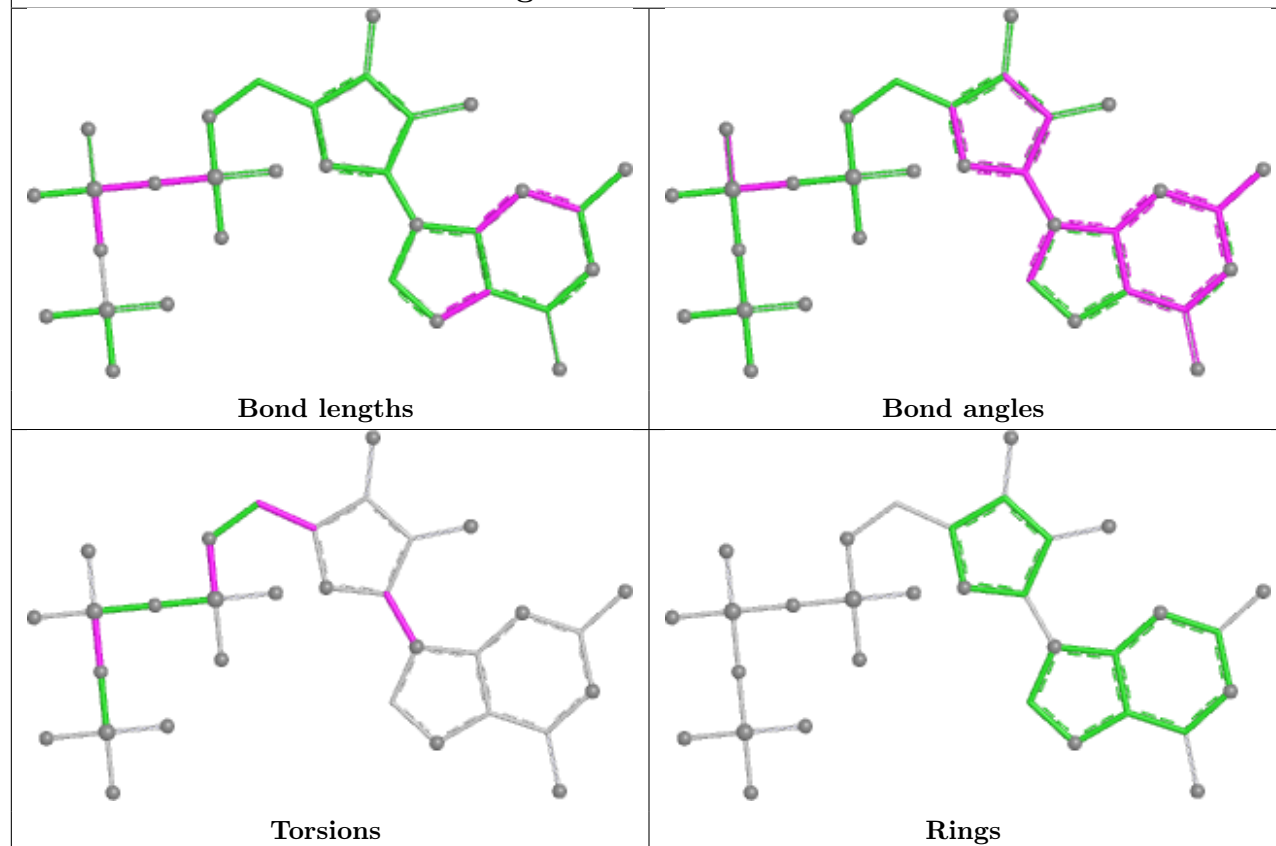
Ligand GTP BF 501



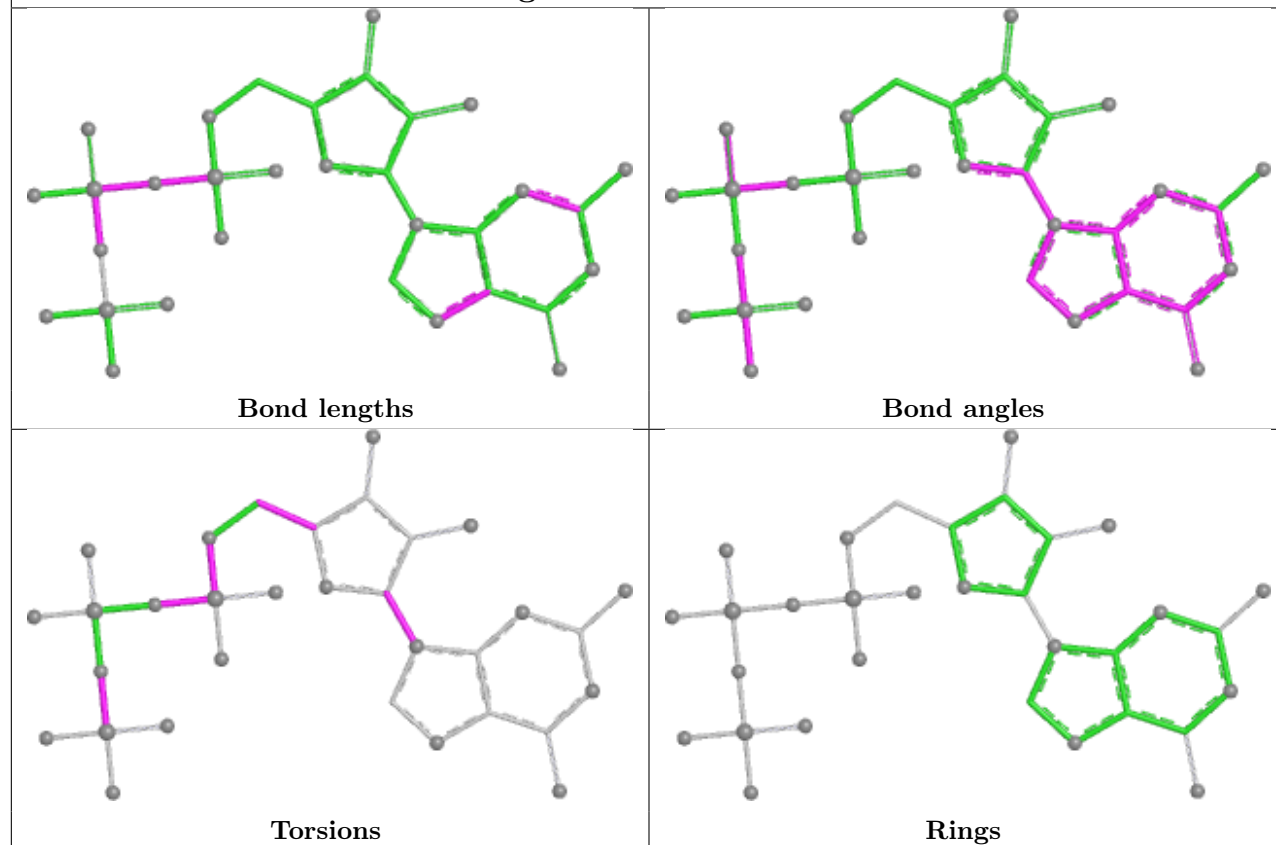
Ligand GTP WF 501



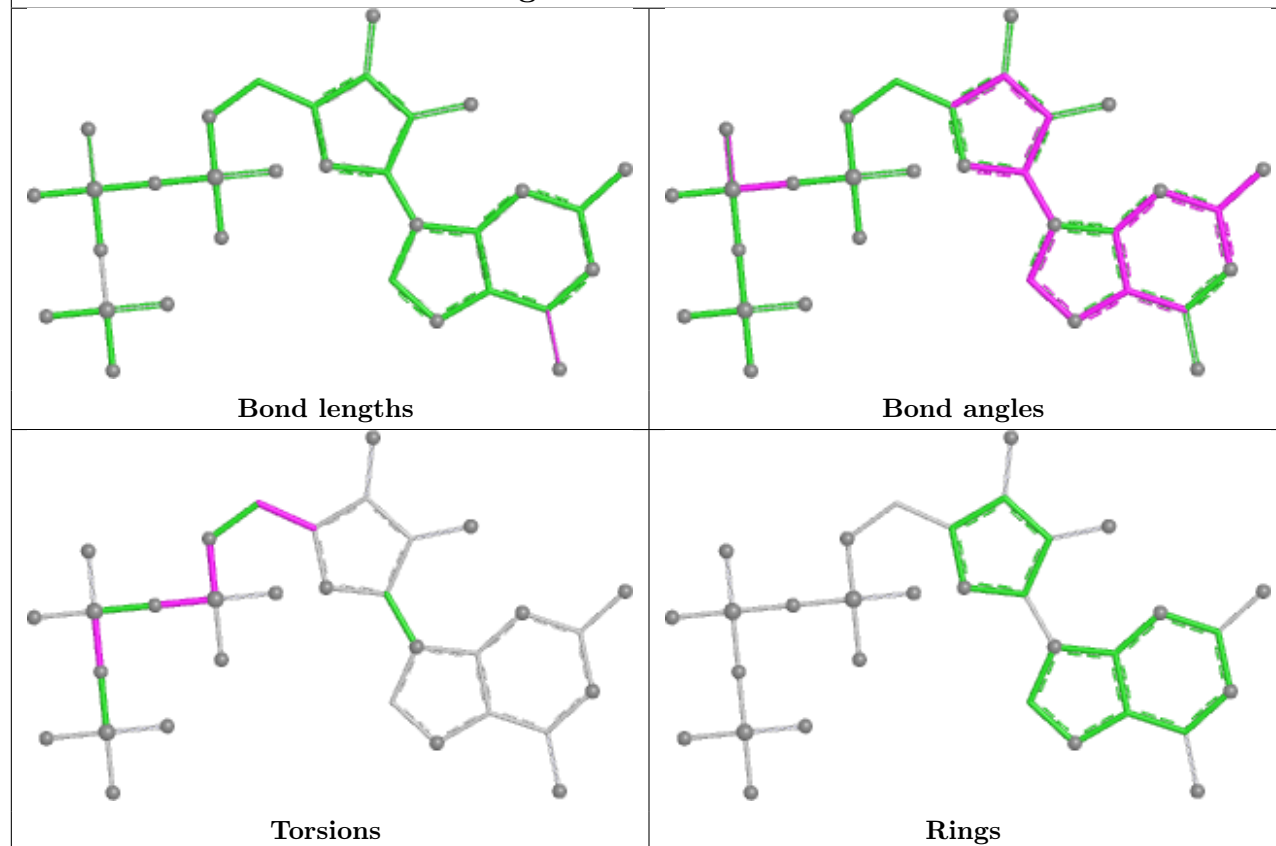
Ligand GTP DD 501



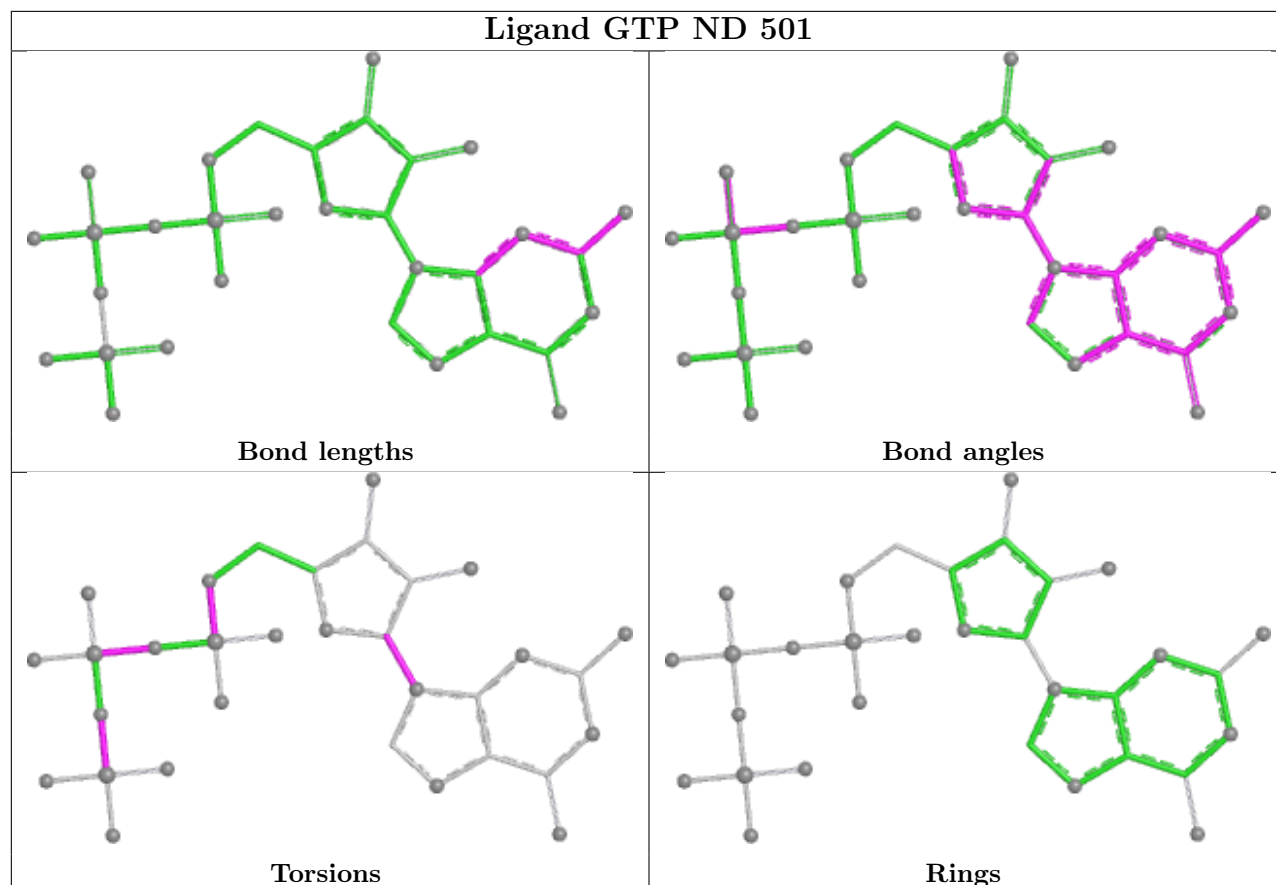
Ligand GTP KF 501



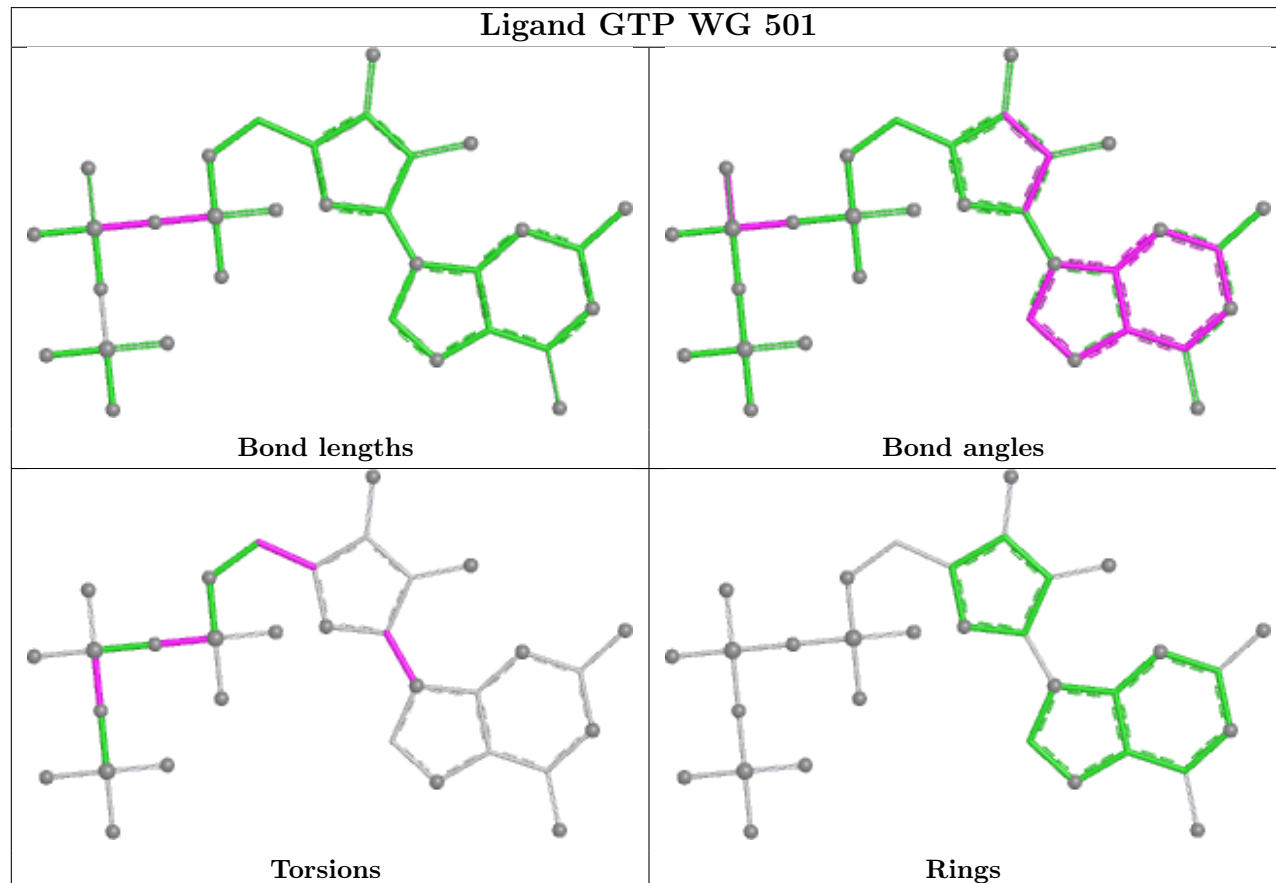
Ligand GTP LG 501



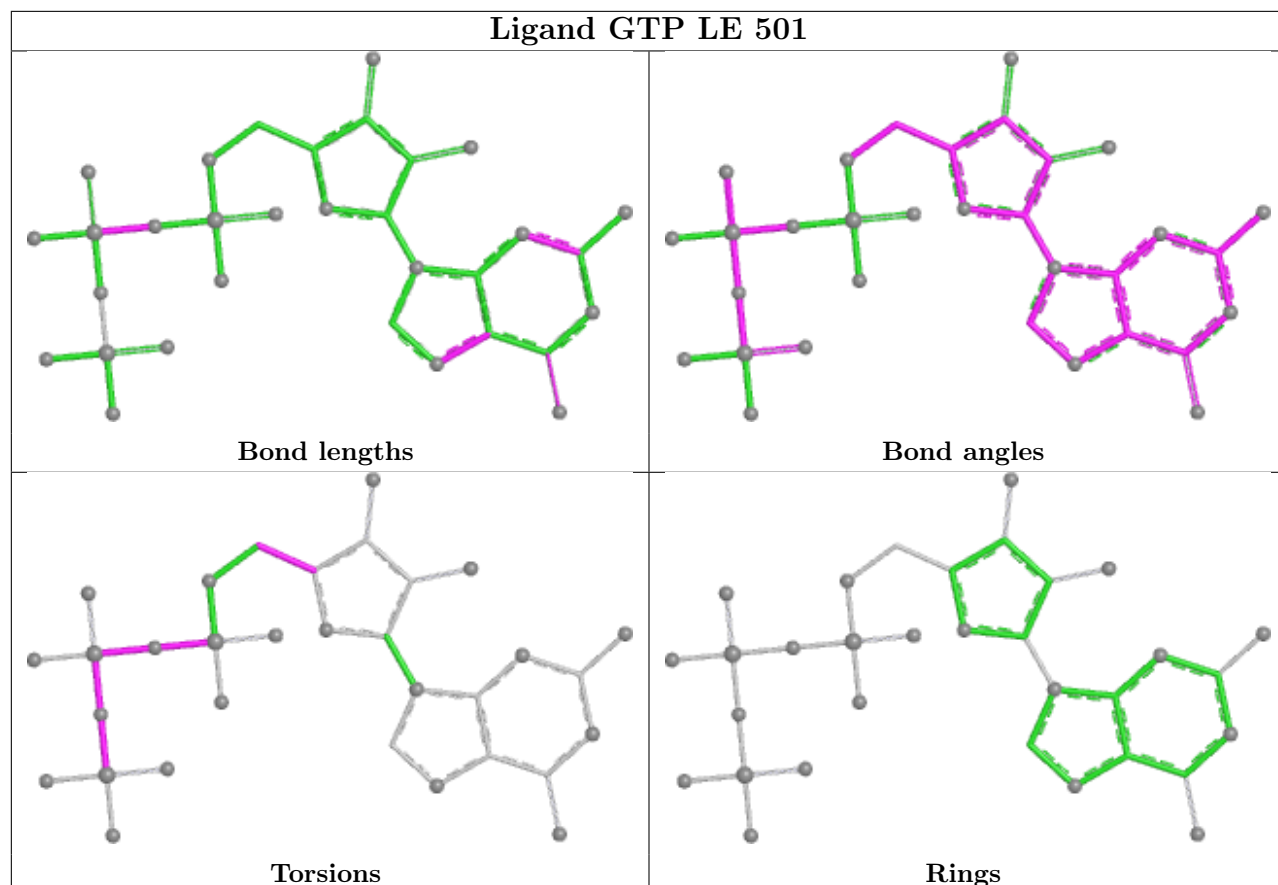
Ligand GTP ND 501



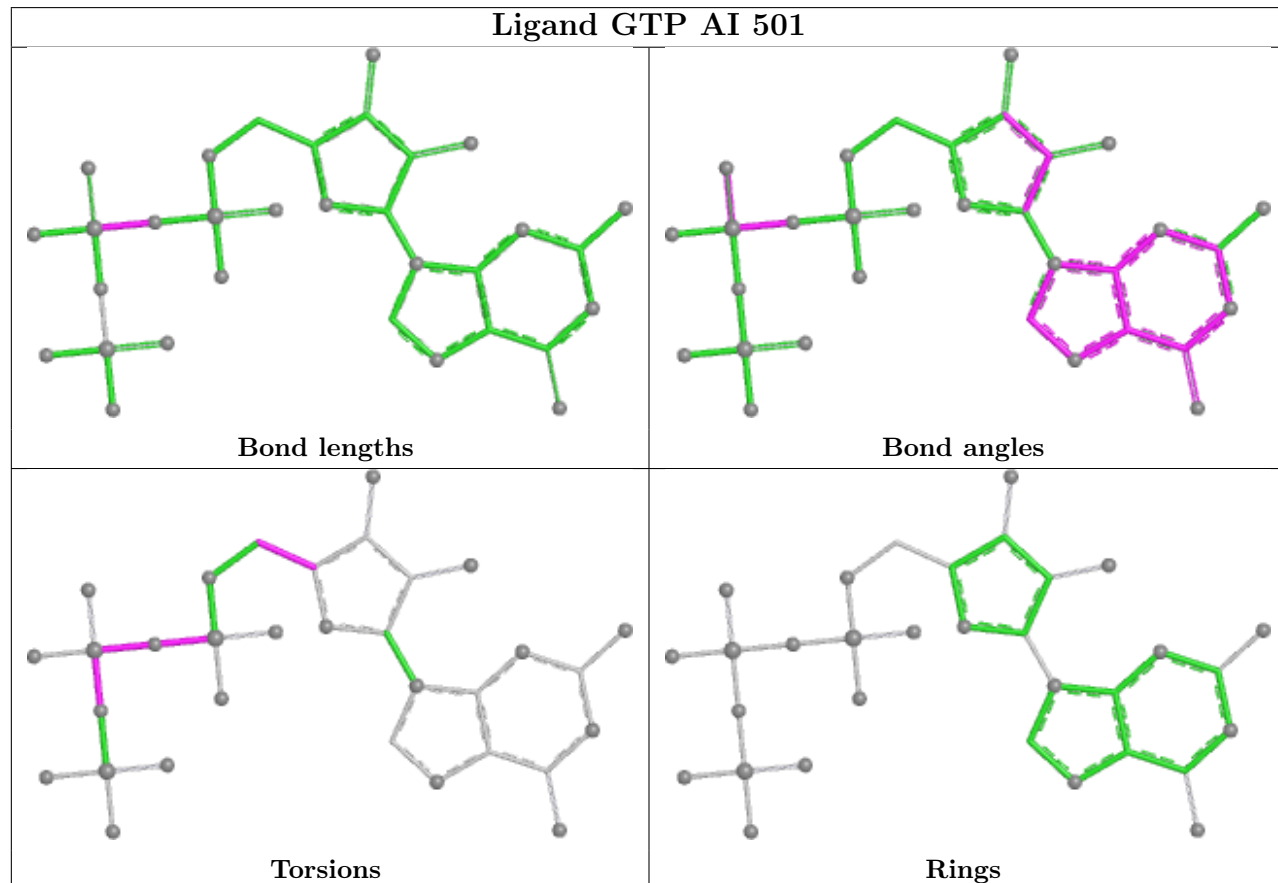
Ligand GTP WG 501



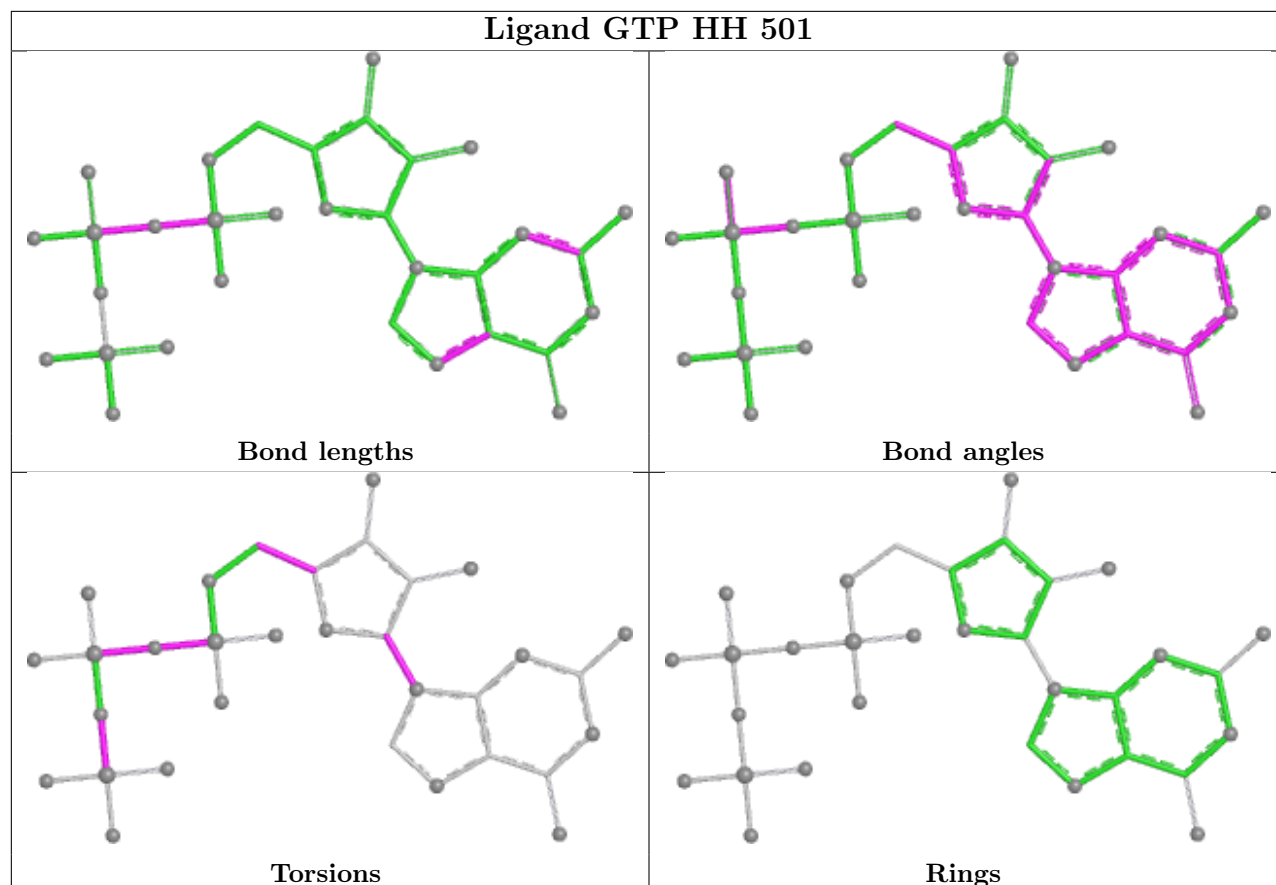
Ligand GTP LE 501



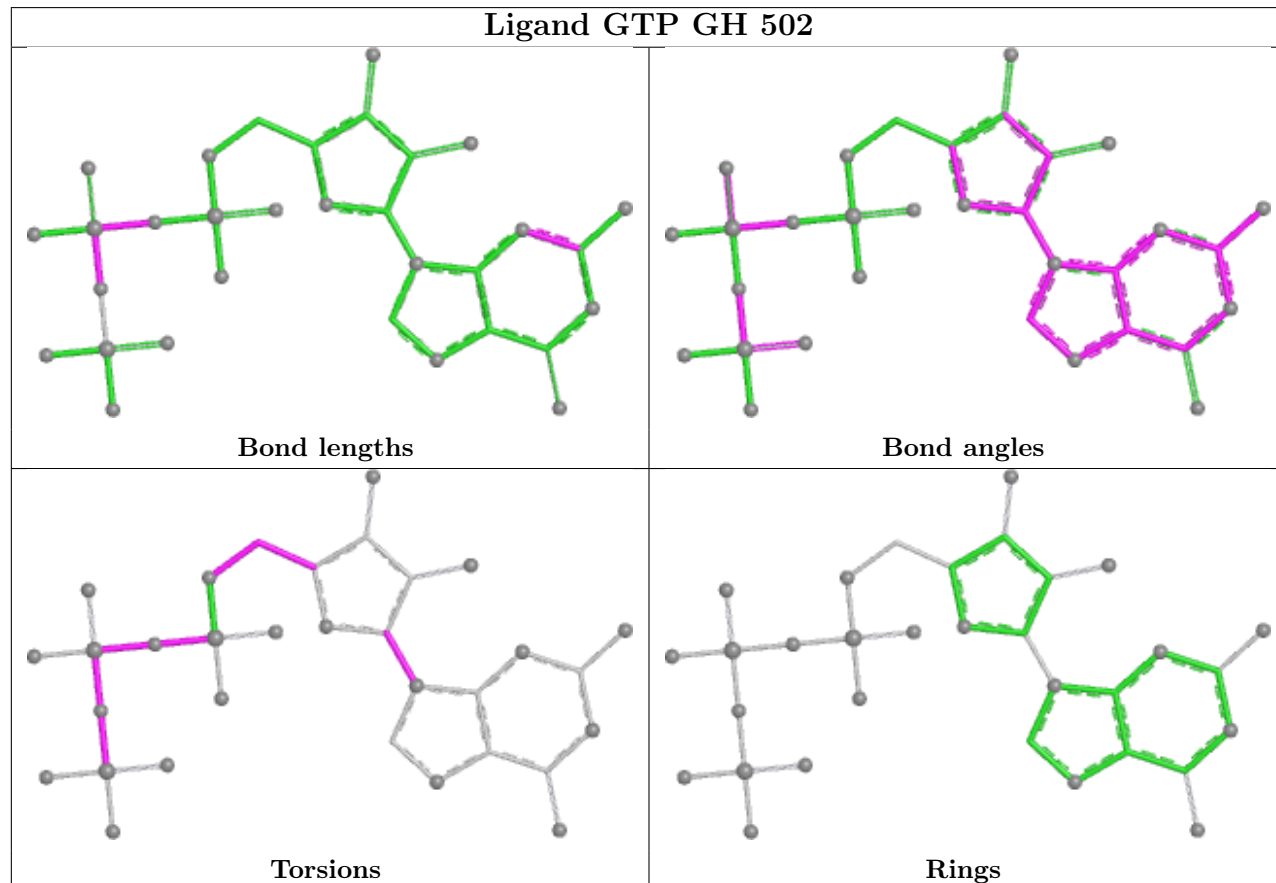
Ligand GTP AI 501



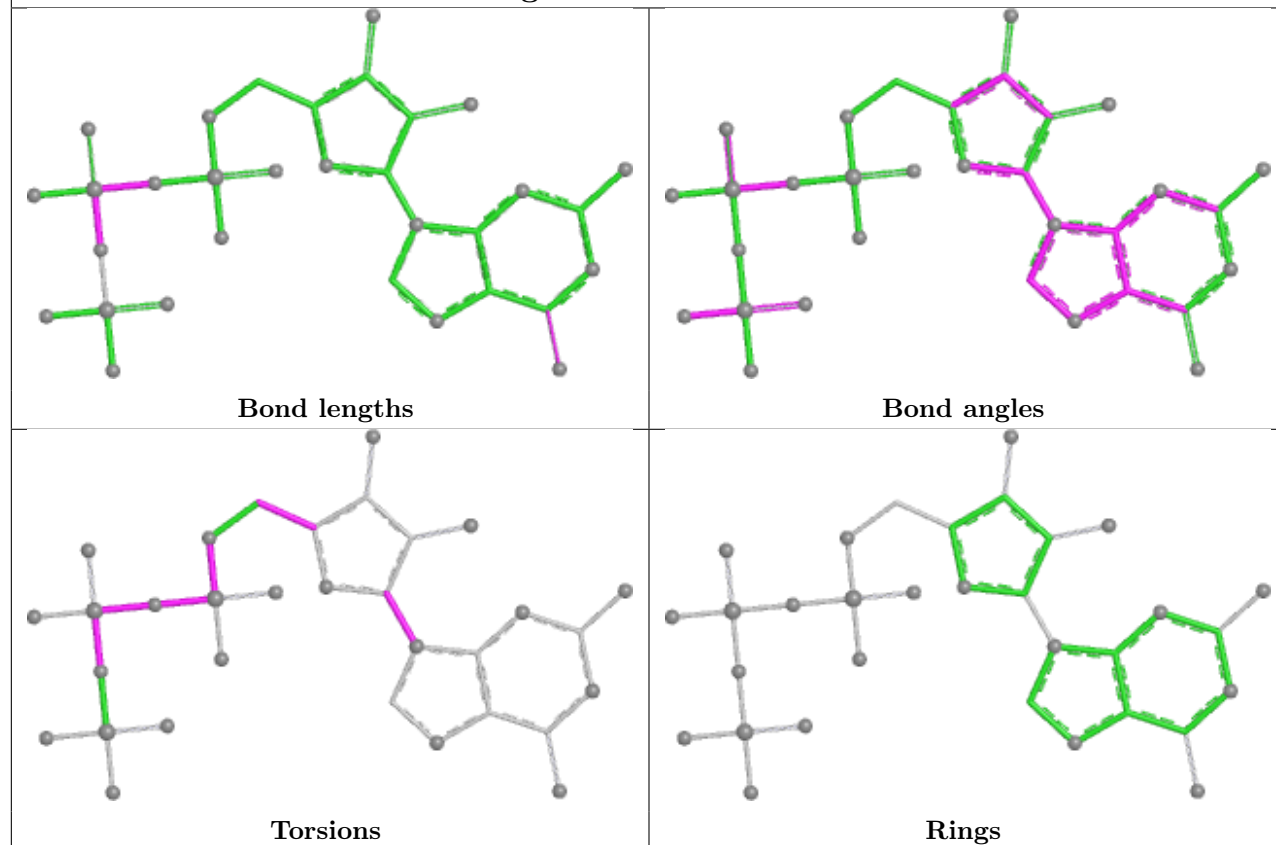
Ligand GTP HH 501



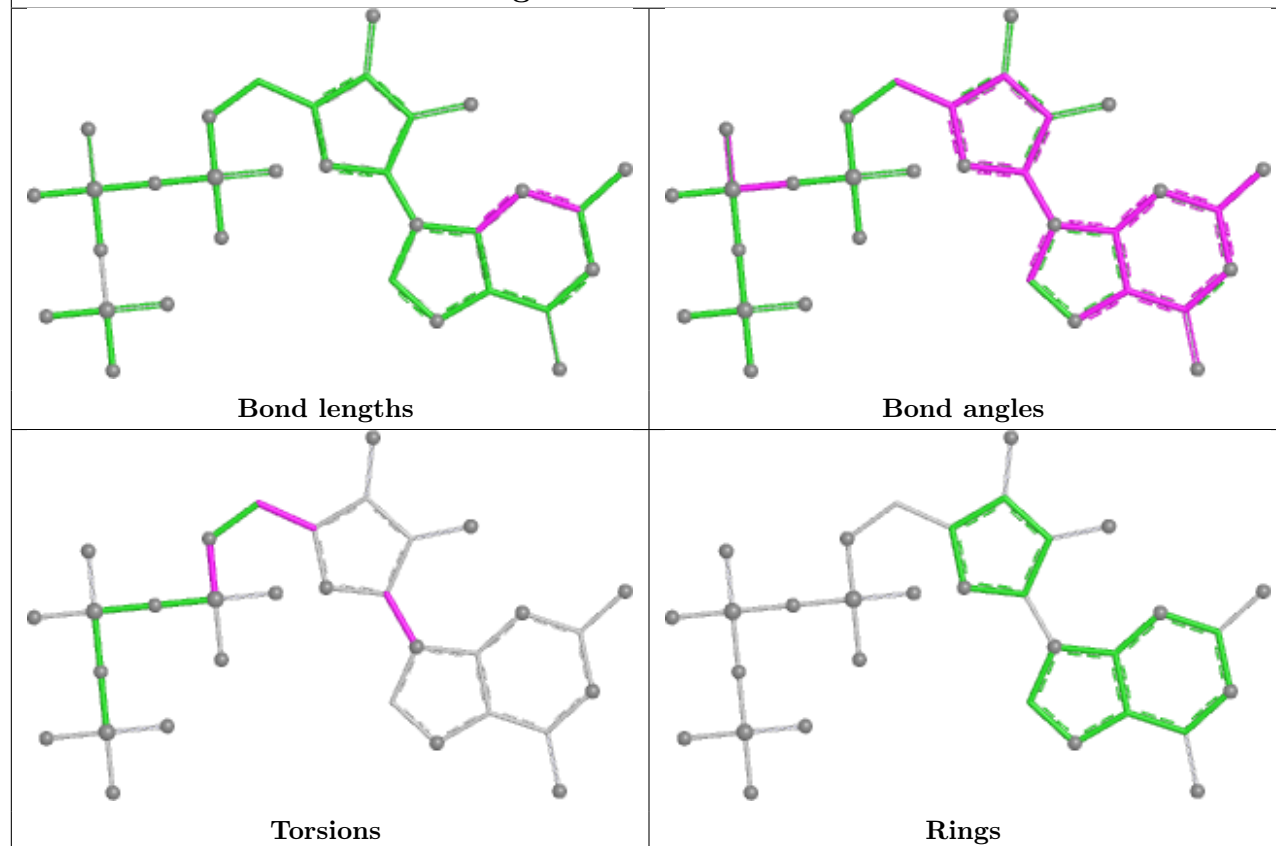
Ligand GTP GH 502



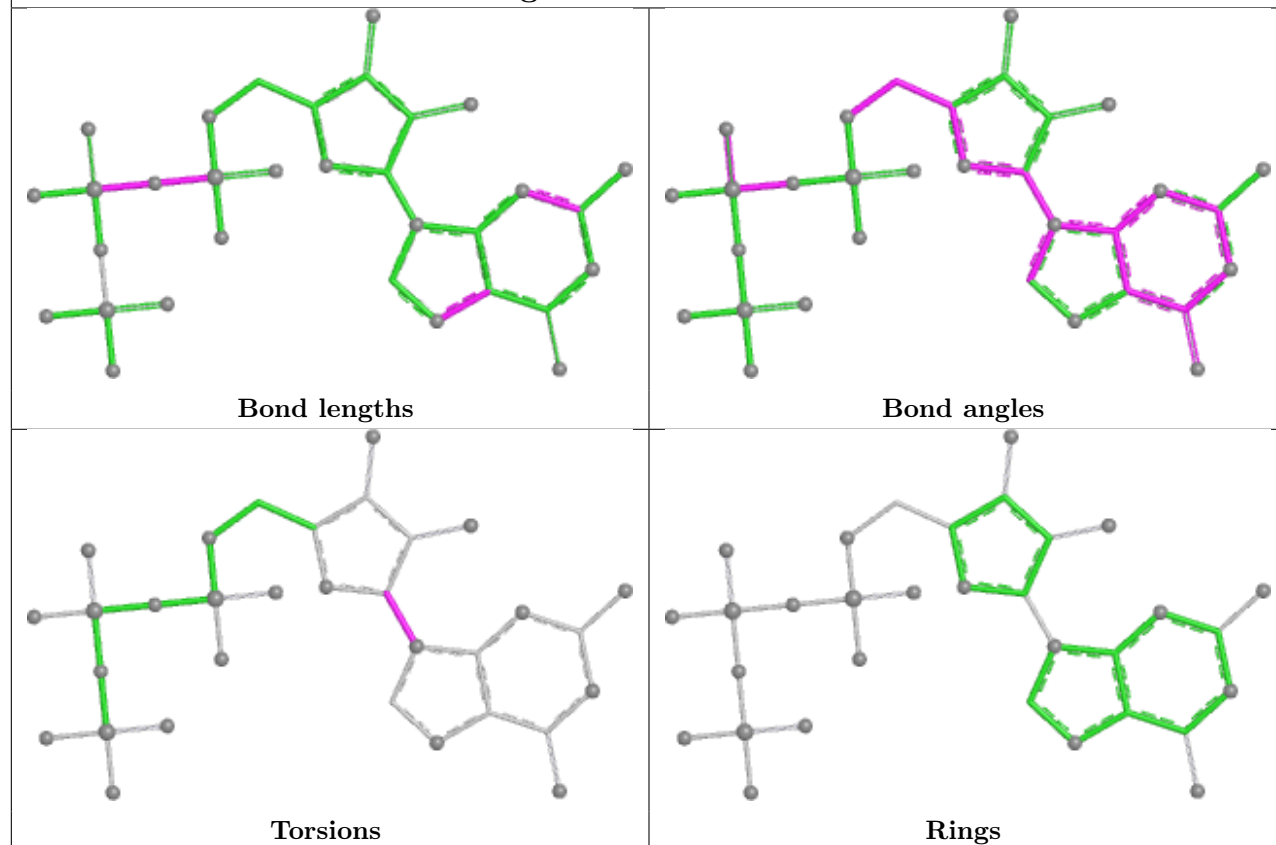
Ligand GTP FF 502



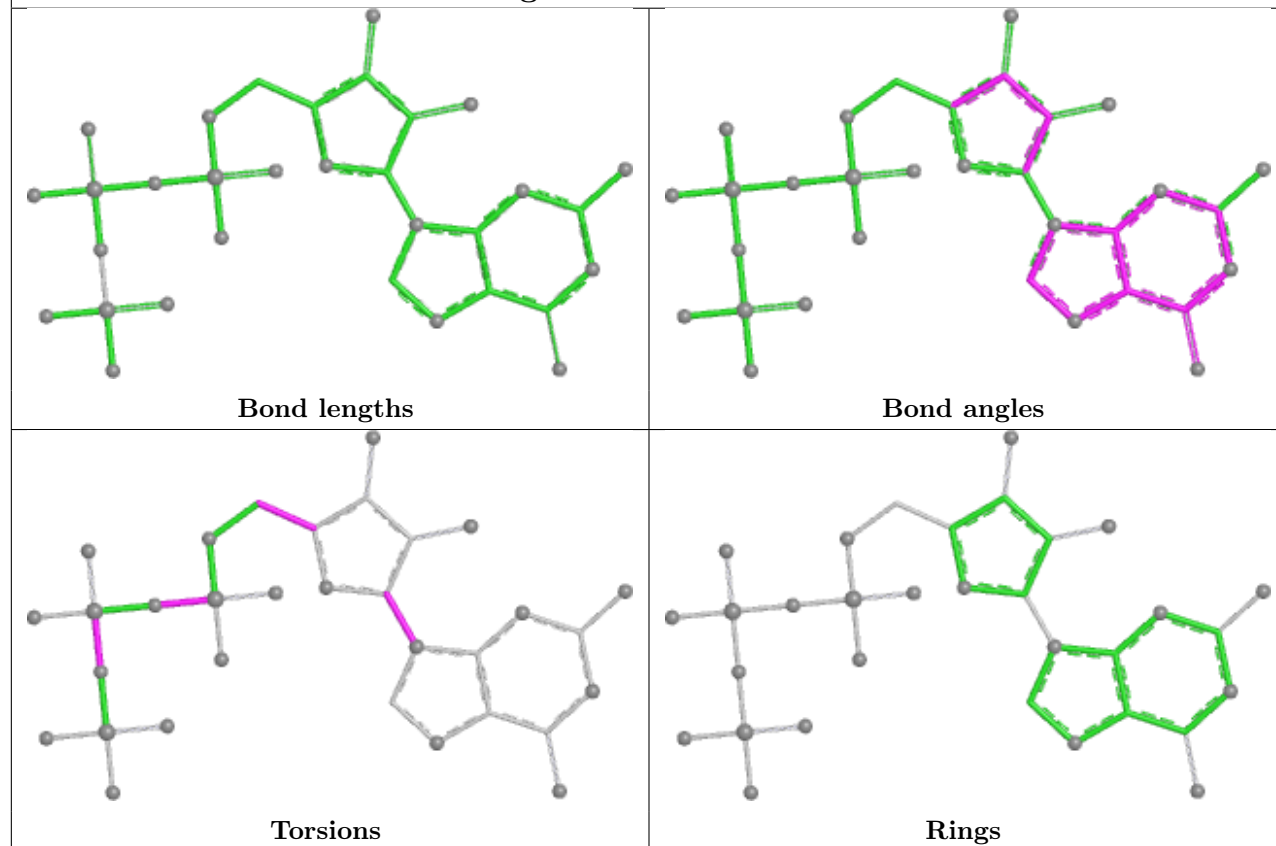
Ligand GTP MH 501



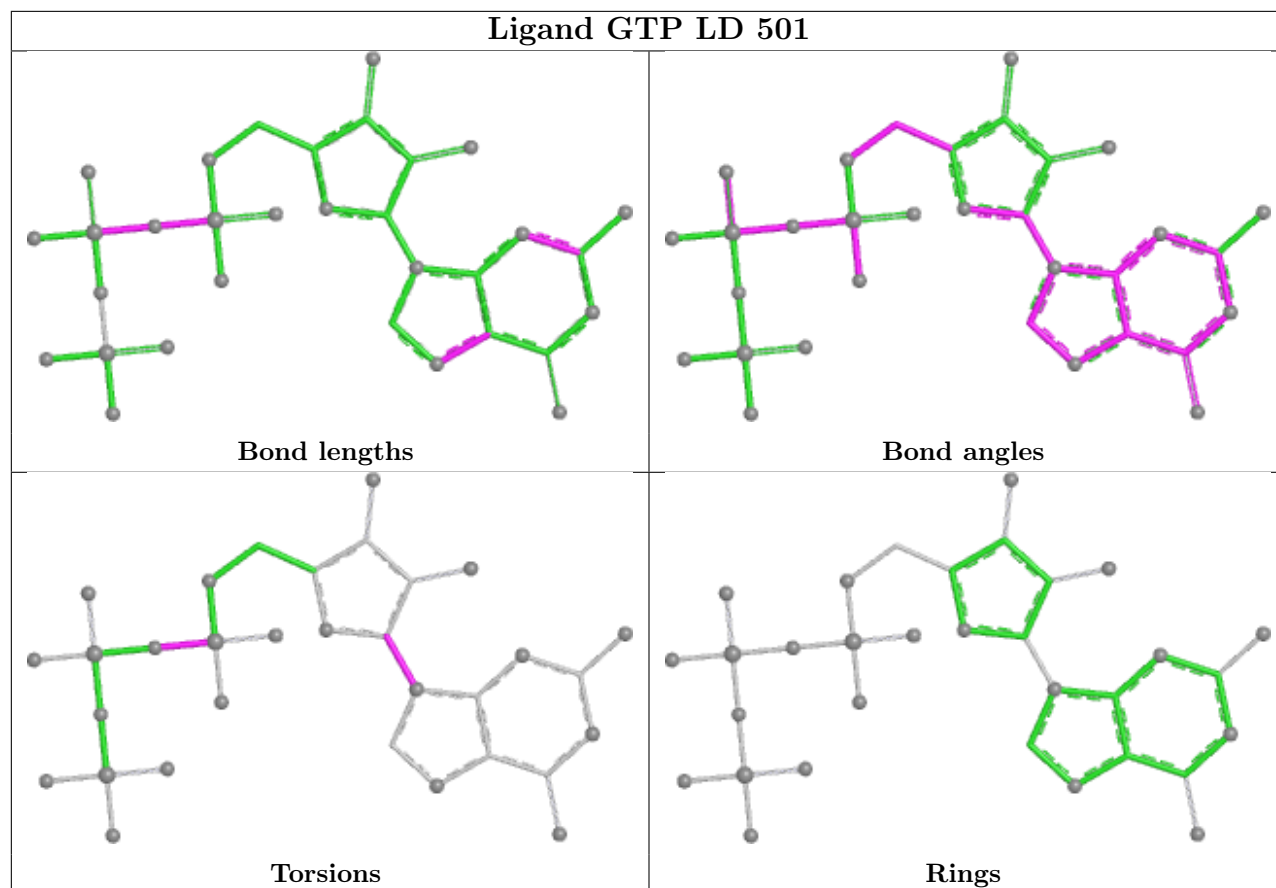
Ligand GTP JH 501



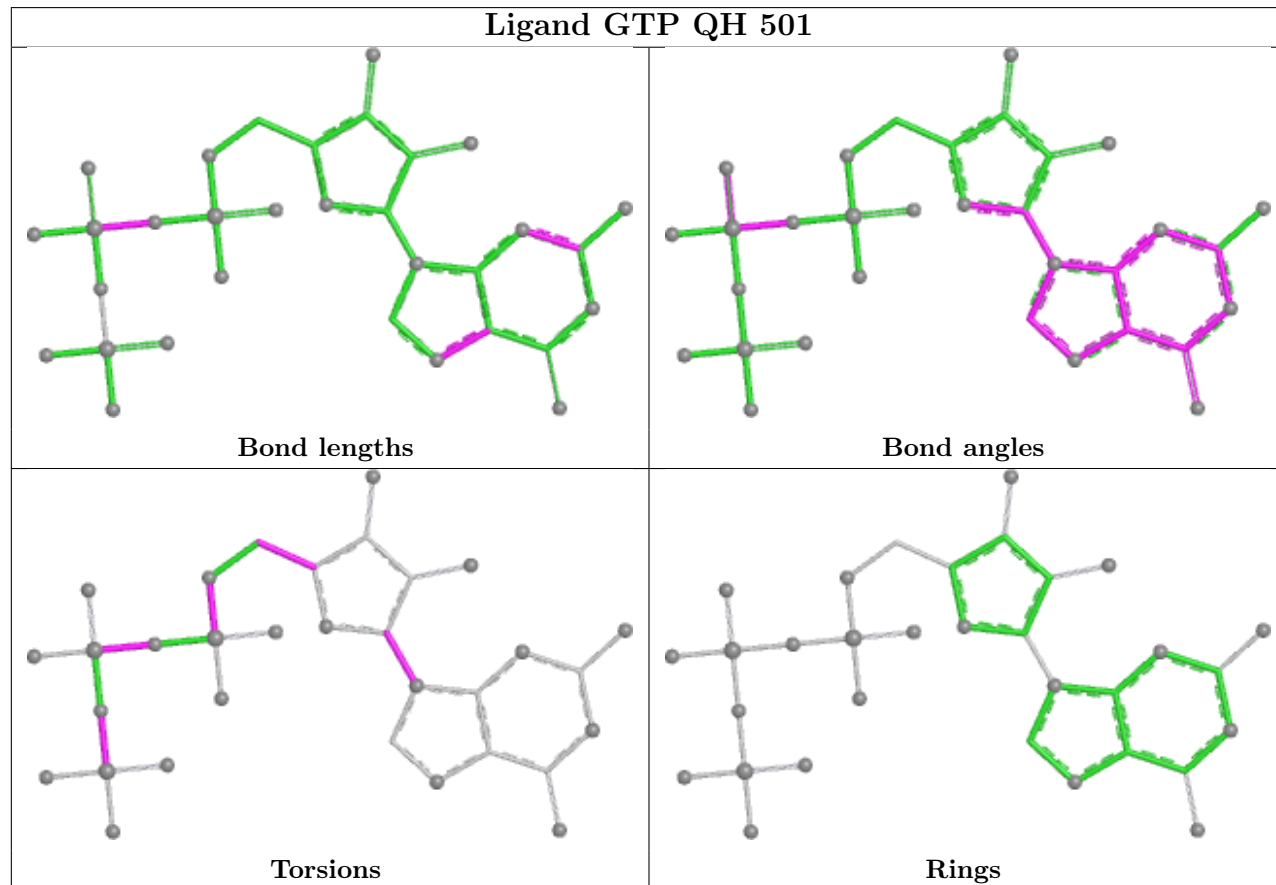
Ligand GTP MI 501



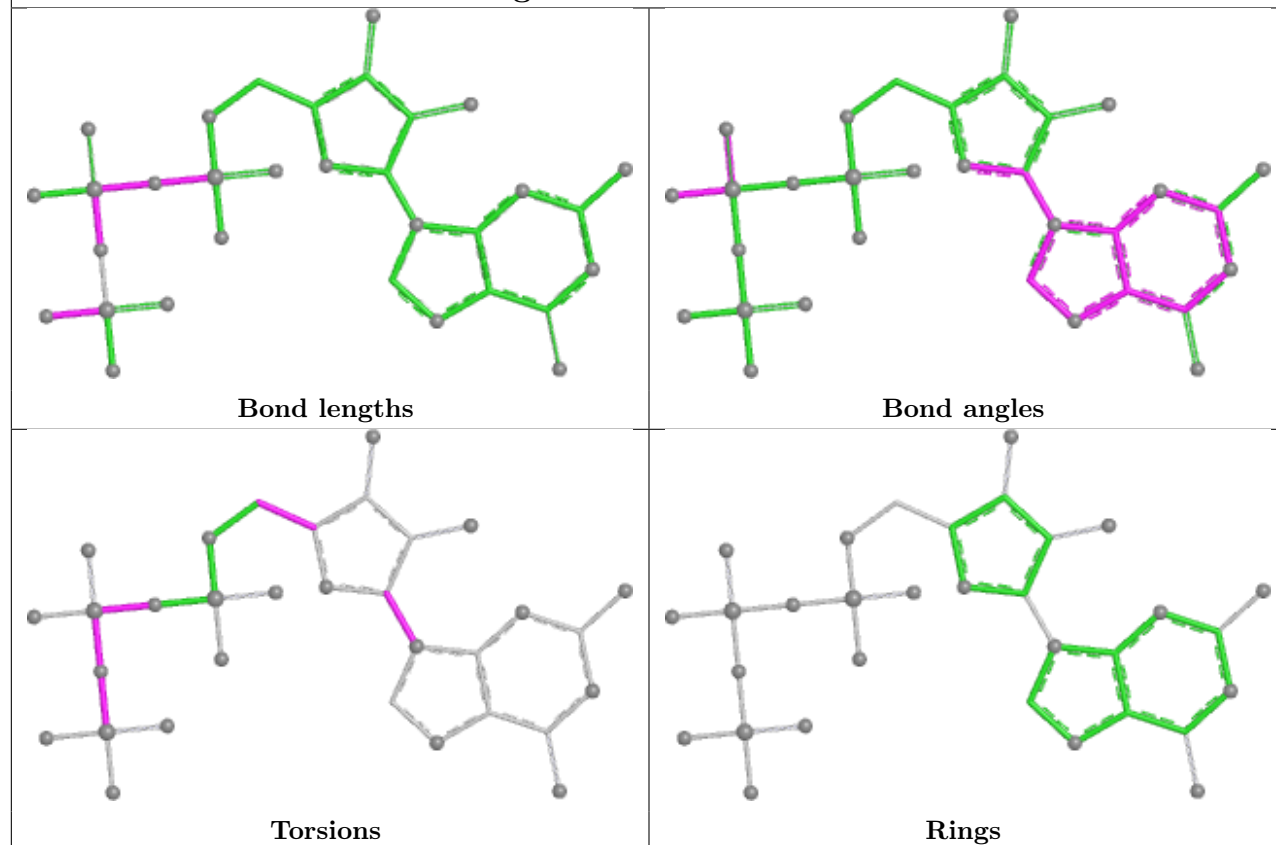
Ligand GTP LD 501



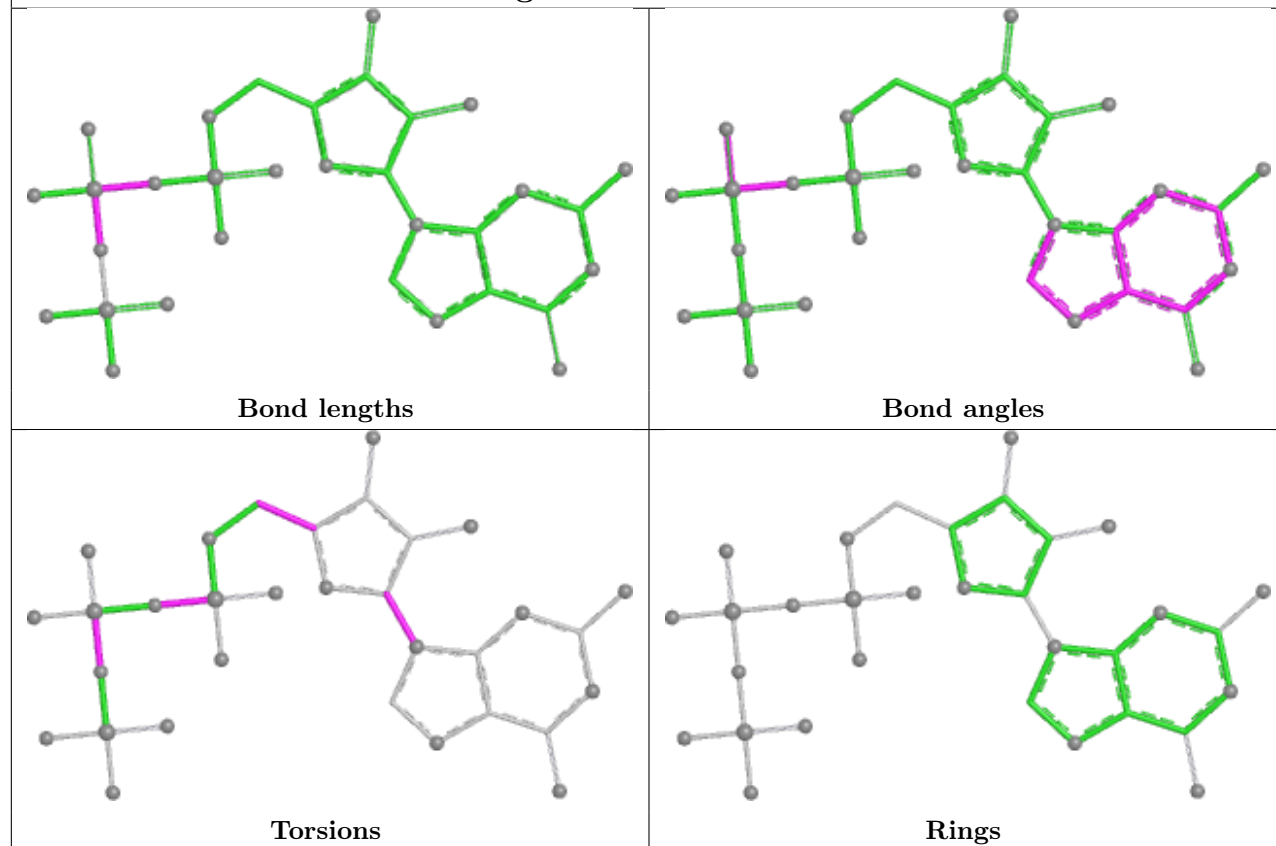
Ligand GTP QH 501



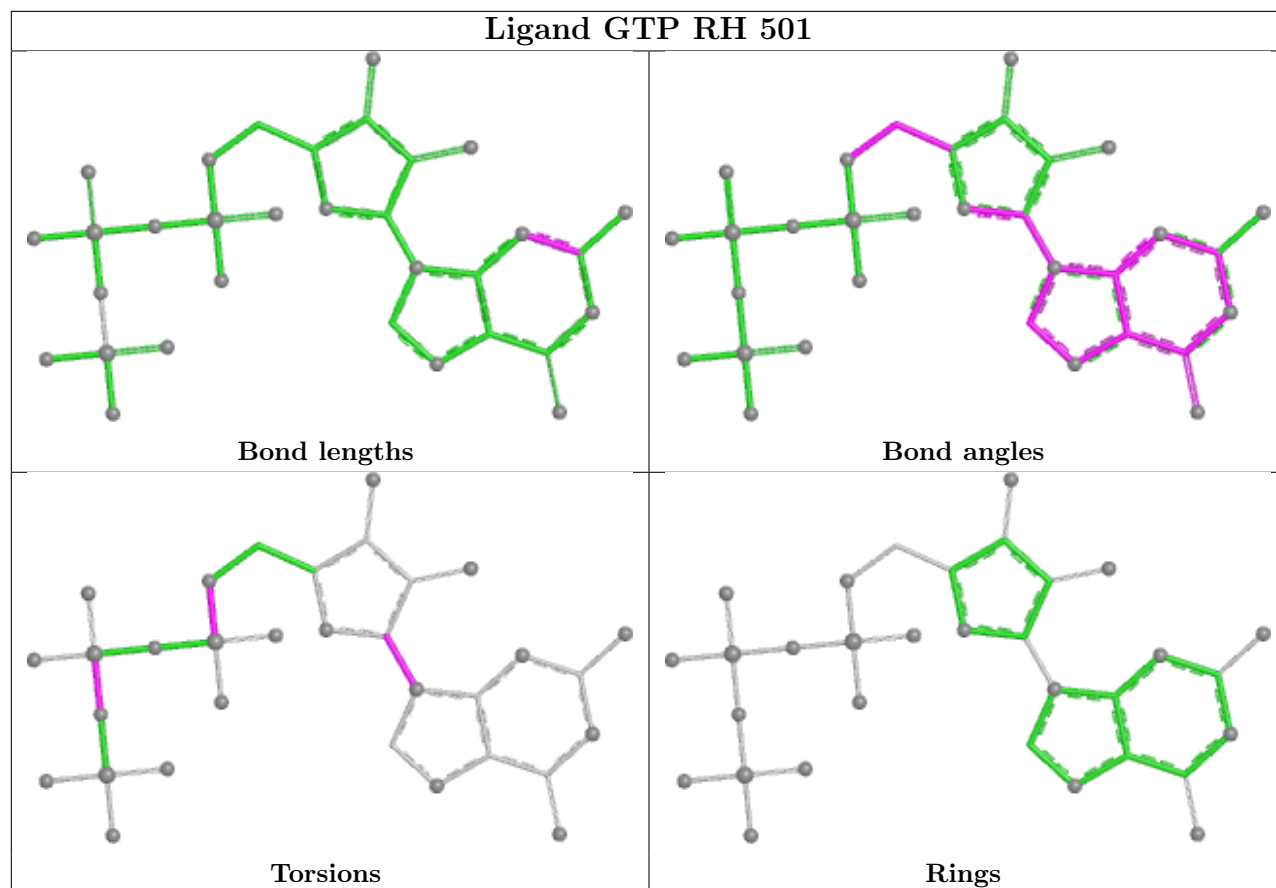
Ligand GTP WE 501



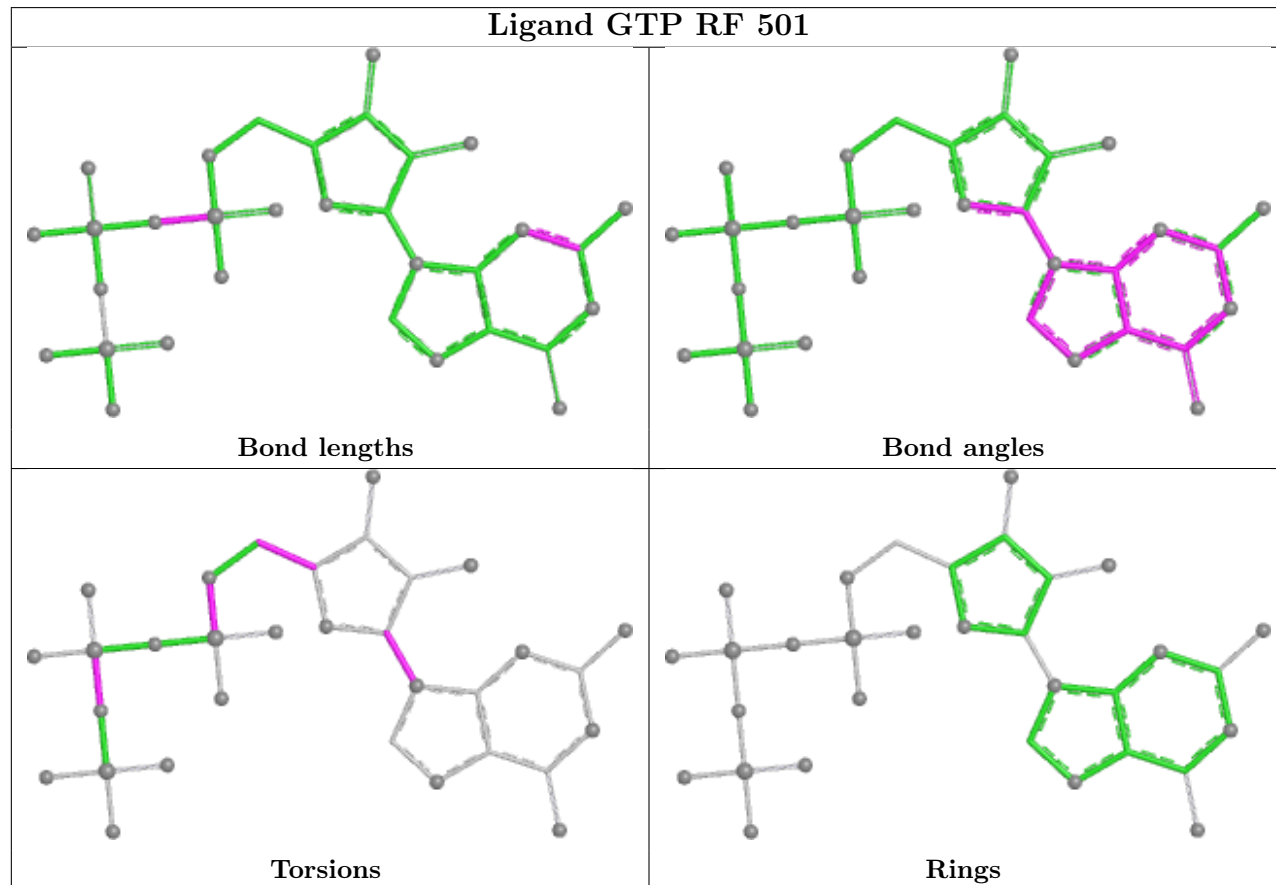
Ligand GTP OG 501



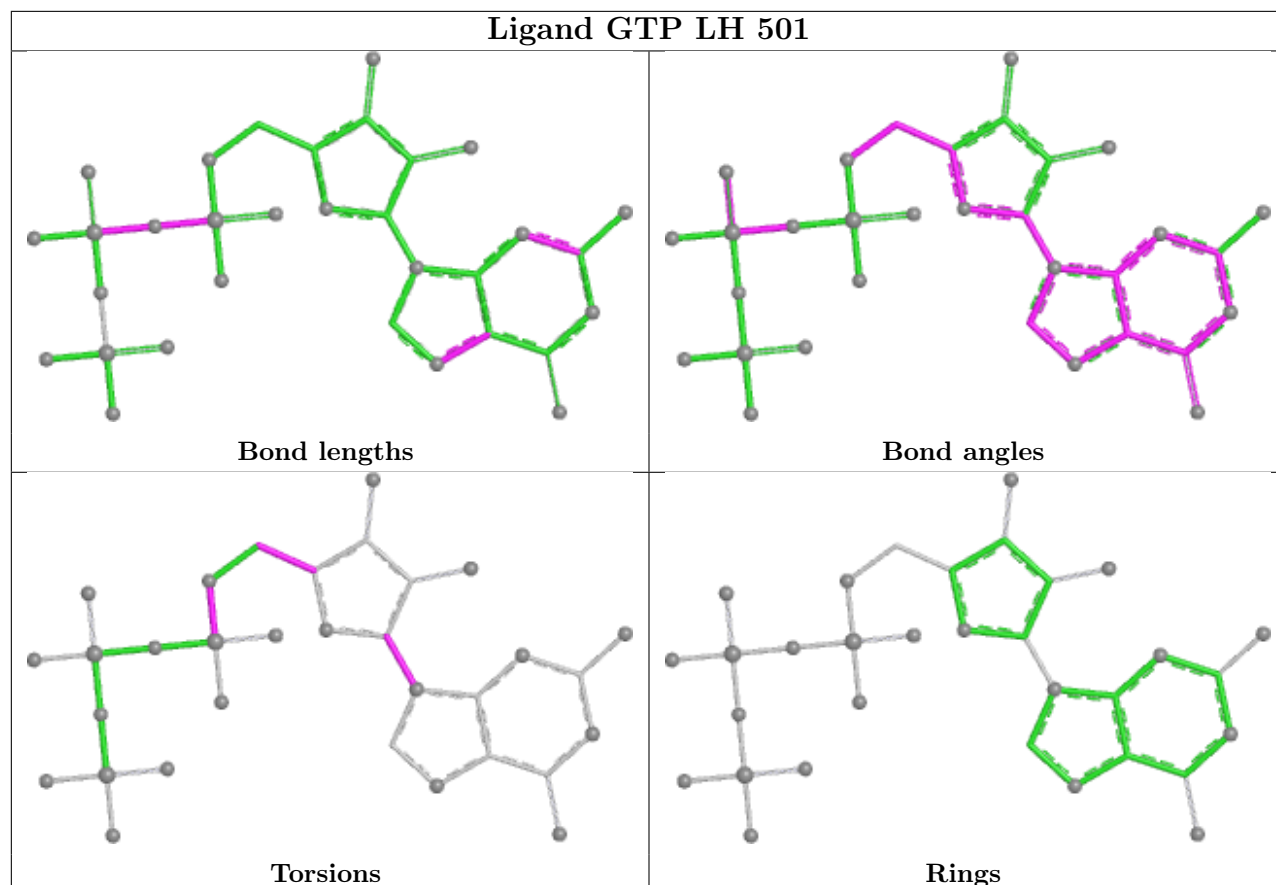
Ligand GTP RH 501



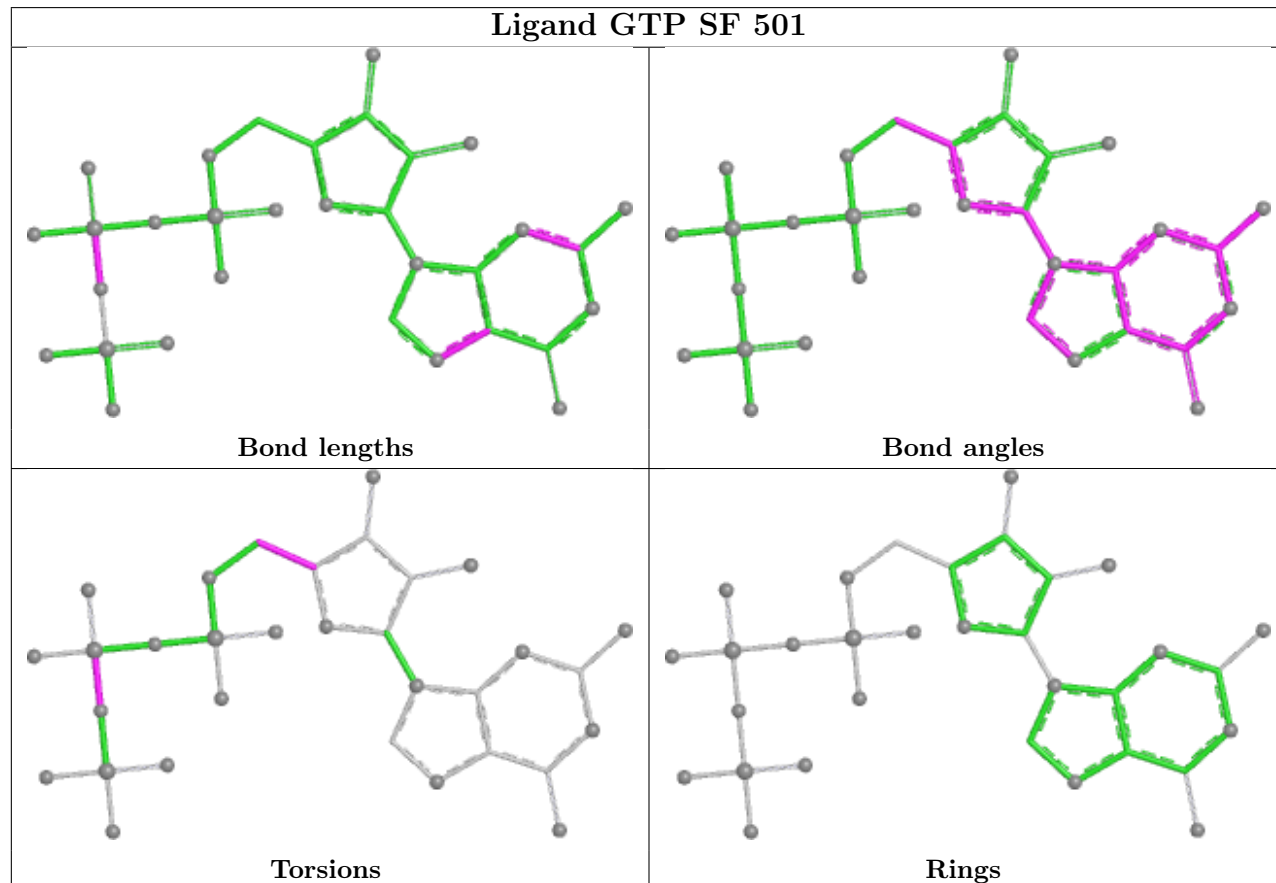
Ligand GTP RF 501



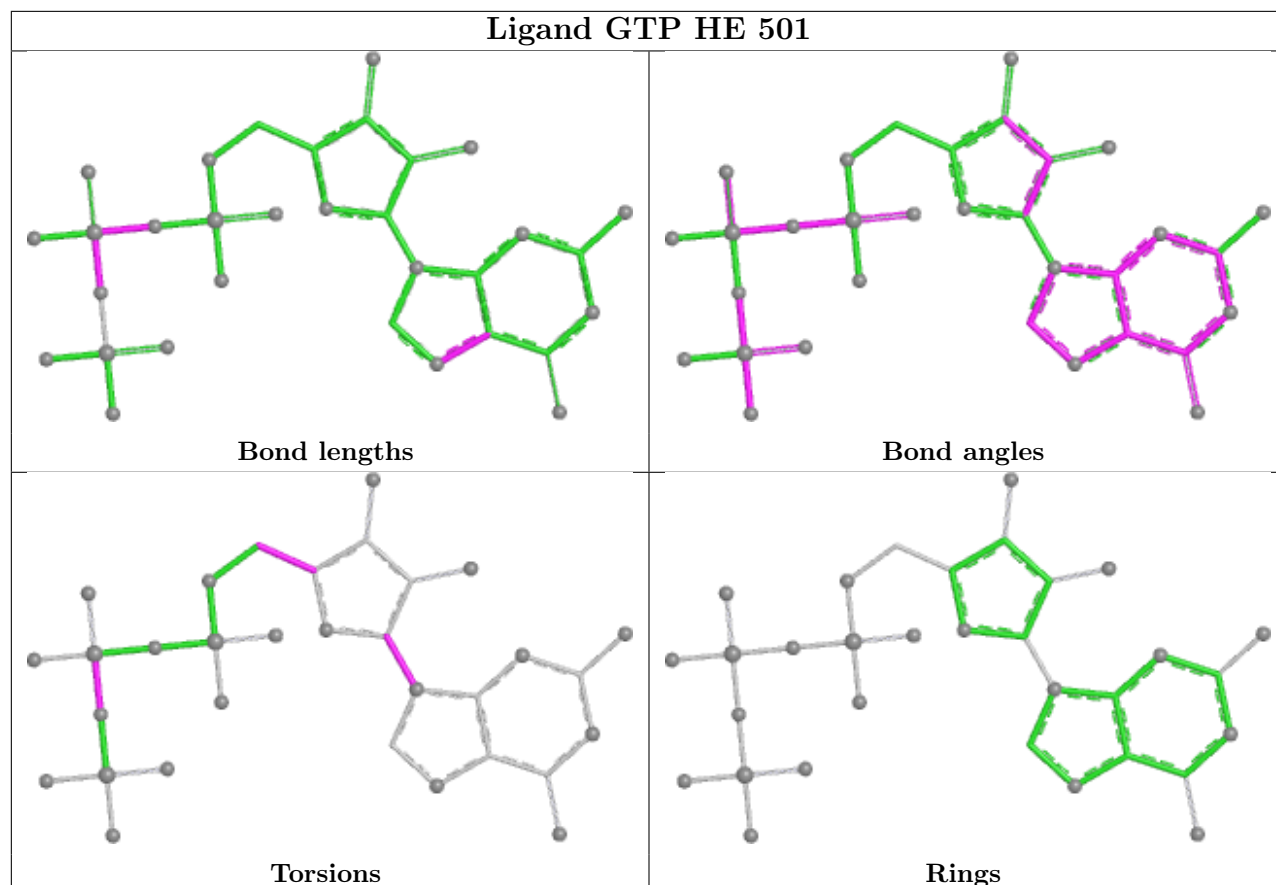
Ligand GTP LH 501



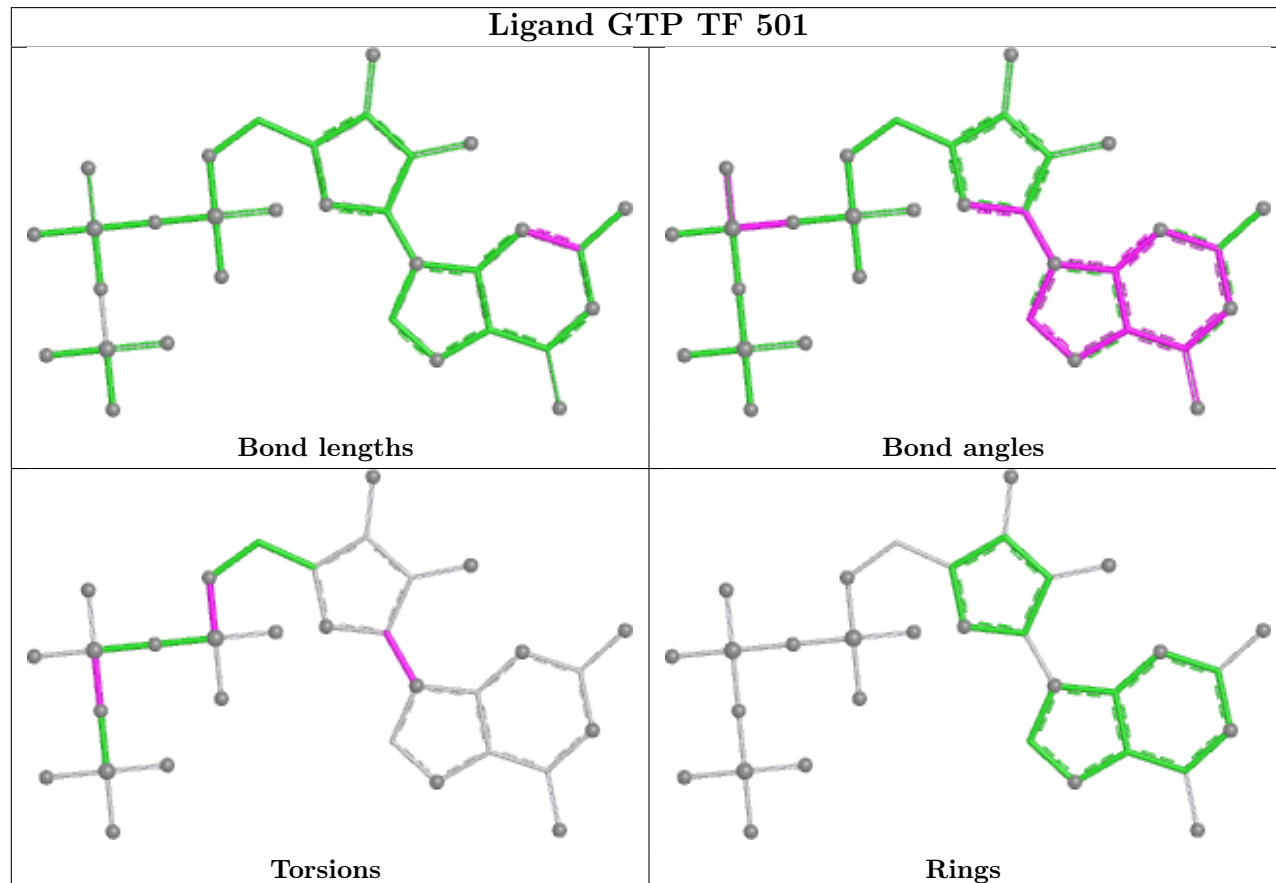
Ligand GTP SF 501

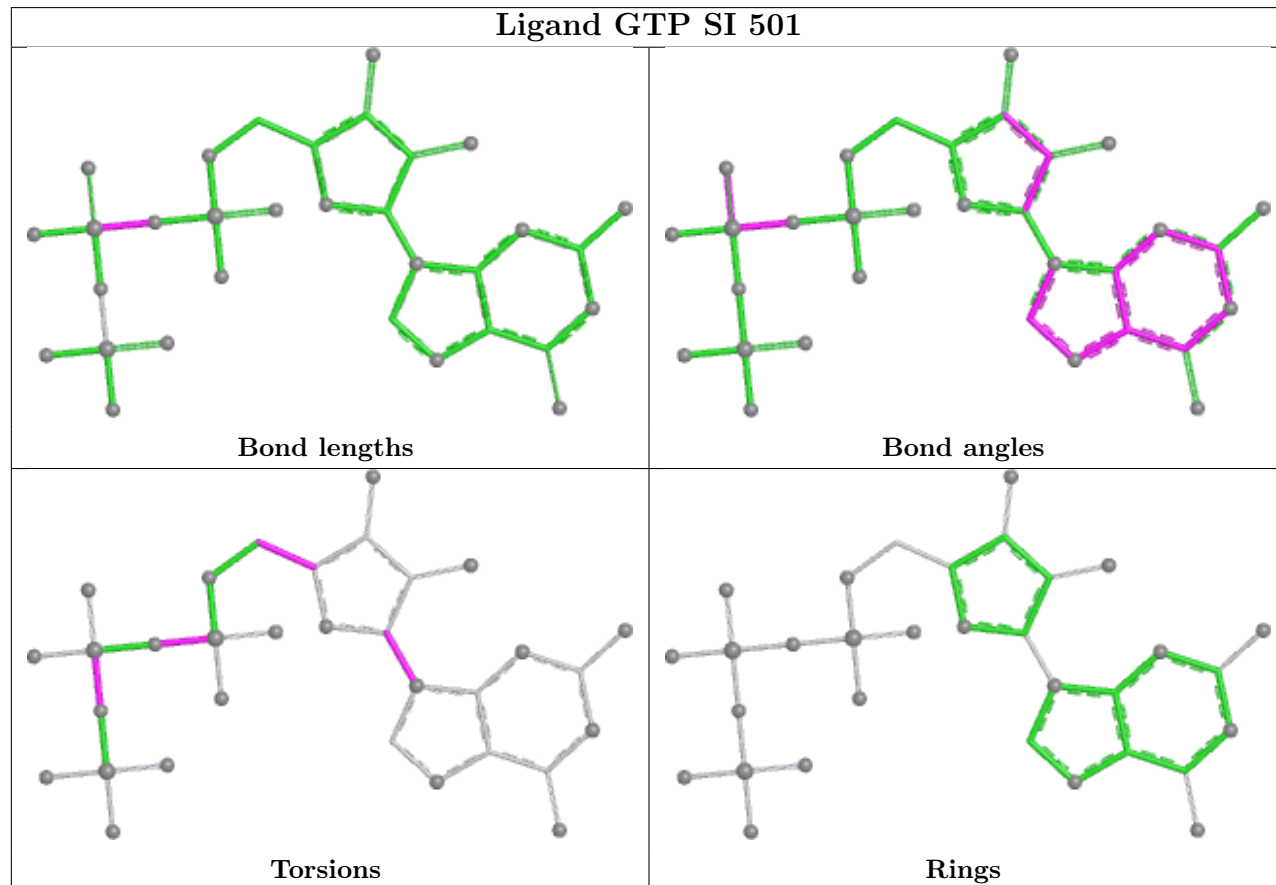
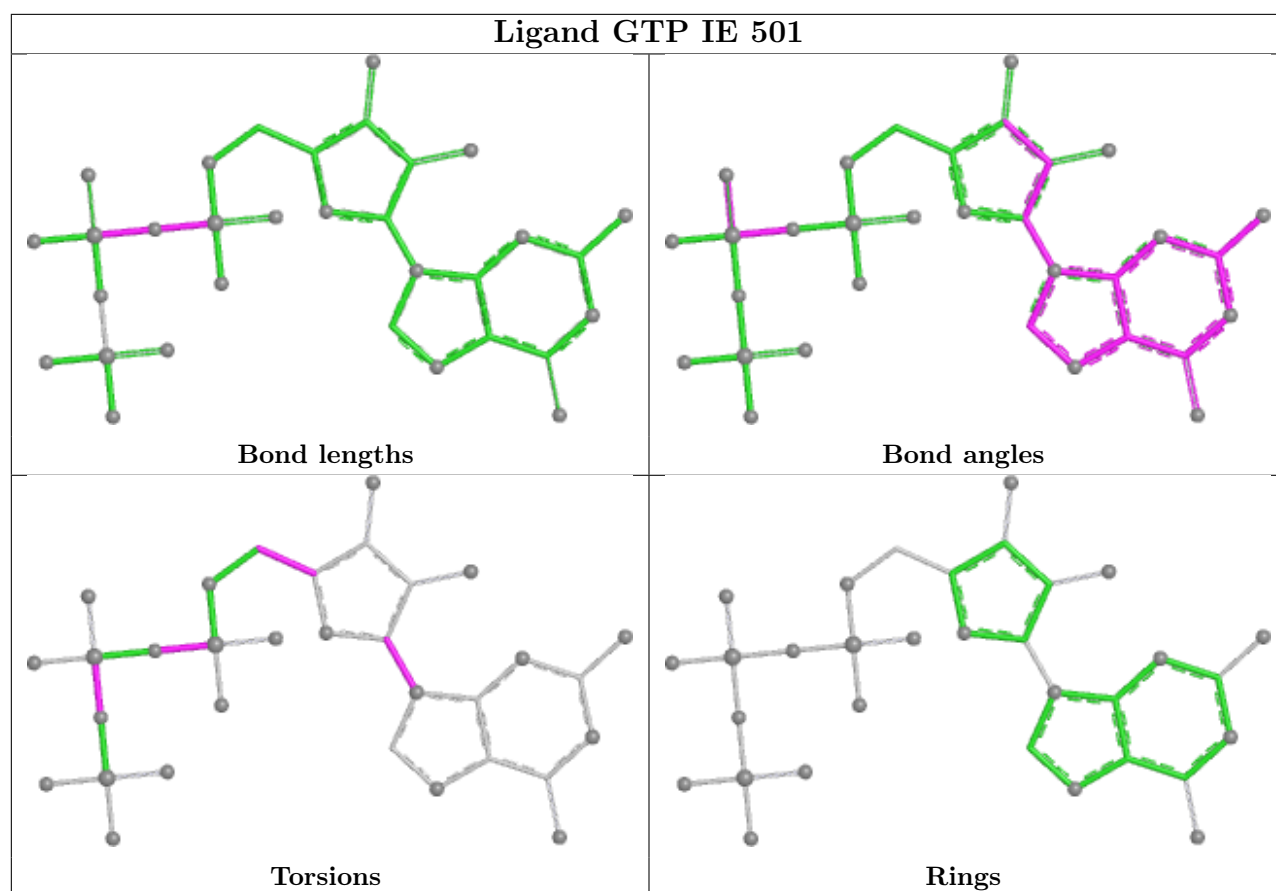


Ligand GTP HE 501

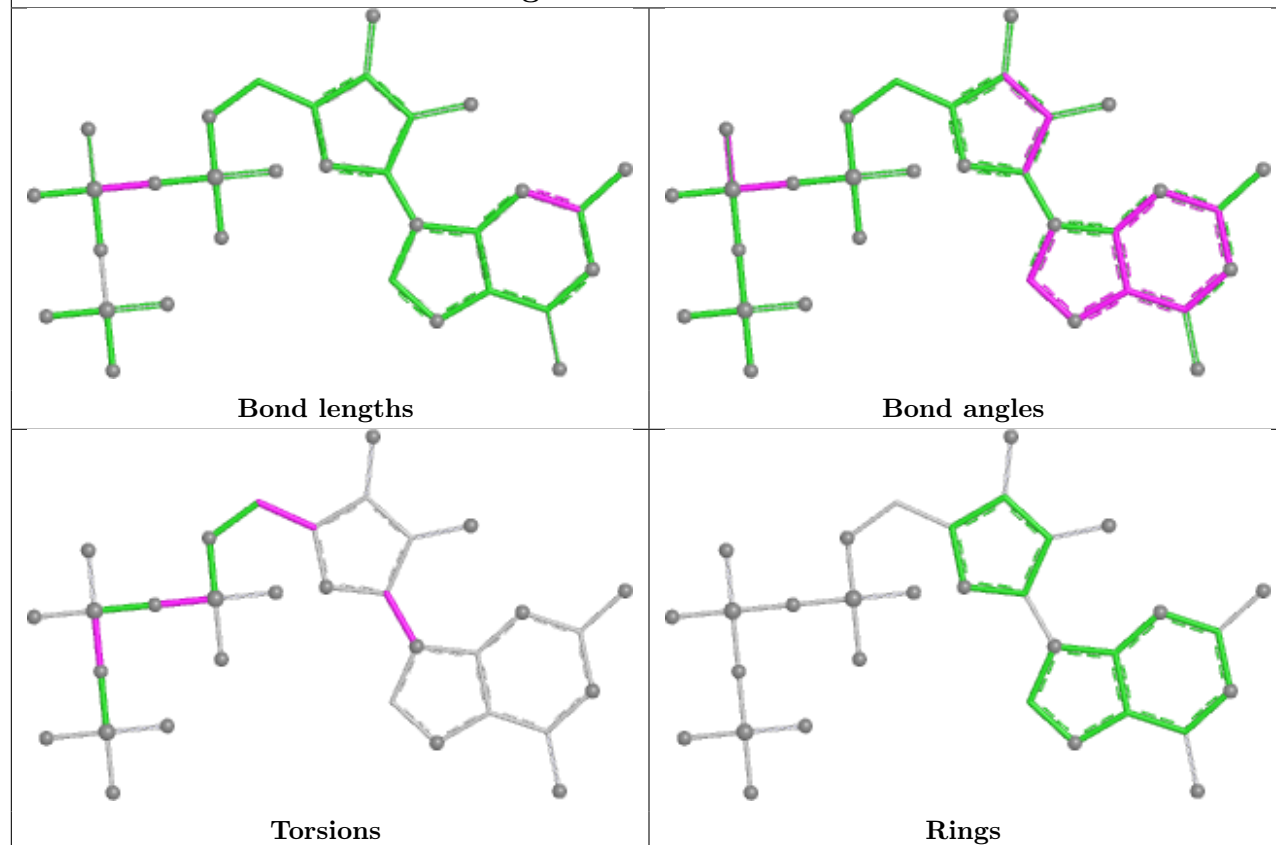


Ligand GTP TF 501

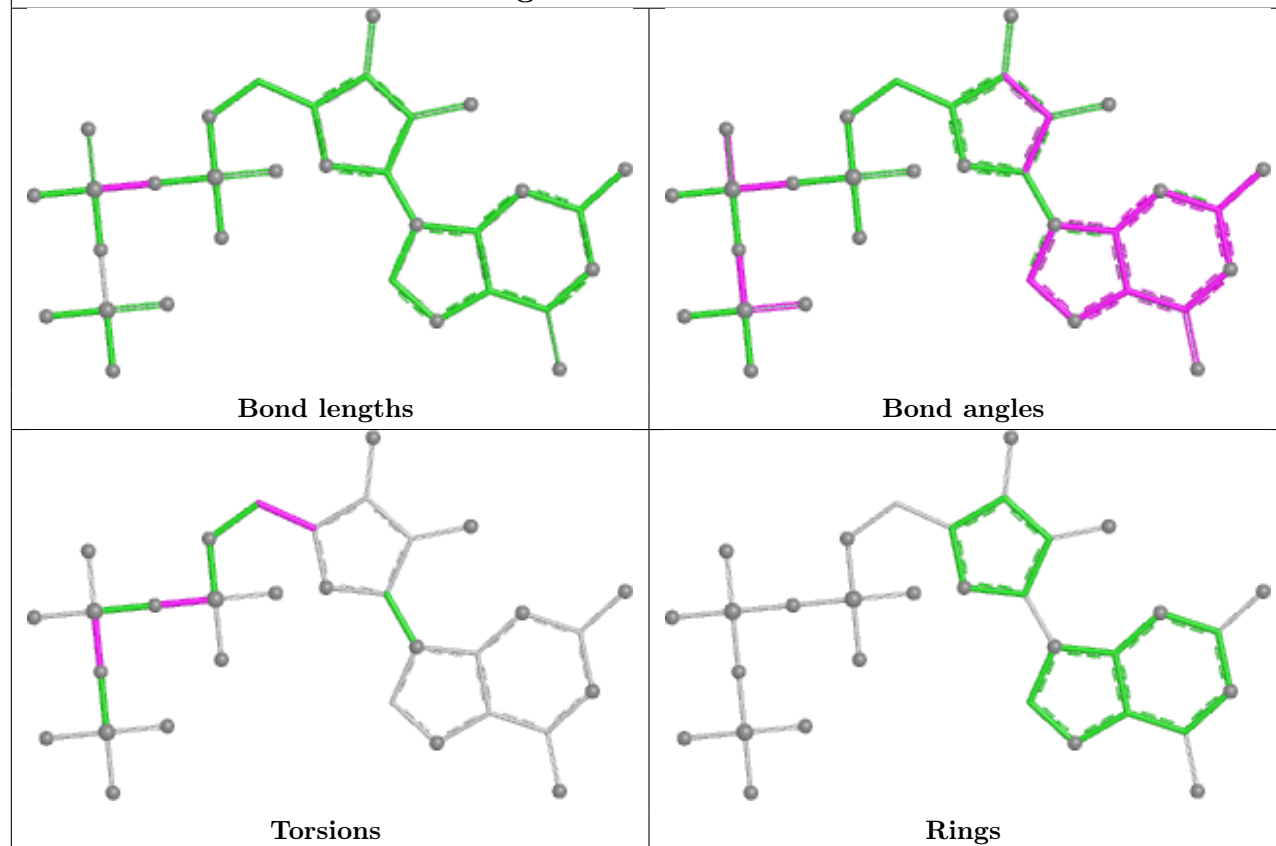




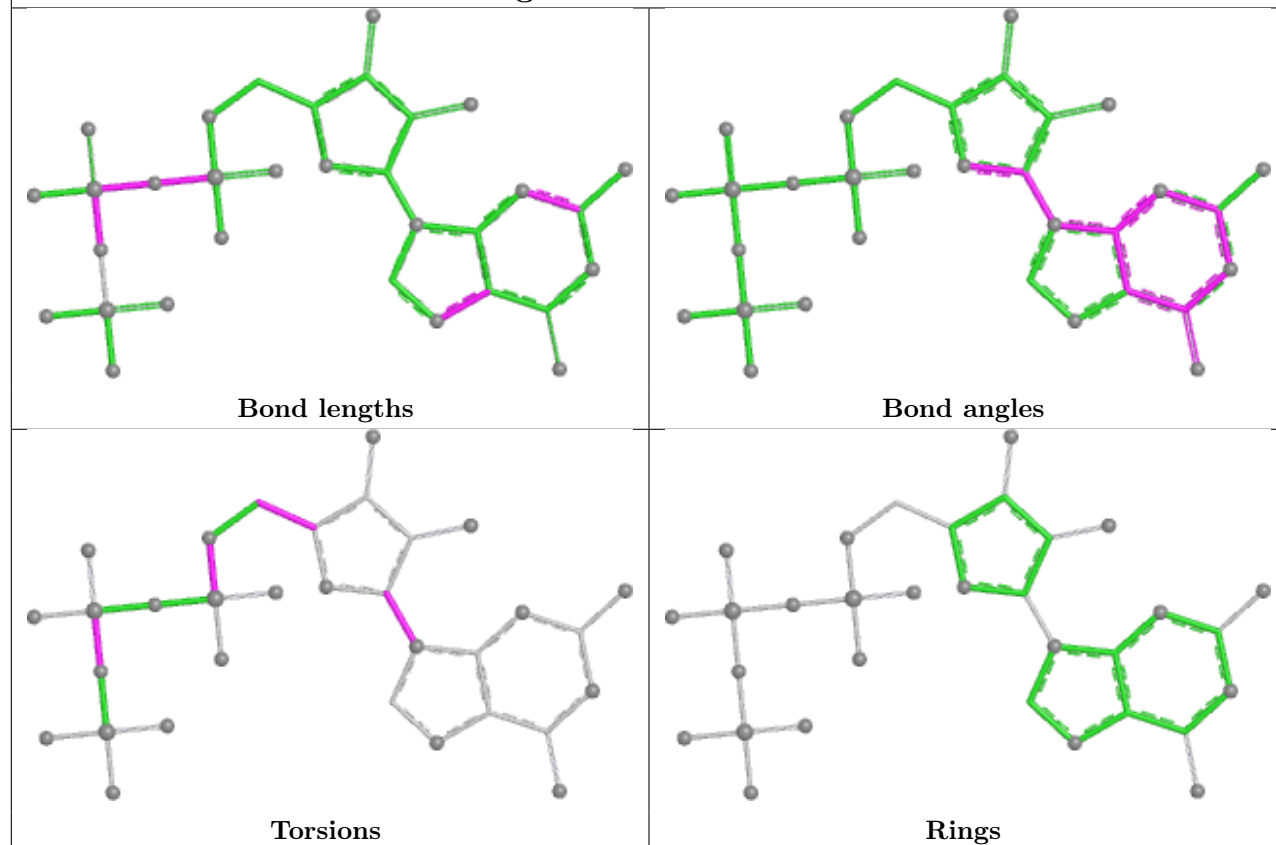
Ligand GTP SE 501



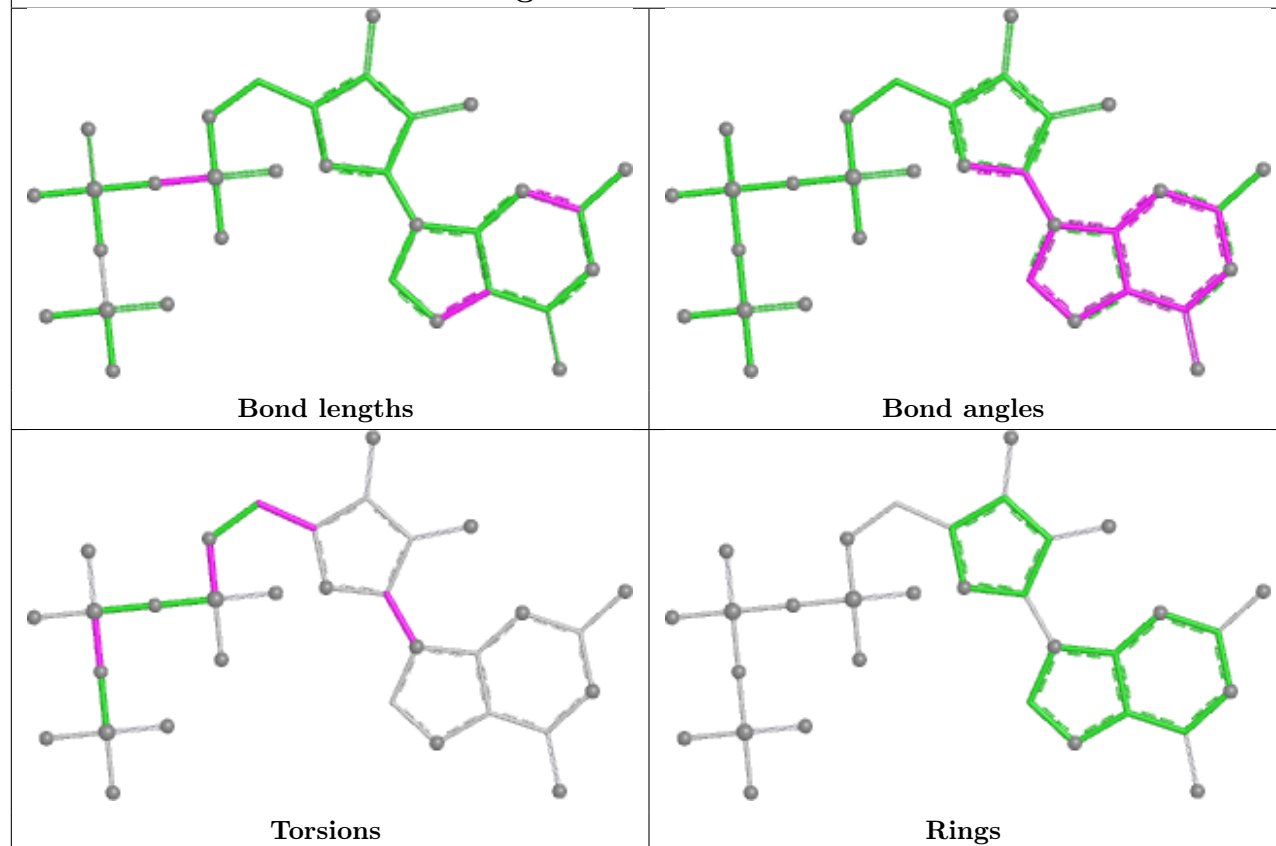
Ligand GTP BG 501



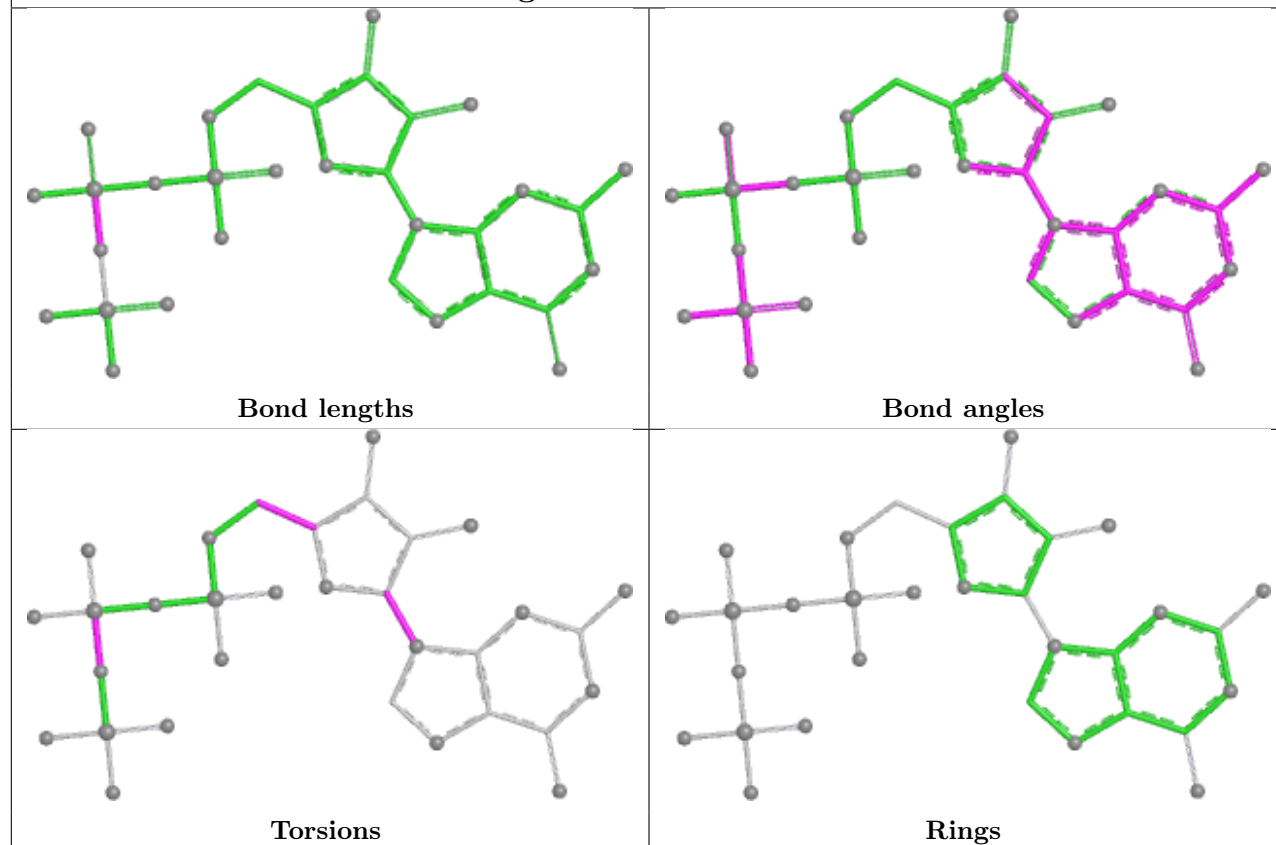
Ligand GTP UD 501



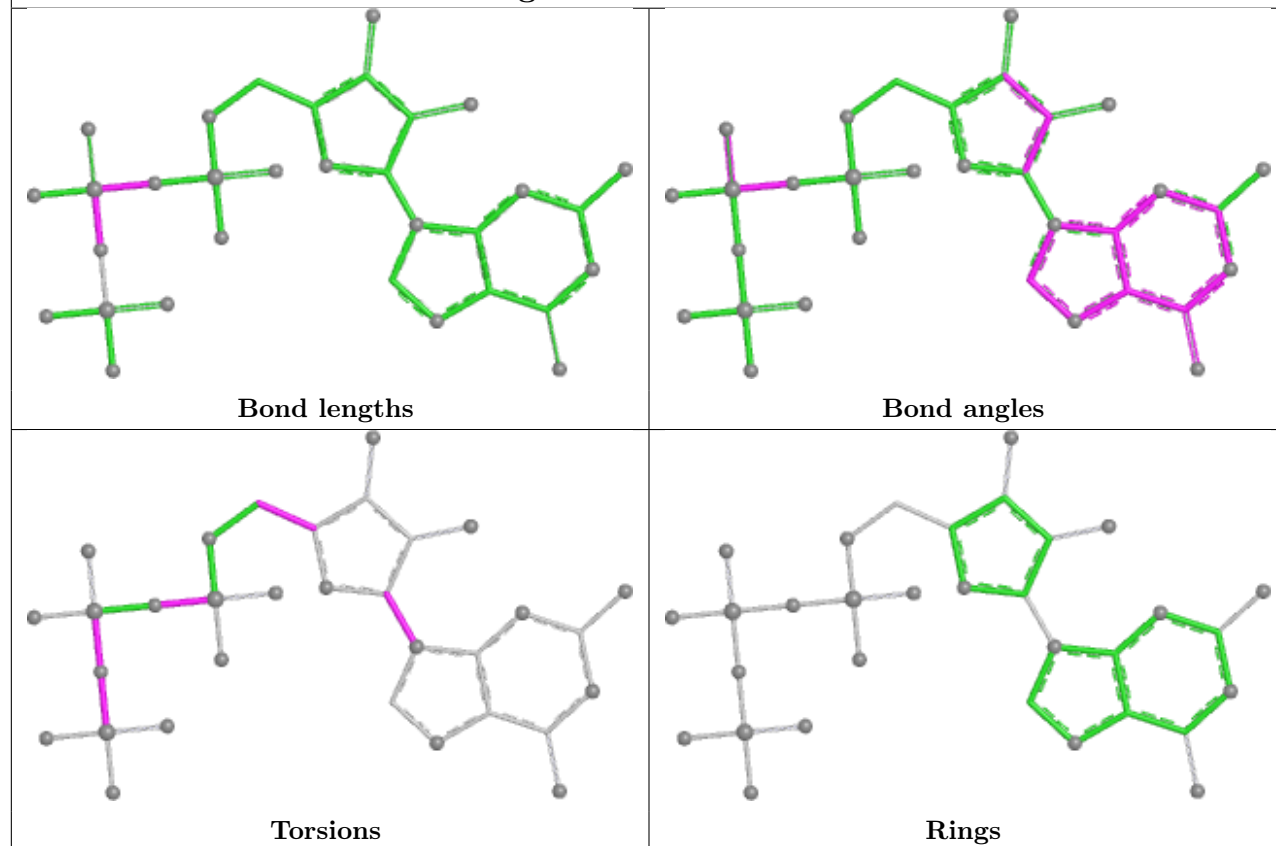
Ligand GTP VD 501



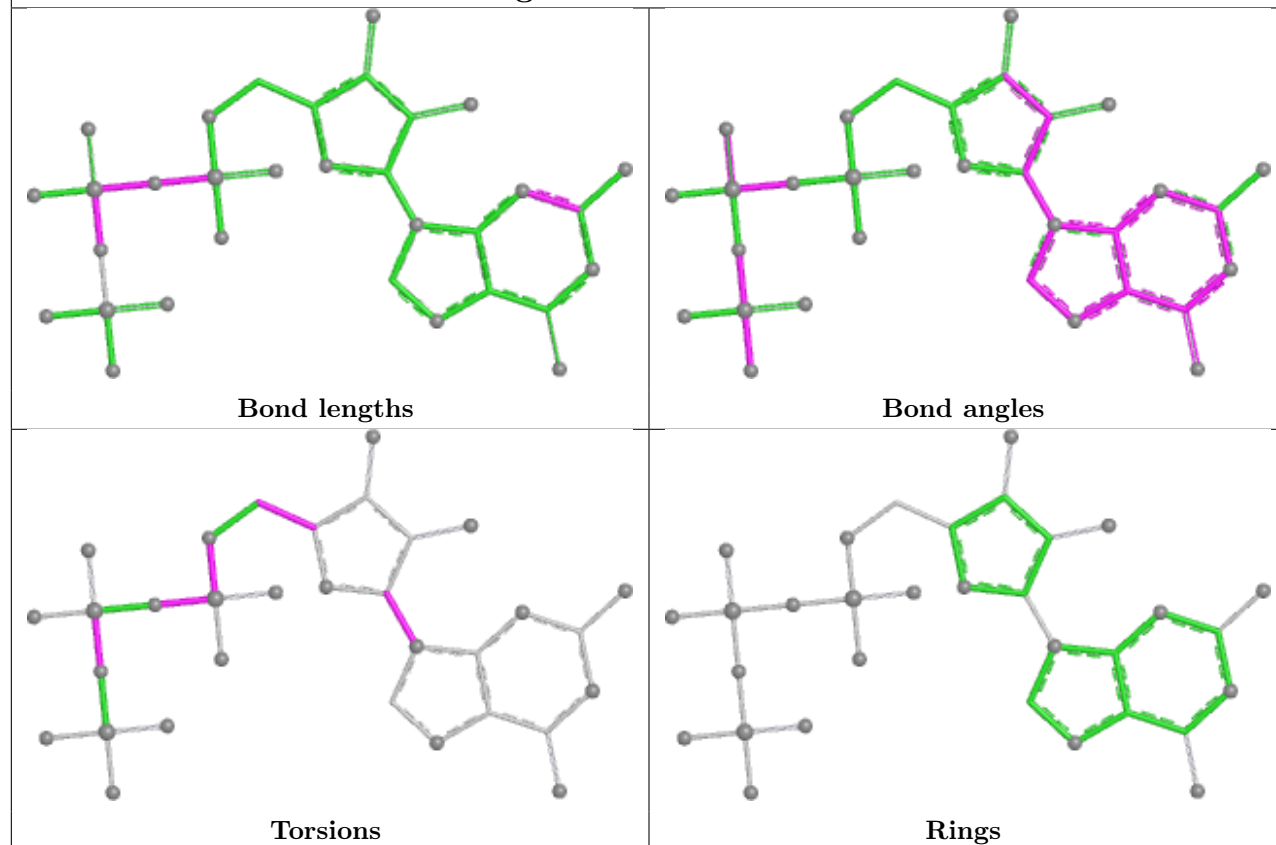
Ligand GTP DE 501



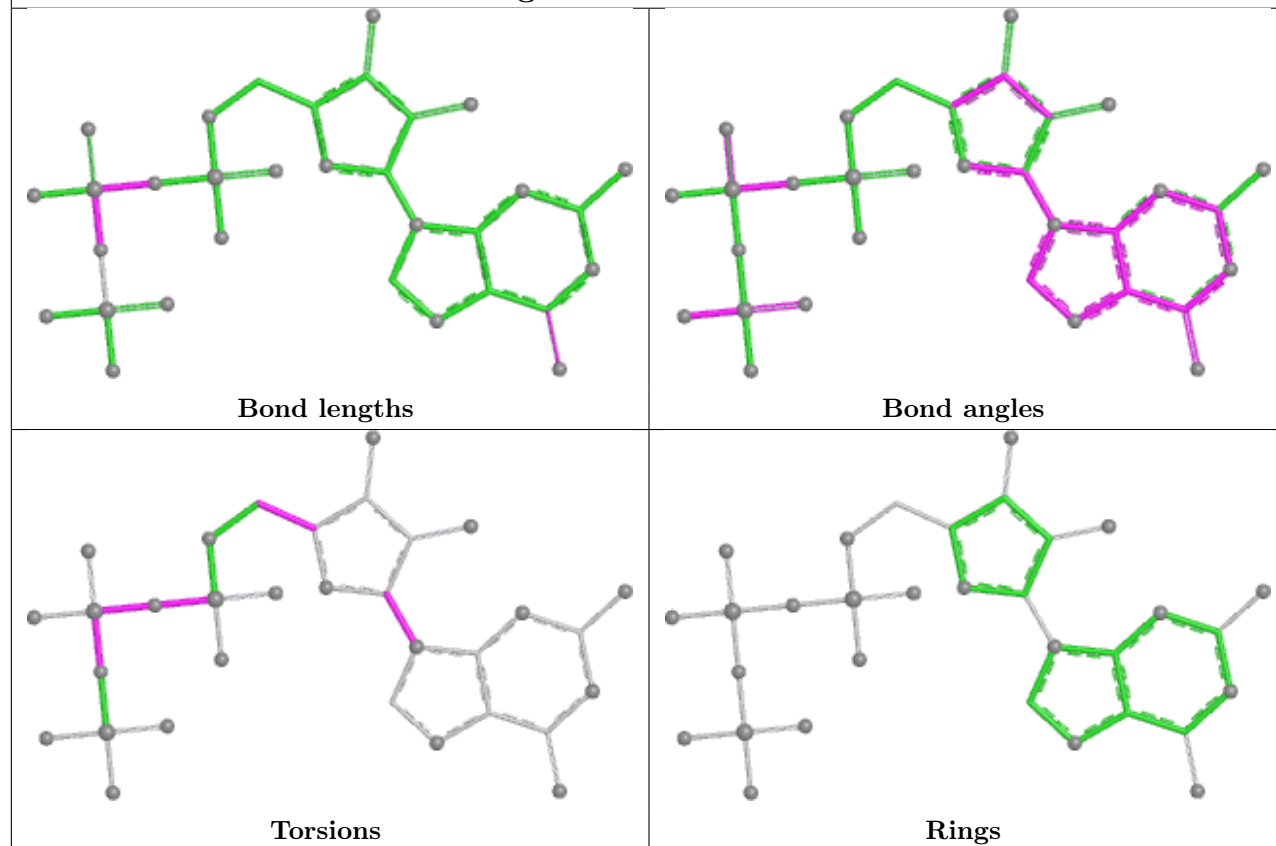
Ligand GTP WI 501



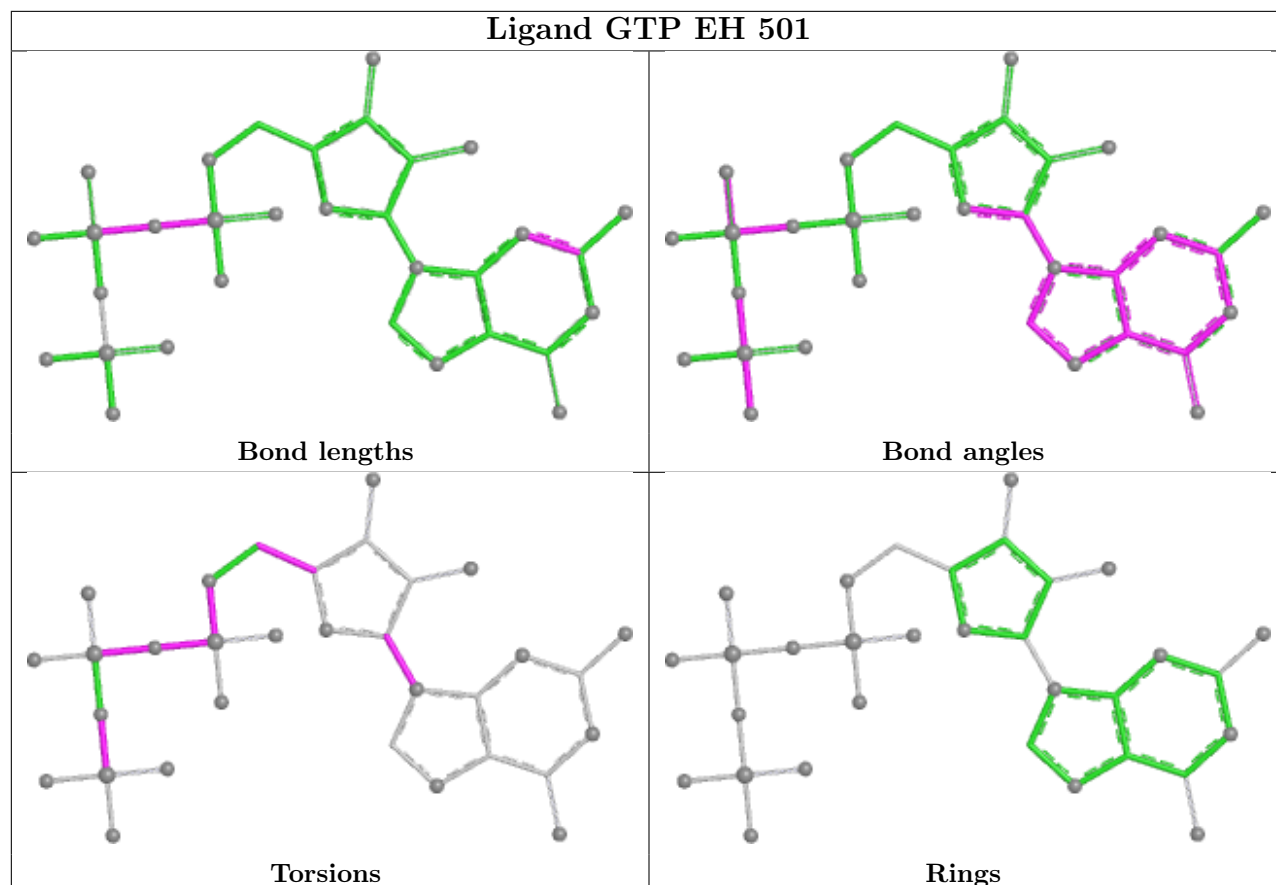
Ligand GTP NG 501



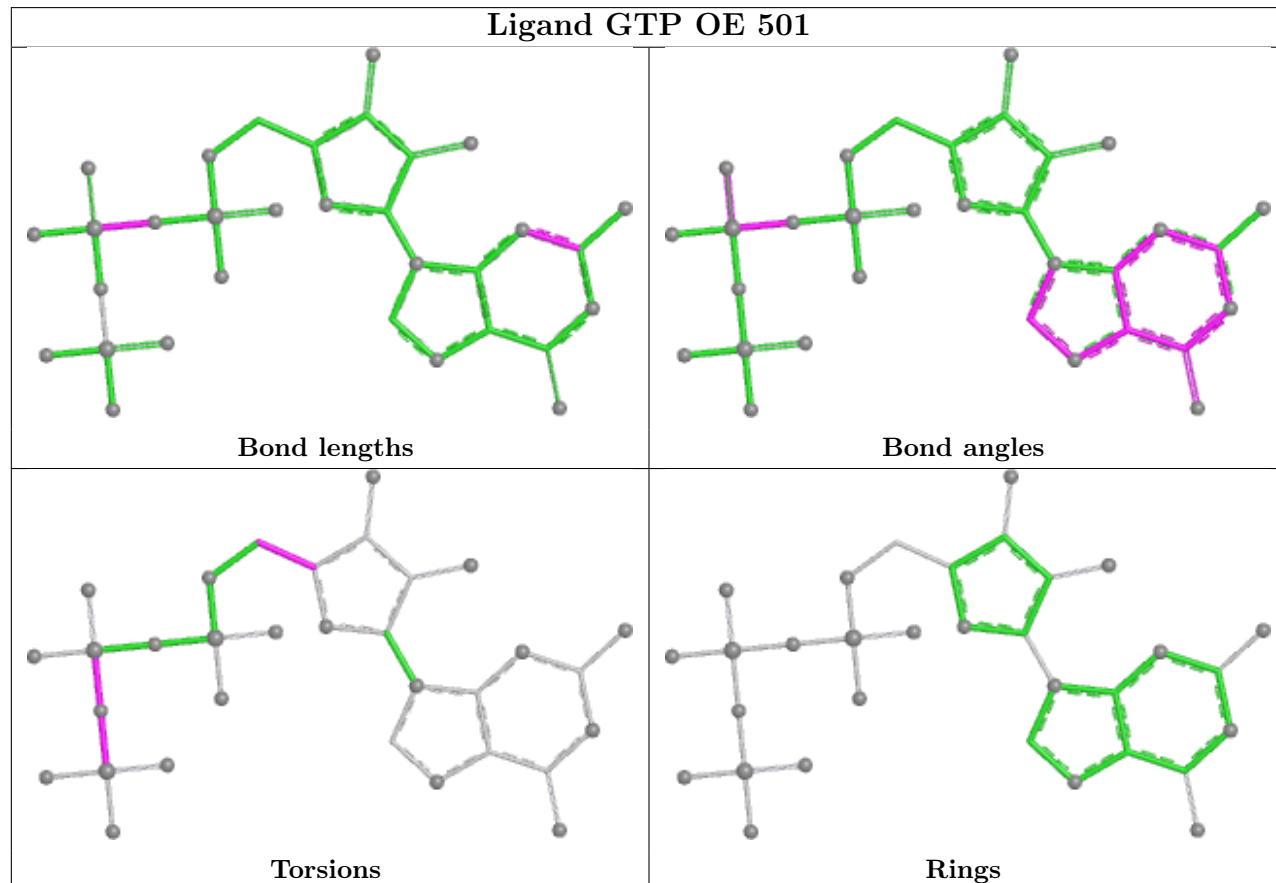
Ligand GTP EG 501



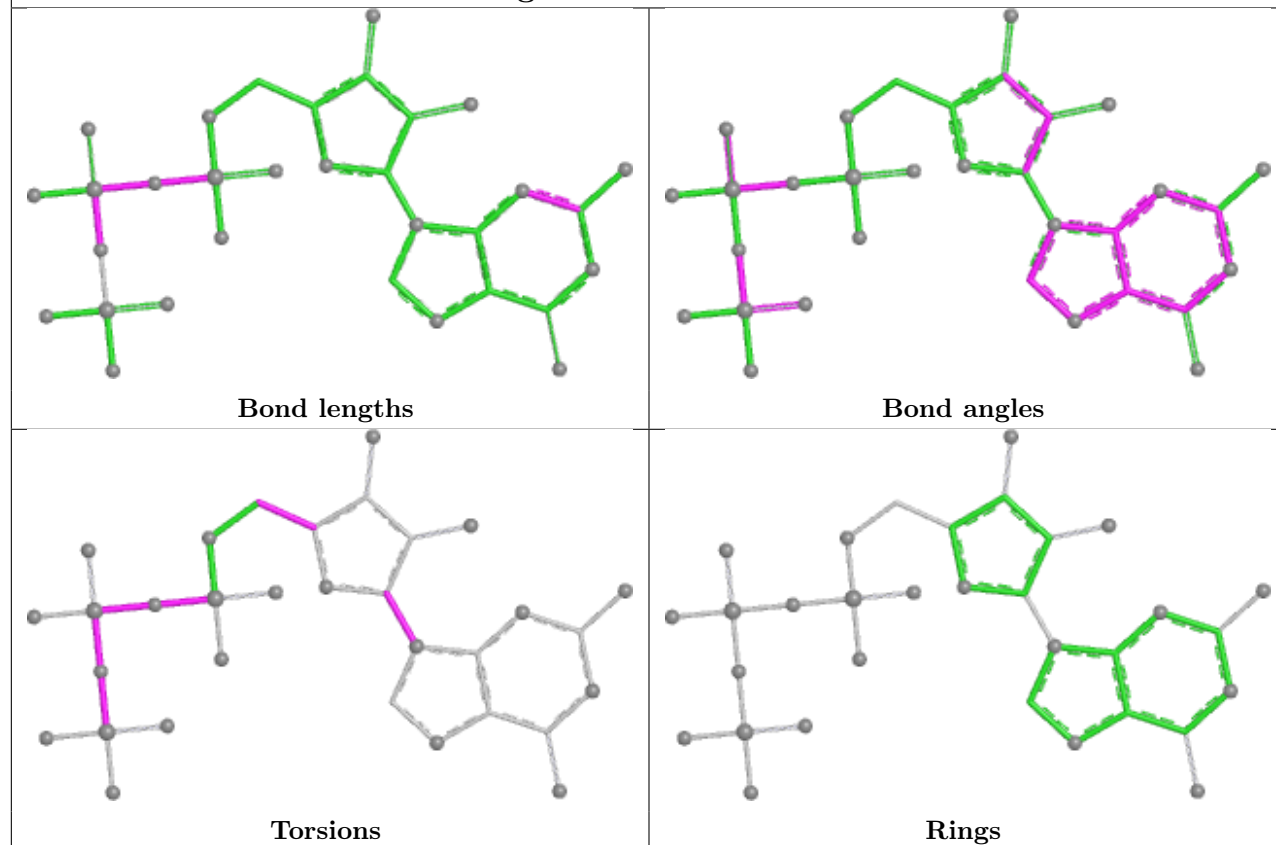
Ligand GTP EH 501



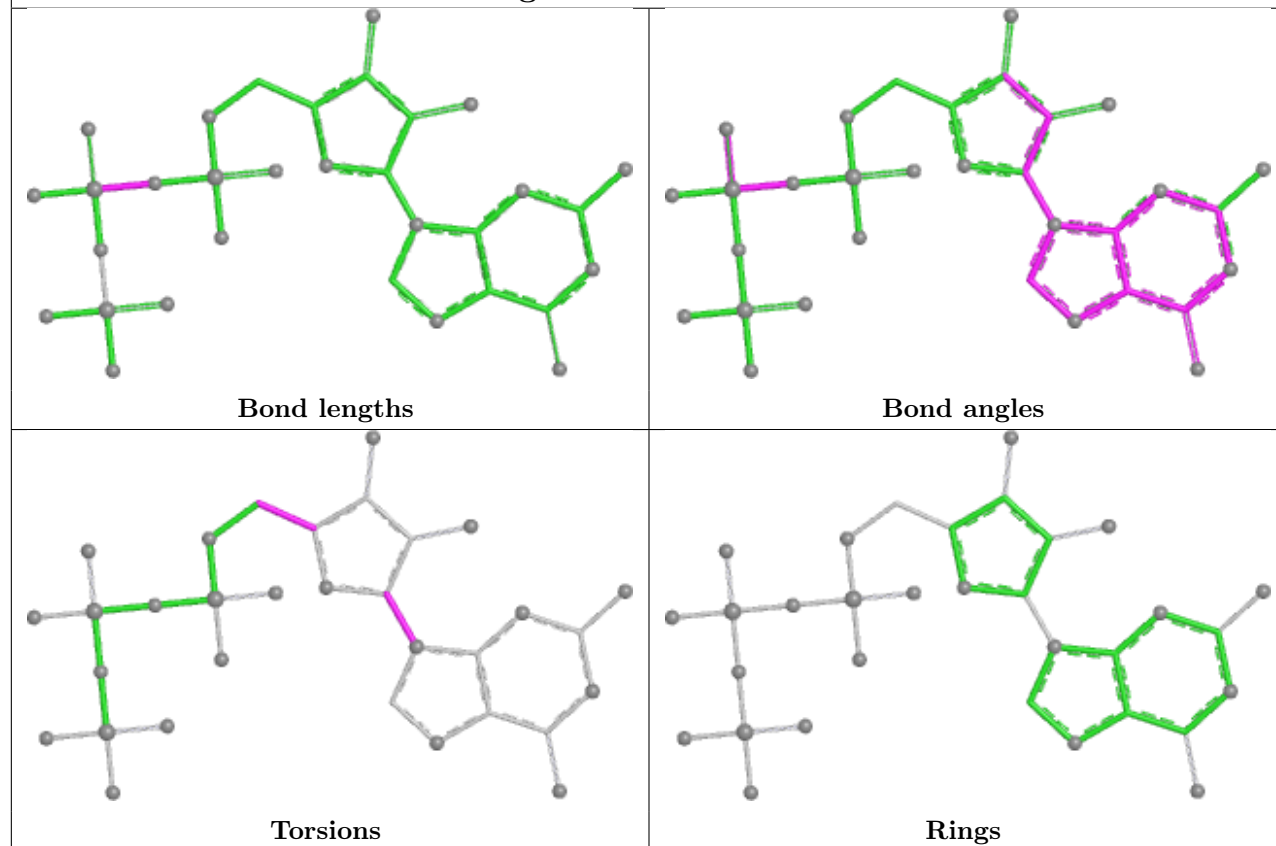
Ligand GTP OE 501



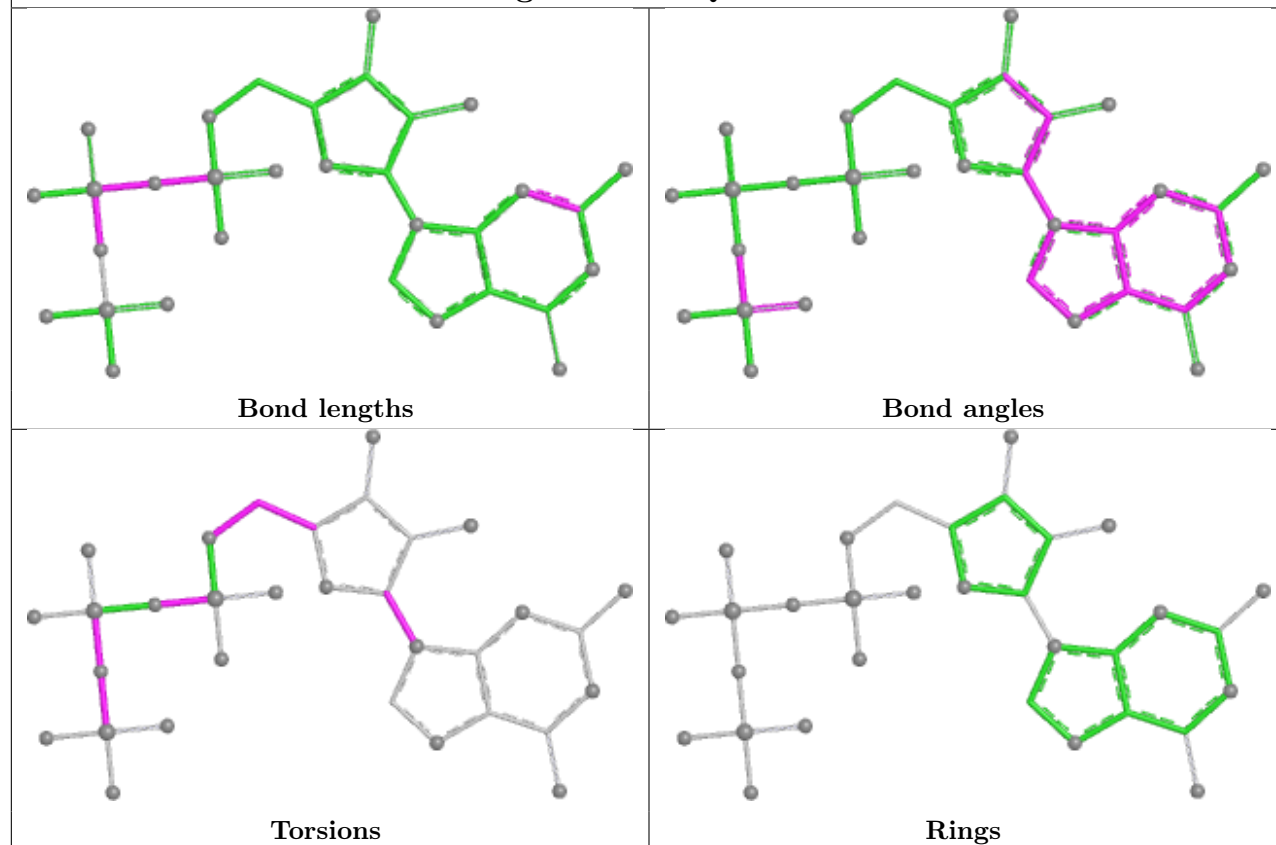
Ligand GTP PG 501



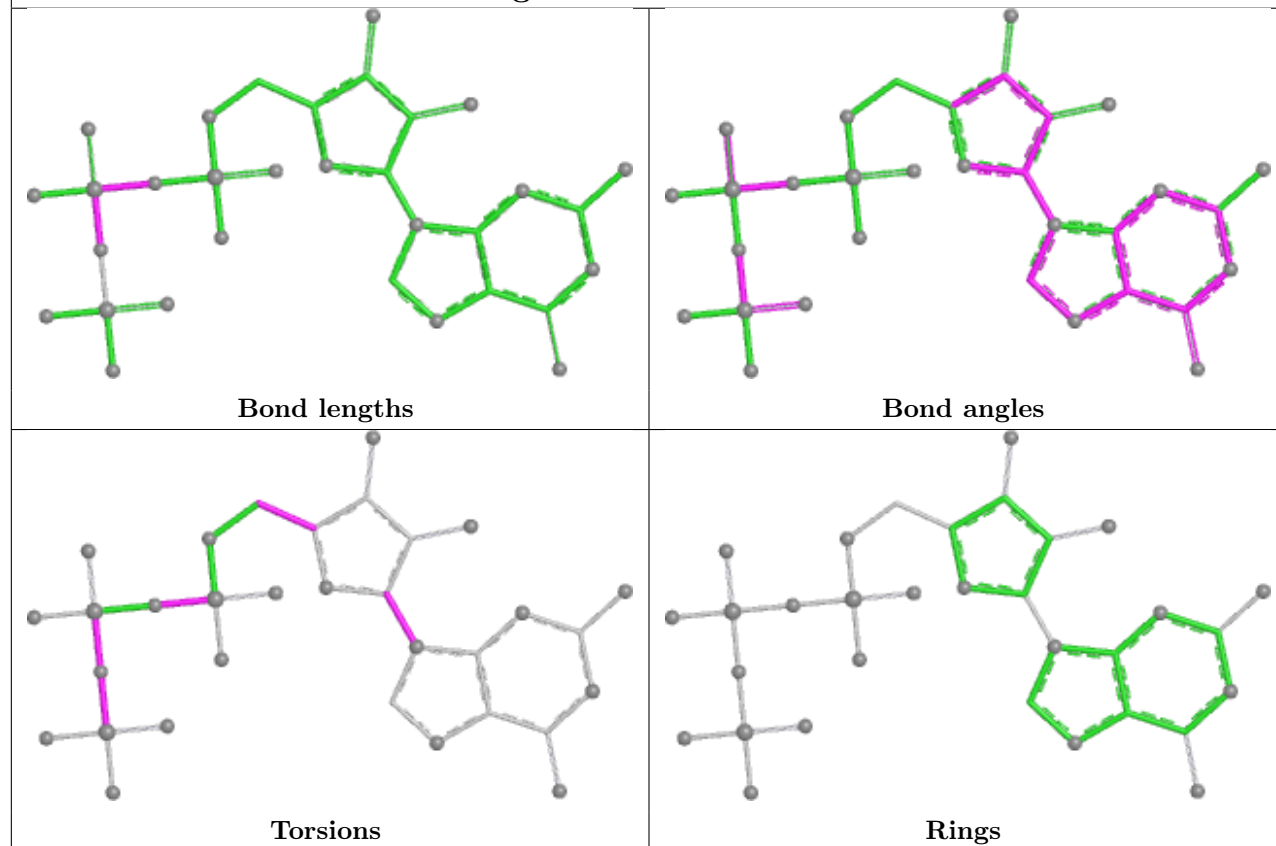
Ligand GTP BE 501



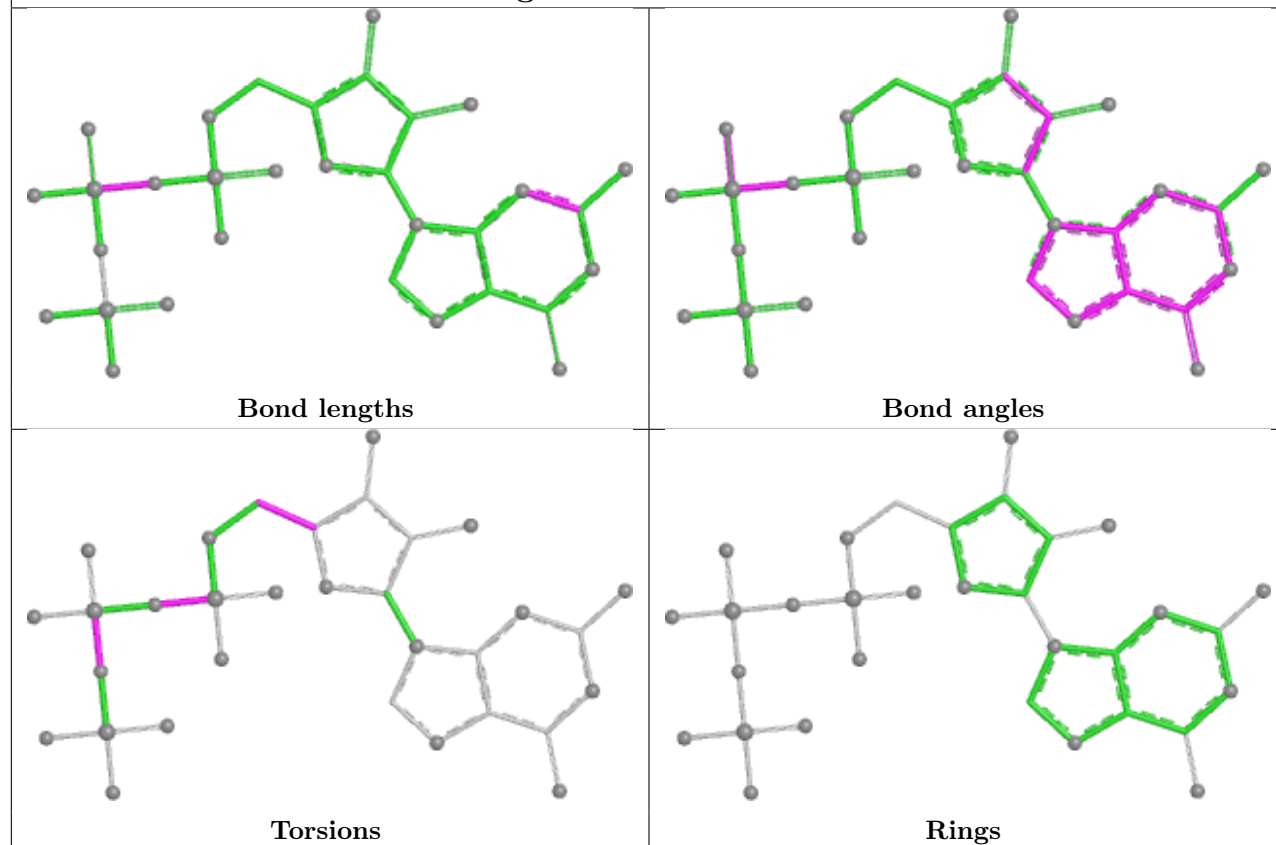
Ligand GTP QG 501



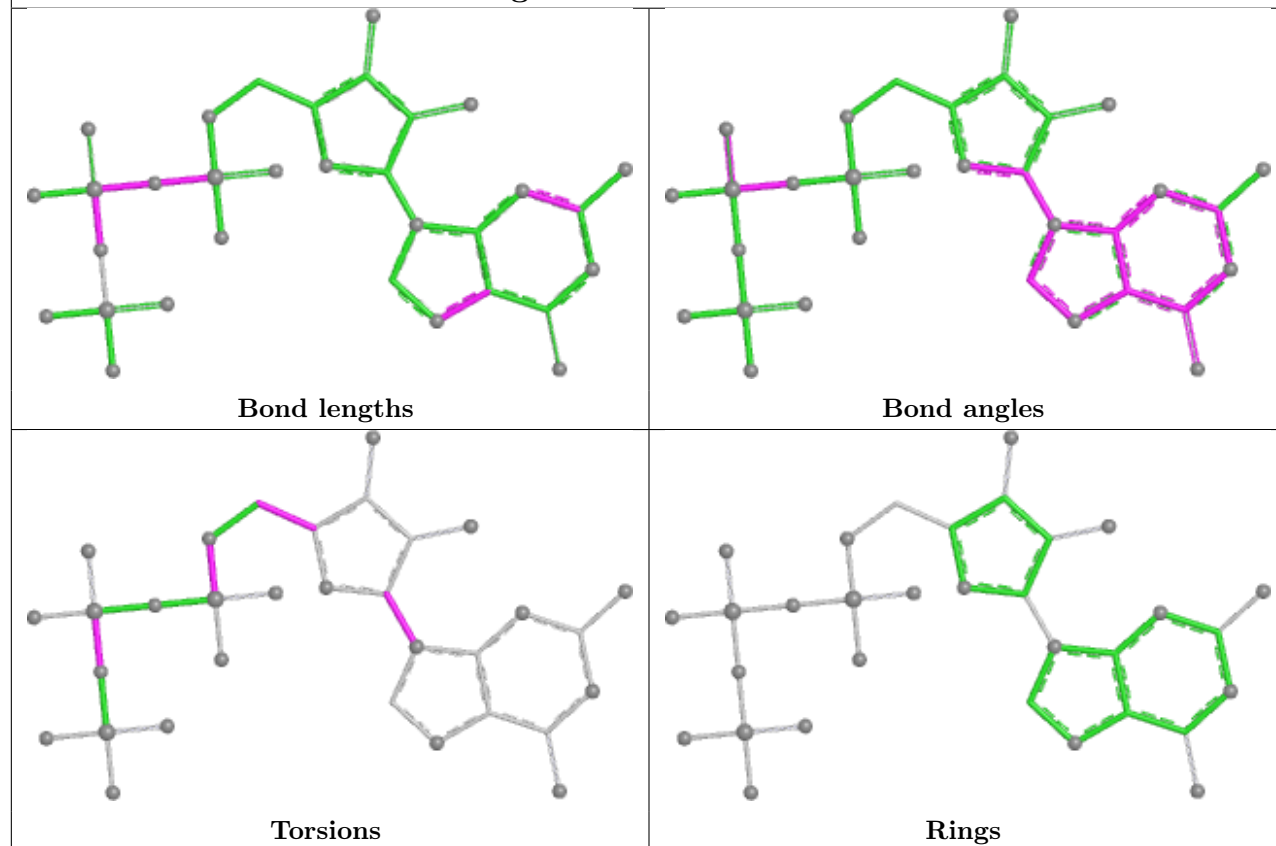
Ligand GTP MG 501



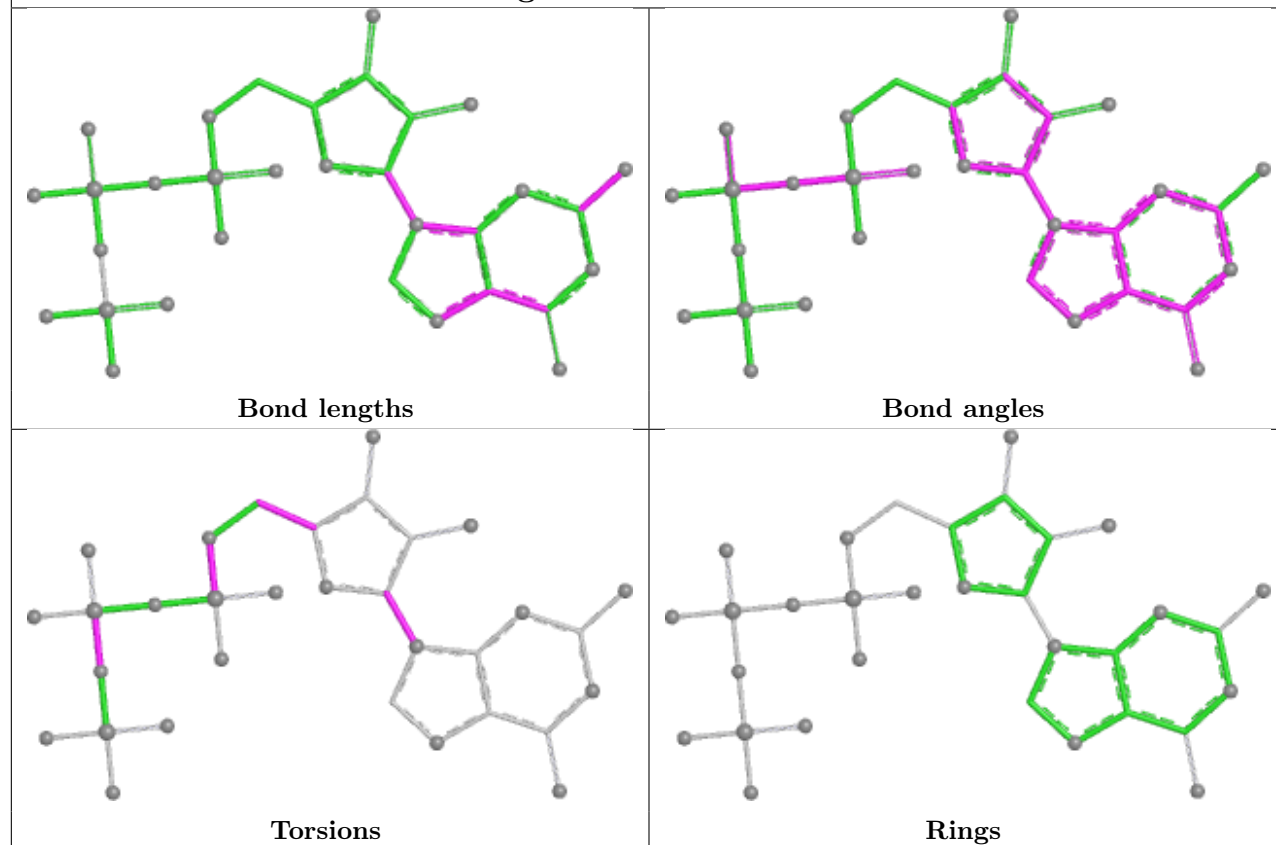
Ligand GTP RG 501



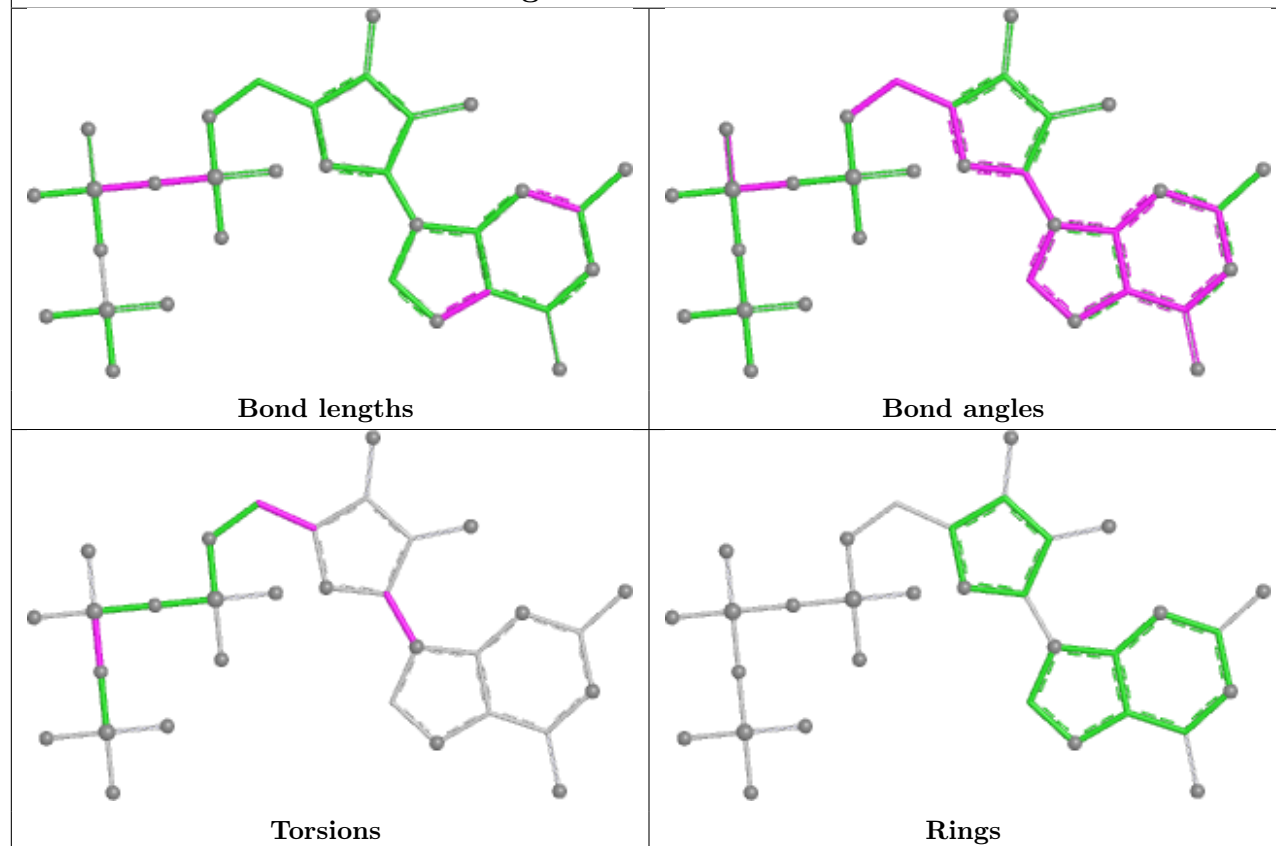
Ligand GTP WH 501



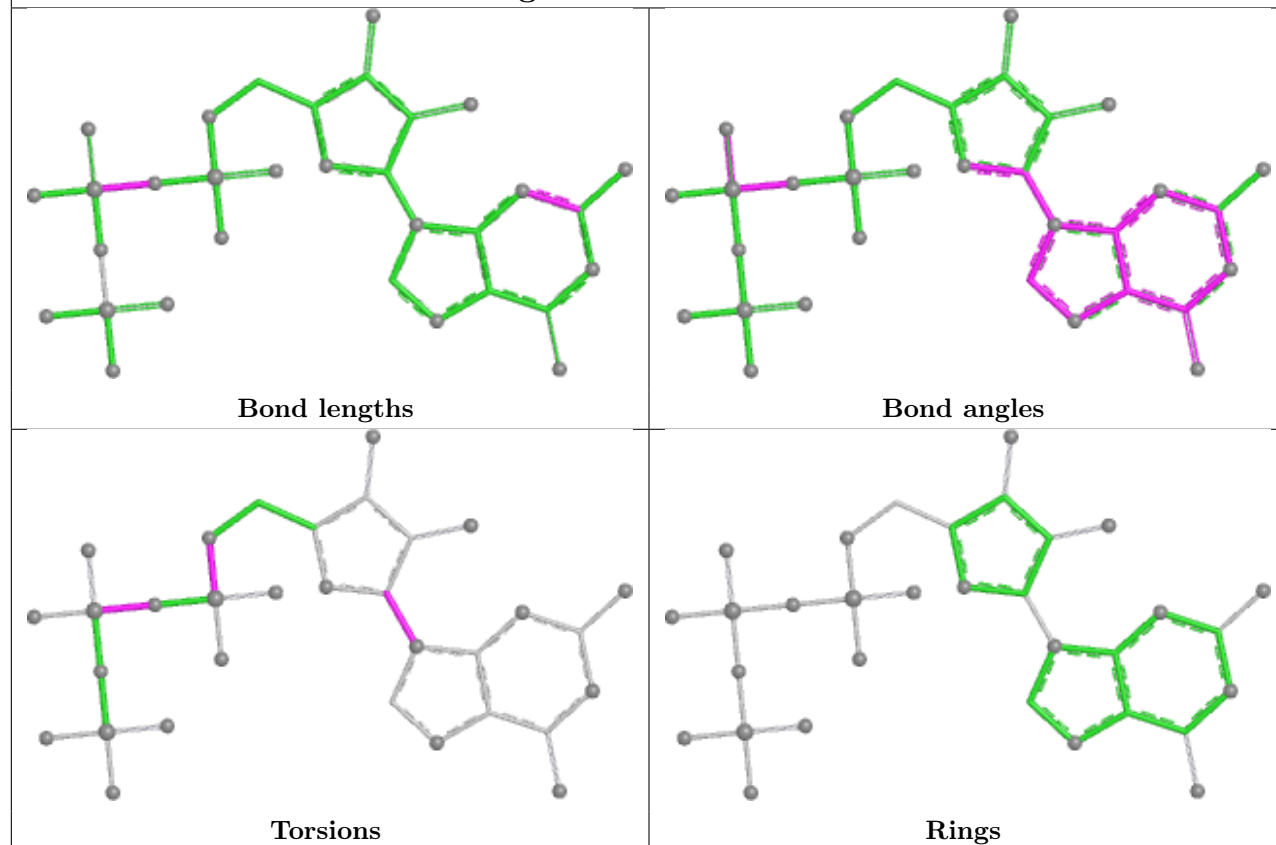
Ligand GTP GE 501



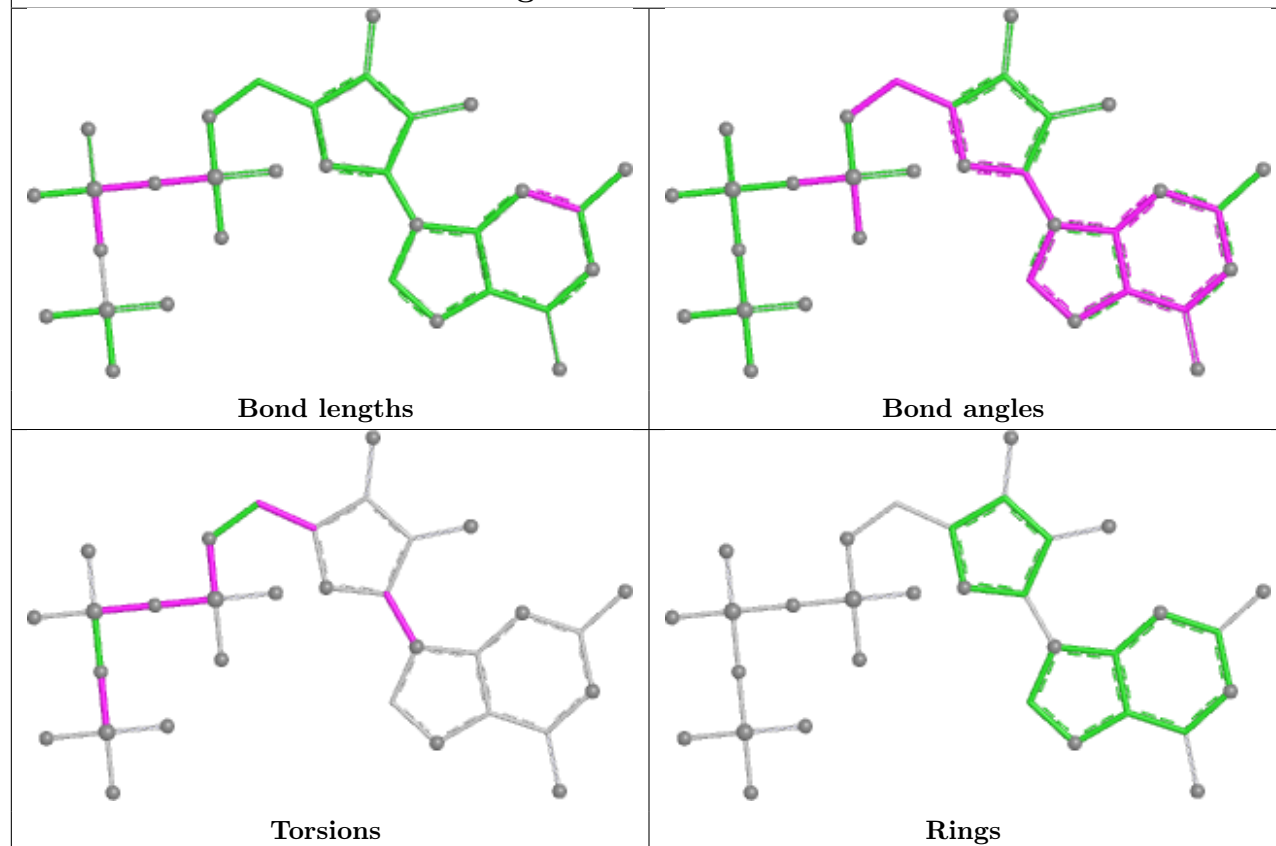
Ligand GTP LF 501



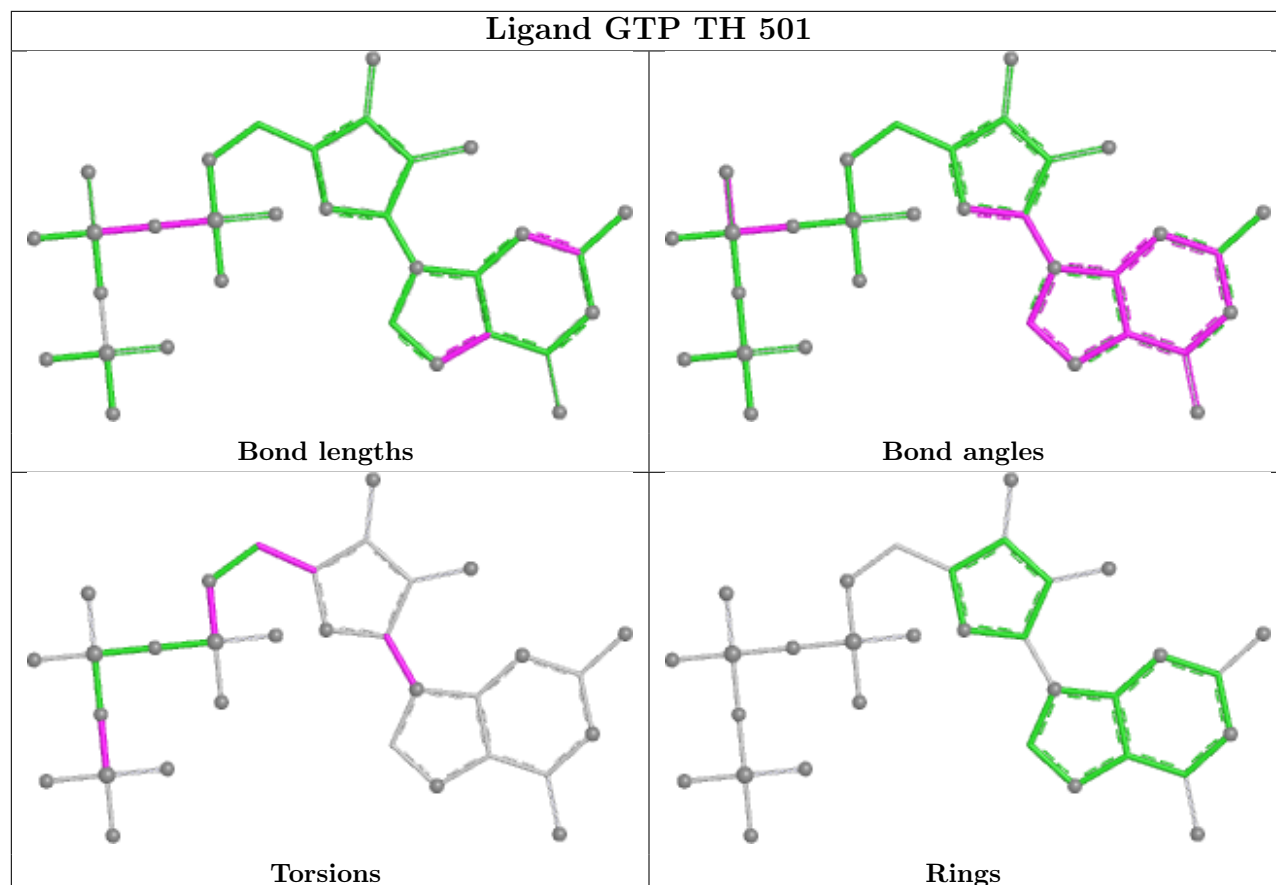
Ligand GTP FD 501



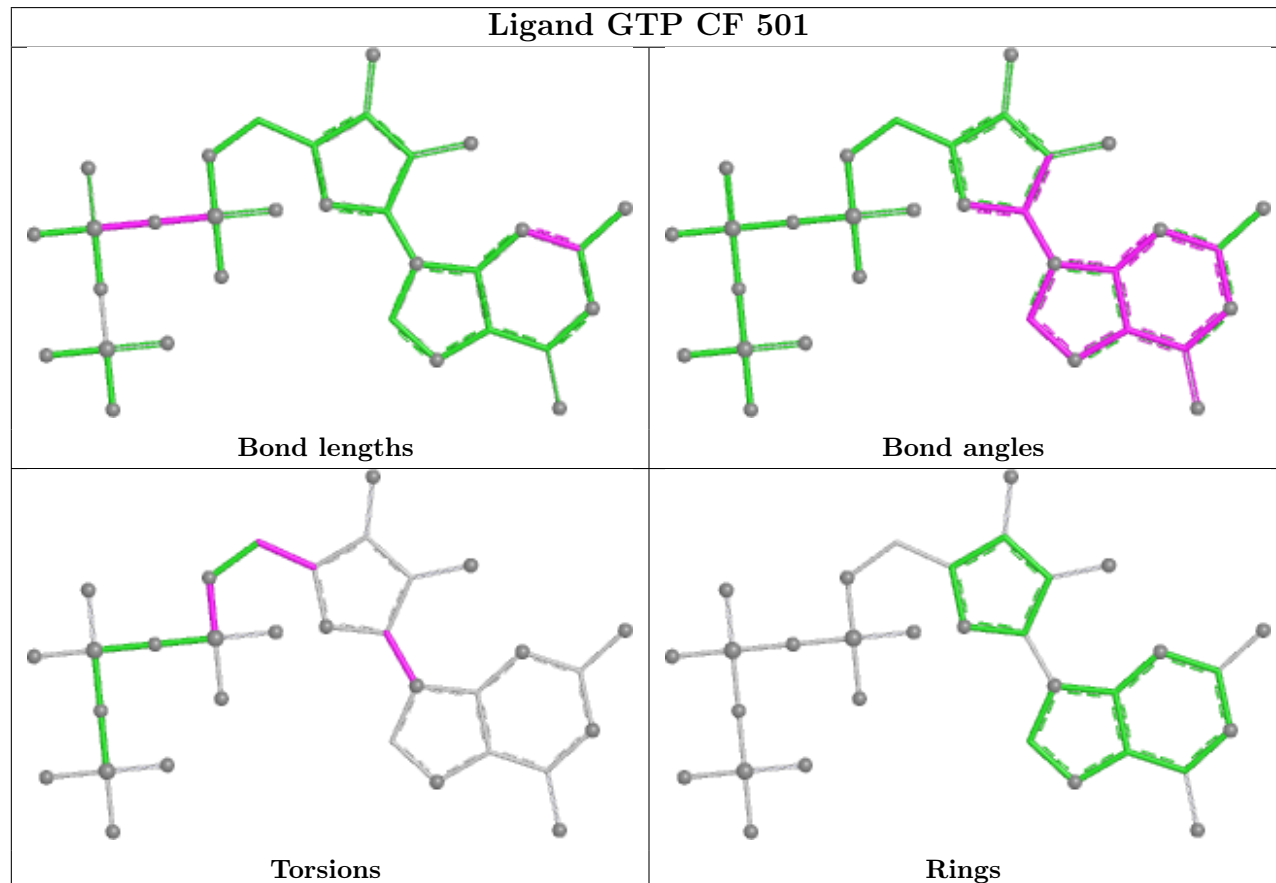
Ligand GTP BH 501



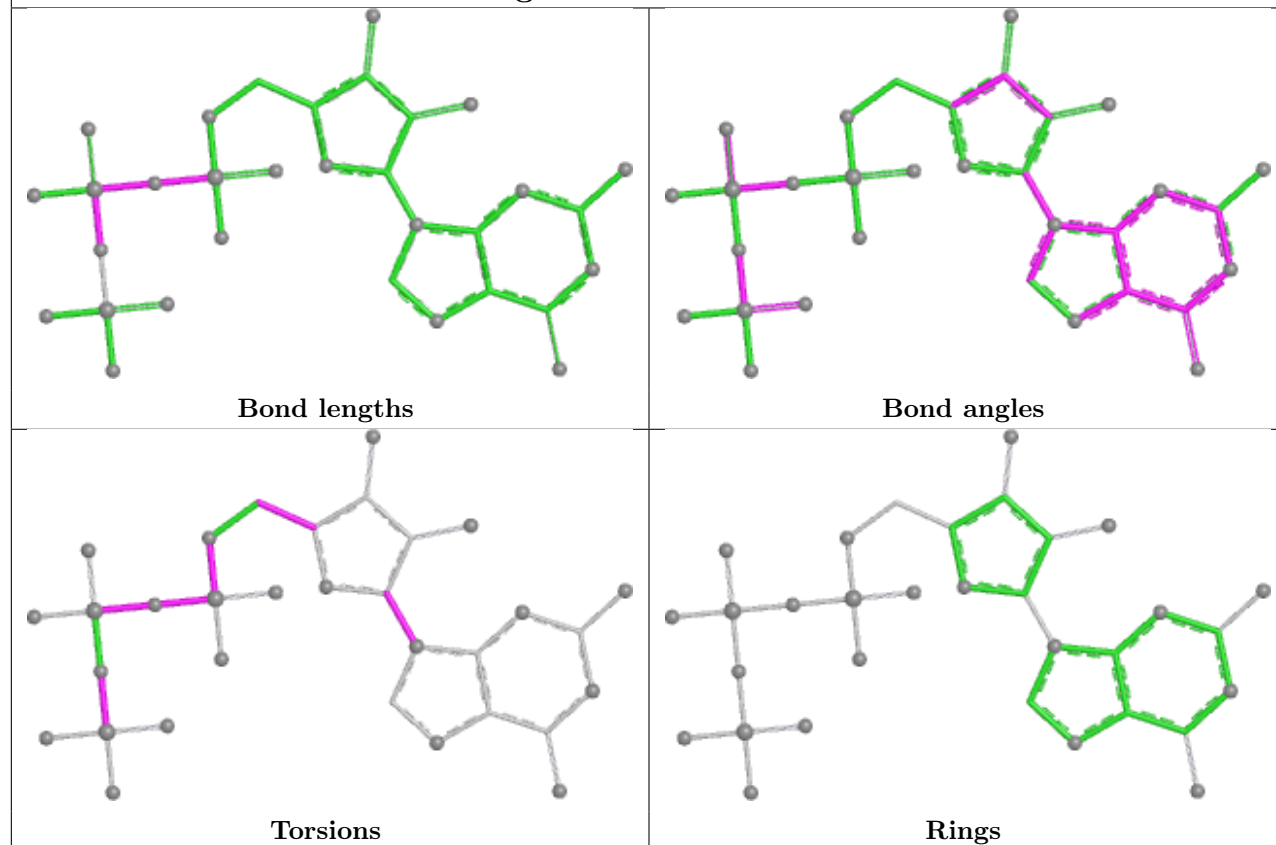
Ligand GTP TH 501



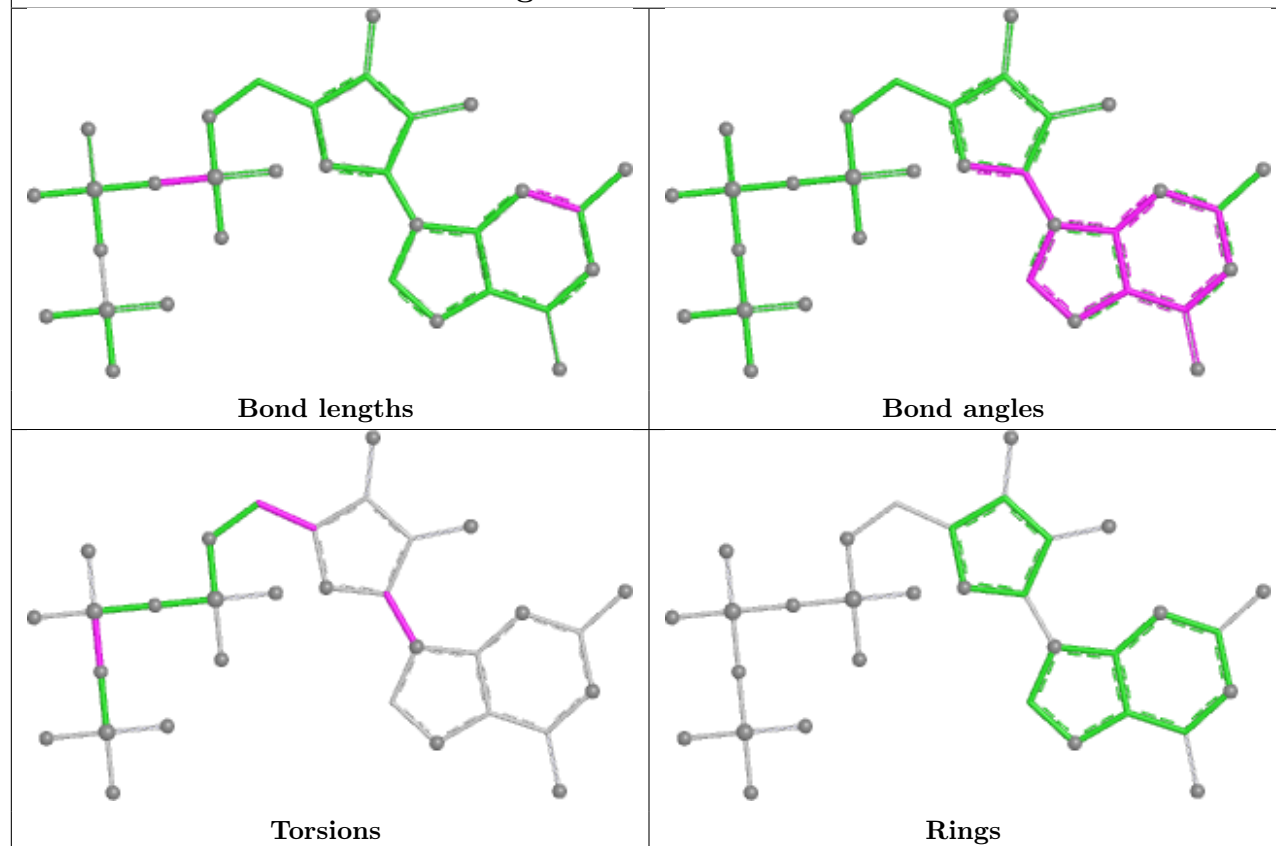
Ligand GTP CF 501



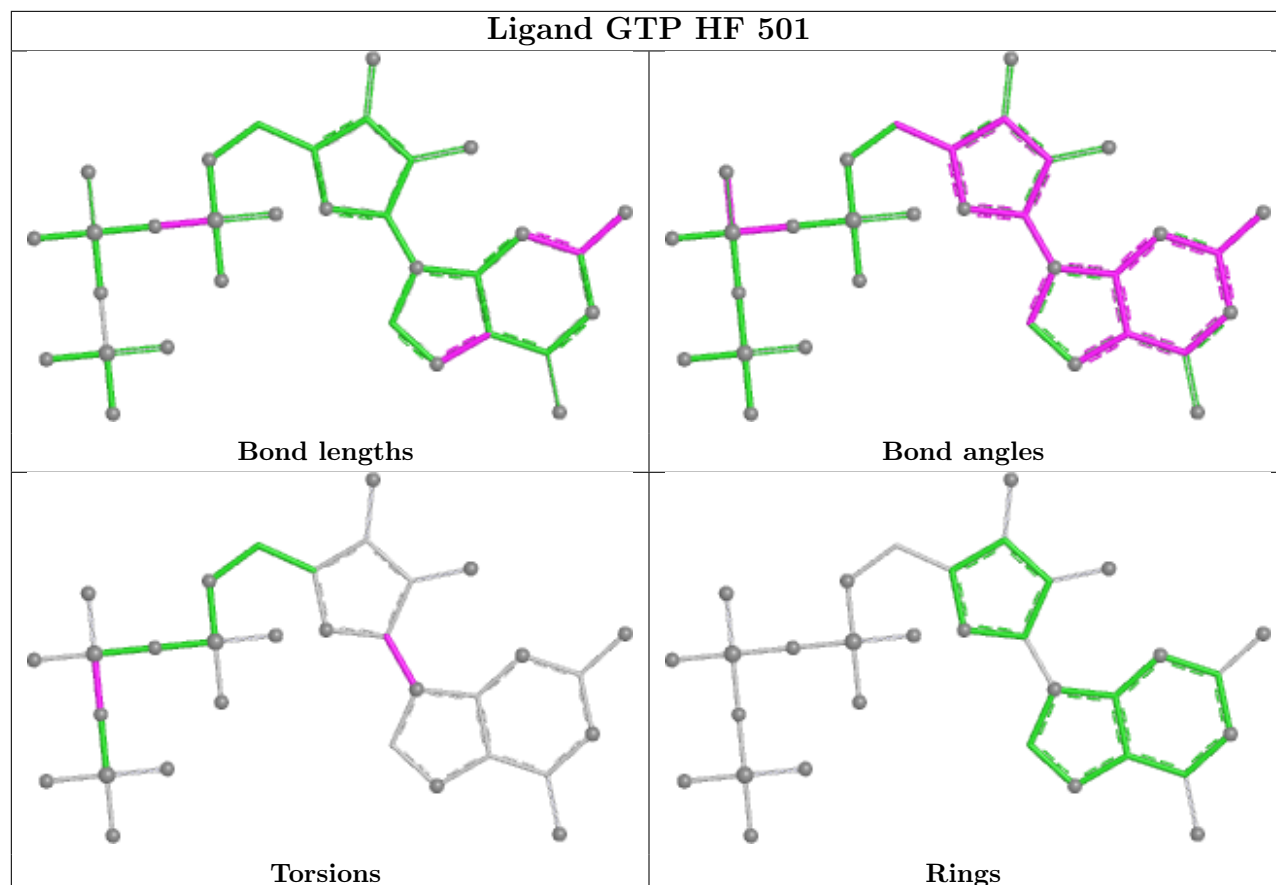
Ligand GTP UG 501



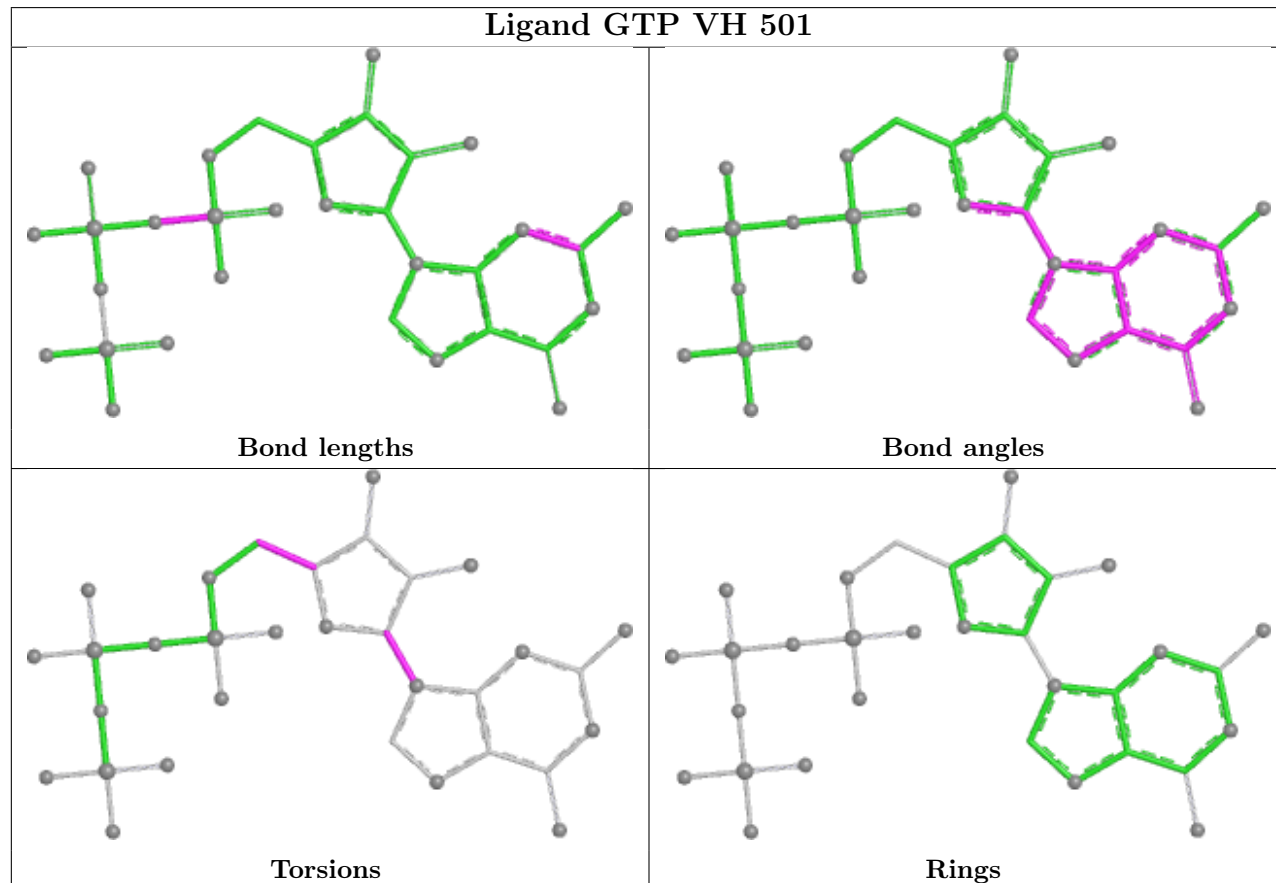
Ligand GTP OH 501



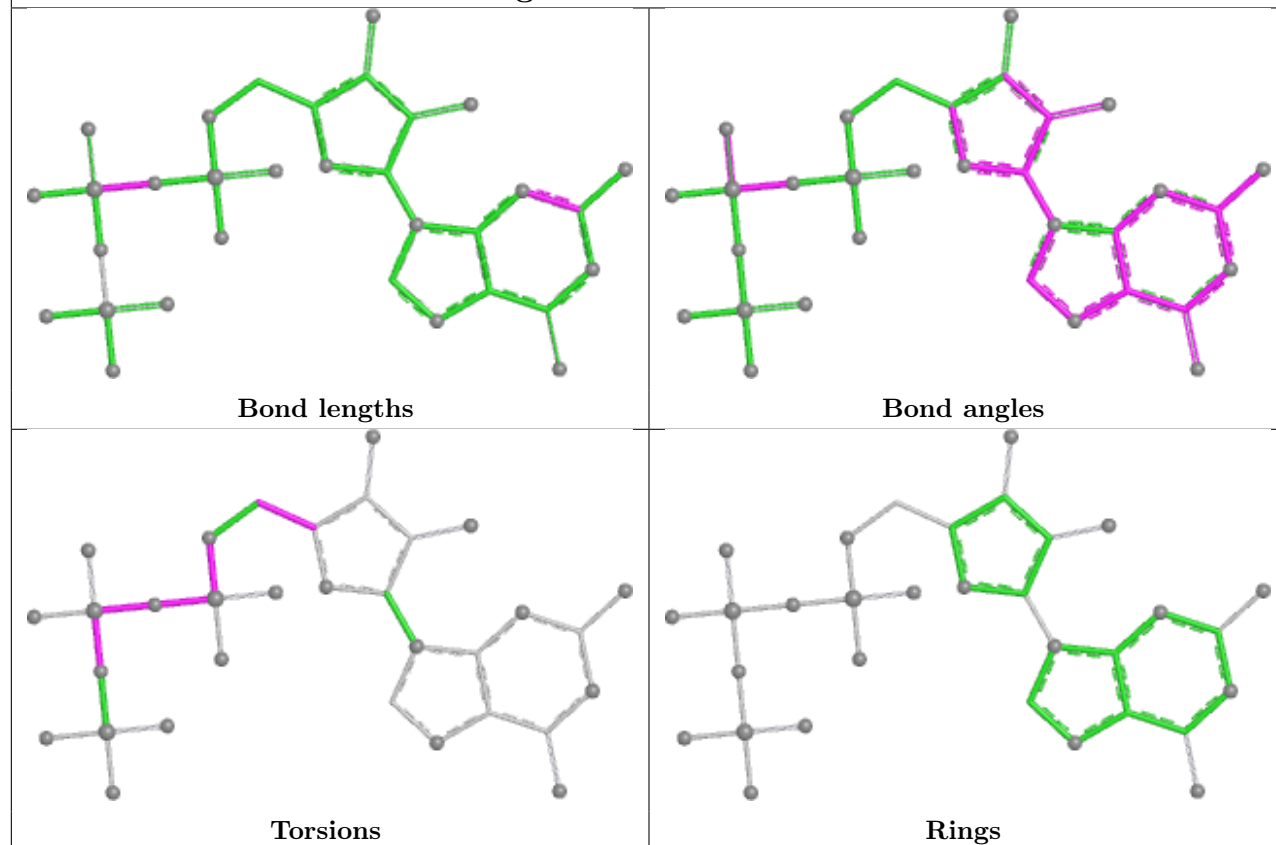
Ligand GTP HF 501



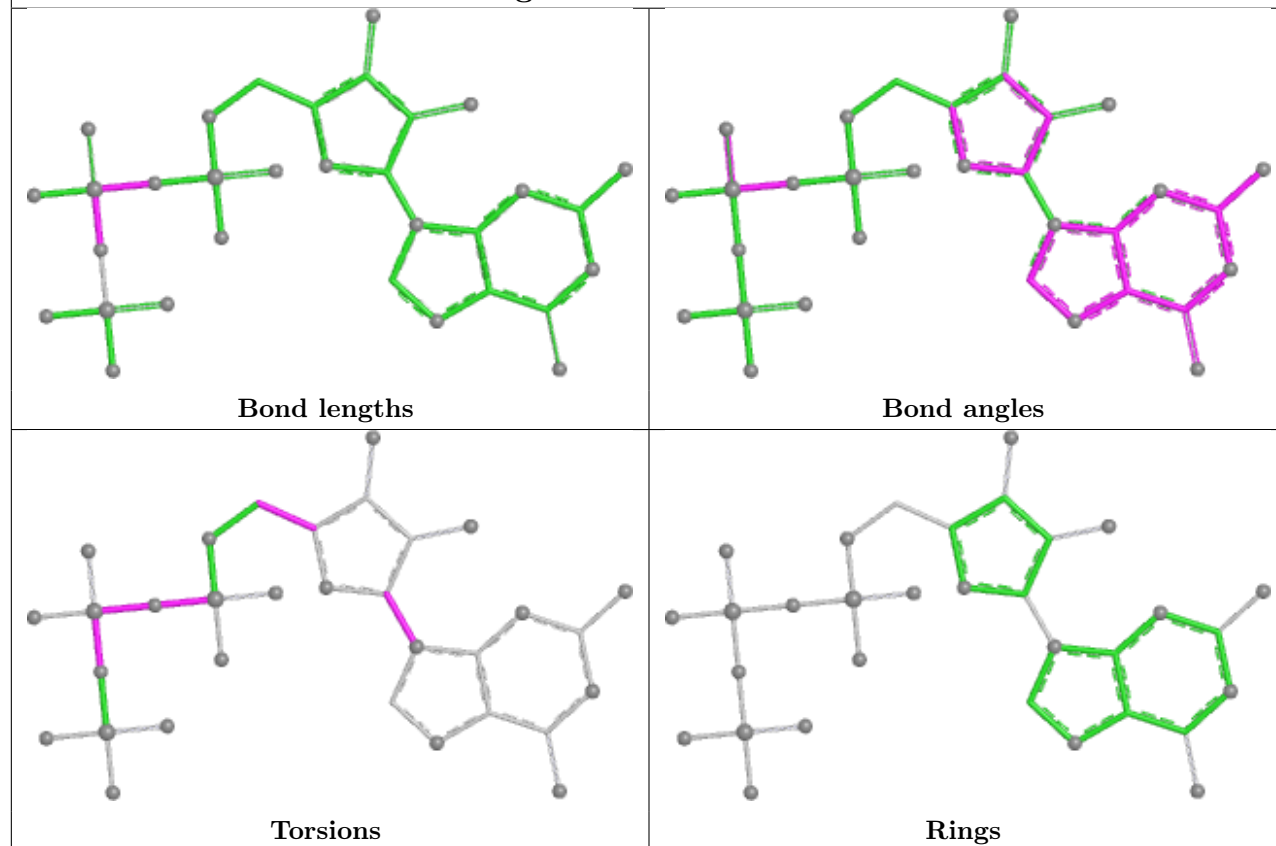
Ligand GTP VH 501



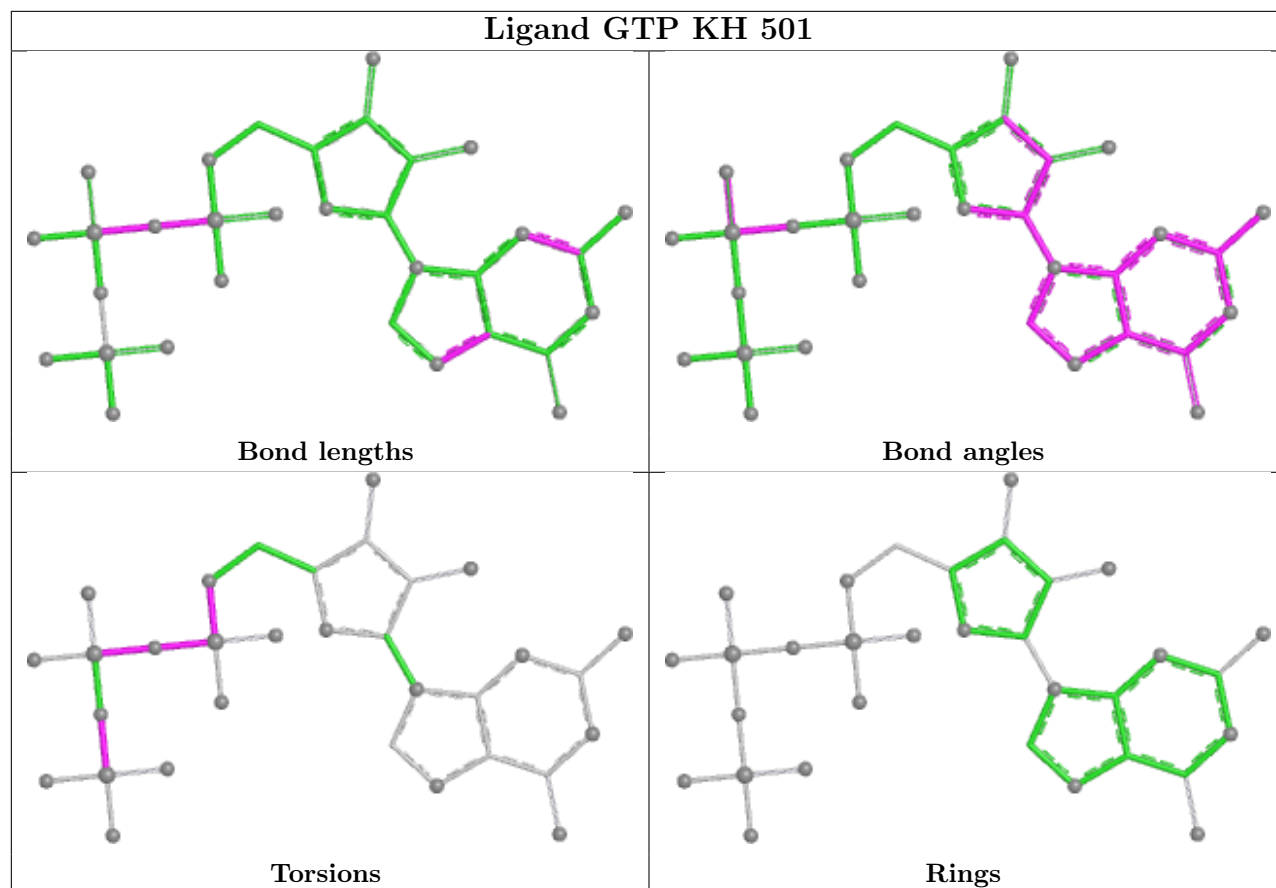
Ligand GTP KG 501



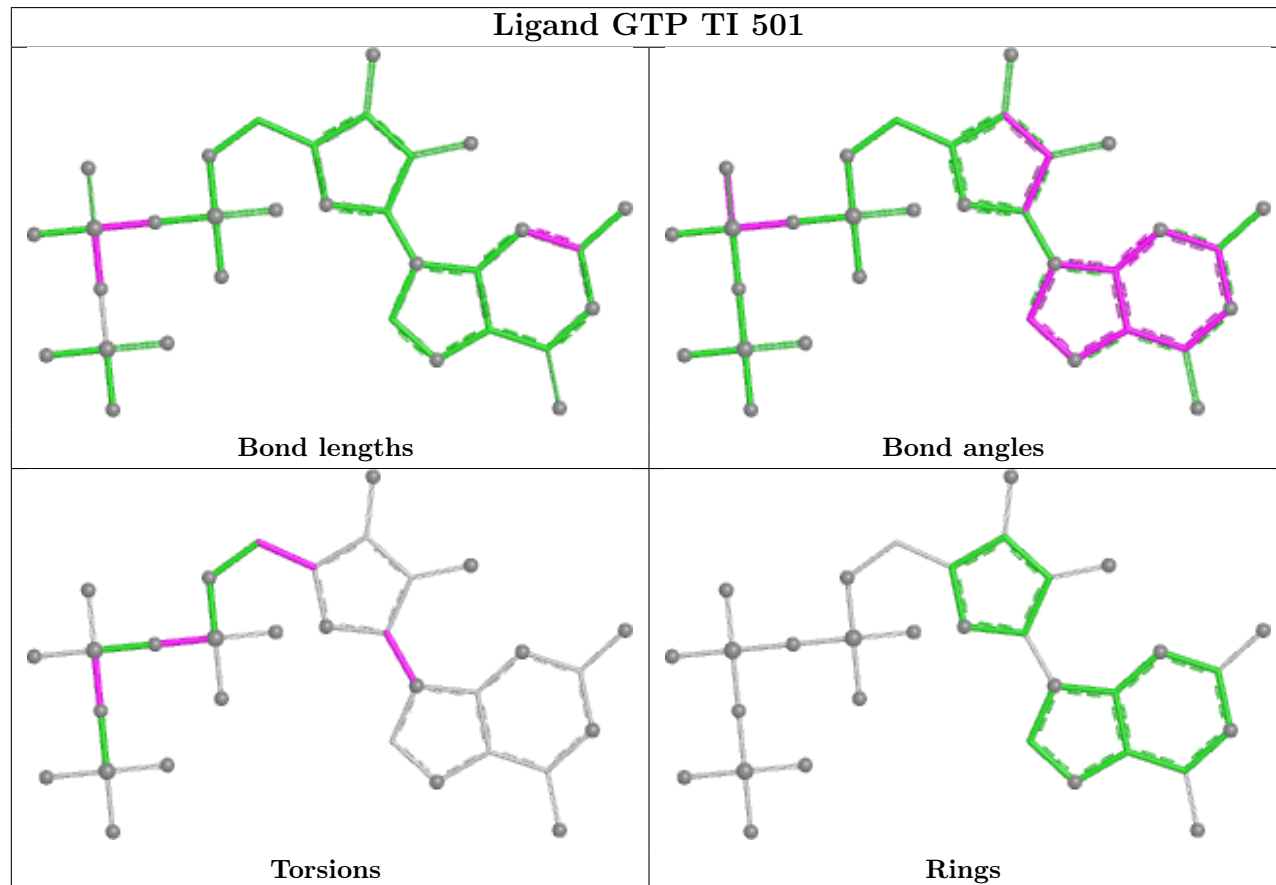
Ligand GTP GG 501



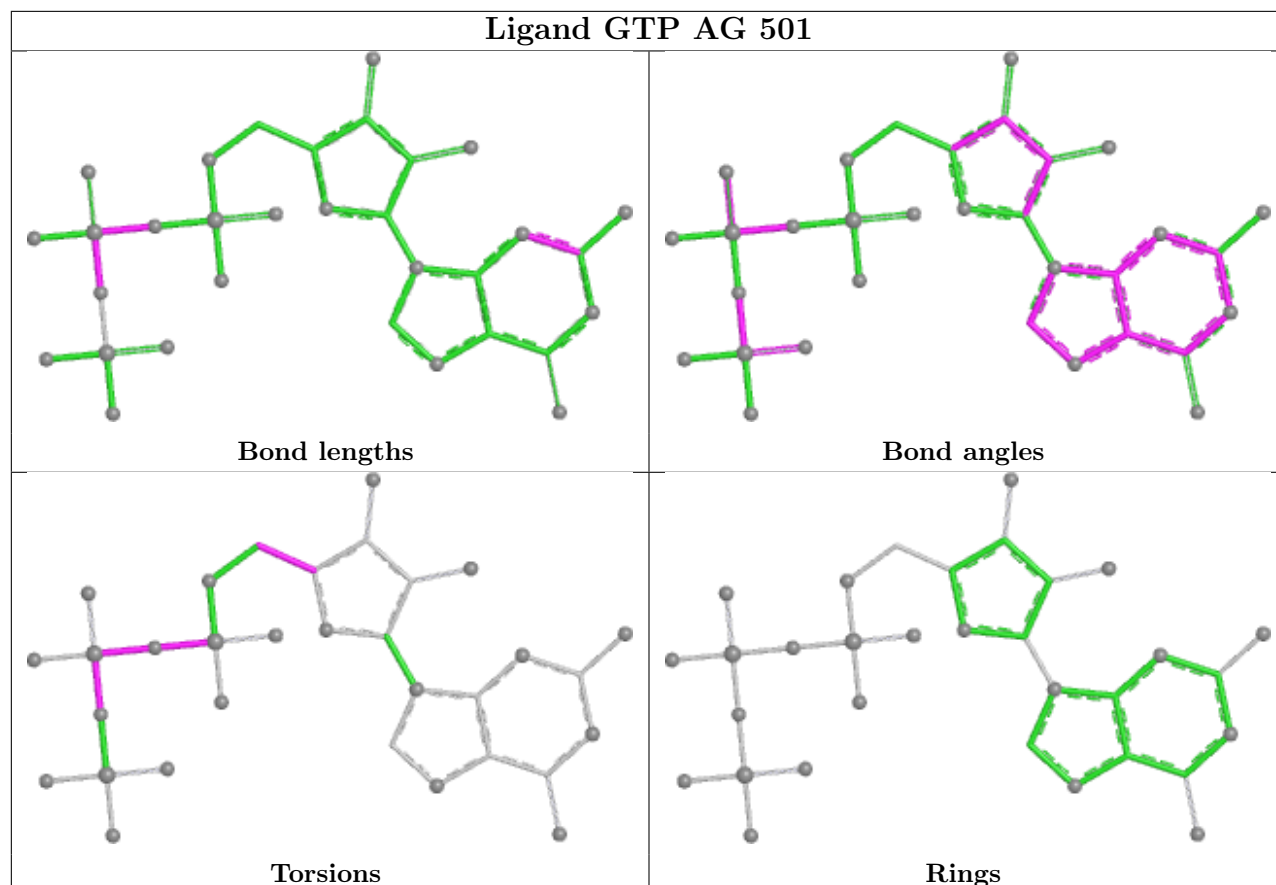
Ligand GTP KH 501



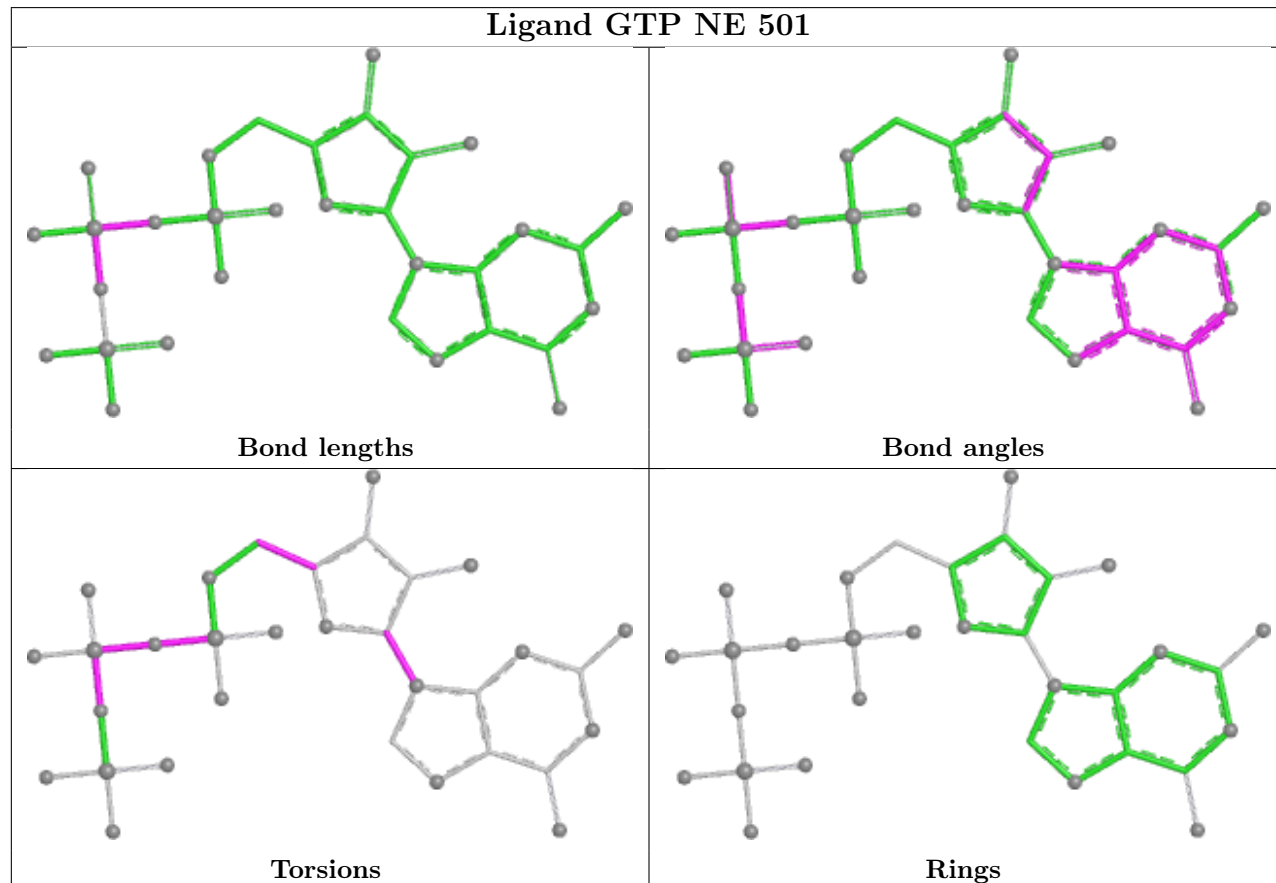
Ligand GTP TI 501



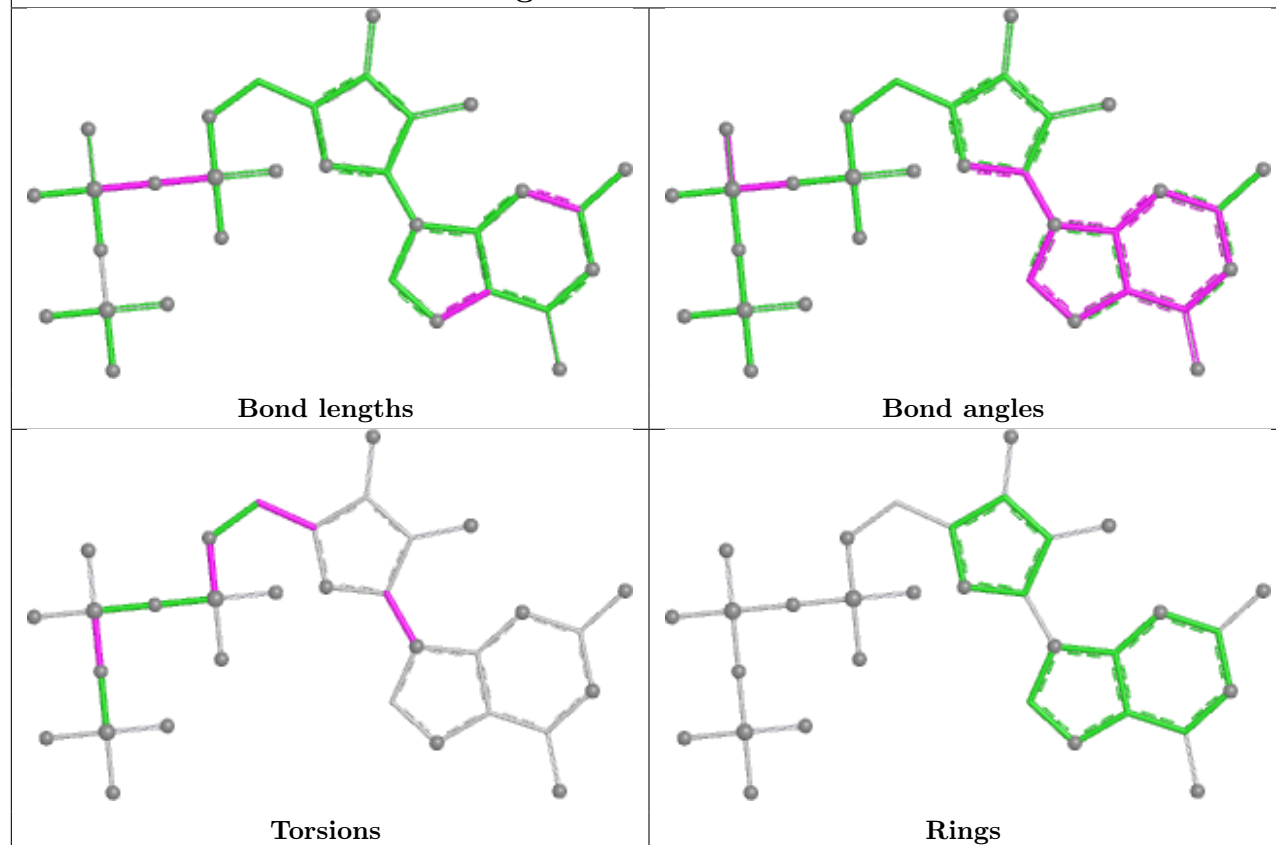
Ligand GTP AG 501



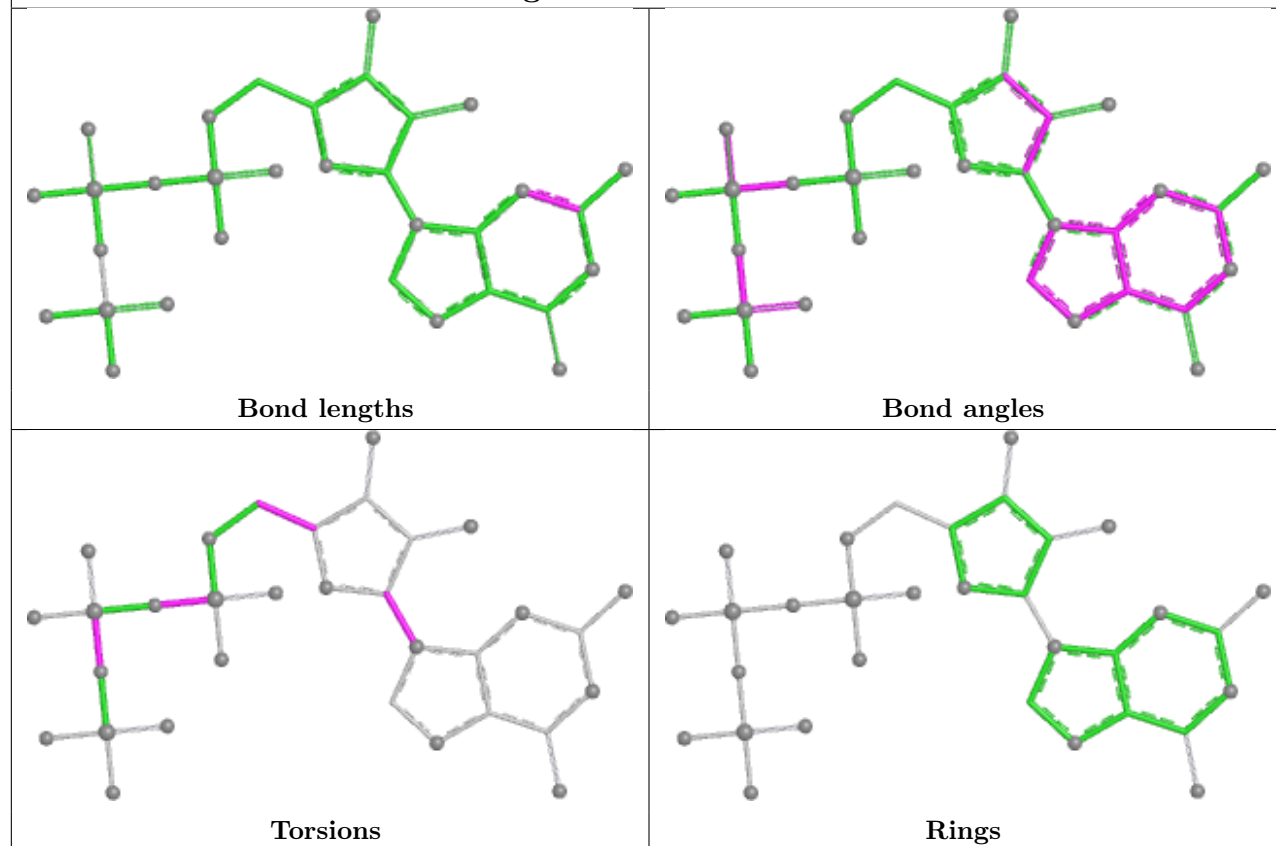
Ligand GTP NE 501



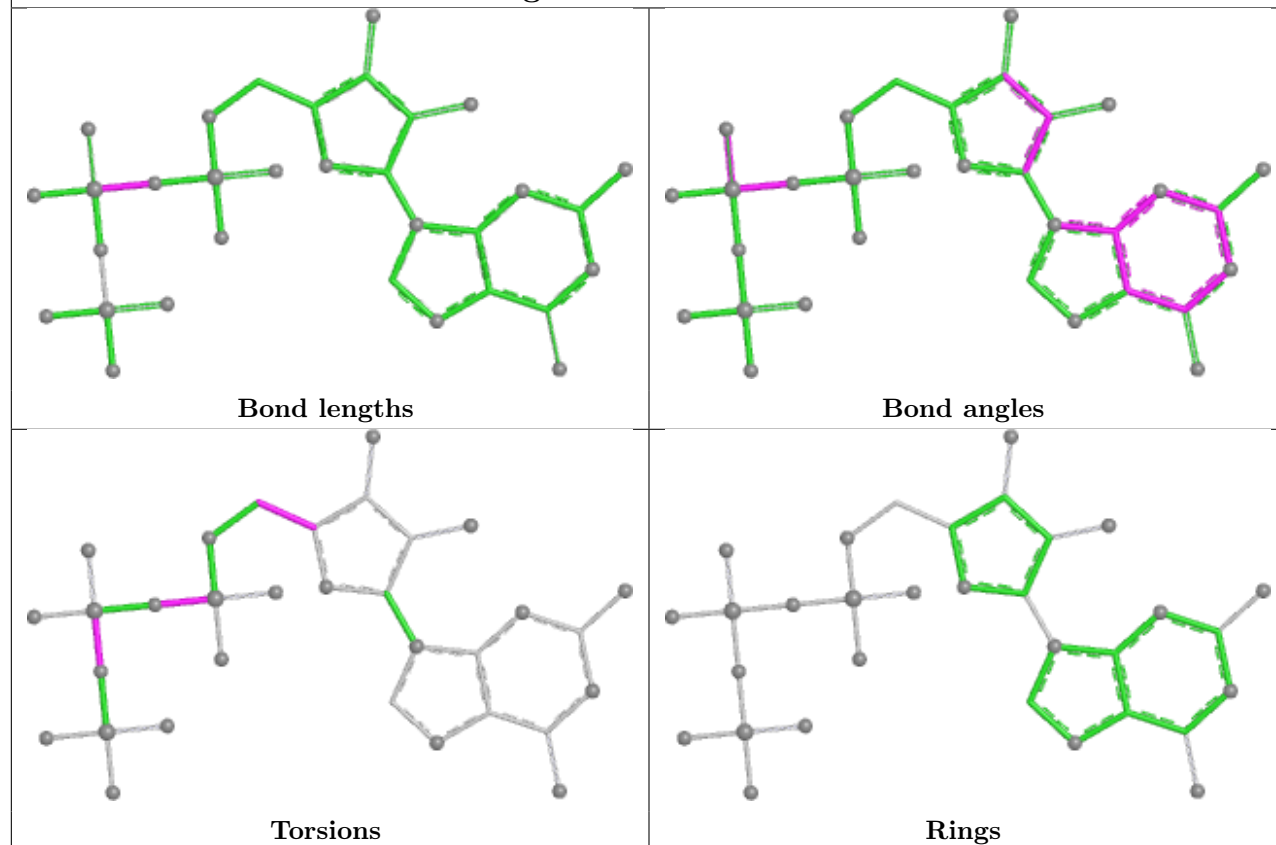
Ligand GTP HD 501



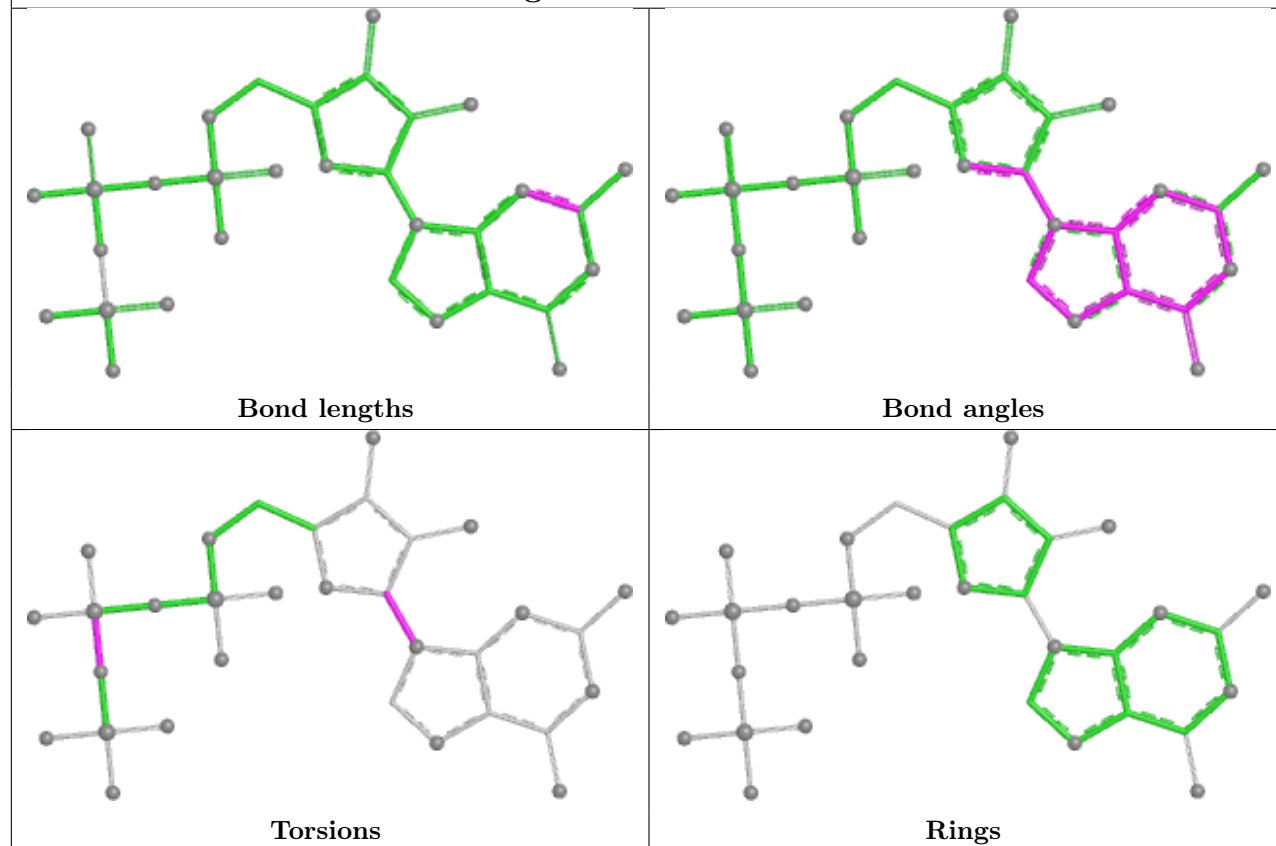
Ligand GTP KI 501



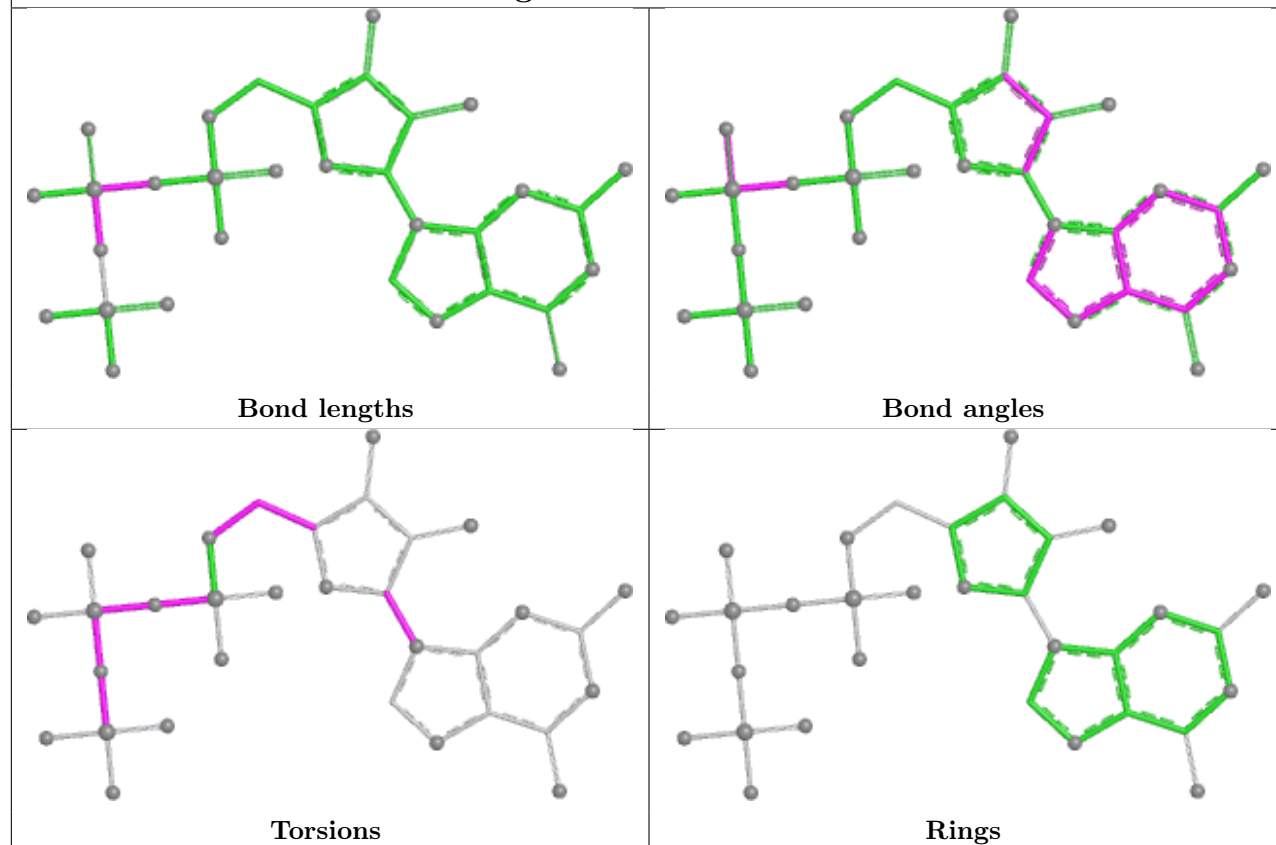
Ligand GTP IG 501



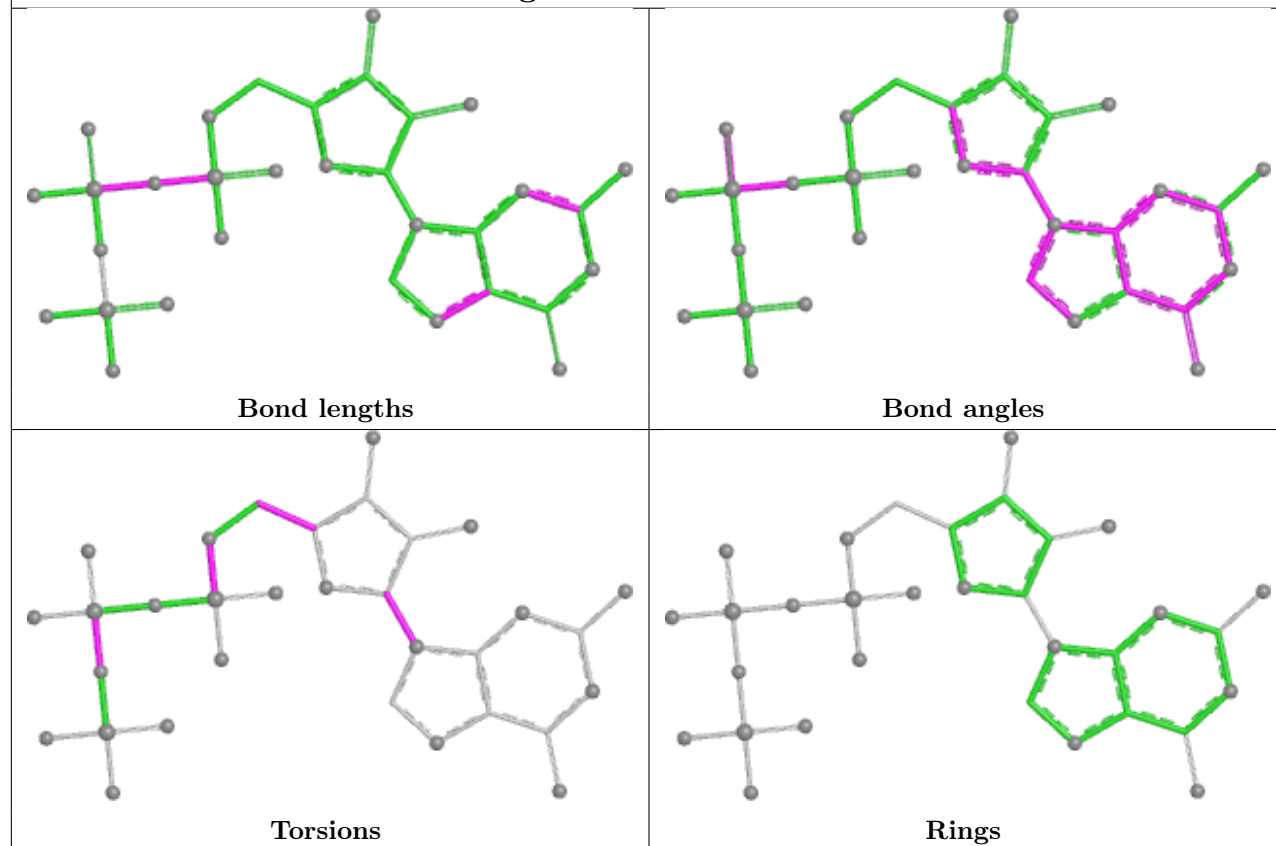
Ligand GTP SJ 501



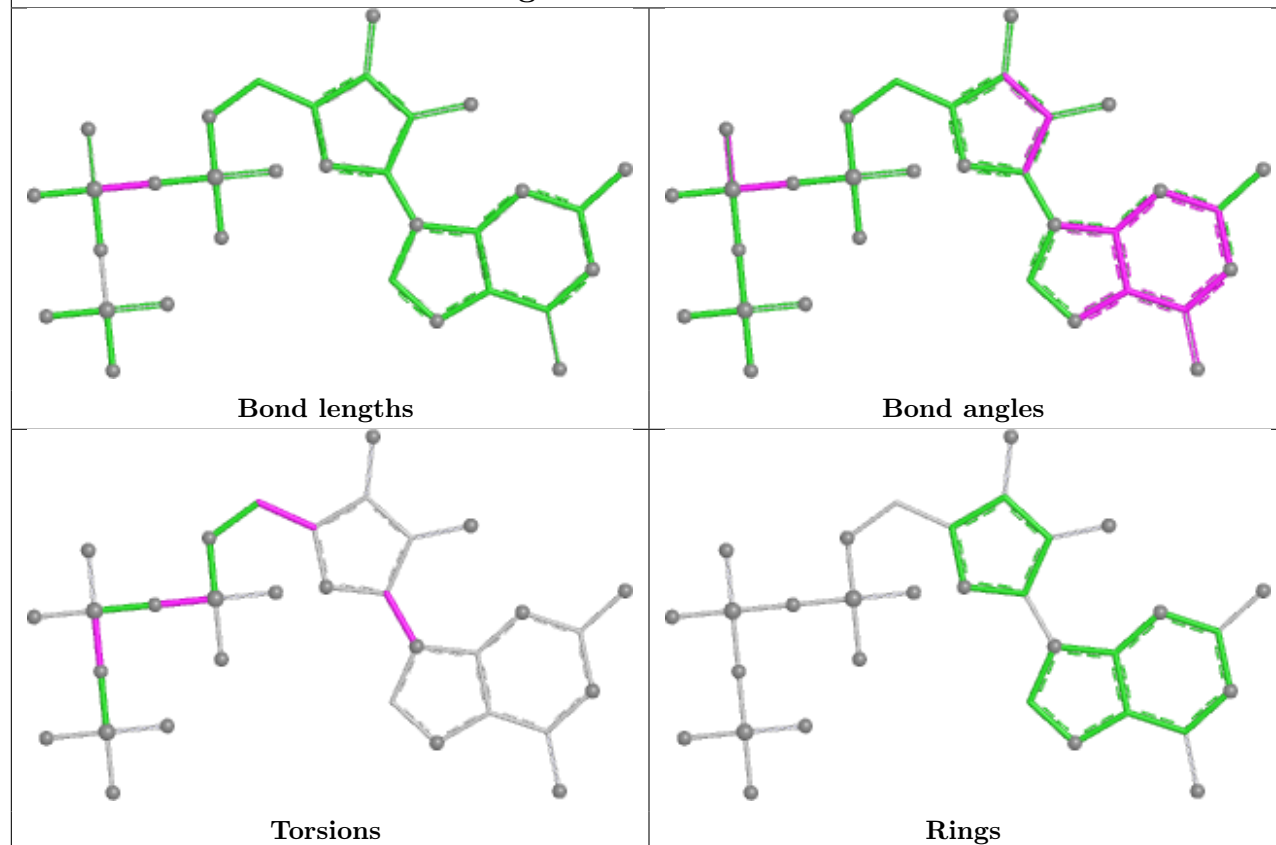
Ligand GTP ME 501



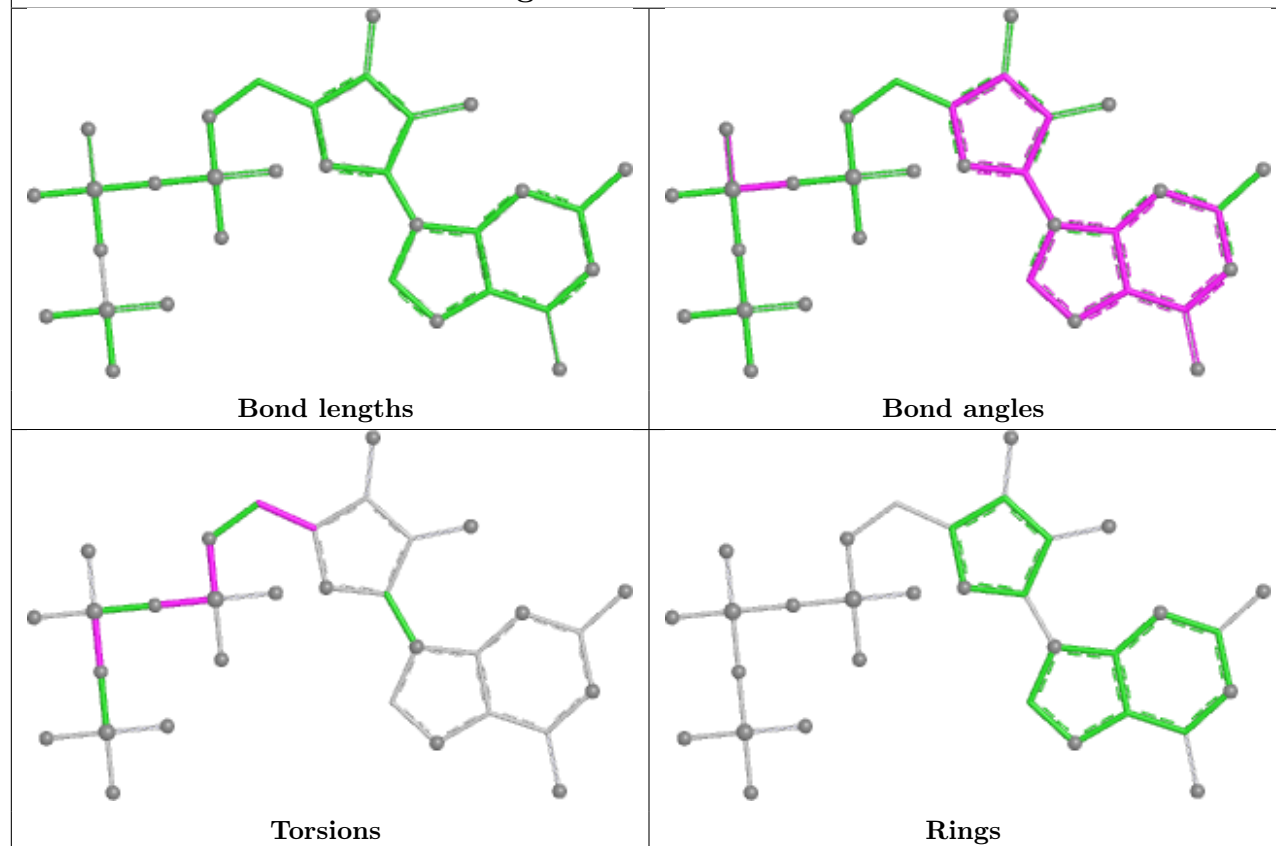
Ligand GTP AF 501

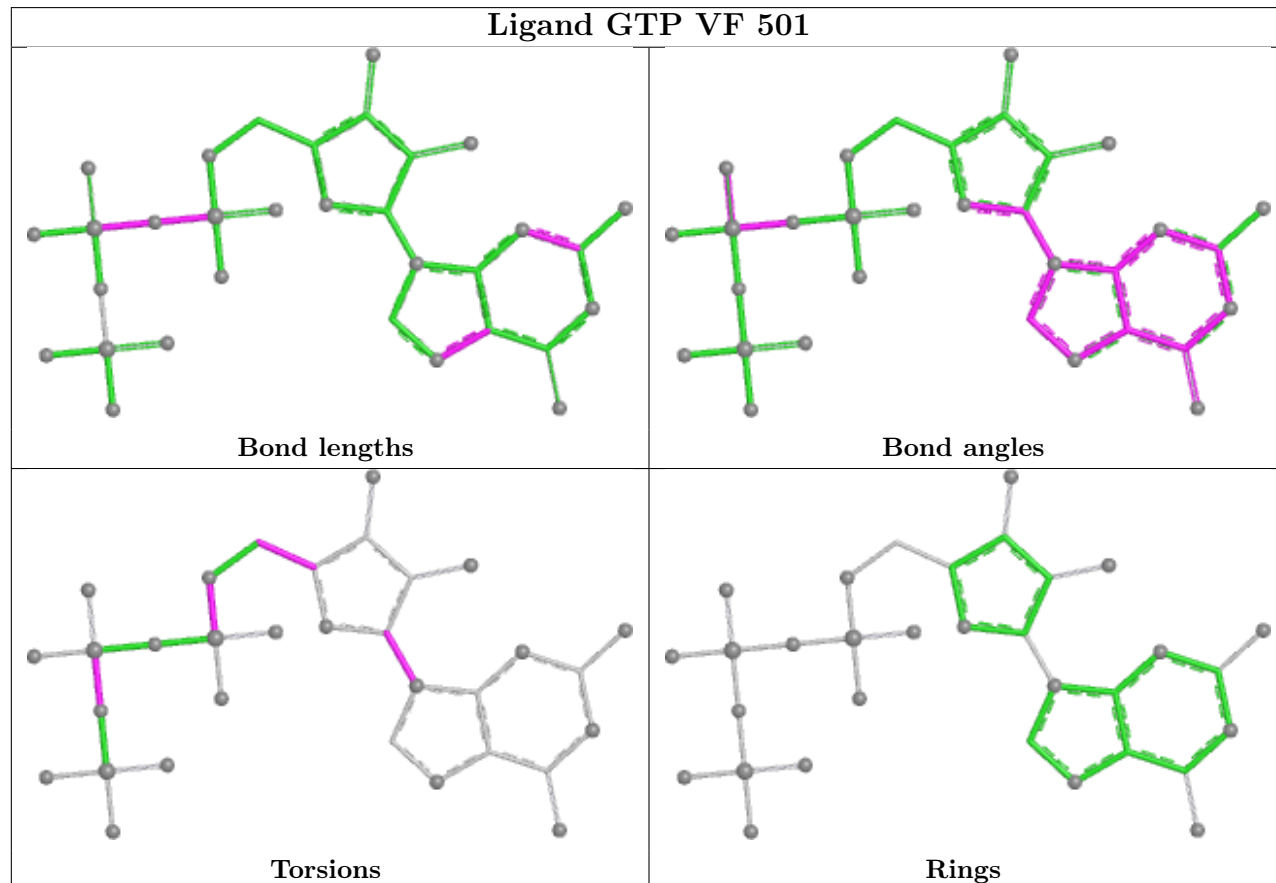
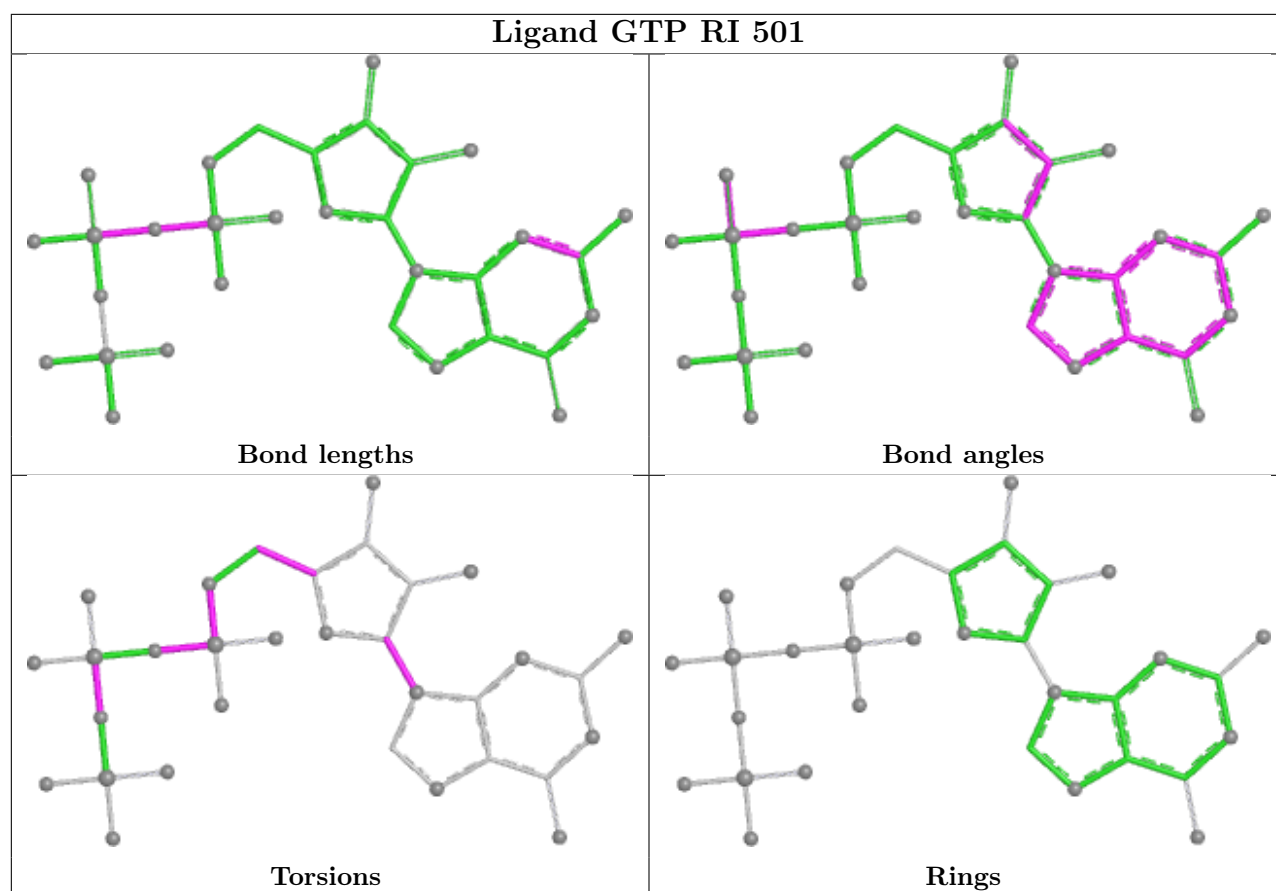


Ligand GTP AE 501

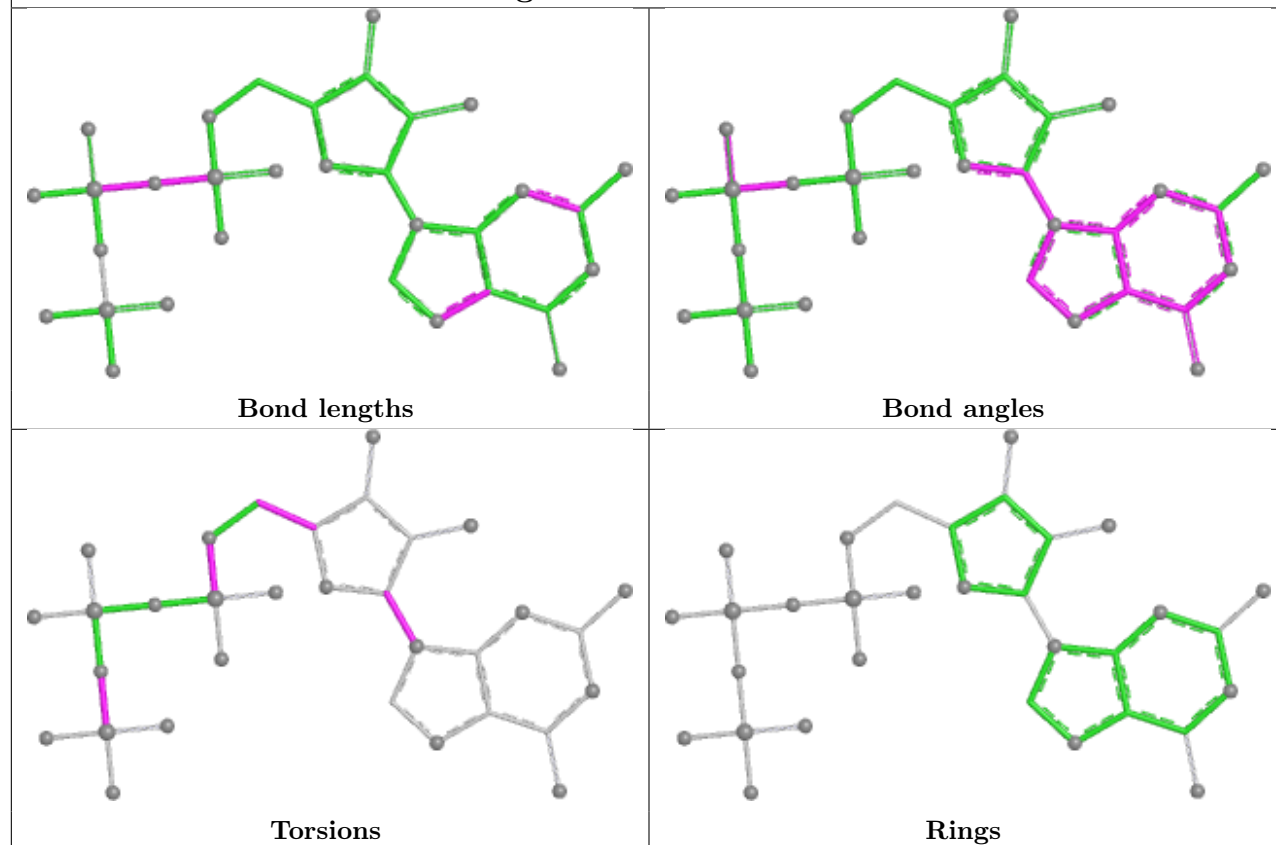


Ligand GTP CG 501

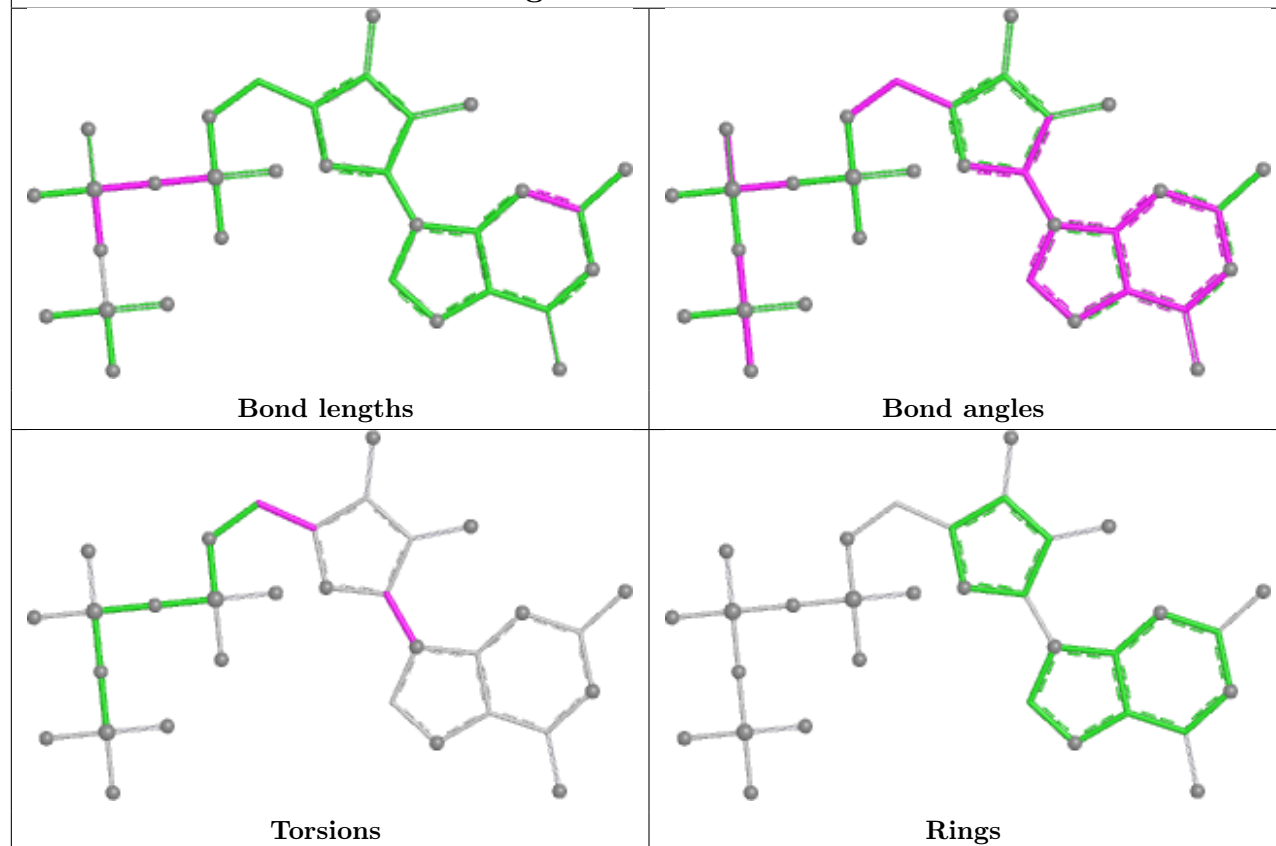




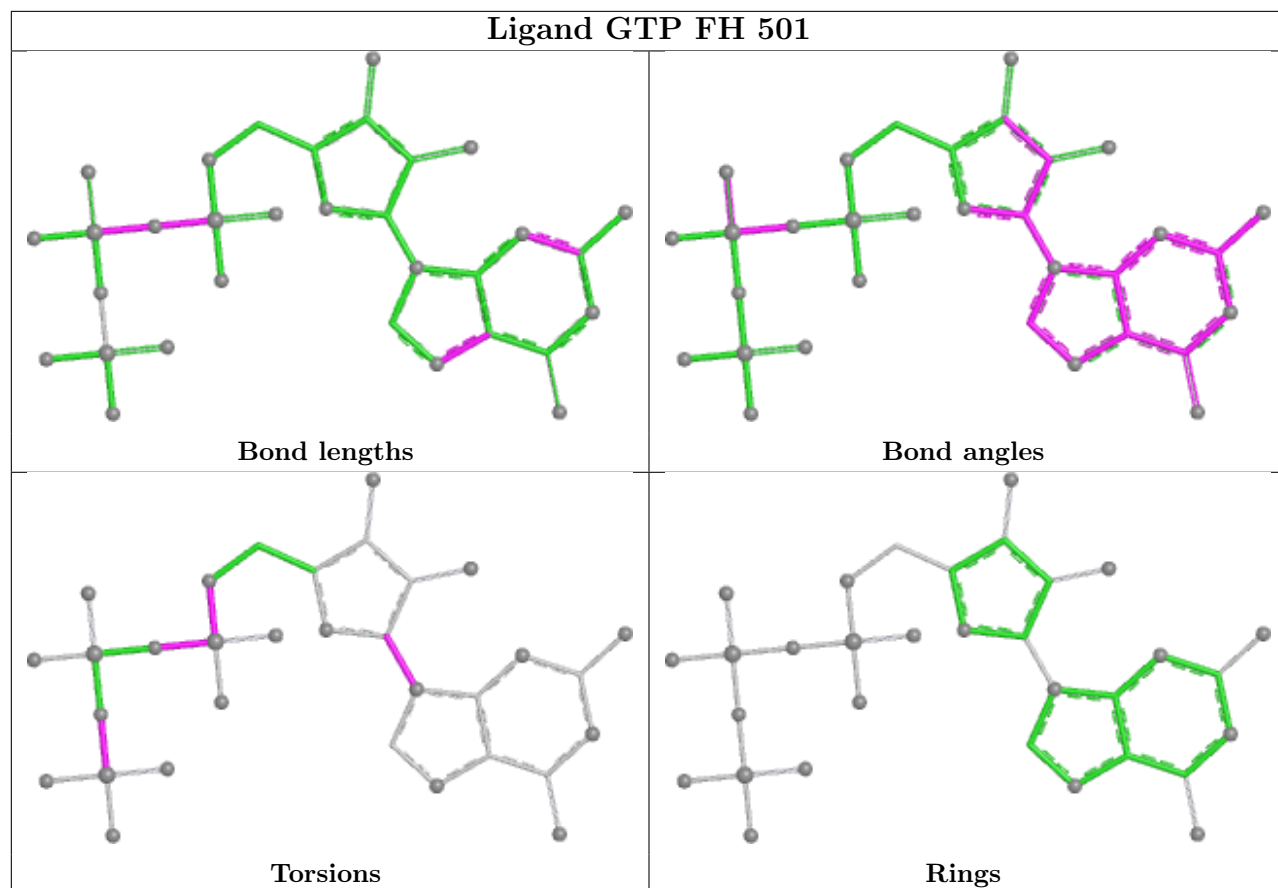
Ligand GTP UH 501



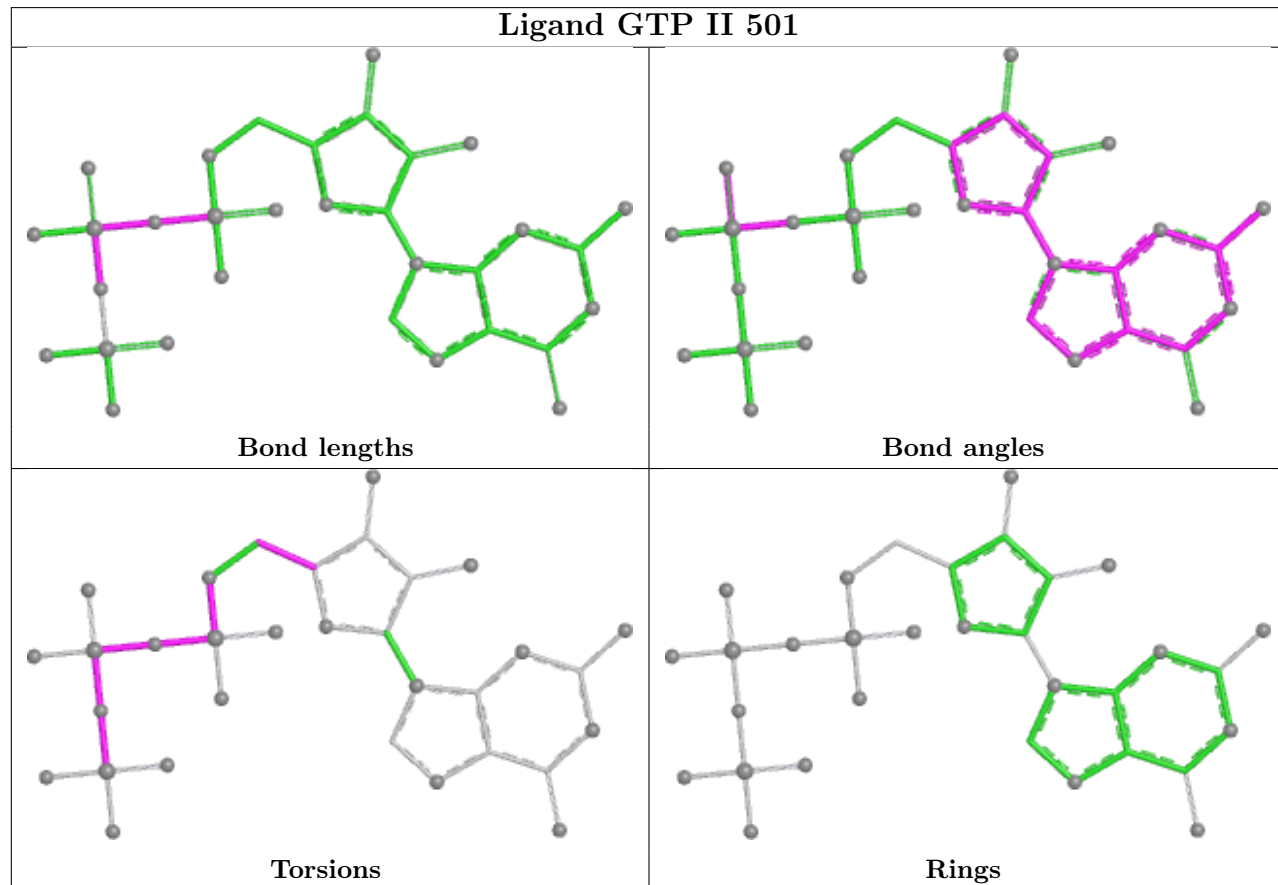
Ligand GTP IF 501



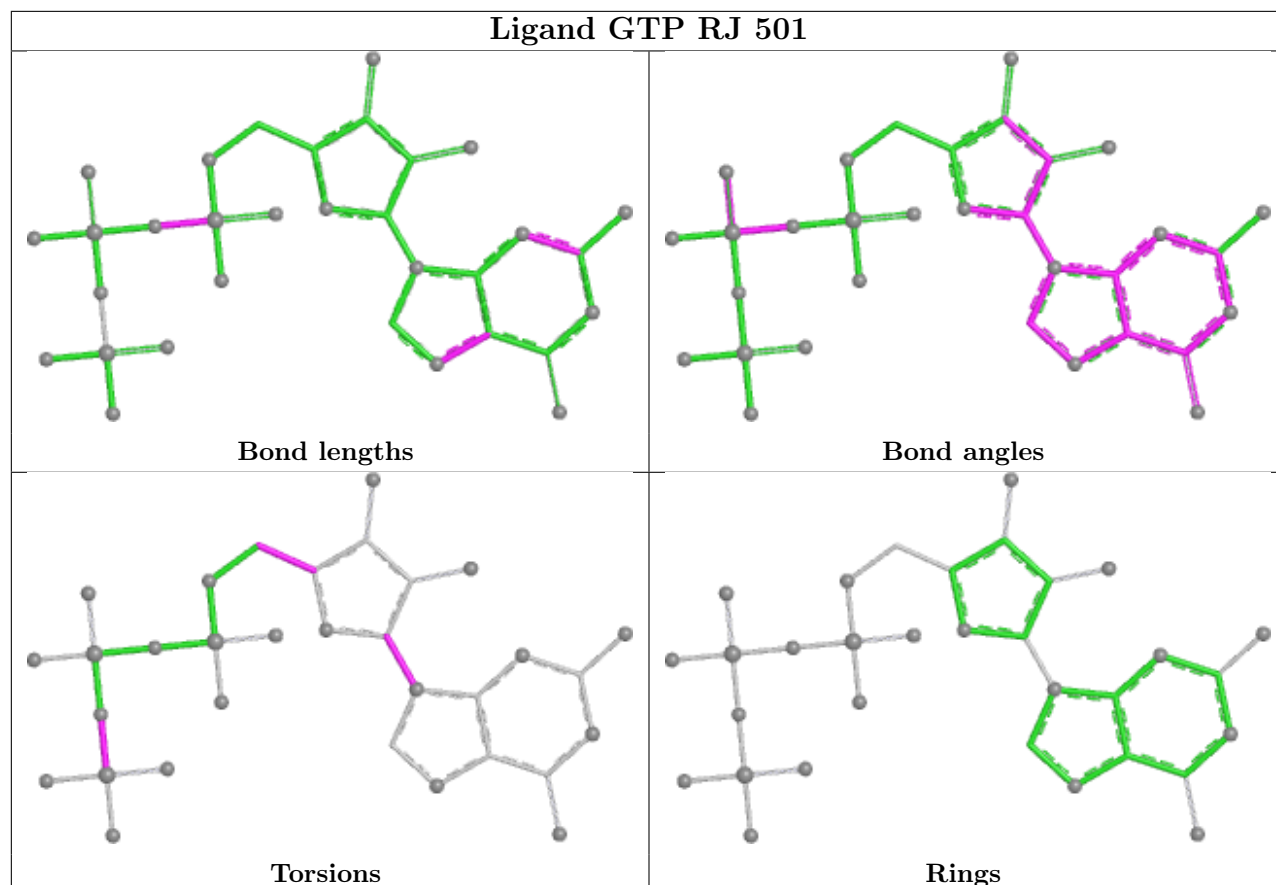
Ligand GTP FH 501



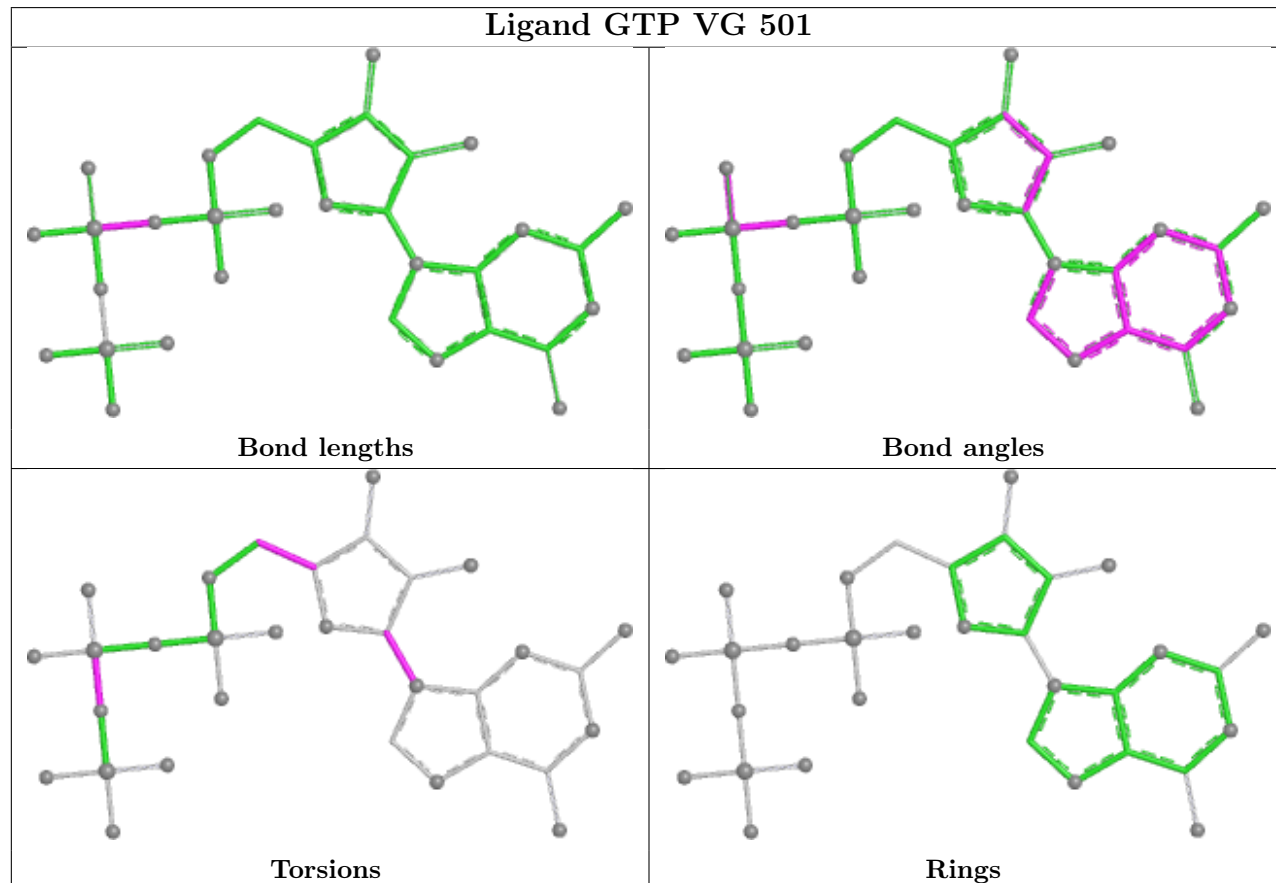
Ligand GTP II 501



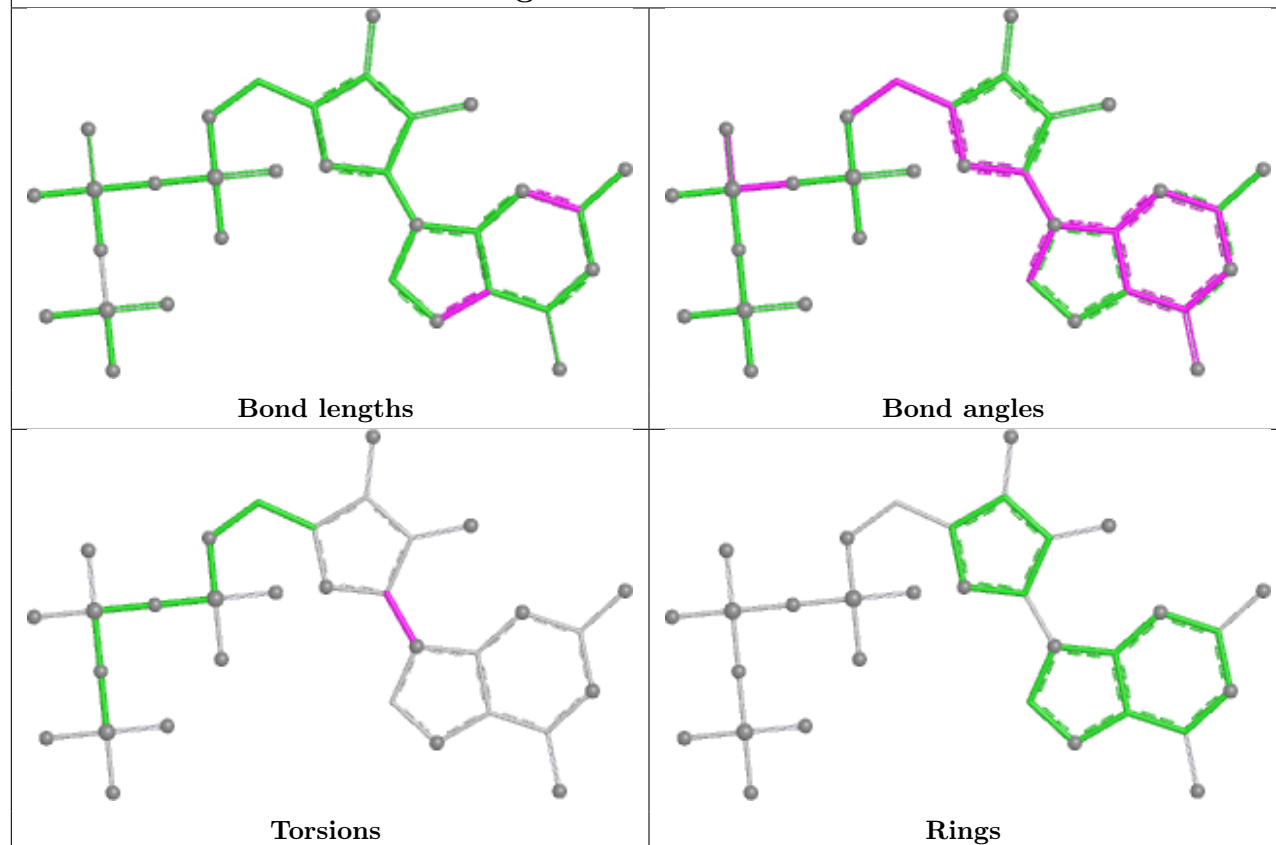
Ligand GTP RJ 501



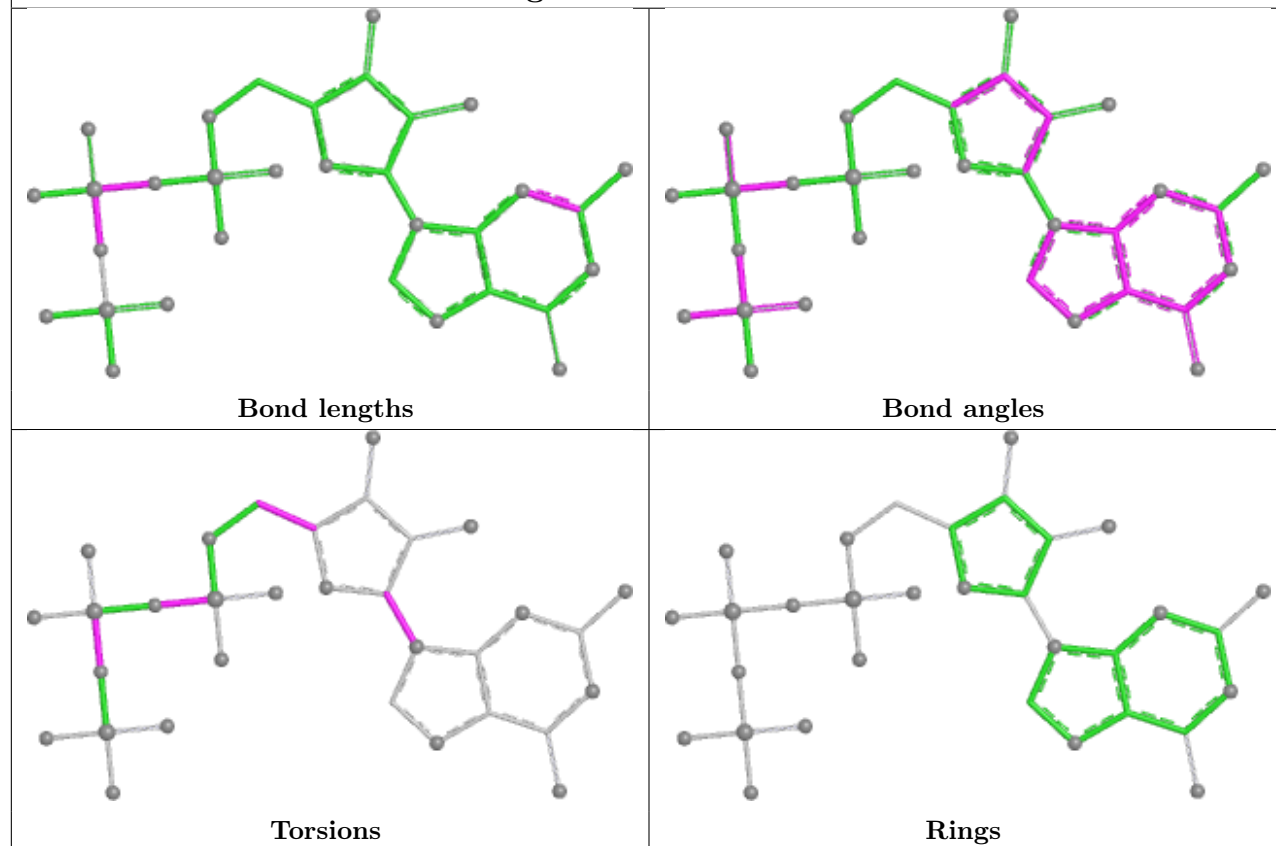
Ligand GTP VG 501



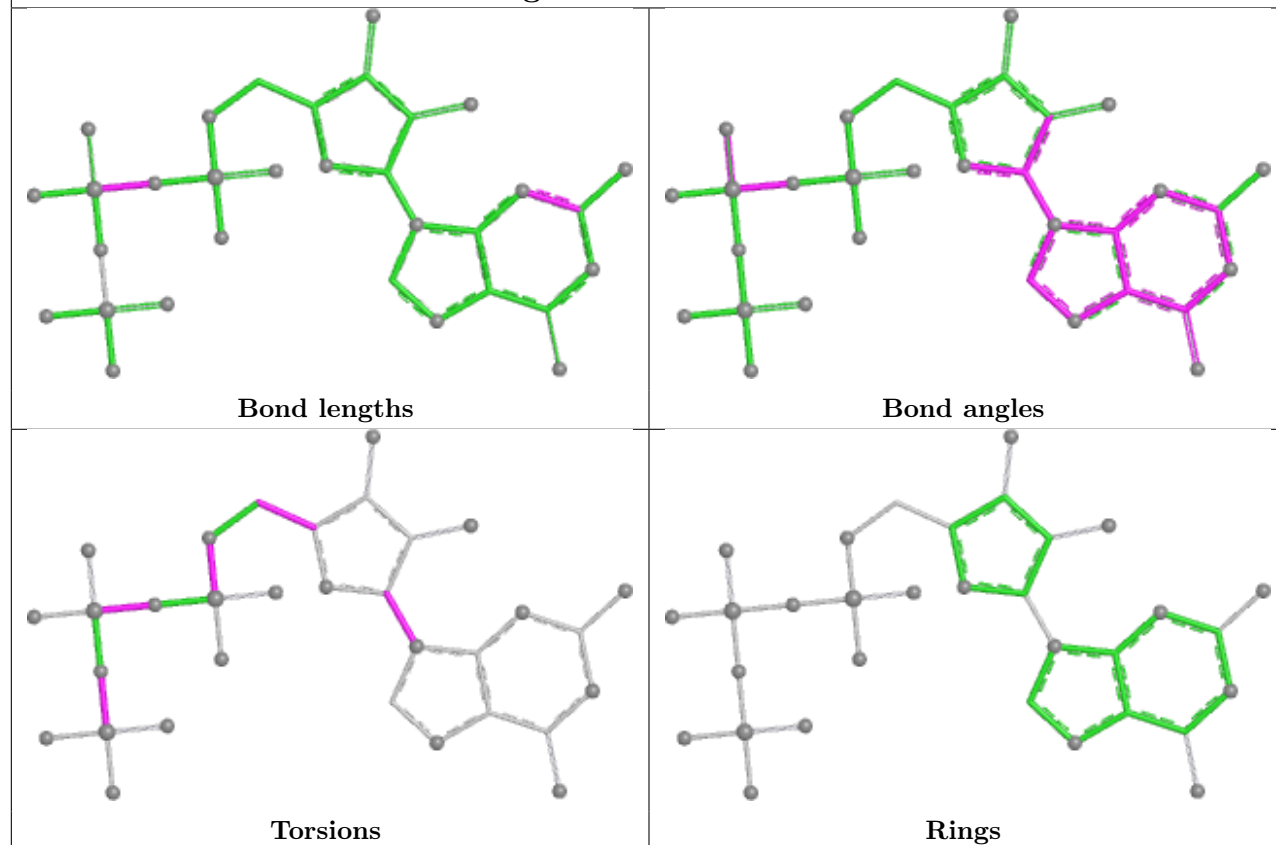
Ligand GTP DH 501



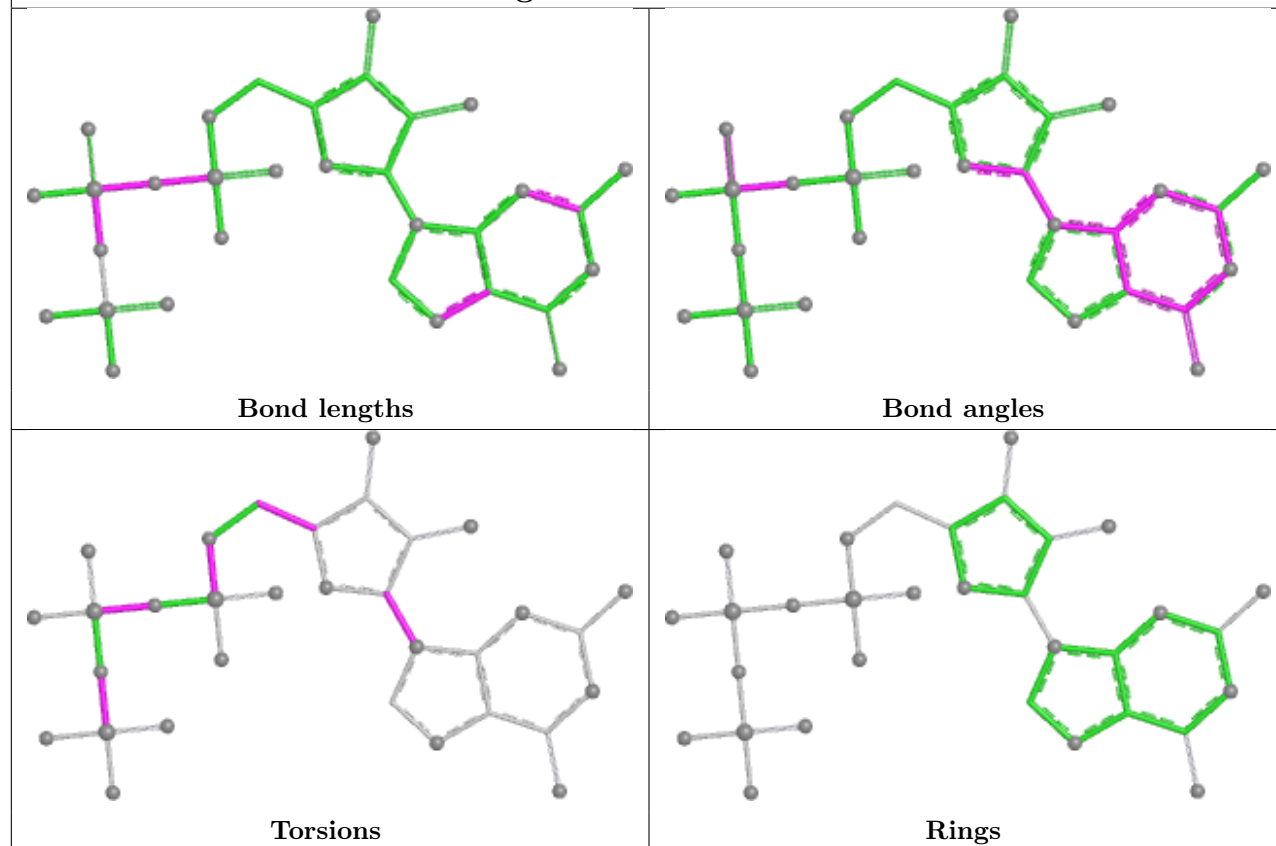
Ligand GTP LI 501



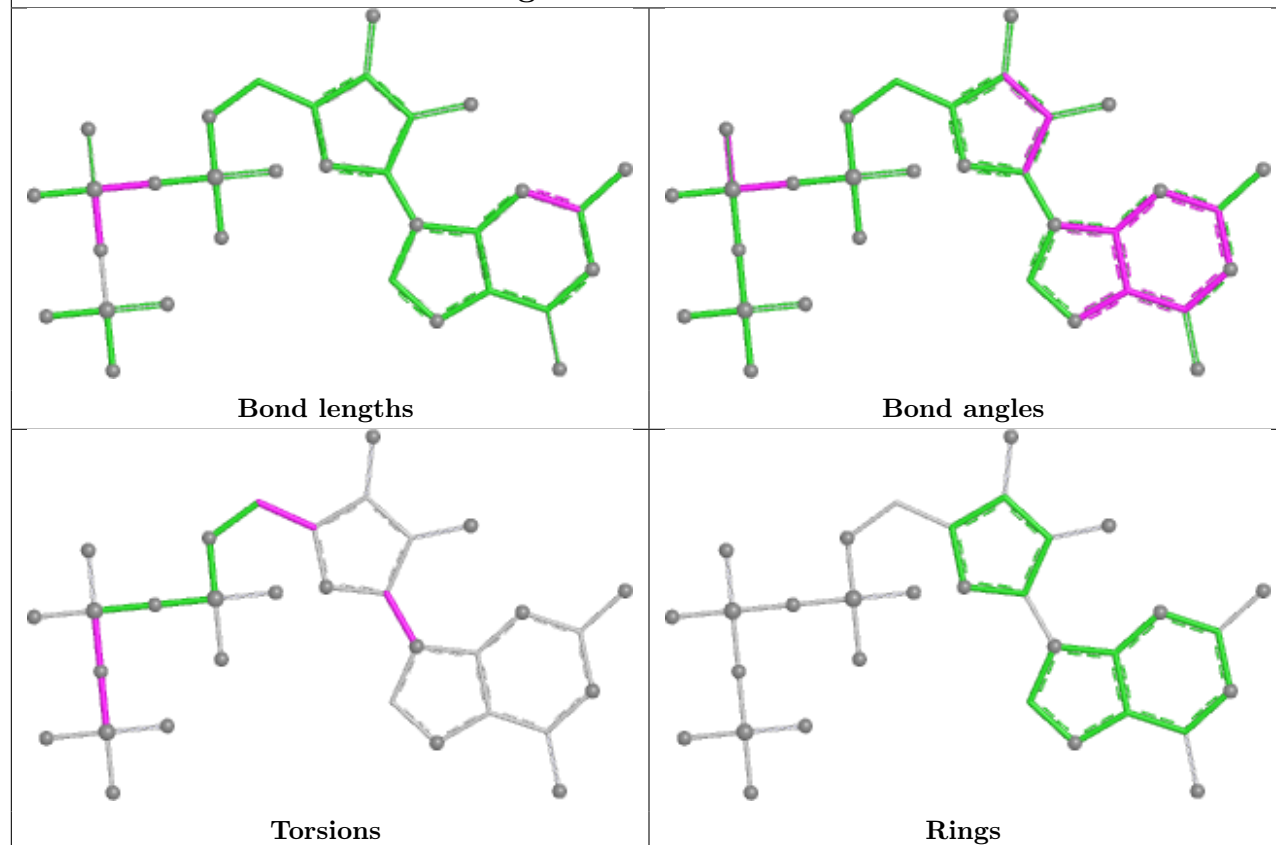
Ligand GTP JF 501



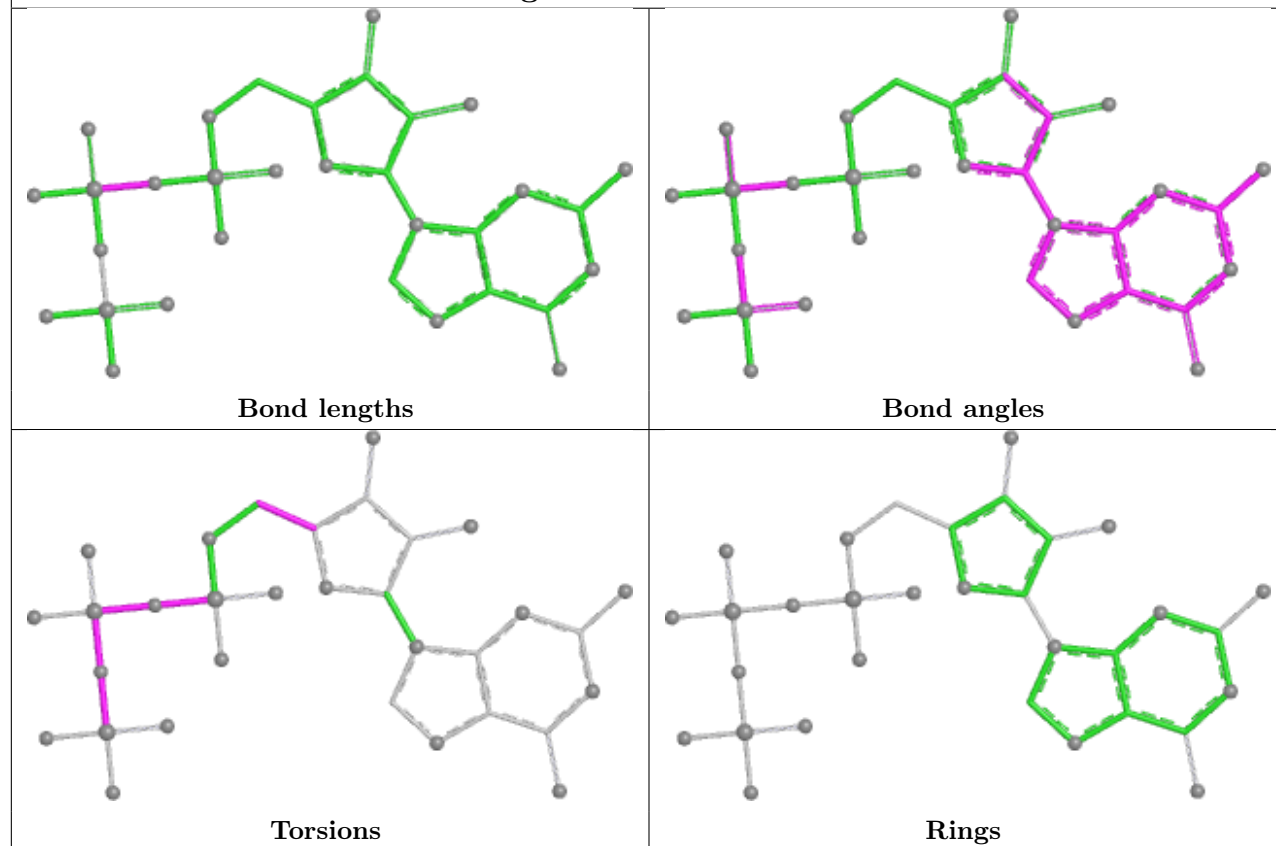
Ligand GTP AH 501



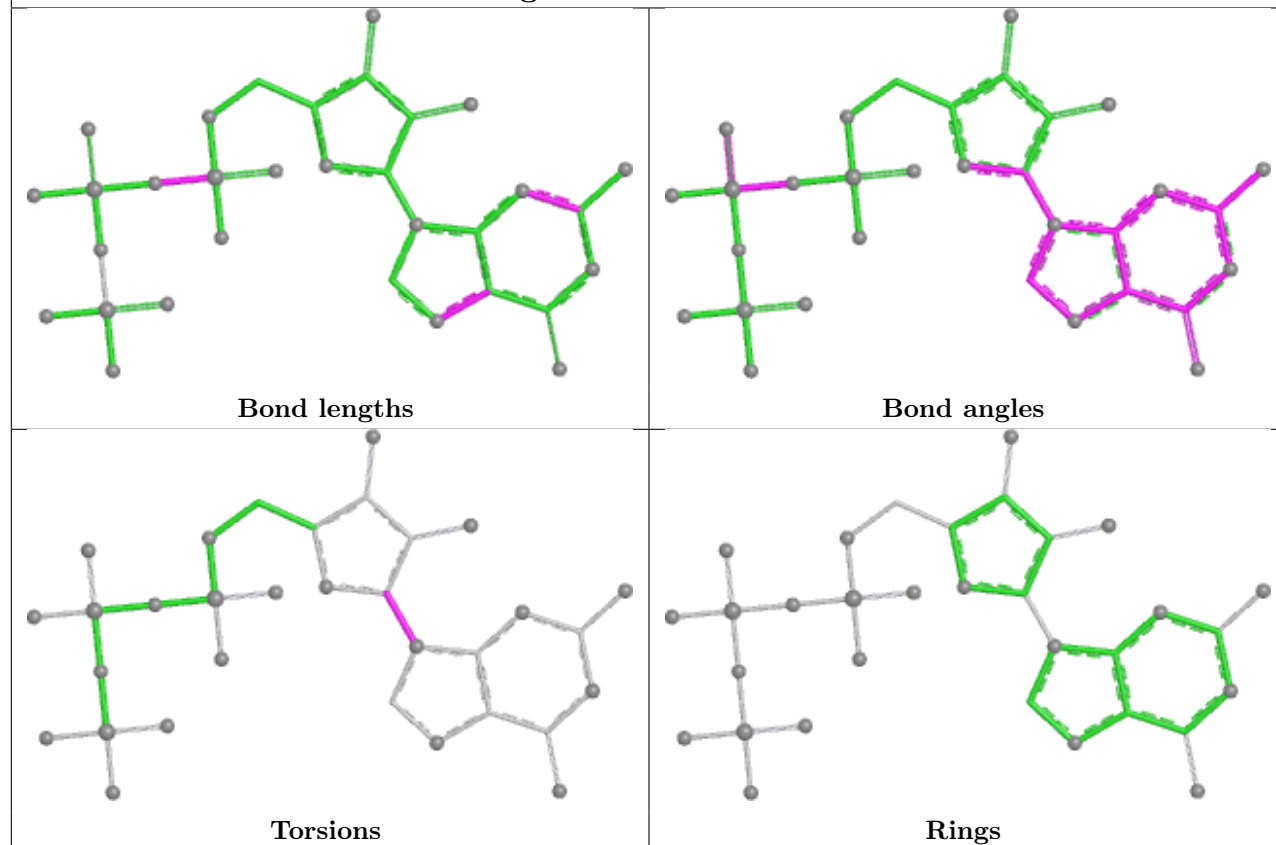
Ligand GTP UE 501



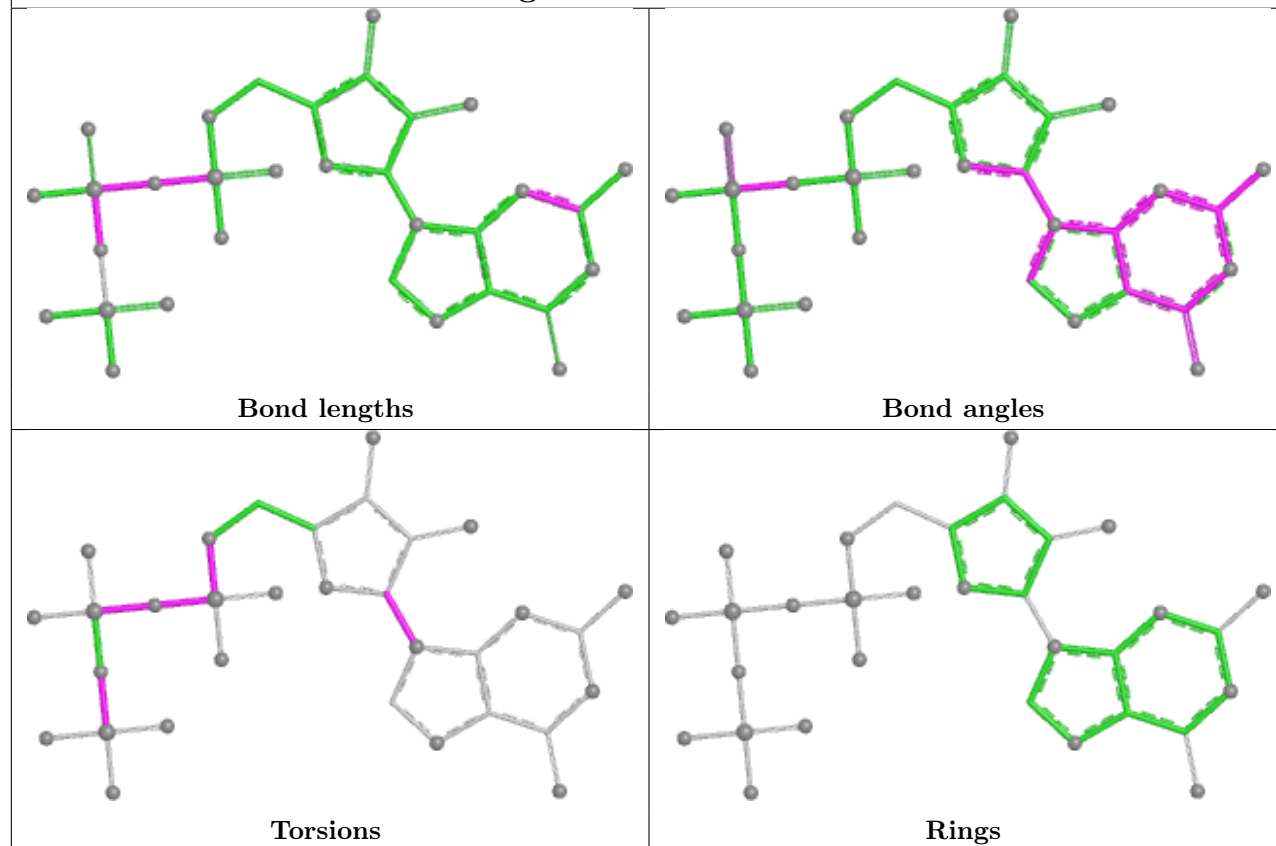
Ligand GTP FE 501



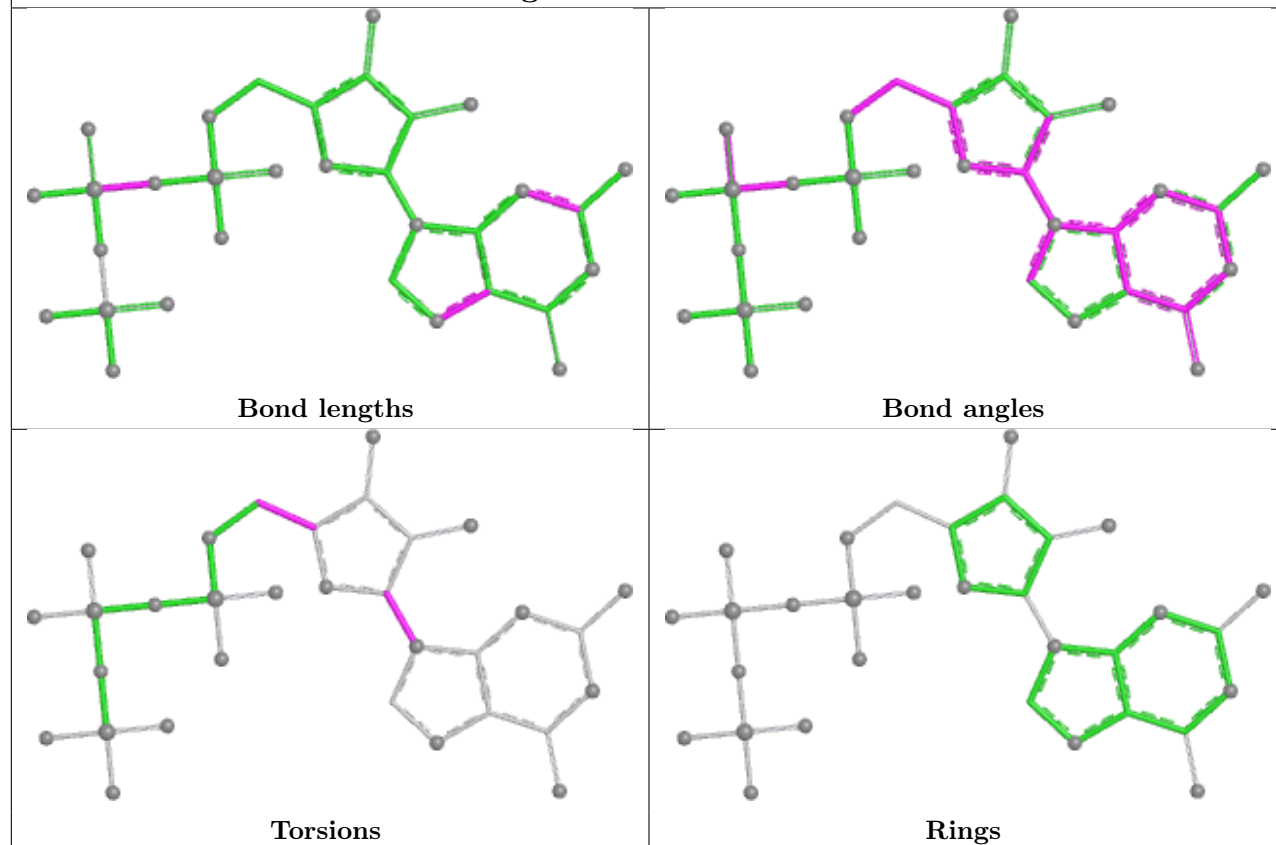
Ligand GTP PF 501



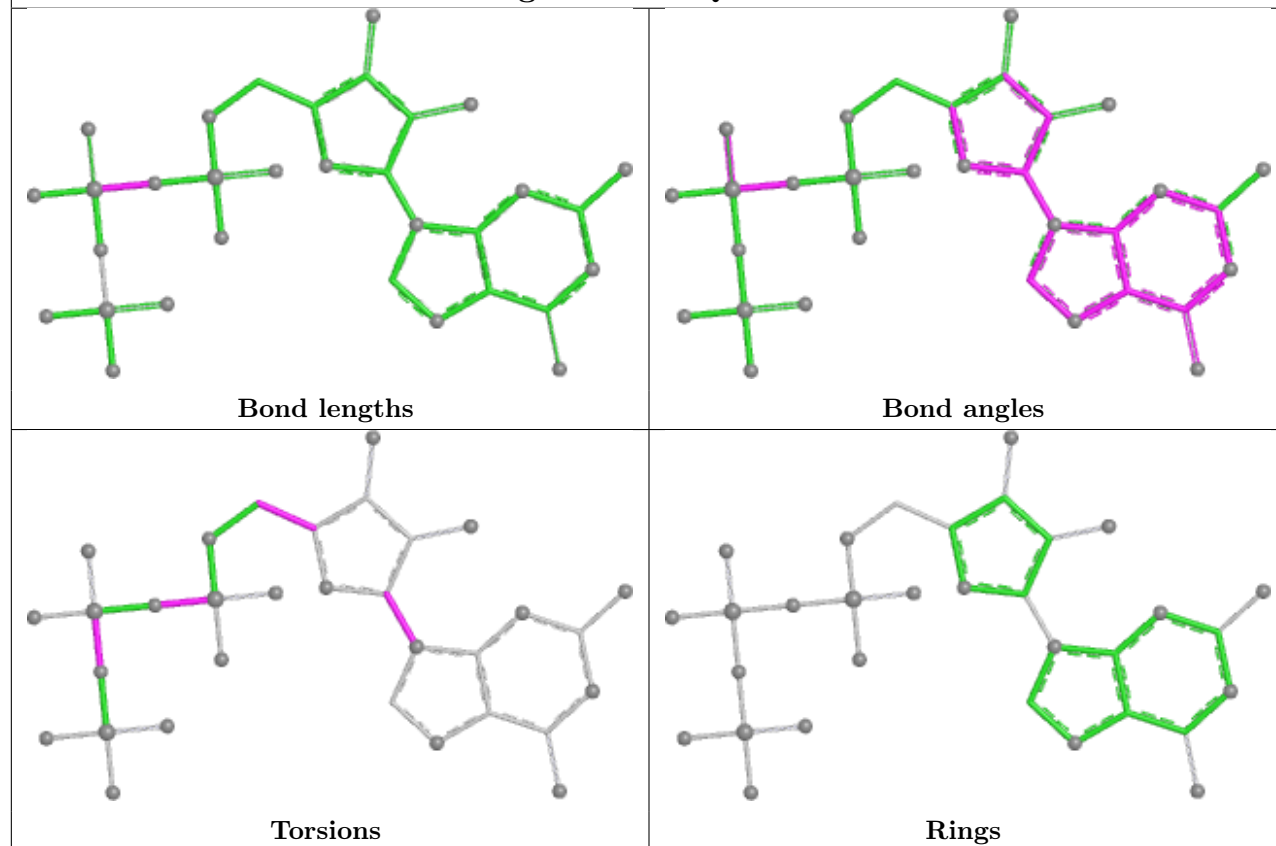
Ligand GTP OF 501



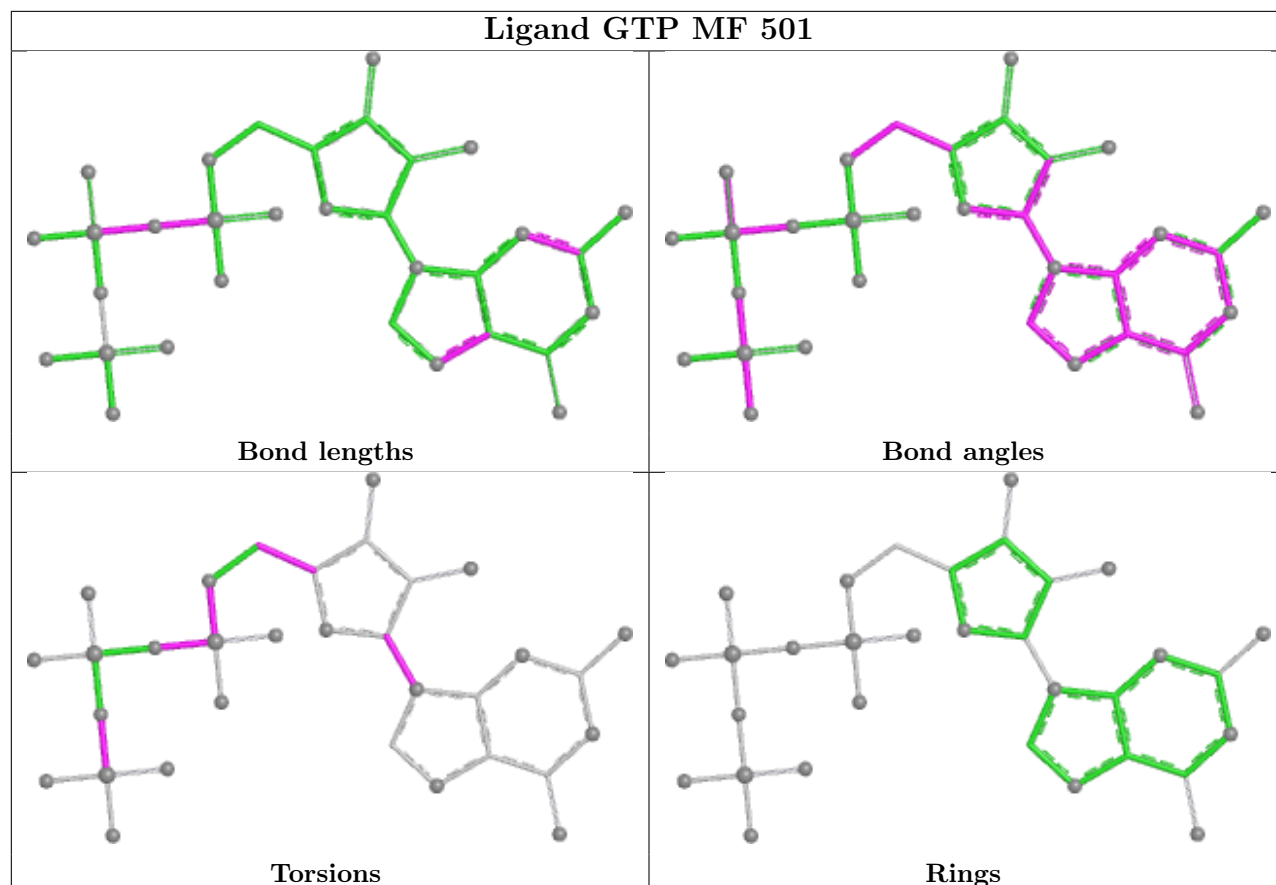
Ligand GTP FF 501



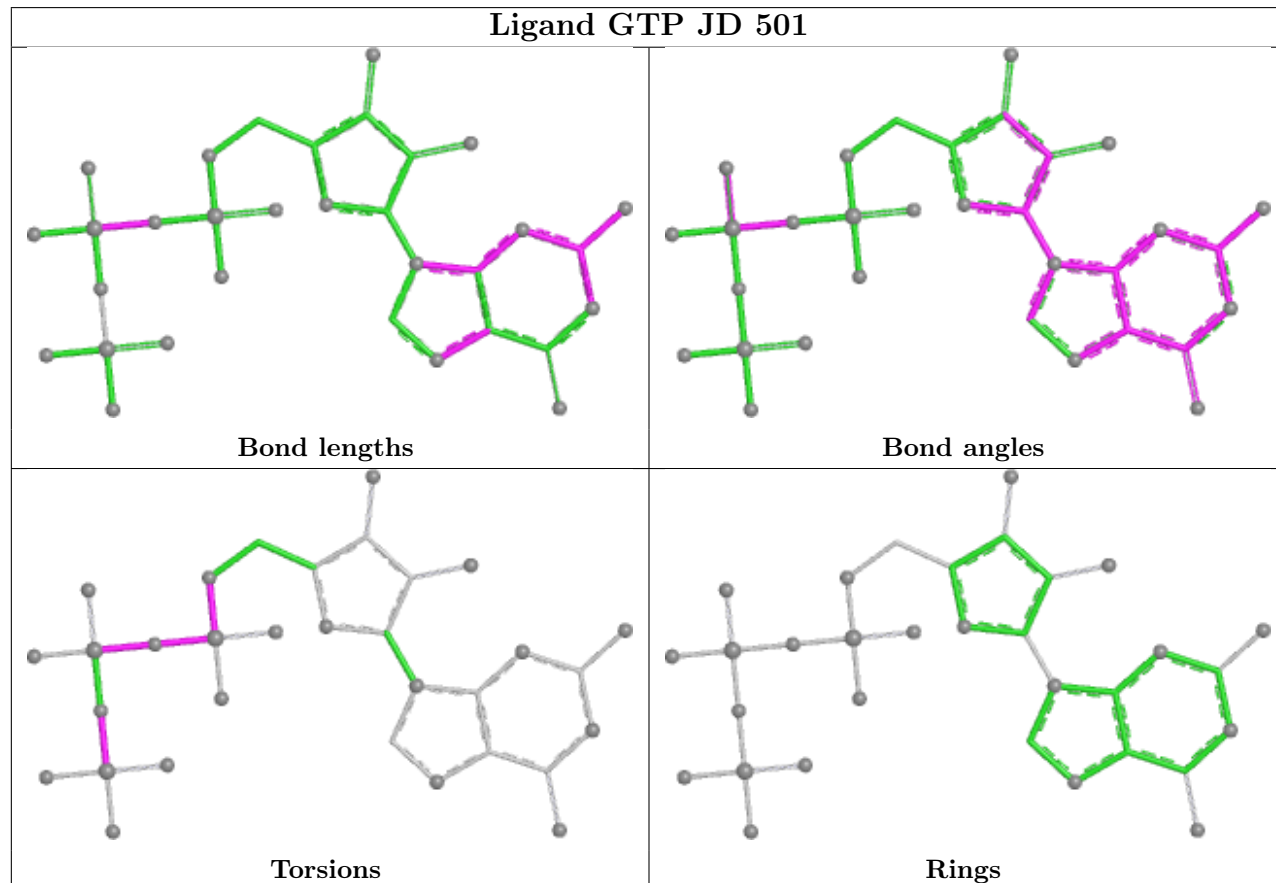
Ligand GTP QE 501



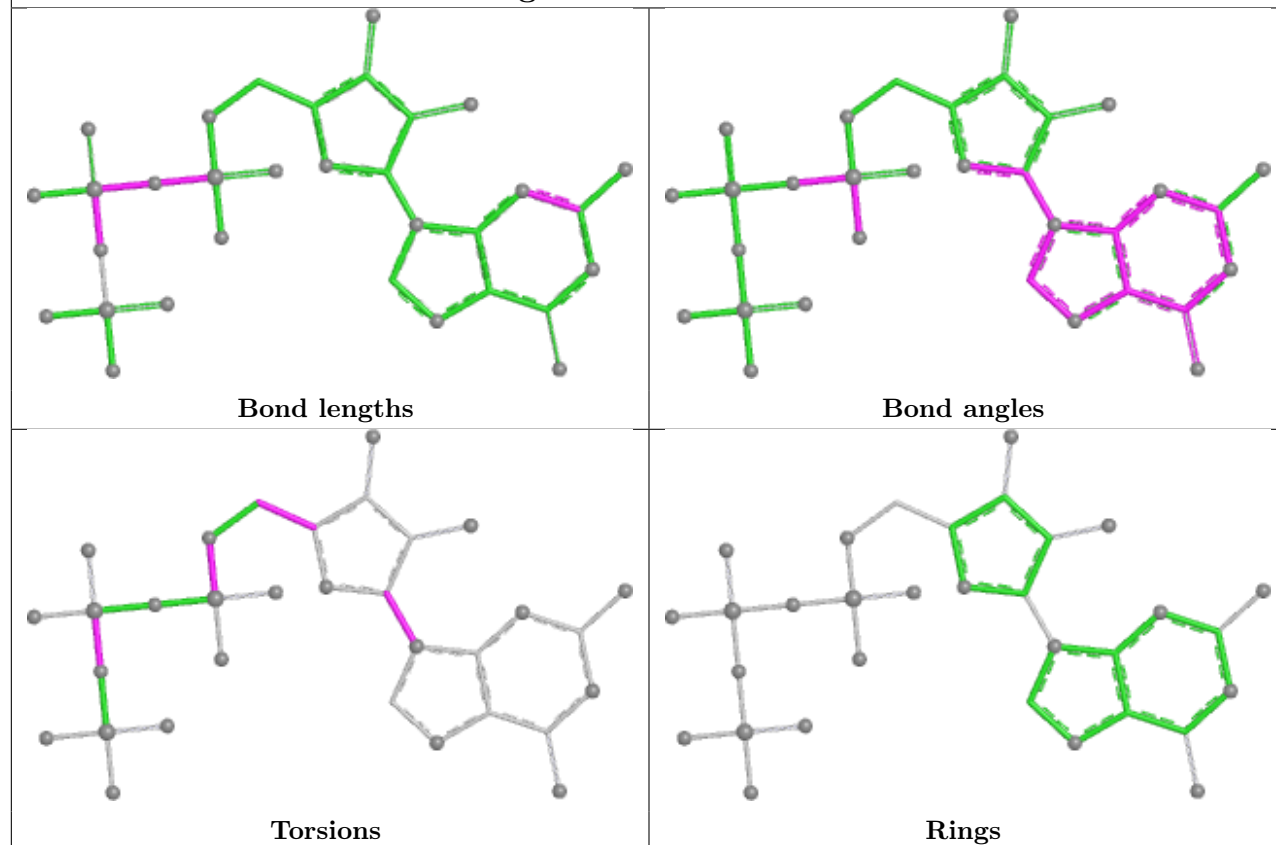
Ligand GTP MF 501



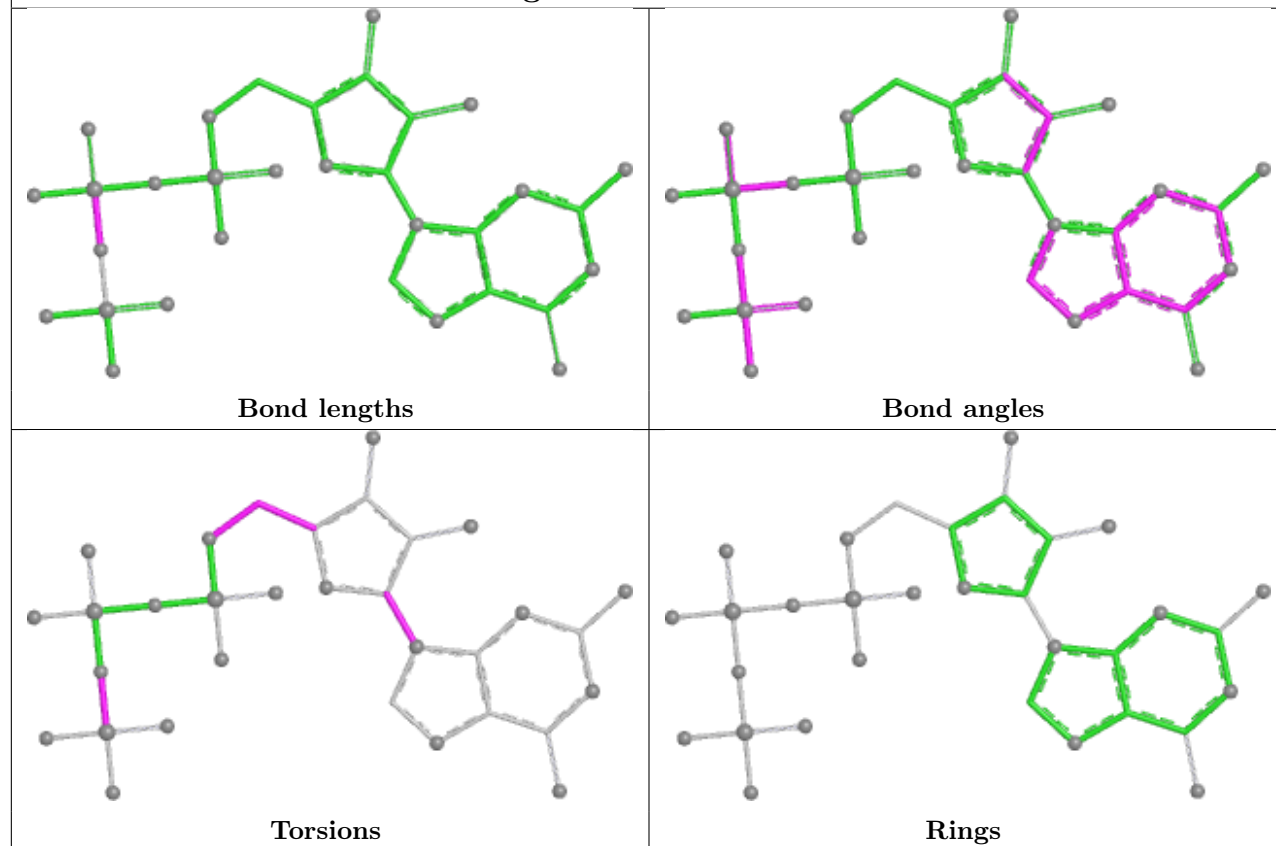
Ligand GTP JD 501



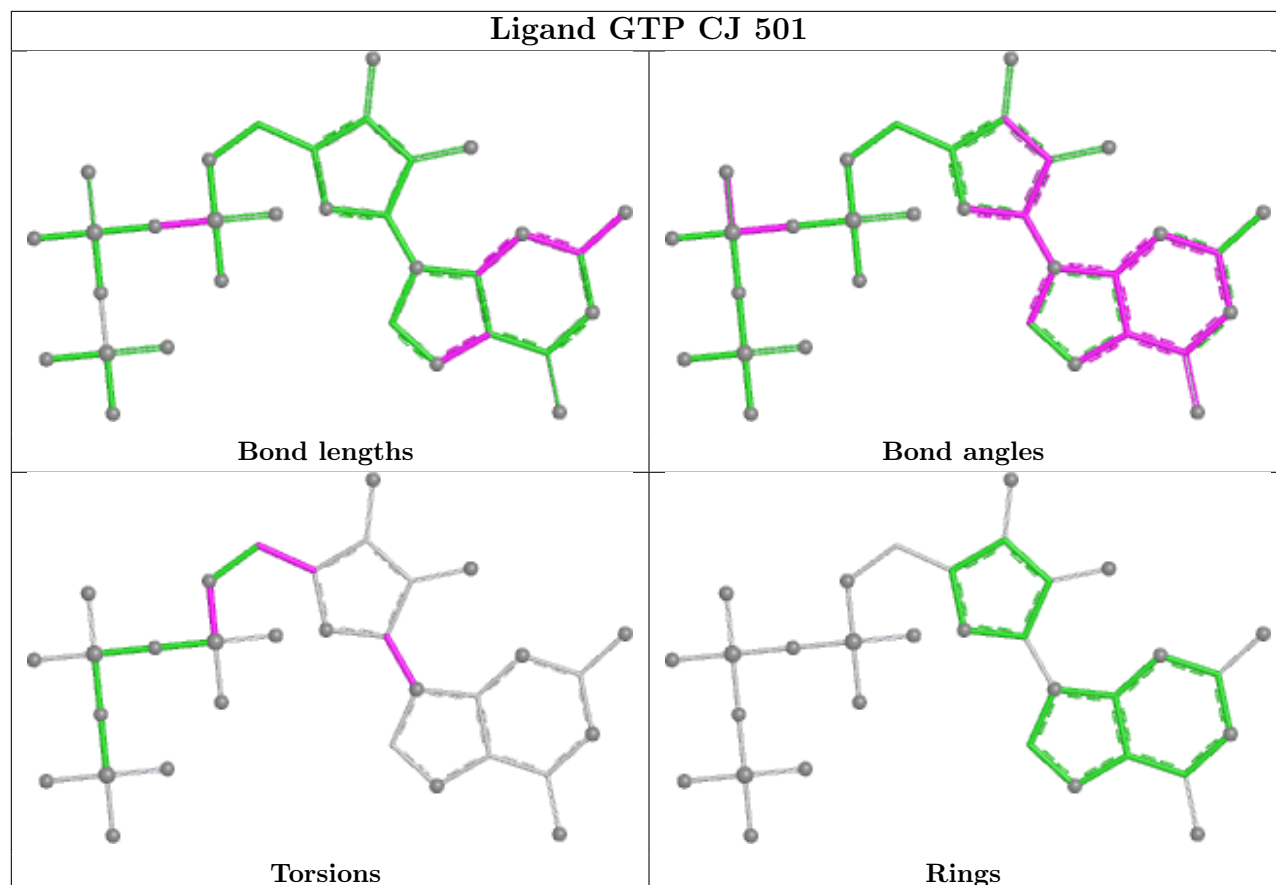
Ligand GTP DF 501



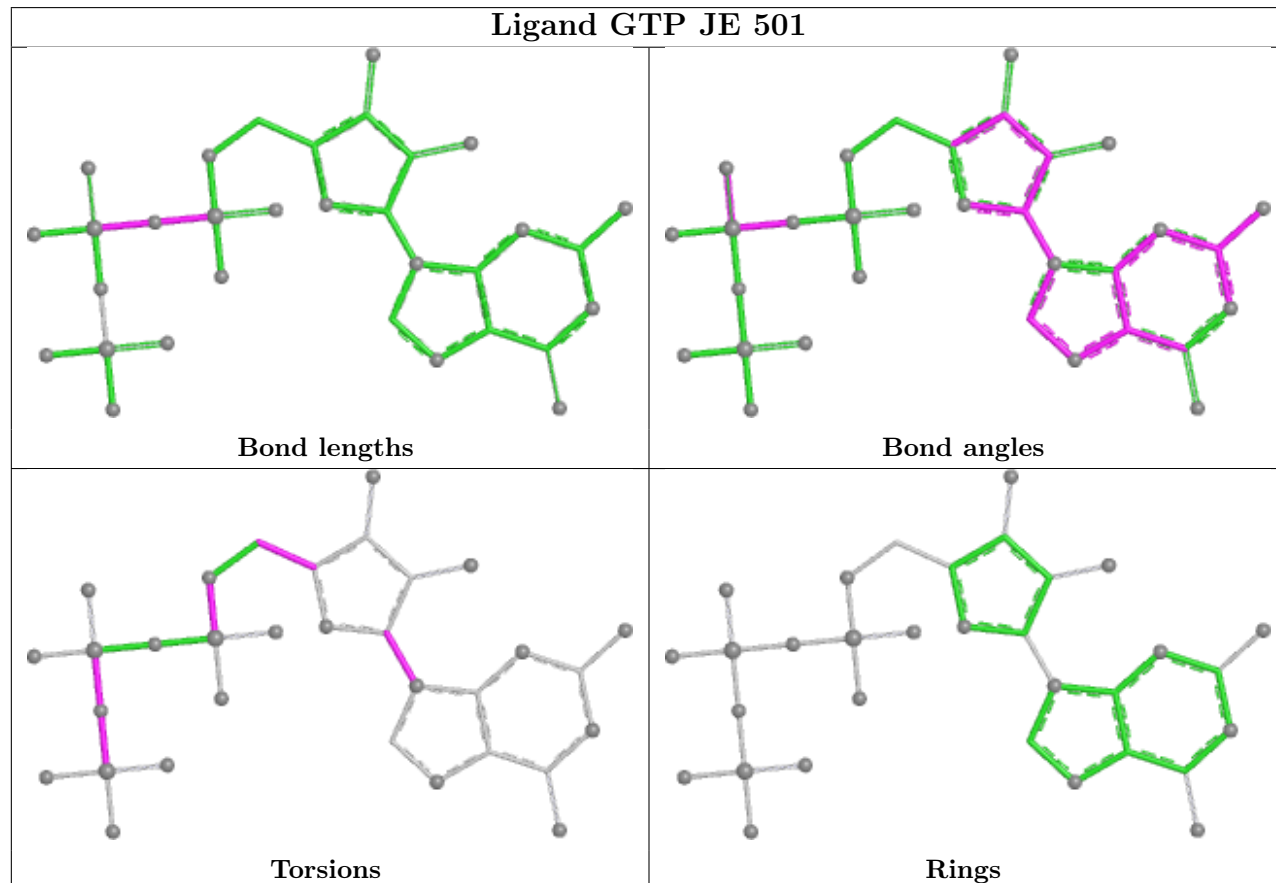
Ligand GTP NI 501



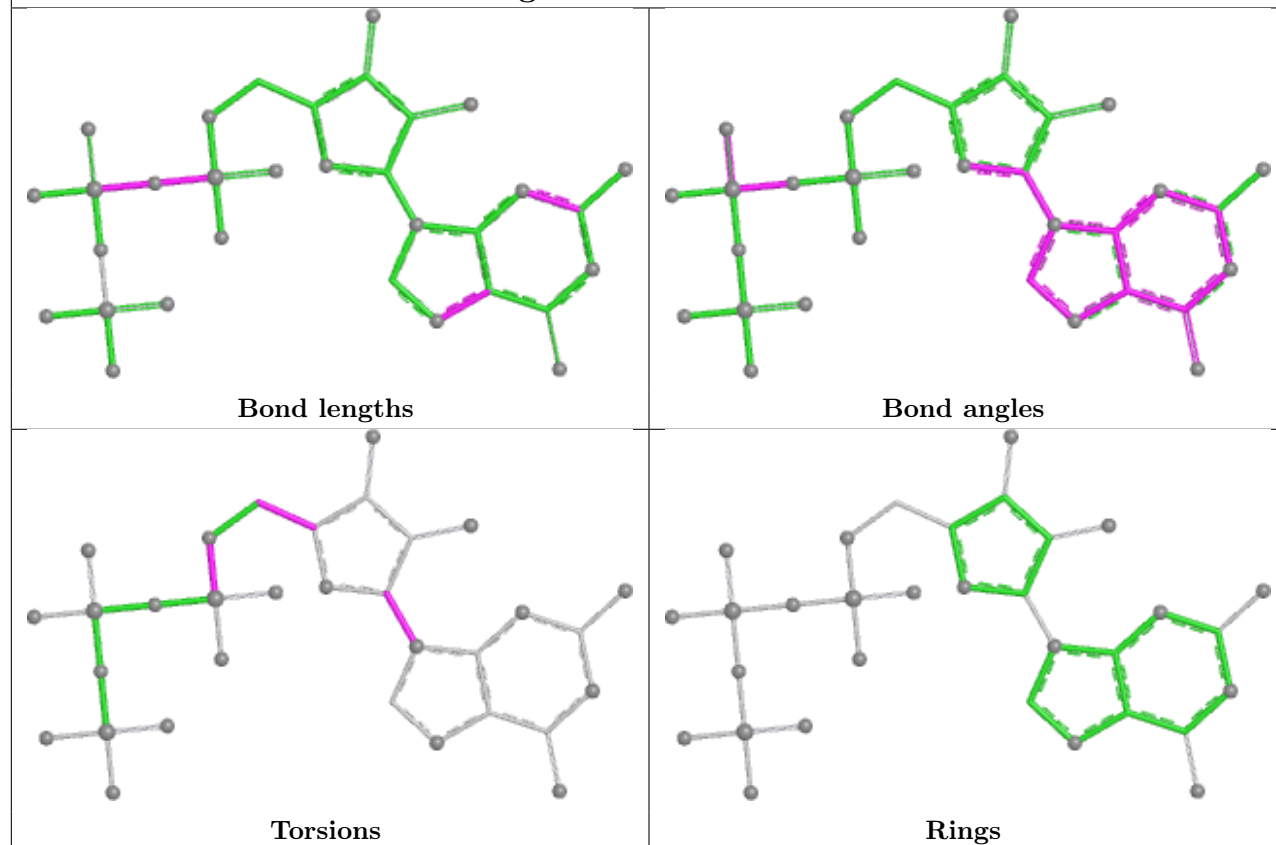
Ligand GTP CJ 501



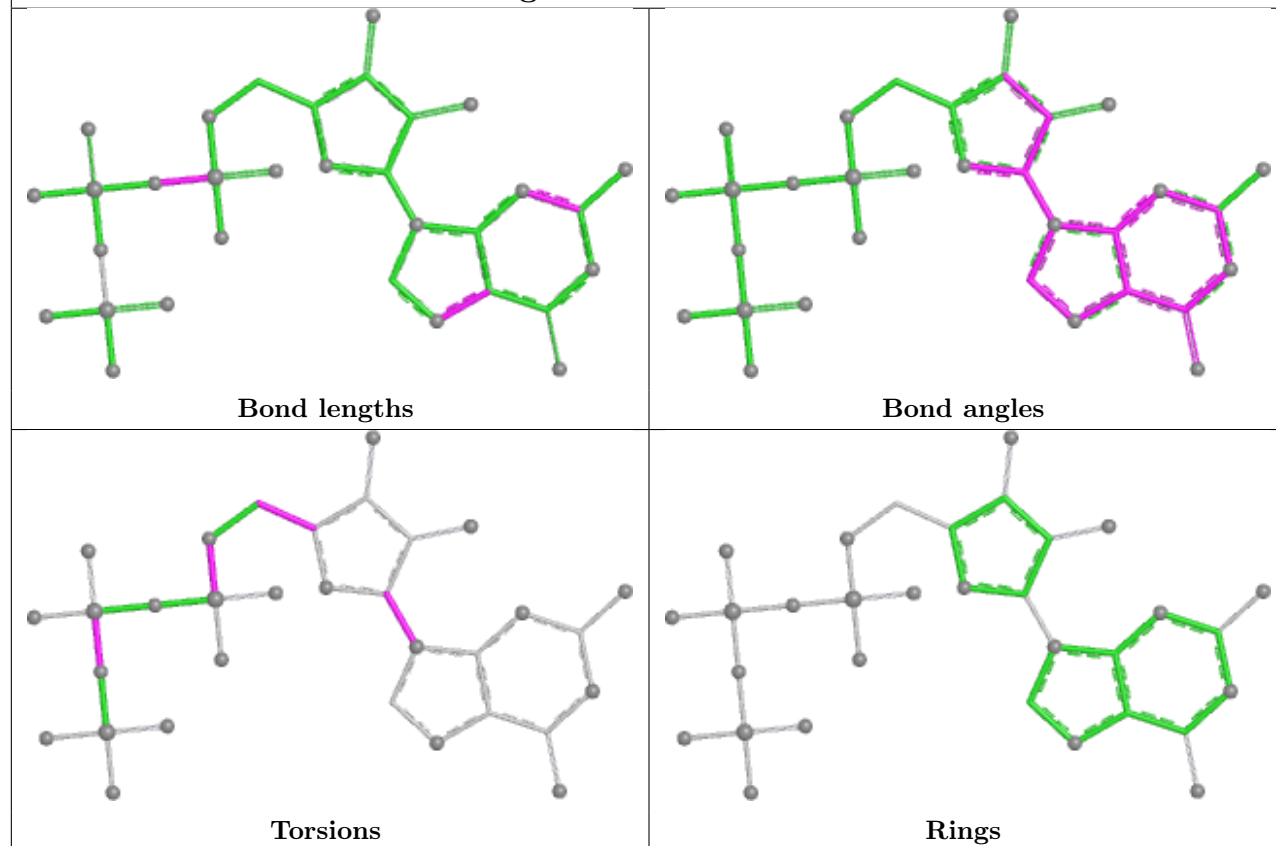
Ligand GTP JE 501



Ligand GTP UF 501



Ligand GTP SH 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

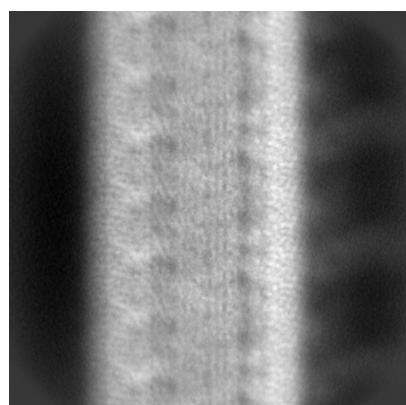
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35229. These allow visual inspection of the internal detail of the map and identification of artifacts.

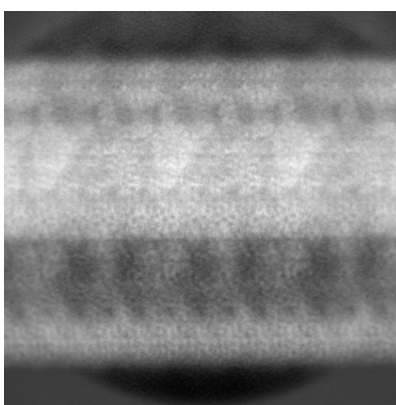
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

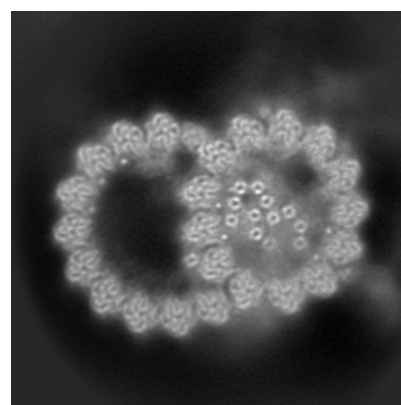
6.1.1 Primary map



X



Y

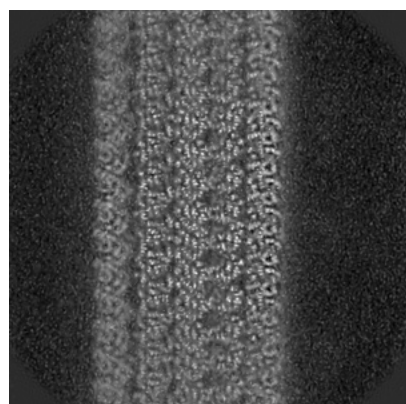


Z

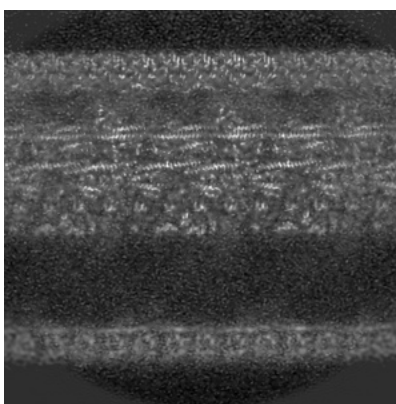
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

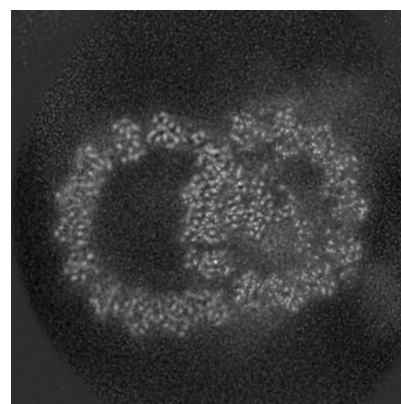
6.2.1 Primary map



X Index: 160



Y Index: 160

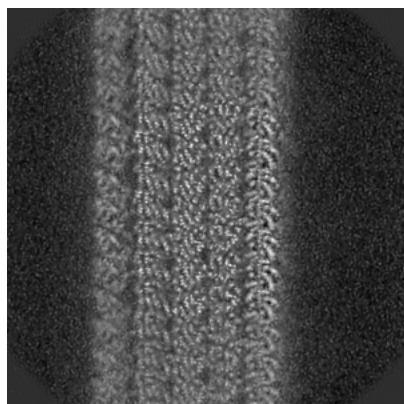


Z Index: 160

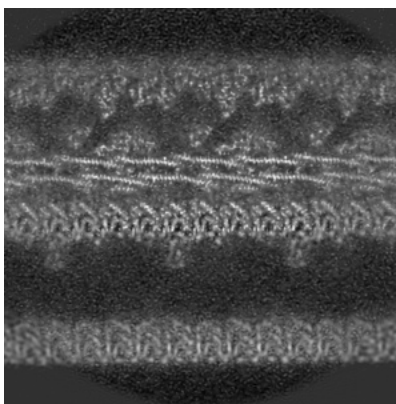
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

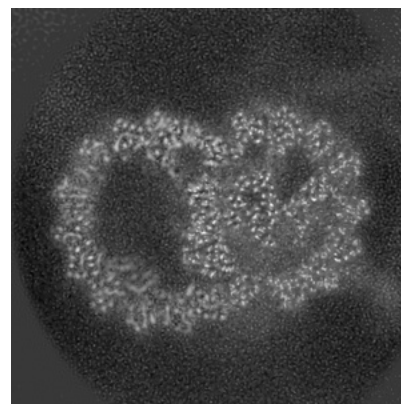
6.3.1 Primary map



X Index: 158



Y Index: 175

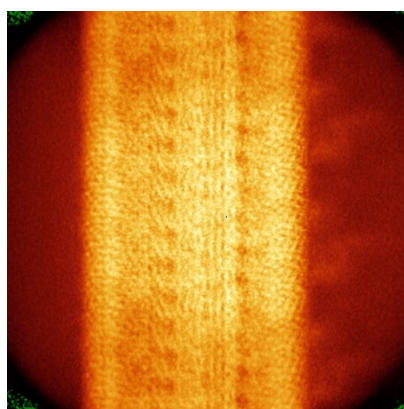


Z Index: 178

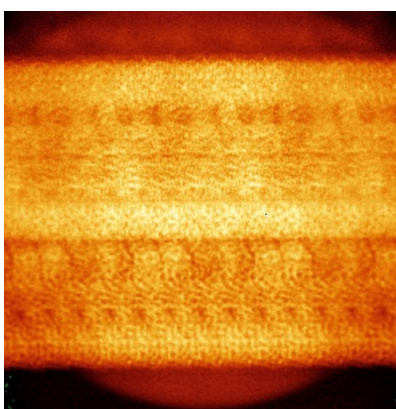
The images above show the largest variance slices of the map in three orthogonal directions.

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

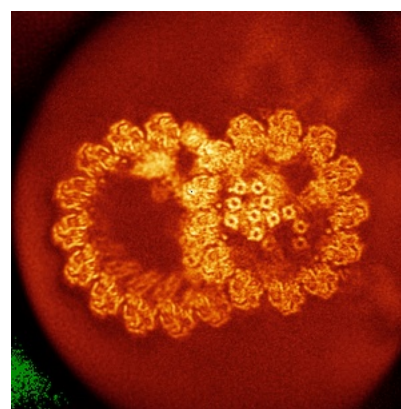
6.4.1 Primary map



X



Y

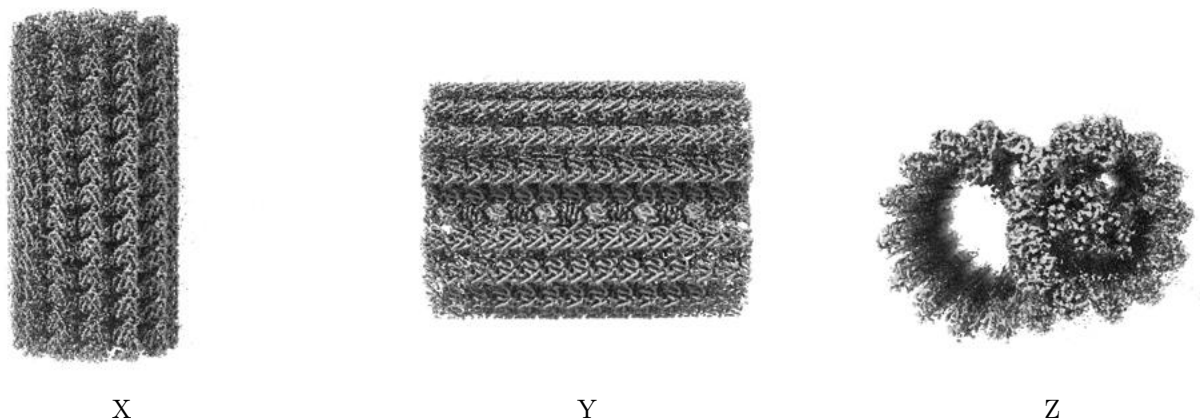


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

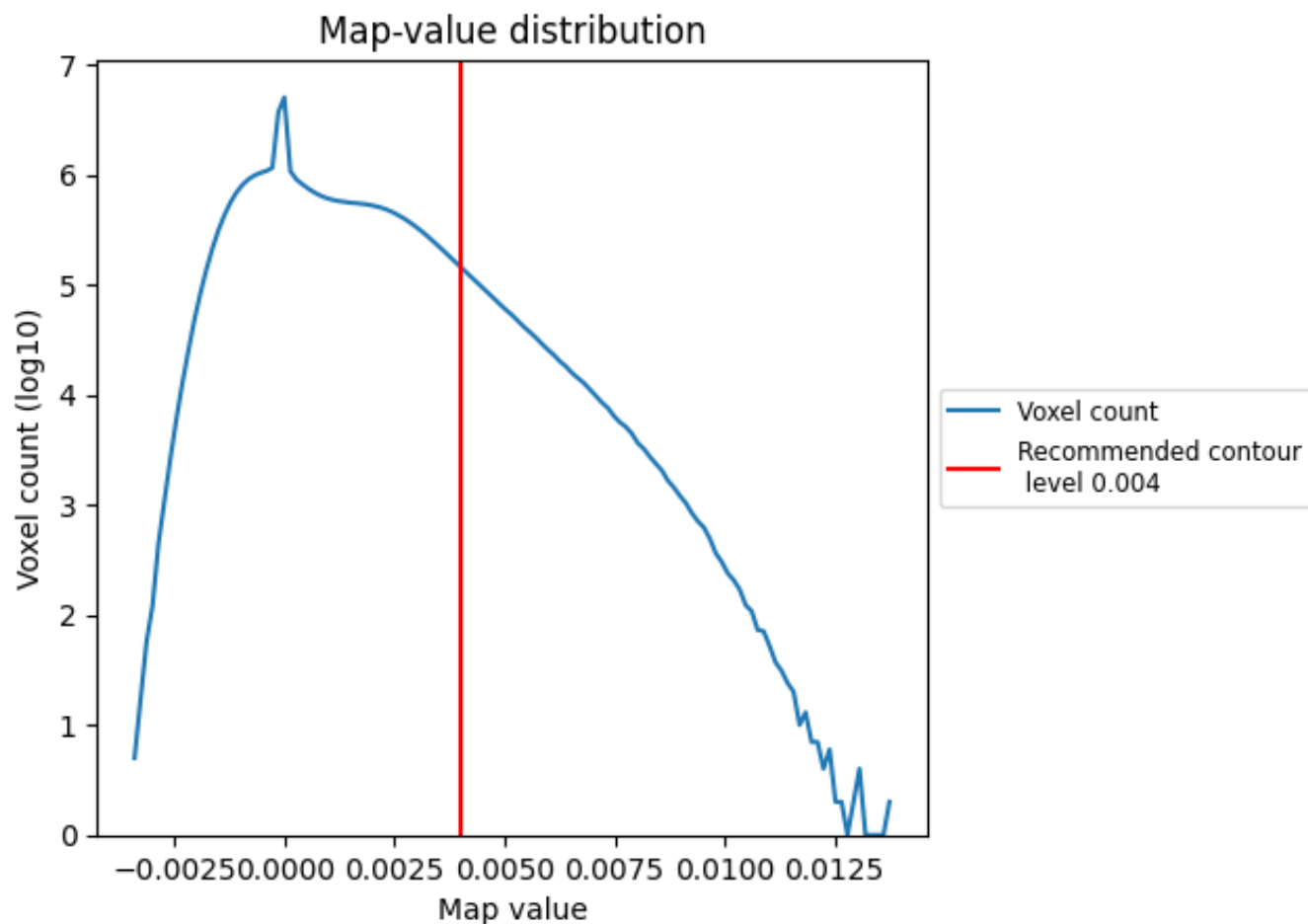
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

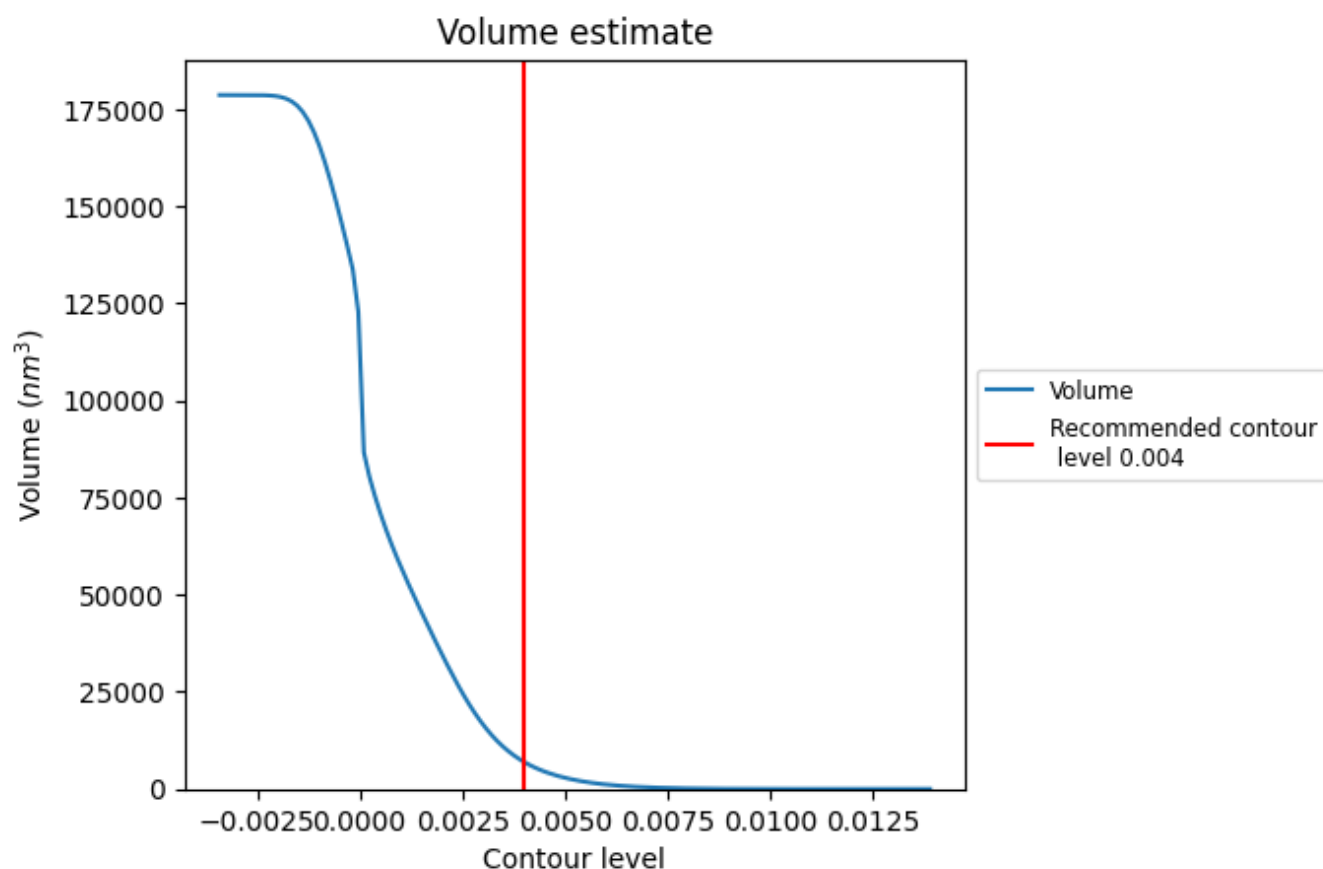
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

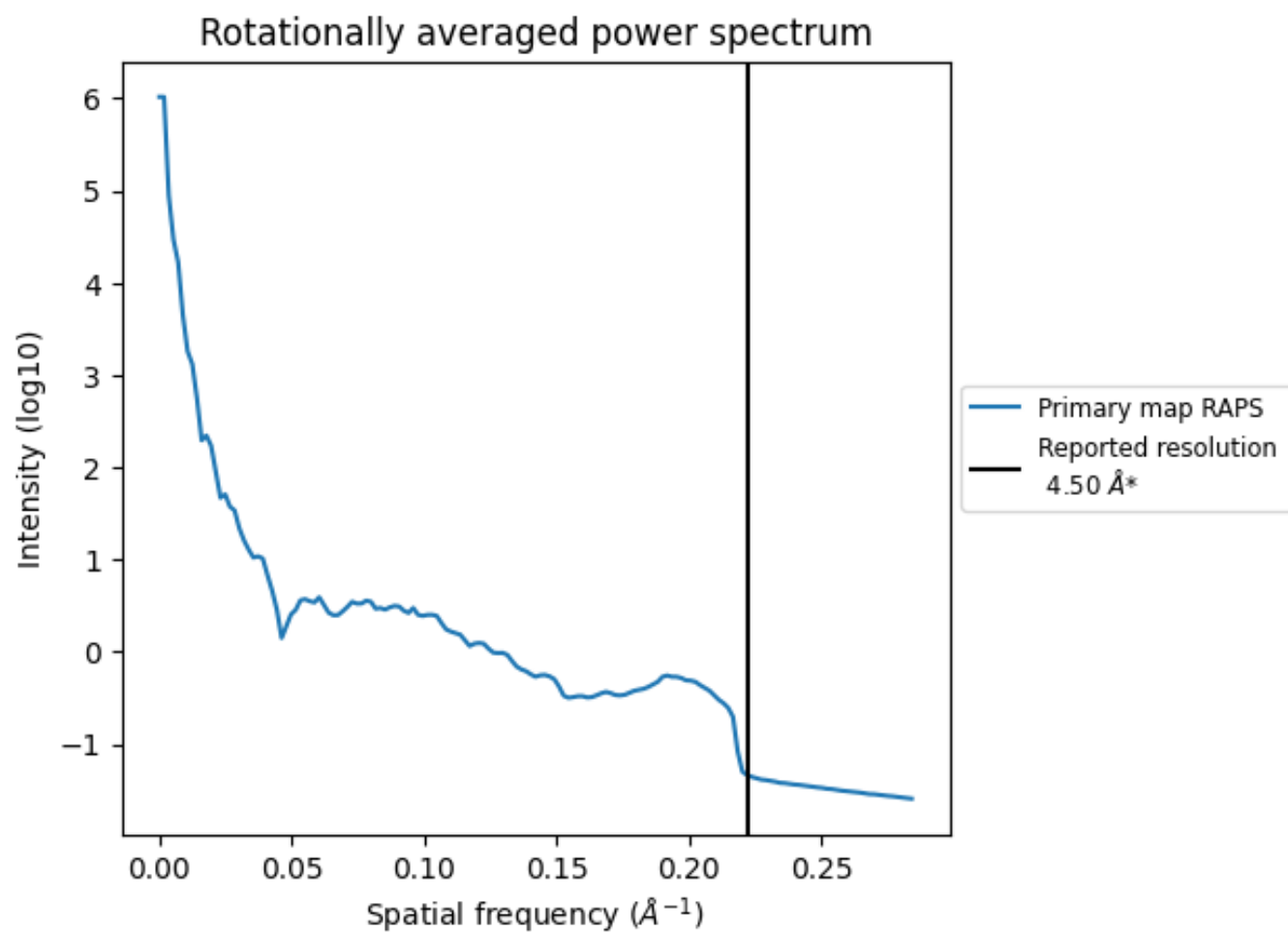
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6982 nm³; this corresponds to an approximate mass of 6307 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 0.222 Å⁻¹

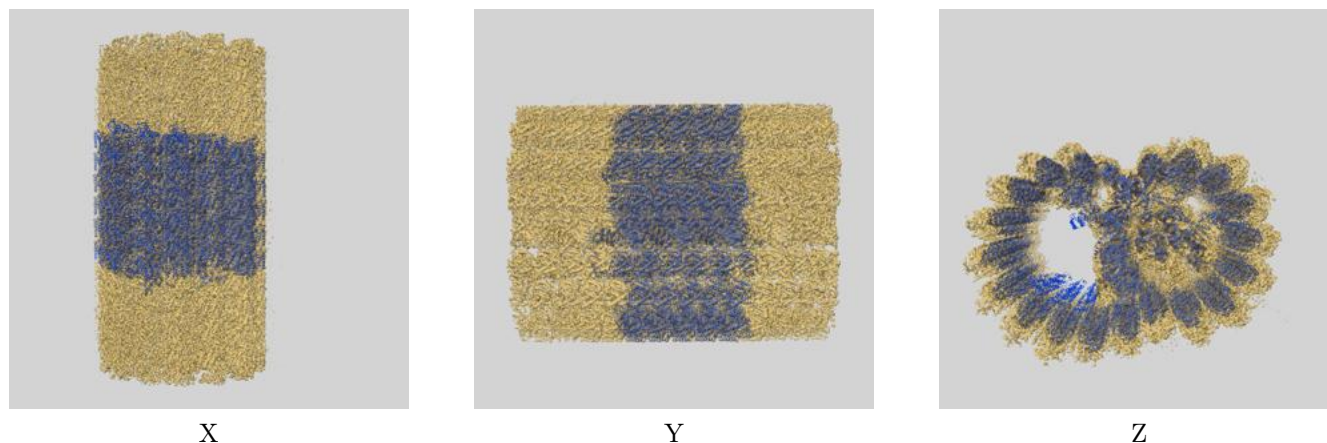
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

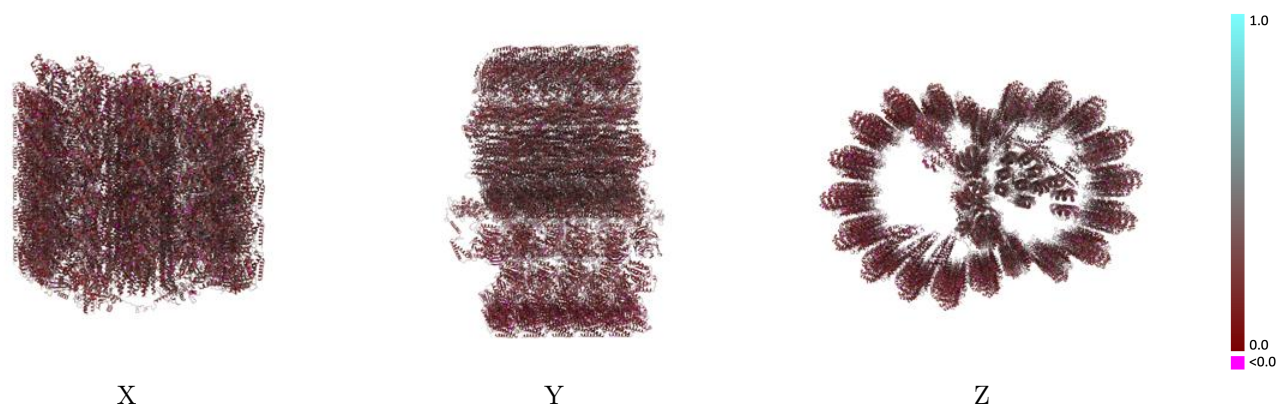
This section contains information regarding the fit between EMDB map EMD-35229 and PDB model 8I7O. Per-residue inclusion information can be found in section 3 on page 30.

9.1 Map-model overlay [i](#)



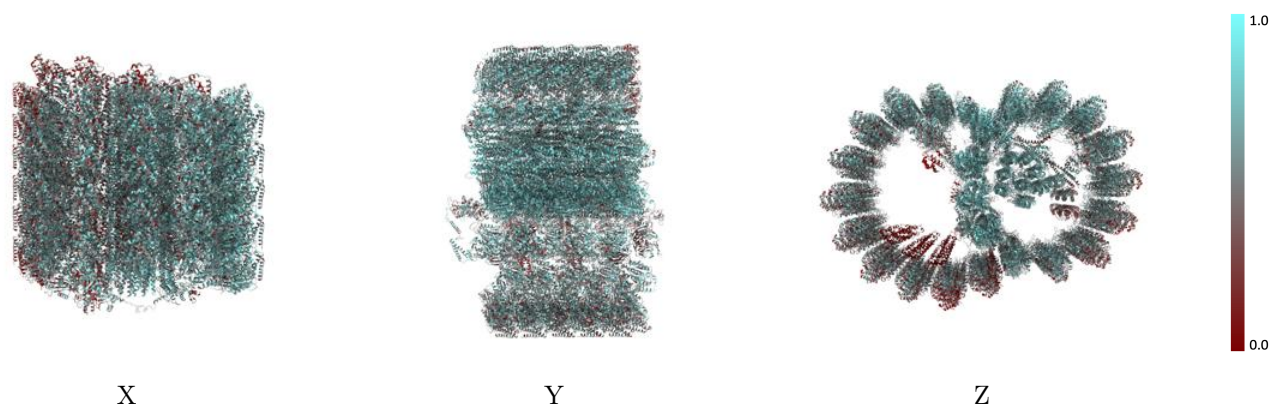
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



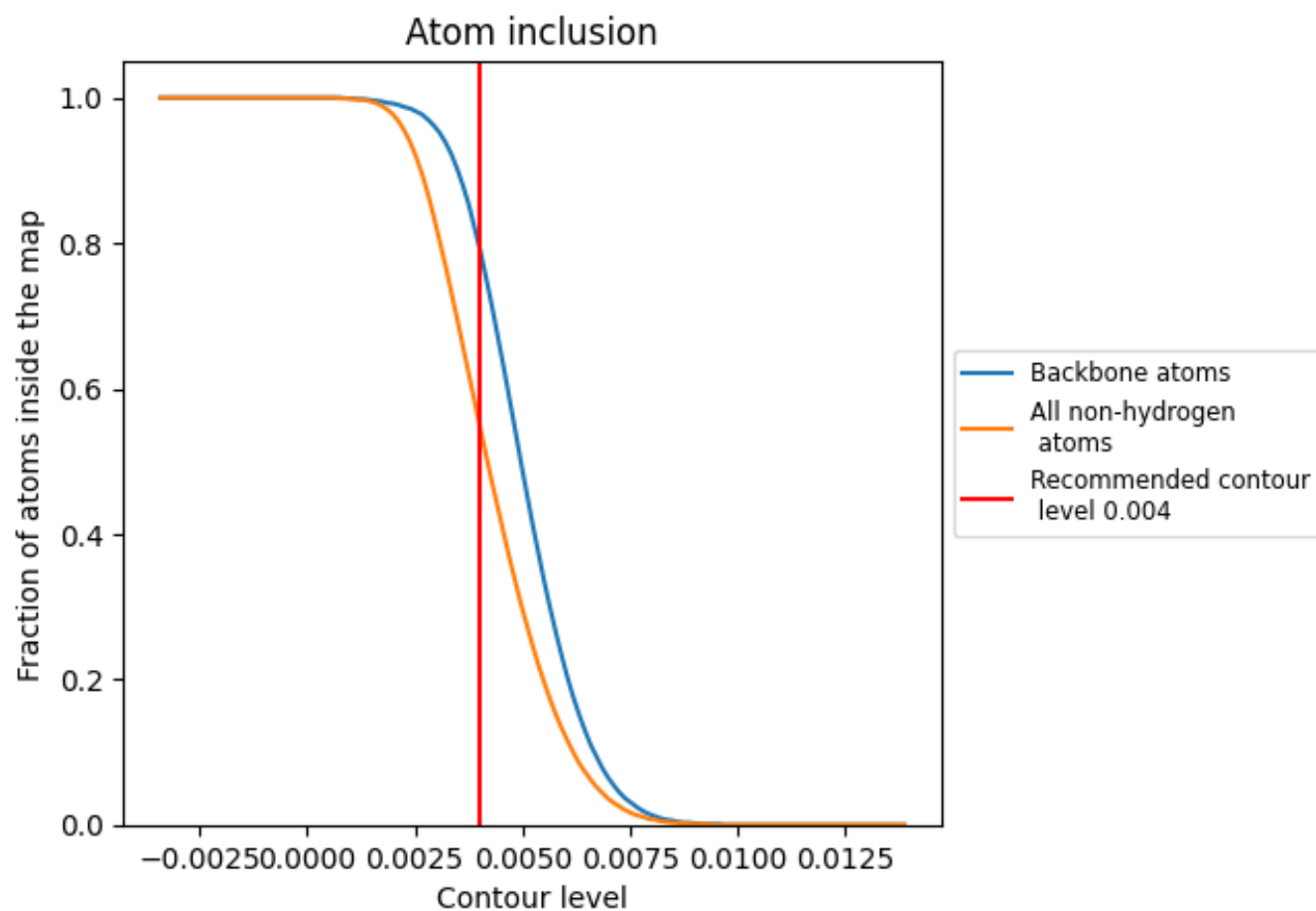
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5520	 0.2480
A2	 0.7070	 0.3000
A3	 0.7070	 0.2980
AE	 0.7160	 0.2840
AF	 0.7460	 0.2980
AG	 0.7370	 0.2930
AH	 0.7440	 0.2910
AI	 0.7520	 0.2930
B2	 0.6820	 0.2930
B3	 0.6960	 0.3000
B7	 0.6930	 0.2900
B8	 0.6950	 0.2860
BE	 0.6430	 0.2790
BF	 0.6820	 0.2850
BG	 0.6560	 0.2810
BH	 0.7020	 0.2970
BI	 0.6880	 0.2850
C2	 0.7060	 0.2860
C3	 0.6990	 0.2850
C4	 0.6920	 0.2790
C7	 0.7150	 0.2910
C8	 0.7000	 0.2910
CF	 0.6440	 0.2760
CG	 0.6470	 0.2790
CH	 0.6620	 0.2820
CI	 0.6480	 0.2790
CJ	 0.6350	 0.2750
Cb	 0.6950	 0.2970
Cc	 0.6990	 0.2900
D2	 0.6950	 0.2980
D3	 0.6970	 0.2880
D4	 0.6930	 0.2970
D7	 0.7030	 0.2630
D8	 0.7010	 0.2810
D9	 0.7080	 0.2940



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
DD	 0.6170	 0.2640
DE	 0.6250	 0.2690
DF	 0.6350	 0.2770
DG	 0.6100	 0.2670
DH	 0.6290	 0.2680
E2	 0.6260	 0.3210
E3	 0.6700	 0.3270
ED	 0.5550	 0.2600
EE	 0.6130	 0.2810
EF	 0.6060	 0.2730
EG	 0.5900	 0.2830
EH	 0.5830	 0.2630
F2	 0.6310	 0.2700
F3	 0.6110	 0.2590
F6	 0.4720	 0.2310
F7	 0.4710	 0.2320
FD	 0.5030	 0.2530
FE	 0.5680	 0.2770
FF	 0.5890	 0.2820
FG	 0.5500	 0.2810
FH	 0.5620	 0.2730
Fa	 0.2860	 0.2000
Fb	 0.3000	 0.2080
Fc	 0.2420	 0.2420
F1	 0.4430	 0.1880
G1	 0.5610	 0.3020
G2	 0.5800	 0.3040
G5	 0.5910	 0.2990
GD	 0.4360	 0.2560
GE	 0.5290	 0.2660
GF	 0.5620	 0.2730
GG	 0.5200	 0.2620
GH	 0.5330	 0.2760
GI	 0.5070	 0.2630
H3	 0.5760	 0.2550
H4	 0.5860	 0.2450
HD	 0.3910	 0.2450
HE	 0.5050	 0.2570
HF	 0.5120	 0.2520
HG	 0.5100	 0.2540
HH	 0.5230	 0.2650
HI	 0.5140	 0.2630

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
I2	 0.6550	 0.2400
I3	 0.6890	 0.2300
IE	 0.5330	 0.2520
IF	 0.5620	 0.2640
IG	 0.5740	 0.2790
IH	 0.5620	 0.2710
II	 0.5550	 0.2650
J2	 0.5660	 0.3040
J3	 0.5450	 0.2850
JD	 0.5770	 0.2520
JE	 0.6010	 0.2650
JF	 0.6100	 0.2710
JG	 0.5810	 0.2730
JH	 0.5910	 0.2540
K2	 0.5810	 0.2560
K3	 0.6100	 0.2730
K4	 0.4550	 0.2670
KD	 0.6470	 0.2750
KE	 0.6490	 0.2820
KF	 0.6630	 0.2990
KG	 0.6460	 0.2900
KH	 0.6590	 0.2820
KI	 0.6330	 0.2760
L2	 0.5330	 0.2460
L3	 0.5210	 0.2470
LD	 0.6700	 0.2830
LE	 0.6830	 0.2990
LF	 0.6820	 0.2890
LG	 0.6900	 0.3000
LH	 0.6900	 0.3040
LI	 0.6770	 0.2910
M2	 0.6020	 0.2980
M3	 0.5410	 0.2840
ME	 0.6860	 0.2940
MF	 0.6900	 0.2970
MG	 0.7330	 0.2980
MH	 0.7450	 0.2950
MI	 0.7060	 0.2970
N2	 0.5800	 0.2630
N3	 0.6110	 0.2630
ND	 0.3420	 0.2050
NE	 0.3840	 0.2110

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
NF	0.4680	0.2120
NG	0.4570	0.2170
NH	0.4520	0.2180
NI	0.3380	0.2110
O1	0.4830	0.2640
O2	0.6020	0.2780
OD	0.3060	0.1950
OE	0.3940	0.1970
OF	0.4100	0.2000
OG	0.3920	0.2020
OH	0.4290	0.2060
OI	0.3920	0.1990
P1	0.4790	0.1940
P2	0.4990	0.1920
PE	0.4140	0.1970
PF	0.4430	0.2040
PG	0.4200	0.2000
PH	0.4430	0.1970
PI	0.4300	0.1980
Q1	0.2420	0.1900
Q2	0.2690	0.1910
QE	0.4140	0.1960
QF	0.4240	0.2020
QG	0.4260	0.1980
QH	0.4370	0.2040
QI	0.4380	0.1930
R2	0.5270	0.2520
RE	0.4260	0.1930
RF	0.4350	0.1970
RG	0.4230	0.2000
RH	0.4360	0.1990
RI	0.4380	0.2010
RJ	0.4420	0.2040
SE	0.4610	0.2000
SF	0.4770	0.2000
SG	0.4710	0.1990
SH	0.4790	0.1970
SI	0.4790	0.2010
SJ	0.4570	0.1980
TF	0.5130	0.1920
TG	0.4860	0.1880
TH	0.4990	0.1970

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
TI	 0.4960	 0.1920
TJ	 0.5110	 0.1990
UD	 0.5090	 0.1920
UE	 0.4970	 0.1980
UF	 0.5280	 0.2000
UG	 0.5340	 0.1870
UH	 0.5290	 0.1960
VD	 0.5790	 0.2070
VE	 0.5510	 0.2070
VF	 0.5780	 0.2140
VG	 0.5630	 0.2130
VH	 0.5980	 0.2070
WE	 0.5950	 0.2280
WF	 0.6200	 0.2300
WG	 0.5870	 0.2340
WH	 0.6110	 0.2280
WI	 0.5920	 0.2190
XC	 0.7050	 0.2590
XD	 0.6980	 0.2660
XE	 0.7130	 0.2630
XJ	 0.5340	 0.2470
XK	 0.6700	 0.2490
XL	 0.5030	 0.2340
YI	 0.0330	 0.1640
YJ	 0.0220	 0.1820
YK	 0.0090	 0.1630
YL	 0.0440	 0.1750
YM	 0.0660	 0.1750
YN	 0.0890	 0.1900