wwPDB EM Validation Summary Report

Nov 29, 2023 – 11:03 PM JST

PDB ID	:	8I7O
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:

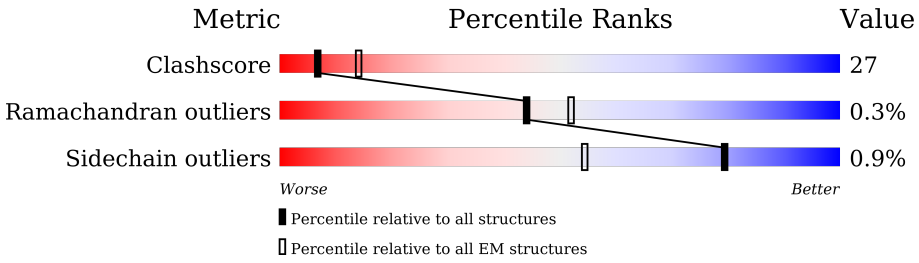
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	45% 39% 16%
1	A3	418	32% 17% 50%
2	AE	438	7% 47% 53%
2	AG	438	47% 51%
2	AI	438	5% 45% 55%
2	BE	438	12% 52% 47%
2	BG	438	11% 48% 50%
2	BI	438	8% 55% 45%

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Mol	Chain	Length	Quality of chain
2	CG	438	11% 52% 47%
2	CI	438	13% 50% 48%
2	DE	438	17% 48% 51%
2	DG	438	16% 50% 50%
2	EE	438	16% 53% 45%
2	EG	438	18% 52% 47%
2	FE	438	23% 50% 49%
2	FG	438	25% 52% 47%
2	GE	438	25% 51% 47%
2	GG	438	32% 50% 49%
2	GI	438	32% 57% 42%
2	HE	438	32% 49% 50%
2	HG	438	32% 53% 46%
2	HI	438	29% 56% 43%
2	IE	438	28% 58% 41%
2	IG	438	25% 53% 46%
2	II	438	23% 52% 47%
2	JE	438	16% 49% 50%
2	JG	438	19% 55% 44%
2	KE	438	11% 47% 52%
2	KG	438	12% 51% 48%
2	KI	438	15% 55% 45%
2	LE	438	7% 55% 44%
2	LG	438	7% 50% 49%
2	LI	438	8% 56% 43%

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Mol	Chain	Length	Quality of chain
2	ME	438	8% 50% 50%
2	MG	438	5% 47% 51%
2	MI	438	8% 52% 47%
2	NE	438	53% 41% 58%
2	NG	438	41% 41% 58%
2	NI	438	61% 42% 56%
2	OE	438	49% 43% 55%
2	OG	438	50% 46% 53%
2	OI	438	50% 42% 57%
2	PE	438	46% 43% 56%
2	PG	438	46% 42% 56%
2	PI	438	42% 42% 57%
2	QE	438	44% 42% 57%
2	QG	438	42% 42% 57%
2	QI	438	40% 42% 58%
2	RE	438	43% 43% 56%
2	RG	438	45% 41% 58%
2	RI	438	42% 36% 63%
2	SE	438	37% 47% 53%
2	SG	438	35% 37% 61%
2	SI	438	34% 40% 59%
2	TG	438	34% 43% 55%
2	TI	438	34% 44% 55%
2	UE	438	34% 43% 56%
2	UG	438	28% 39% 59%

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Mol	Chain	Length	Quality of chain
2	VE	438	22% 42% 57%
2	VG	438	21% 40% 58%
2	WE	438	18% 39% 60%
2	WG	438	19% 38% 61%
2	WI	438	18% 36% 63%
3	AF	427	49% 50%
3	AH	427	48% 52%
3	BF	427	8% 53% 46%
3	BH	427	6% 51% 48%
3	CF	427	9% 52% 47%
3	CH	427	8% 54% 46%
3	CJ	427	12% 53% 47%
3	DD	427	14% 53% 47%
3	DF	427	11% 49% 51%
3	DH	427	12% 54% 45%
3	ED	427	25% 57% 42%
3	EF	427	15% 52% 48%
3	EH	427	22% 56% 44%
3	FD	427	32% 59% 41%
3	FF	427	18% 56% 44%
3	FH	427	22% 59% 41%
3	GD	427	45% 54% 45%
3	GF	427	23% 52% 48%
3	GH	427	29% 53% 47%
3	HD	427	52% 58% 41%

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Mol	Chain	Length	Quality of chain
3	HF	427	33% 54% 46%
3	HH	427	27% 52% 47%
3	IF	427	23% 51% 49%
3	IH	427	22% 52% 48%
3	JD	427	17% 53% 46%
3	JF	427	17% 55% 45%
3	JH	427	18% 56% 43%
3	KD	427	9% 55% 45%
3	KF	427	8% 56% 43%
3	KH	427	9% 55% 45%
3	LD	427	8% 53% 46%
3	LF	427	6% 50% 49%
3	LH	427	6% 52% 47%
3	MF	427	7% 54% 46%
3	MH	427	45% 54%
3	ND	427	61% 52% 47%
3	NF	427	37% 47% 53%
3	NH	427	41% 47% 52%
3	OD	427	63% 53% 47%
3	OF	427	45% 53% 46%
3	OH	427	44% 42% 57%
3	PF	427	39% 46% 53%
3	PH	427	38% 46% 53%
3	QF	427	43% 44% 56%
3	QH	427	40% 46% 54%

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Mol	Chain	Length	Quality of chain
3	RF	427	43% 42% 58%
3	RH	427	44% 43% 56%
3	RJ	427	39% 46% 54%
3	SF	427	33% 44% 56%
3	SH	427	34% 43% 56%
3	SJ	427	37% 41% 58%
3	TF	427	28% 46% 54%
3	TH	427	33% 50% 49%
3	TJ	427	30% 49% 51%
3	UD	427	29% 48% 52%
3	UF	427	24% 43% 56%
3	UH	427	27% 48% 52%
3	VD	427	15% 43% 56%
3	VF	427	17% 45% 55%
3	VH	427	14% 44% 56%
3	WF	427	12% 44% 55%
3	WH	427	13% 50% 49%
4	B2	430	40% 18% 42%
4	B3	430	46% 34% 20%
4	B7	430	53% 33% 13%
4	B8	430	20% 21% 59%
5	C2	490	16% 13% 71%
5	C3	490	43% 32% 25%
5	C4	490	7% 9% 83%
5	C7	490	32% 18% 50%

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Mol	Chain	Length	Quality of chain
5	C8	490	39% 24% 36%
5	Cb	490	53% 47%
5	Cc	490	54% 46%
6	D2	447	11% 5% 84%
6	D3	447	55% 33% 12%
6	D4	447	19% 11% 70%
6	D7	447	9% 13% 77%
6	D8	447	52% 35% 13%
6	D9	447	14% 9% 77%
7	E2	206	20% 54% 34% 9%
7	E3	206	23% 7% 69%
8	F2	557	34% 24% 42%
8	F3	557	6% 23% 18% 58%
8	F6	557	20% 35% 19% 45%
8	F7	557	16% 24% 20% 56%
8	Fa	557	27% 38% 62%
8	Fb	557	40% 57% 42%
8	Fc	557	5% 95%
8	Fl	557	23% 59% 40%
9	G1	648	21% 47% 31% 21%
9	G2	648	19% 46% 30% 24%
10	G5	750	19% 55% 43%
11	H3	319	9% 18% 24% 55%
11	H4	319	10% 14% 24% 57%
12	I2	200	10% 8% 81%

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Mol	Chain	Length	Quality of chain
12	I3	200	12% 7% 81%
13	J2	189	22% 53% 37% 10%
13	J3	189	23% 55% 35% 10%
14	K2	499	7% 17% 24% 58%
14	K3	499	14% 40% 43% 14%
14	K4	499	15% 21% 12% 66%
15	L2	255	24% 40% 50% 7%
15	L3	255	24% 46% 45% 7%
16	M2	141	9% 18% 26% 56%
16	M3	141	13% 23% 21% 56%
17	N2	168	8% 17% 23% 60%
17	N3	168	7% 20% 20% 60%
18	O1	189	25% 30% 26% 44%
18	O2	189	12% 23% 31% 44%
19	P1	620	39% 44% 53%
19	P2	620	35% 41% 56%
20	Q1	1516	8% 5% 7% 88%
20	Q2	1516	8% 7% 88%
21	R2	283	8% 11% 14% 74%
22	XC	193	34% 61%
22	XD	193	39% 55%
22	XE	193	32% 64%
23	XJ	241	17% 34% 39% 26%
23	XK	241	7% 32% 41% 26%
23	XL	241	20% 34% 39% 26%

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Mol	Chain	Length	Quality of chain
24	YI	168	98% 35% 64%
24	YJ	168	99% 43% 55%
24	YK	168	99% 47% 52%
24	YL	168	97% 49% 50%
24	YM	168	97% 48% 51%
24	YN	168	93% 42% 58%

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	BH	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	HI	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	-
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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	GTP	RJ	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		

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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

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

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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		

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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		

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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		

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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		

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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		

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

- 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 4192 2708 704 763 17	0	0
9	G2	495	Total C N O S 4081 2634 687 743 17	0	0

- 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 6169 3983 1027 1130 29	0	0

- Molecule 11 is a protein called Protein FAM166A.

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

- Molecule 12 is a protein called Protein FAM166C.

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

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

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

- 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	0	0
			535	335	95	105		
17	N3	68	Total	C	N	O	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		

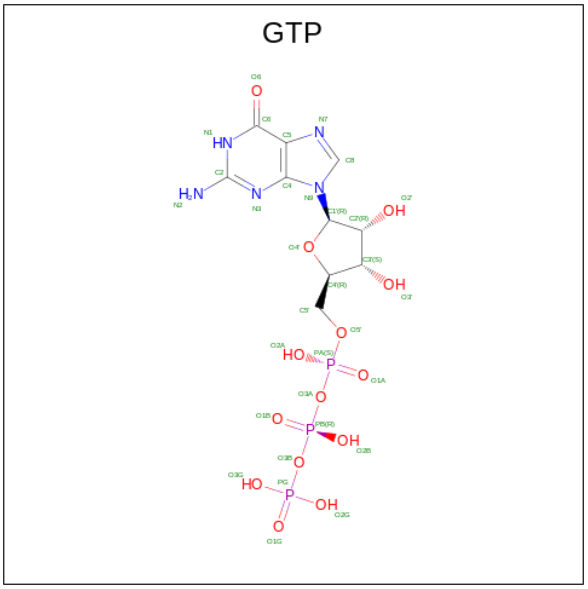
- Molecule 23 is a protein called Parkin coregulated gene protein homolog.

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 (three-letter code: 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	

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

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

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

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

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

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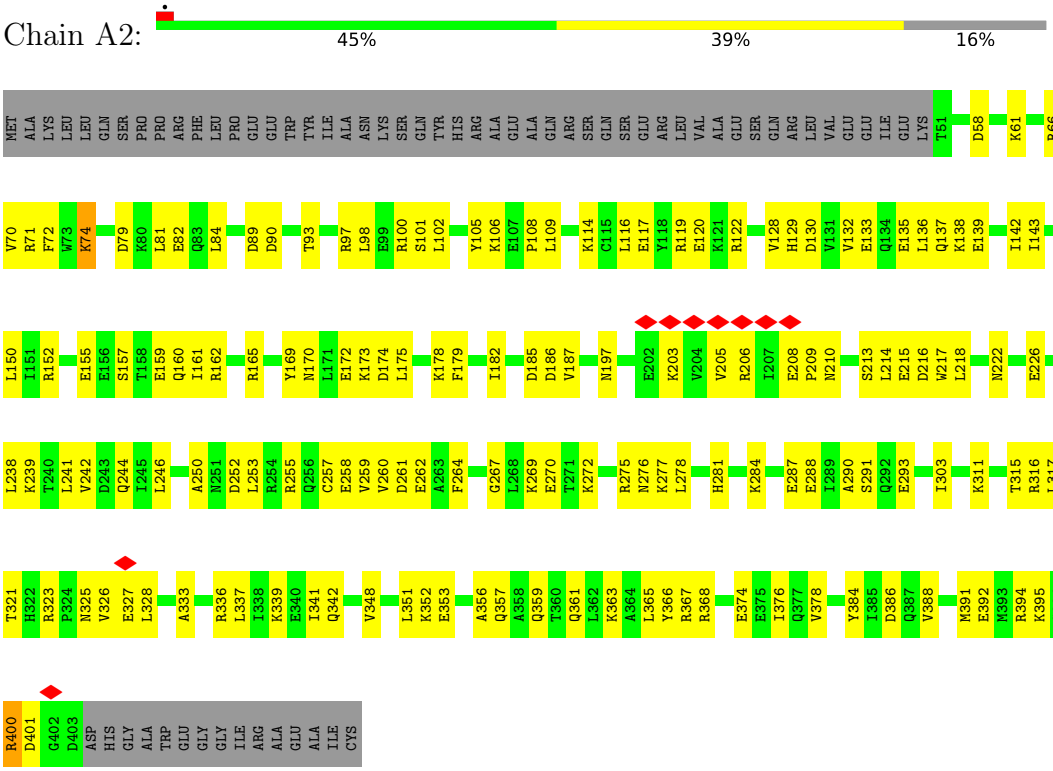
Mol	Chain	Residues	Atoms					AltConf
25	UF	1	Total	C	N	O	P	0
			32	10	5	14	3	
25	UG	1	Total	C	N	O	P	0
			32	10	5	14	3	
25	UH	1	Total	C	N	O	P	0
			32	10	5	14	3	
25	VD	1	Total	C	N	O	P	0
			32	10	5	14	3	
25	VE	1	Total	C	N	O	P	0
			32	10	5	14	3	
25	VF	1	Total	C	N	O	P	0
			32	10	5	14	3	
25	VG	1	Total	C	N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

3 Residue-property plots (i)

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

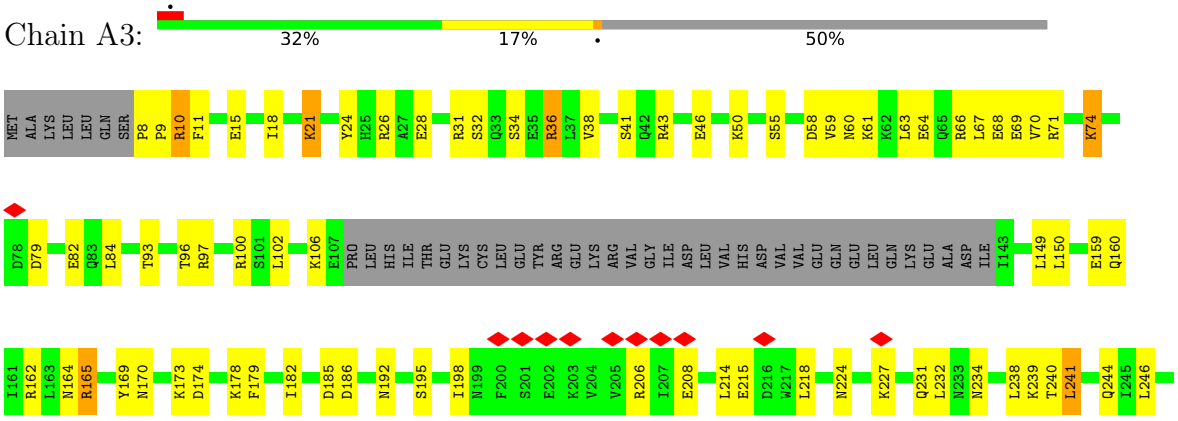
• Molecule 1: Tektin-1

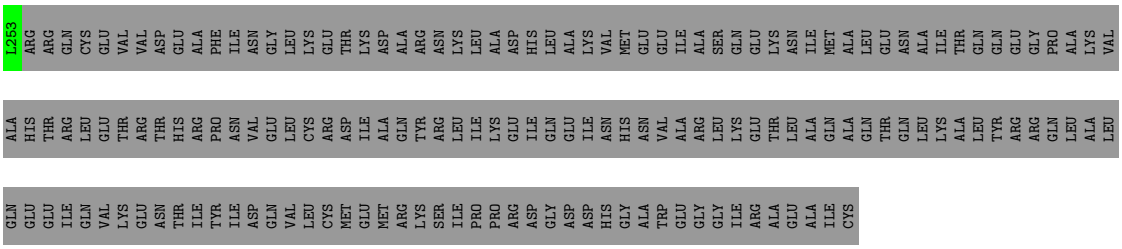
Chain A2:



• Molecule 1: Tektin-1

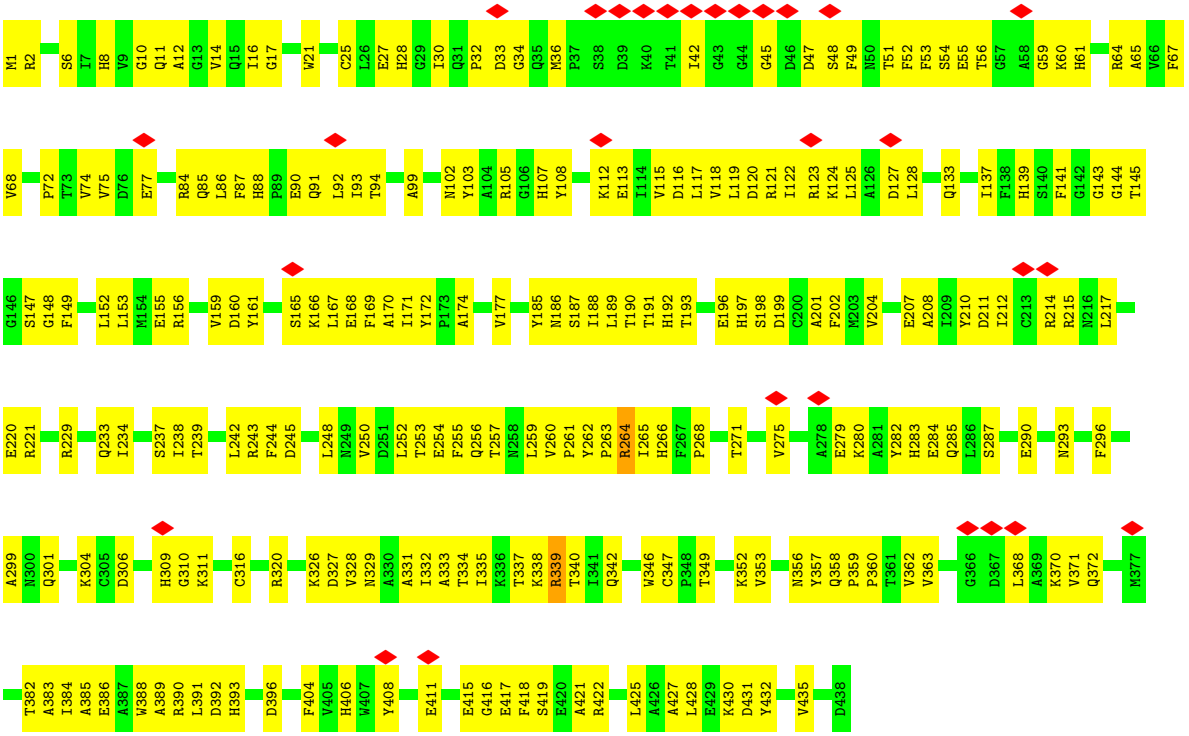
Chain A3:





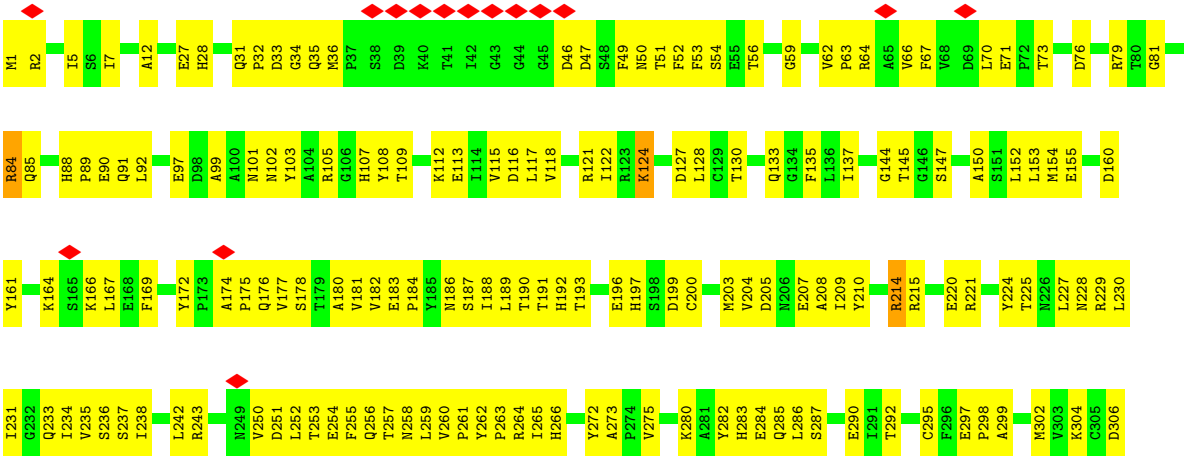
• Molecule 2: Detyrosinated tubulin alpha-3 chain

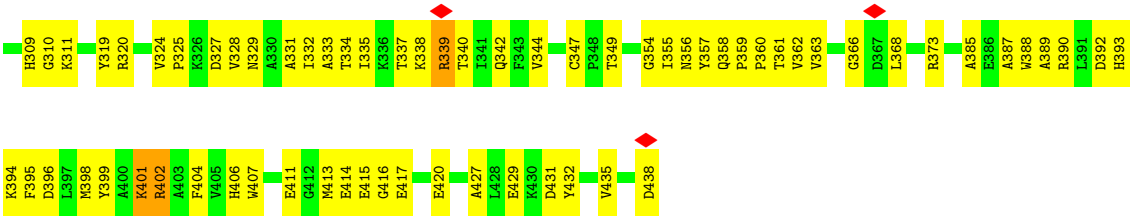
Chain AE:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

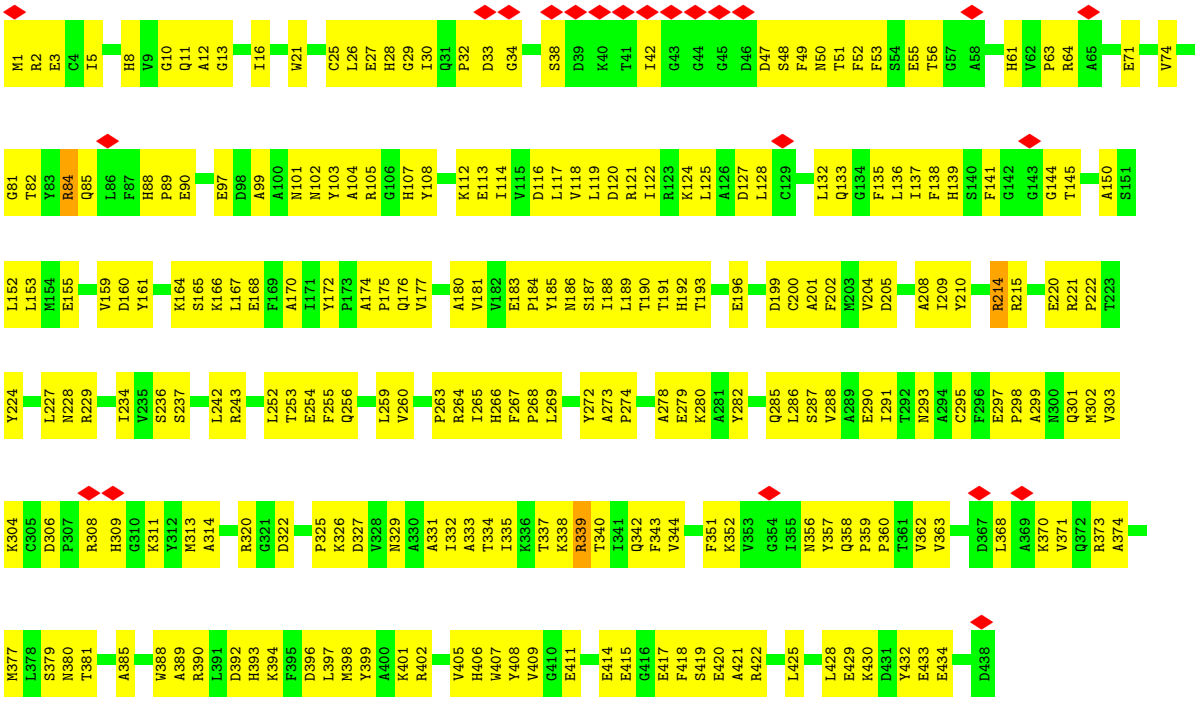
Chain AG:





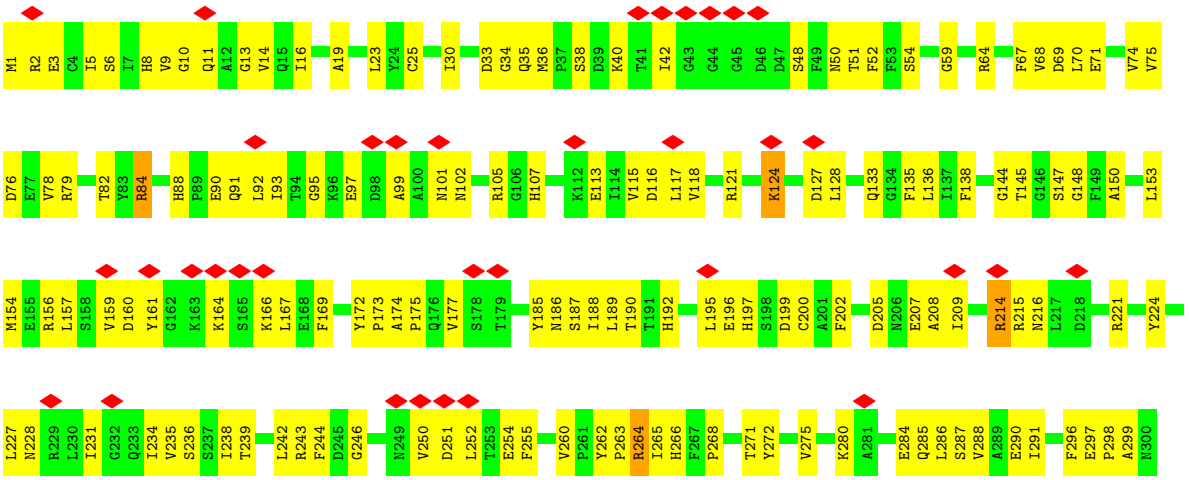
• Molecule 2: Detyrosinated tubulin alpha-3 chain

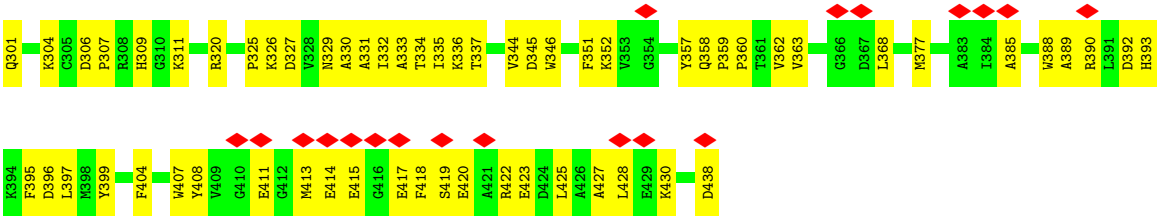
Chain AI:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

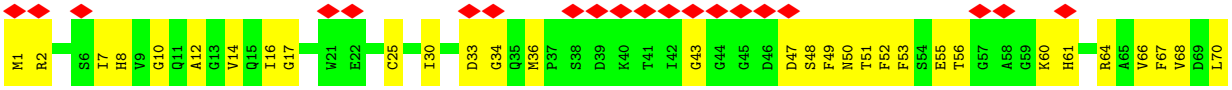
Chain BE:

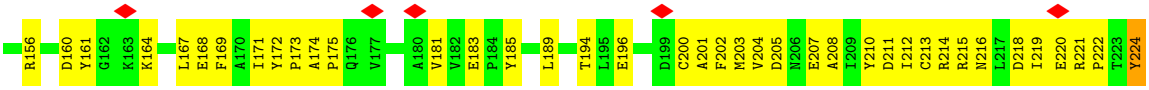


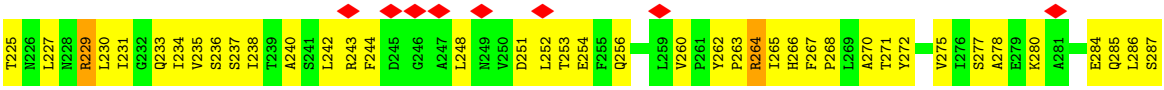


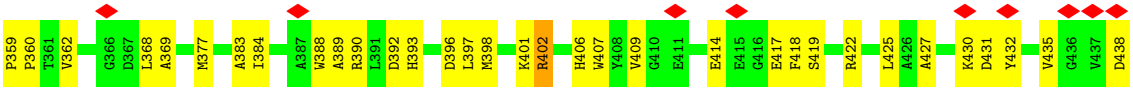
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain BG:



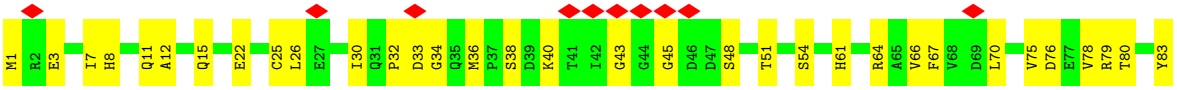


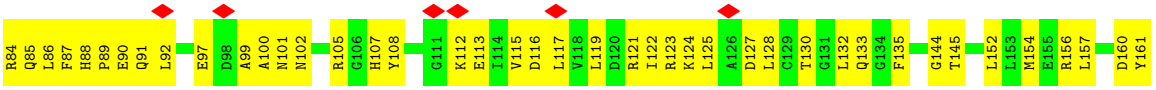


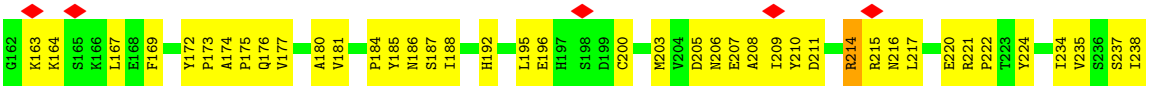


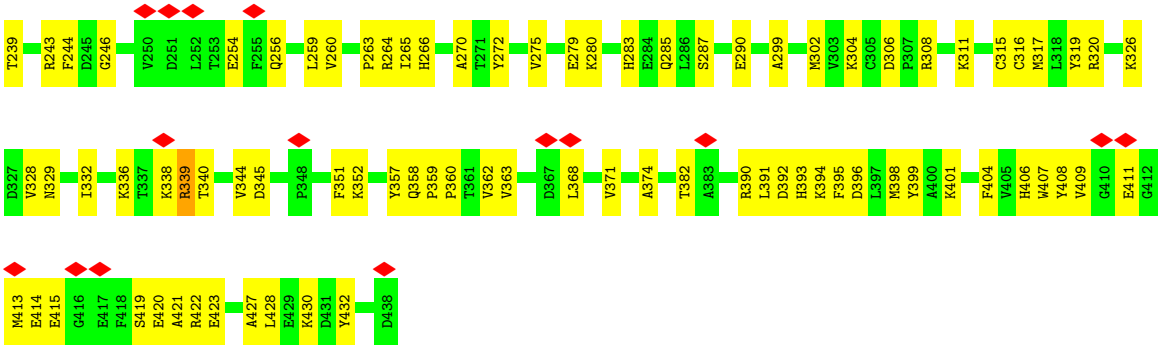
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain BI:

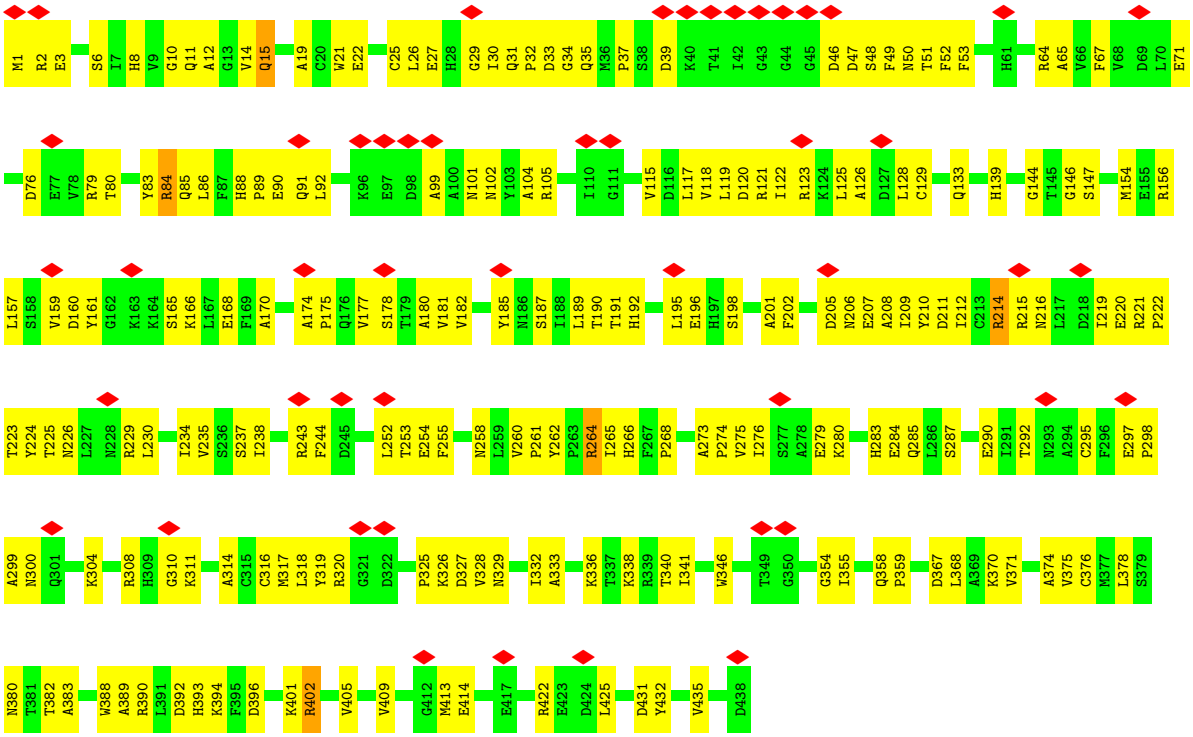




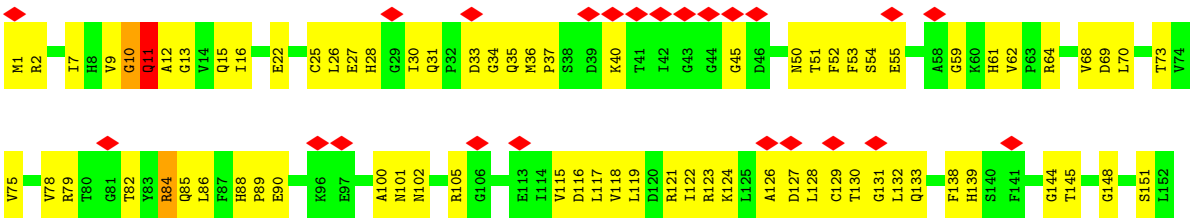


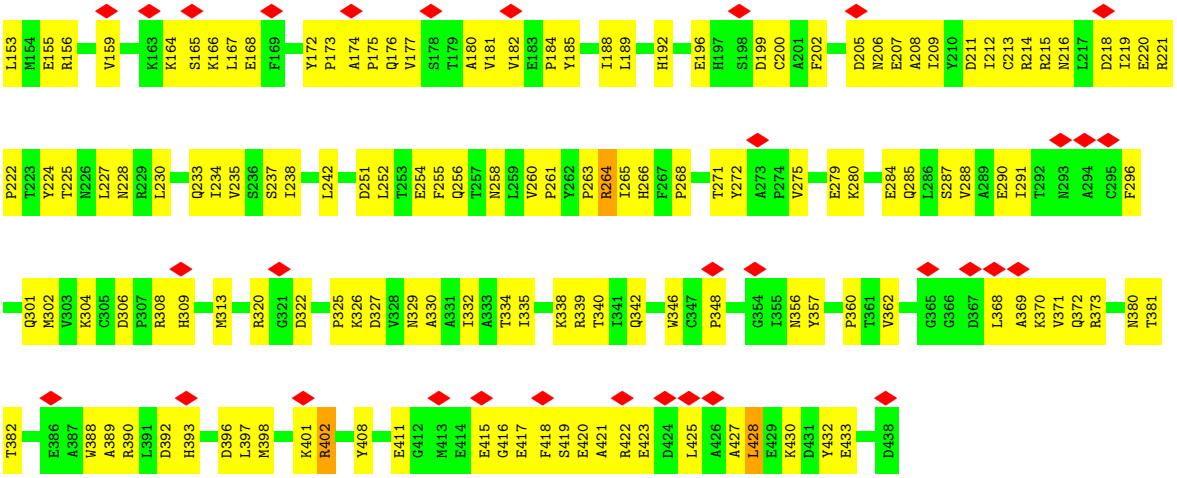


• Molecule 2: Detyrosinated tubulin alpha-3 chain



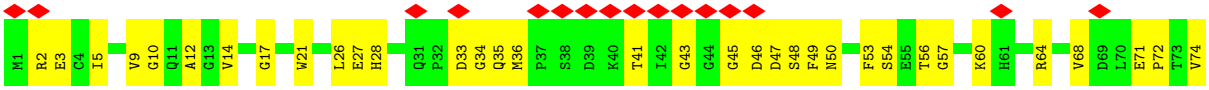
• Molecule 2: Detyrosinated tubulin alpha-3 chain





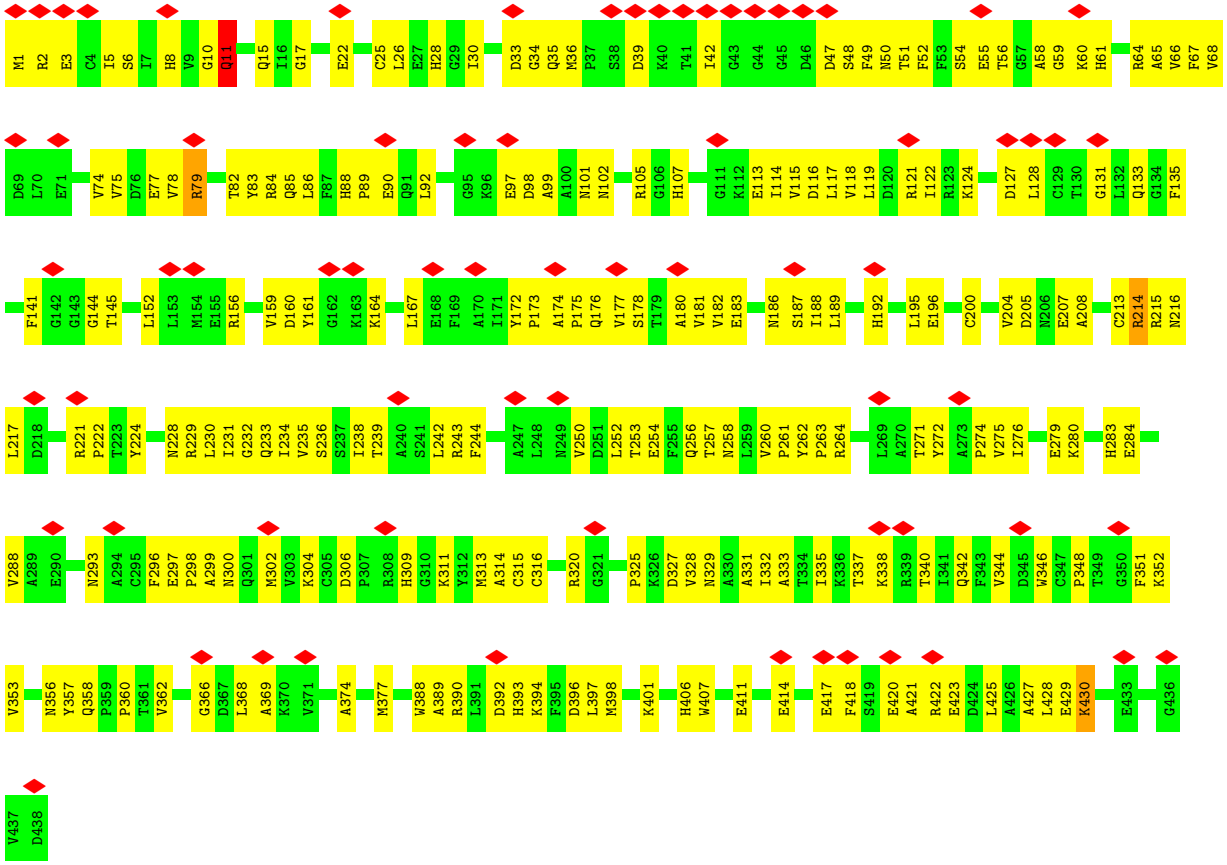
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain DE:



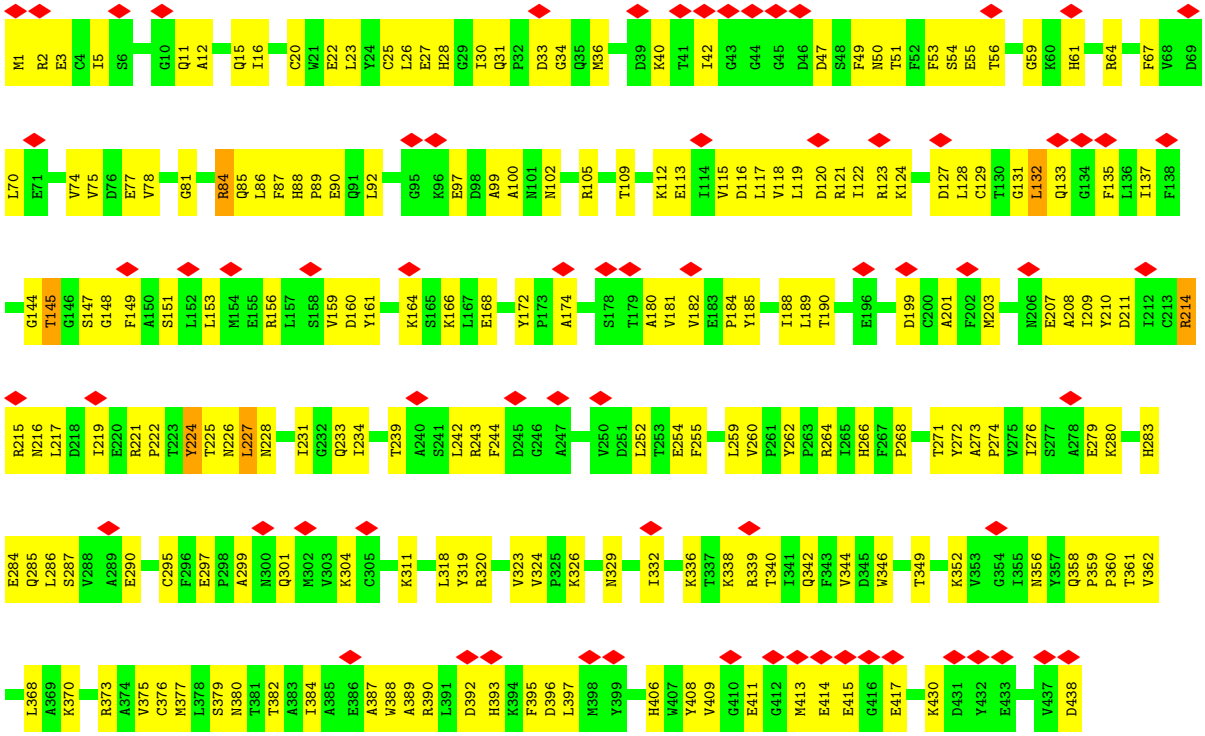
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain DG:



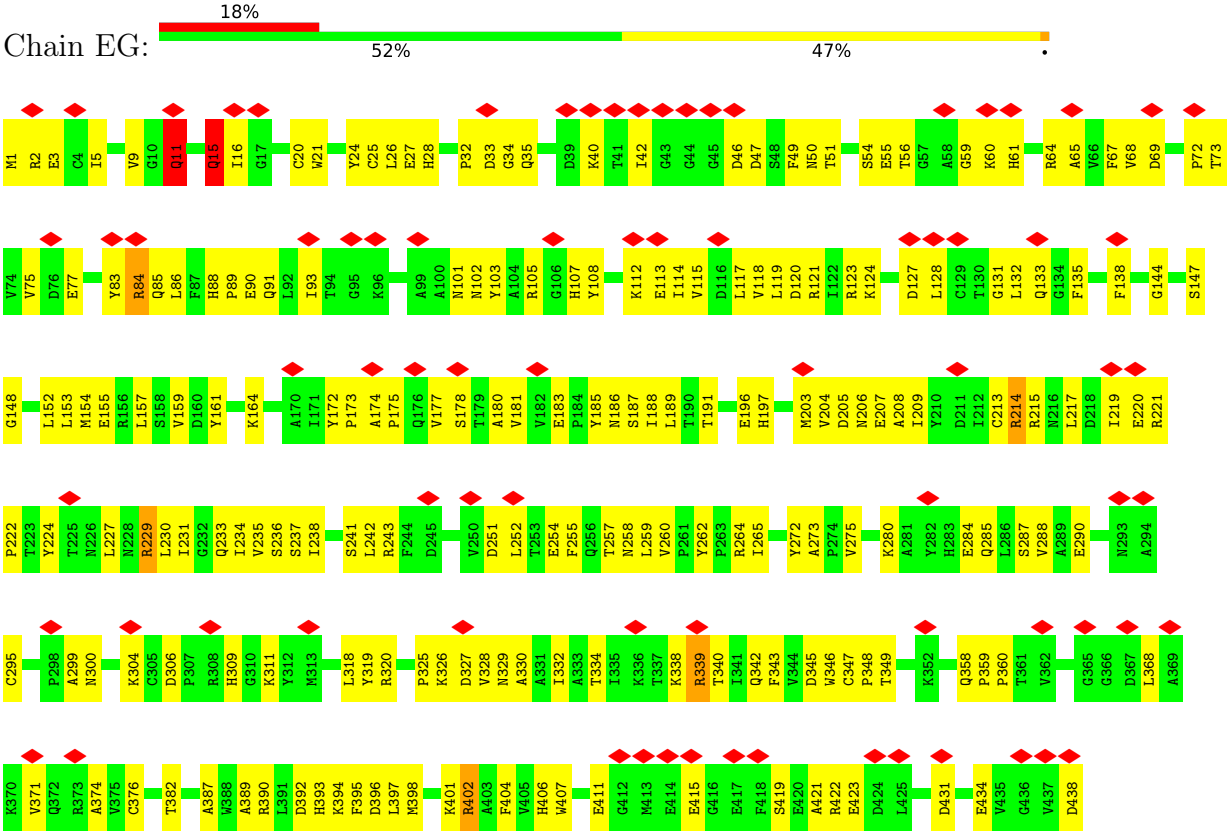
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain EE:



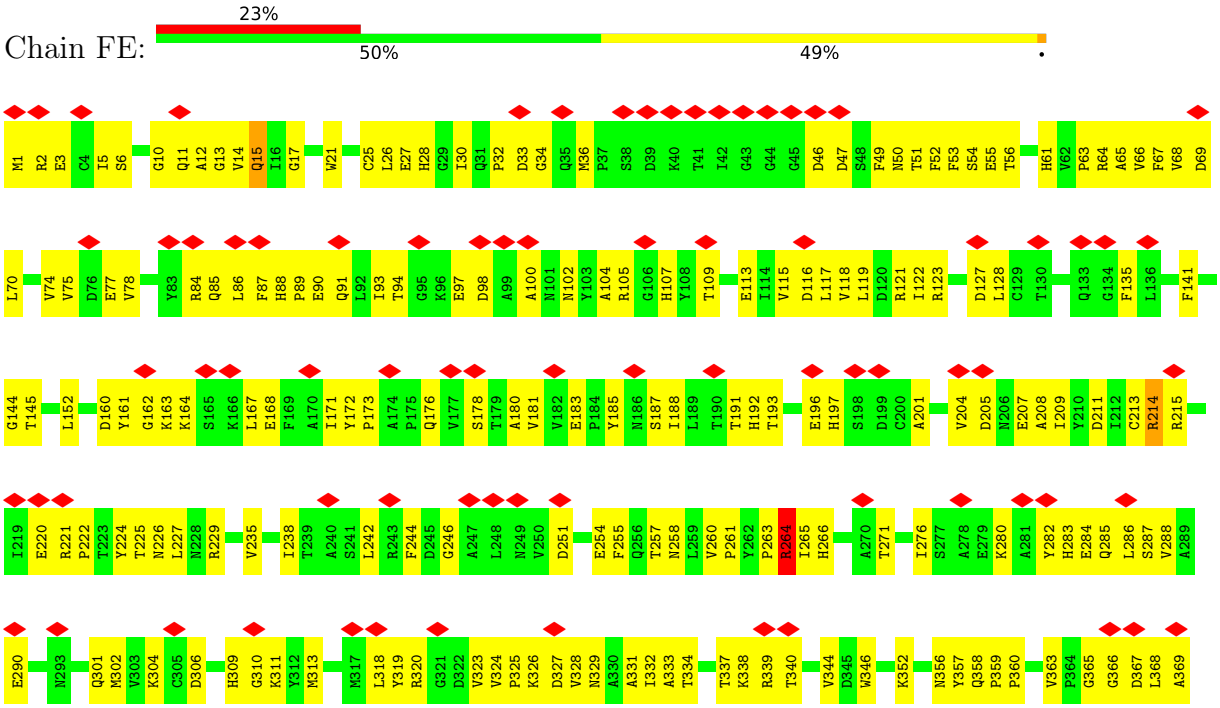
• Molecule 2: Detyrosinated tubulin alpha-3 chain

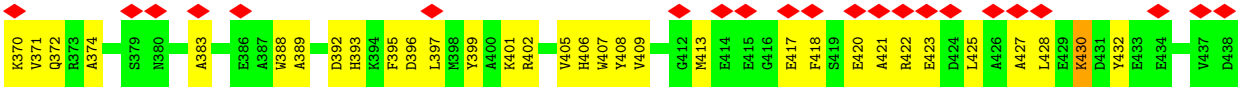
Chain EG:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

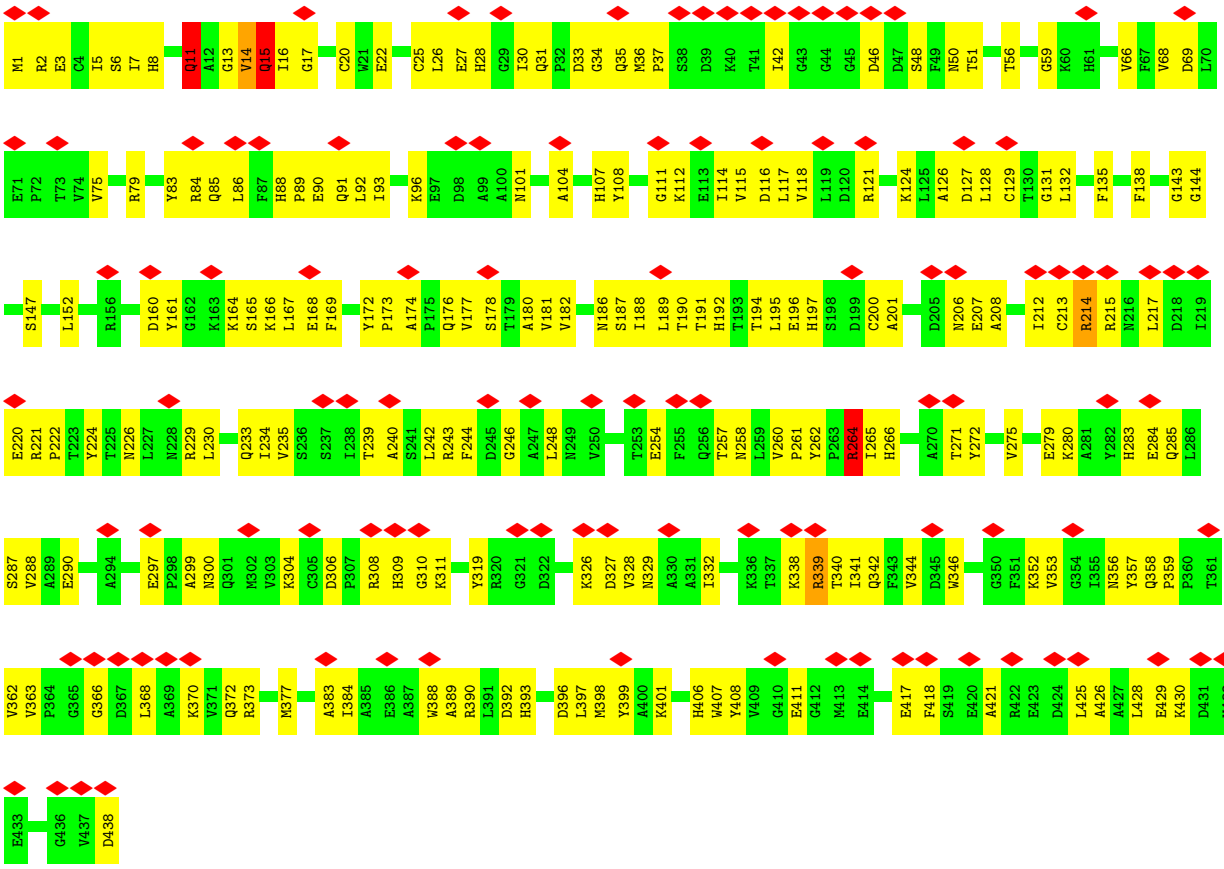
Chain FE:





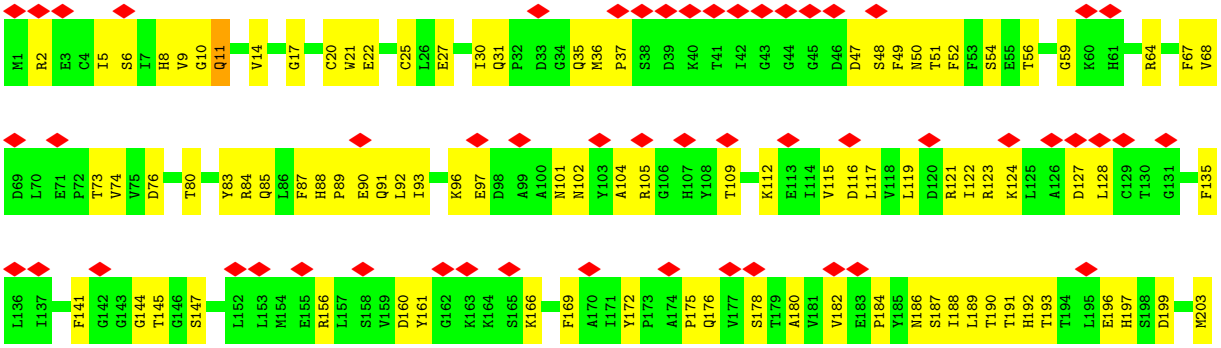
• Molecule 2: Detyrosinated tubulin alpha-3 chain

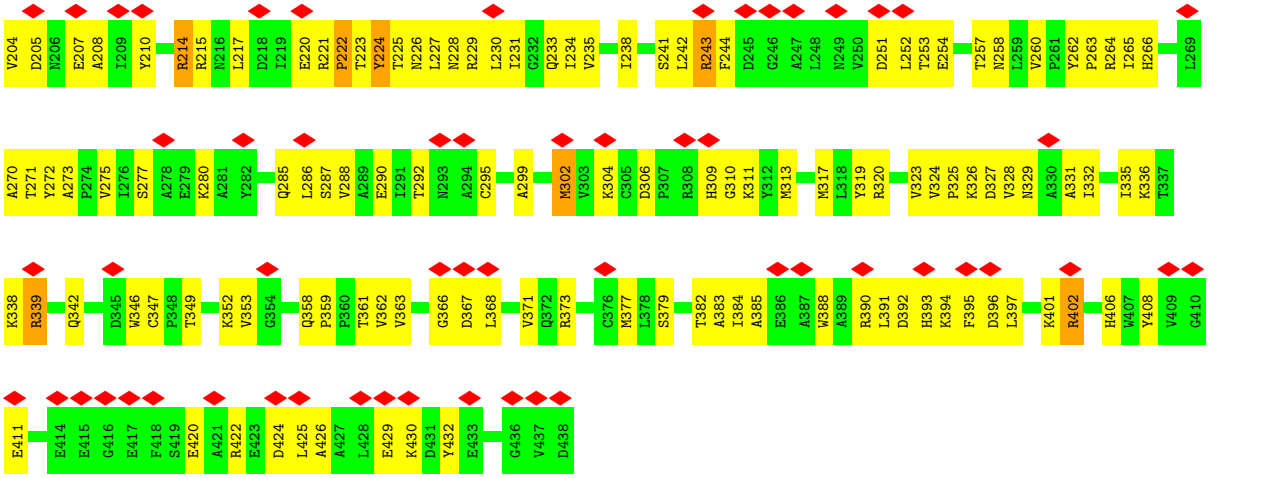
Chain FG:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

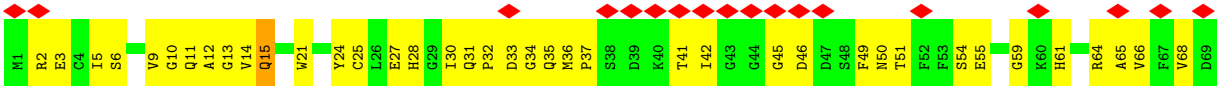
Chain GE:

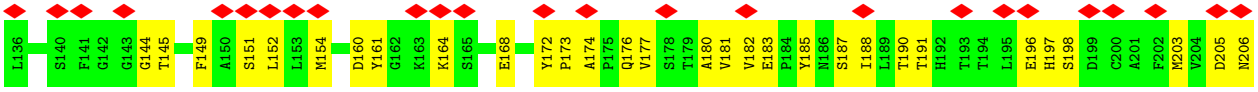


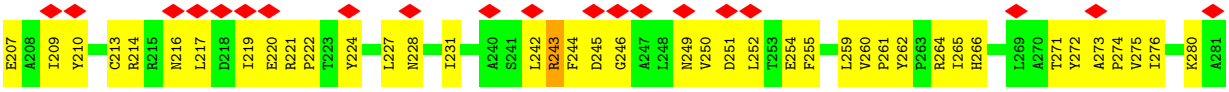


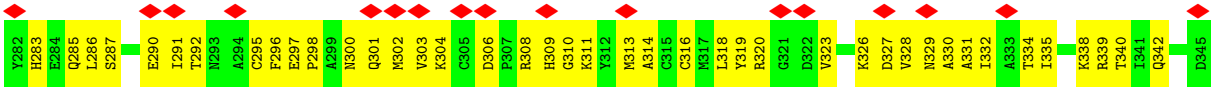
• Molecule 2: Detyrosinated tubulin alpha-3 chain

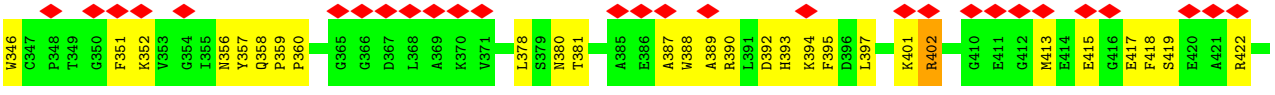
Chain GG:

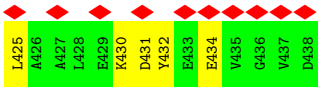






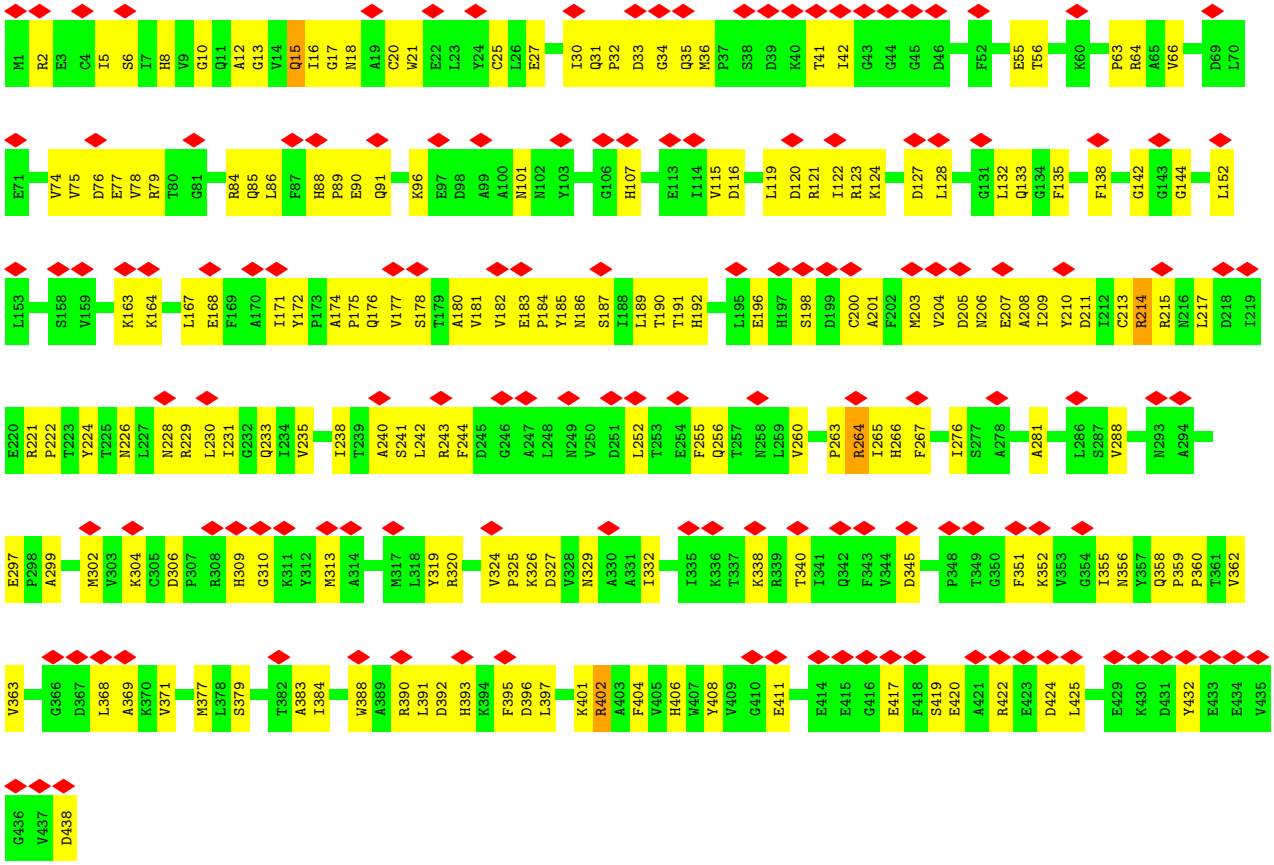






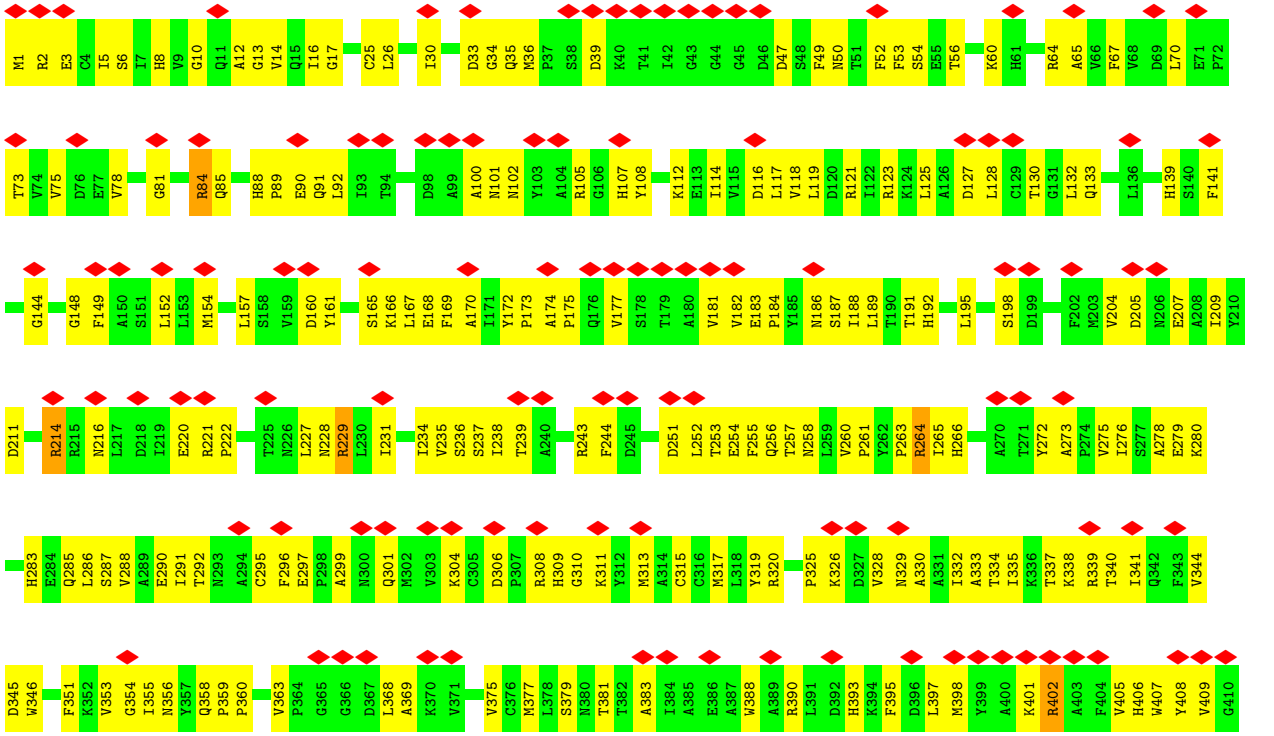
• Molecule 2: Detyrosinated tubulin alpha-3 chain

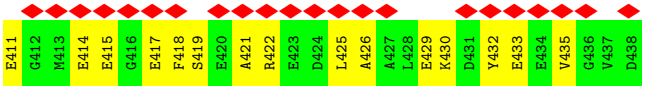
Chain GI:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain HE:



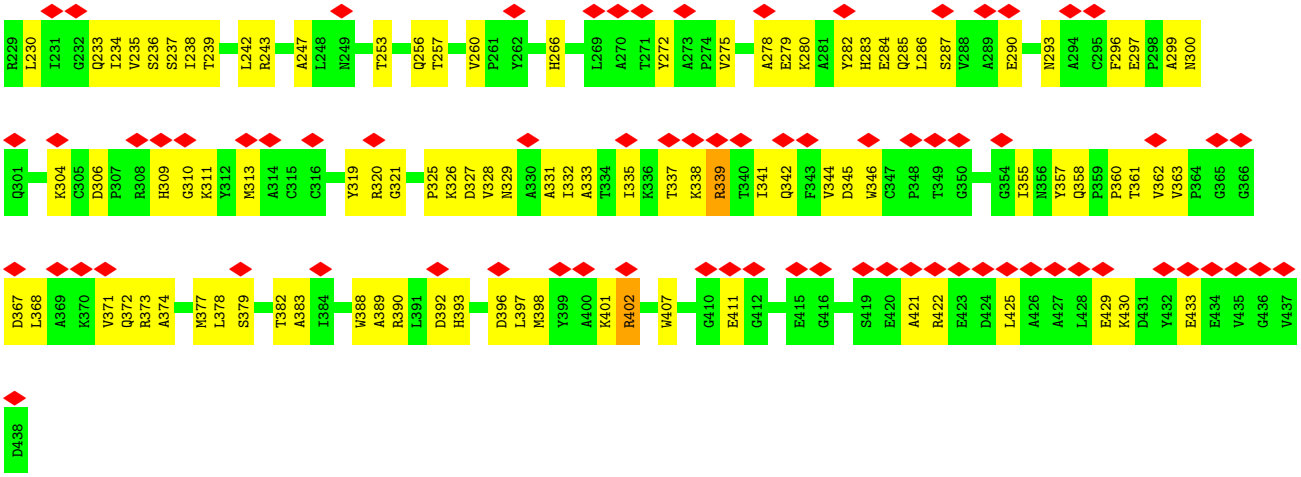


• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain HG:

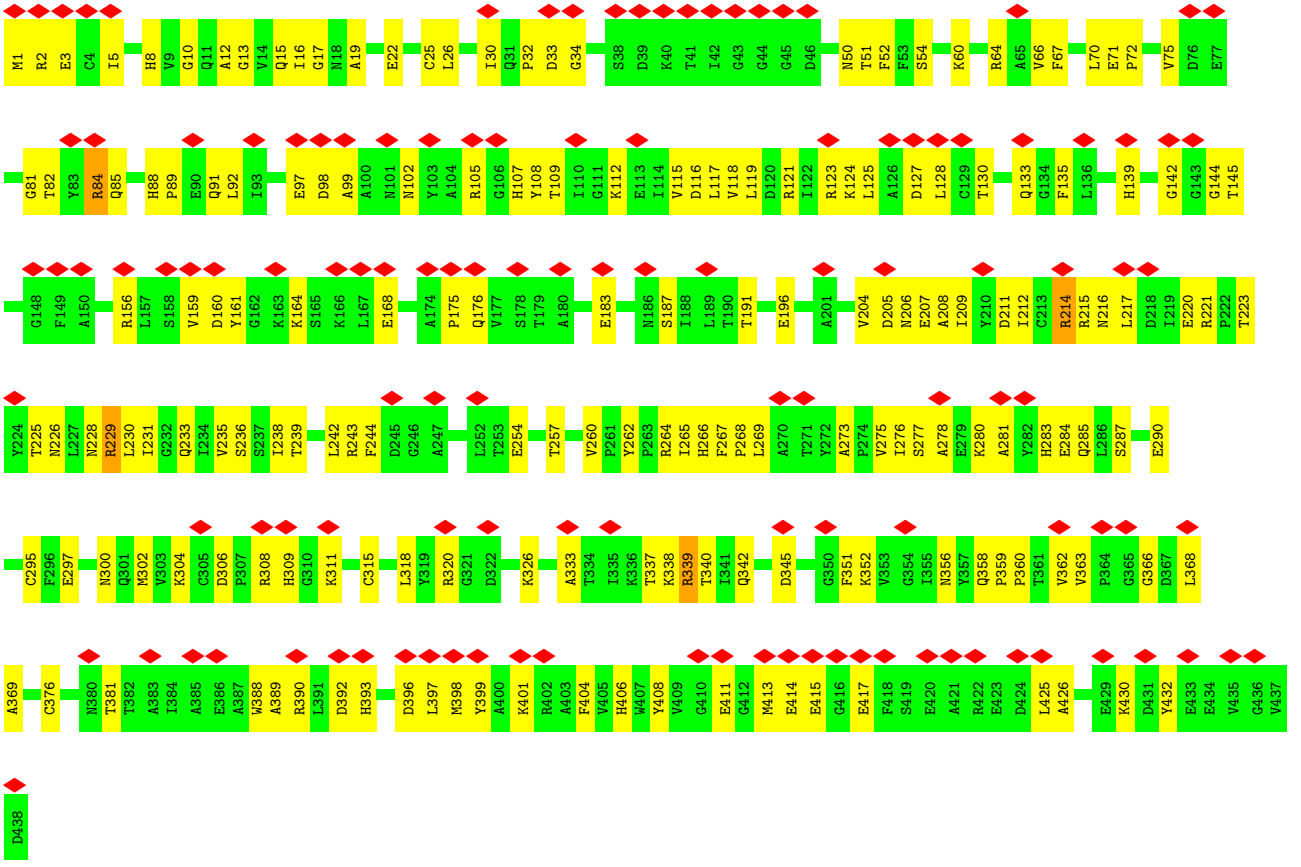
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain HI:



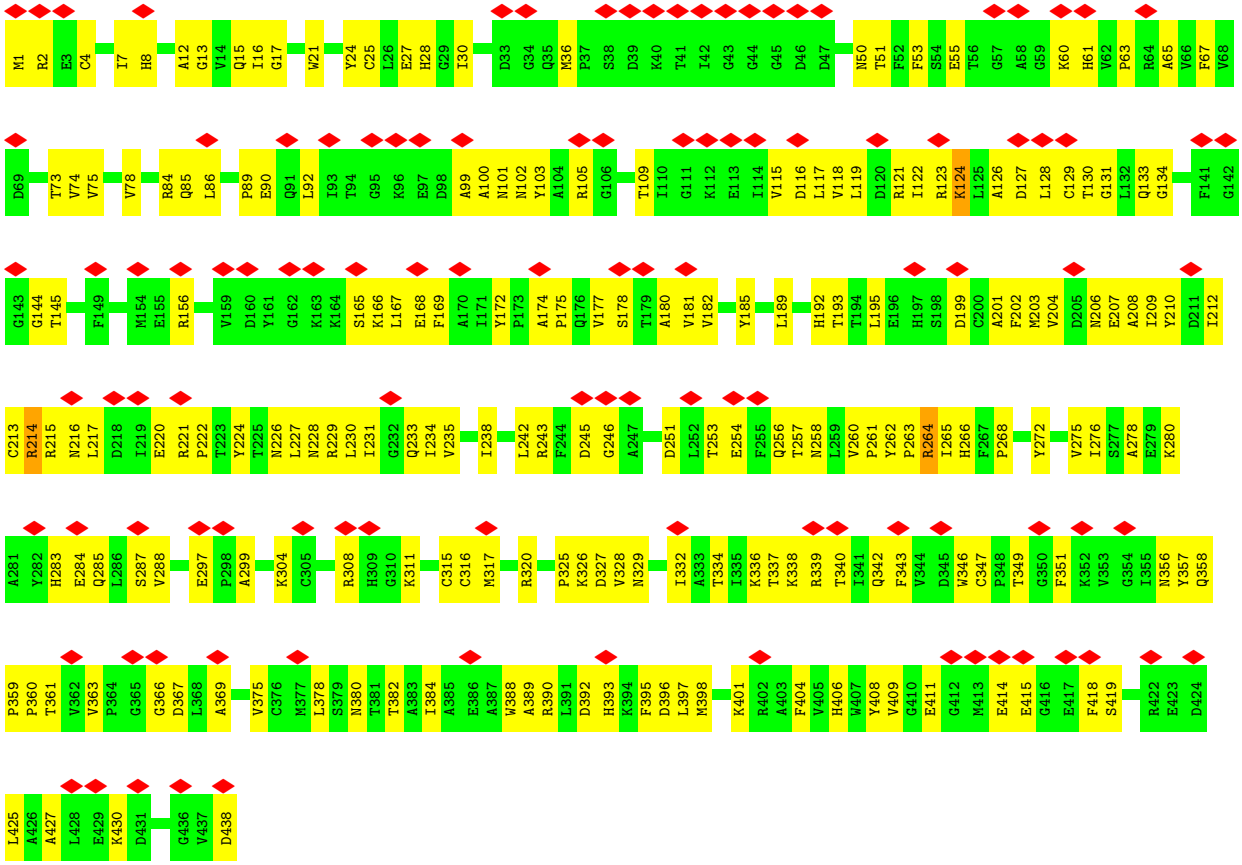
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain IE:



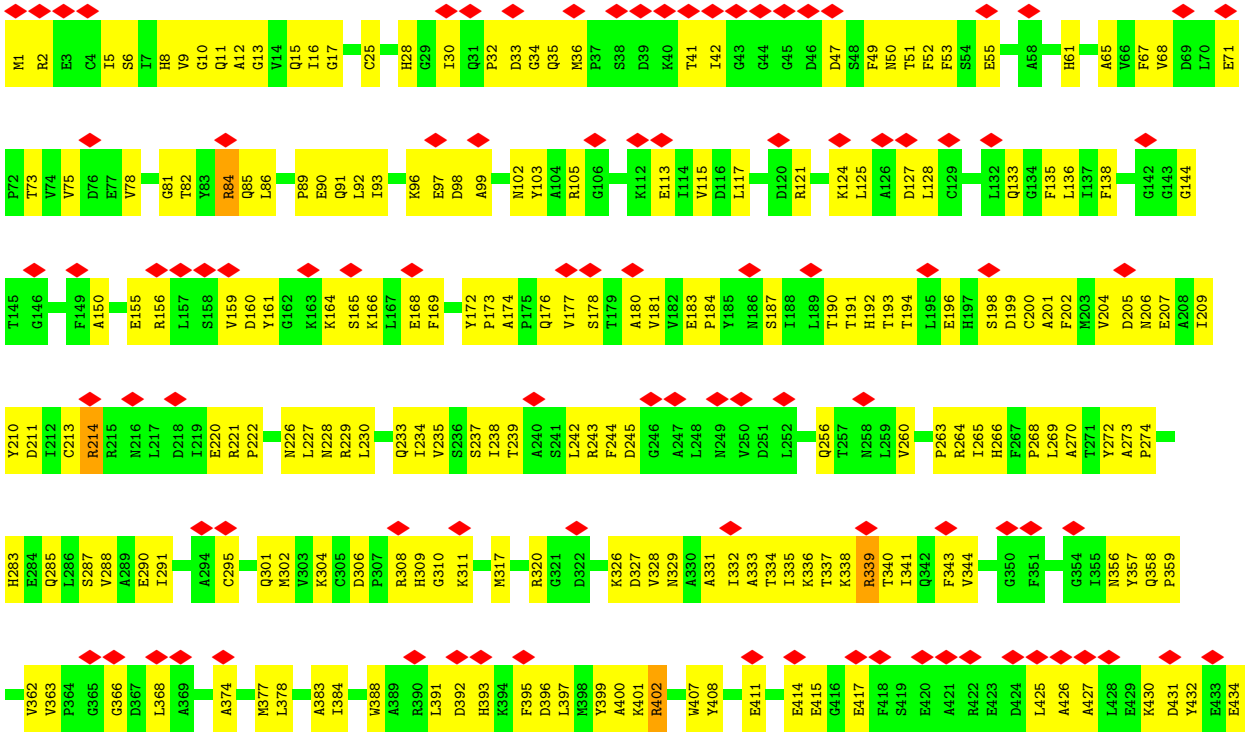
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain IG:



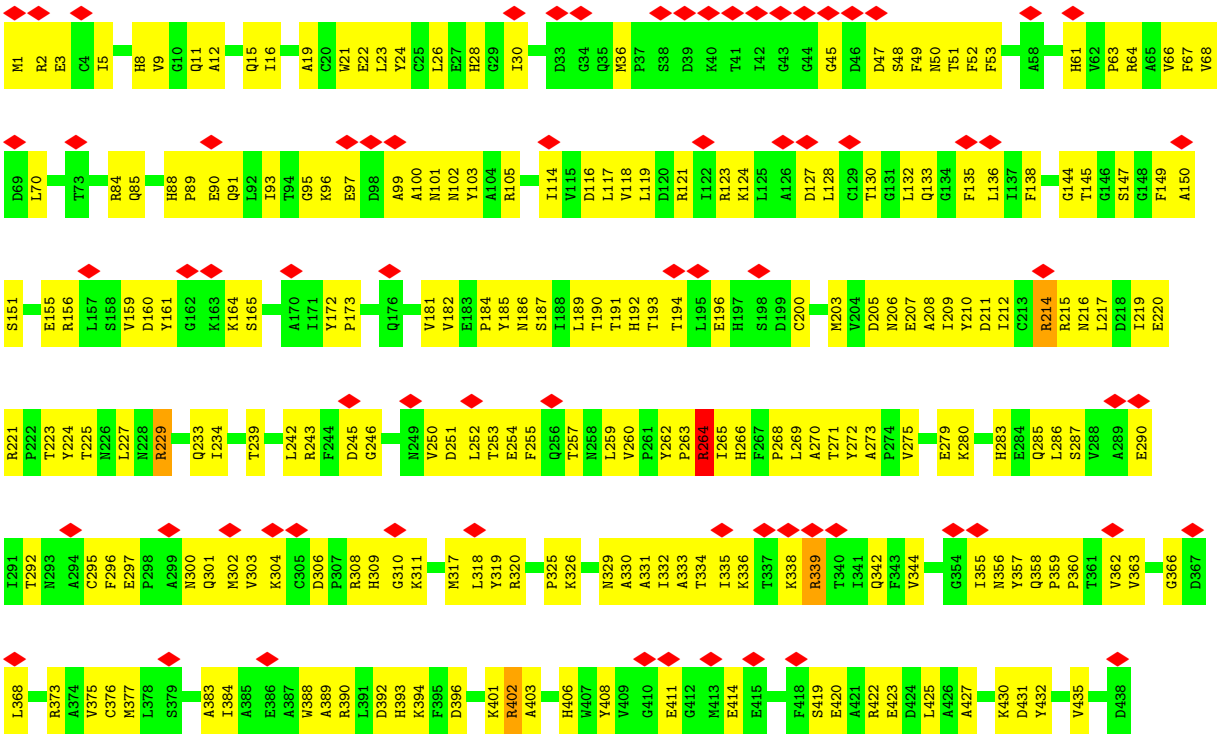
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain II:



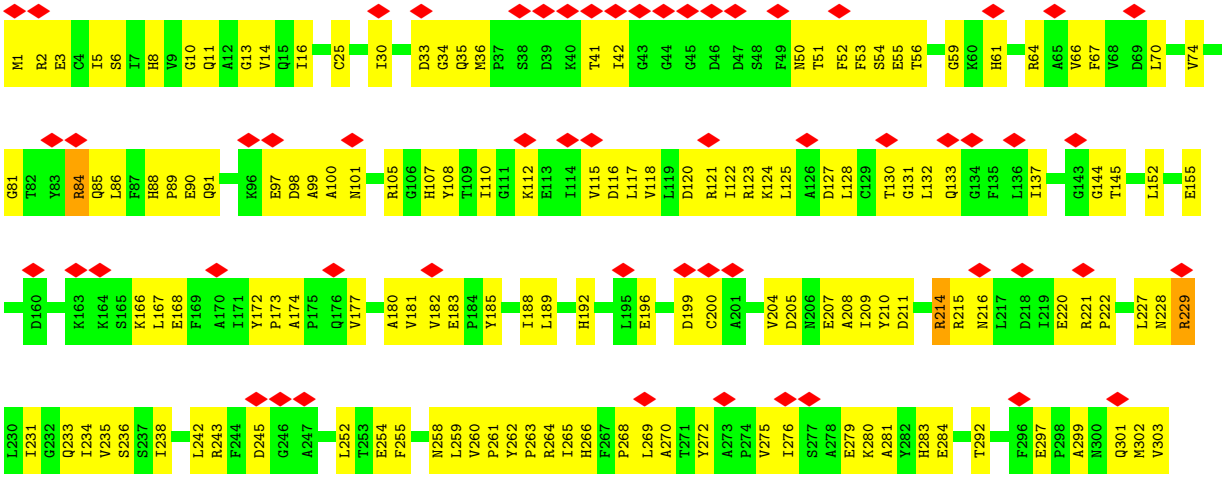
• Molecule 2: Detyrosinated tubulin alpha-3 chain

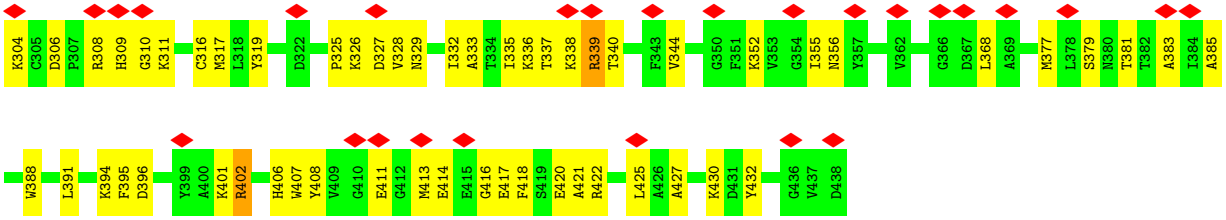
Chain JE:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

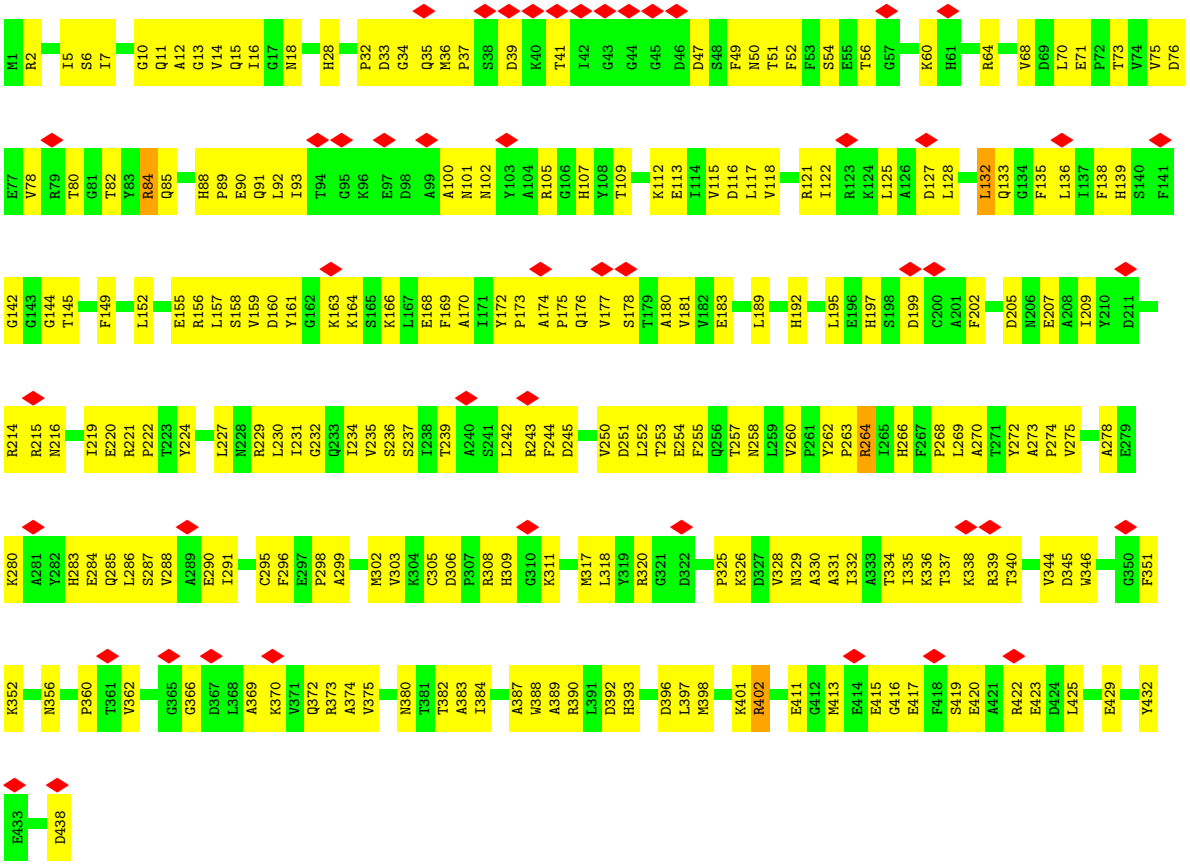
Chain JG:





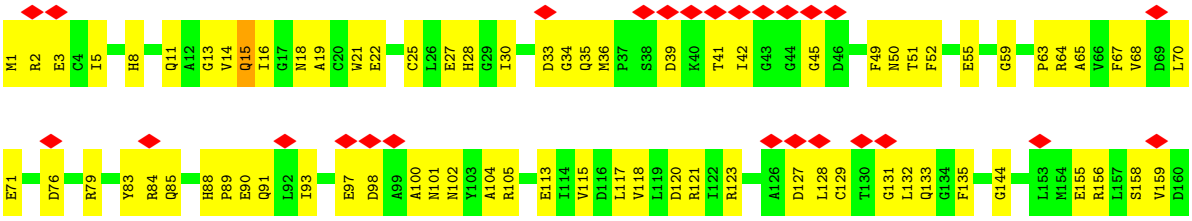
• Molecule 2: Detyrosinated tubulin alpha-3 chain

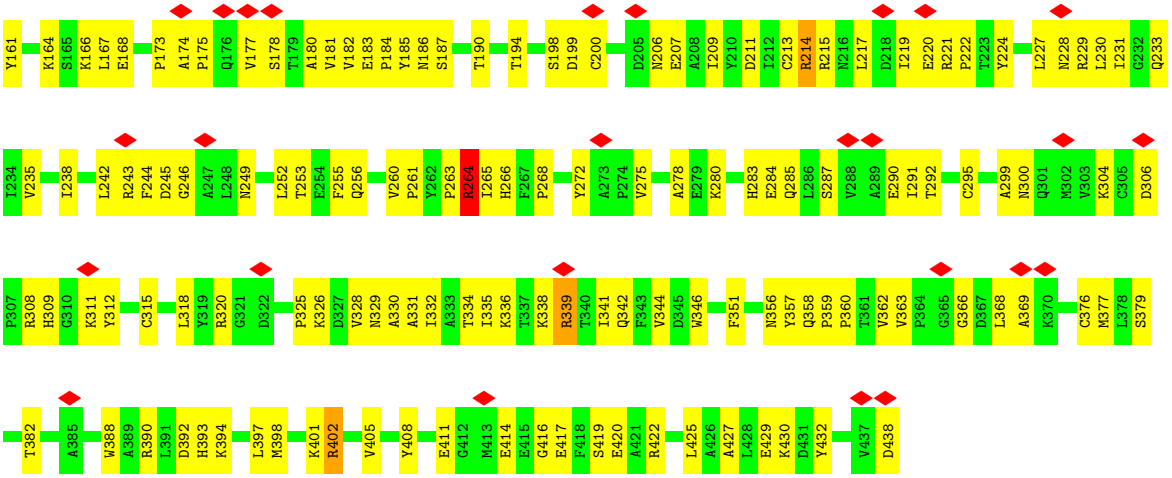
Chain KE:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

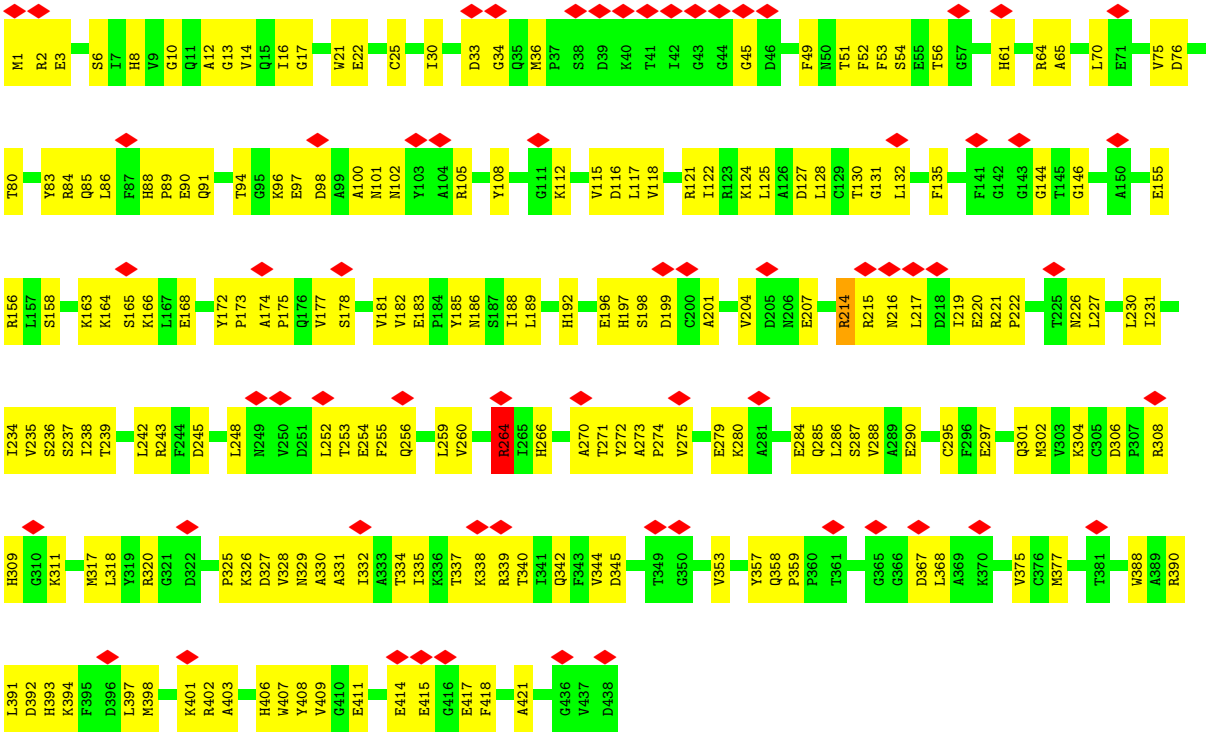
Chain KG:





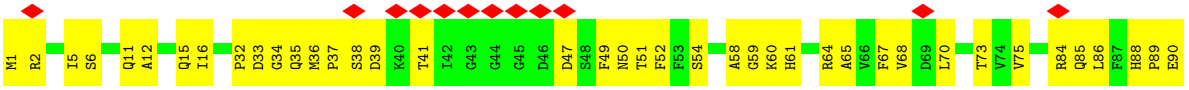
• Molecule 2: Detyrosinated tubulin alpha-3 chain

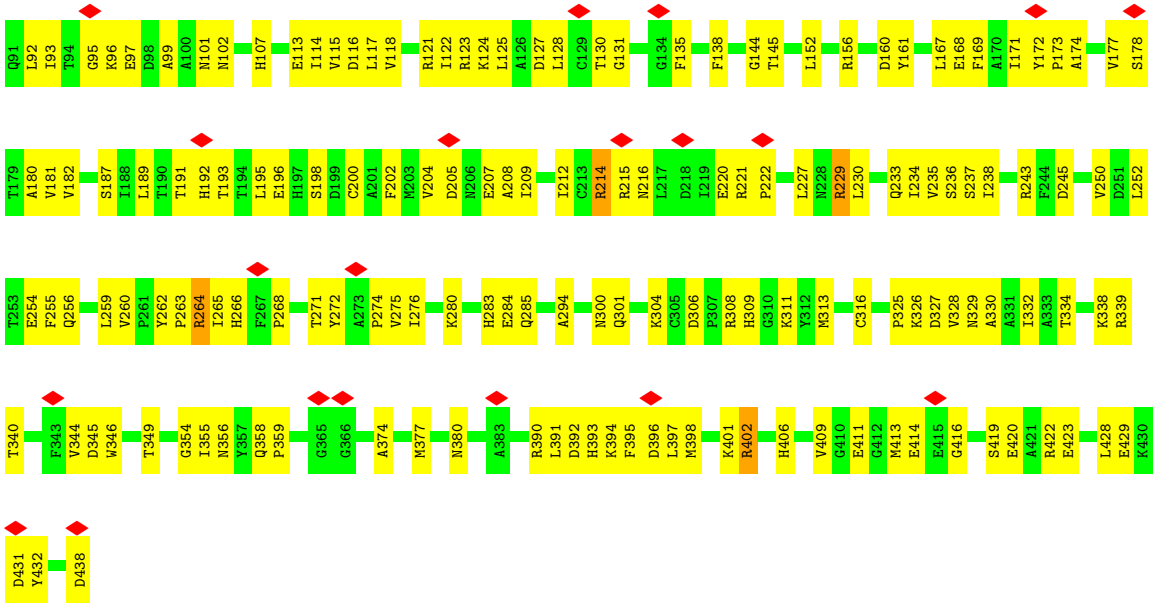
Chain KI:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

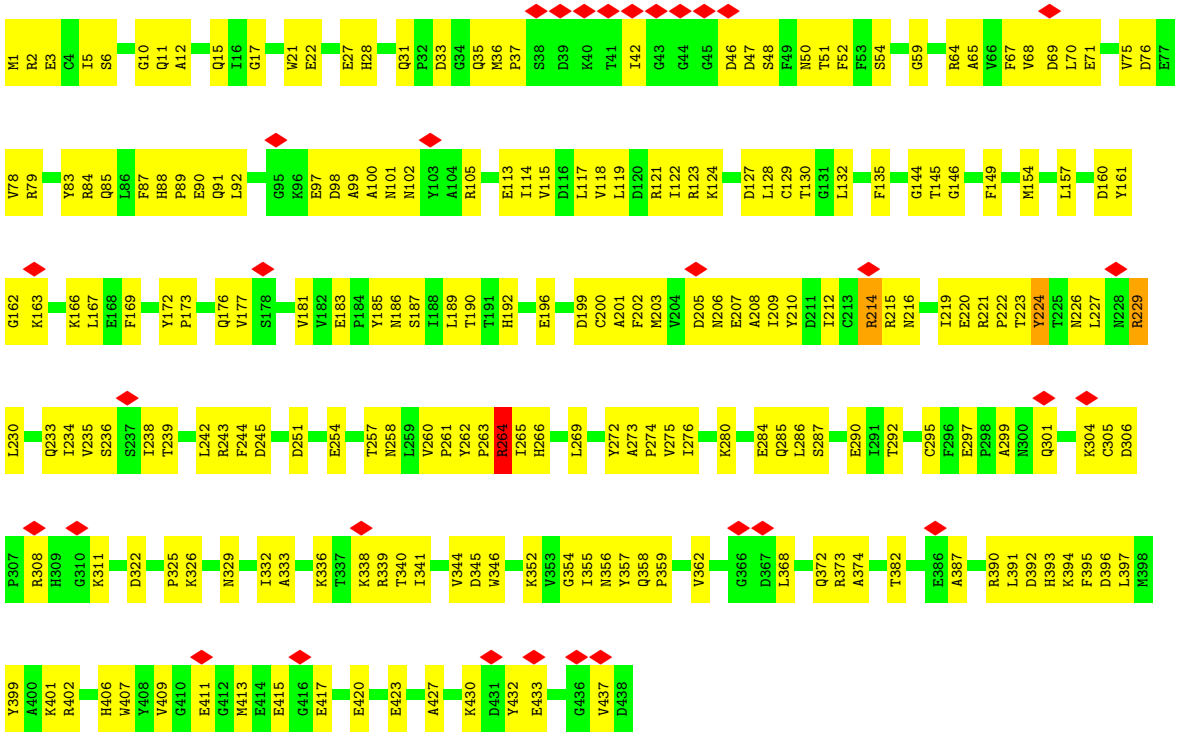
Chain LE:





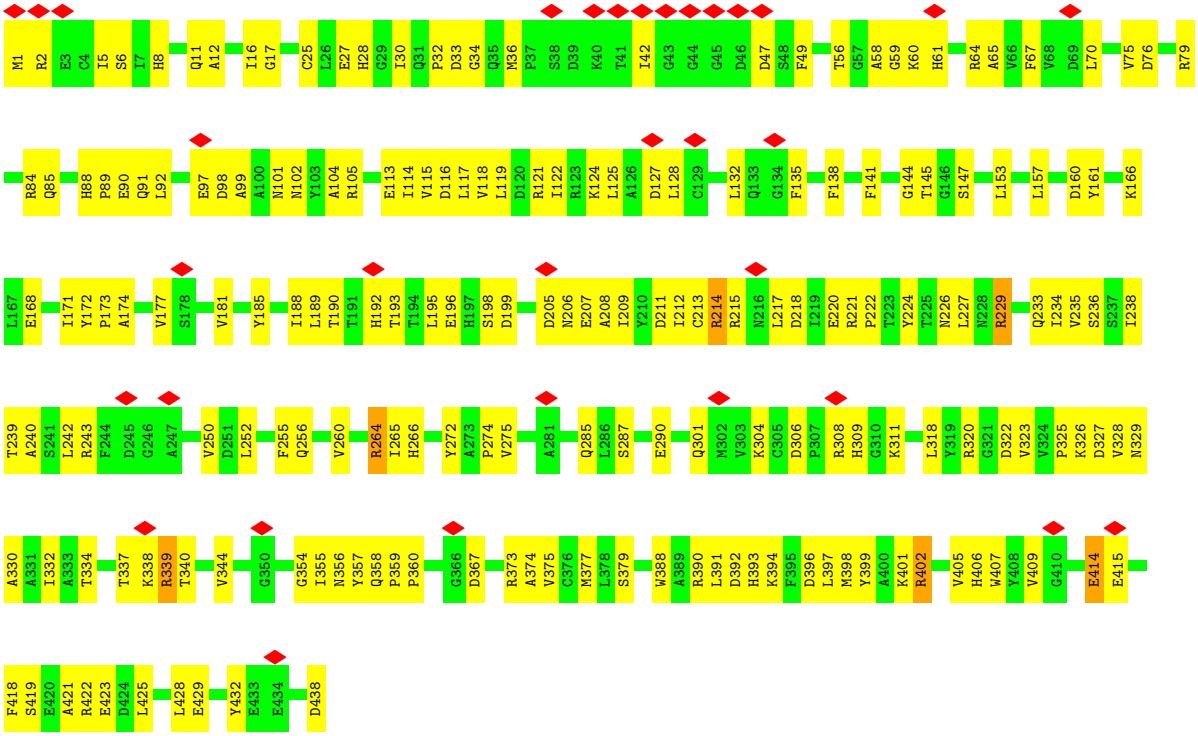
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain LG:



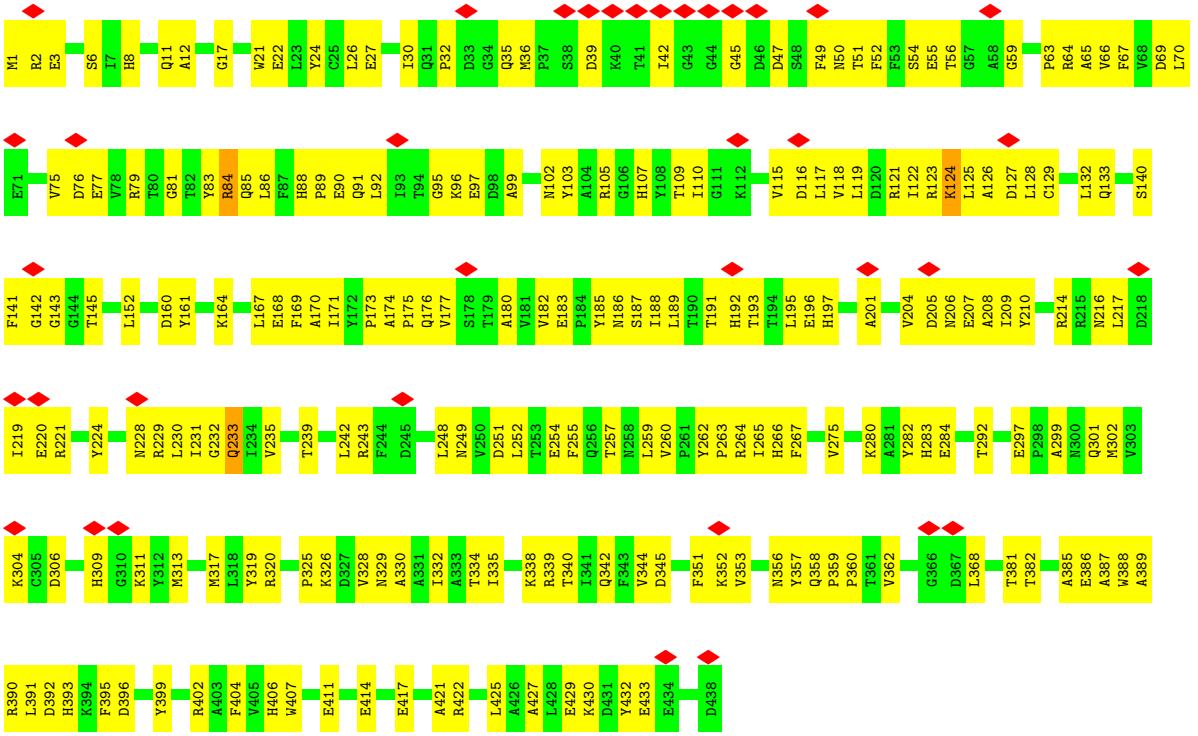
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain LI:



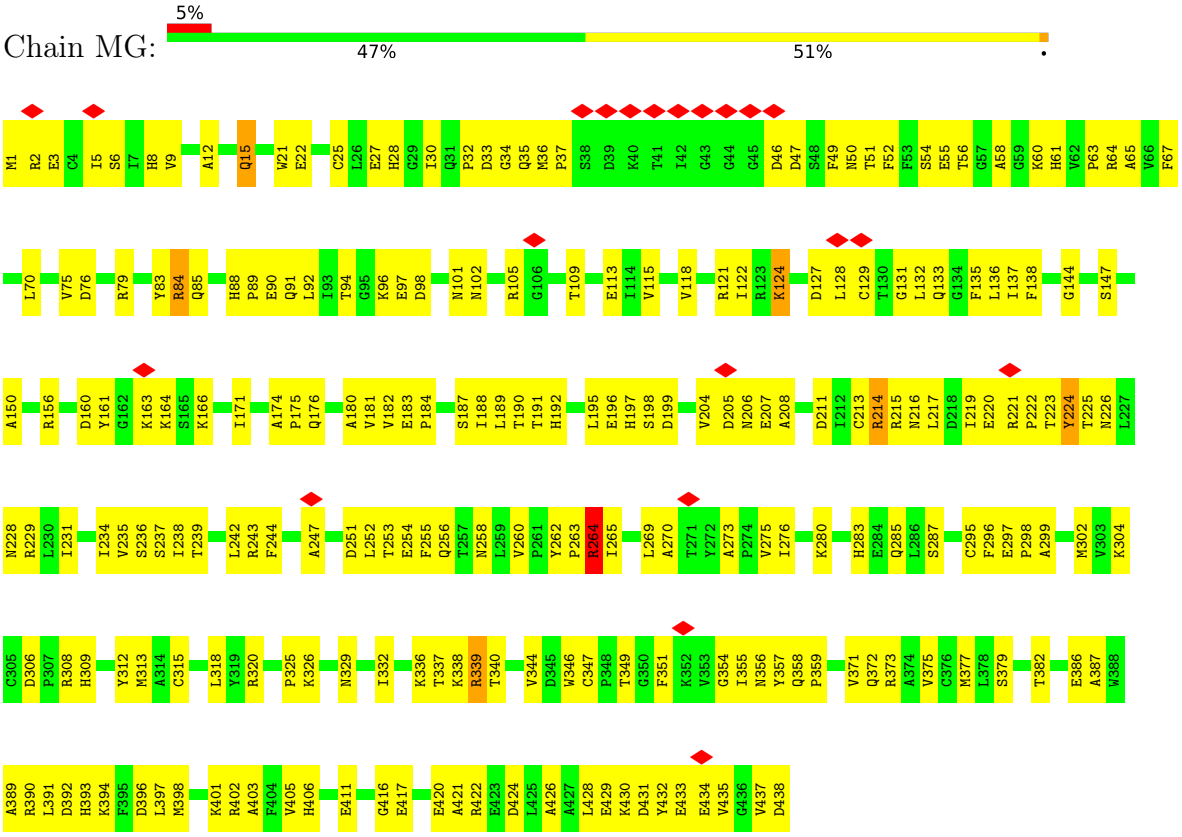
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain ME:



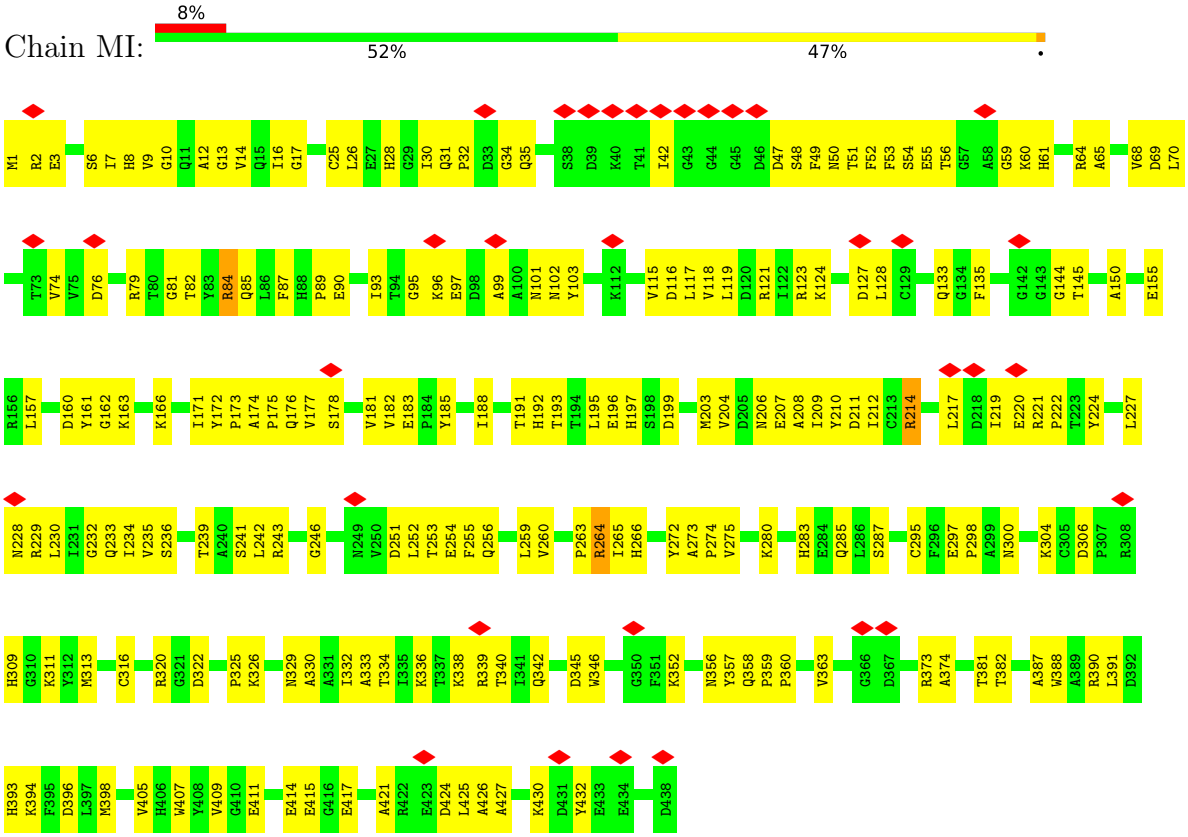
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain MG:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain MI:

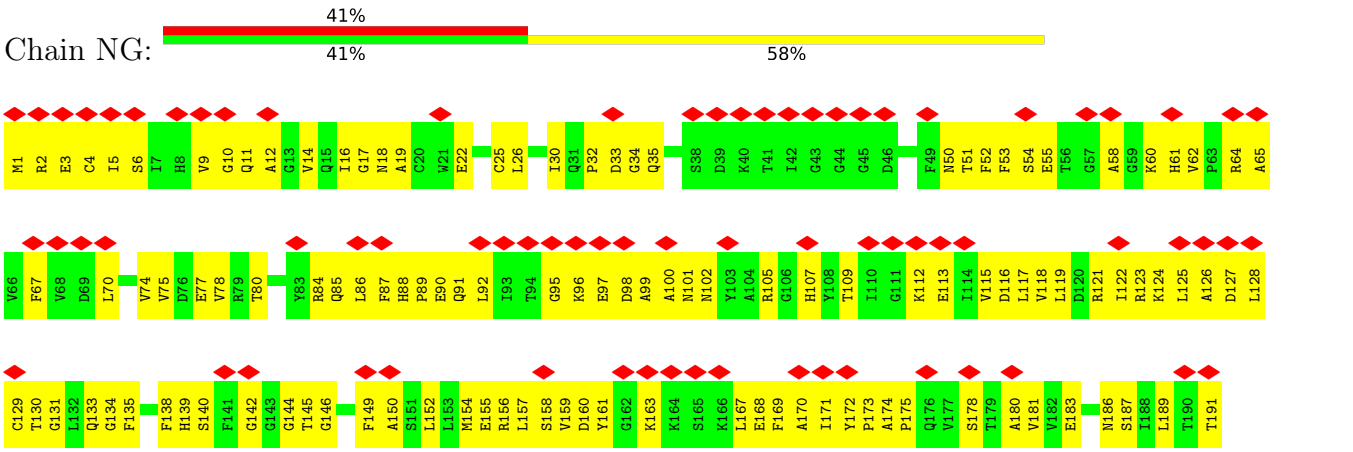


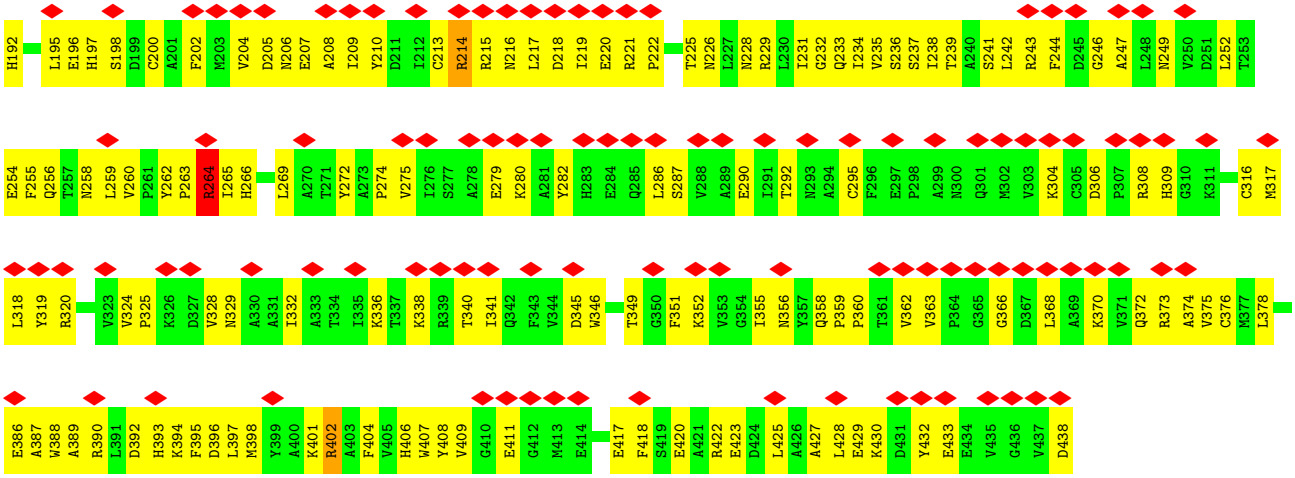
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain NE:

• Molecule 2: Detyrosinated tubulin alpha-3 chain

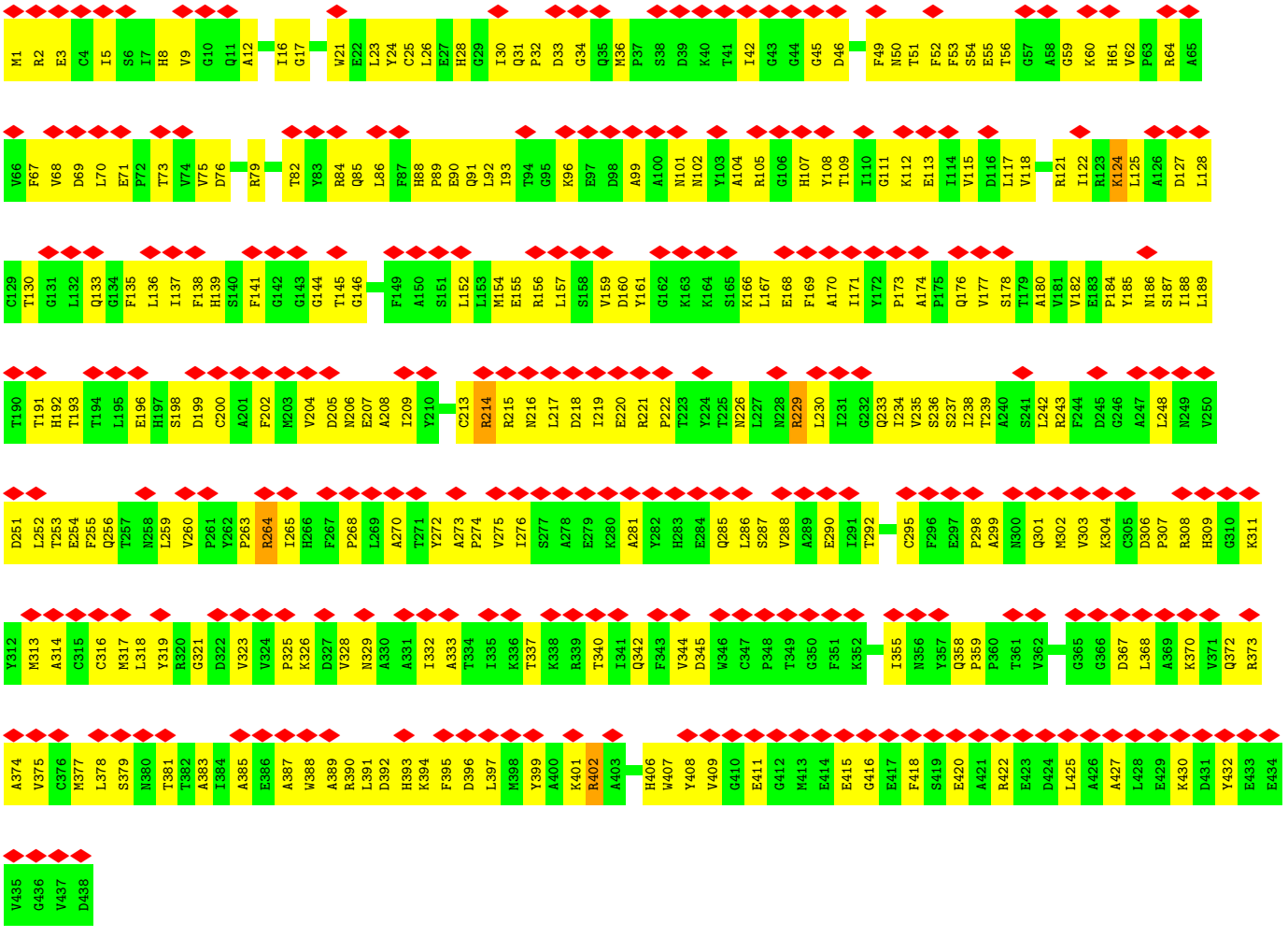
Chain NG:





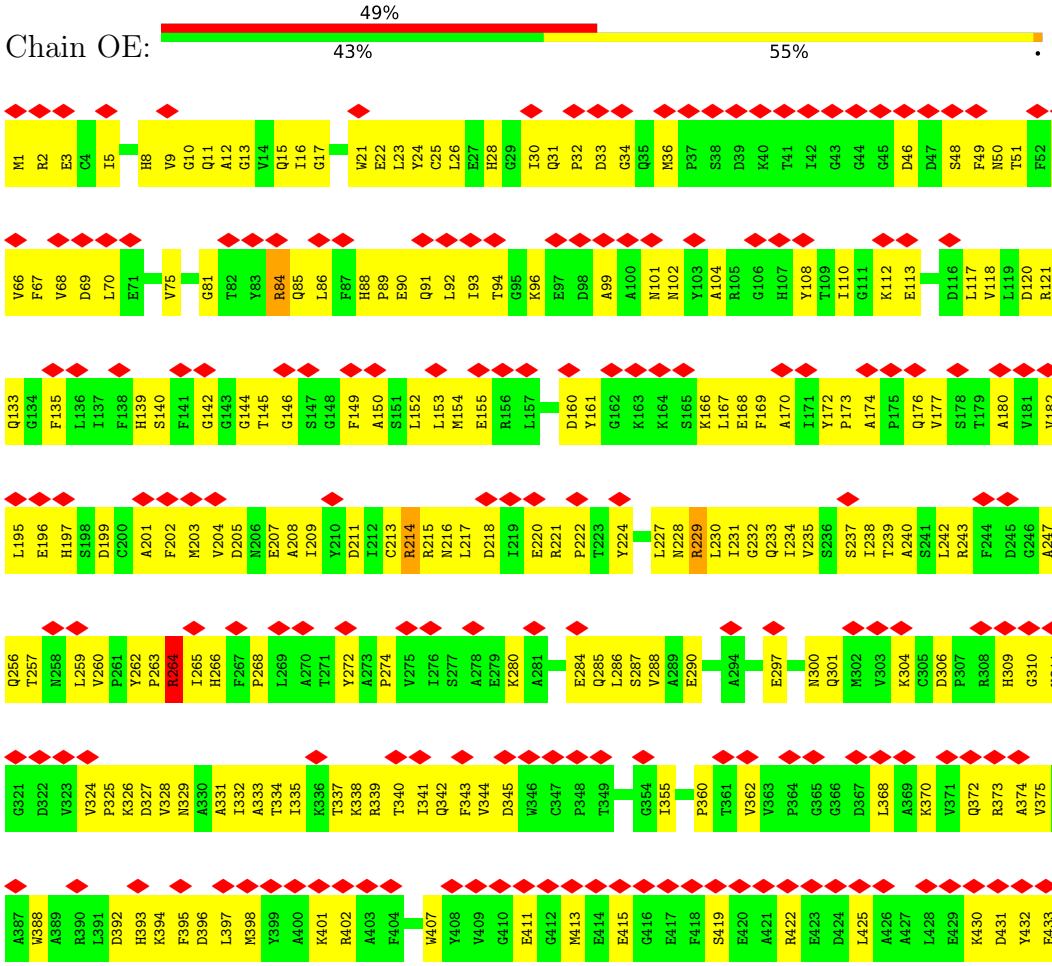
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain NI:



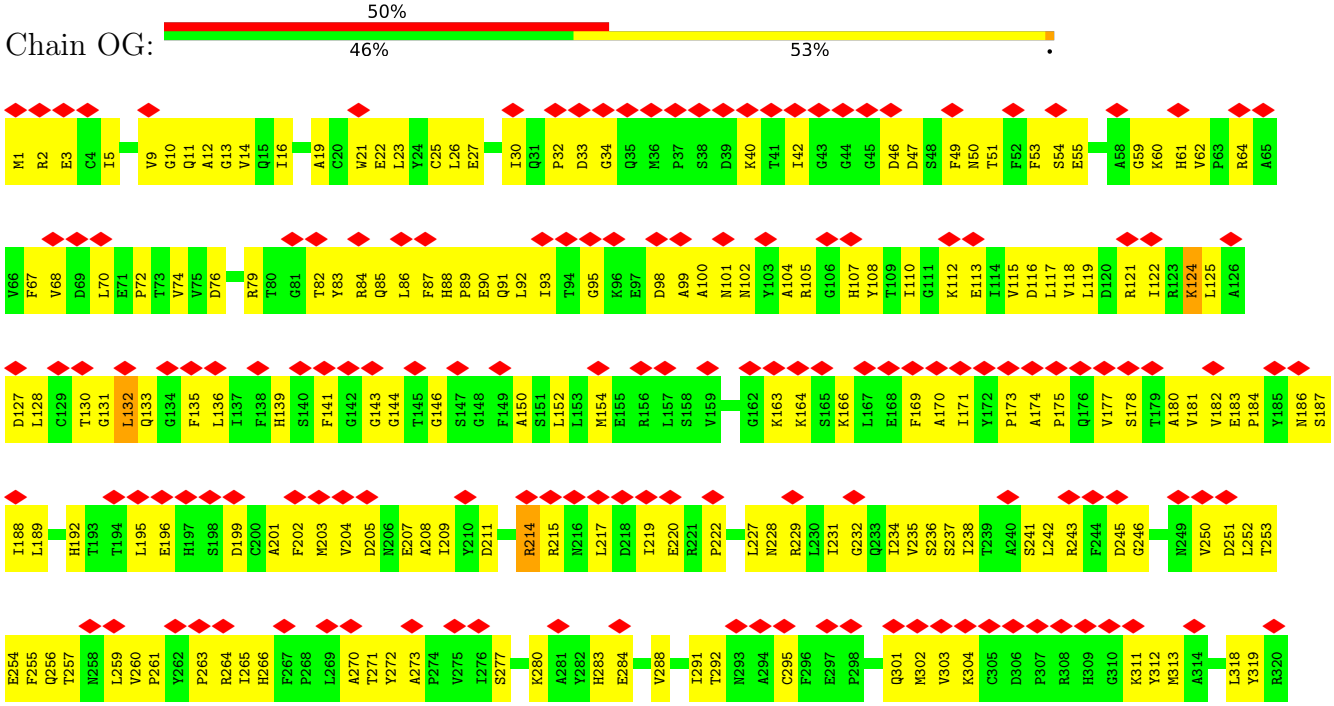
• Molecule 2: Detyrosinated tubulin alpha-3 chain

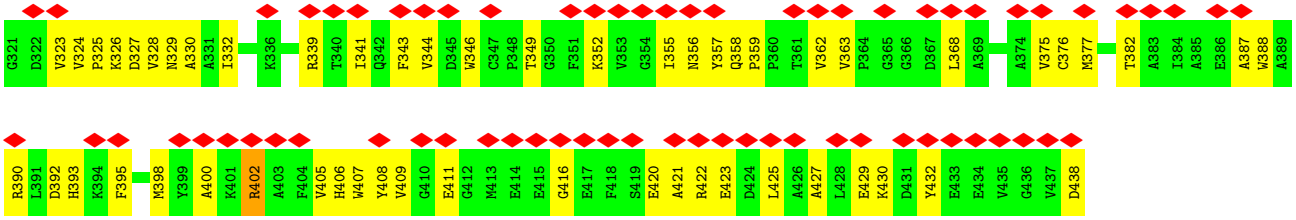
Chain OE:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

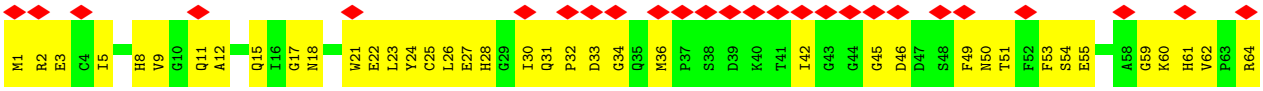
Chain OG:

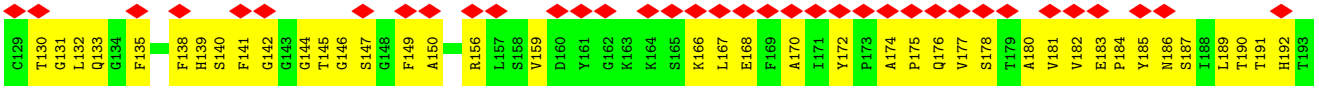


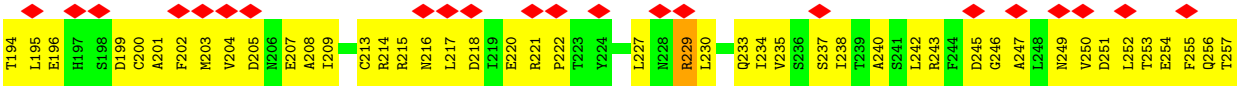


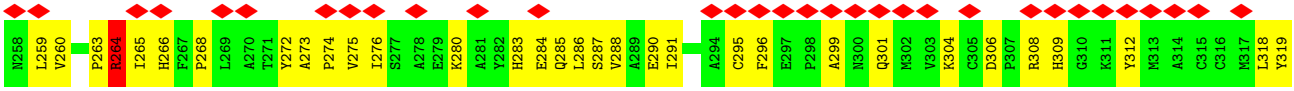
• Molecule 2: Detyrosinated tubulin alpha-3 chain

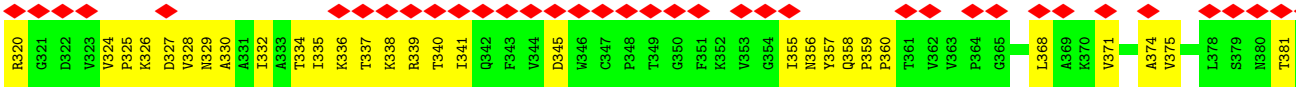
Chain OI:

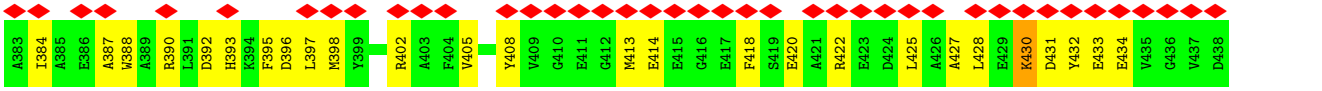


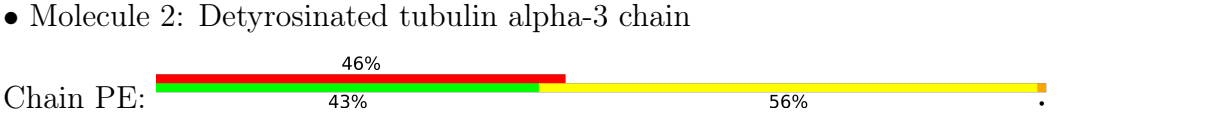






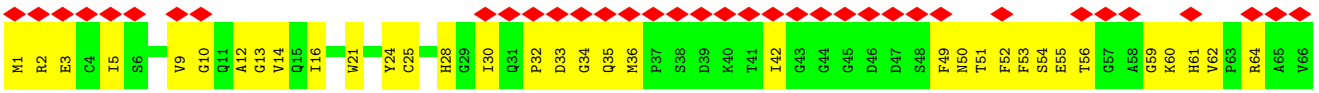


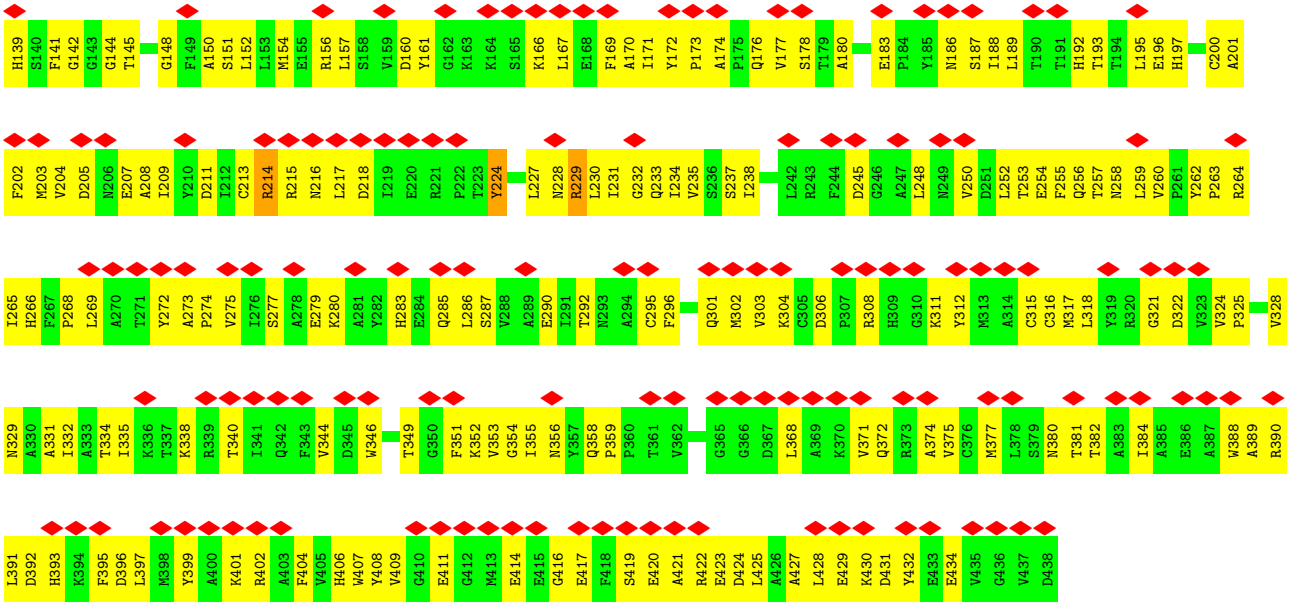




• Molecule 2: Detyrosinated tubulin alpha-3 chain

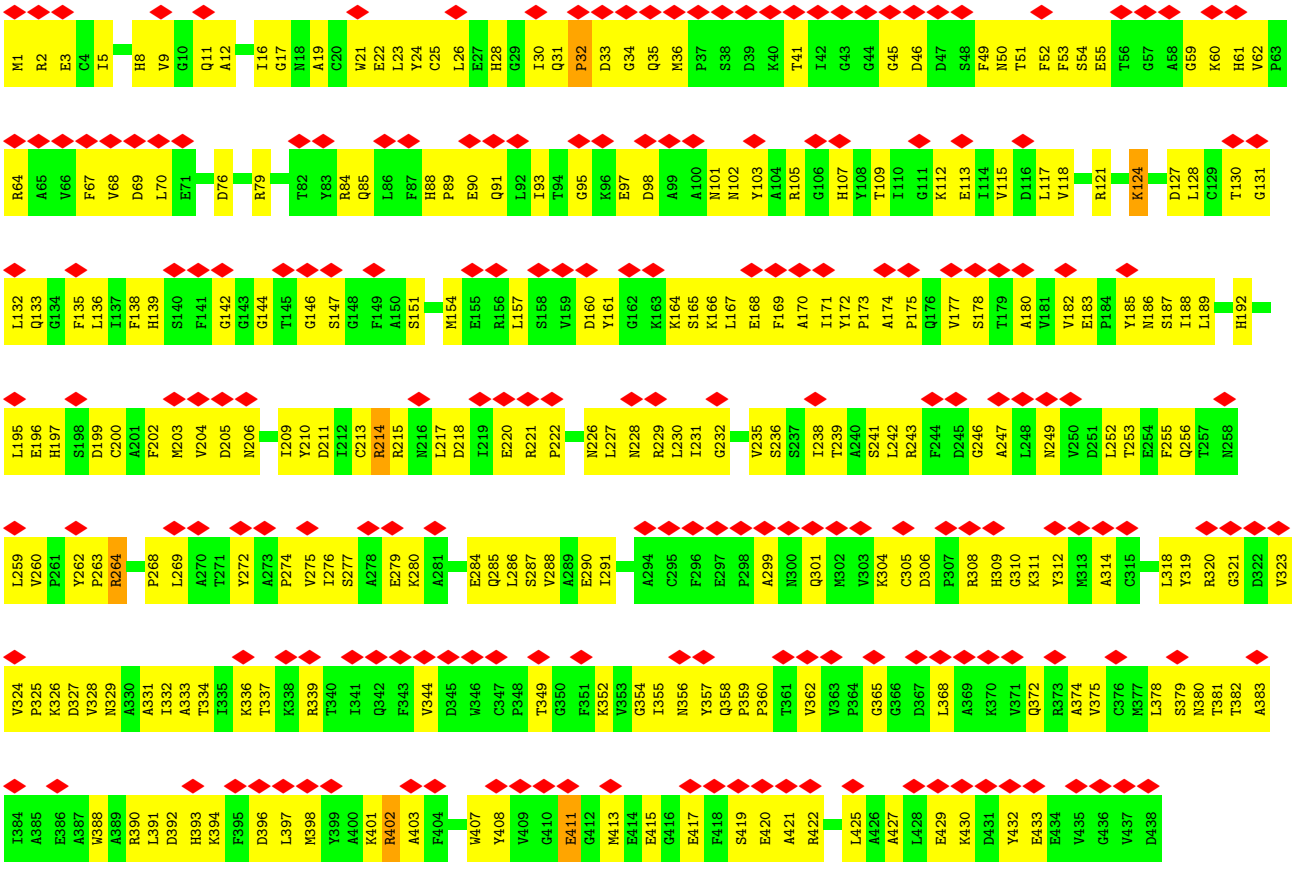
Chain PE:





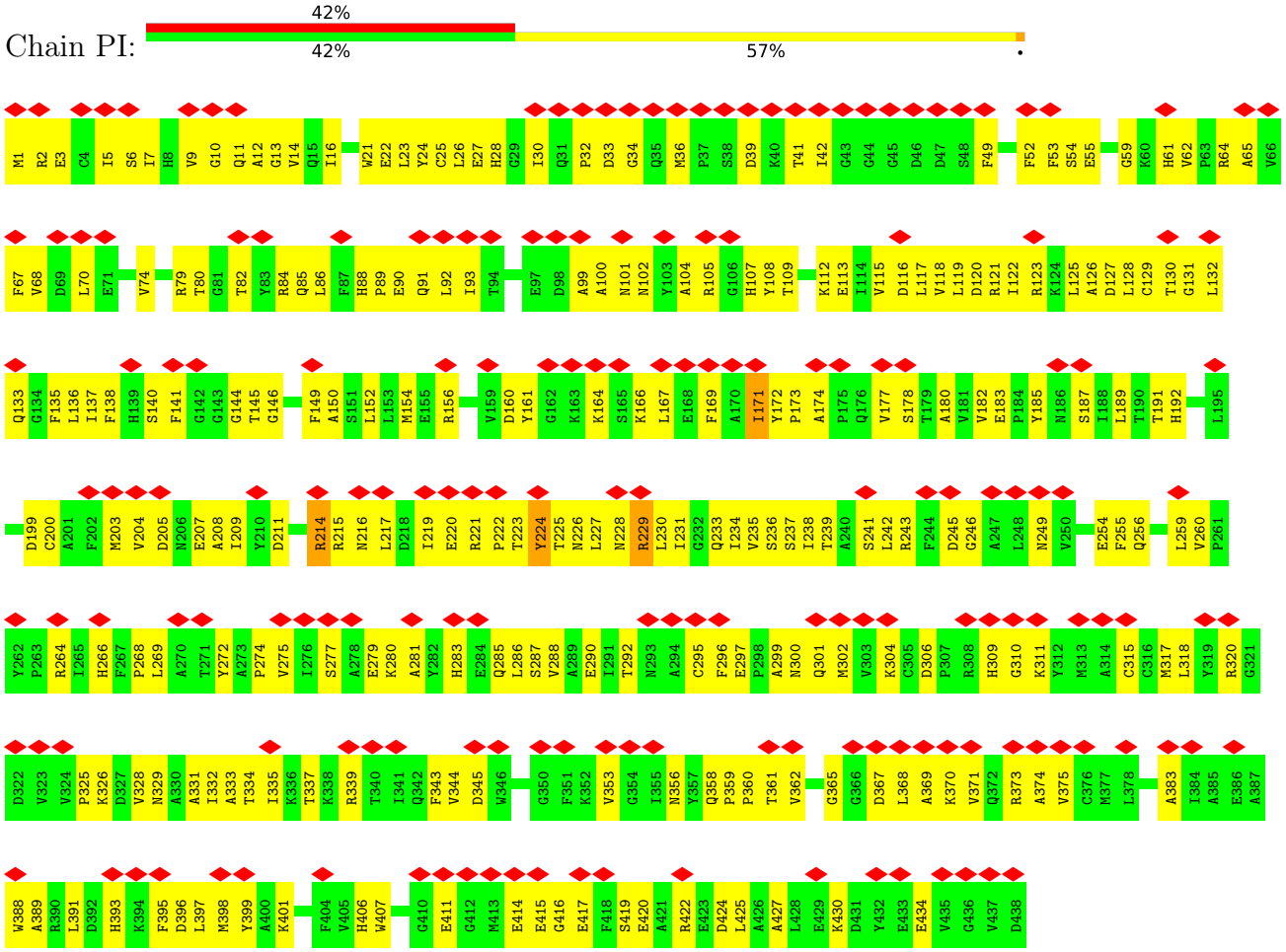
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain PG:



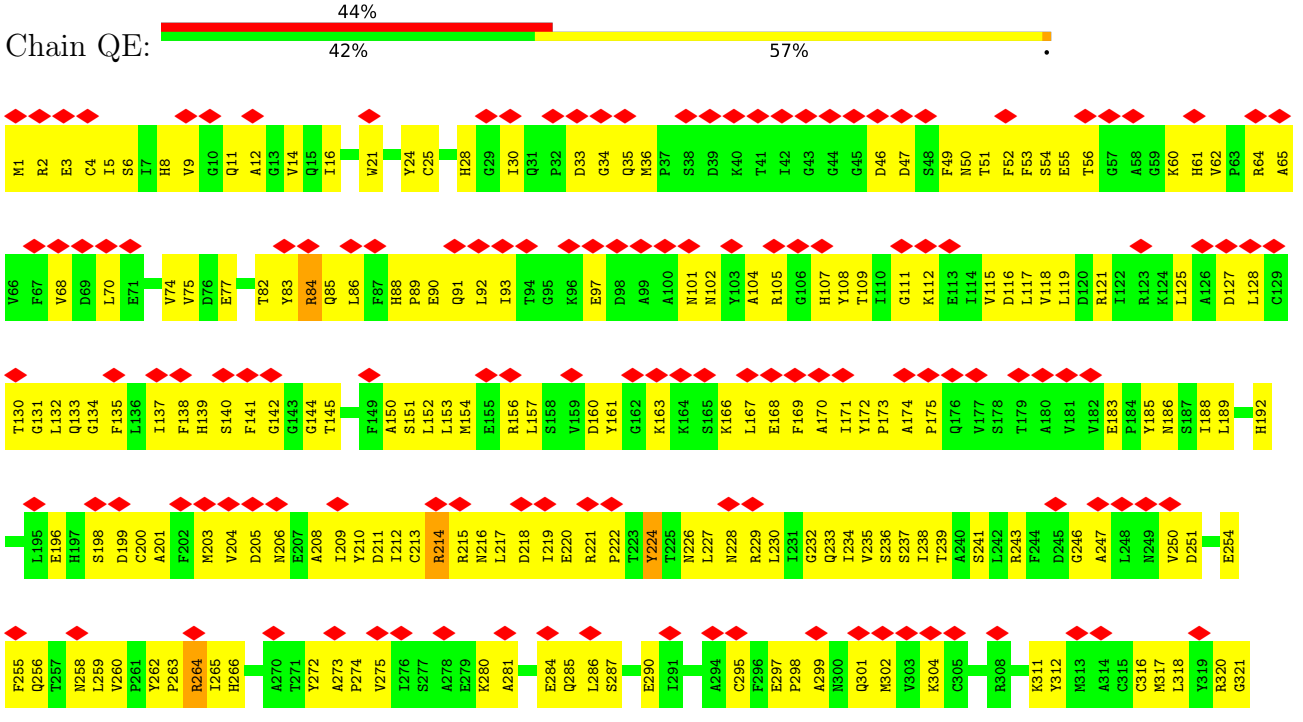
• Molecule 2: Detyrosinated tubulin alpha-3 chain

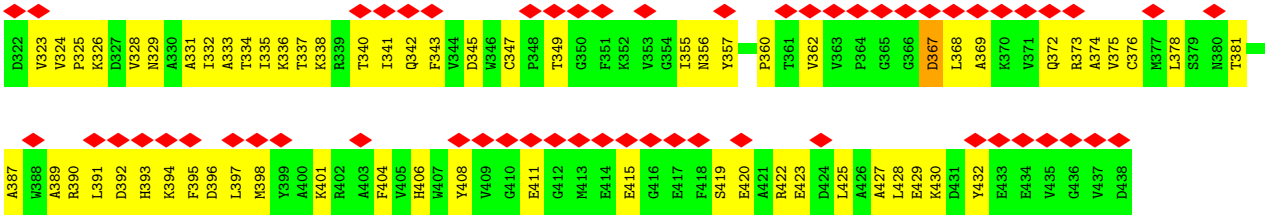
Chain PI:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

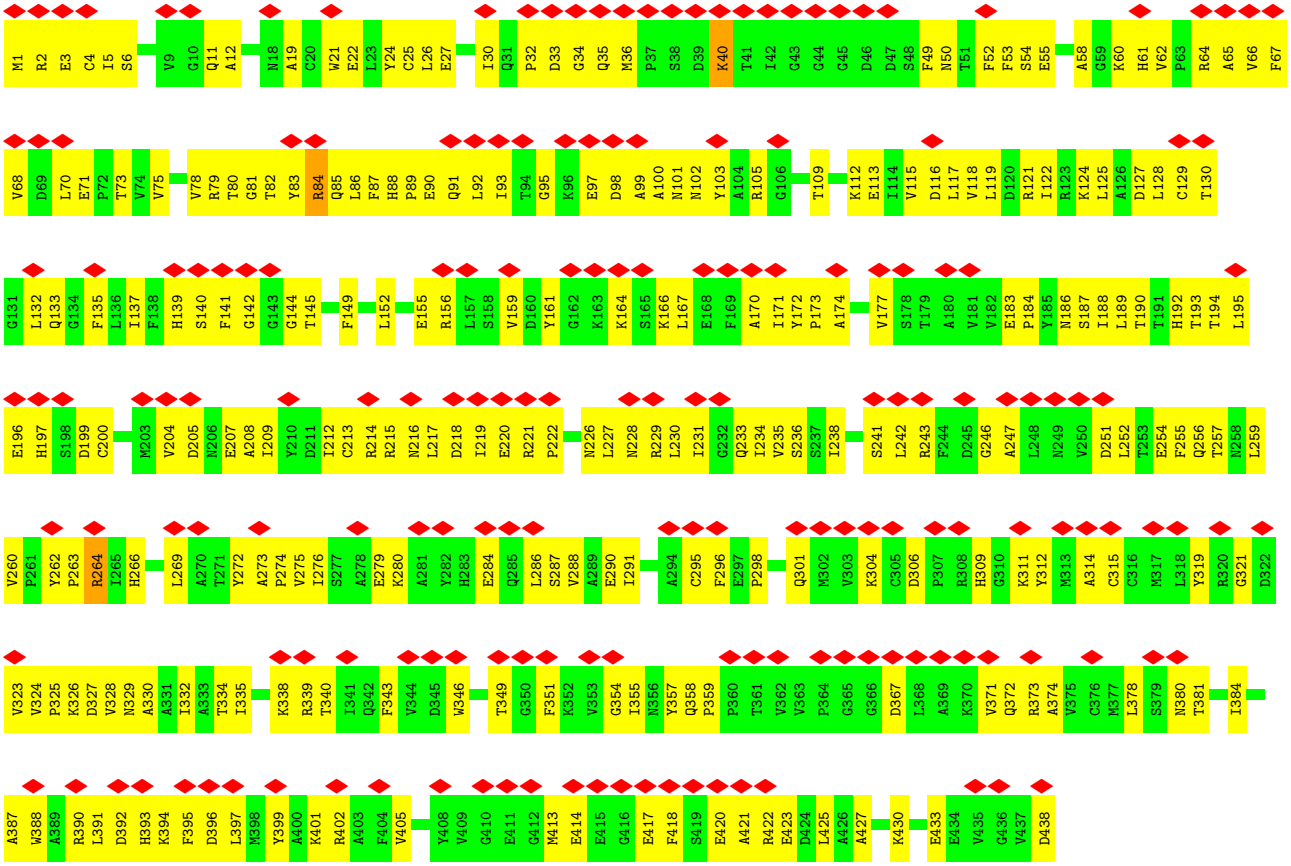
Chain QE:





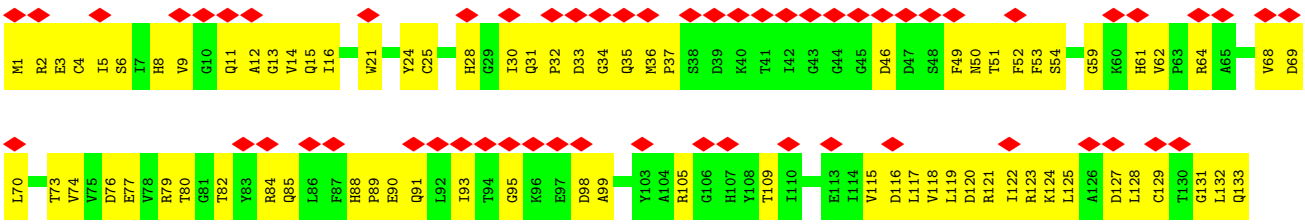
• Molecule 2: Detyrosinated tubulin alpha-3 chain

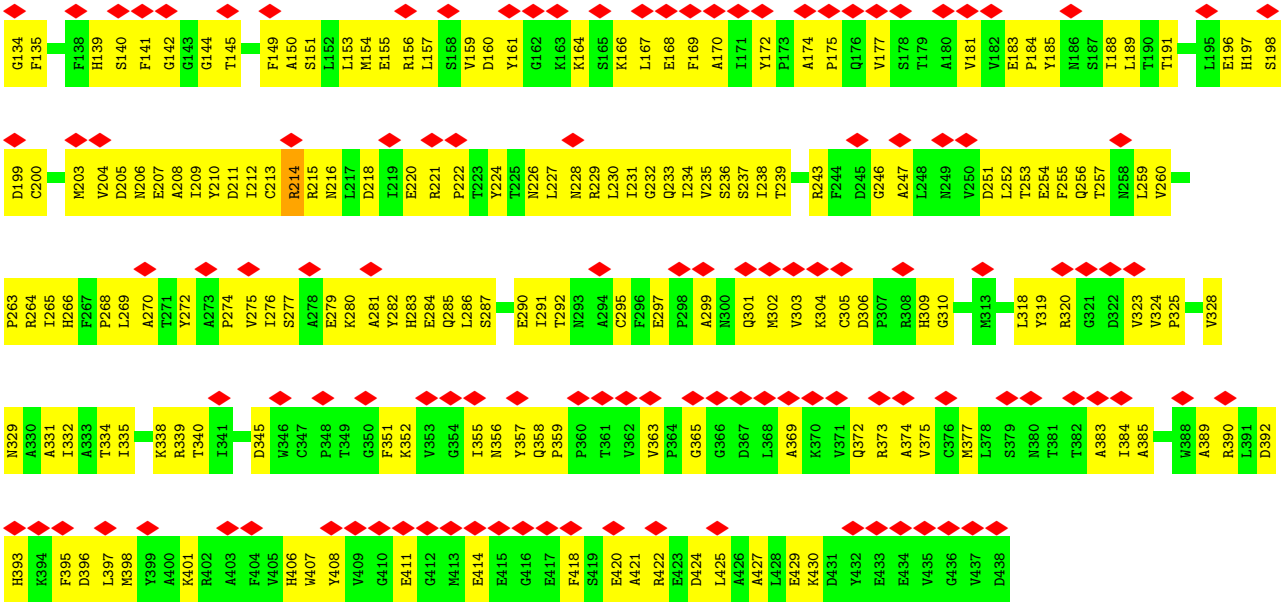
Chain QG:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

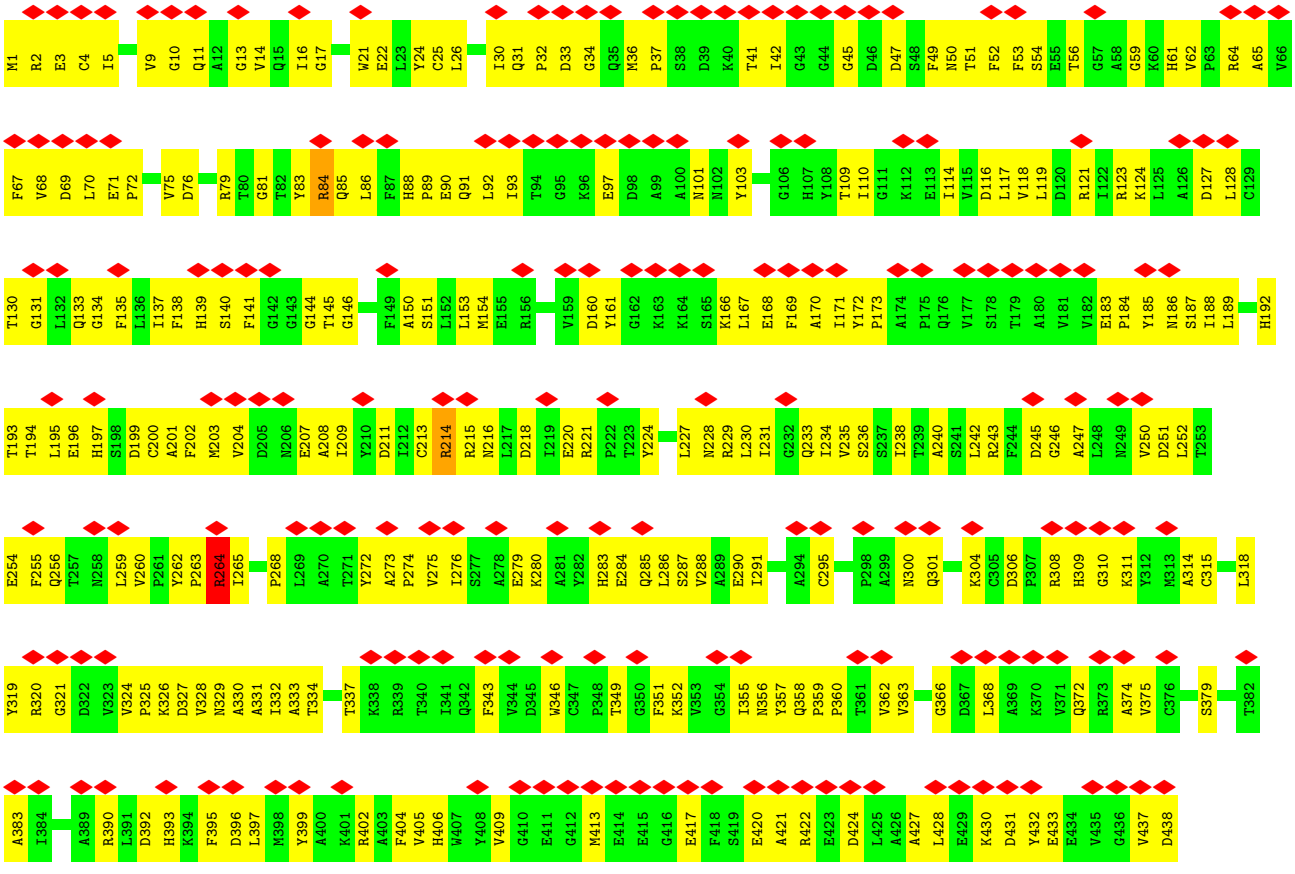
Chain QI:





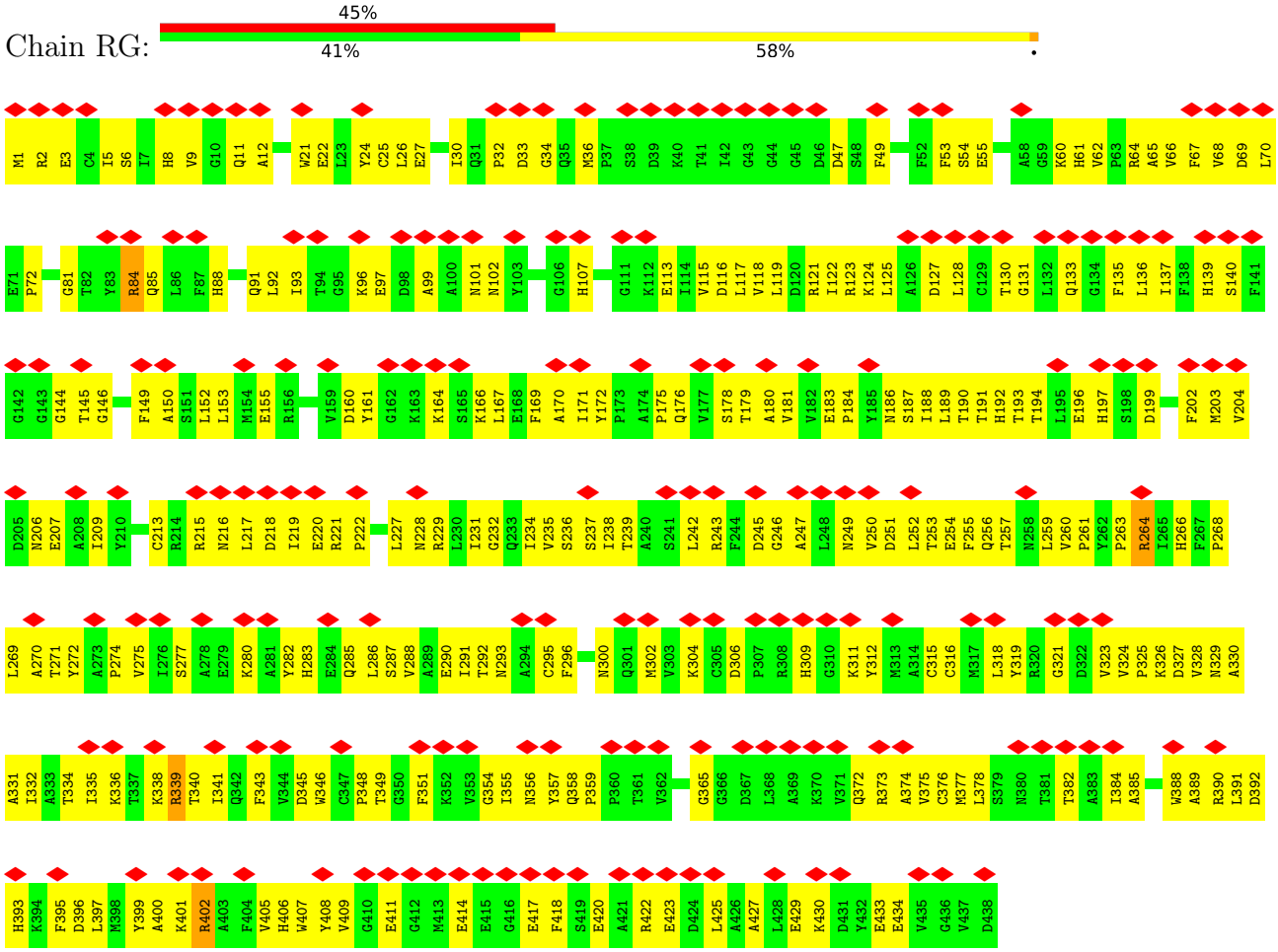
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain RE:



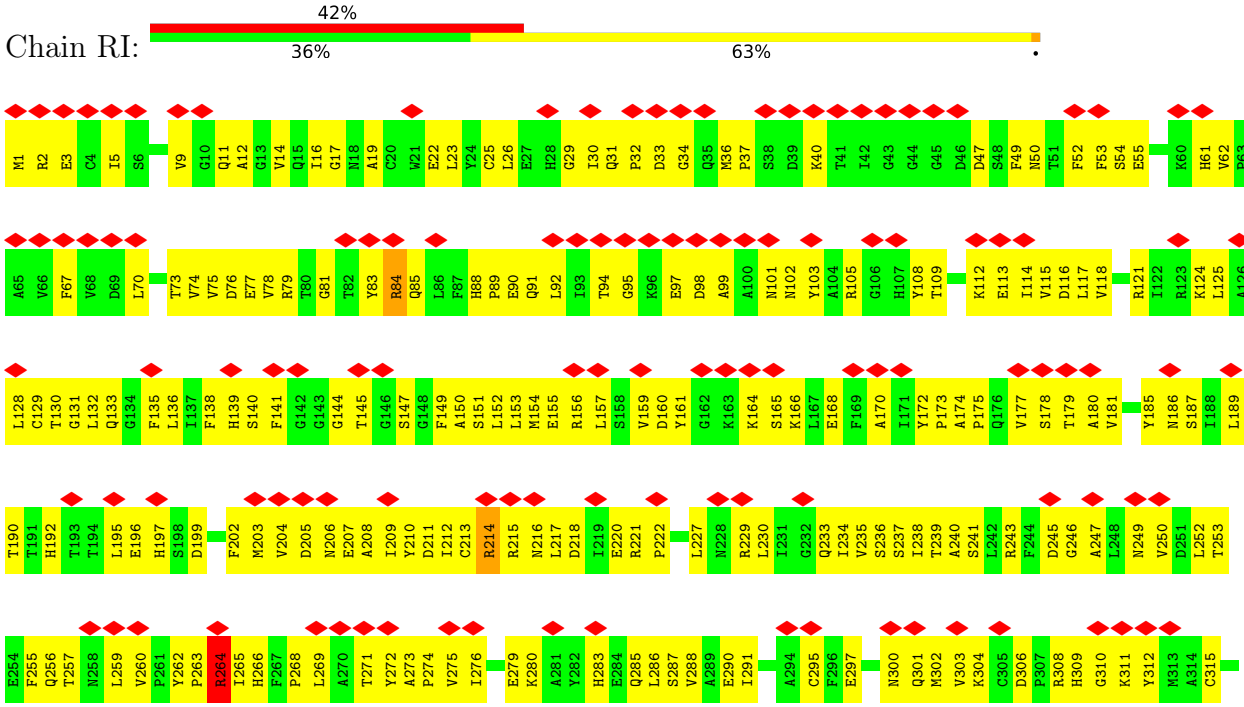
• Molecule 2: Detyrosinated tubulin alpha-3 chain

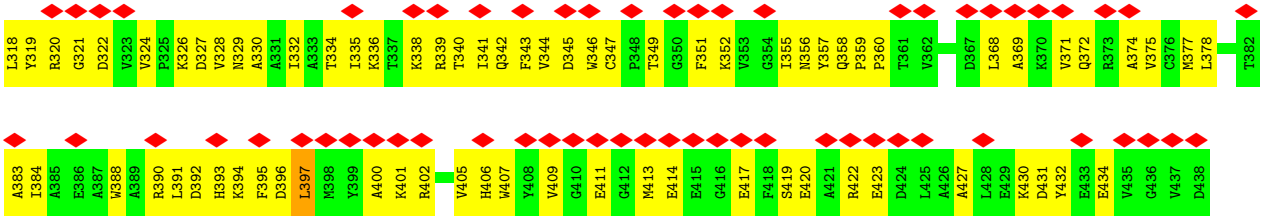
Chain RG:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

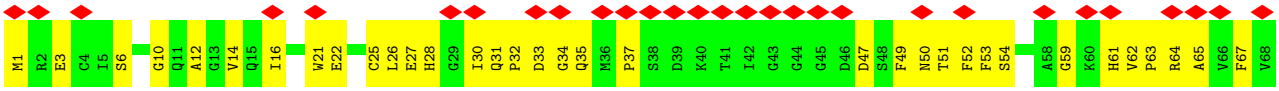
Chain RI:

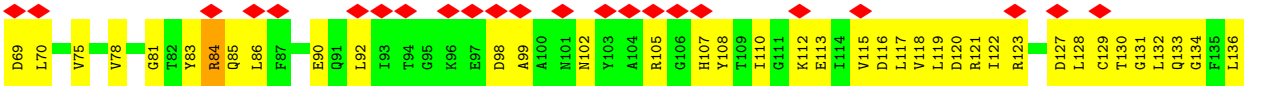


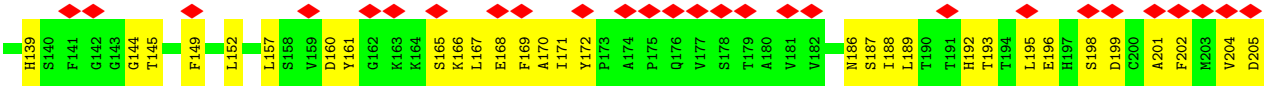


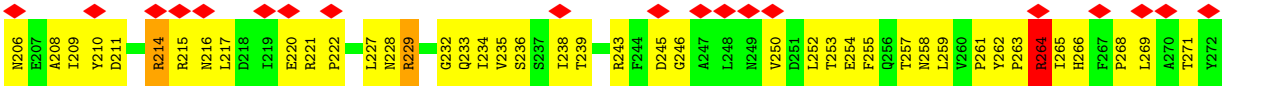
• Molecule 2: Detyrosinated tubulin alpha-3 chain

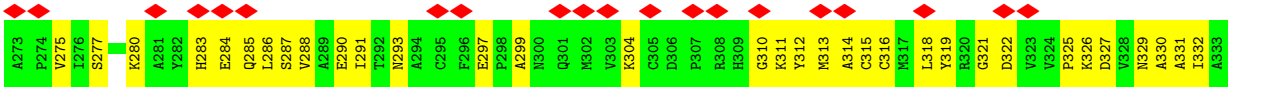
Chain SE:

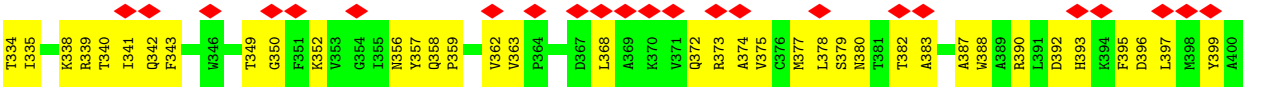


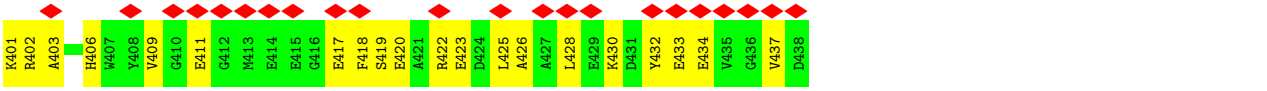


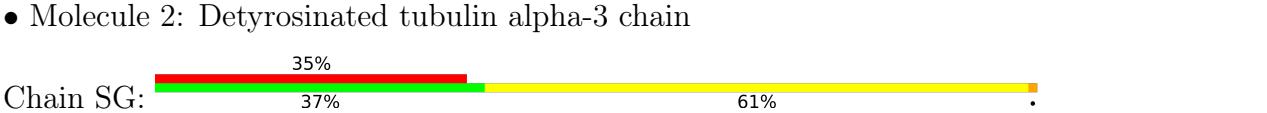


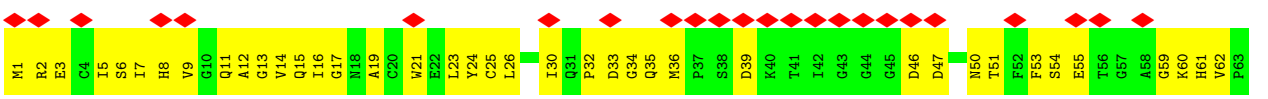






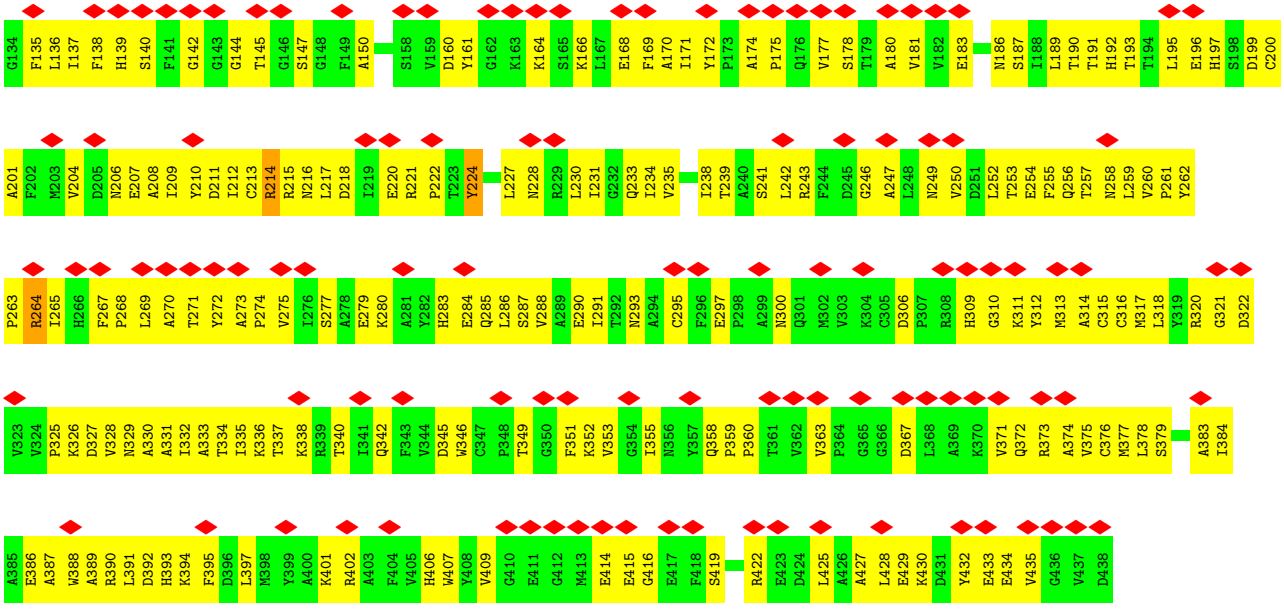






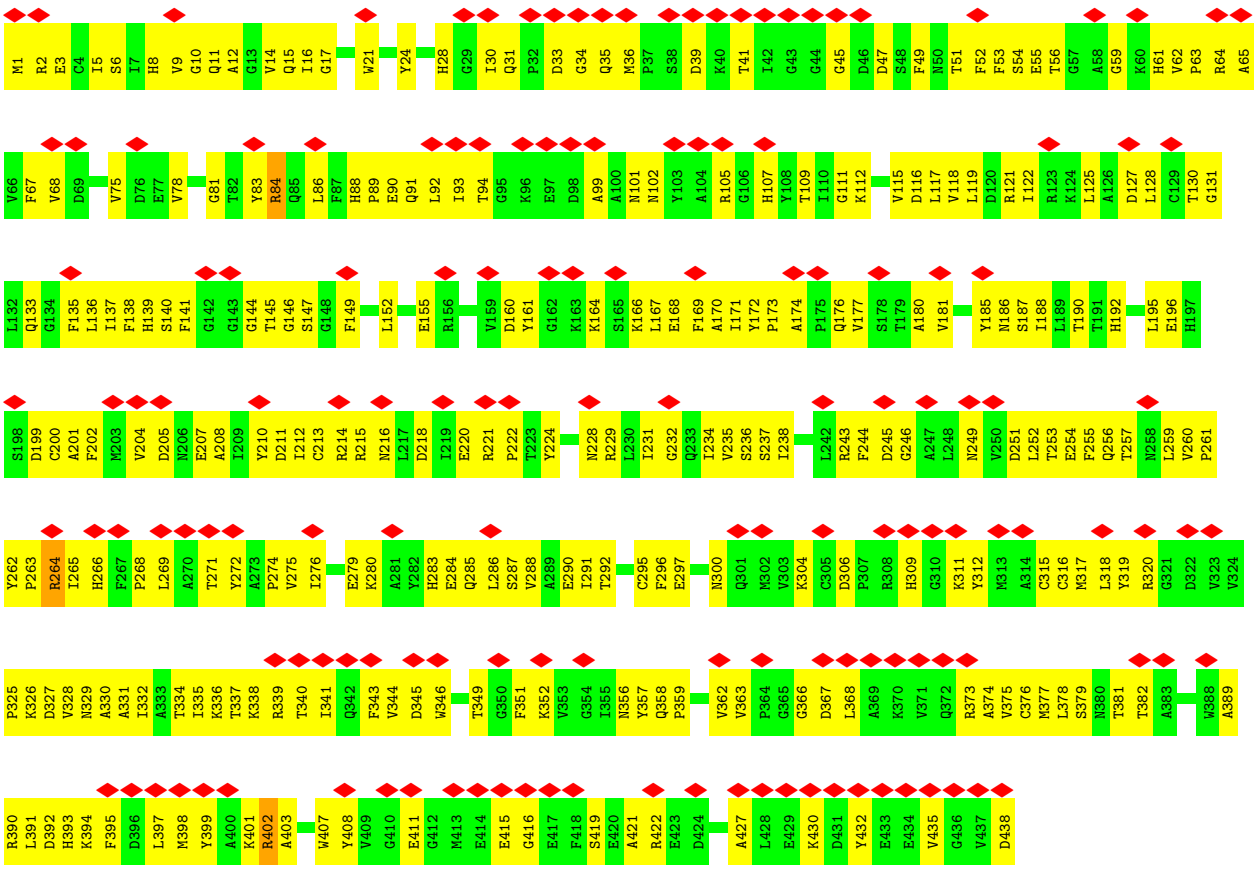
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain SG:



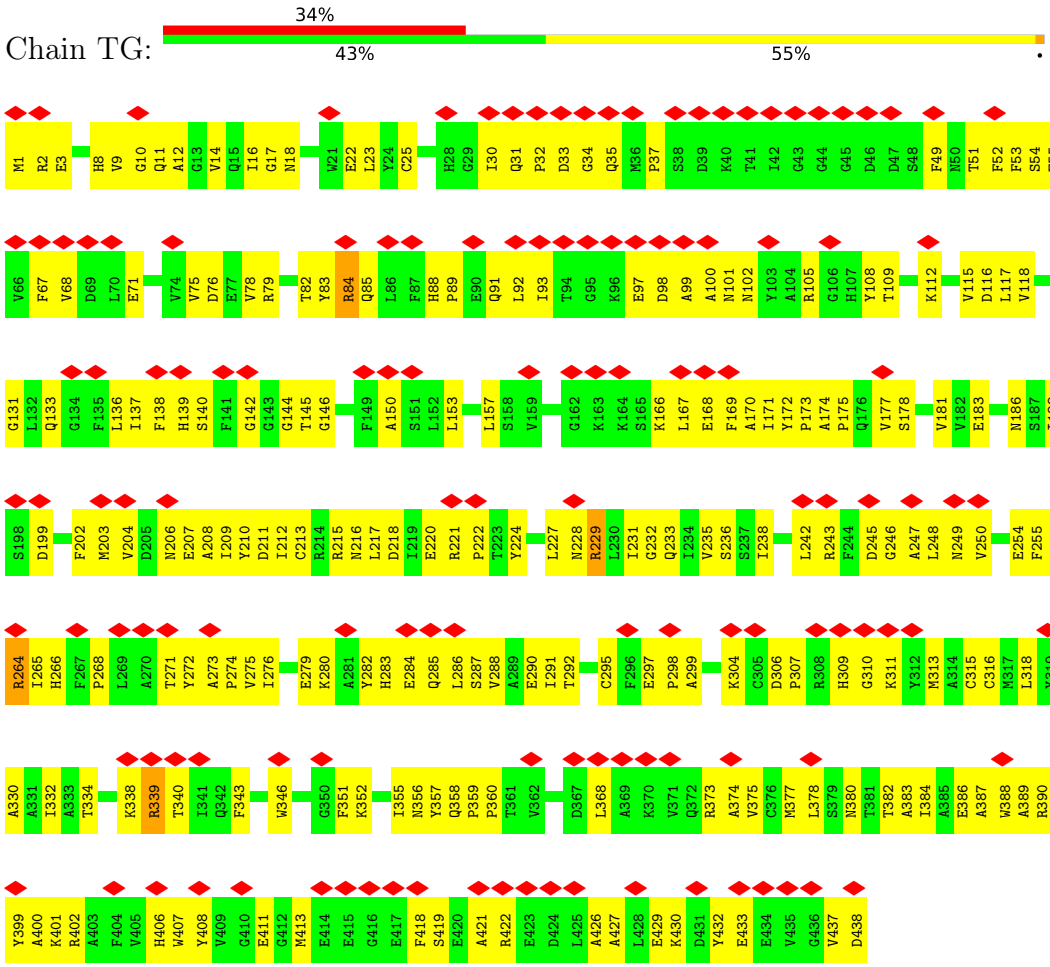
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain SI:



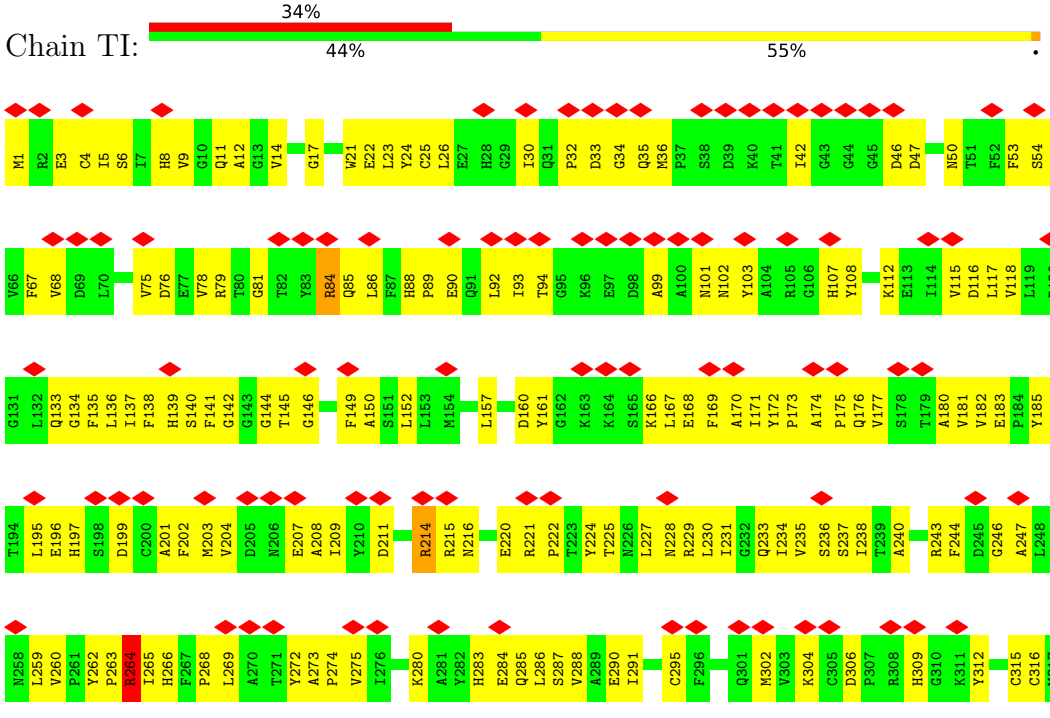
• Molecule 2: Detyrosinated tubulin alpha-3 chain

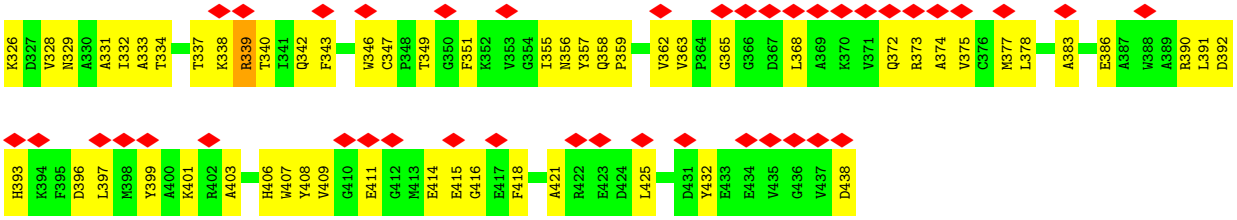
Chain TG:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain TI:



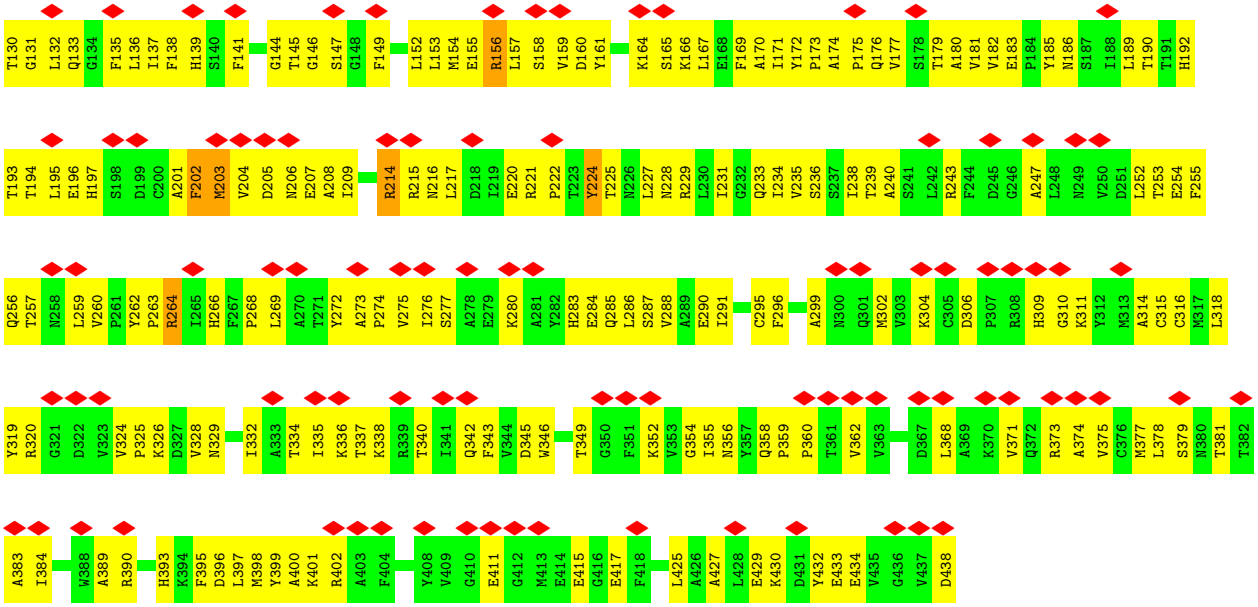


• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain UE:

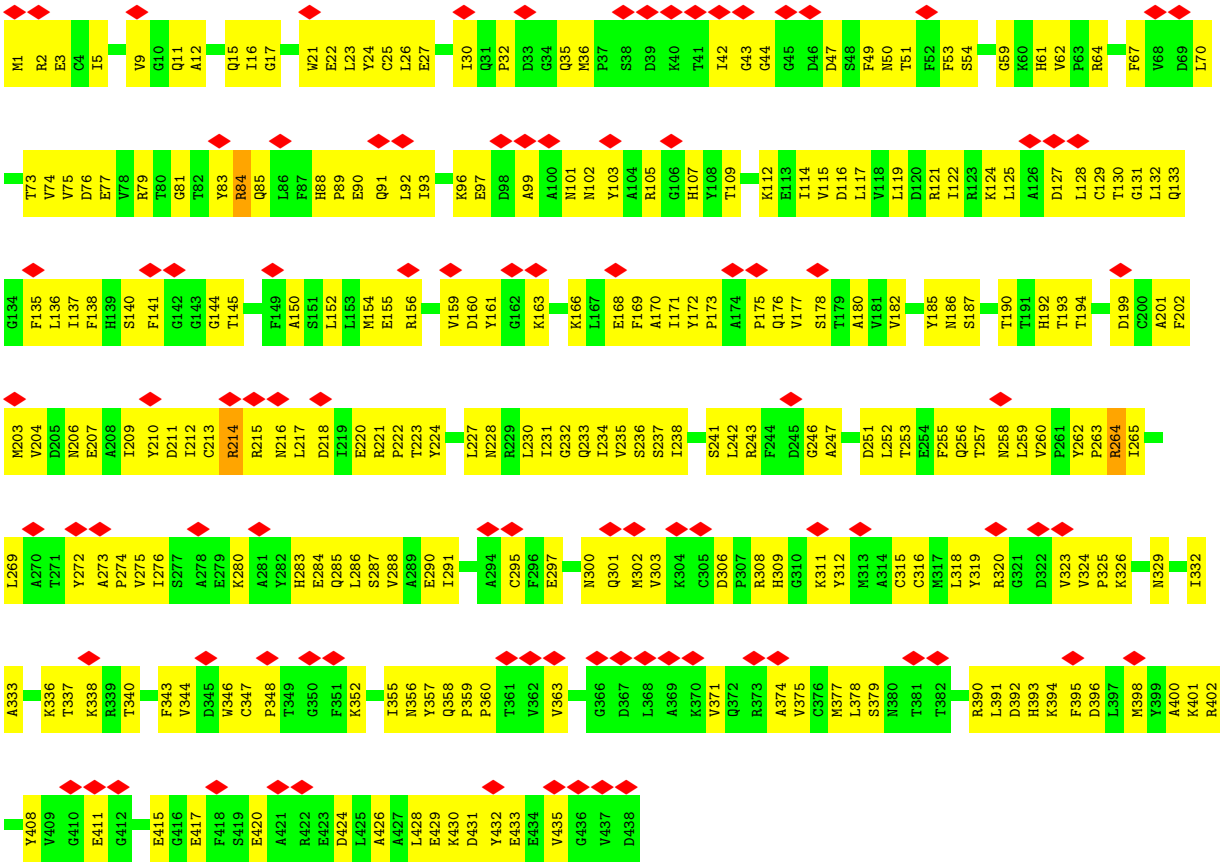
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain UG:



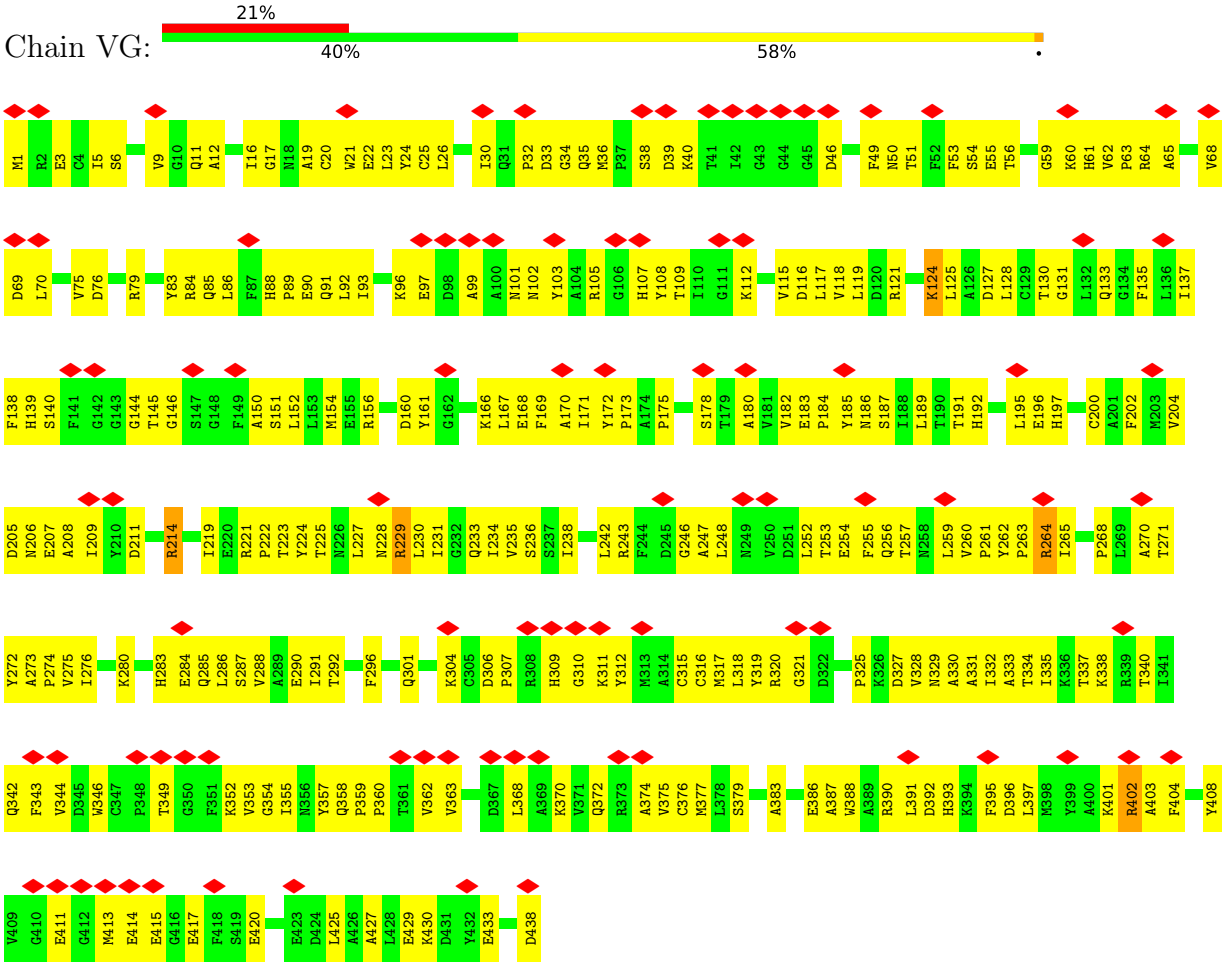
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain VE:



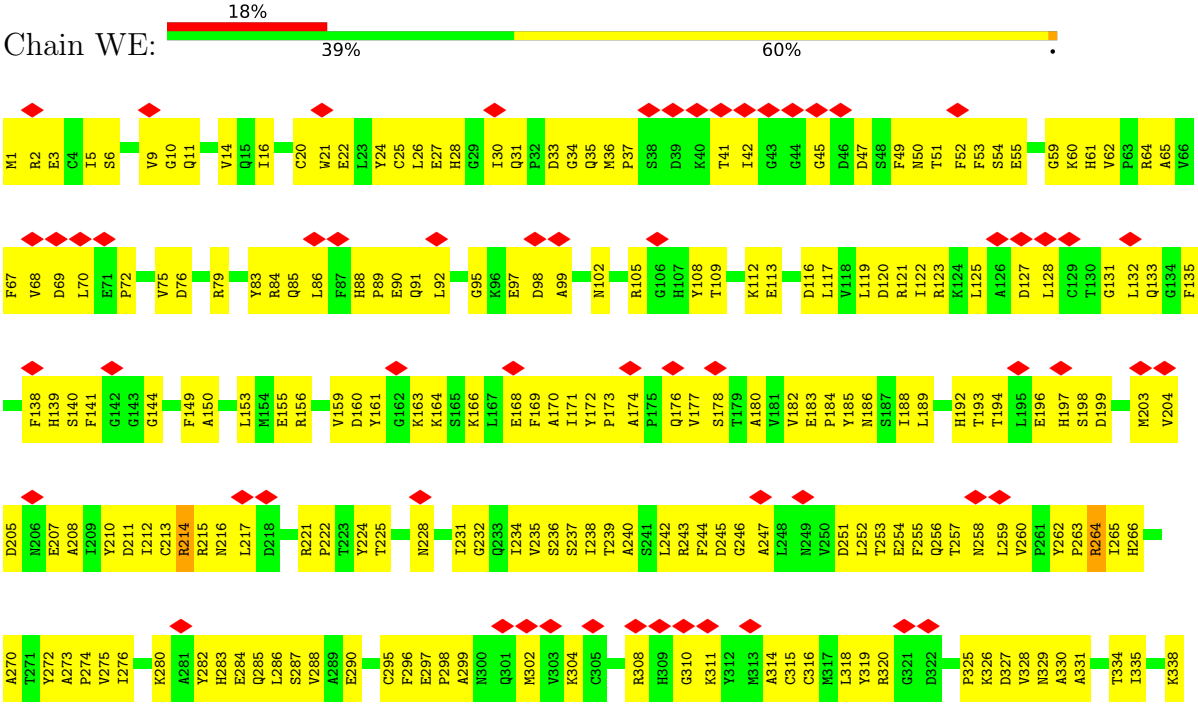
• Molecule 2: Detyrosinated tubulin alpha-3 chain

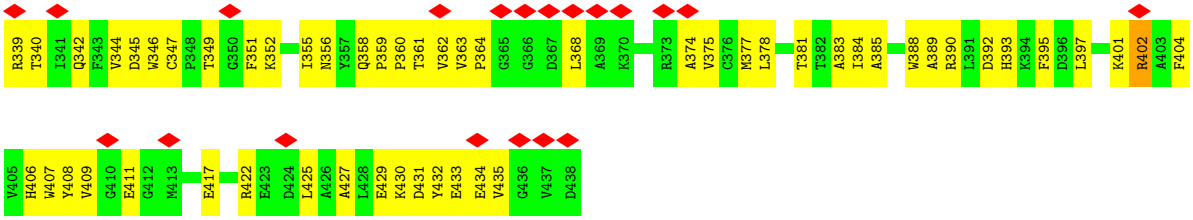
Chain VG:



• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain WE:



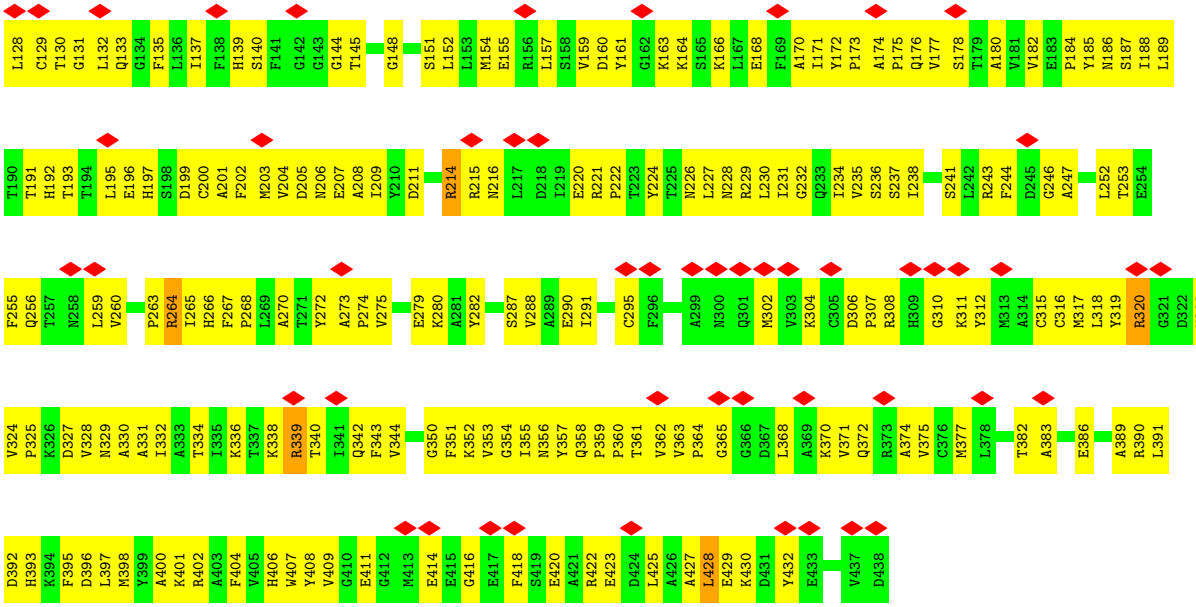


• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain WG:

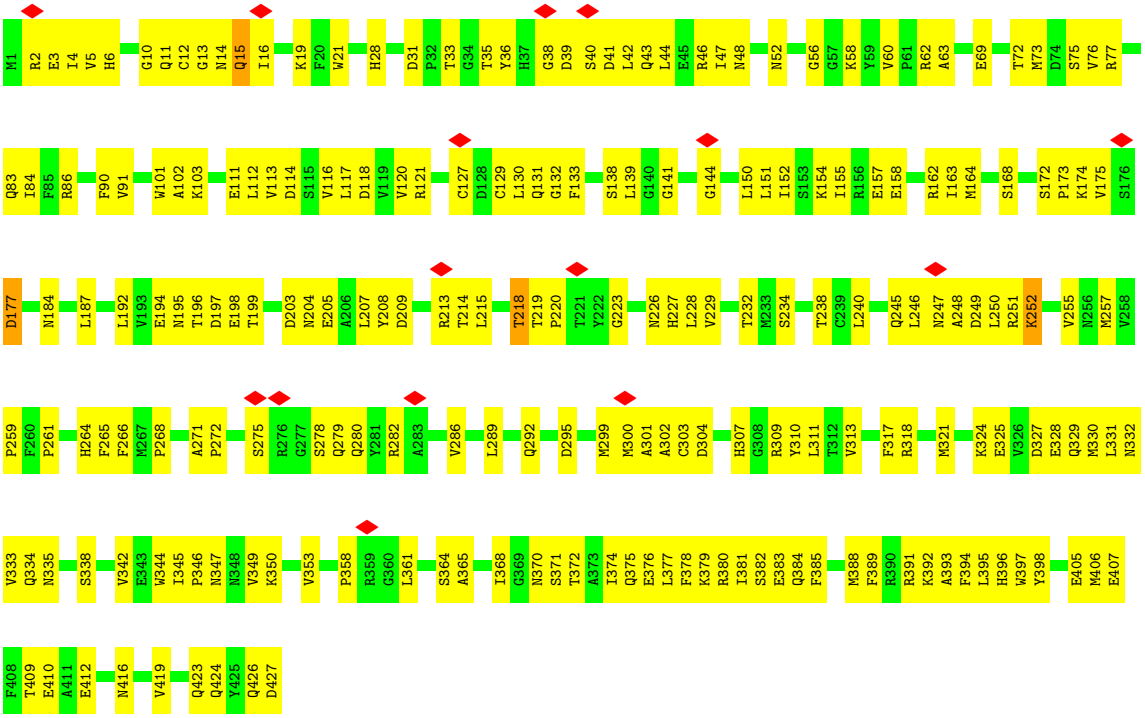
• Molecule 2: Detyrosinated tubulin alpha-3 chain

Chain WI:



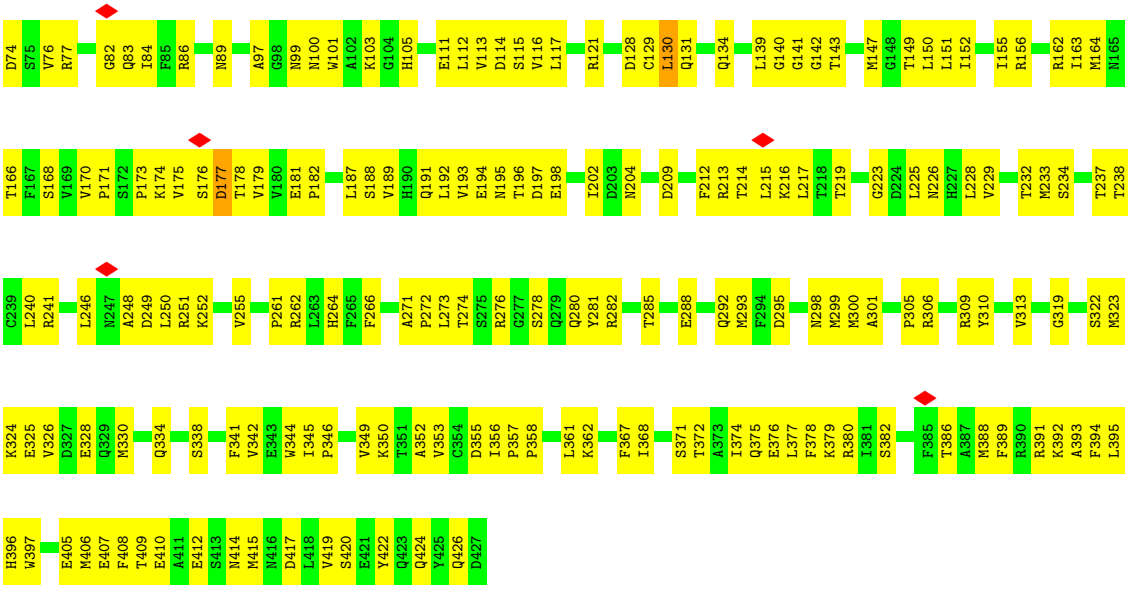
• Molecule 3: Tubulin beta-4B chain

Chain AF:



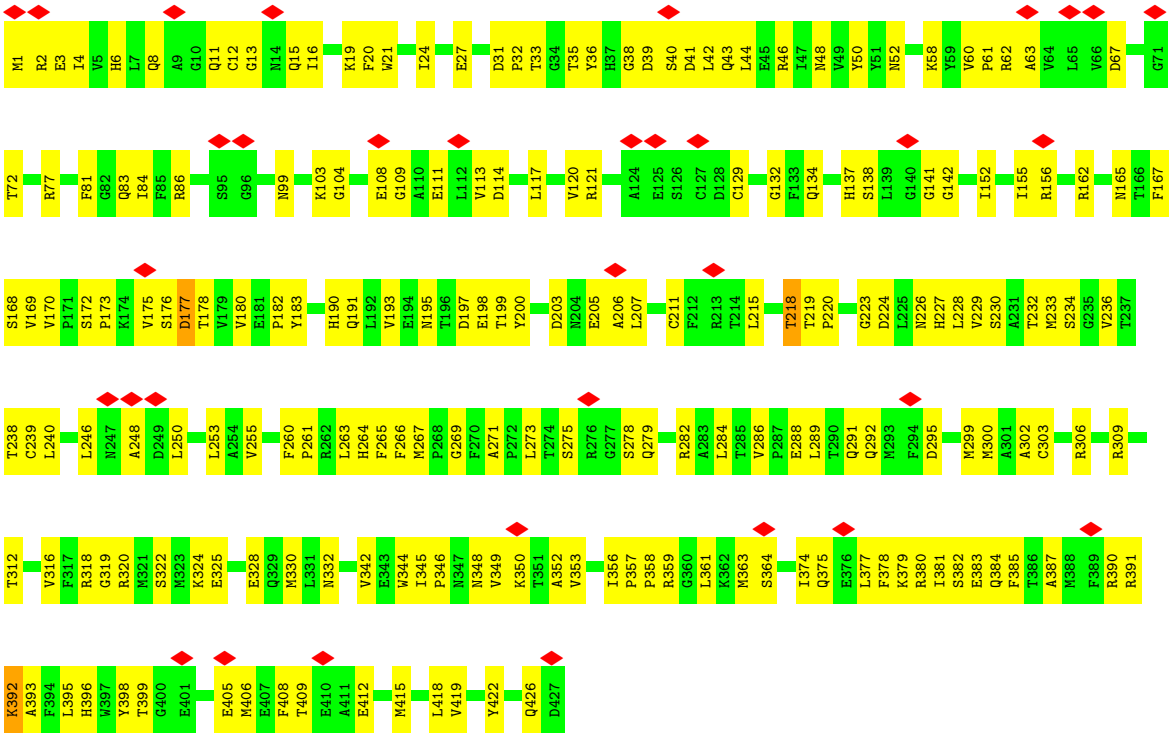
• Molecule 3: Tubulin beta-4B chain

Chain AH:



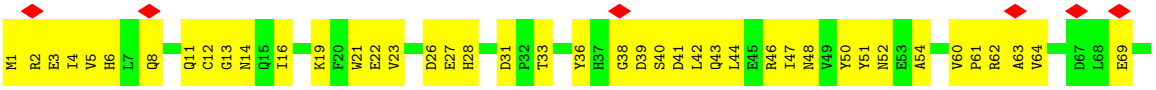
• Molecule 3: Tubulin beta-4B chain

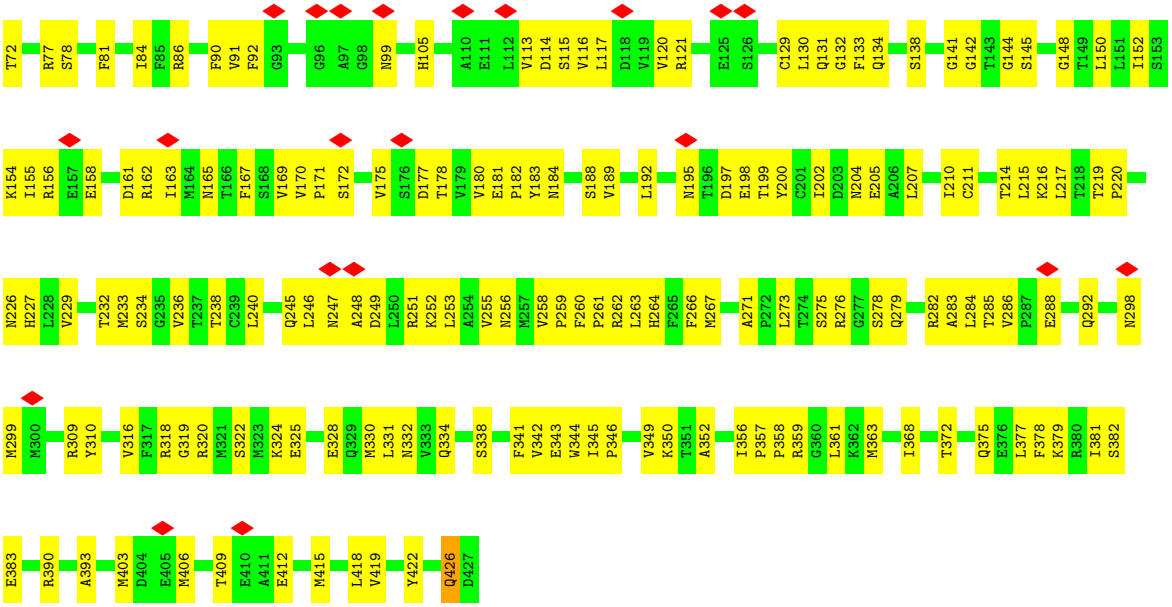
Chain BF:



• Molecule 3: Tubulin beta-4B chain

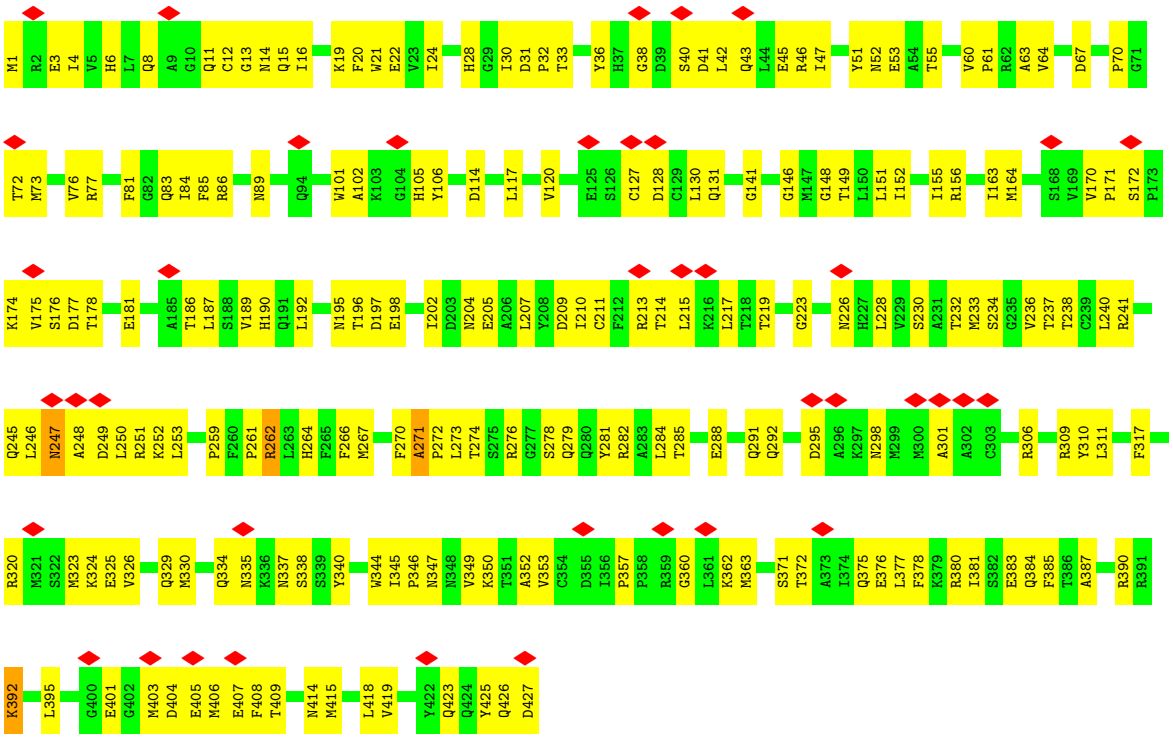
Chain BH:





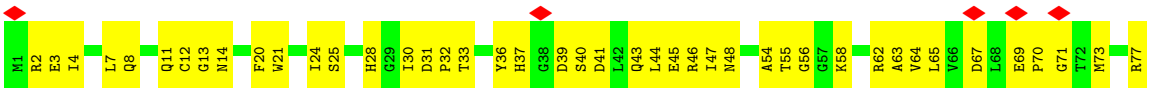
• Molecule 3: Tubulin beta-4B chain

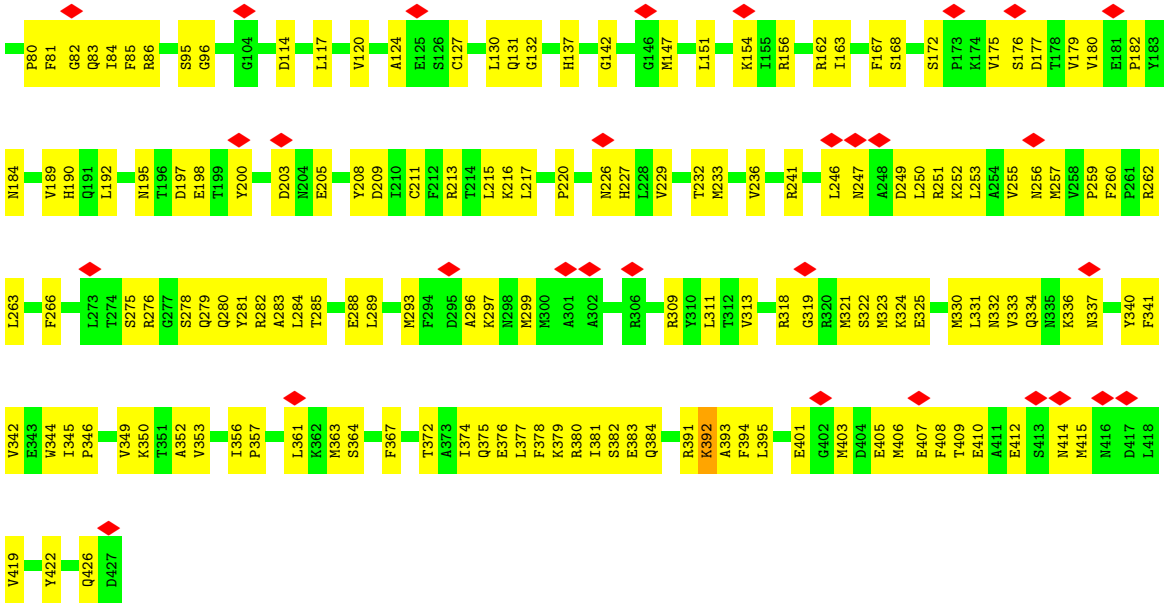
Chain CF:



• Molecule 3: Tubulin beta-4B chain

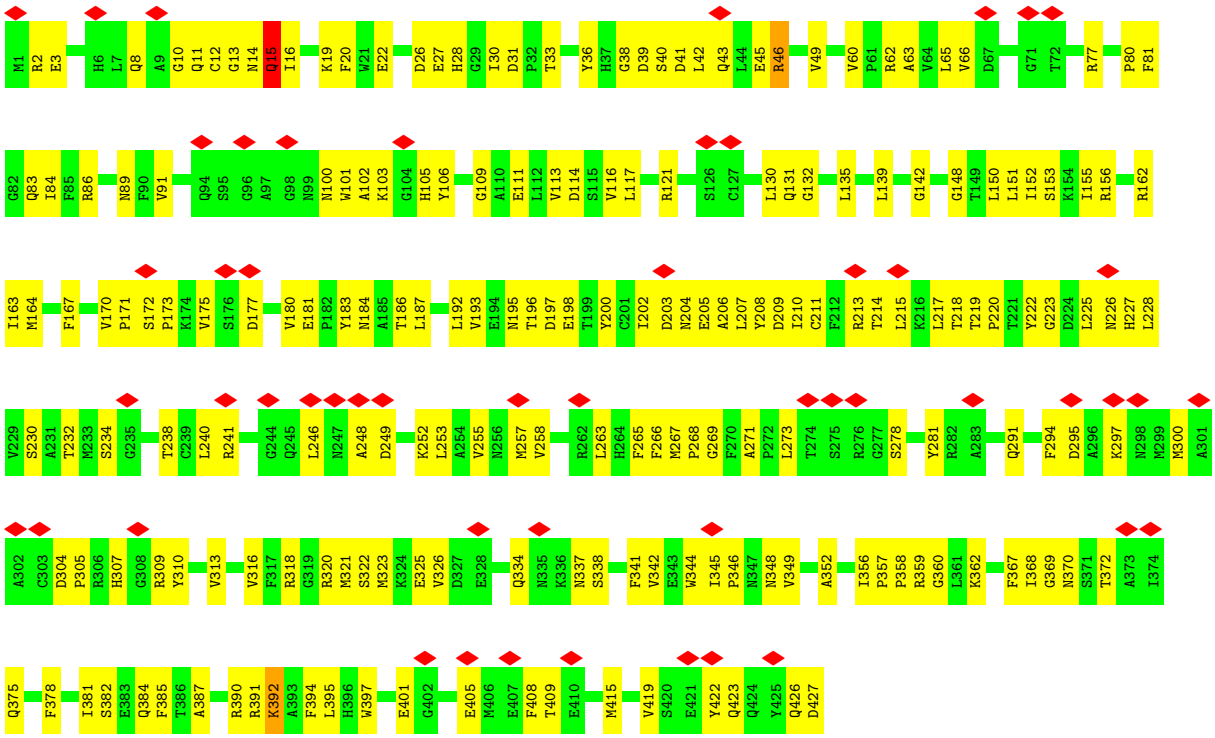
Chain CH:





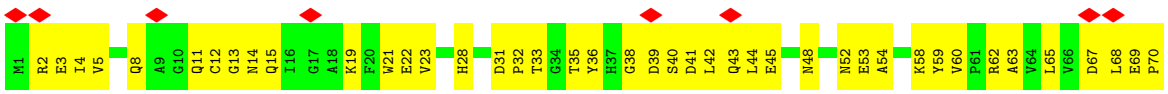
• Molecule 3: Tubulin beta-4B chain

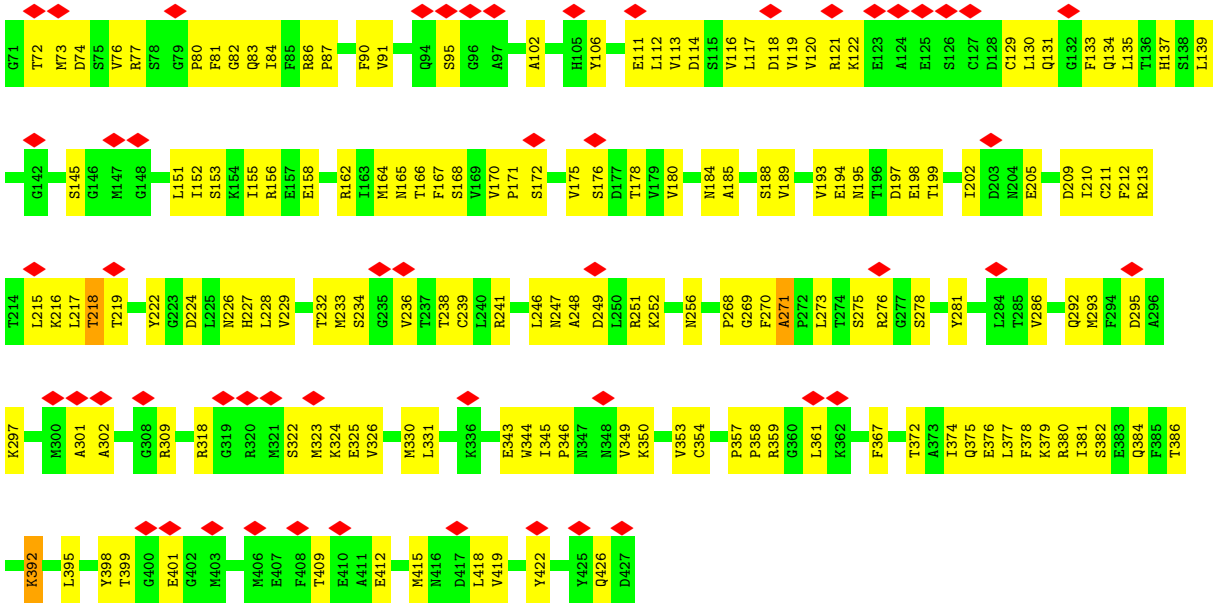
Chain CJ:



• Molecule 3: Tubulin beta-4B chain

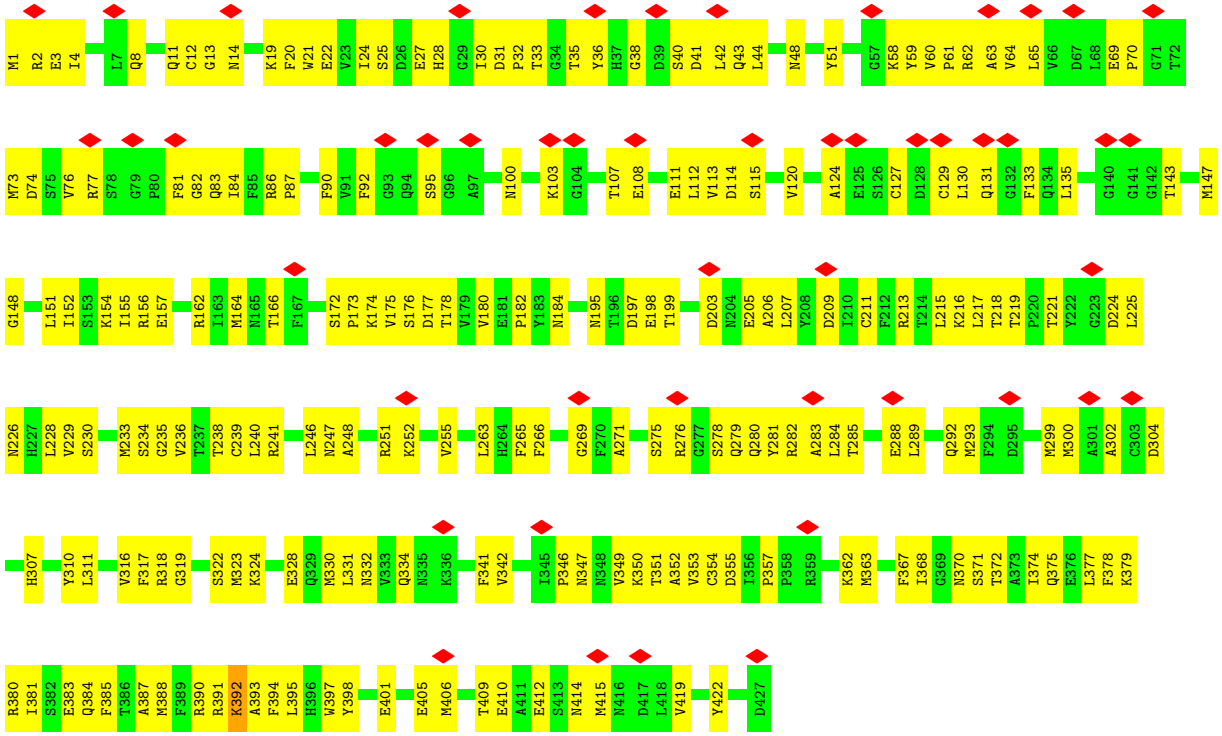
Chain DD:





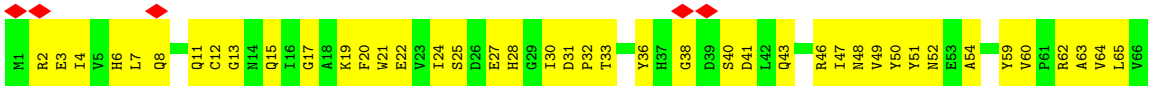
• Molecule 3: Tubulin beta-4B chain

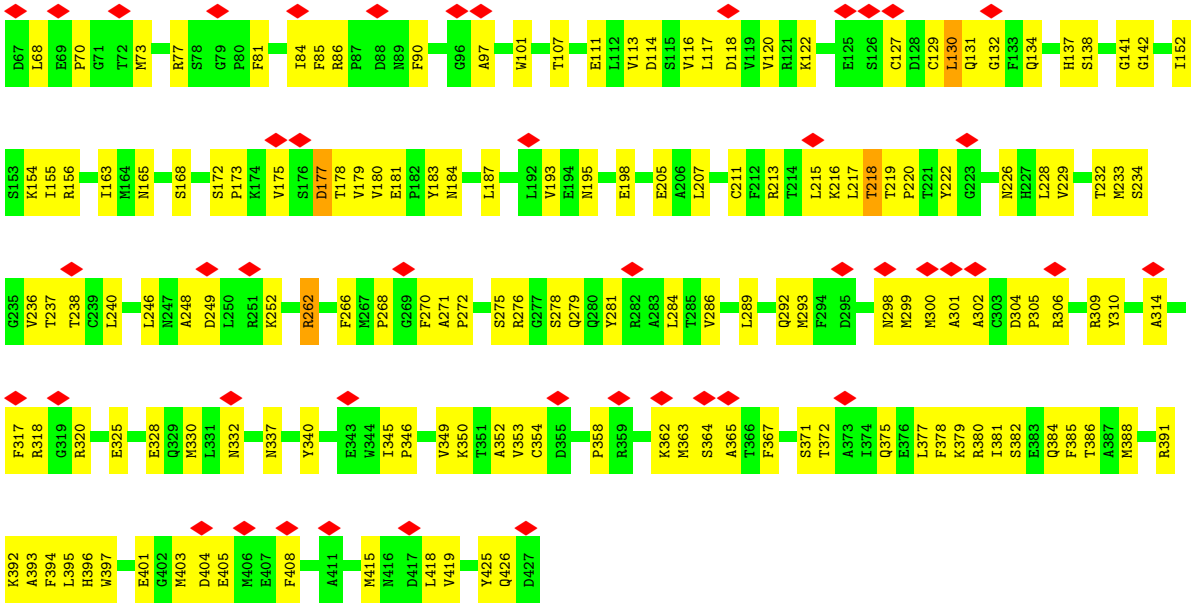
Chain DF:



• Molecule 3: Tubulin beta-4B chain

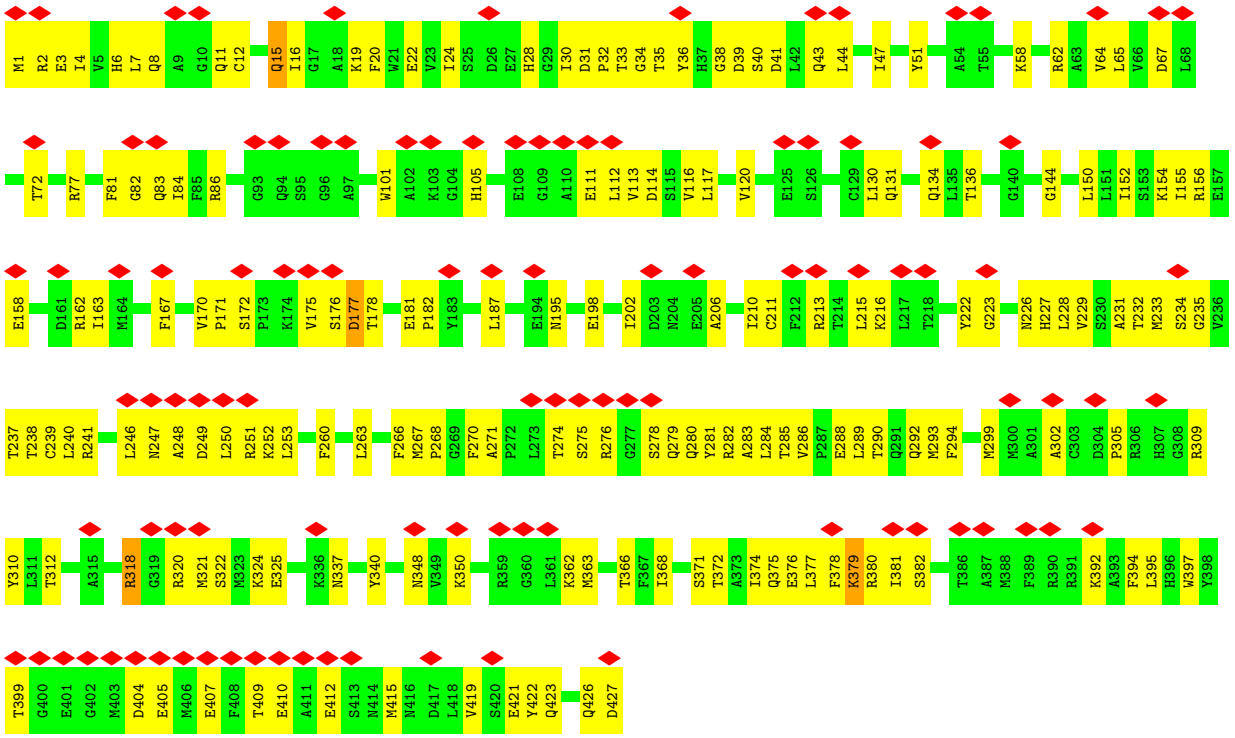
Chain DH:





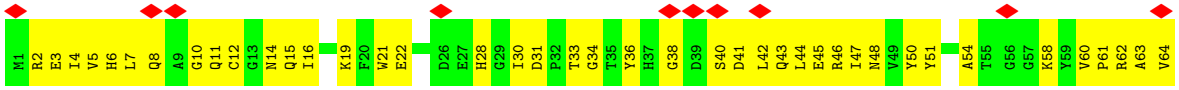
• Molecule 3: Tubulin beta-4B chain

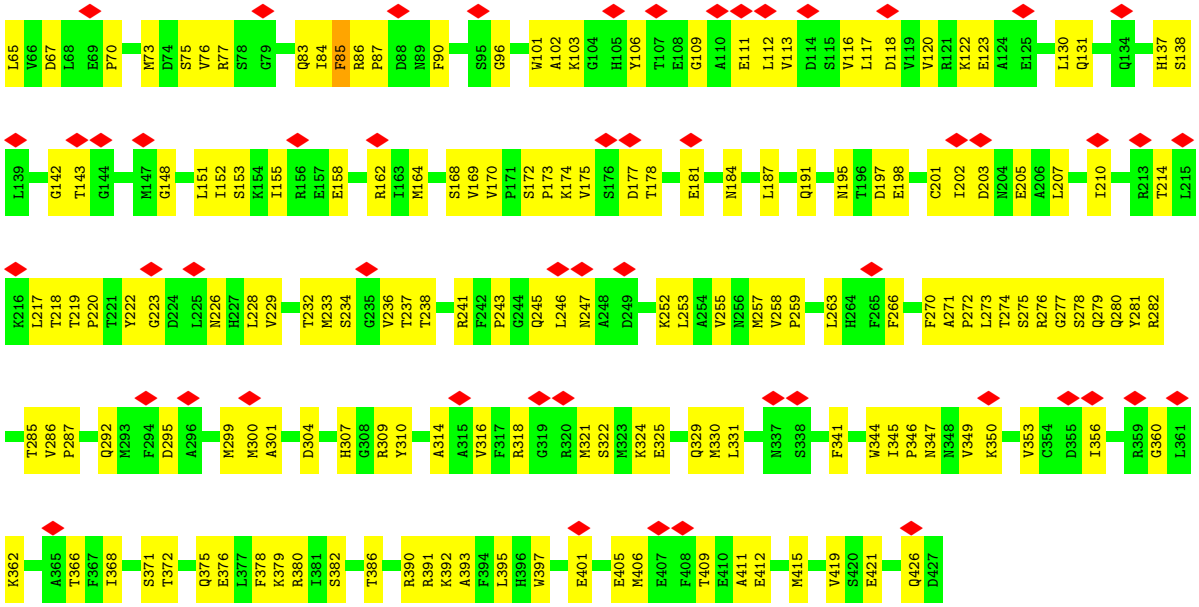
Chain ED:



• Molecule 3: Tubulin beta-4B chain

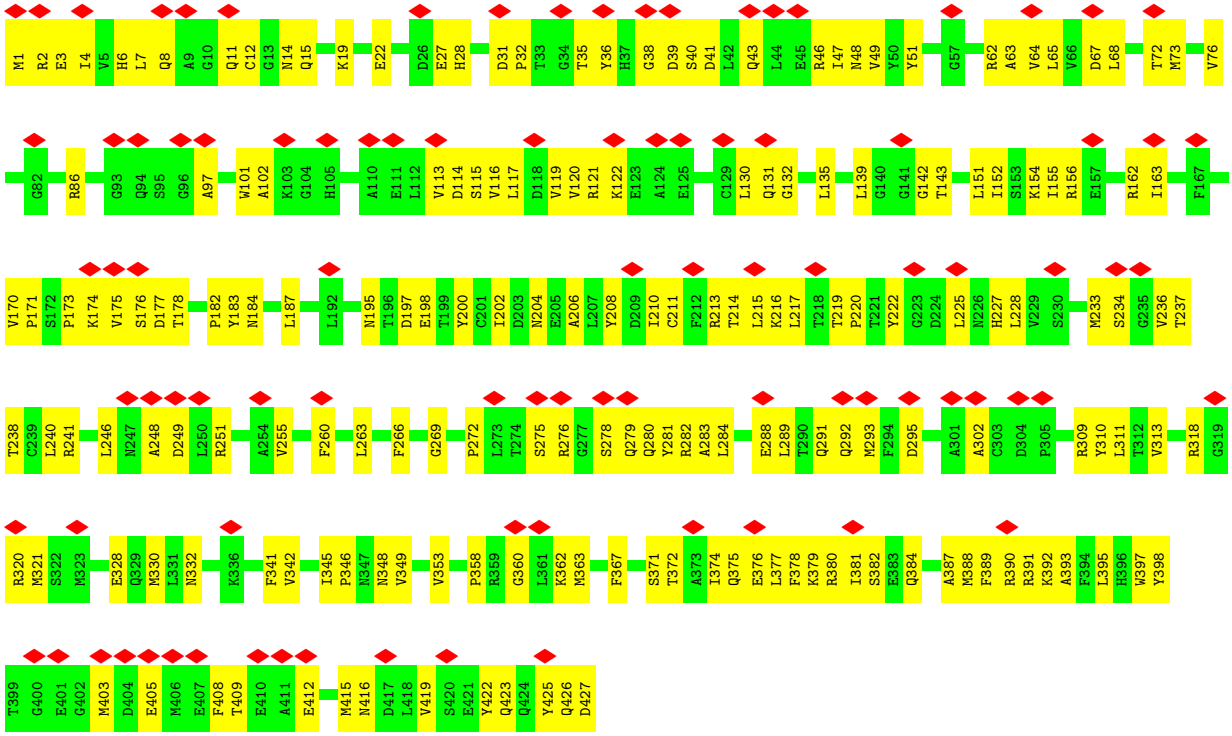
Chain EF:





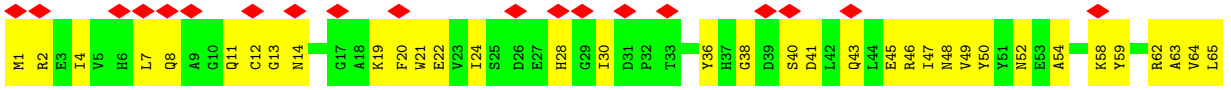
• Molecule 3: Tubulin beta-4B chain

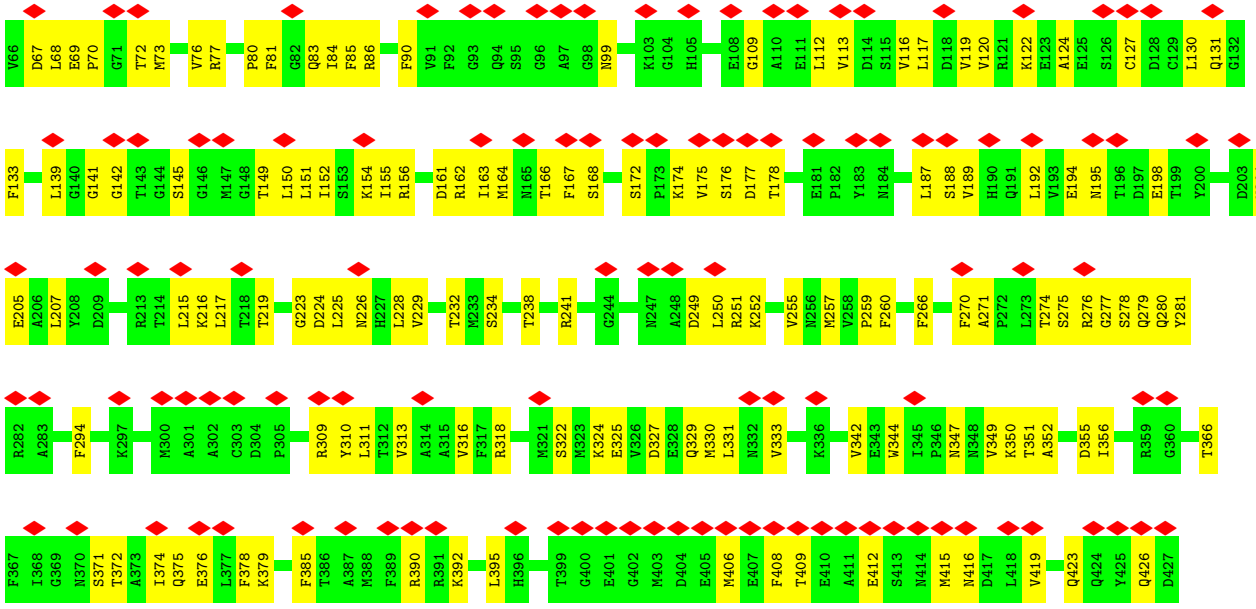
Chain EH:



• Molecule 3: Tubulin beta-4B chain

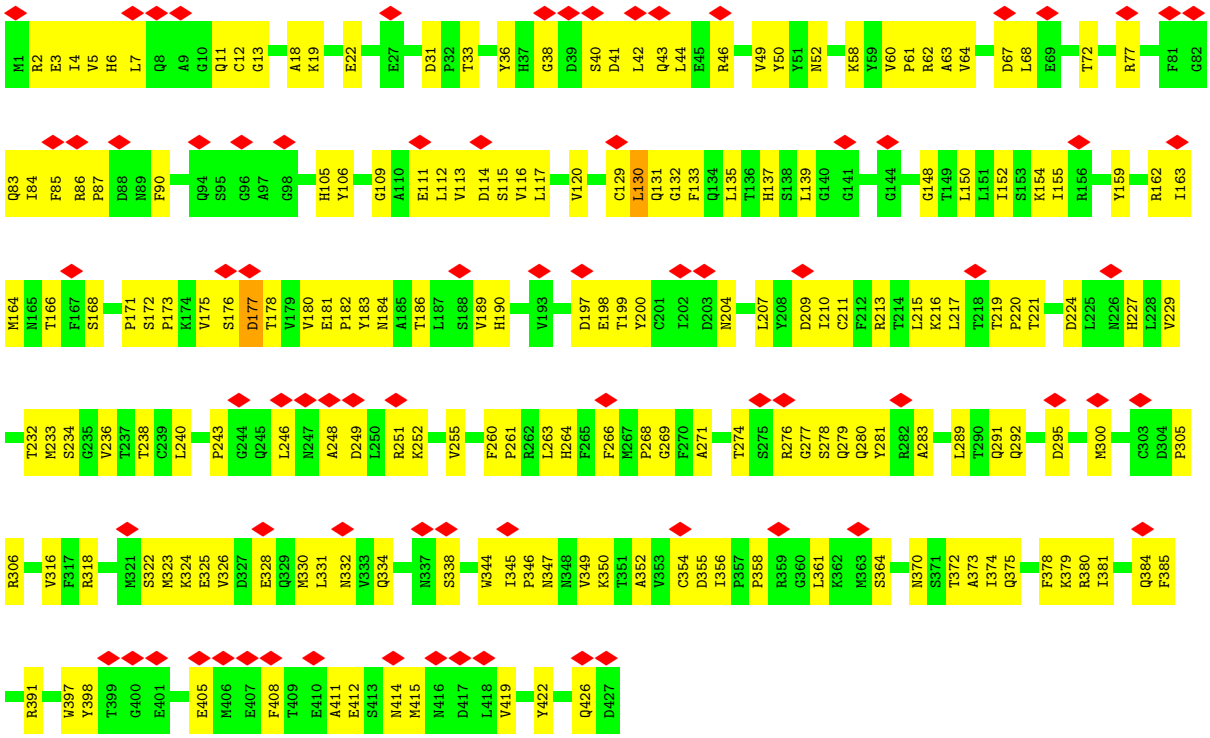
Chain FD:





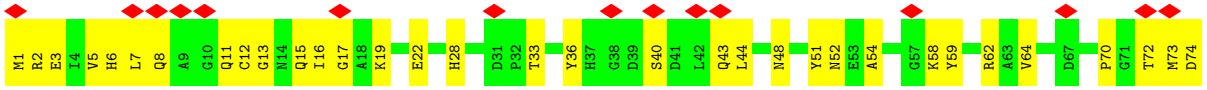
• Molecule 3: Tubulin beta-4B chain

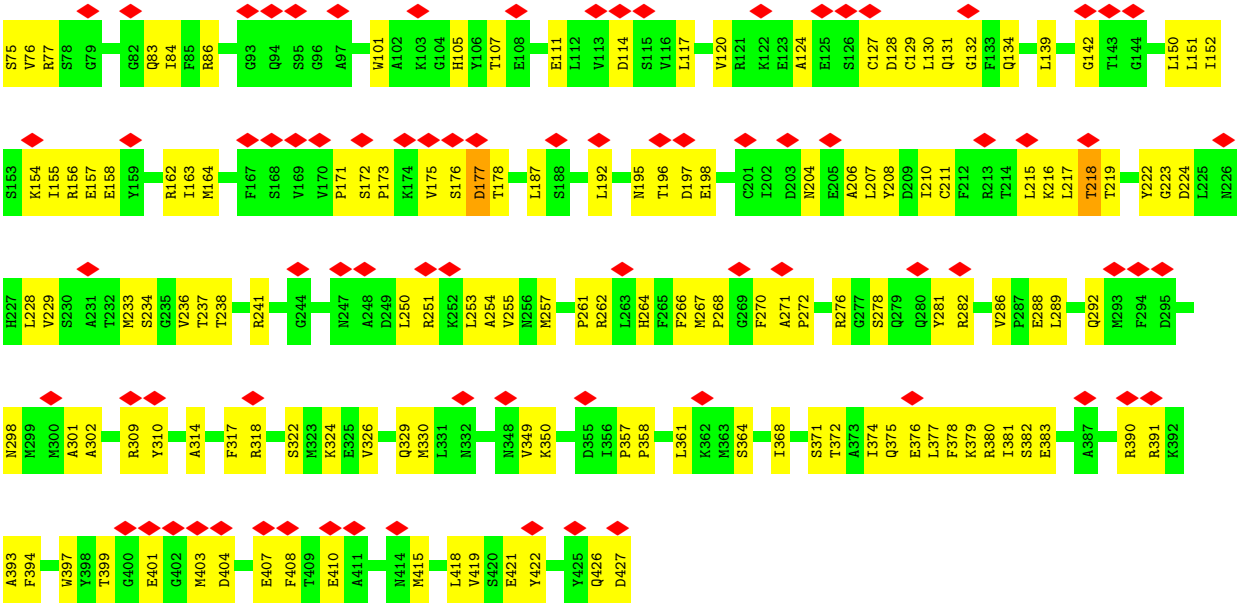
Chain FF:



• Molecule 3: Tubulin beta-4B chain

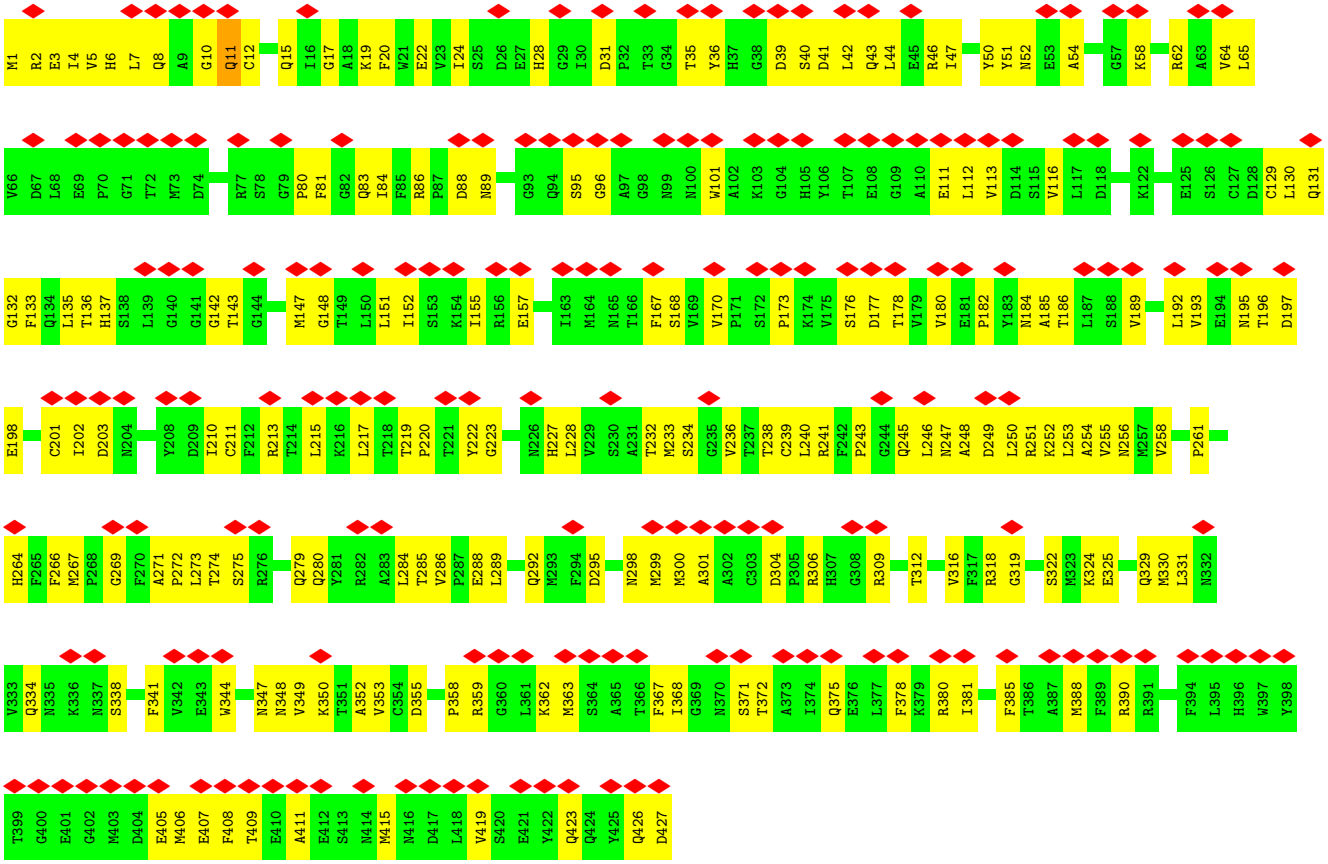
Chain FH:





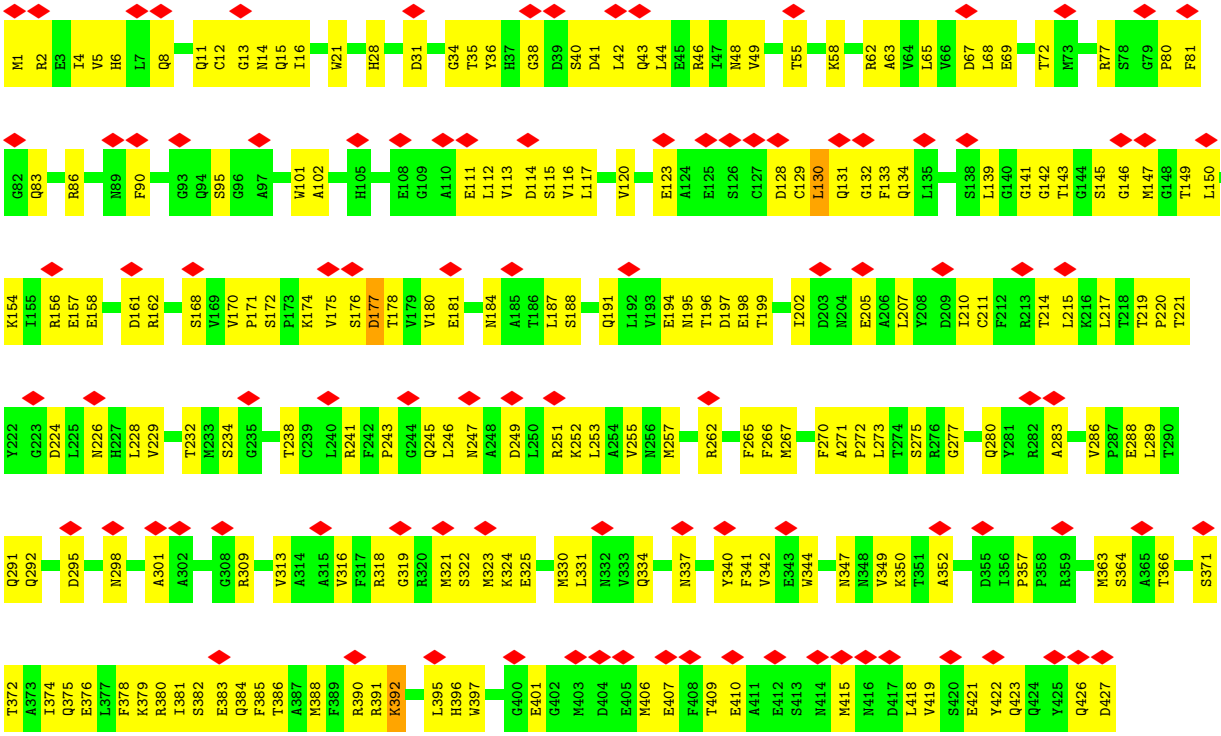
• Molecule 3: Tubulin beta-4B chain

Chain GD:



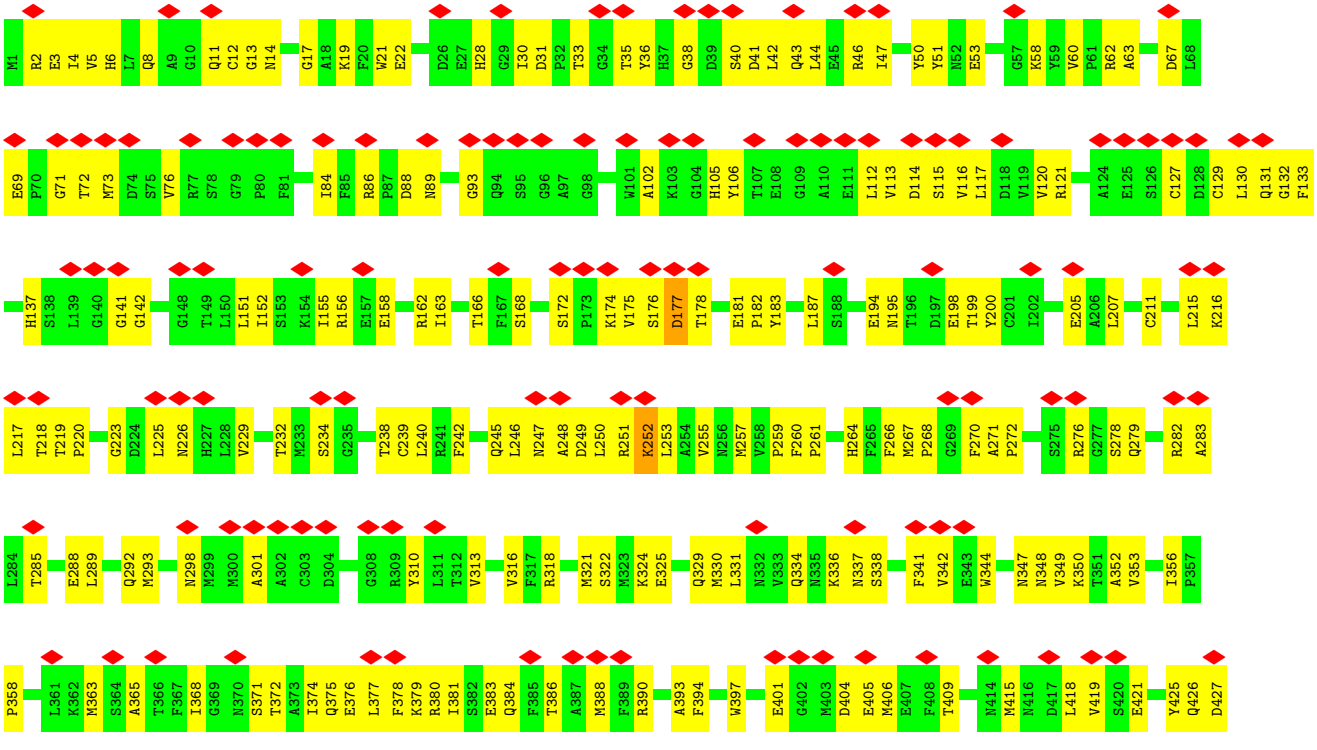
• Molecule 3: Tubulin beta-4B chain

Chain GF:



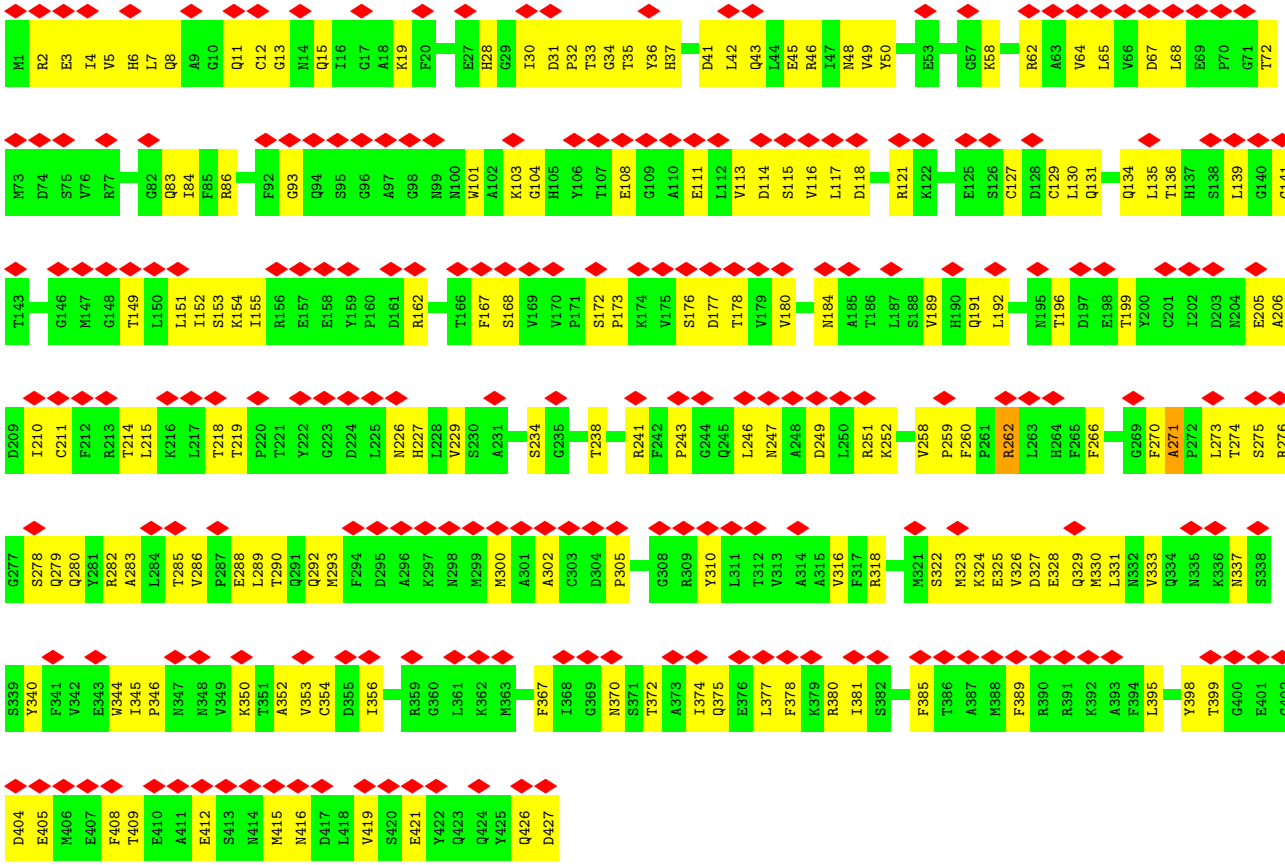
• Molecule 3: Tubulin beta-4B chain

Chain GH:



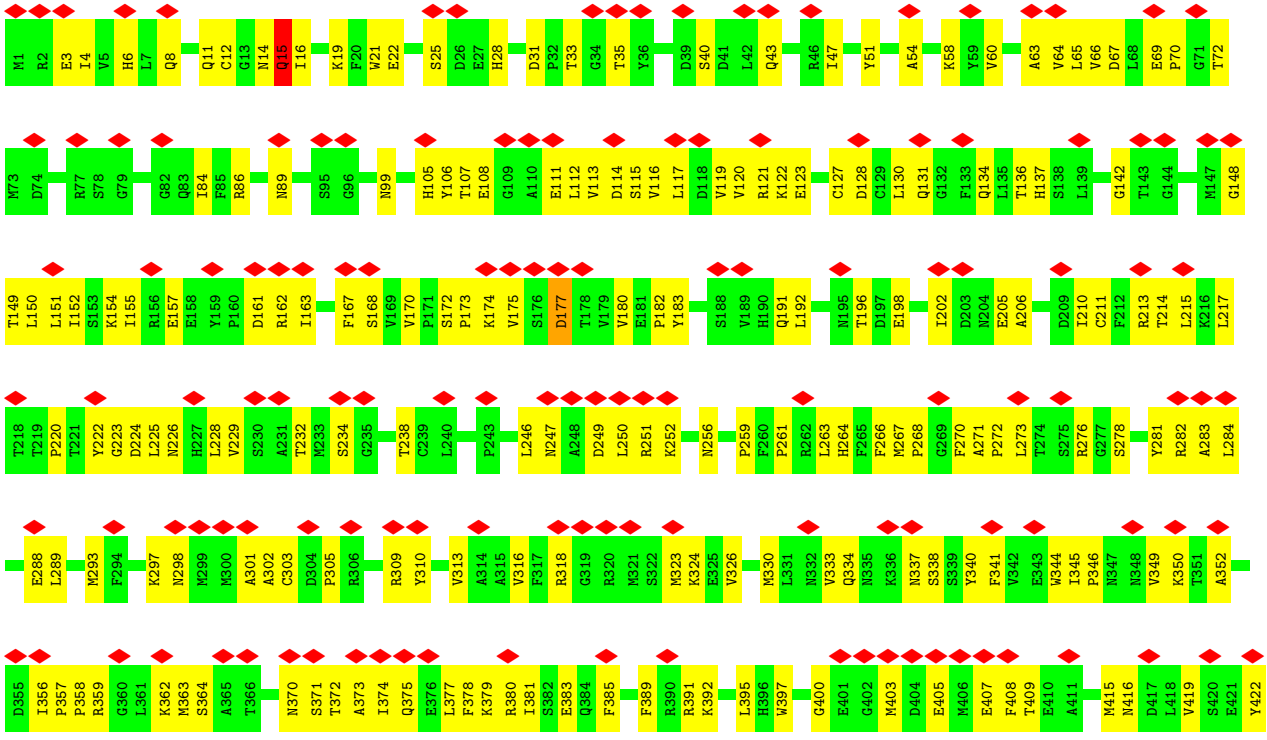
• Molecule 3: Tubulin beta-4B chain

Chain HD:



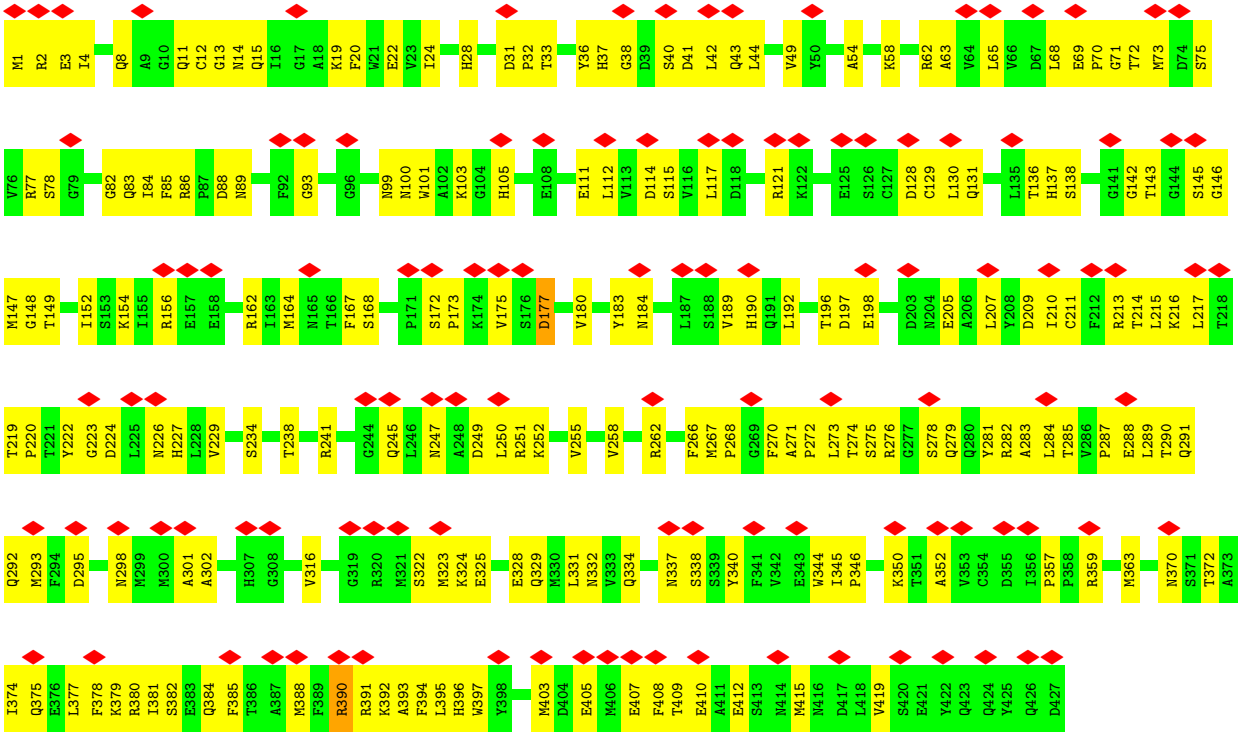
• Molecule 3: Tubulin beta-4B chain

Chain HF:



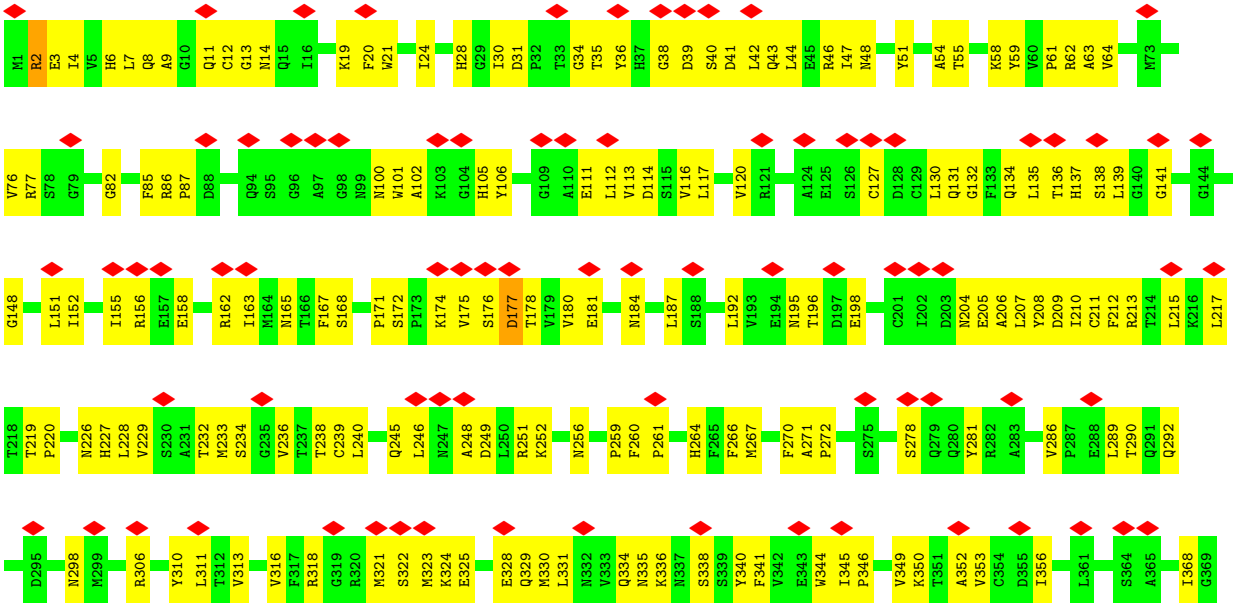
• Molecule 3: Tubulin beta-4B chain

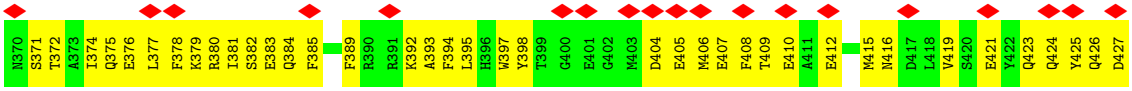
Chain HH:



• Molecule 3: Tubulin beta-4B chain

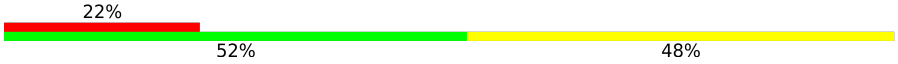
Chain IF:

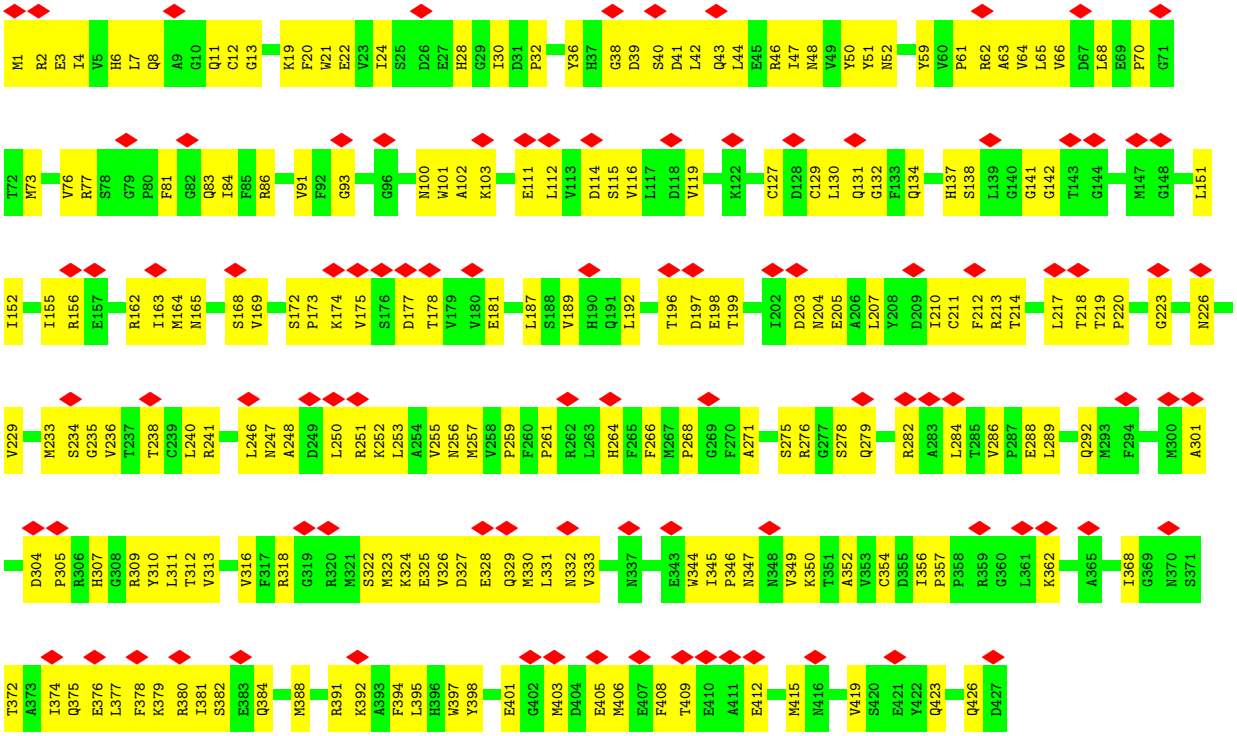




• Molecule 3: Tubulin beta-4B chain

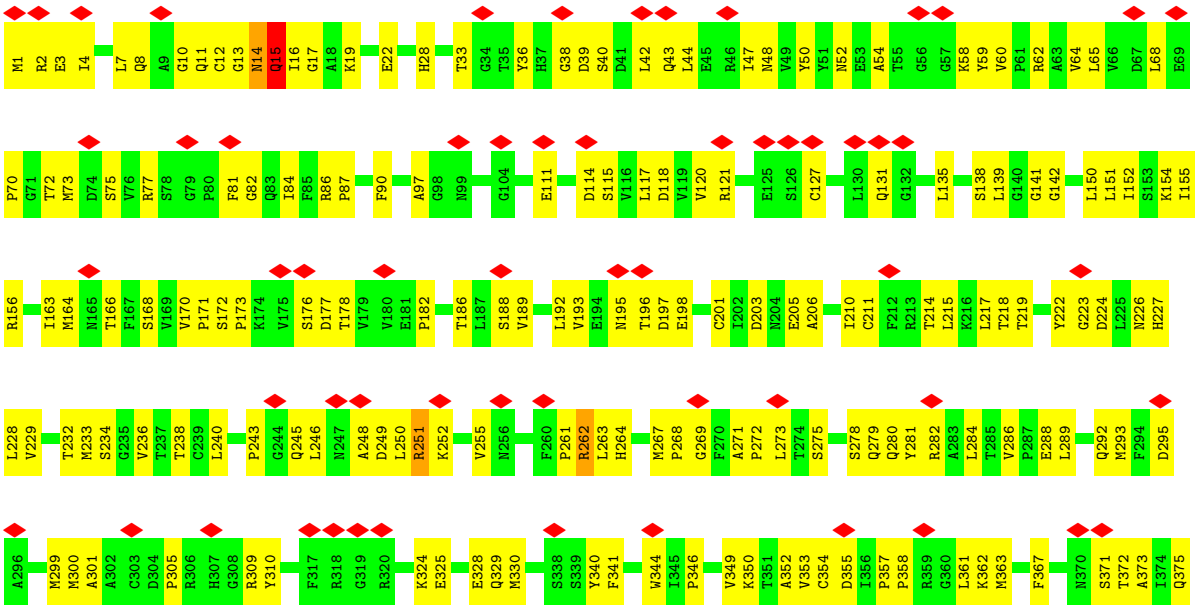
Chain IH:

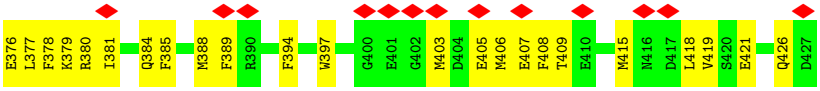




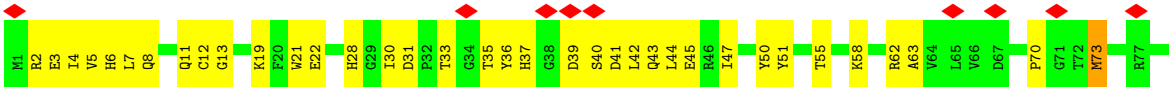
• Molecule 3: Tubulin beta-4B chain

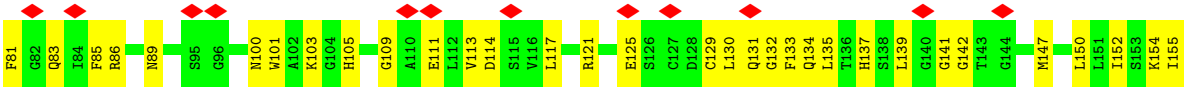
Chain JD:

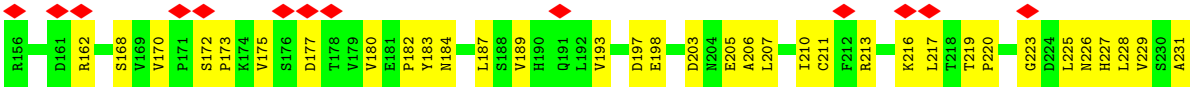


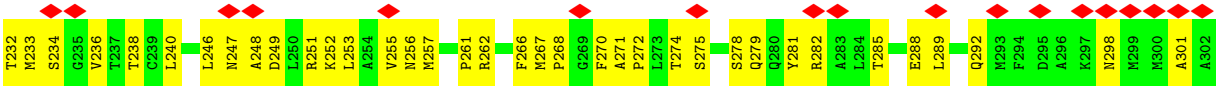


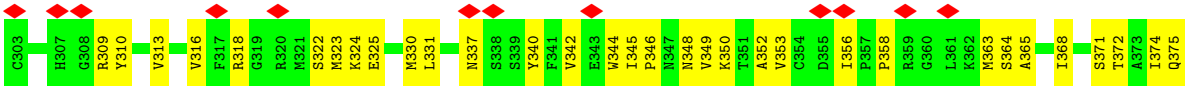
• Molecule 3: Tubulin beta-4B chain

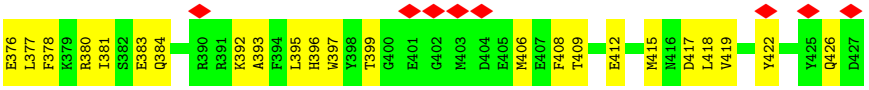




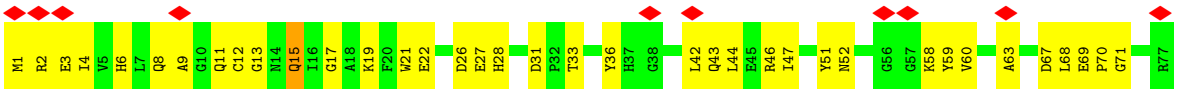


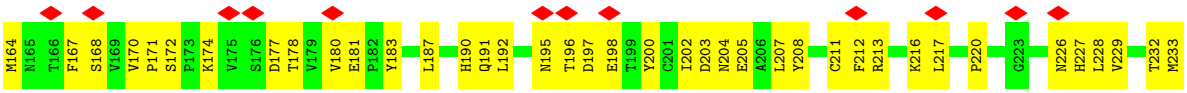


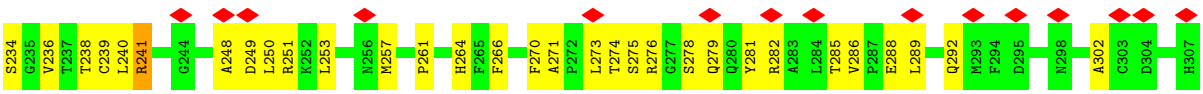


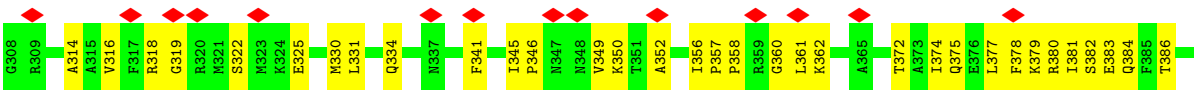


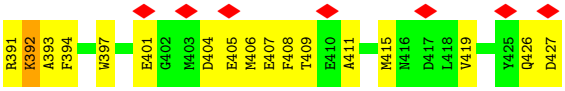
• Molecule 3: Tubulin beta-4B chain





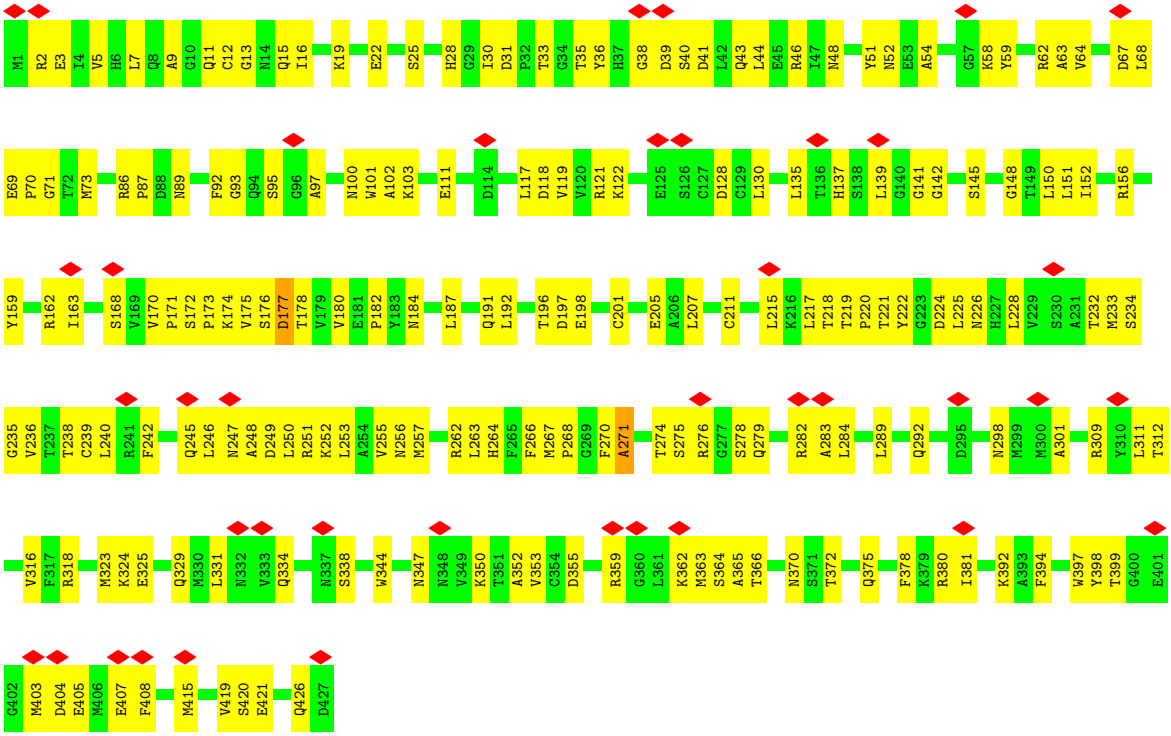






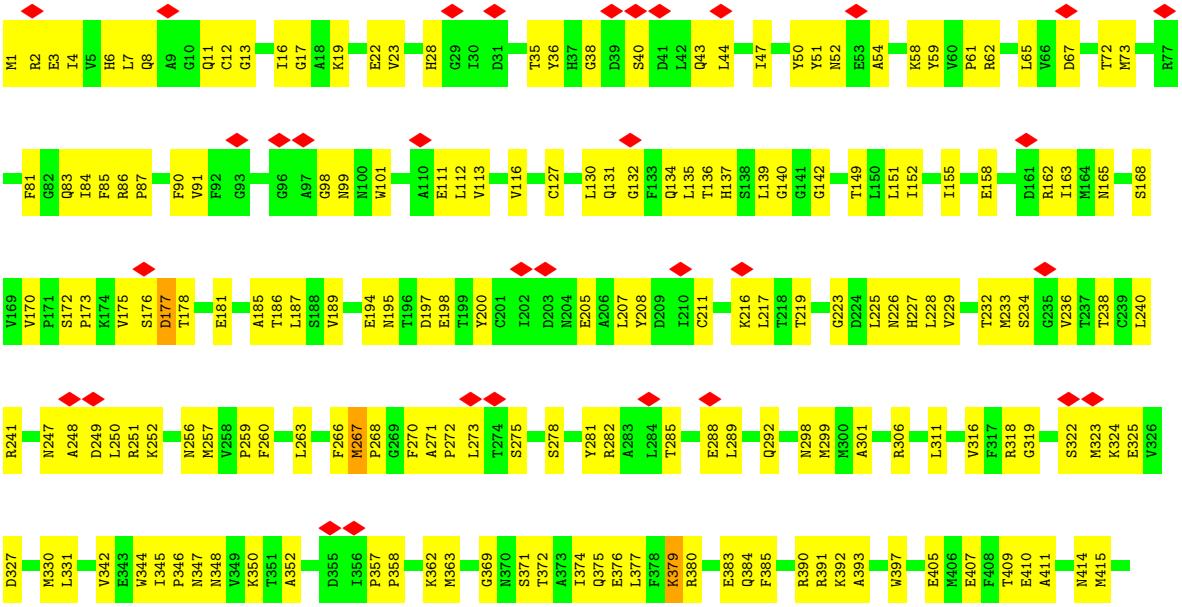
• Molecule 3: Tubulin beta-4B chain

Chain KD:



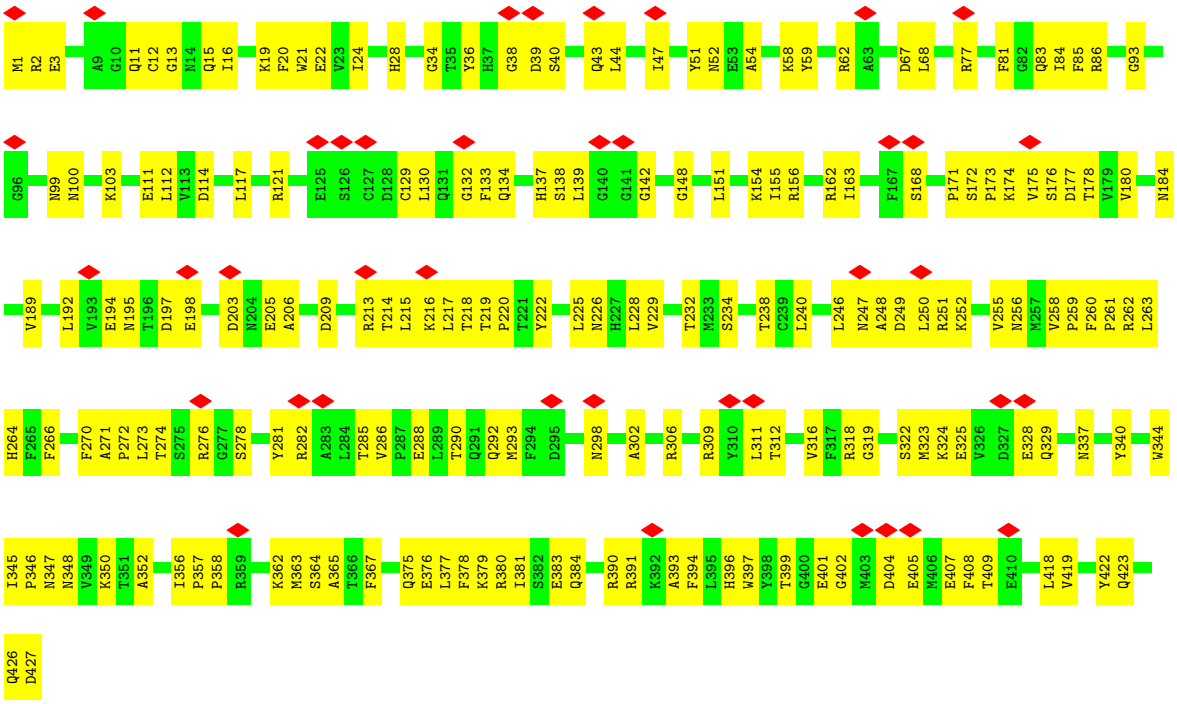
• Molecule 3: Tubulin beta-4B chain

Chain KF:



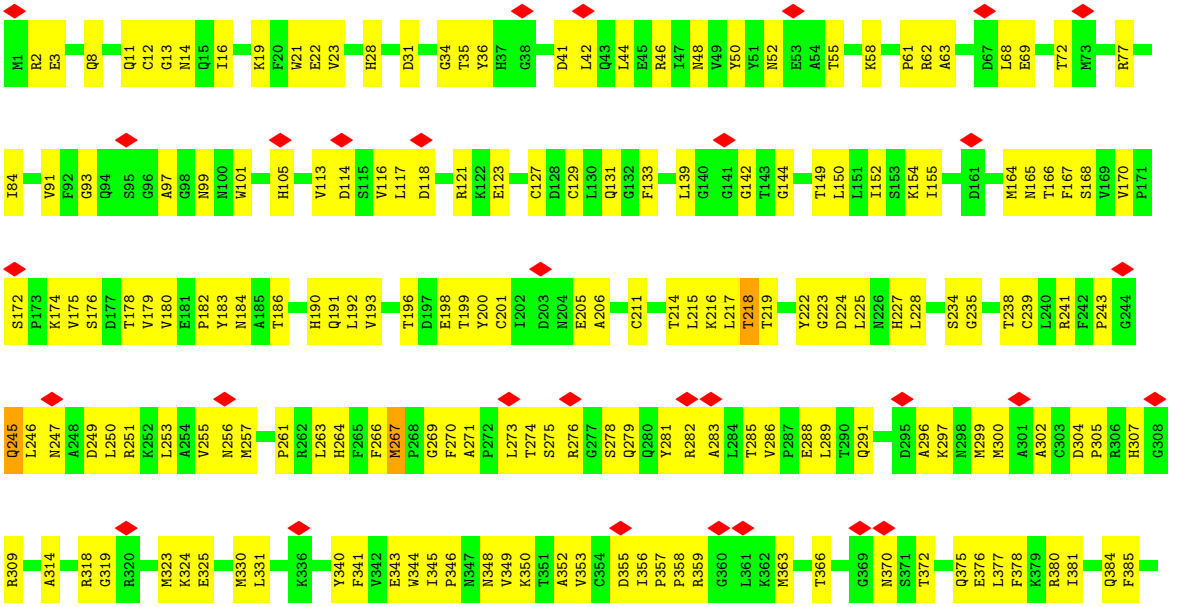
• Molecule 3: Tubulin beta-4B chain

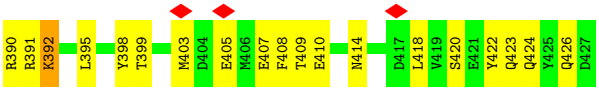
Chain KH:



• Molecule 3: Tubulin beta-4B chain

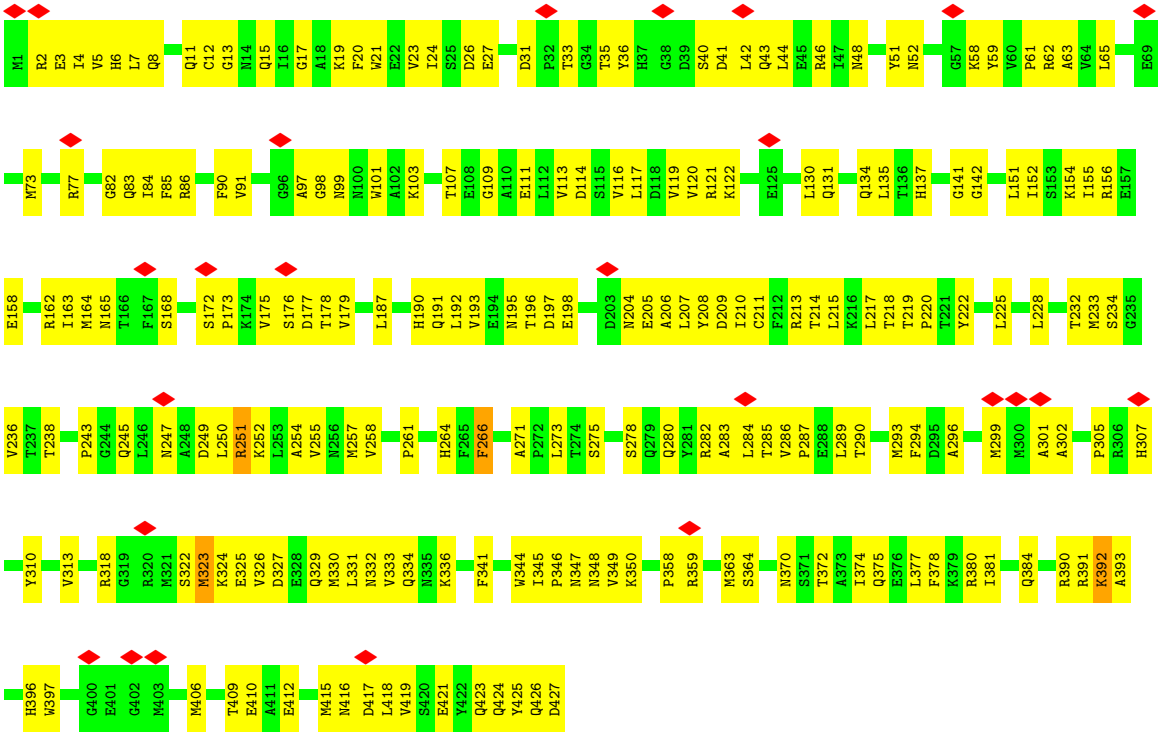
Chain LD:





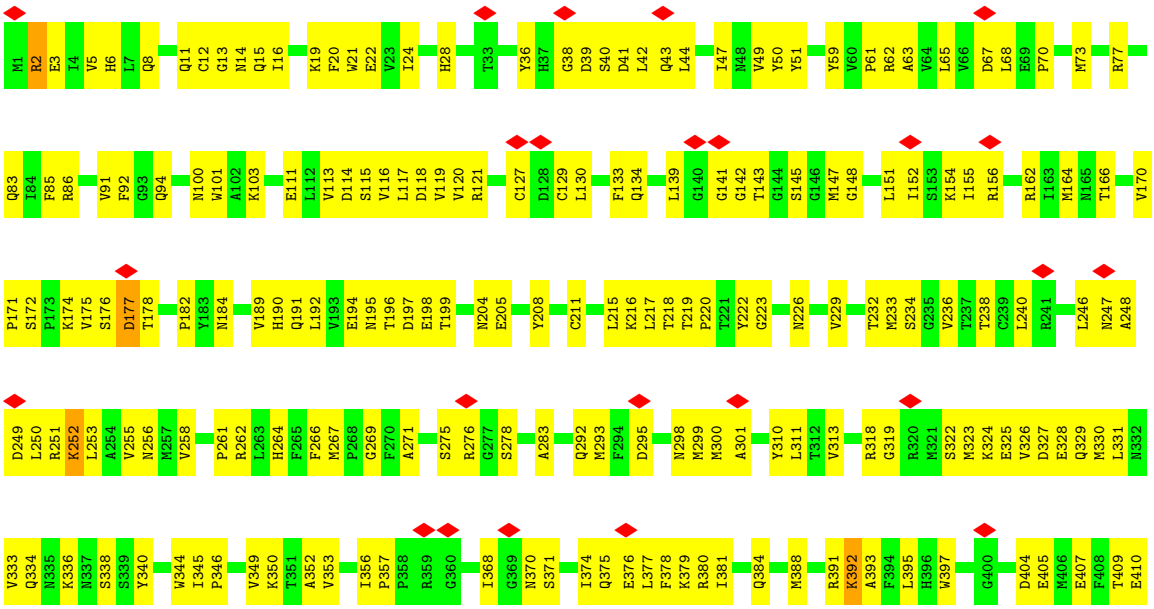
• Molecule 3: Tubulin beta-4B chain

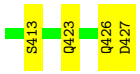
Chain LF:



• Molecule 3: Tubulin beta-4B chain

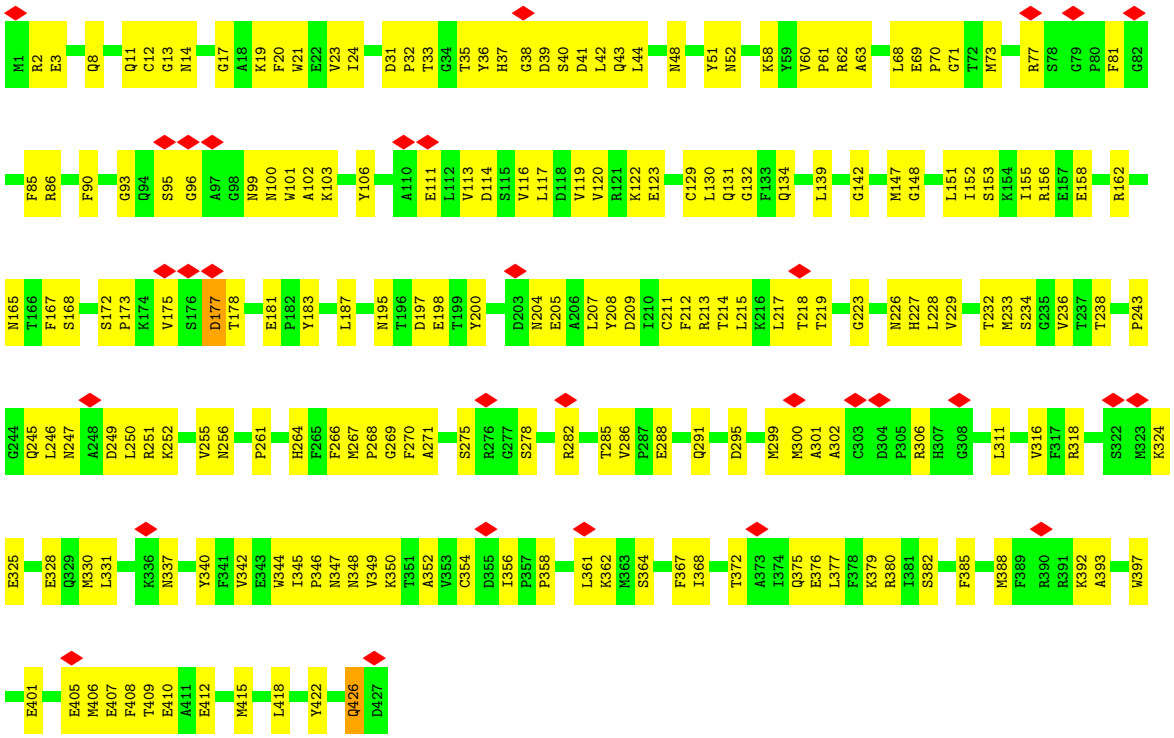
Chain LH:





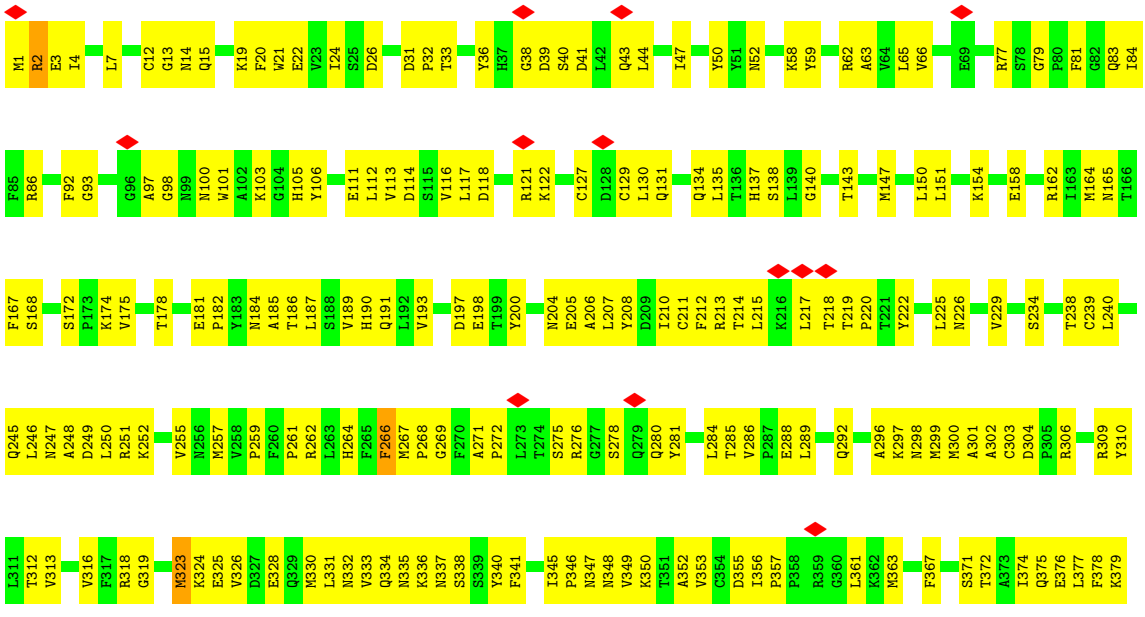
• Molecule 3: Tubulin beta-4B chain

Chain MF:



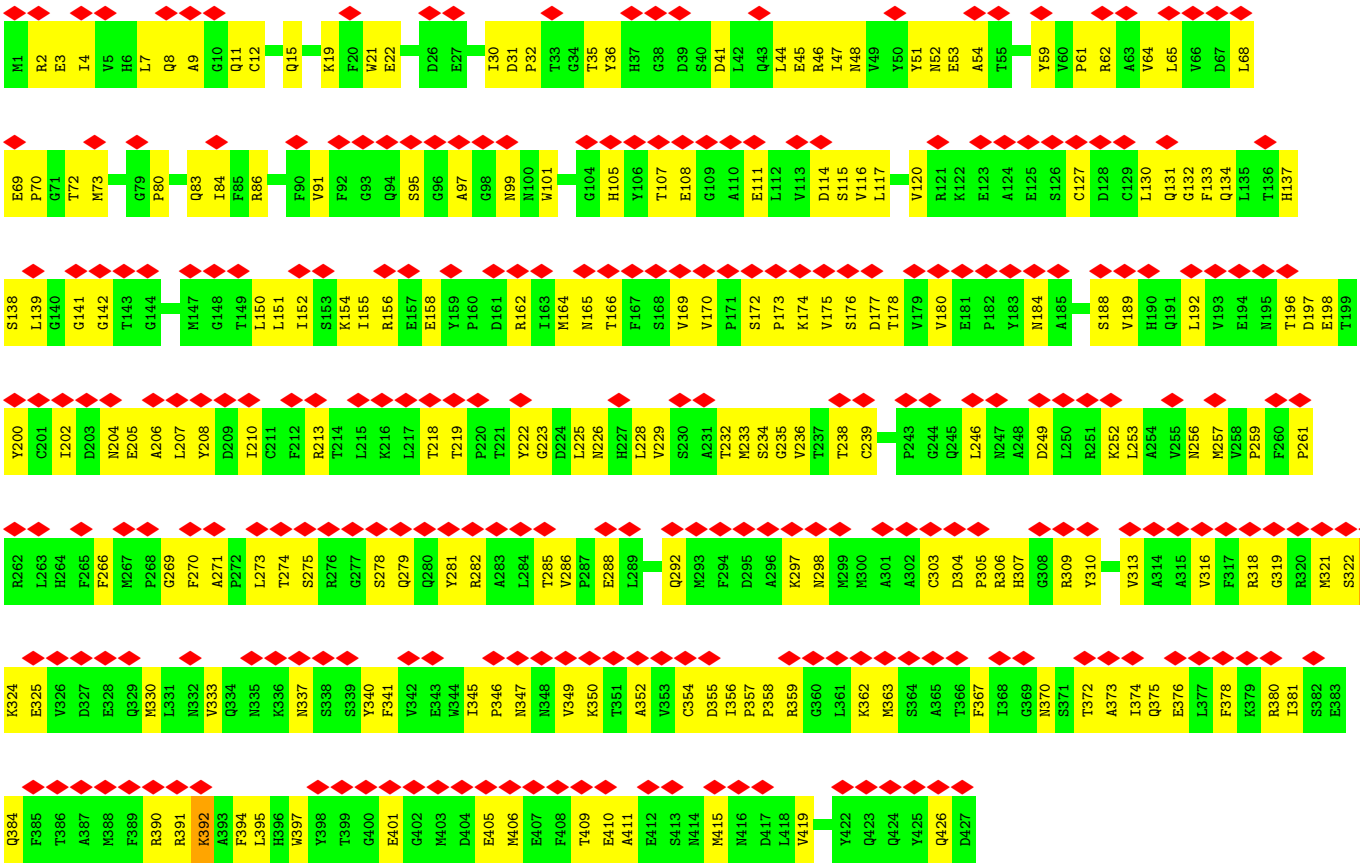
• Molecule 3: Tubulin beta-4B chain

Chain MH:



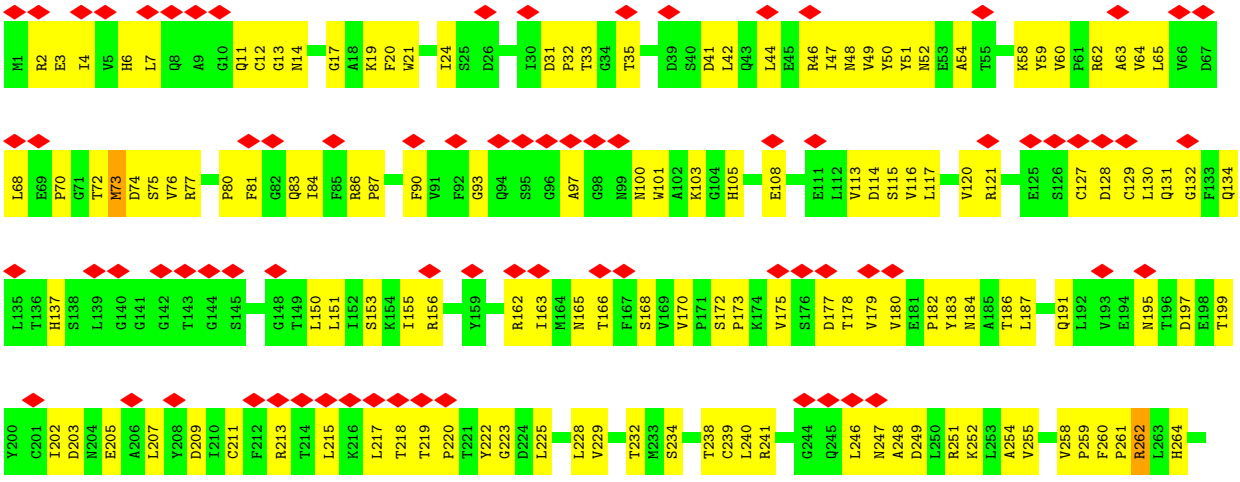
• Molecule 3: Tubulin beta-4B chain

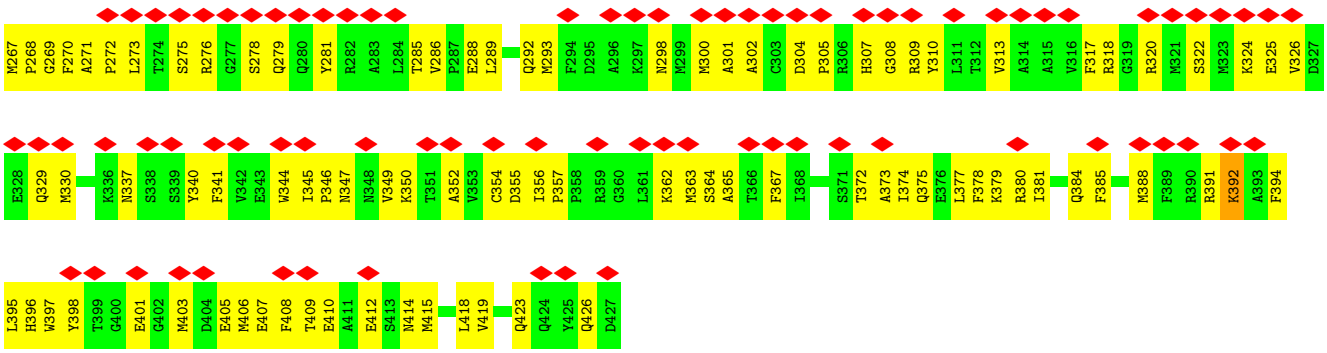
Chain ND:



• Molecule 3: Tubulin beta-4B chain

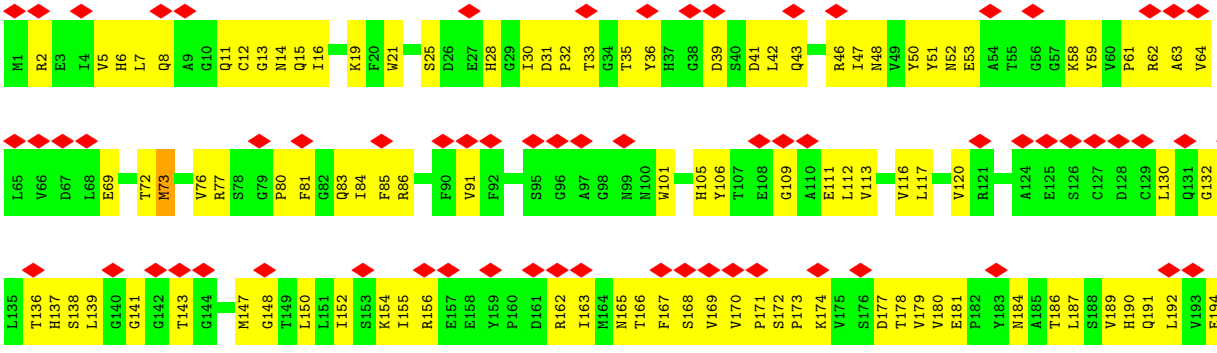
Chain NF:





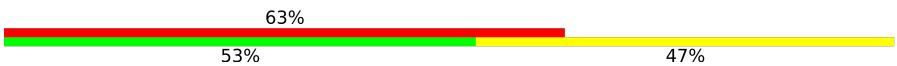
• Molecule 3: Tubulin beta-4B chain

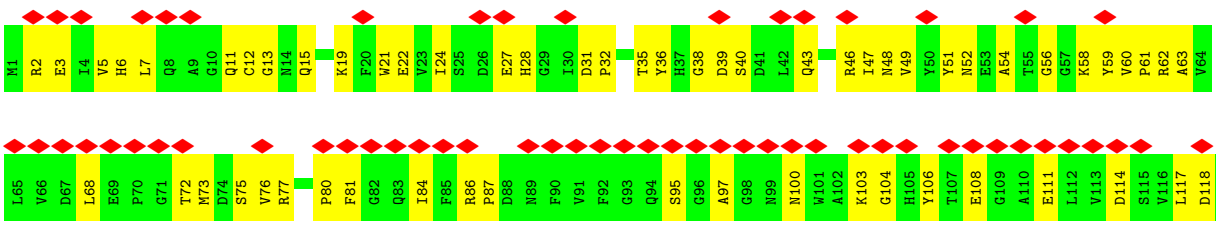
Chain NH:

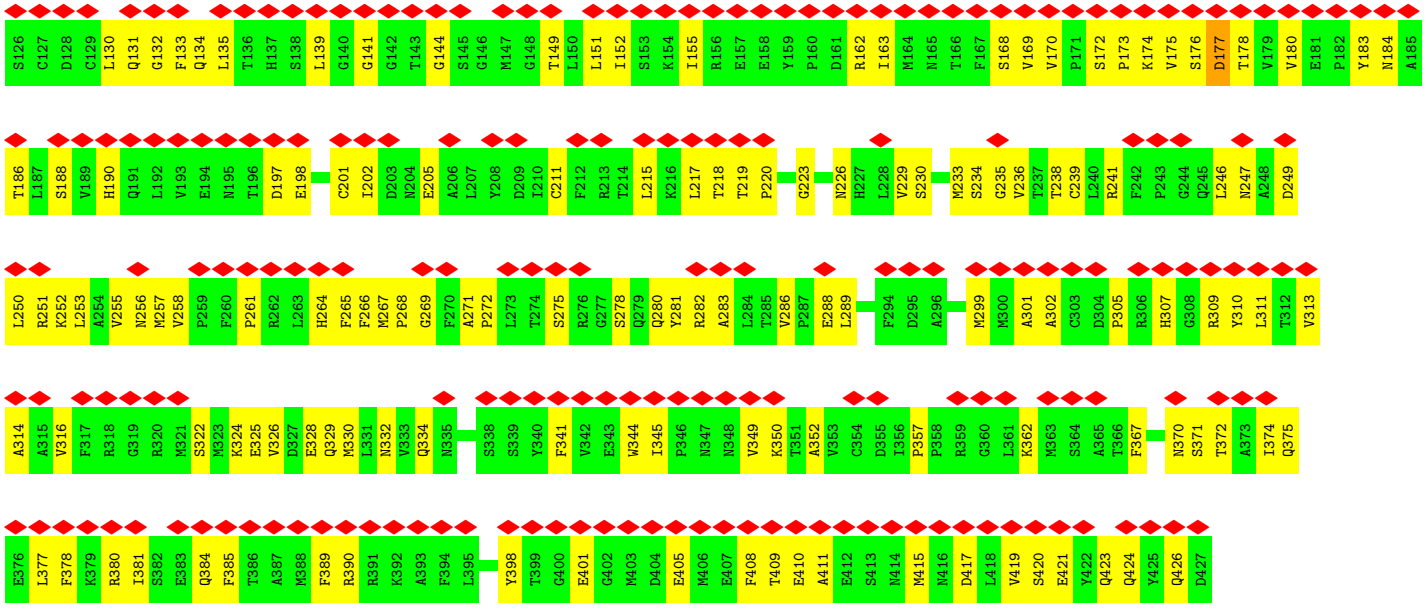


• Molecule 3: Tubulin beta-4B chain

Chain OD:

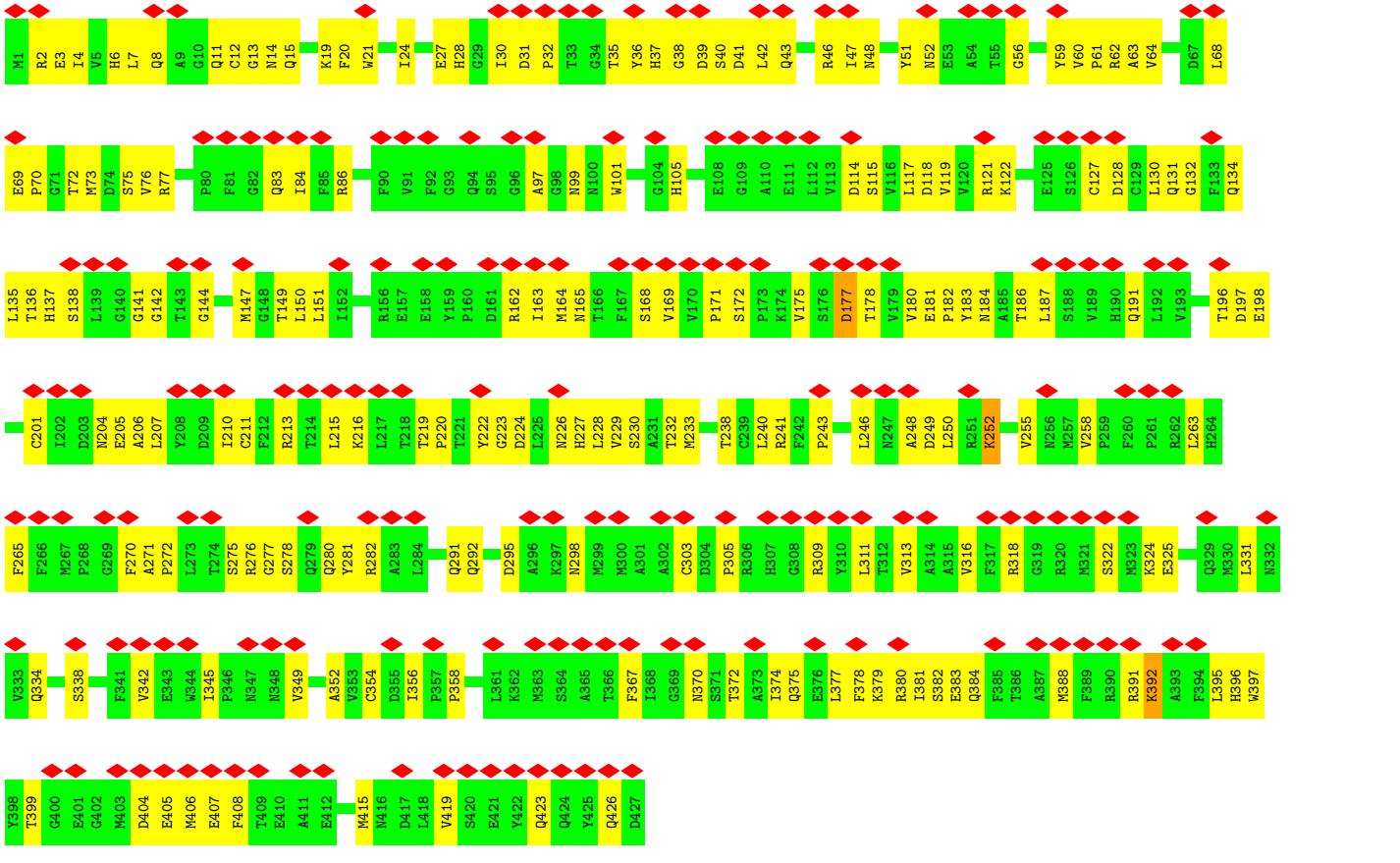






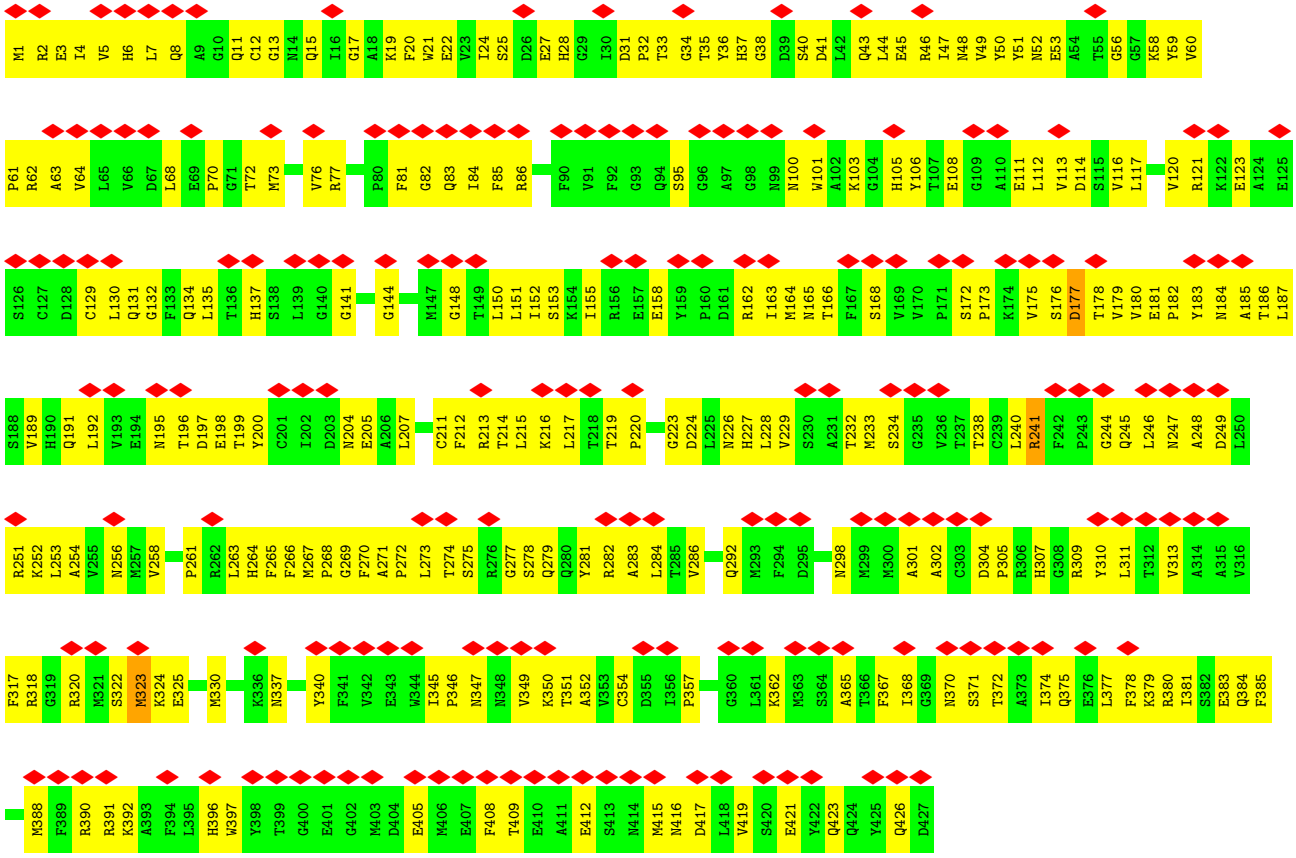
• Molecule 3: Tubulin beta-4B chain

Chain OF:



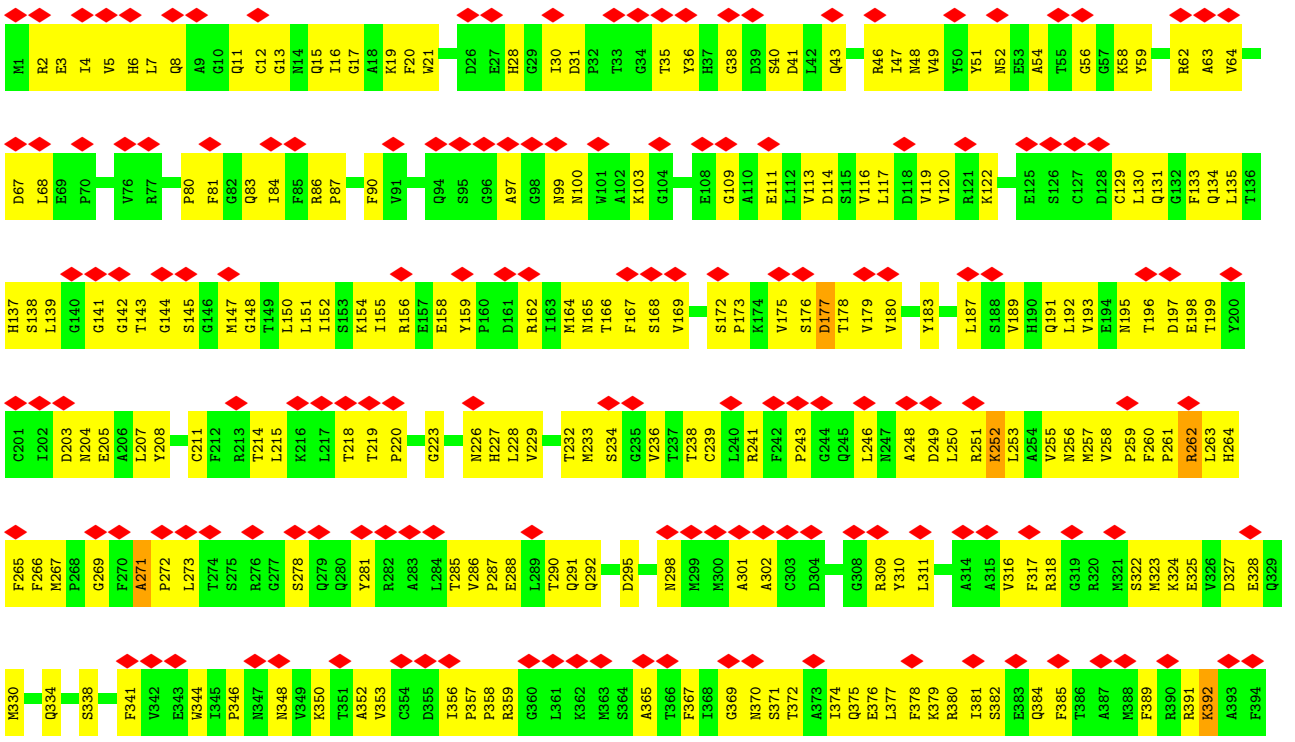
• Molecule 3: Tubulin beta-4B chain

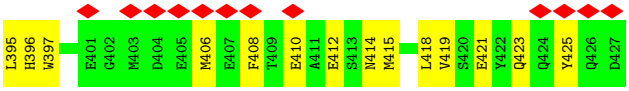
Chain OH:



• Molecule 3: Tubulin beta-4B chain

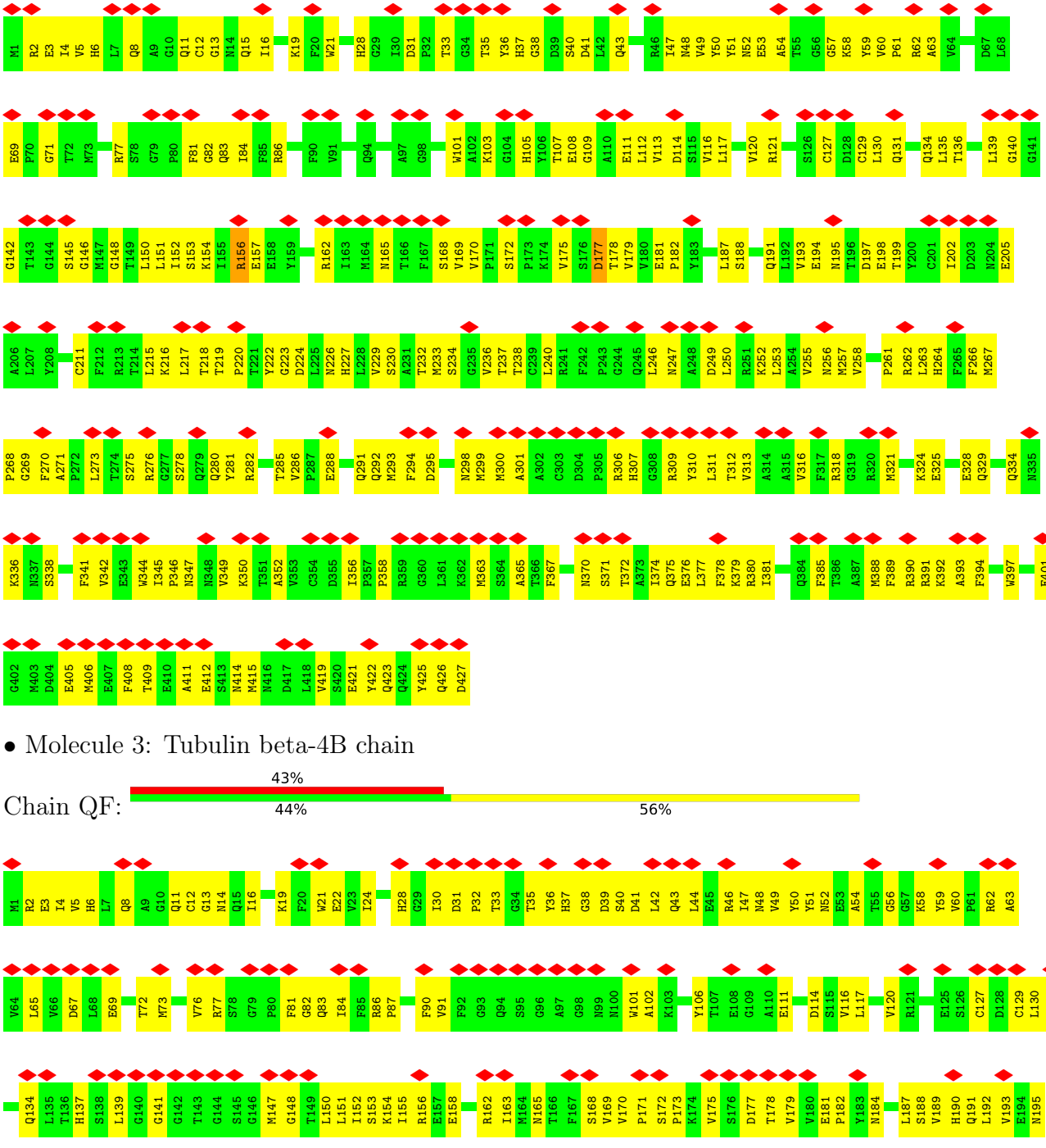
Chain PF:





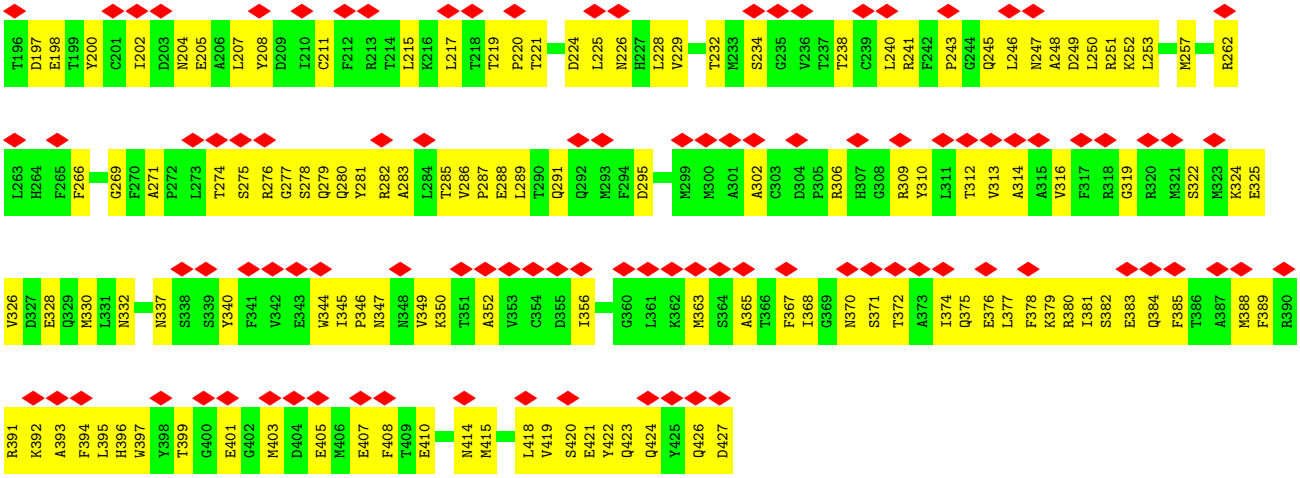
• Molecule 3: Tubulin beta-4B chain

Chain PH:



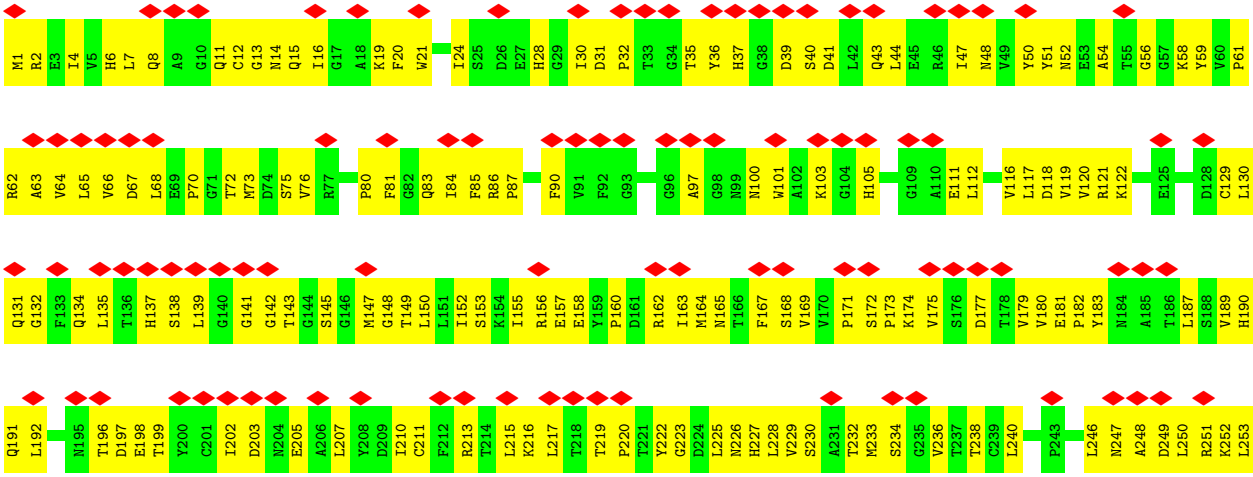
• Molecule 3: Tubulin beta-4B chain

Chain QF:



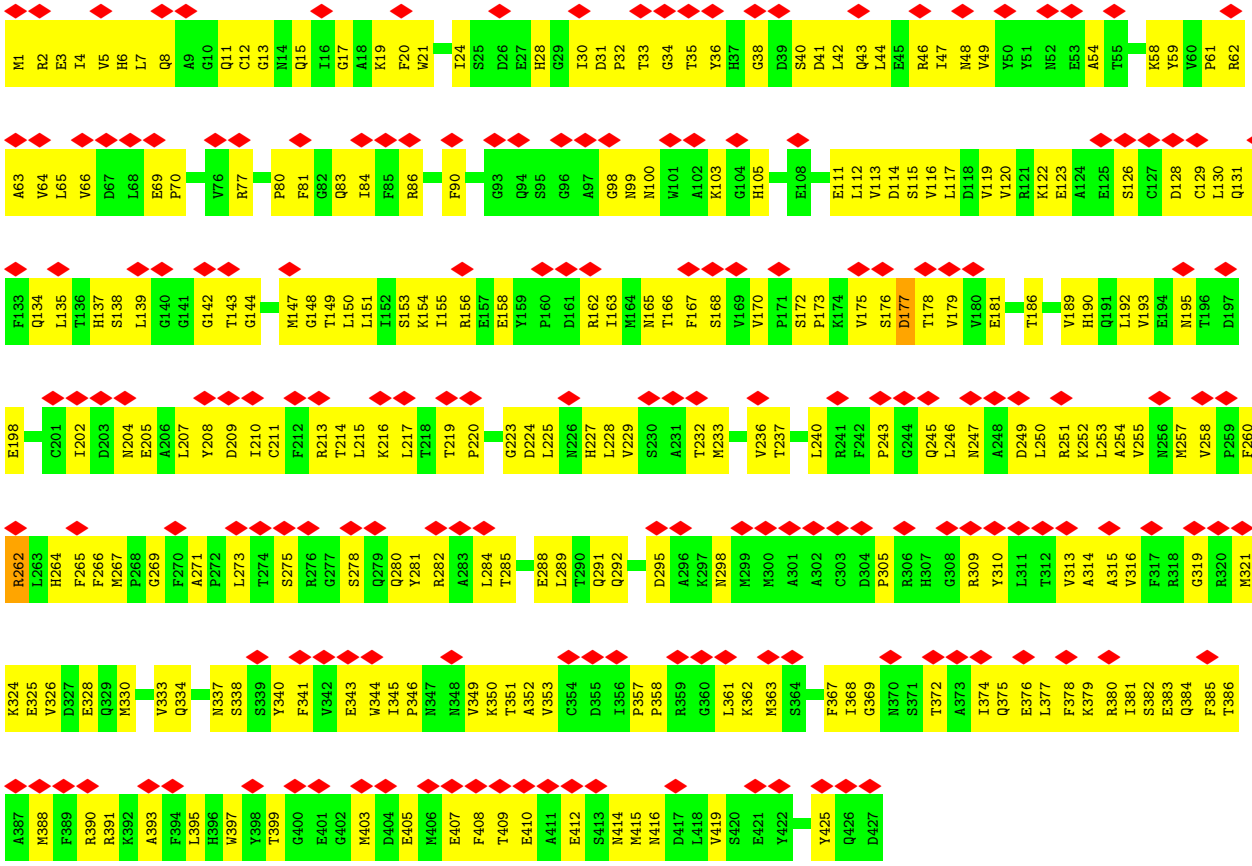
• Molecule 3: Tubulin beta-4B chain

Chain QH:



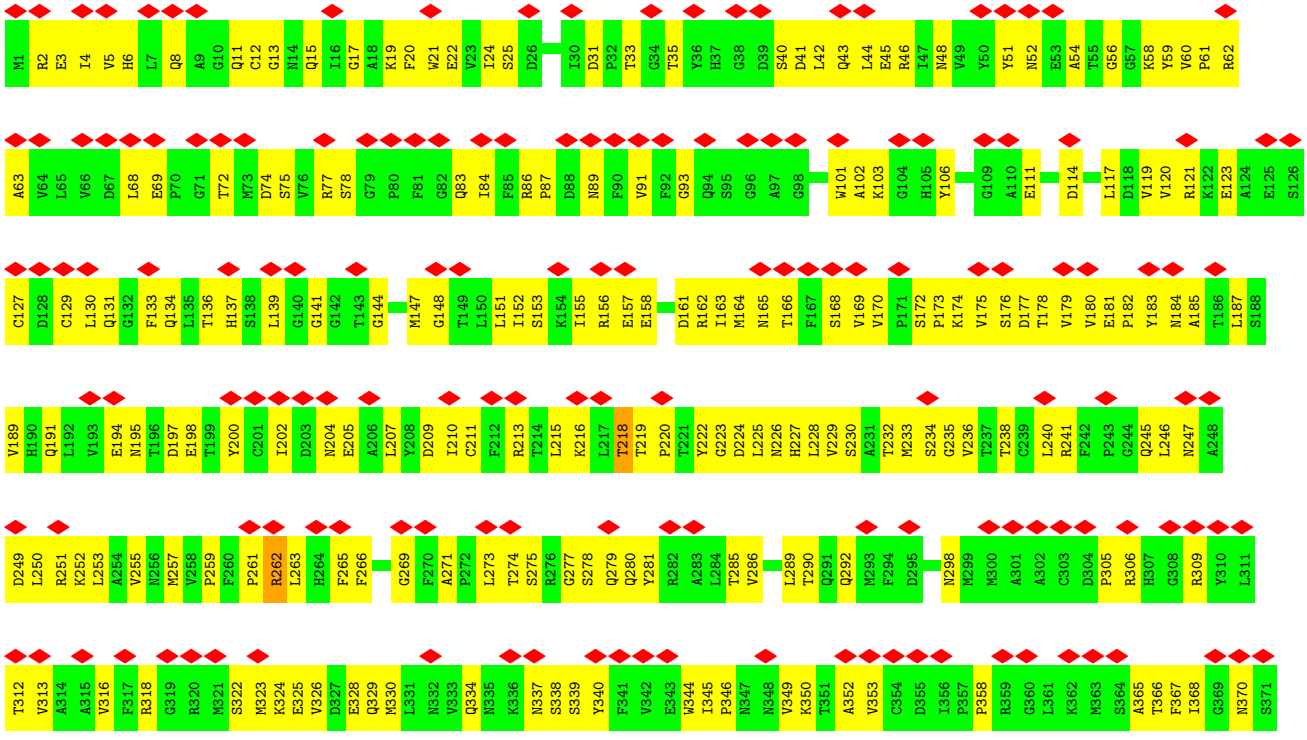
• Molecule 3: Tubulin beta-4B chain

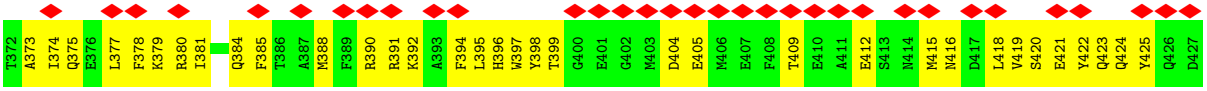
Chain RF:



• Molecule 3: Tubulin beta-4B chain

Chain RH:



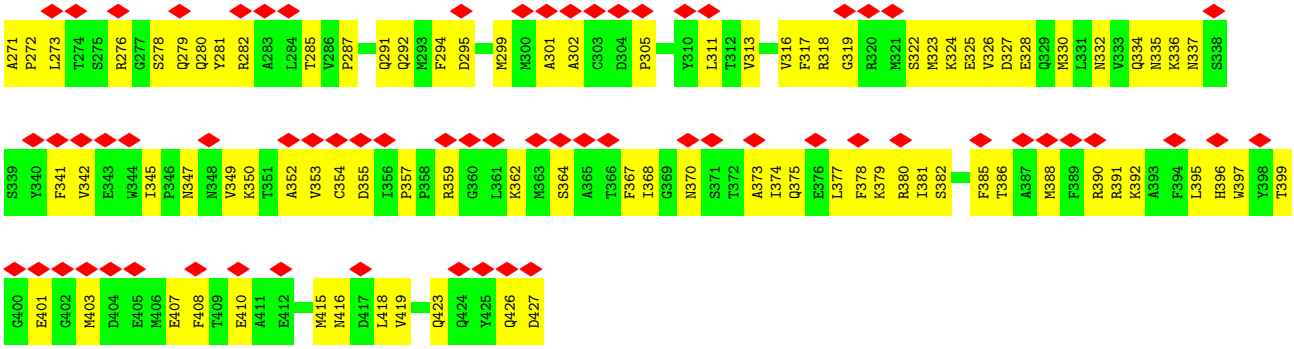


• Molecule 3: Tubulin beta-4B chain

Chain RJ:

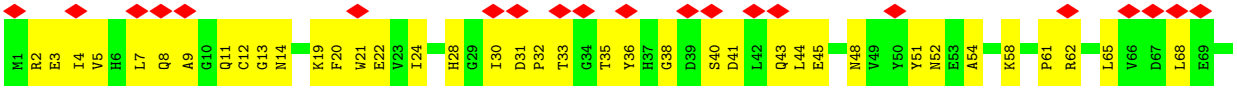
• Molecule 3: Tubulin beta-4B chain

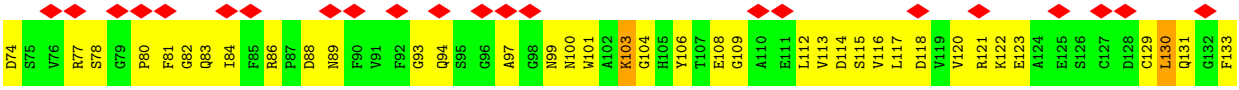
Chain SF:

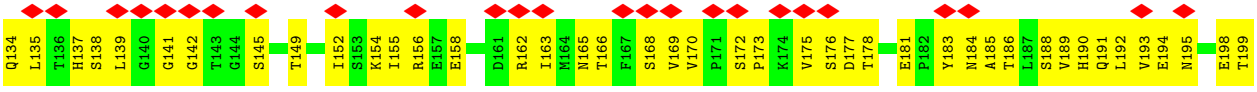


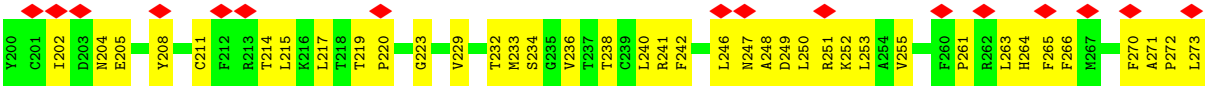
• Molecule 3: Tubulin beta-4B chain

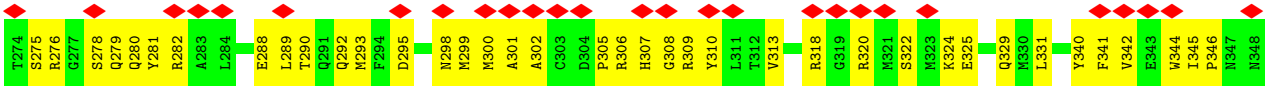
Chain SH:

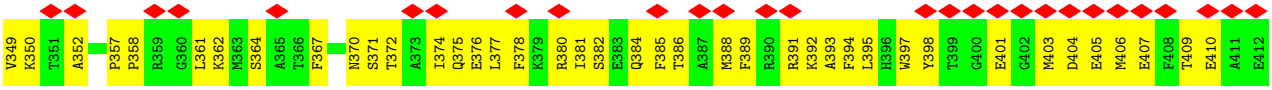


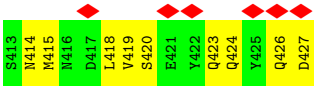






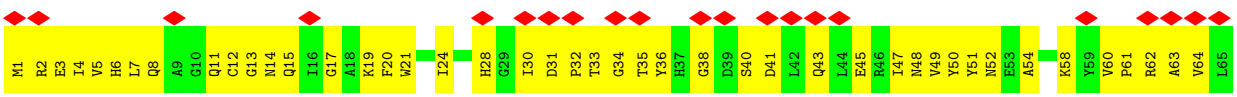


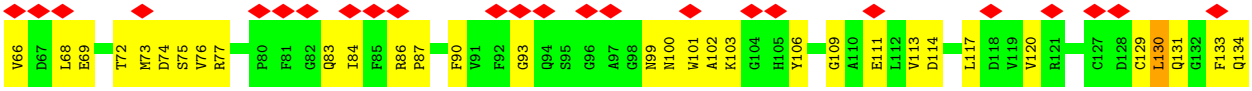


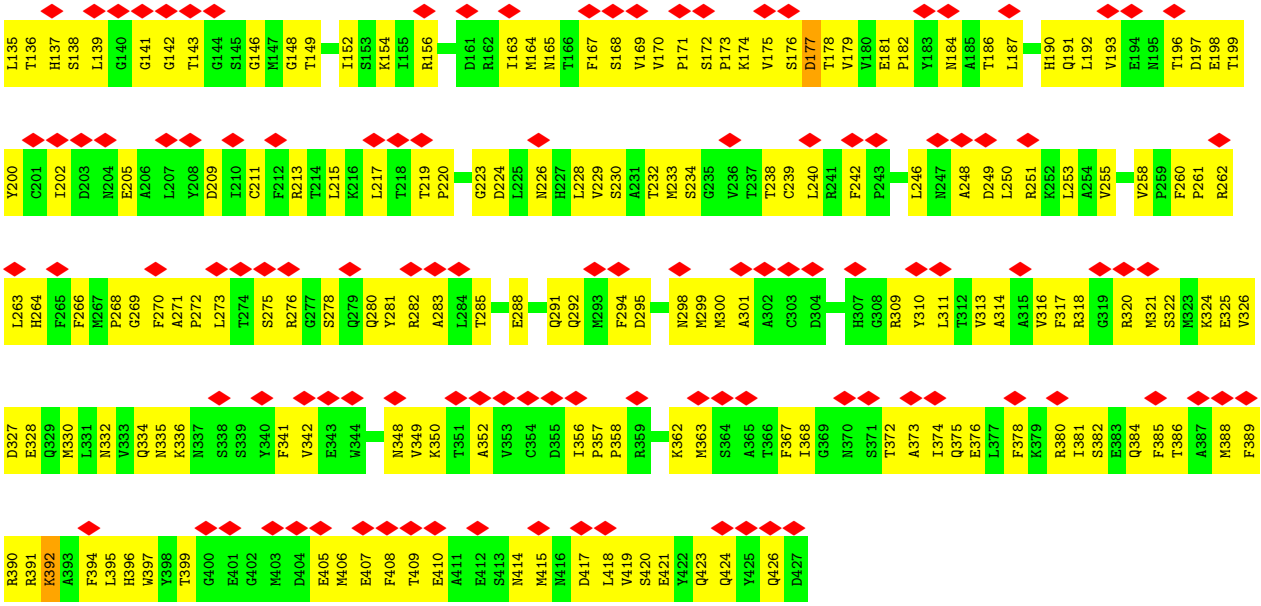


• Molecule 3: Tubulin beta-4B chain

Chain SJ:

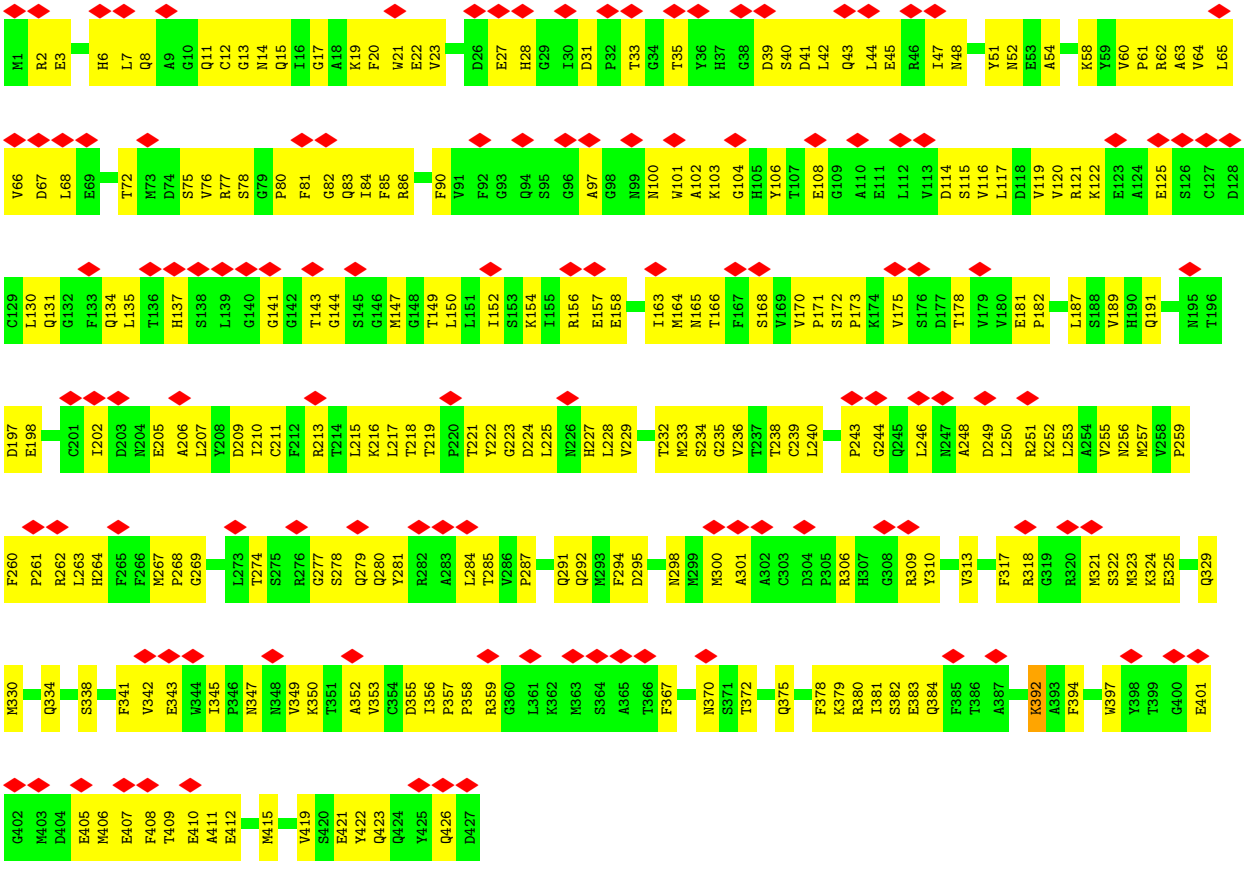






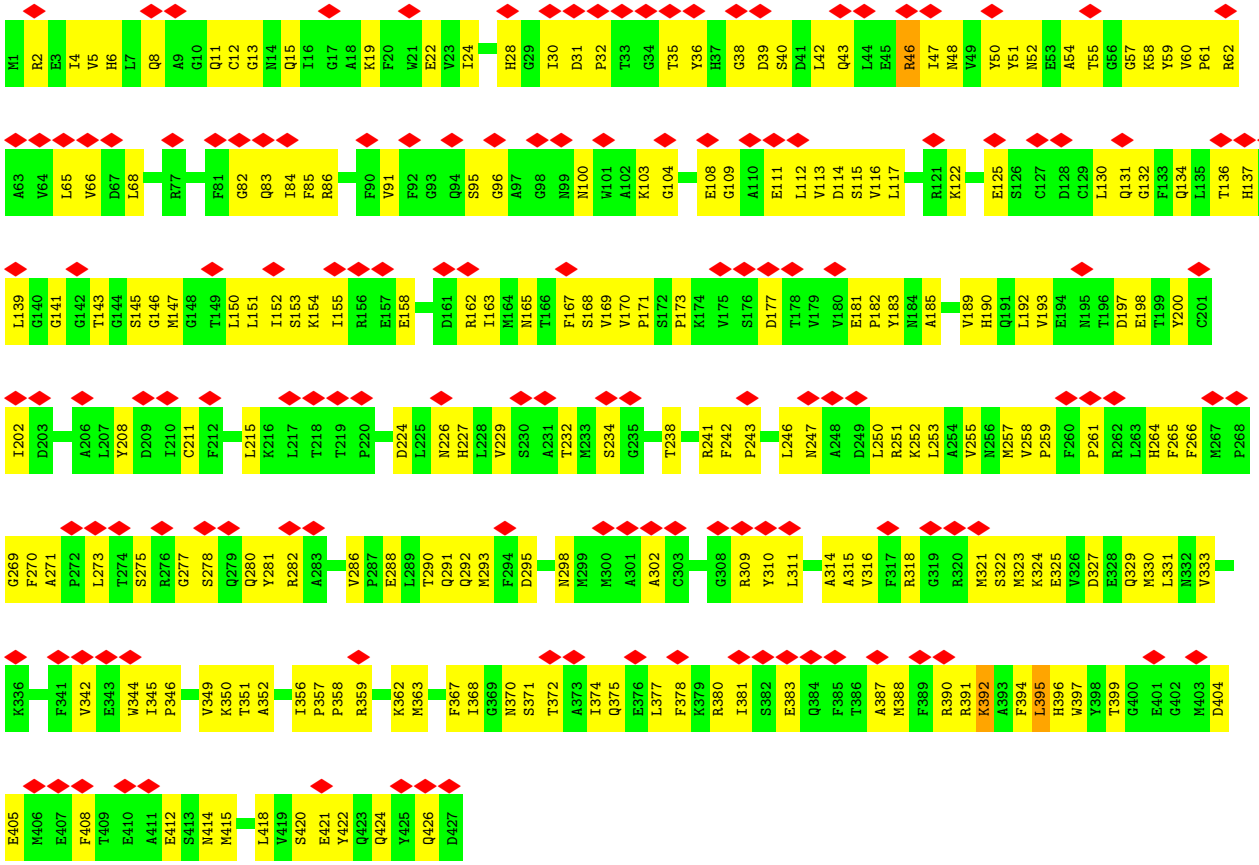
• Molecule 3: Tubulin beta-4B chain

Chain TF:



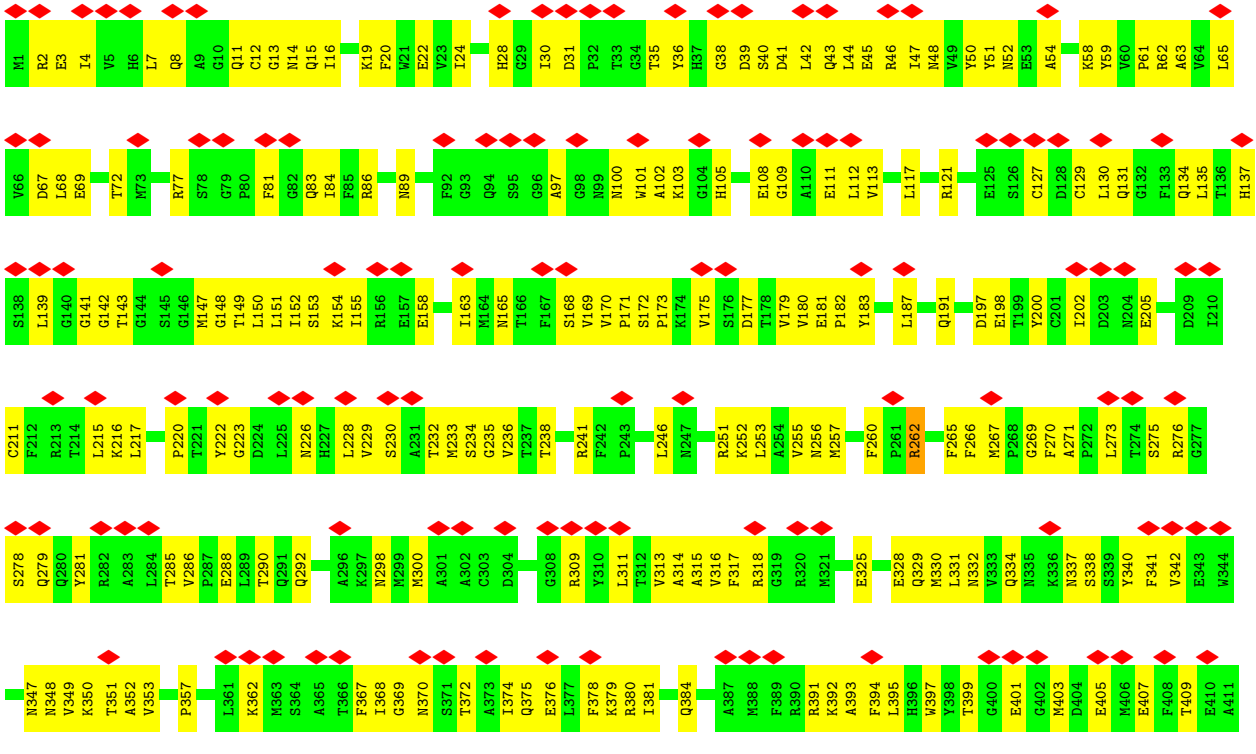
• Molecule 3: Tubulin beta-4B chain

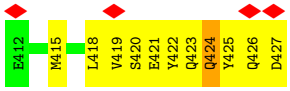
Chain TH:



• Molecule 3: Tubulin beta-4B chain

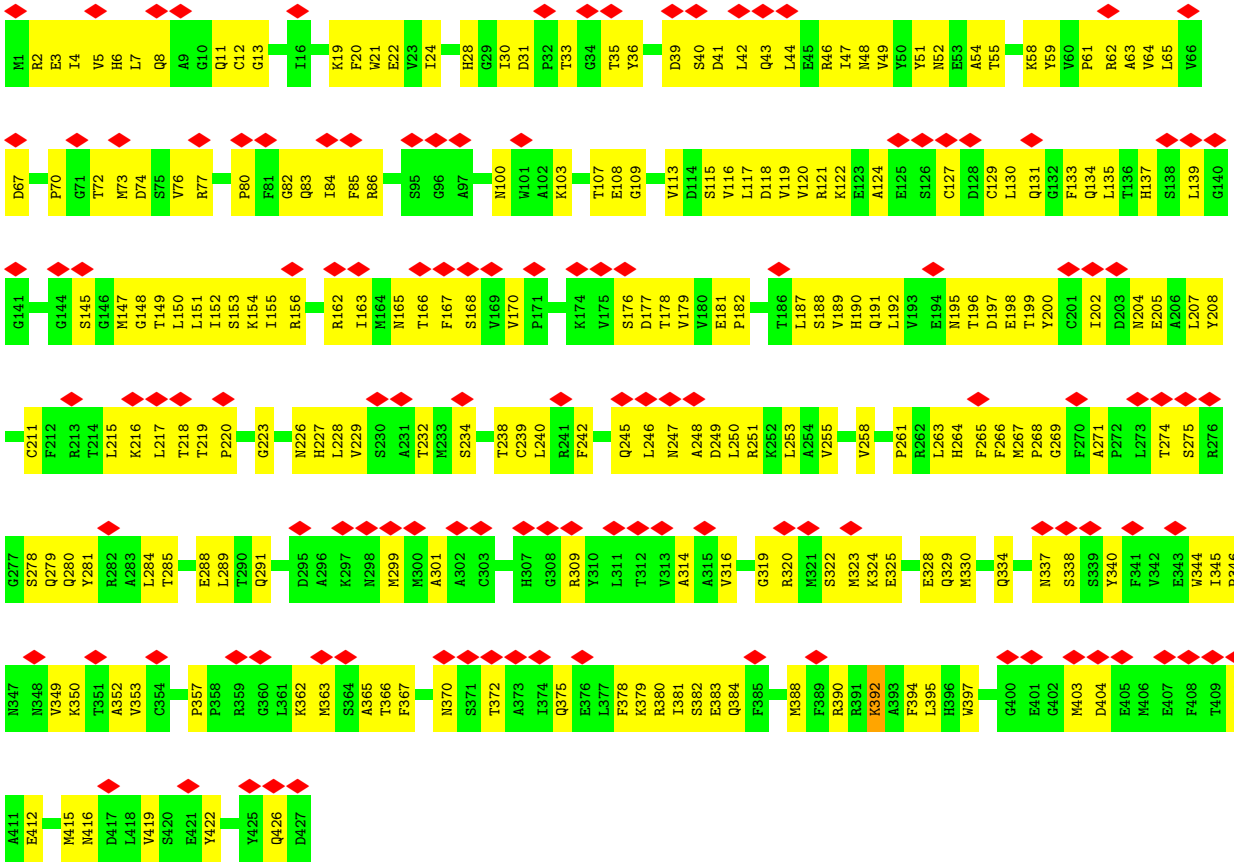
Chain TJ:





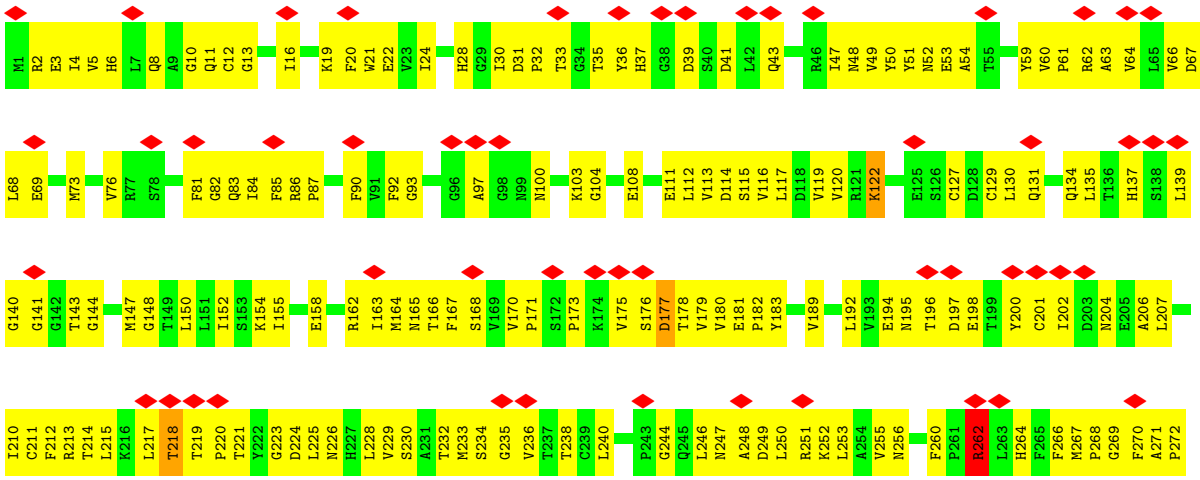
• Molecule 3: Tubulin beta-4B chain

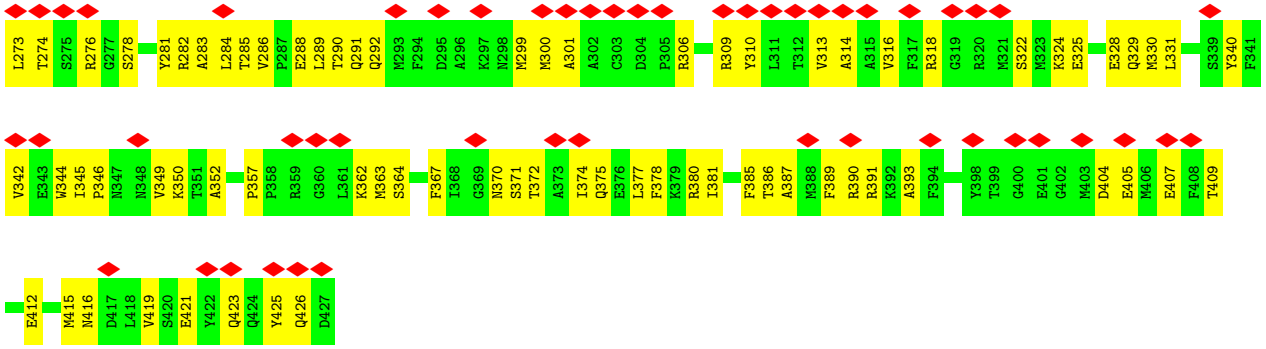
Chain UD:



• Molecule 3: Tubulin beta-4B chain

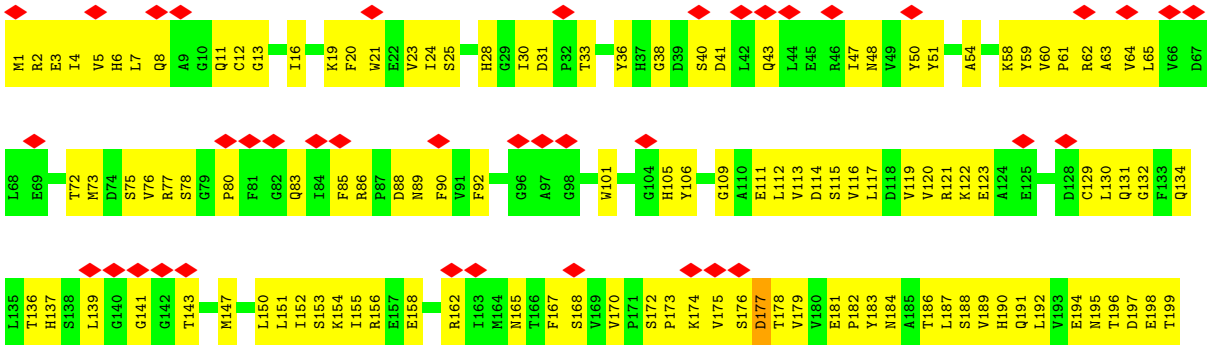
Chain UF:





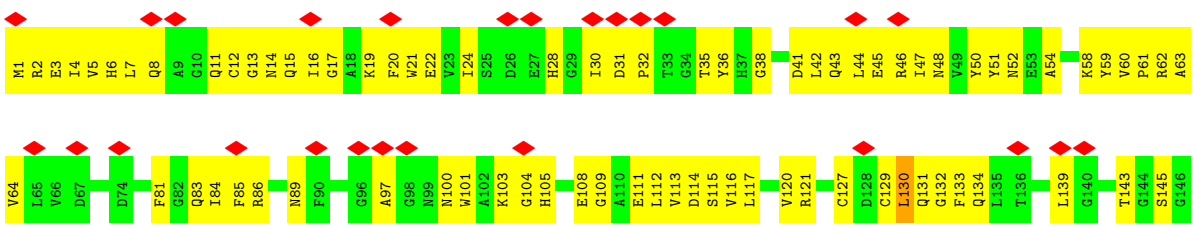
• Molecule 3: Tubulin beta-4B chain

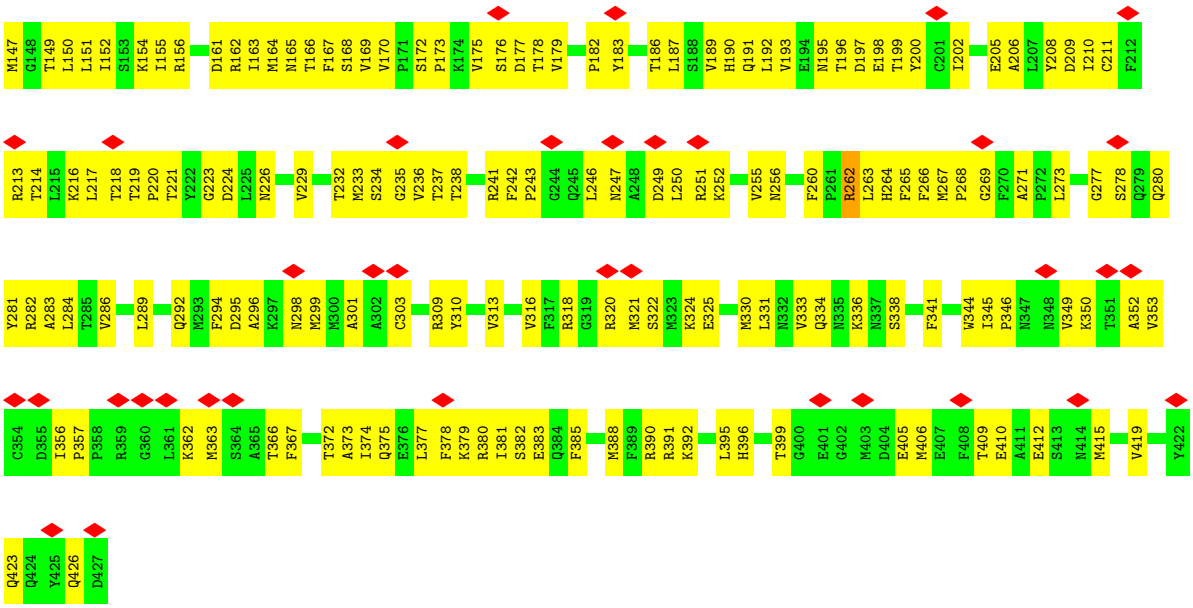
Chain UH:



• Molecule 3: Tubulin beta-4B chain

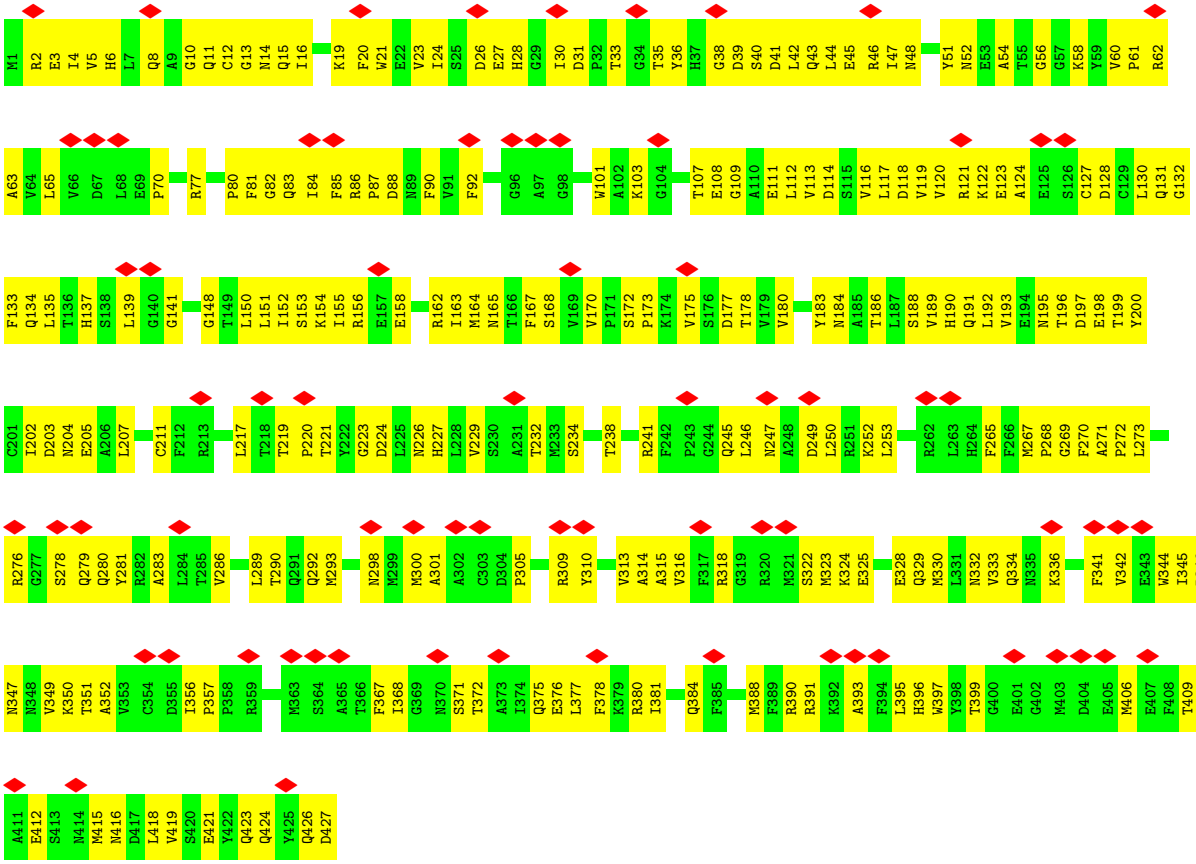
Chain VD:





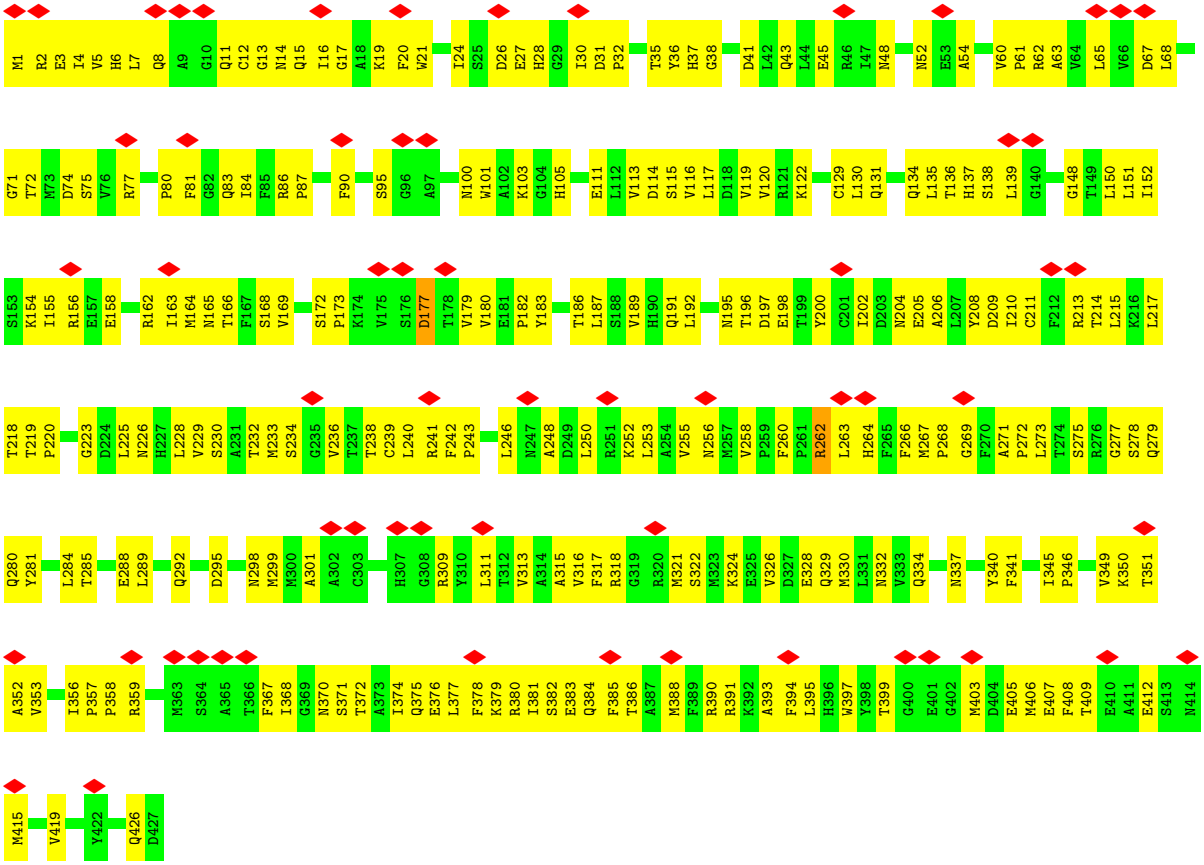
• Molecule 3: Tubulin beta-4B chain

Chain VF:



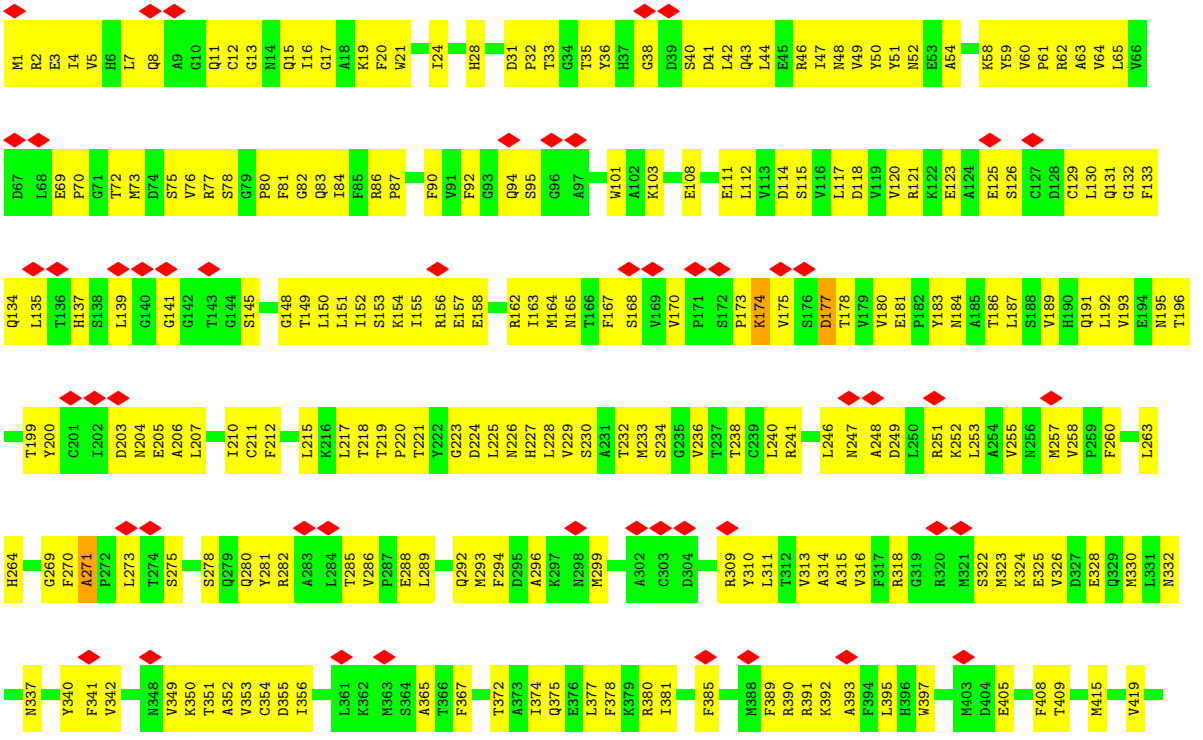
• Molecule 3: Tubulin beta-4B chain

Chain VH:



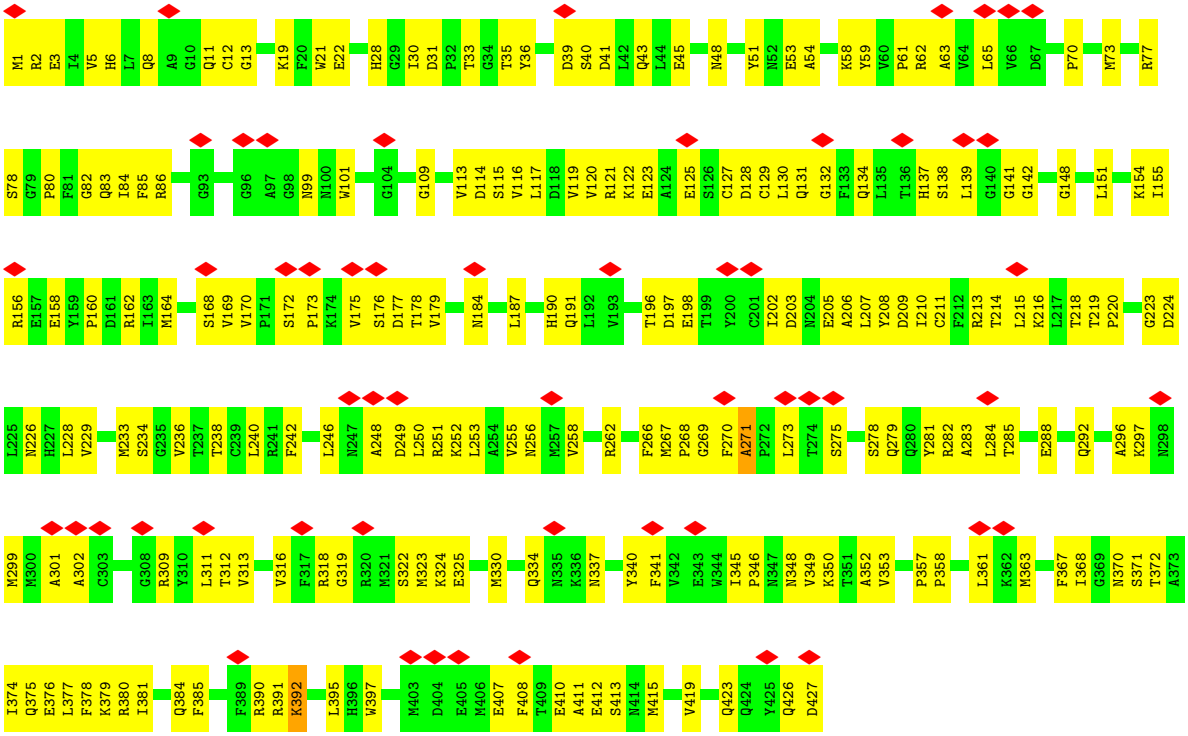
• Molecule 3: Tubulin beta-4B chain

Chain WF: 12% 44% 55%



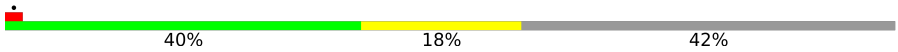
• Molecule 3: Tubulin beta-4B chain

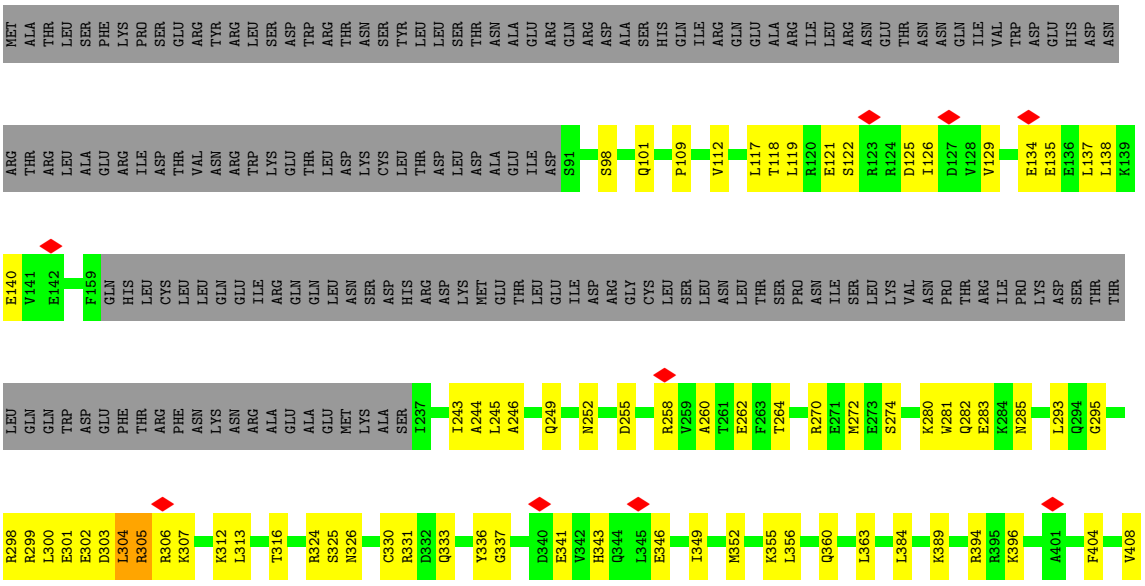
Chain WH:

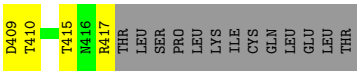


• Molecule 4: Tektin-2

Chain B2:

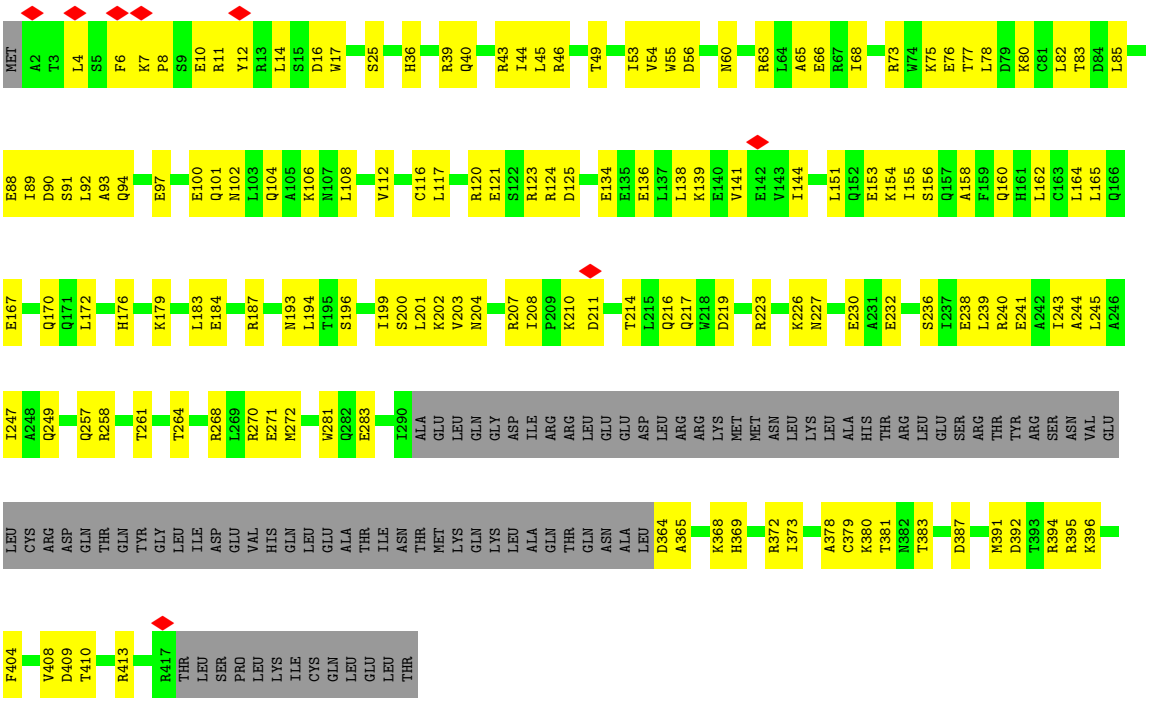






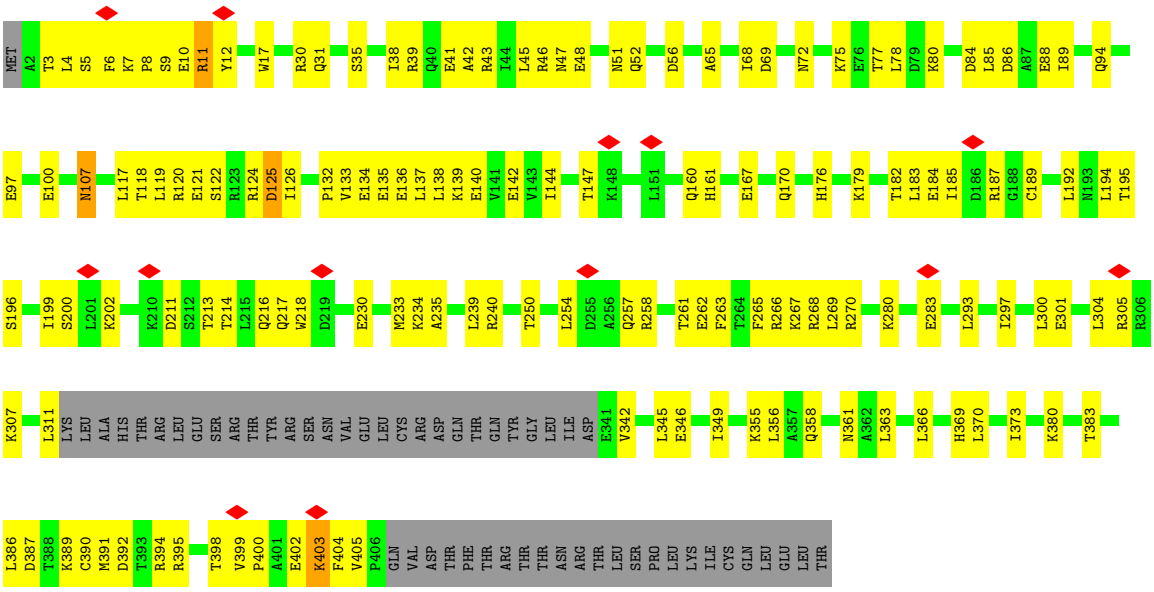
• Molecule 4: Tektin-2

Chain B3:



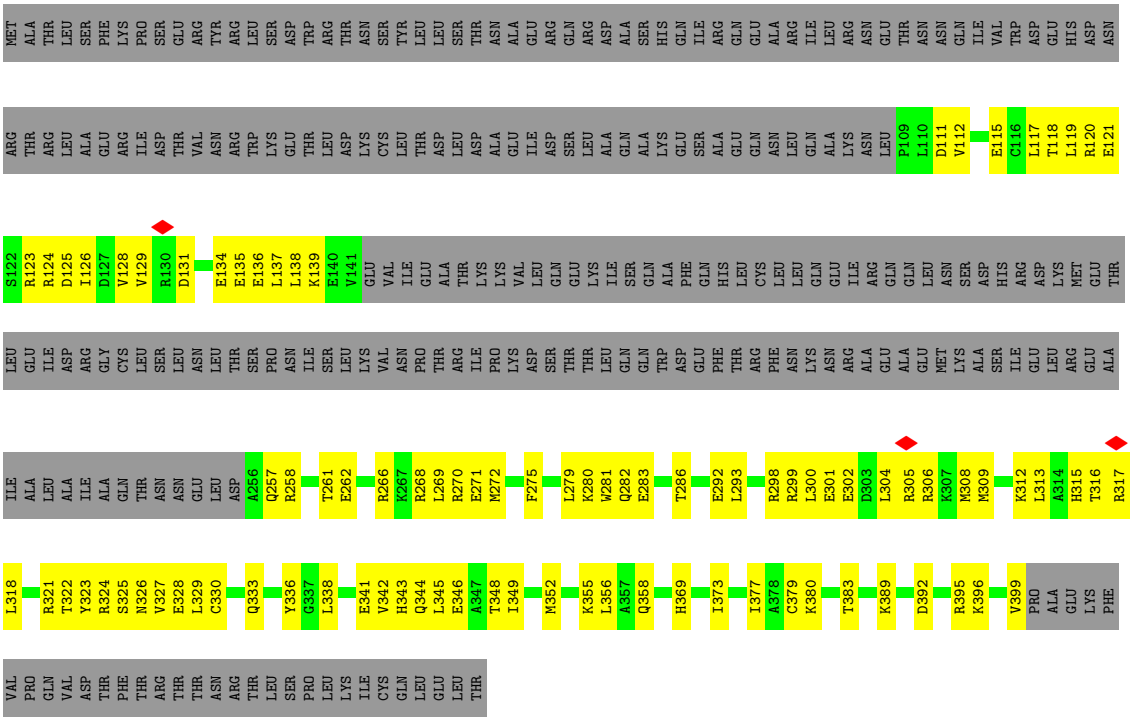
• Molecule 4: Tektin-2

Chain B7:



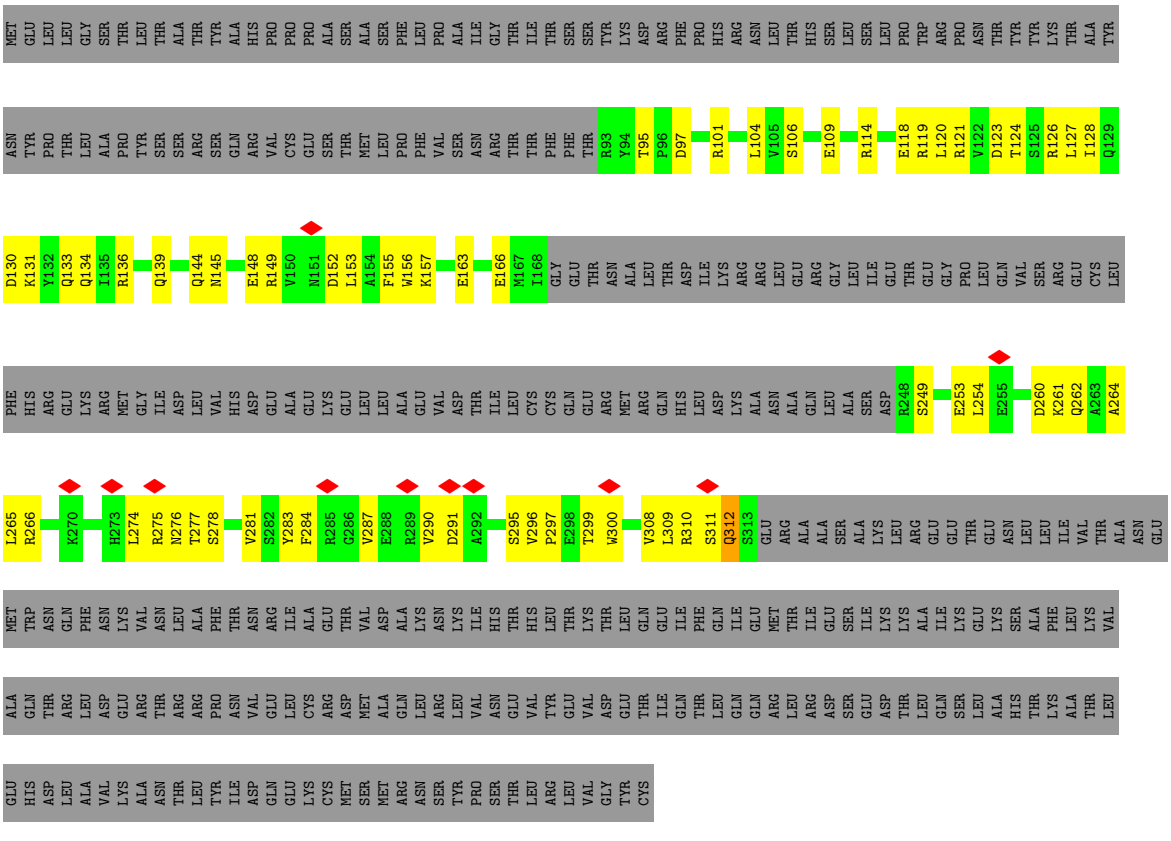
• Molecule 4: Tektin-2

Chain B8:



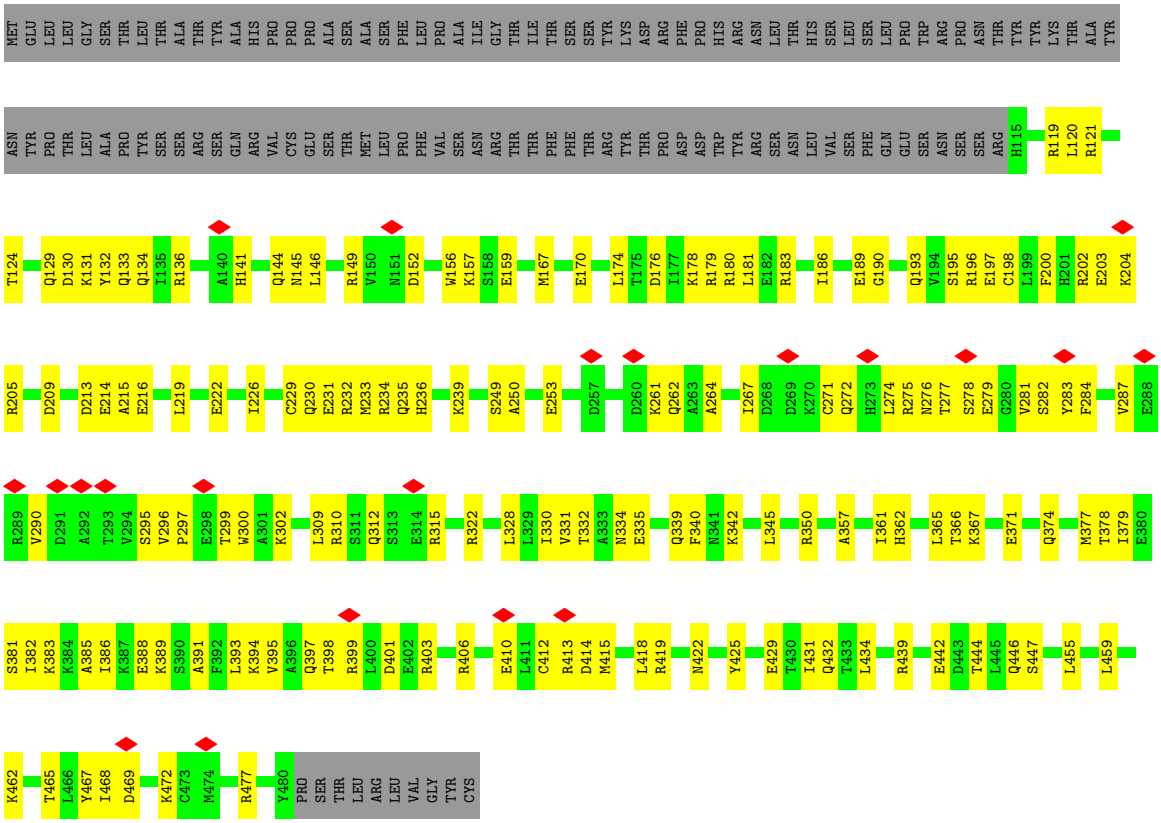
• Molecule 5: Tektin-3

Chain C2:



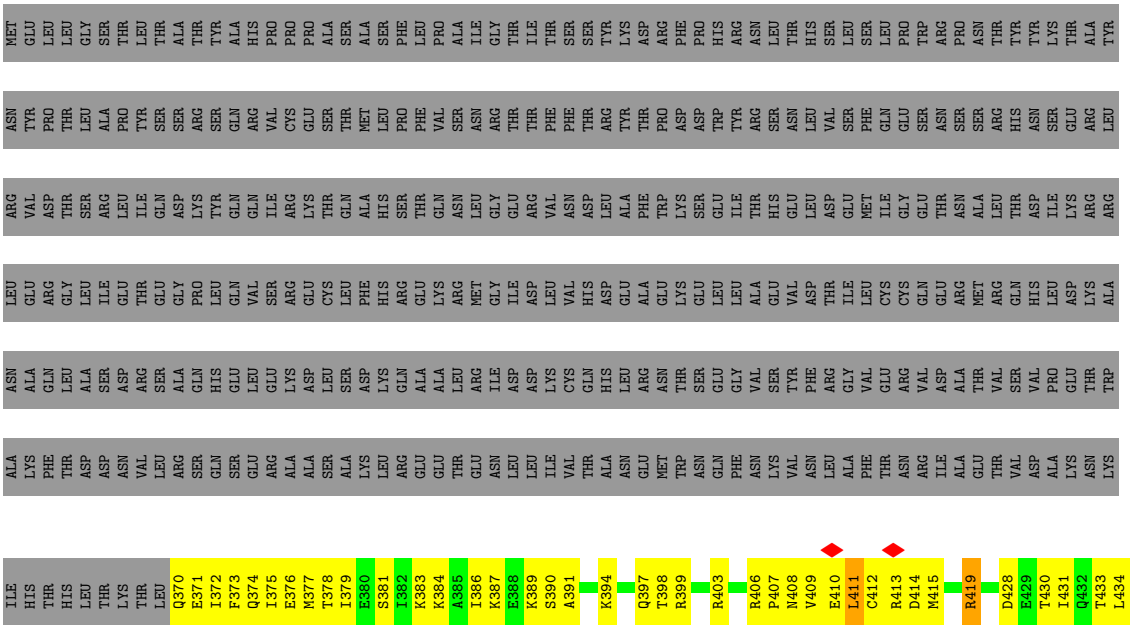
• Molecule 5: Tektin-3

Chain C3:



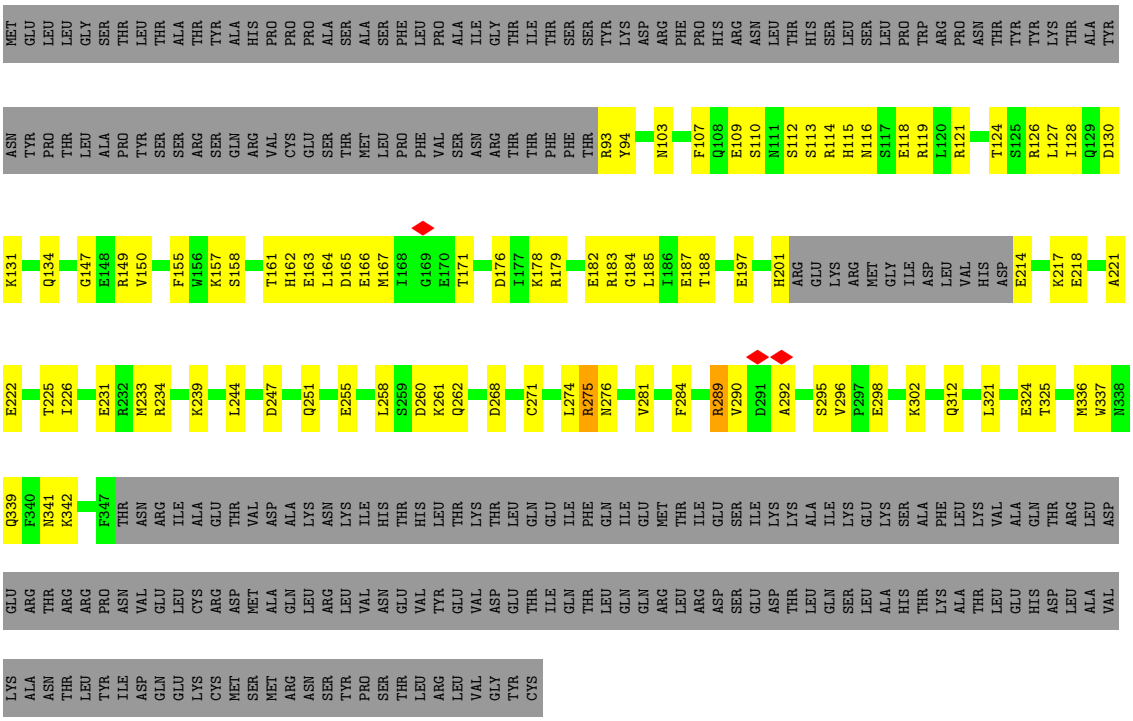
• Molecule 5: Tektin-3

Chain C4:



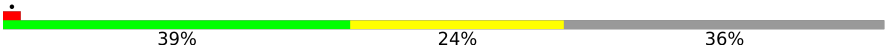
• Molecule 5: Tektin-3

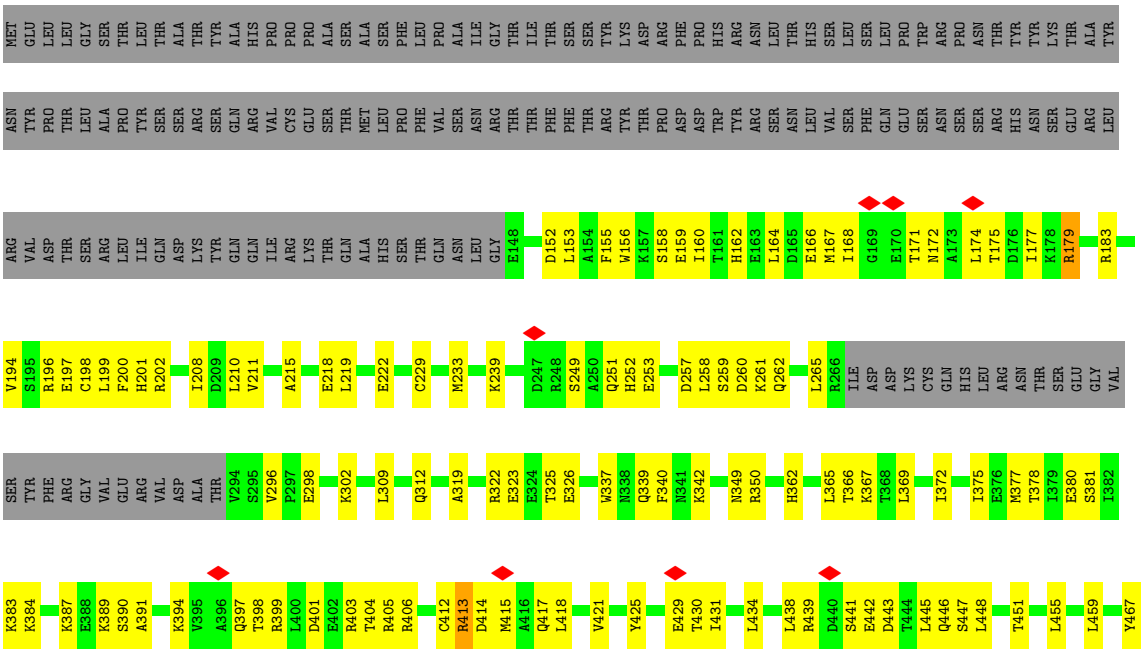
Chain C7:

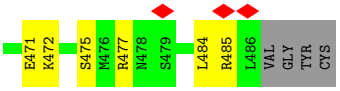


• Molecule 5: Tektin-3

Chain C8:

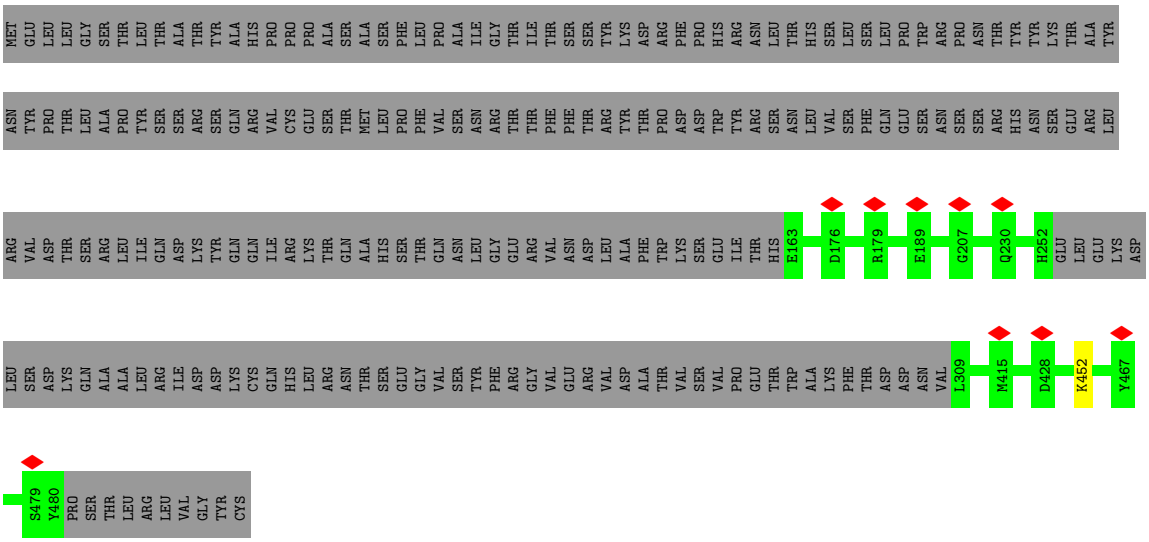






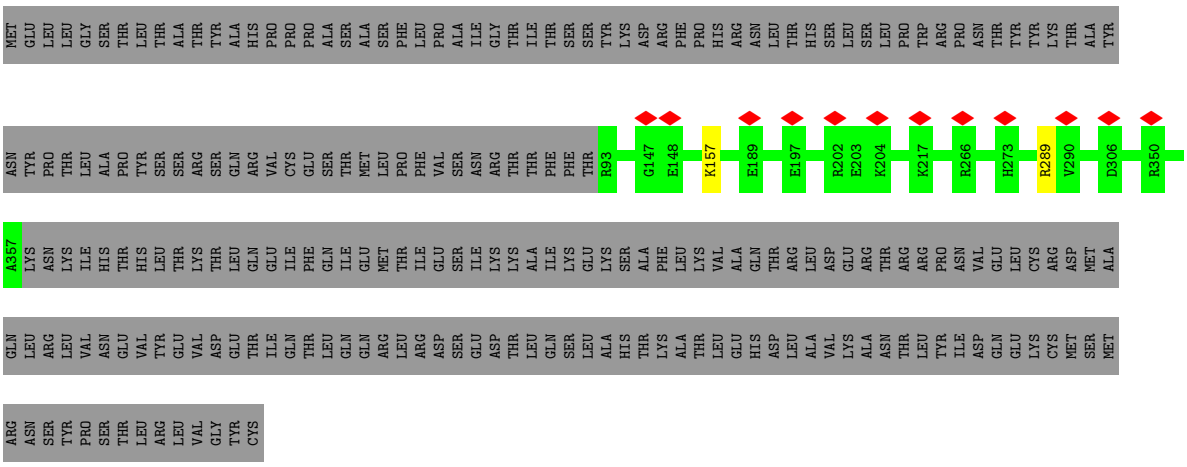
• Molecule 5: Tektin-3

Chain Cb:



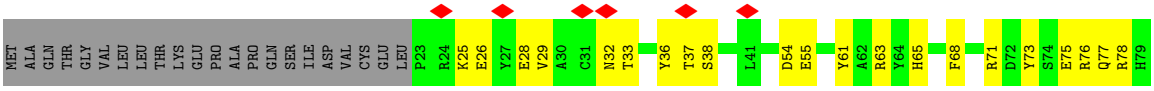
• Molecule 5: Tektin-3

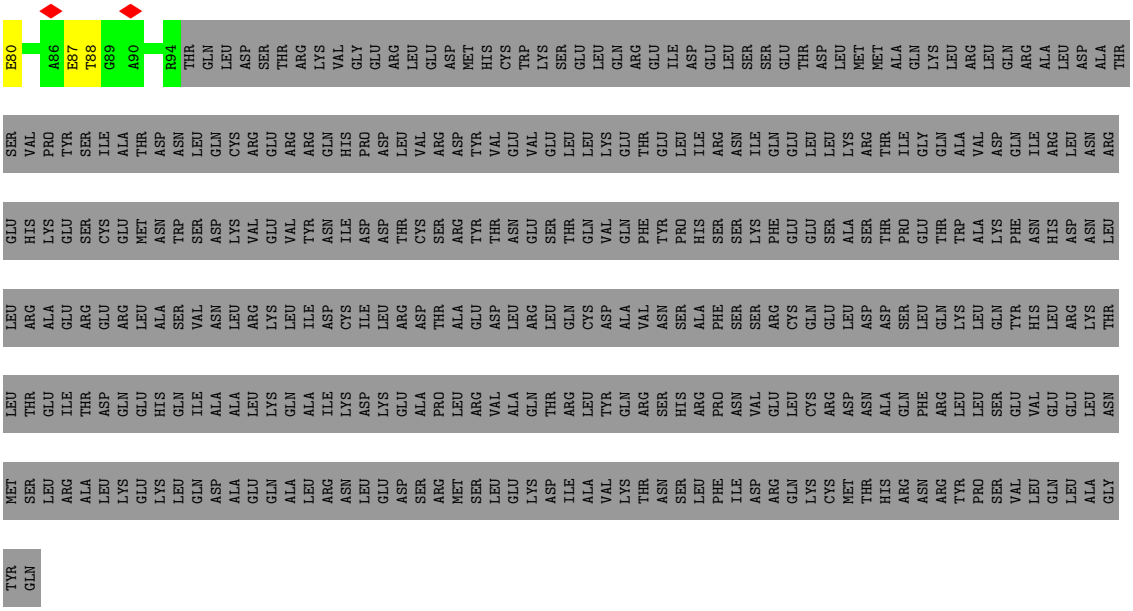
Chain Cc:



• Molecule 6: Tektin-4

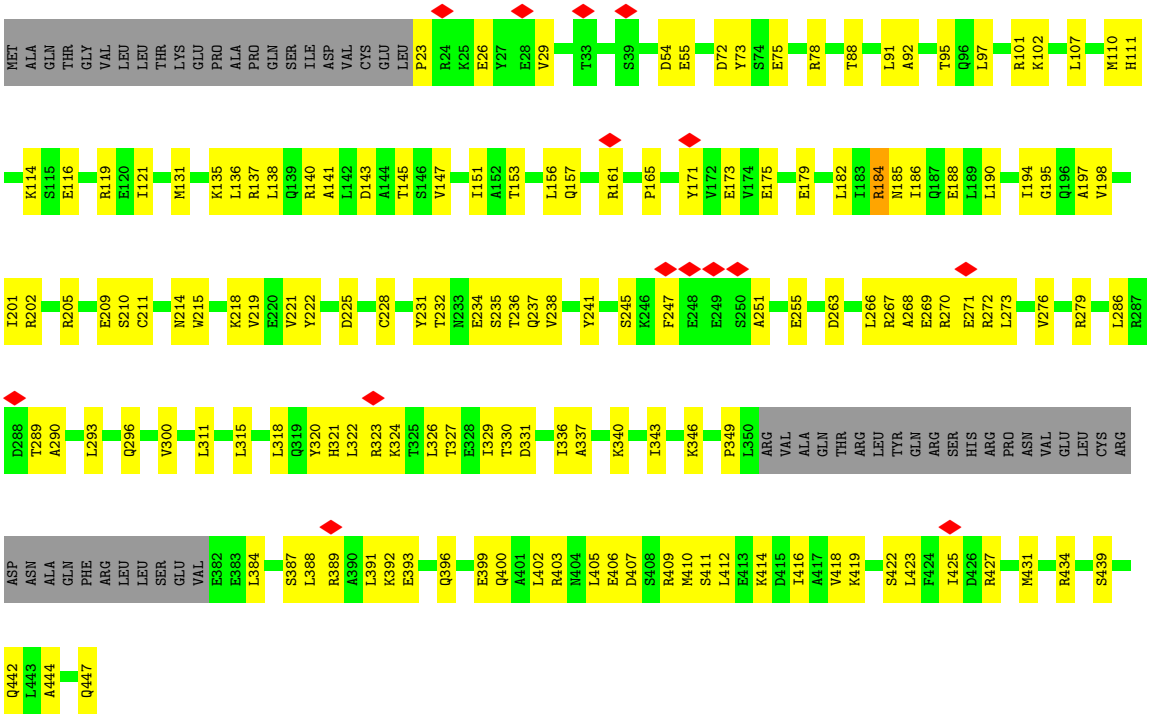
Chain D2:





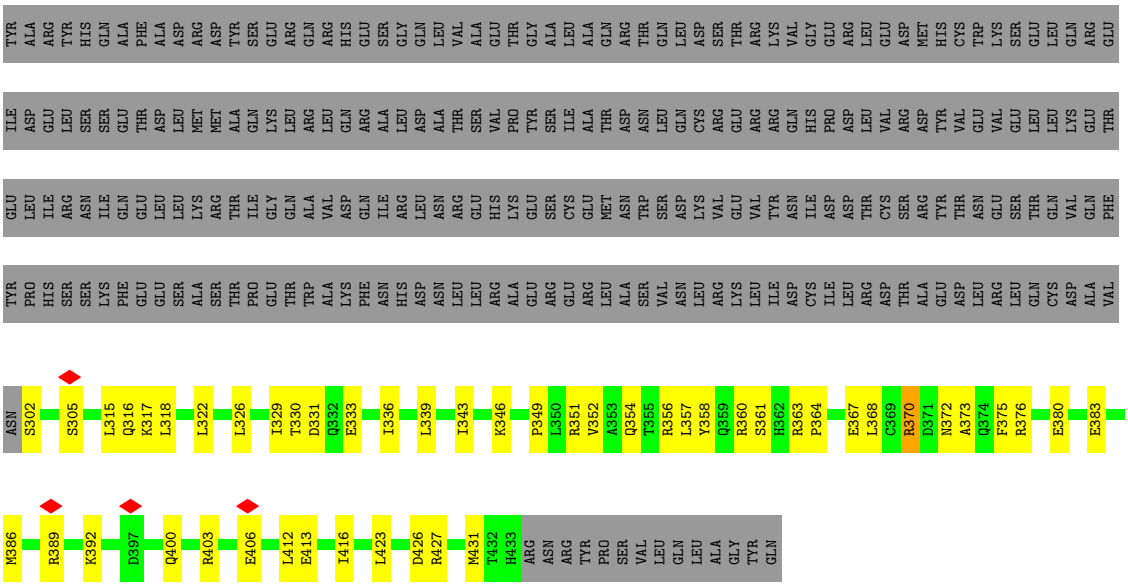
• Molecule 6: Tektin-4

Chain D3:



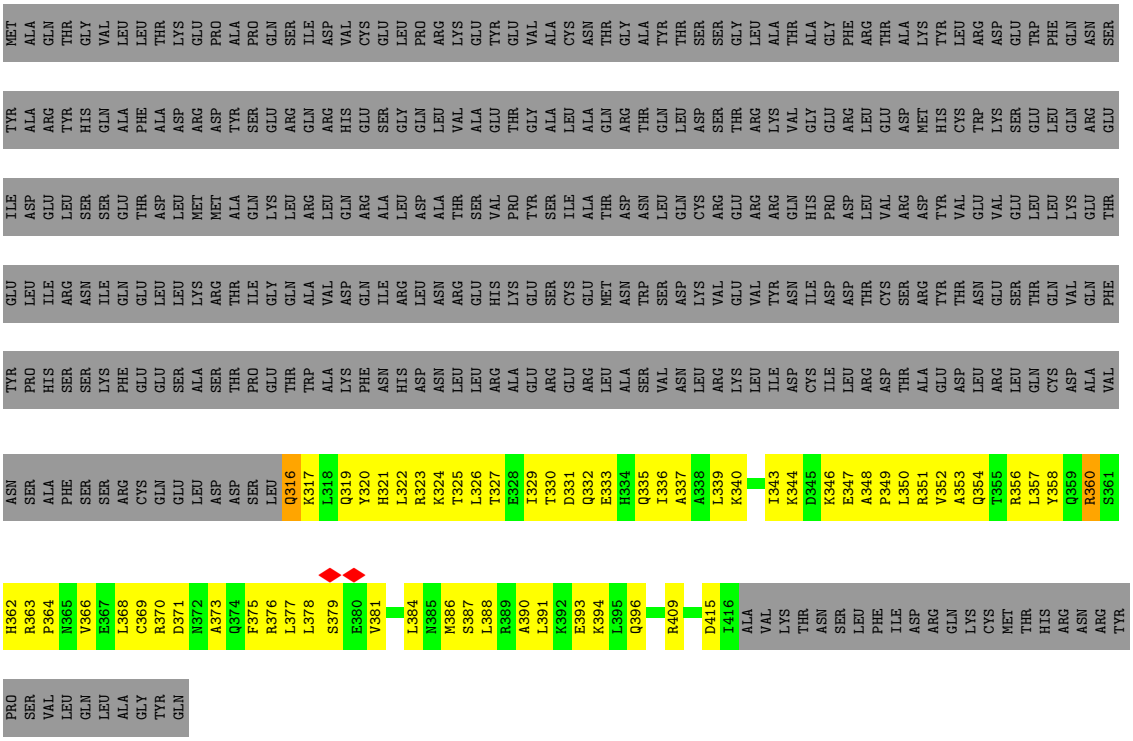
• Molecule 6: Tektin-4

Chain D4:



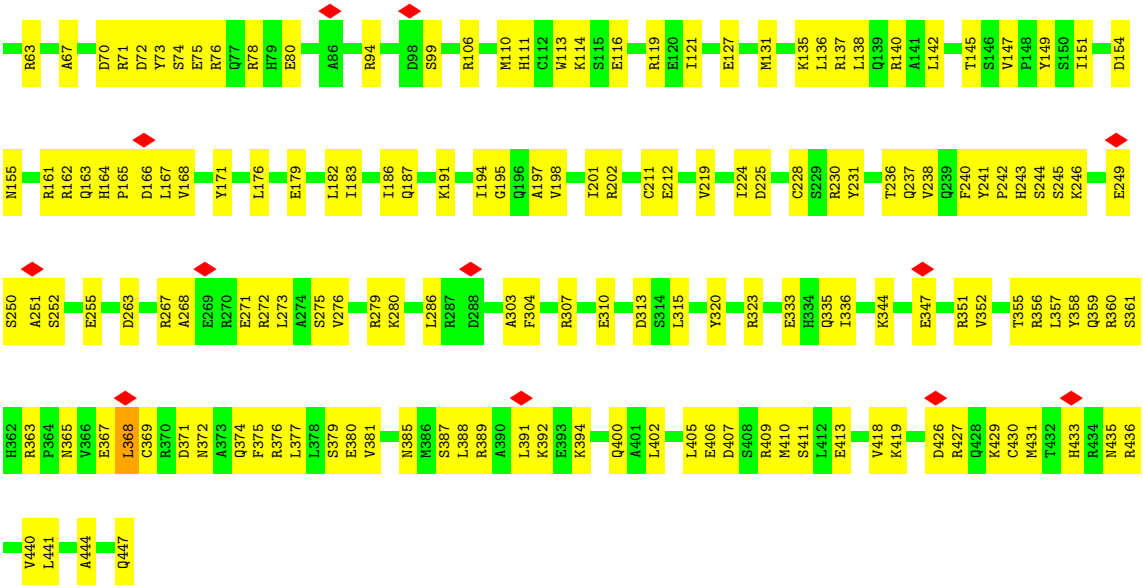
• Molecule 6: Tektin-4

Chain D7:



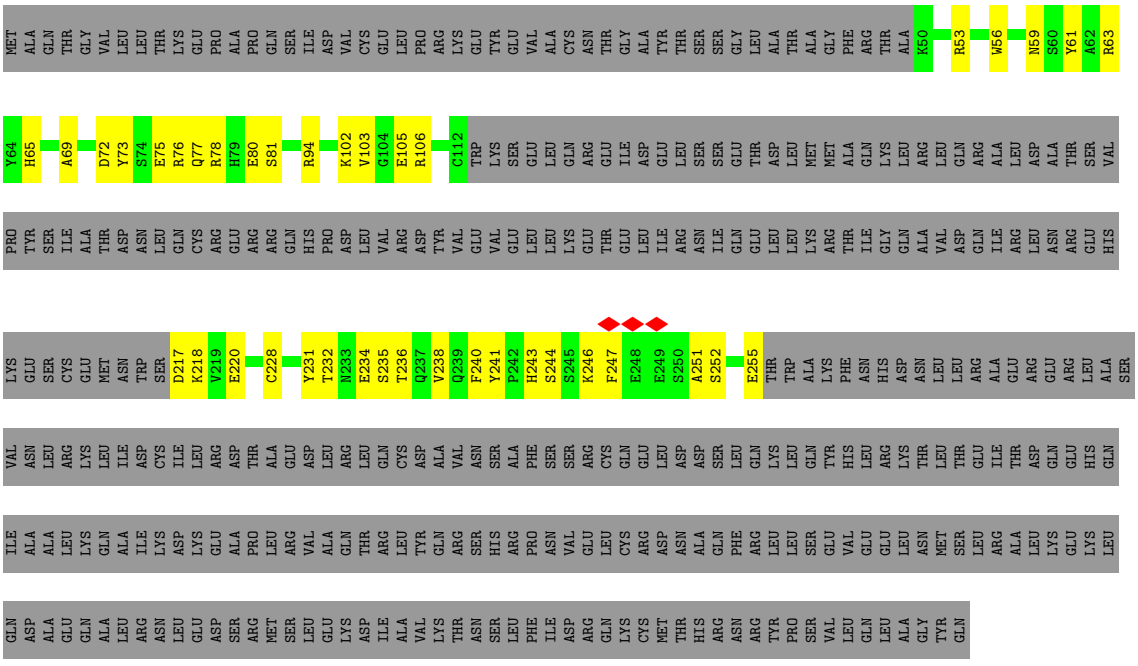
• Molecule 6: Tektin-4

Chain D8:



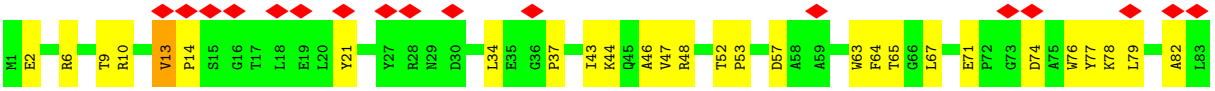
• Molecule 6: Tektin-4

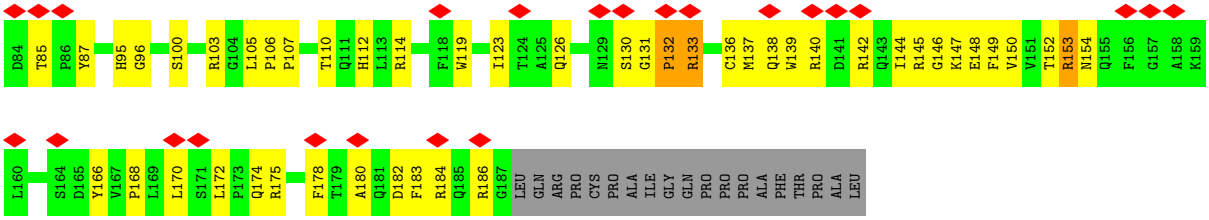
Chain D9:



• Molecule 7: Tektin bundle-interacting protein 1

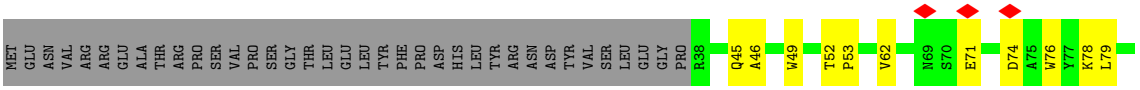
Chain E2:

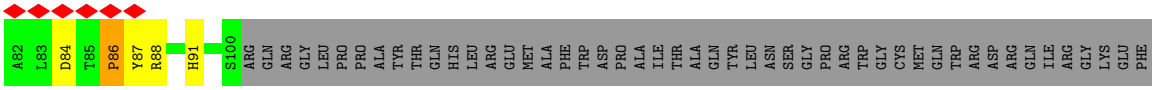




• Molecule 7: Tektin bundle-interacting protein 1

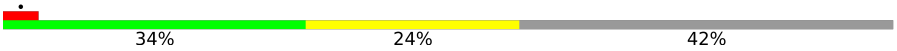
Chain E3:

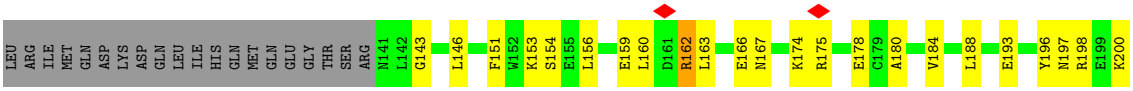


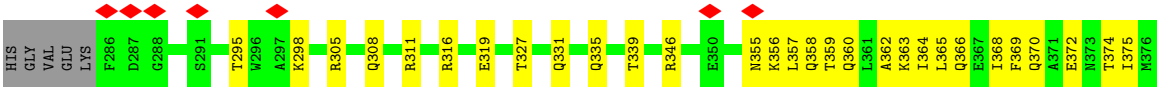


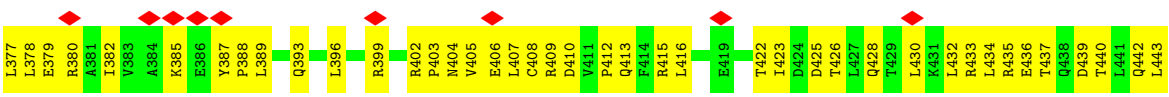
• Molecule 8: Tektin-5

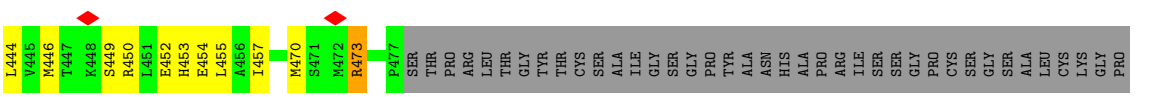
Chain F2:





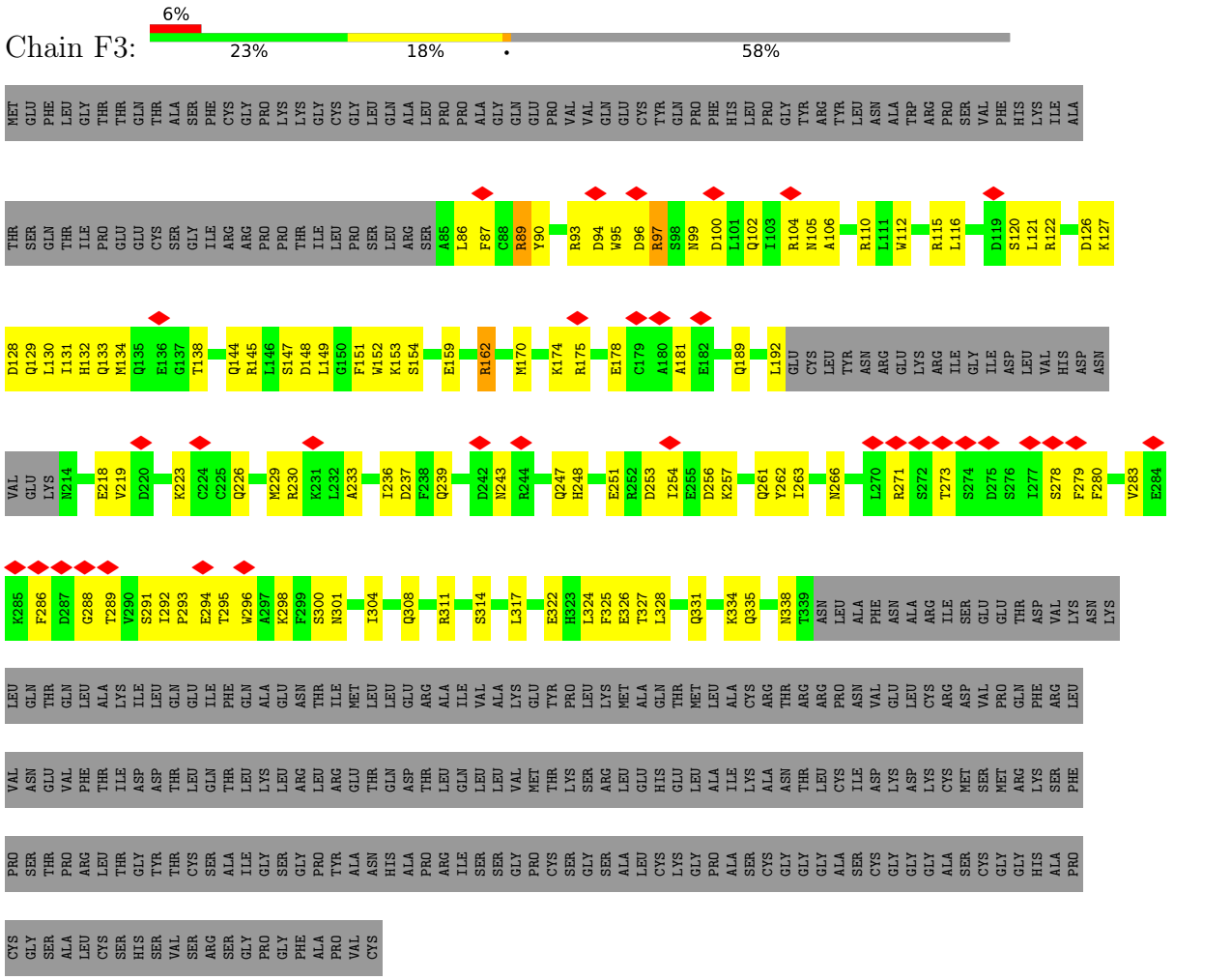






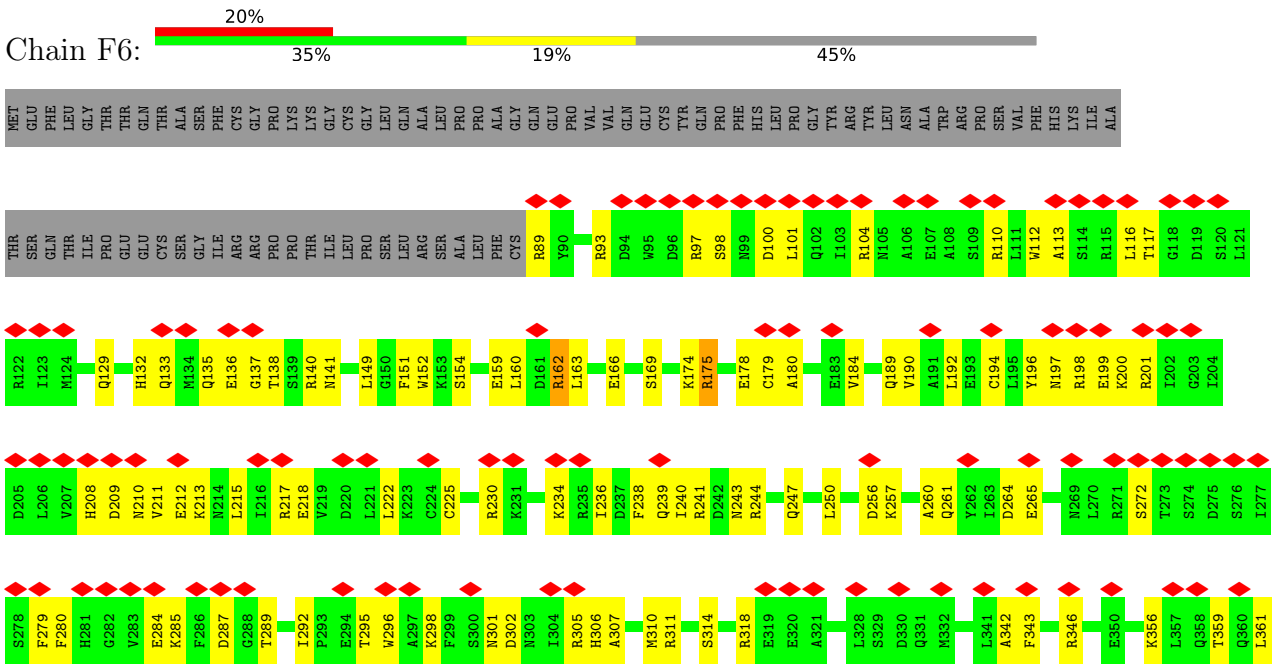
• Molecule 8: Tektin-5

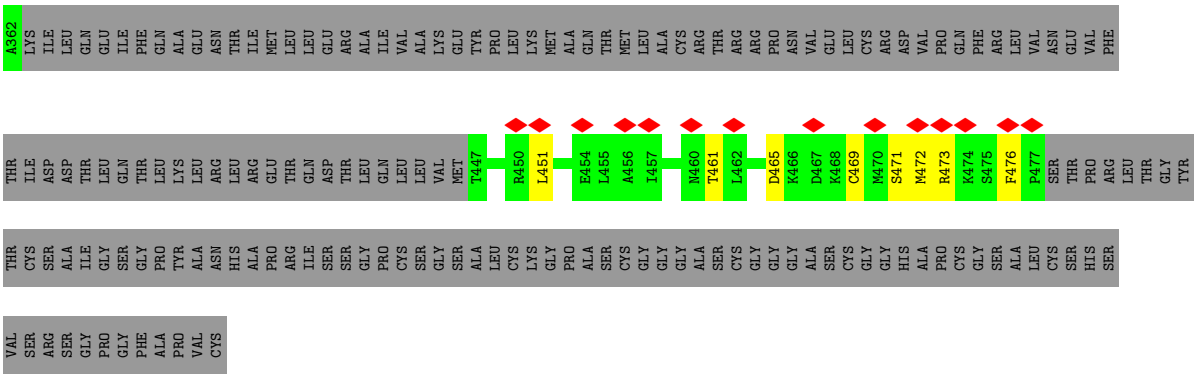
Chain F3:



• Molecule 8: Tektin-5

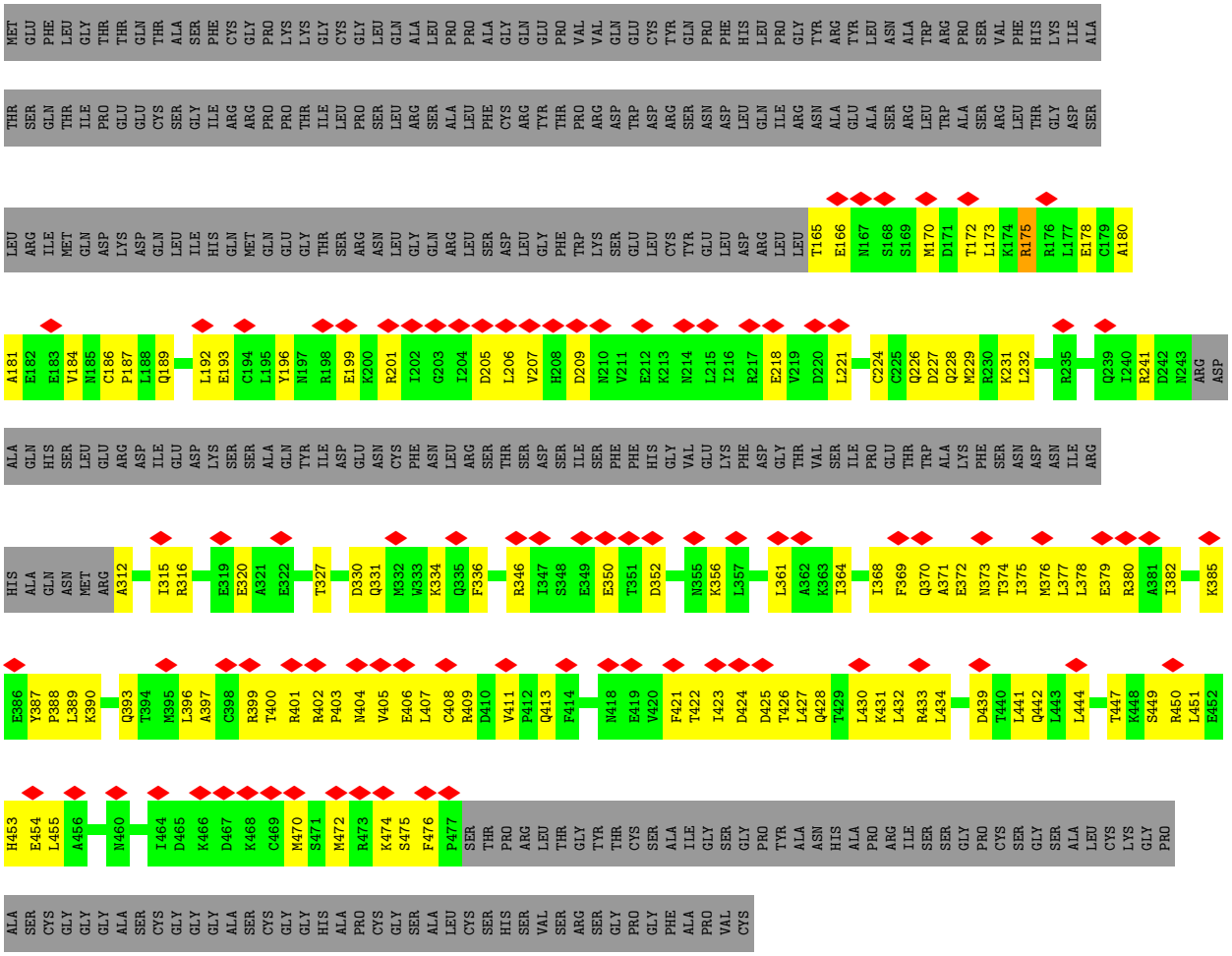
Chain F6:





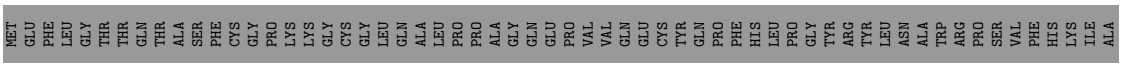
• Molecule 8: Tektin-5

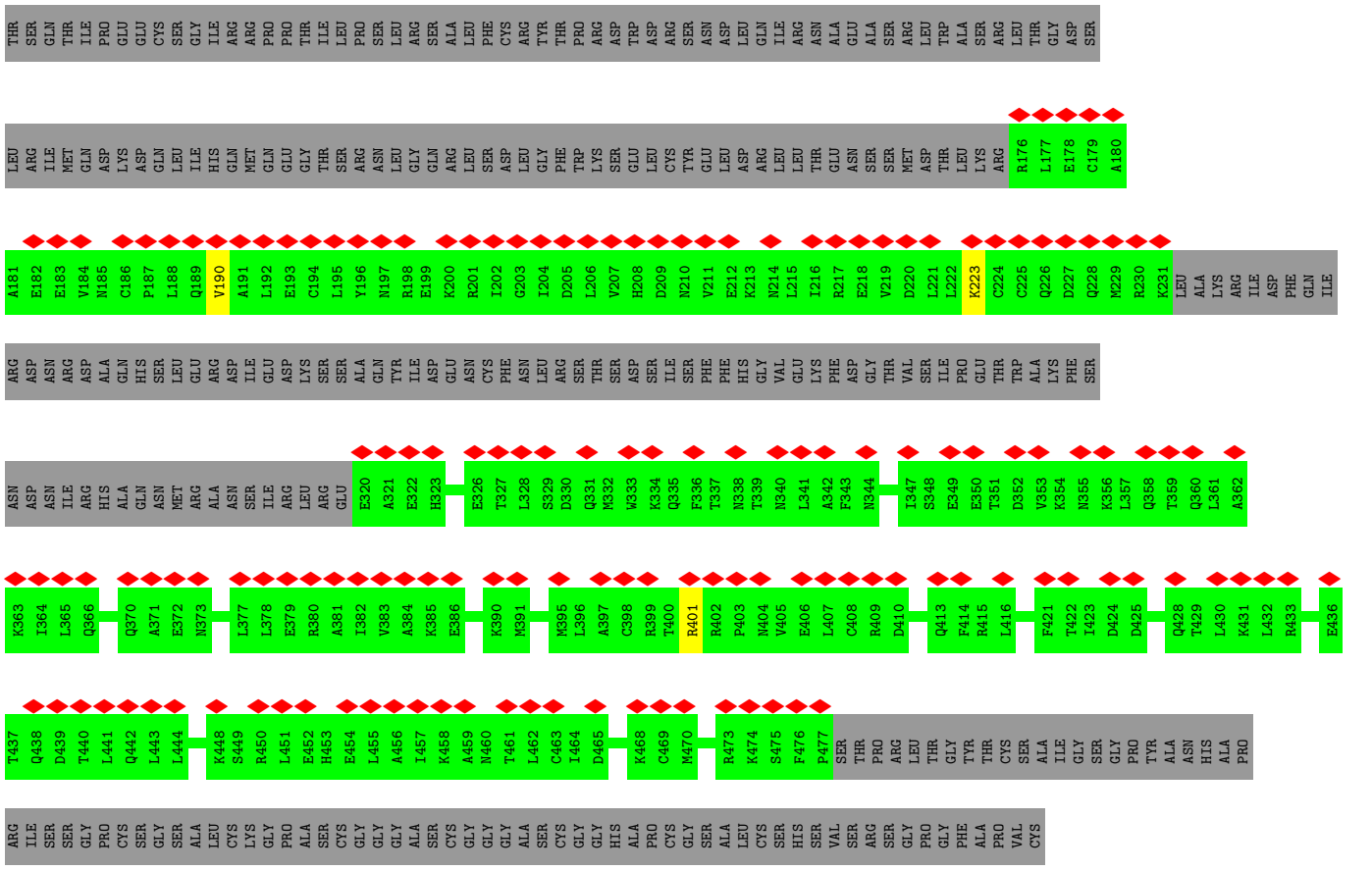
Chain F7:



• Molecule 8: Tektin-5

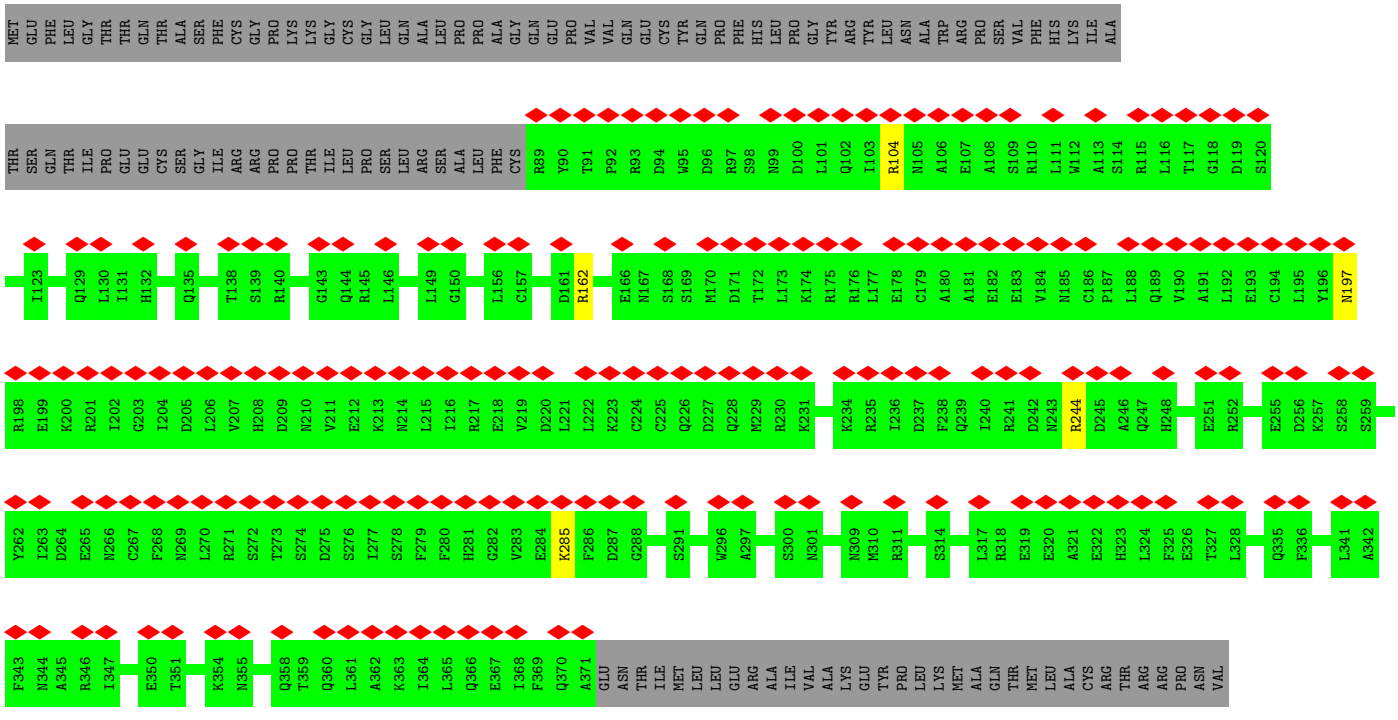
Chain Fa:

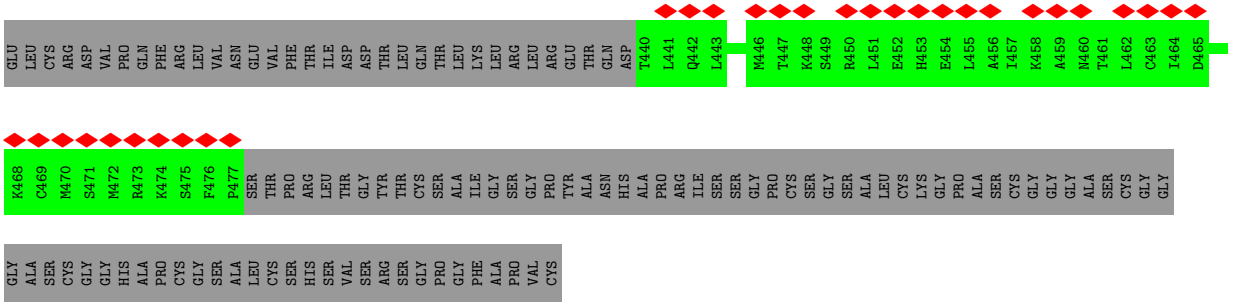




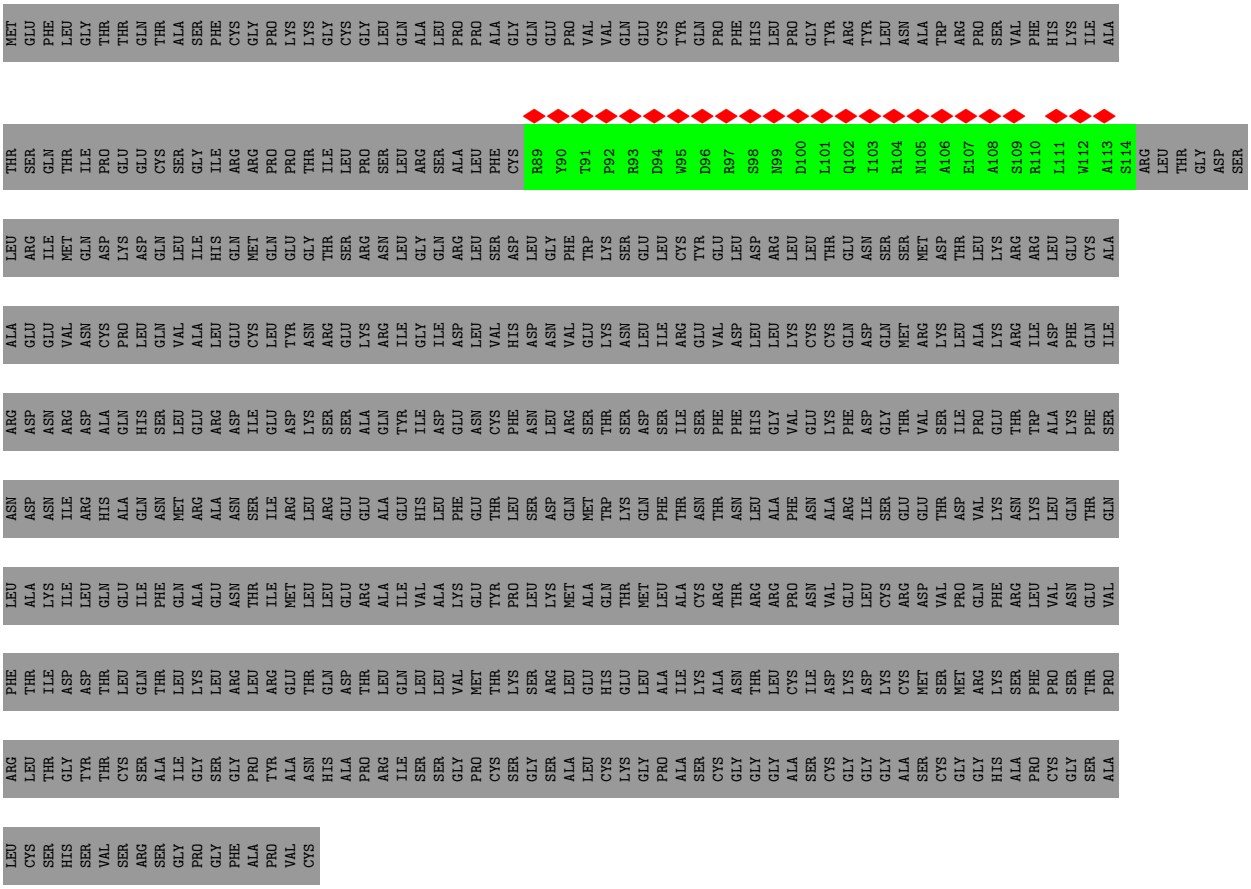
• Molecule 8: Tektin-5

Chain Fb:

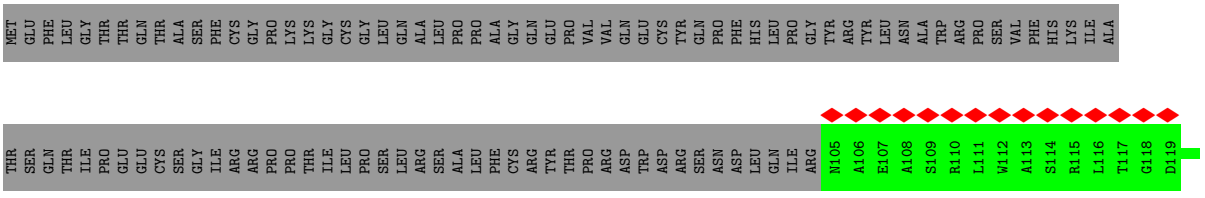


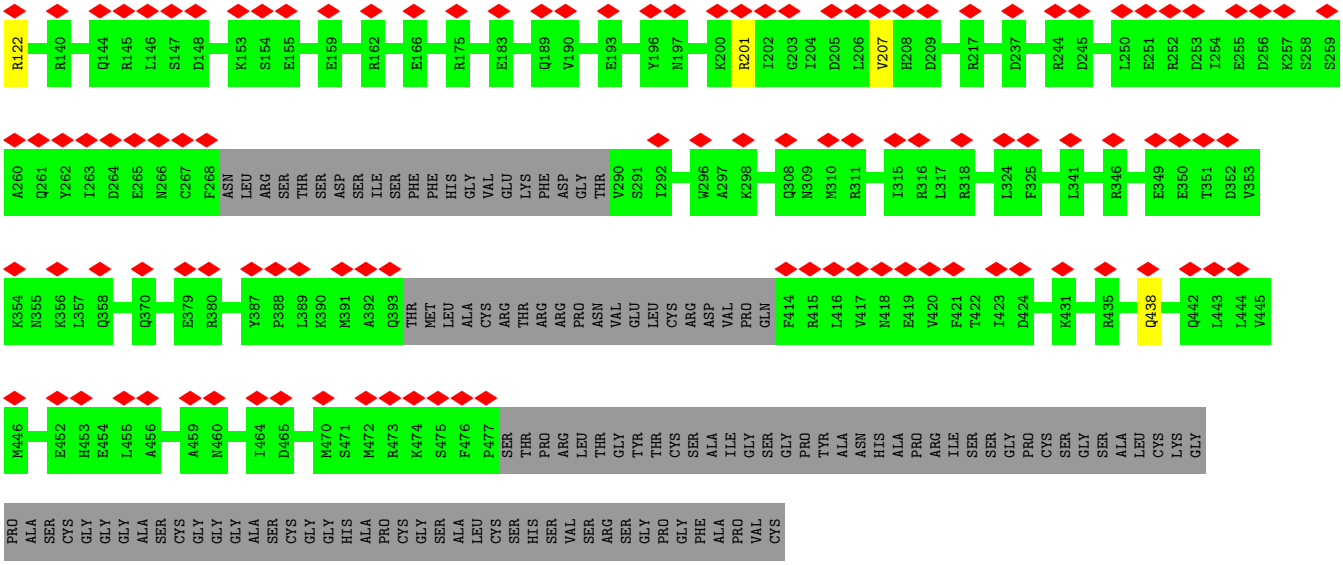


• Molecule 8: Tektin-5



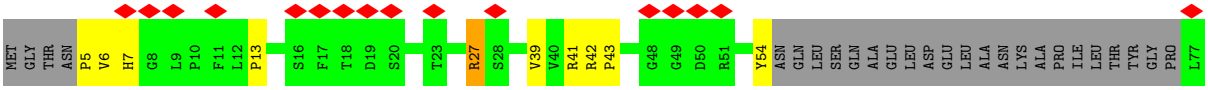
• Molecule 8: Tektin-5

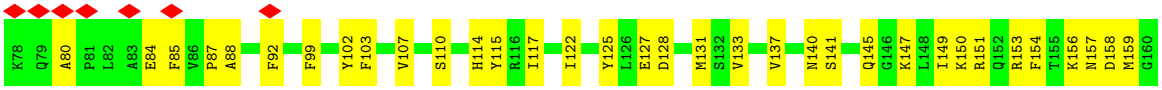


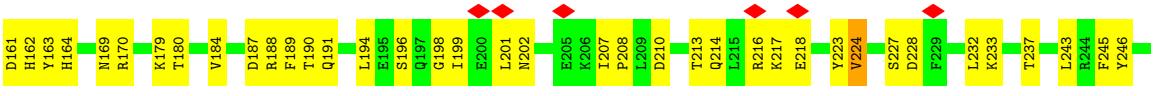


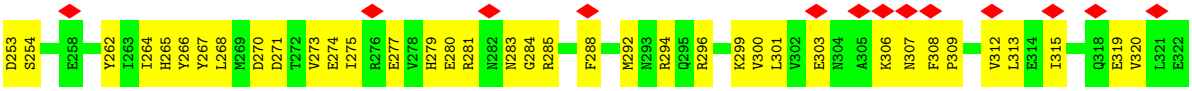
• Molecule 9: EF-hand domain-containing protein 1

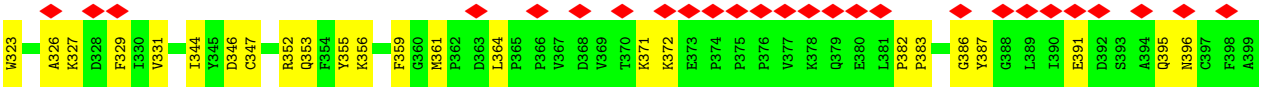
Chain G1:

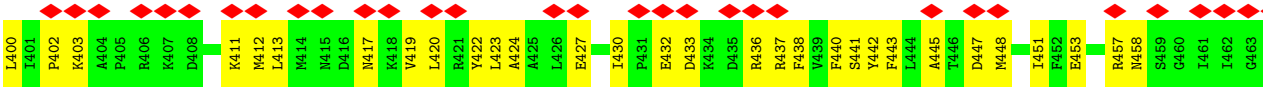


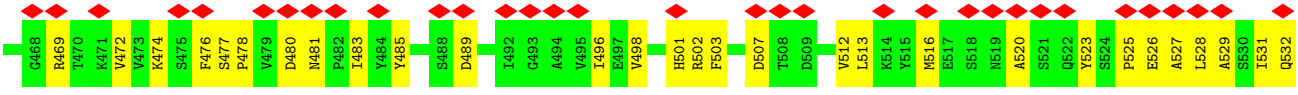


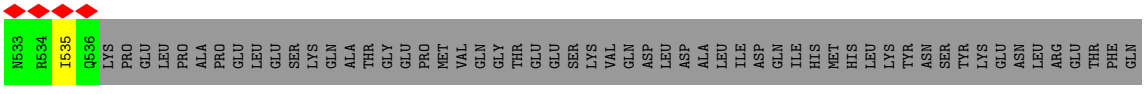






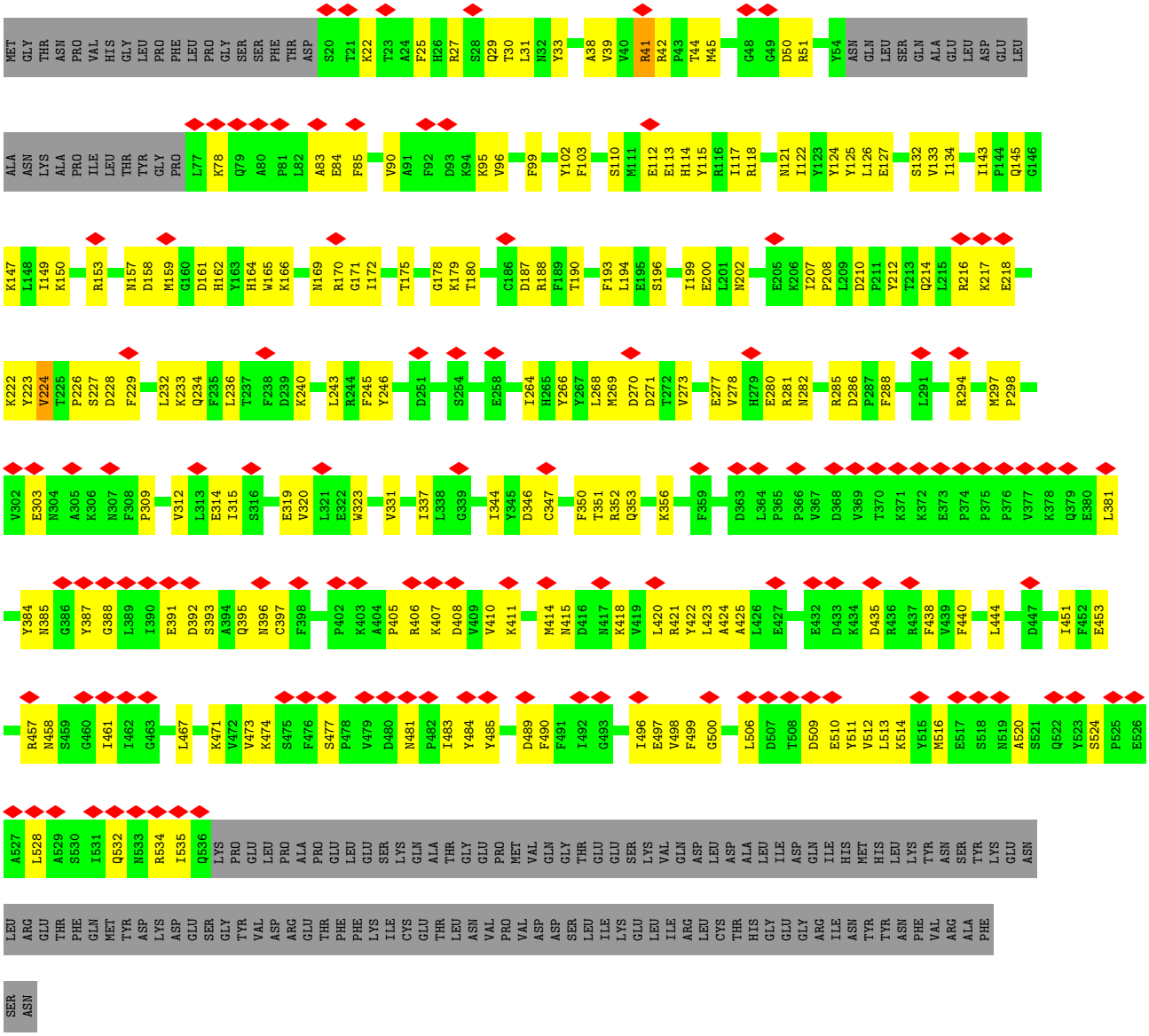






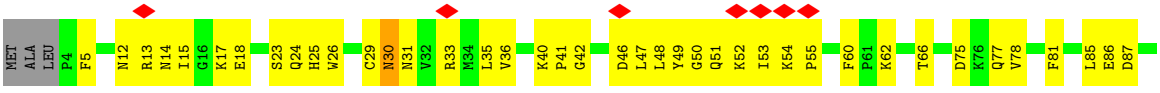
• Molecule 9: EF-hand domain-containing protein 1

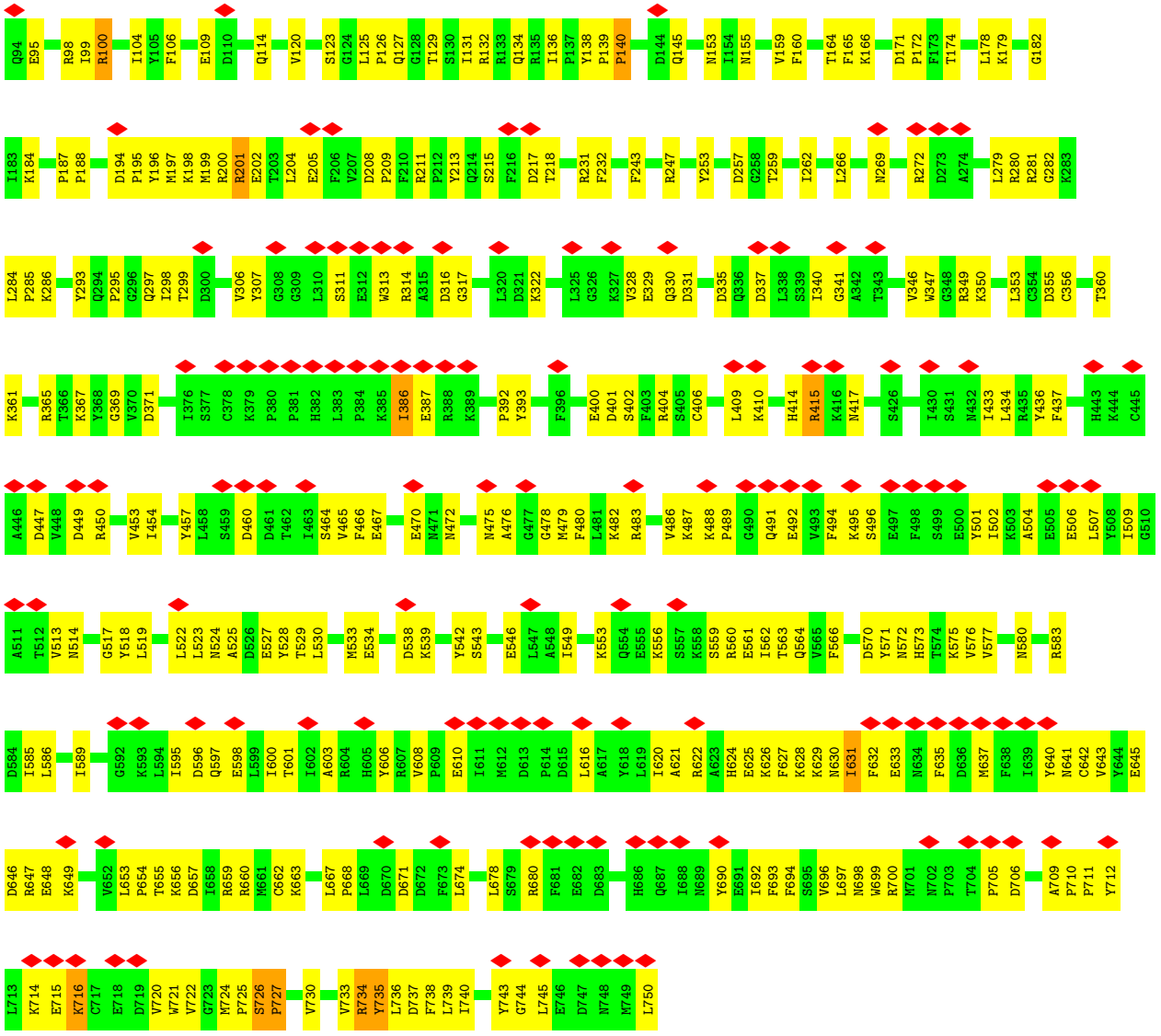
Chain G2:



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

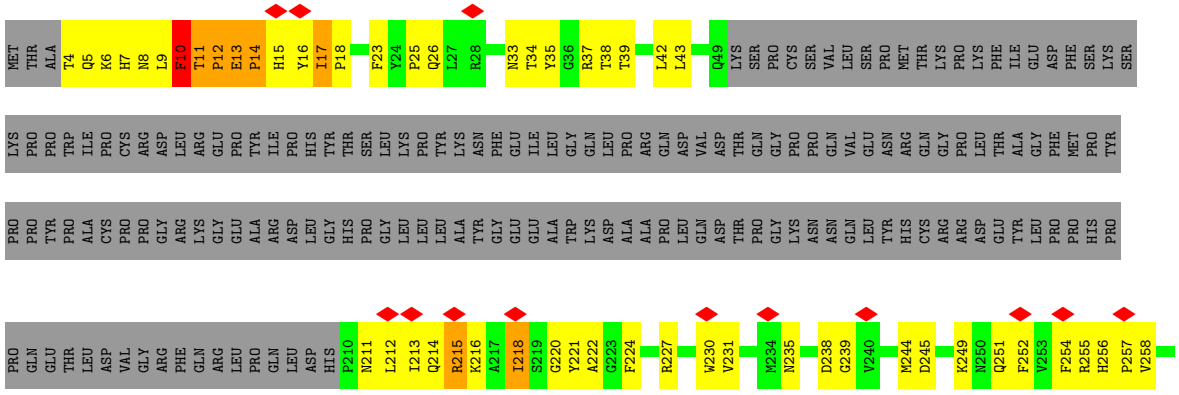
Chain G5:

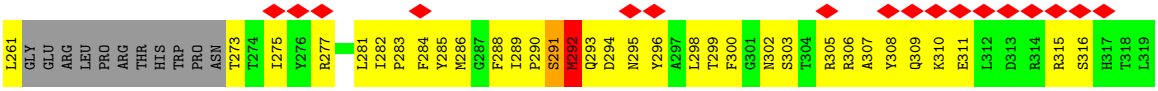




• Molecule 11: Protein FAM166A

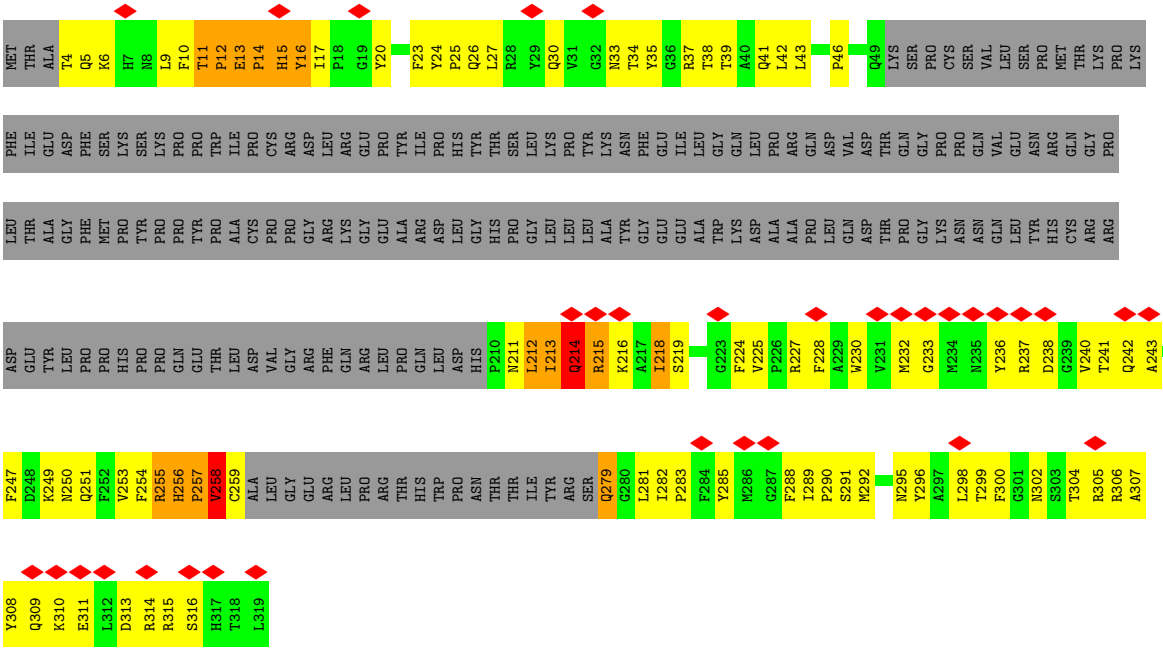
Chain H3:





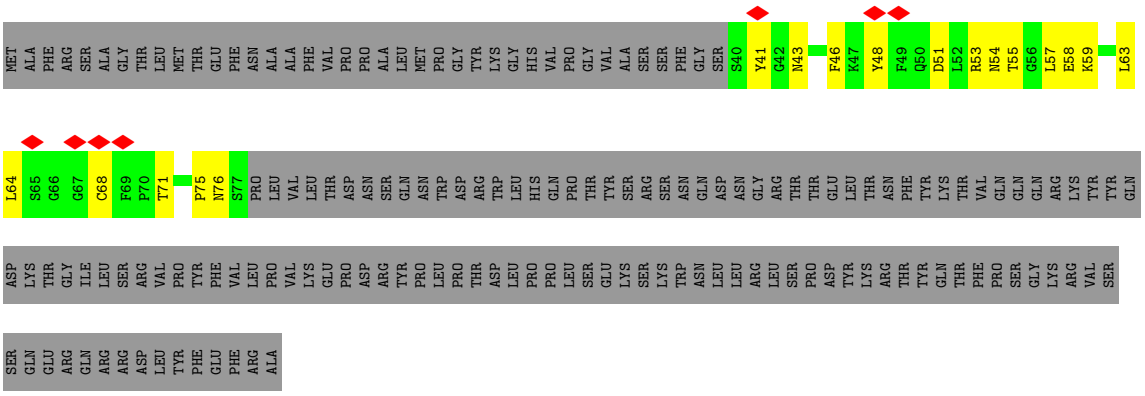
• Molecule 11: Protein FAM166A

Chain H4:



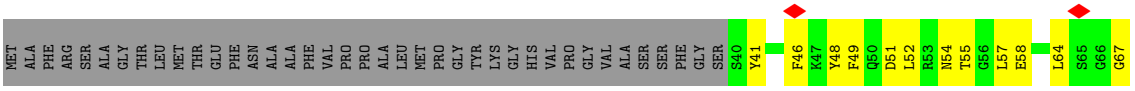
• Molecule 12: Protein FAM166C

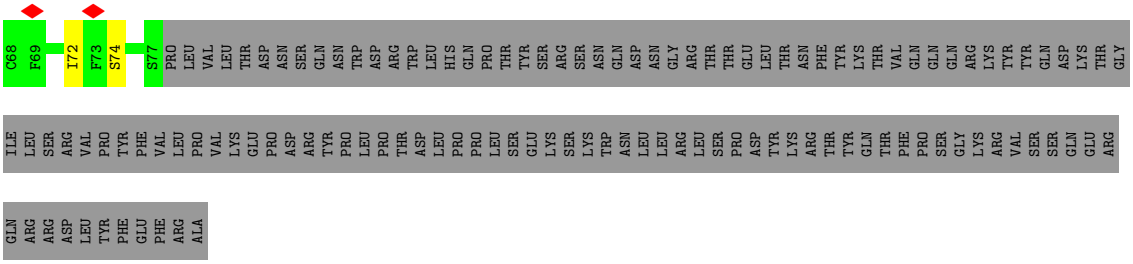
Chain I2:



• Molecule 12: Protein FAM166C

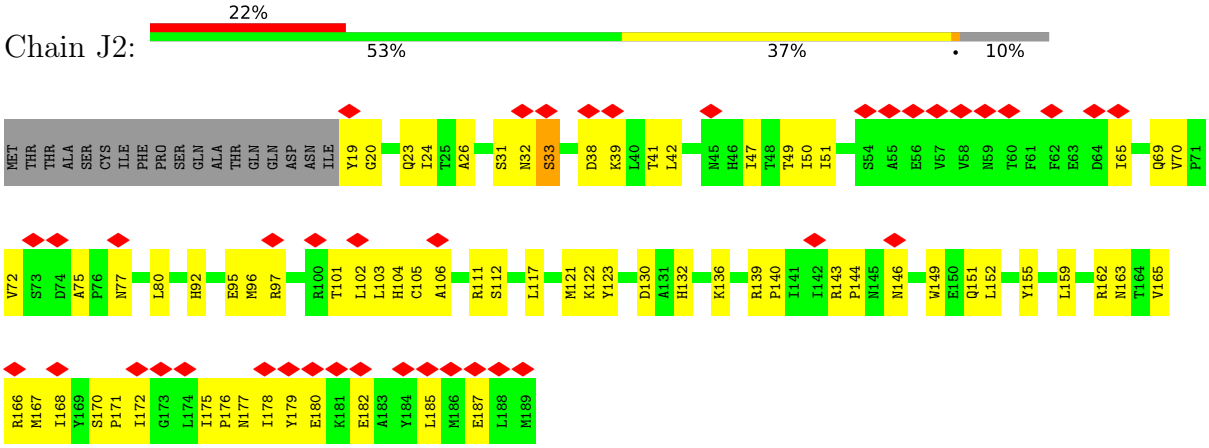
Chain I3:





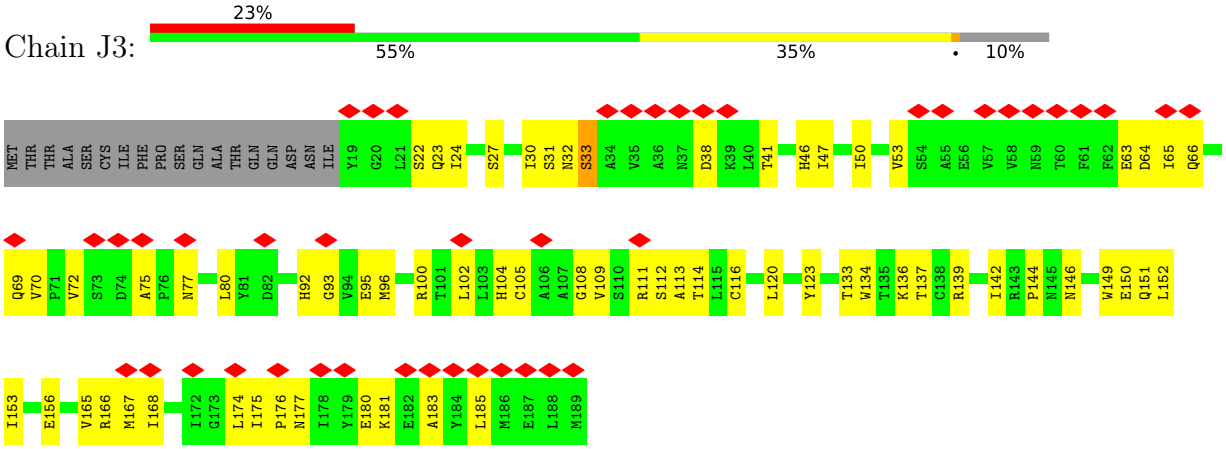
• Molecule 13: Dual specificity phosphatase 21

Chain J2:



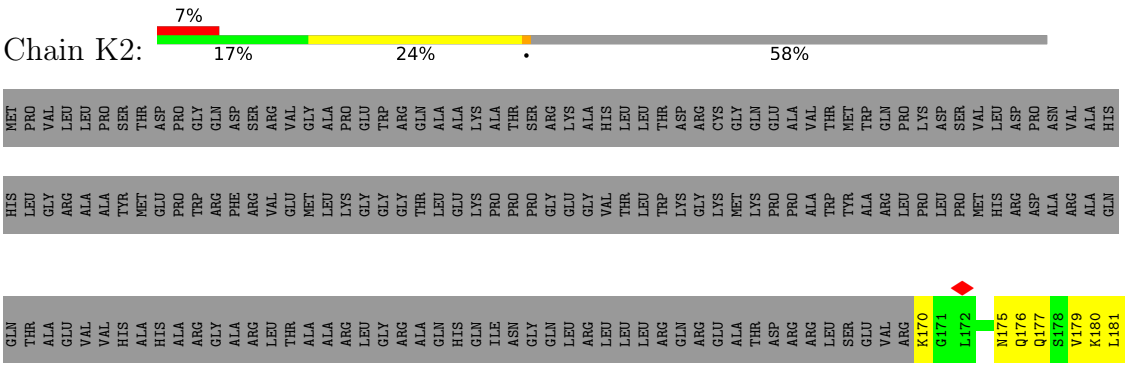
• Molecule 13: Dual specificity phosphatase 21

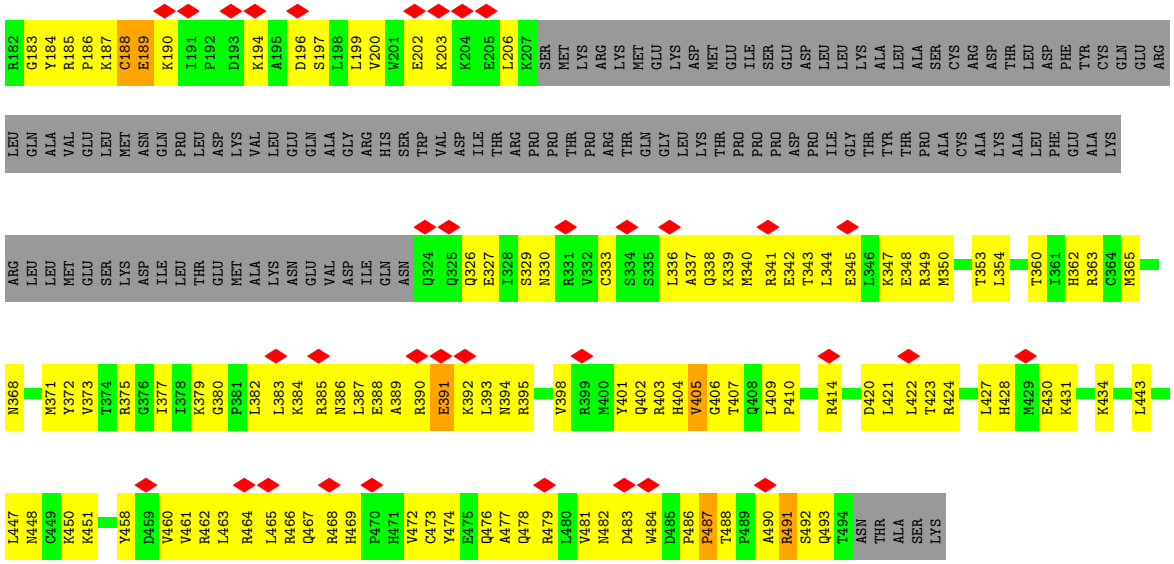
Chain J3:



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

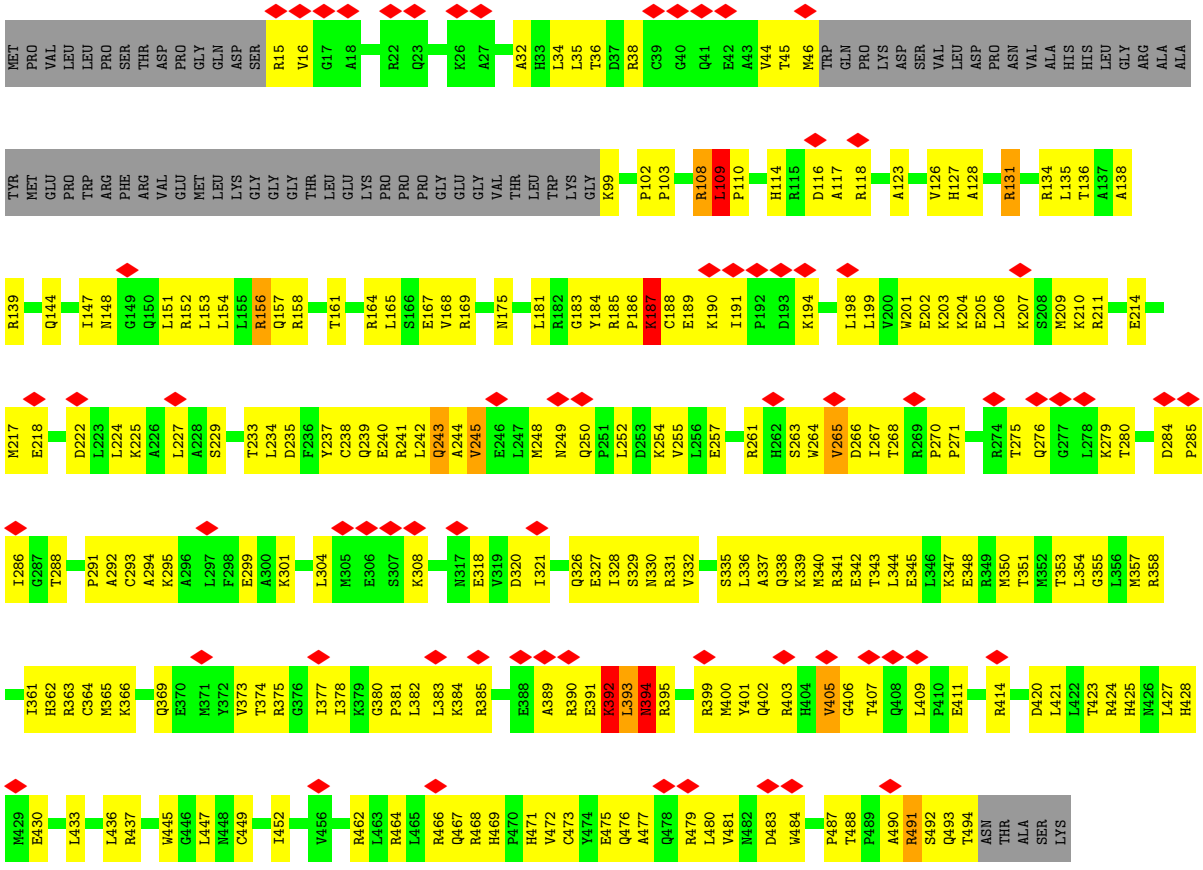
Chain K2:





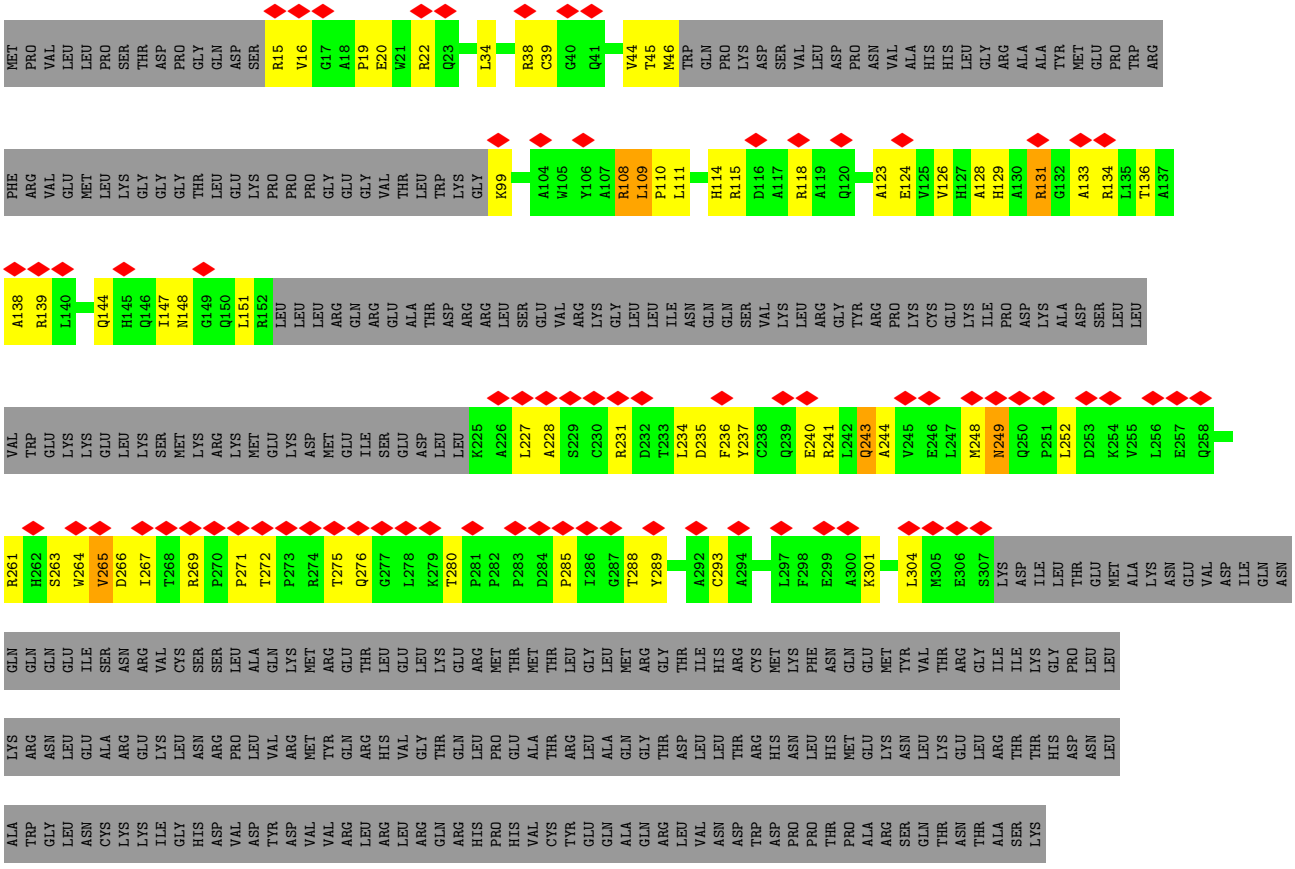
• Molecule 14: Coiled-coil domain-containing protein 105

Chain K3:



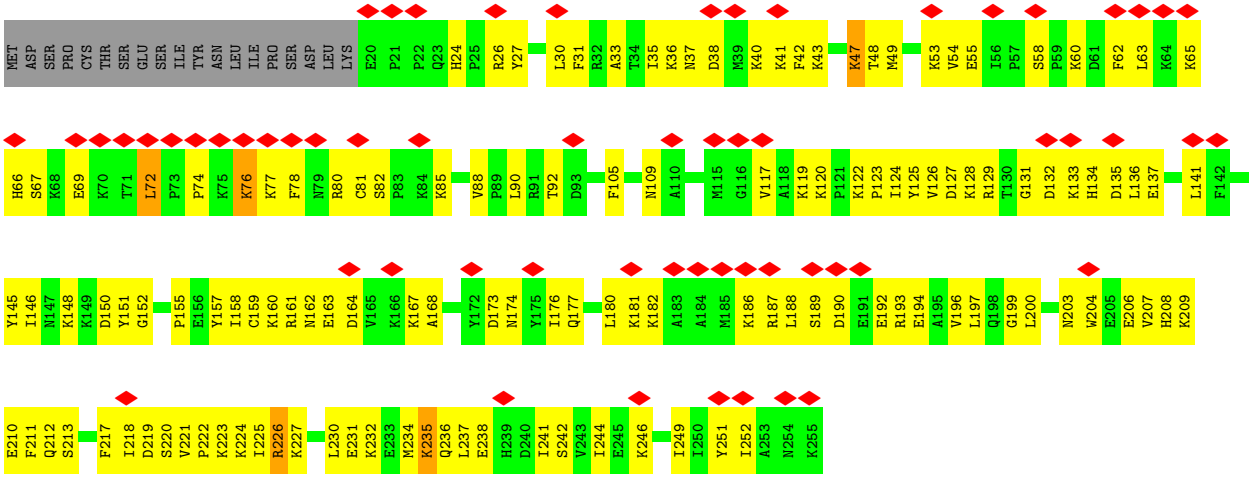
• Molecule 14: Coiled-coil domain-containing protein 105

Chain K4:



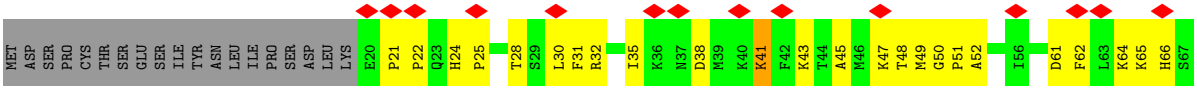
• Molecule 15: Enkurin

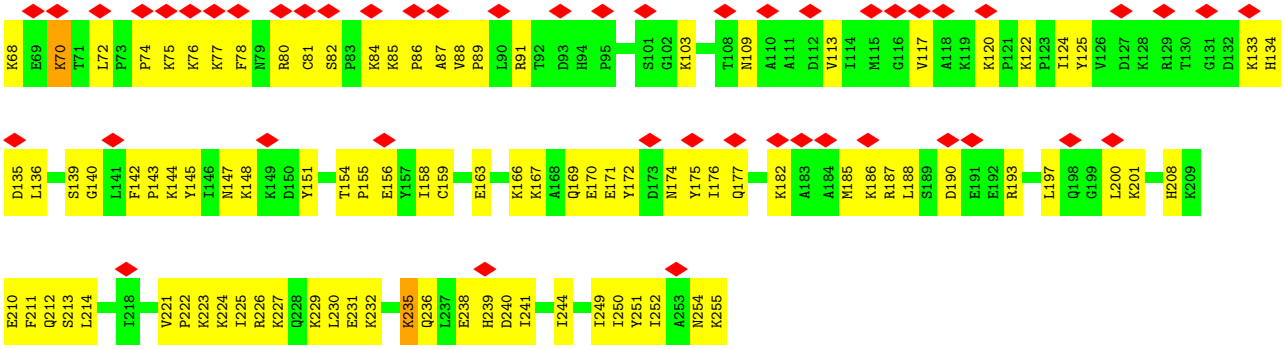
Chain L2:



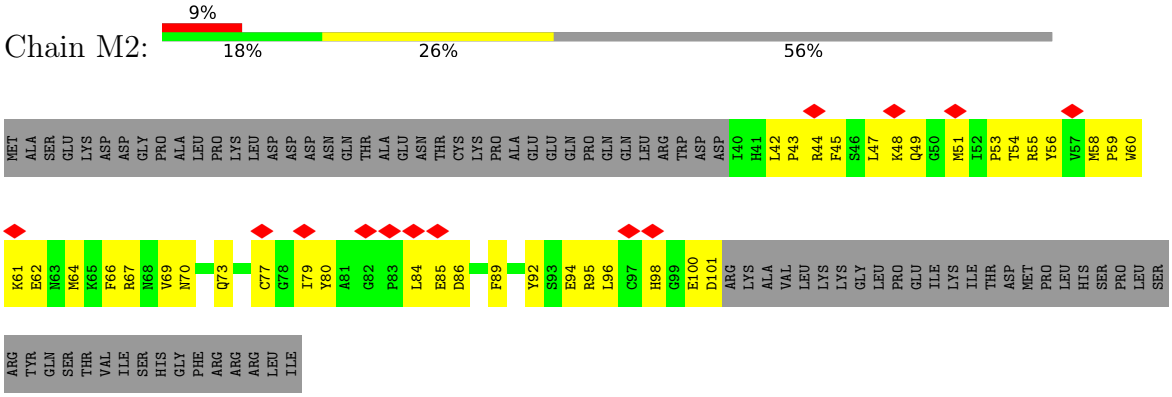
• Molecule 15: Enkurin

Chain L3:

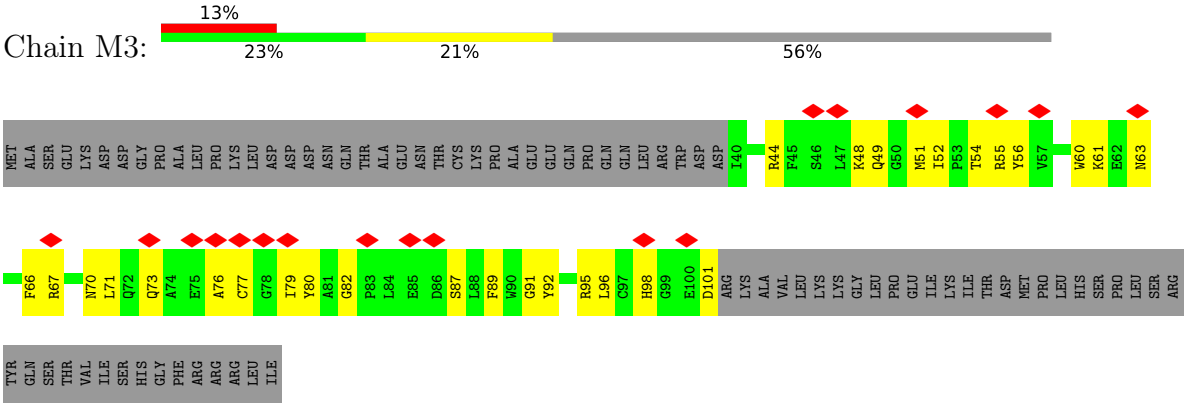




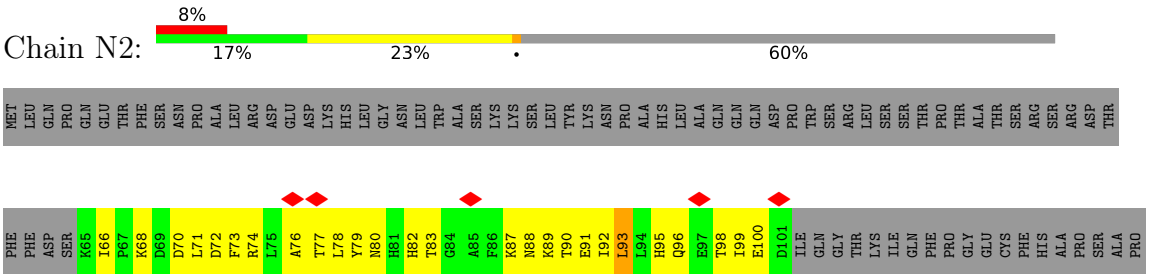
• Molecule 16: Testis-expressed protein 43

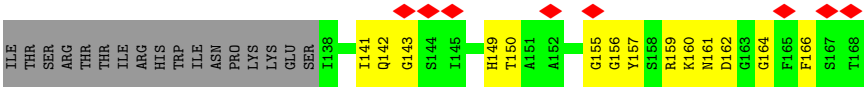


• Molecule 16: Testis-expressed protein 43



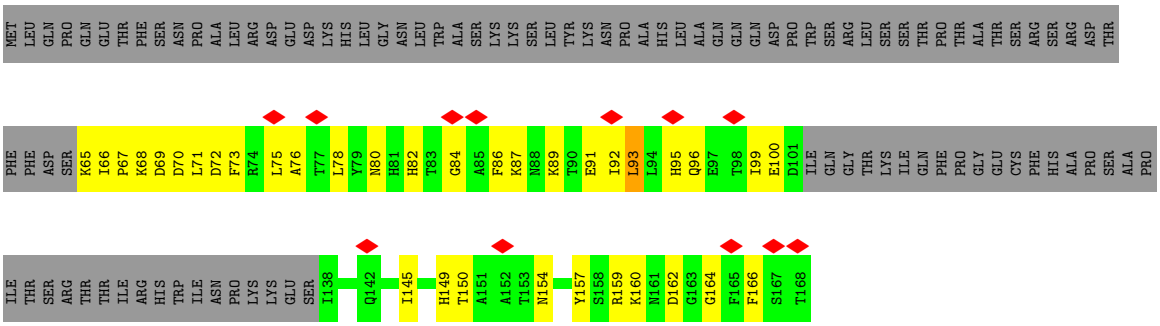
• Molecule 17: Cilia- and flagella-associated protein 276





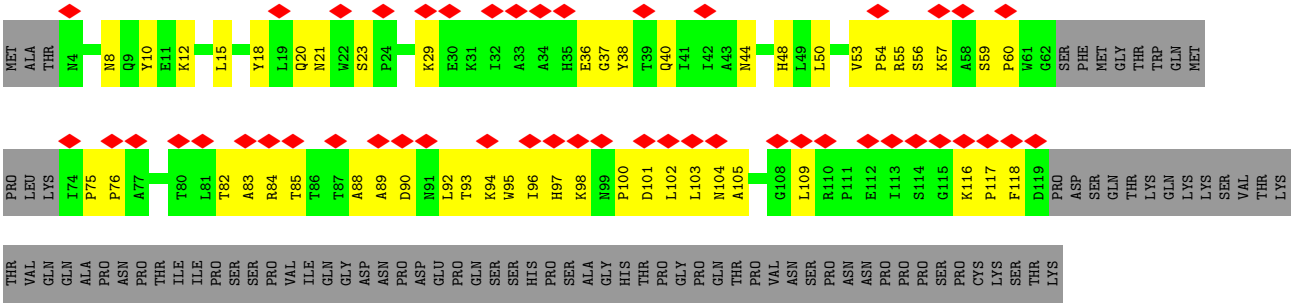
• Molecule 17: Cilia- and flagella-associated protein 276

Chain N3:



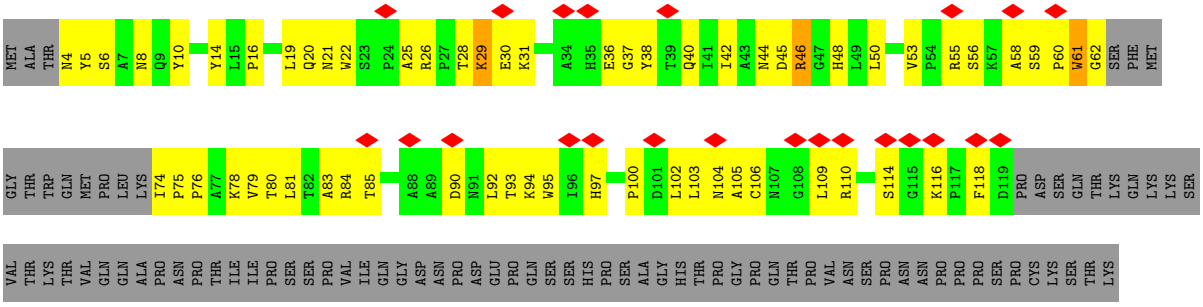
• Molecule 18: Protein Flattop

Chain O1:



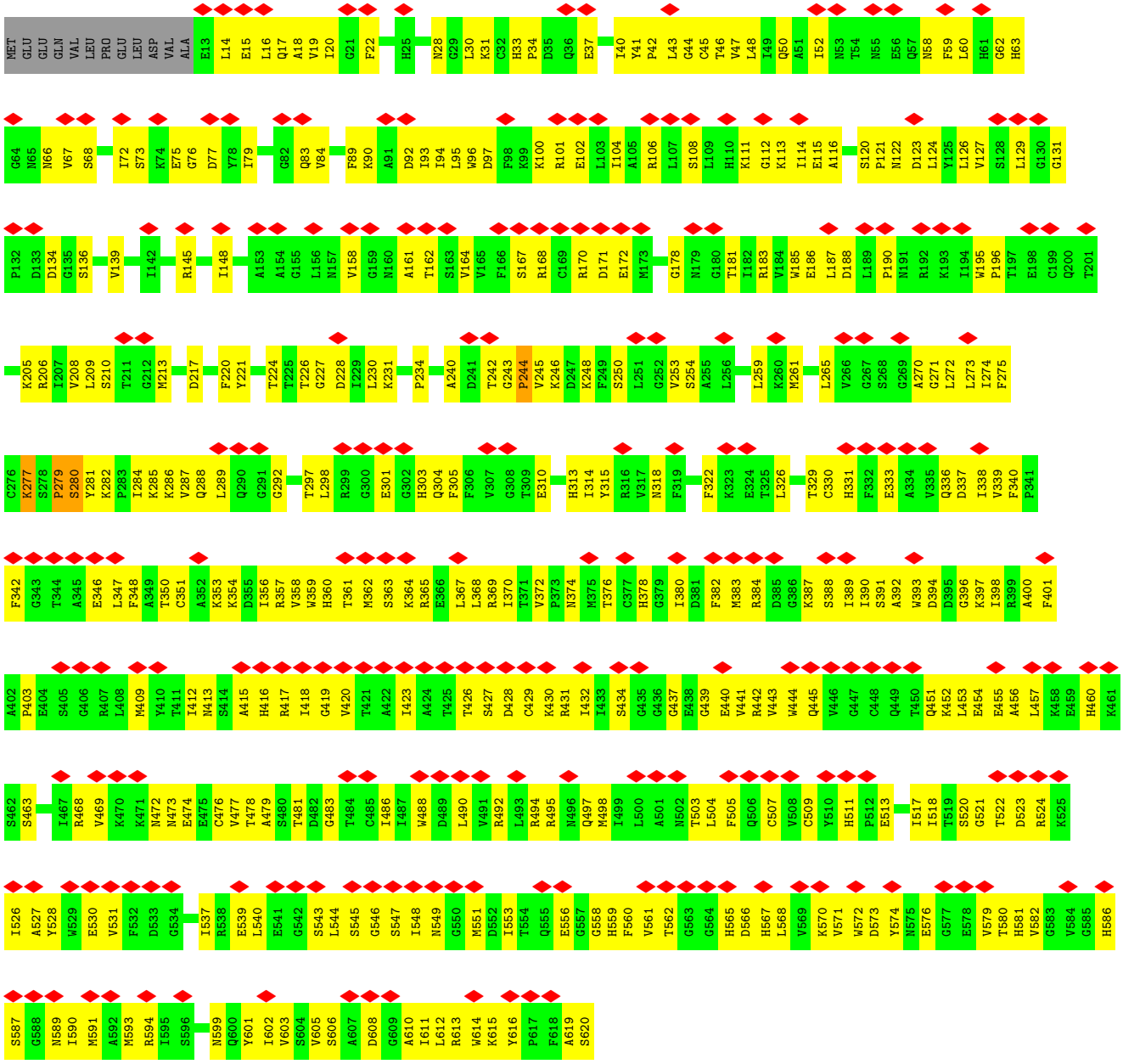
• Molecule 18: Protein Flattop

Chain O2:



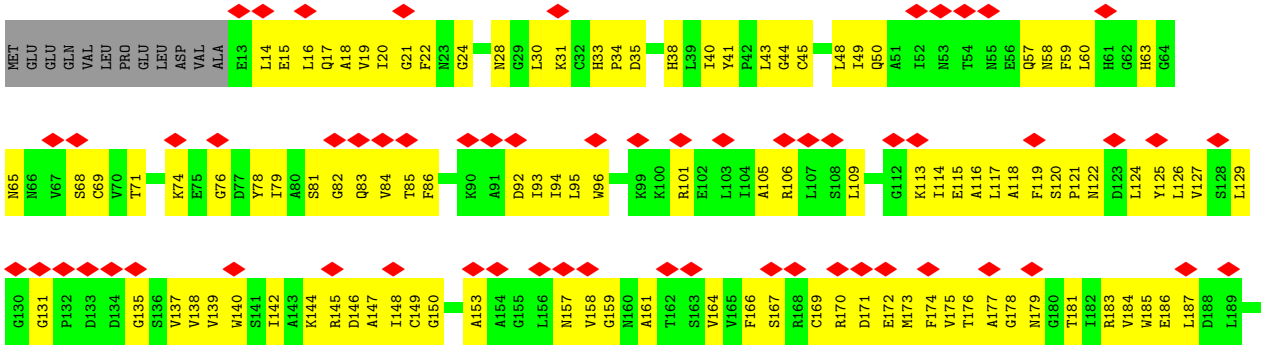
• Molecule 19: Cilia- and flagella-associated protein 52

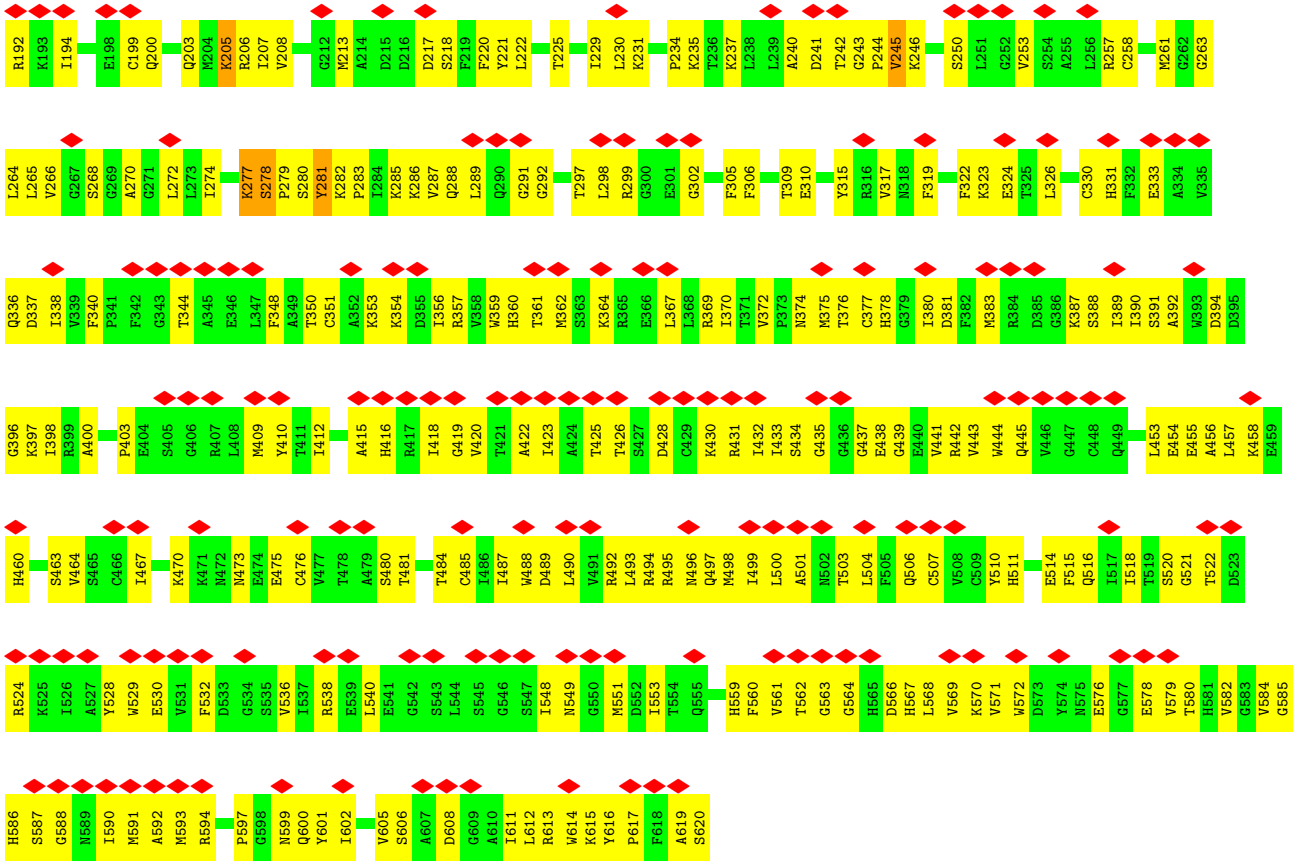
Chain P1:



• Molecule 19: Cilia- and flagella-associated protein 52

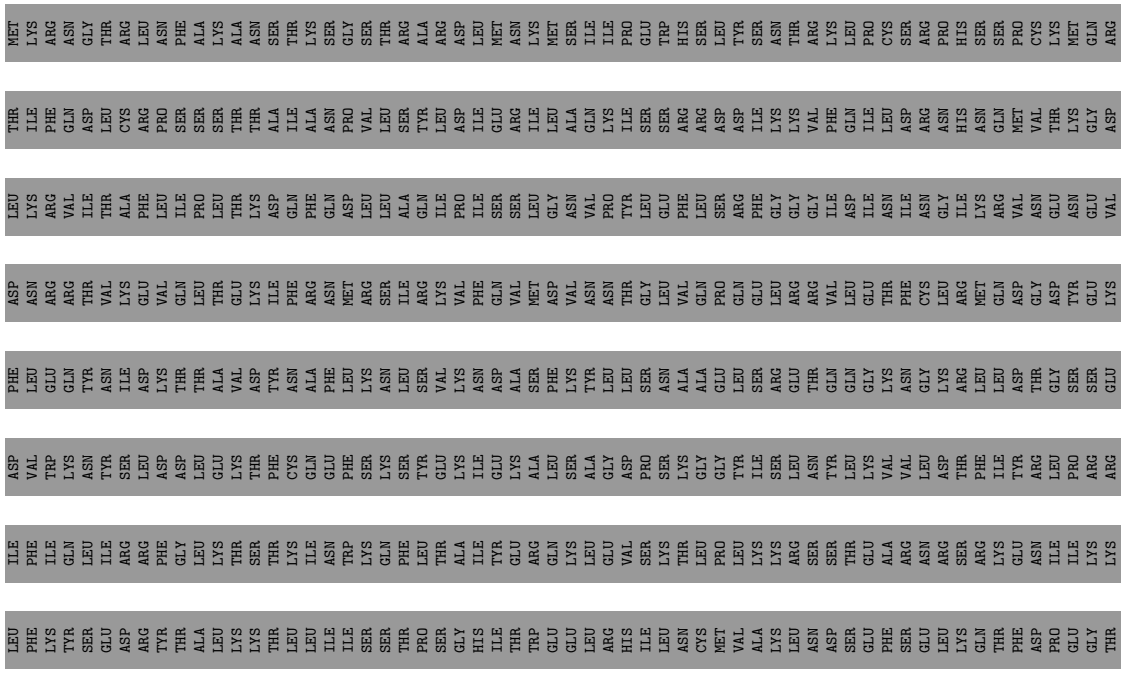
Chain P2:

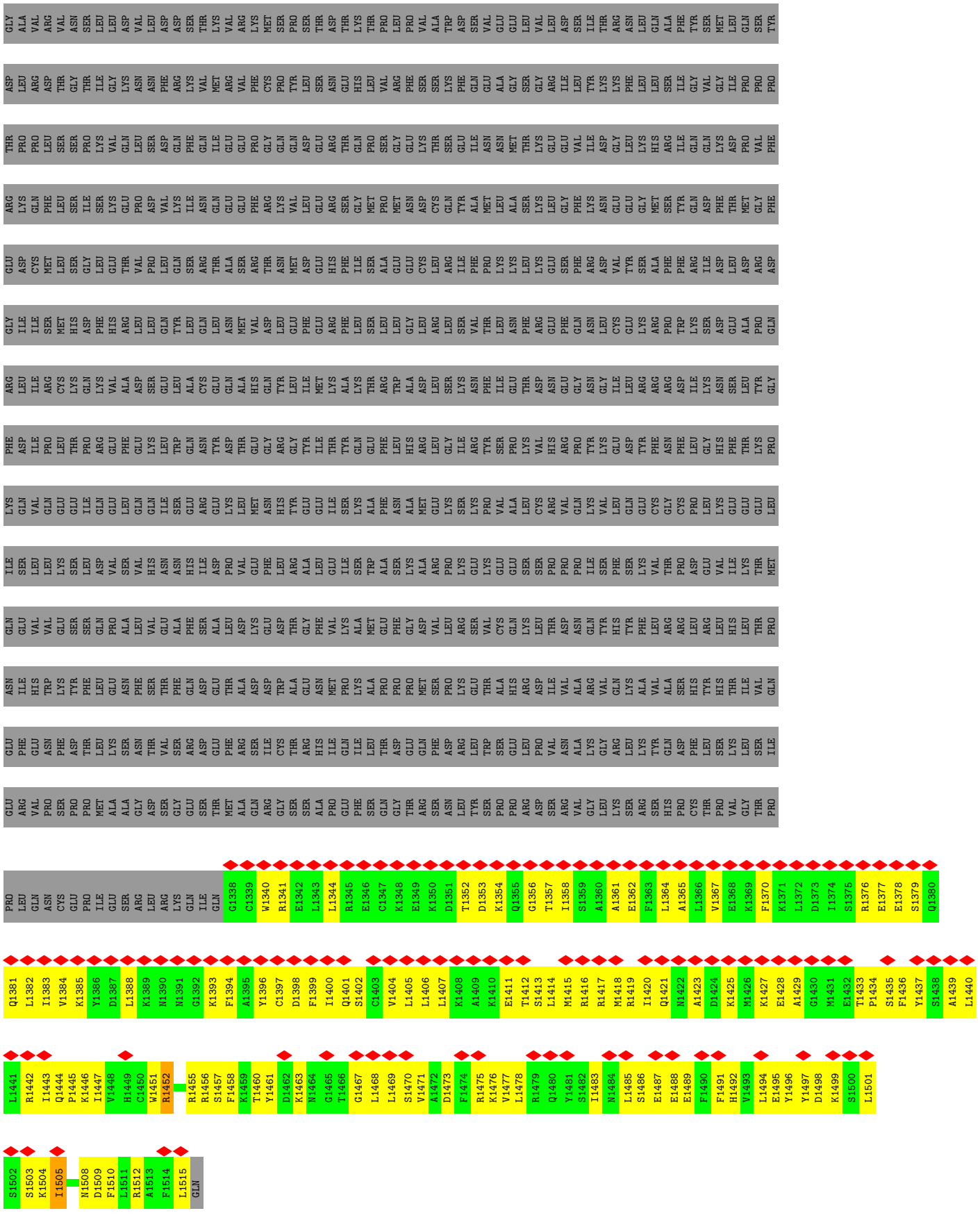




• Molecule 20: EF-hand calcium-binding domain-containing protein 6

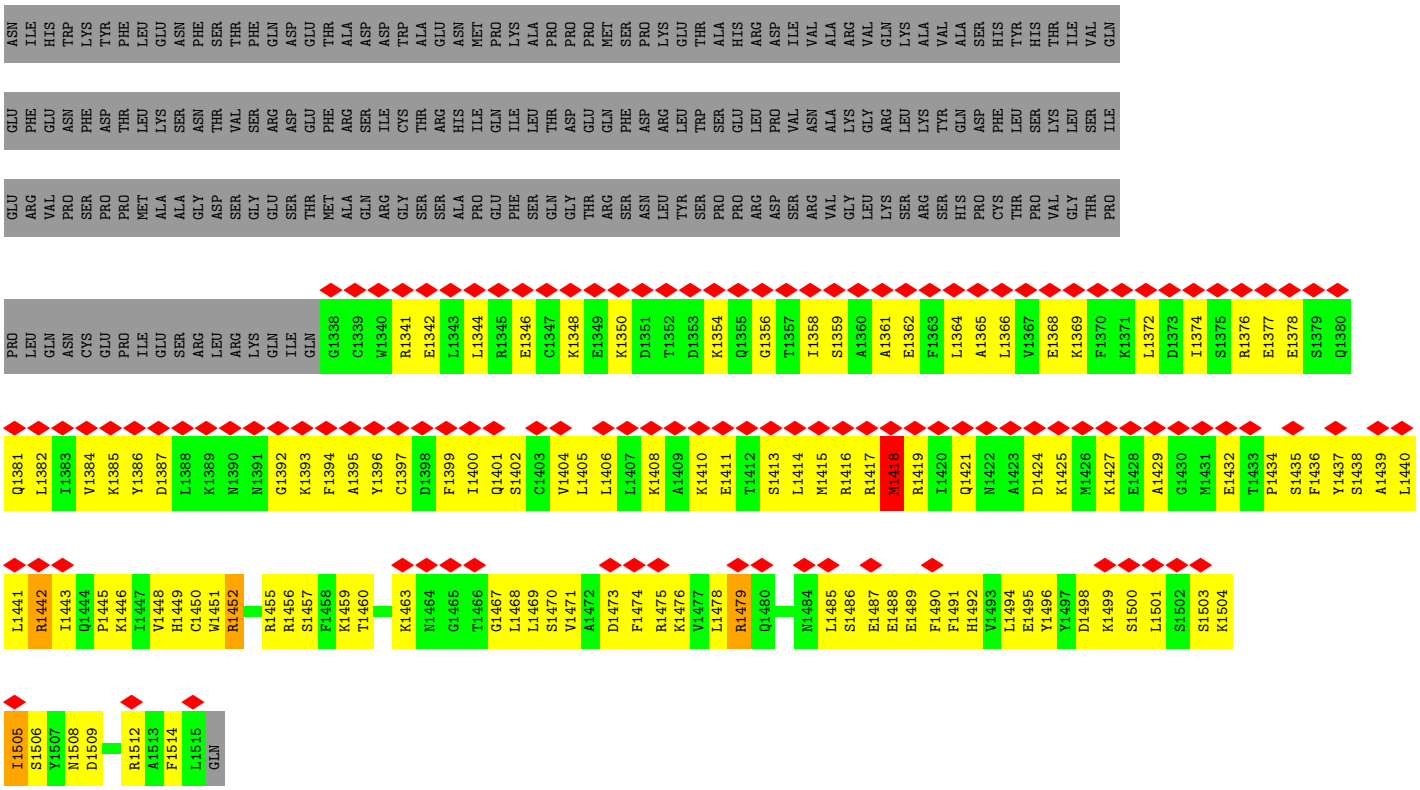
Chain Q1:





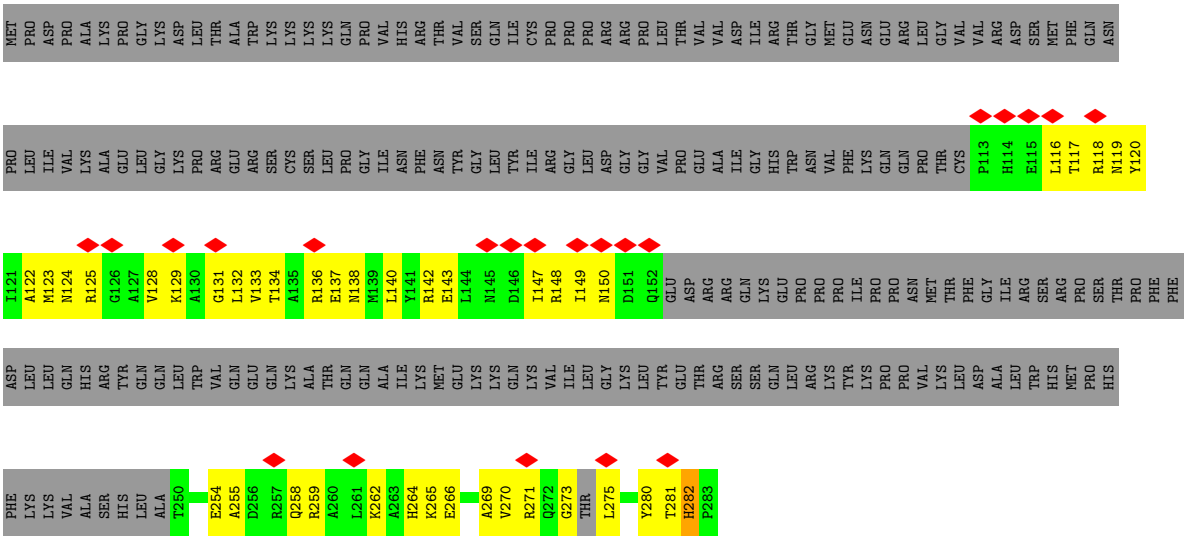
• Molecule 20: EF-hand calcium-binding domain-containing protein 6

Chain Q2:



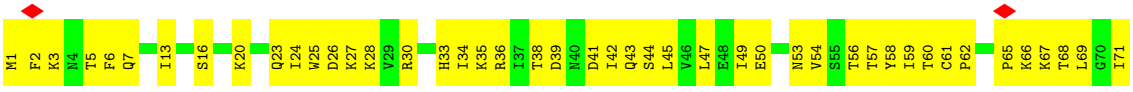
• Molecule 21: Cilia and flagella-associated protein 77

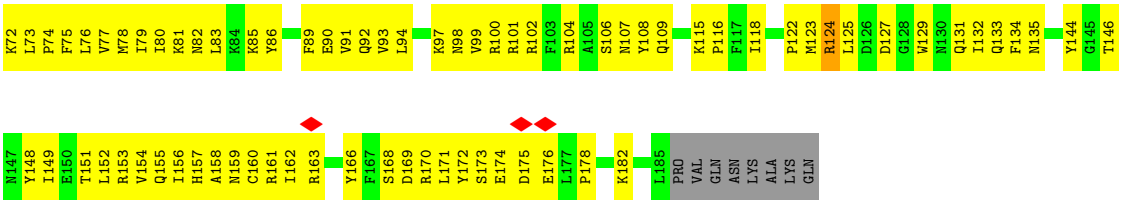
Chain R2:



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

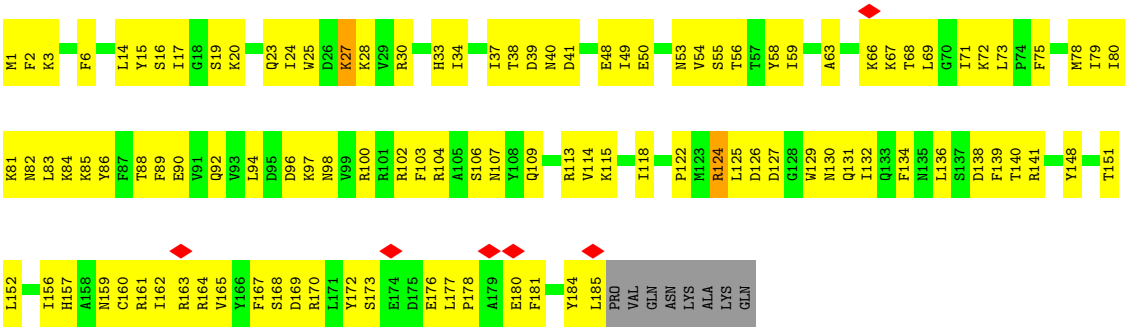
Chain XC:





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

Chain XD:

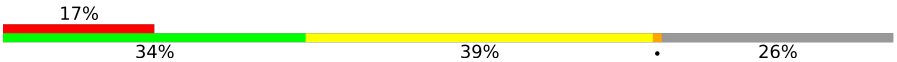


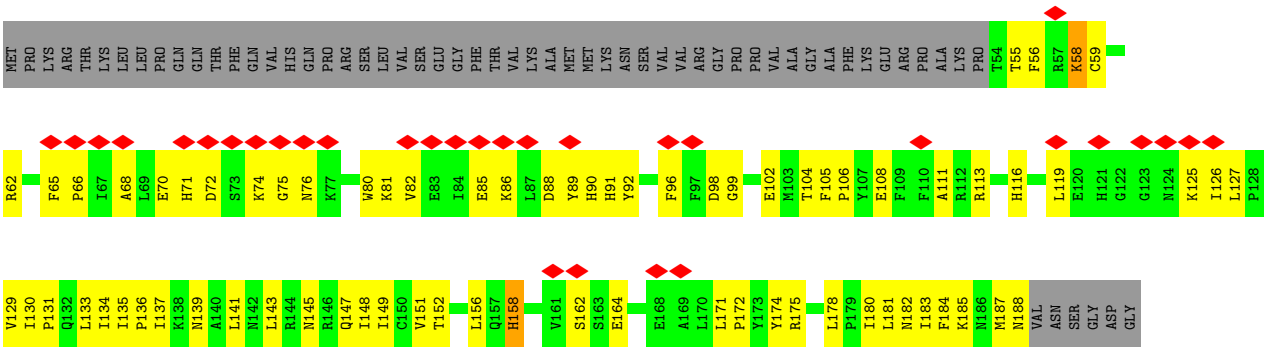
• Molecule 22: Cilia- and flagella-associated protein 20

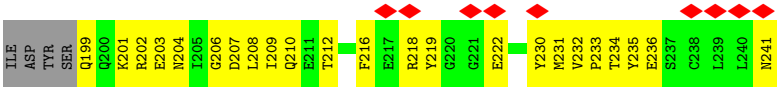
Chain XE:

• Molecule 23: Parkin coregulated gene protein homolog

Chain XJ:

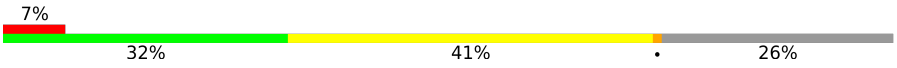


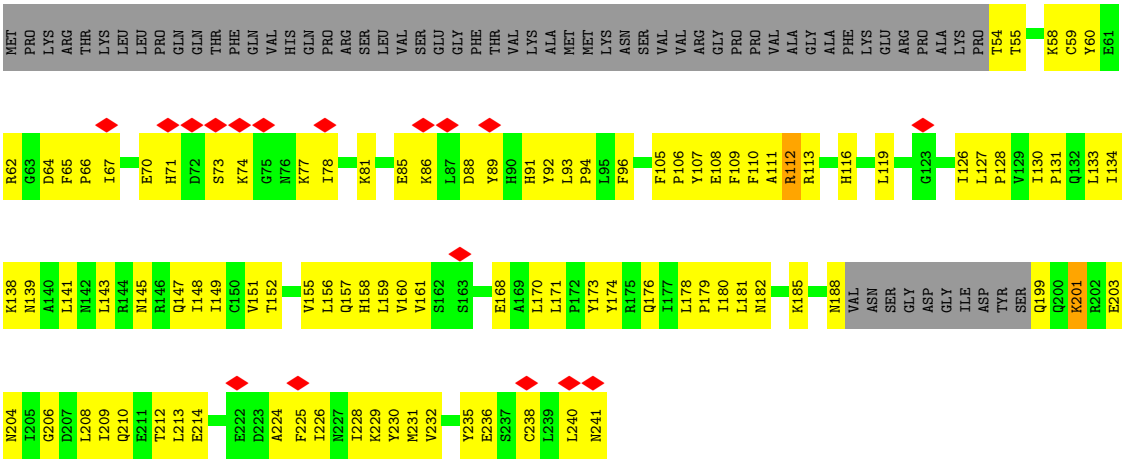




• Molecule 23: Parkin coregulated gene protein homolog

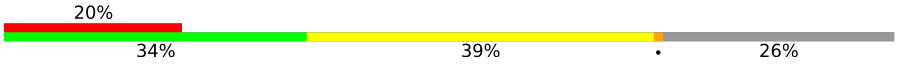
Chain XK:

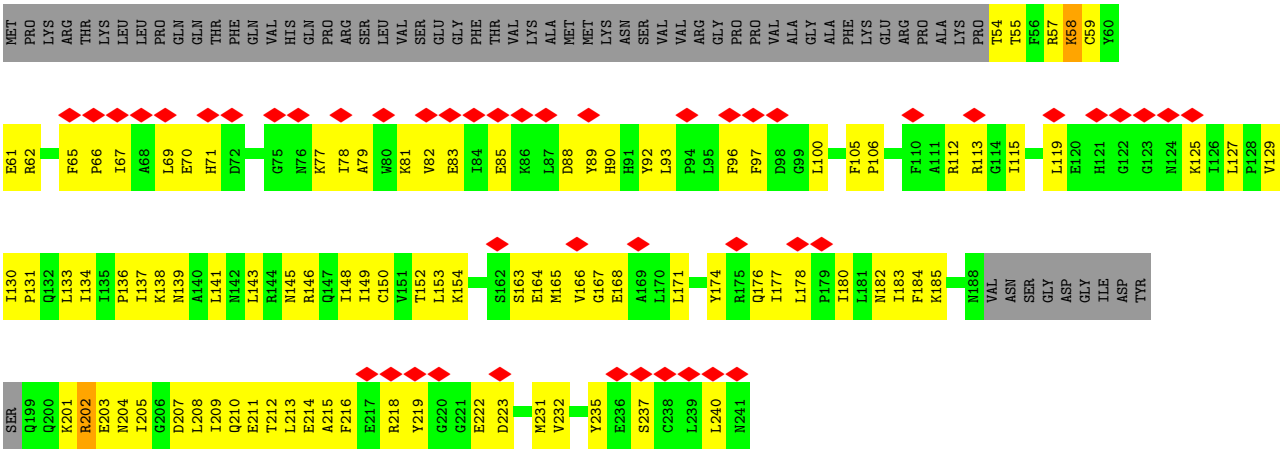




• Molecule 23: Parkin coregulated gene protein homolog

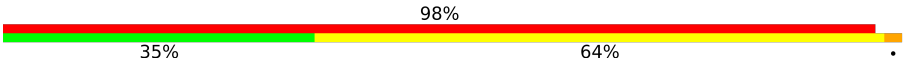
Chain XL:

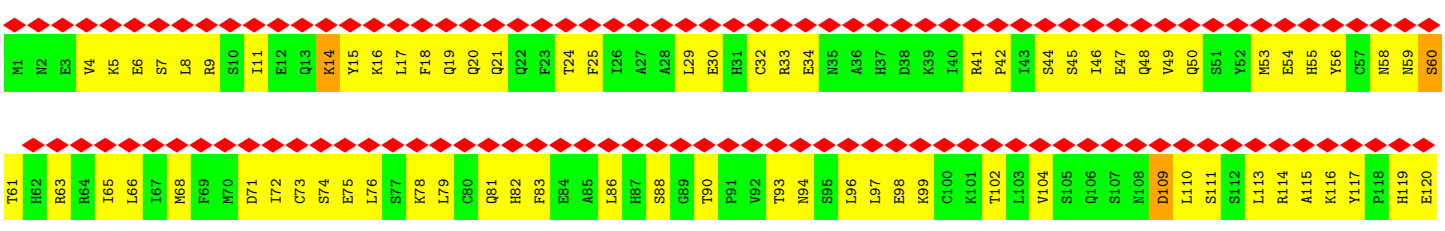




• Molecule 24: Sperm acrosome-associated protein 9

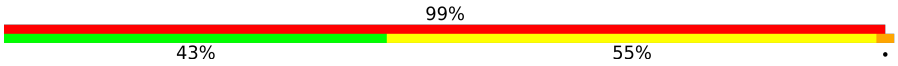
Chain YI:

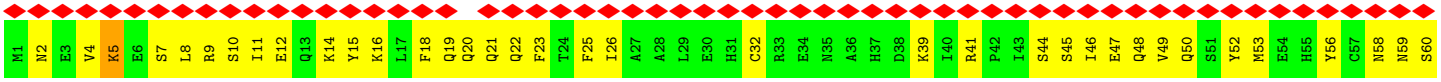


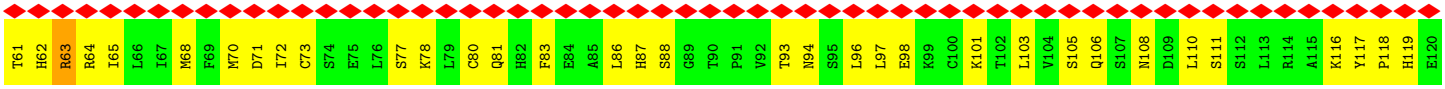


• Molecule 24: Sperm acrosome-associated protein 9

Chain YJ:

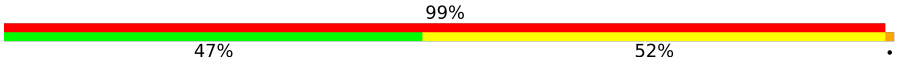


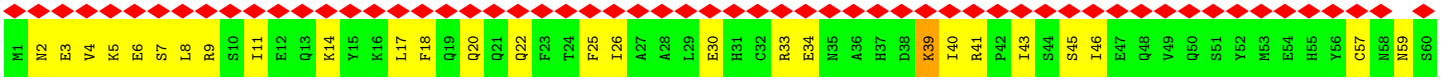


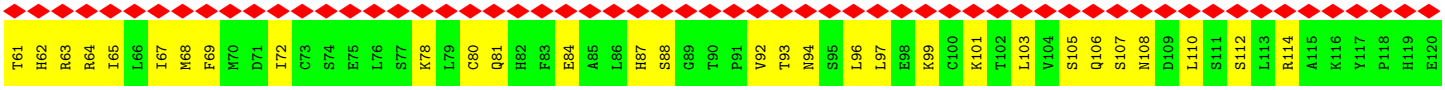


• Molecule 24: Sperm acrosome-associated protein 9

Chain YK:

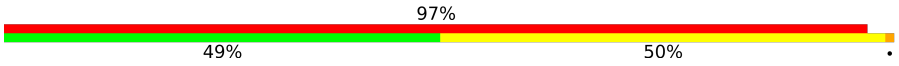


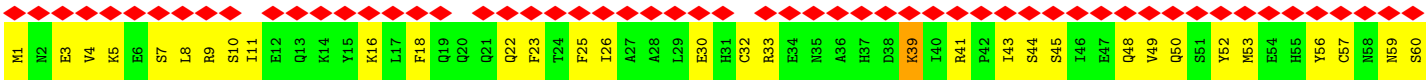


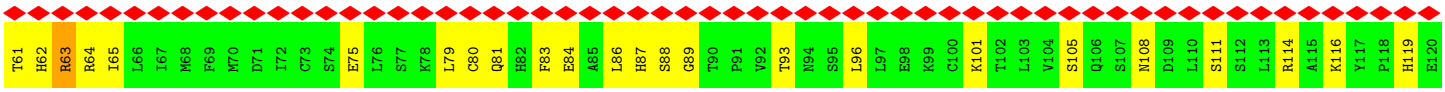


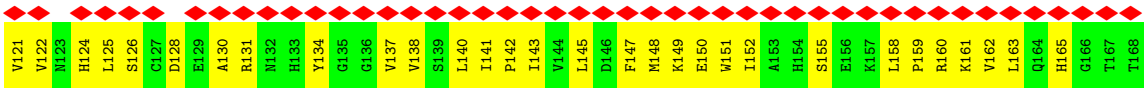
• Molecule 24: Sperm acrosome-associated protein 9

Chain YL:



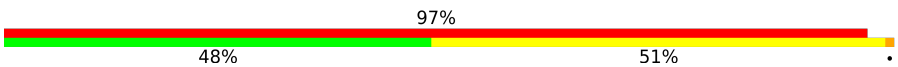






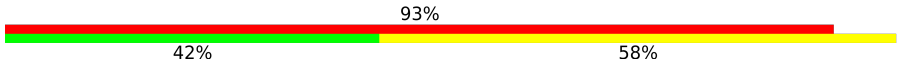
• Molecule 24: Sperm acrosome-associated protein 9

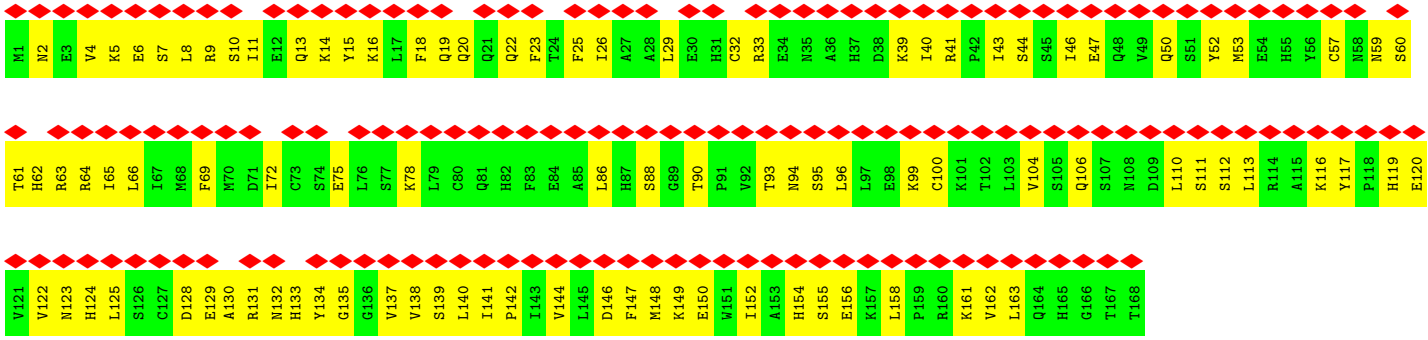
Chain YM:



• Molecule 24: Sperm acrosome-associated protein 9

Chain YN:





4 Experimental information (i)

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 ($e^-/Å^2$)	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

5.1 Standard geometry

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	0.34	0/2914	0.60	0/3926
1	A3	0.36	0/1767	0.60	1/2381 (0.0%)
2	AE	0.33	0/3496	0.58	0/4747
2	AG	0.34	0/3496	0.60	0/4747
2	AI	0.33	0/3496	0.60	0/4747
2	BE	0.31	0/3496	0.58	0/4747
2	BG	0.32	0/3496	0.59	1/4747 (0.0%)
2	BI	0.31	0/3496	0.57	0/4747
2	CG	0.32	0/3496	0.60	1/4747 (0.0%)
2	CI	0.33	0/3496	0.62	3/4747 (0.1%)
2	DE	0.35	1/3496 (0.0%)	0.68	5/4747 (0.1%)
2	DG	0.31	0/3496	0.59	2/4747 (0.0%)
2	EE	0.32	0/3496	0.62	2/4747 (0.0%)
2	EG	0.32	0/3496	0.61	3/4747 (0.1%)
2	FE	0.32	0/3496	0.60	2/4747 (0.0%)
2	FG	0.33	0/3496	0.63	3/4747 (0.1%)
2	GE	0.45	5/3496 (0.1%)	0.64	3/4747 (0.1%)
2	GG	0.32	0/3496	0.60	1/4747 (0.0%)
2	GI	0.32	0/3496	0.62	3/4747 (0.1%)
2	HE	0.30	0/3496	0.57	0/4747
2	HG	0.32	0/3496	0.59	0/4747
2	HI	0.30	0/3496	0.58	0/4747
2	IE	0.30	0/3496	0.56	0/4747
2	IG	0.31	0/3496	0.58	0/4747
2	II	0.30	0/3496	0.57	0/4747
2	JE	0.31	0/3496	0.57	0/4747
2	JG	0.31	0/3496	0.58	0/4747
2	KE	0.31	0/3496	0.59	1/4747 (0.0%)
2	KG	0.34	0/3496	0.61	1/4747 (0.0%)
2	KI	0.32	0/3496	0.60	0/4747
2	LE	0.32	0/3496	0.59	0/4747
2	LG	0.33	0/3496	0.59	0/4747

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	LI	0.33	0/3496	0.58	0/4747
2	ME	0.31	0/3496	0.57	0/4747
2	MG	0.37	1/3496 (0.0%)	0.64	3/4747 (0.1%)
2	MI	0.33	0/3496	0.58	1/4747 (0.0%)
2	NE	0.29	0/3496	0.57	1/4747 (0.0%)
2	NG	0.29	0/3496	0.55	0/4747
2	NI	0.28	0/3496	0.58	0/4747
2	OE	0.29	0/3496	0.58	1/4747 (0.0%)
2	OG	0.28	0/3496	0.57	1/4747 (0.0%)
2	OI	0.29	0/3496	0.56	0/4747
2	PE	0.30	0/3496	0.57	2/4747 (0.0%)
2	PG	0.37	1/3496 (0.0%)	0.66	4/4747 (0.1%)
2	PI	0.31	0/3496	0.60	3/4747 (0.1%)
2	QE	0.30	0/3496	0.59	3/4747 (0.1%)
2	QG	0.29	0/3496	0.58	0/4747
2	QI	0.29	0/3496	0.57	0/4747
2	RE	0.29	0/3496	0.57	0/4747
2	RG	0.29	0/3496	0.56	0/4747
2	RI	0.29	0/3496	0.59	1/4747 (0.0%)
2	SE	0.28	0/3496	0.55	0/4747
2	SG	0.30	0/3496	0.59	2/4747 (0.0%)
2	SI	0.30	0/3496	0.58	0/4747
2	TG	0.28	0/3496	0.55	0/4747
2	TI	0.29	0/3496	0.55	0/4747
2	UE	0.29	0/3496	0.58	1/4747 (0.0%)
2	UG	0.31	1/3496 (0.0%)	0.59	2/4747 (0.0%)
2	VE	0.30	0/3496	0.56	0/4747
2	VG	0.30	0/3496	0.58	0/4747
2	WE	0.32	0/3496	0.58	0/4747
2	WG	0.32	1/3496 (0.0%)	0.60	2/4747 (0.0%)
2	WI	0.30	0/3496	0.60	1/4747 (0.0%)
3	AF	0.33	0/3431	0.62	2/4649 (0.0%)
3	AH	0.33	0/3431	0.59	0/4649
3	BF	0.31	0/3431	0.57	0/4649
3	BH	0.32	0/3431	0.59	0/4649
3	CF	0.30	0/3431	0.60	0/4649
3	CH	0.32	0/3431	0.60	0/4649
3	CJ	0.32	0/3431	0.65	3/4649 (0.1%)
3	DD	0.31	0/3431	0.58	0/4649
3	DF	0.31	0/3431	0.58	0/4649
3	DH	0.30	0/3431	0.58	0/4649
3	ED	0.31	0/3431	0.60	0/4649
3	EF	0.31	0/3431	0.61	1/4649 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	EH	0.30	0/3431	0.57	0/4649
3	FD	0.30	0/3431	0.60	1/4649 (0.0%)
3	FF	0.31	0/3431	0.58	0/4649
3	FH	0.31	0/3431	0.58	0/4649
3	GD	0.32	0/3431	0.60	0/4649
3	GF	0.31	0/3431	0.60	0/4649
3	GH	0.32	0/3431	0.60	3/4649 (0.1%)
3	HD	0.29	0/3431	0.57	0/4649
3	HF	0.33	0/3431	0.61	1/4649 (0.0%)
3	HH	0.30	0/3431	0.57	0/4649
3	IF	0.32	0/3431	0.57	0/4649
3	IH	0.30	0/3431	0.58	0/4649
3	JD	0.31	0/3431	0.62	3/4649 (0.1%)
3	JF	0.31	0/3431	0.58	0/4649
3	JH	0.31	0/3431	0.60	2/4649 (0.0%)
3	KD	0.32	0/3431	0.58	0/4649
3	KF	0.32	0/3431	0.60	1/4649 (0.0%)
3	KH	0.31	0/3431	0.58	0/4649
3	LD	0.34	0/3431	0.64	2/4649 (0.0%)
3	LF	0.33	0/3431	0.63	2/4649 (0.0%)
3	LH	0.33	0/3431	0.63	3/4649 (0.1%)
3	MF	0.33	0/3431	0.58	1/4649 (0.0%)
3	MH	0.35	0/3431	0.60	1/4649 (0.0%)
3	ND	0.29	0/3431	0.57	0/4649
3	NF	0.29	0/3431	0.57	0/4649
3	NH	0.29	0/3431	0.60	1/4649 (0.0%)
3	OD	0.28	0/3431	0.54	0/4649
3	OF	0.30	0/3431	0.59	1/4649 (0.0%)
3	OH	0.29	0/3431	0.58	1/4649 (0.0%)
3	PF	0.29	0/3431	0.57	1/4649 (0.0%)
3	PH	0.28	0/3431	0.56	0/4649
3	QF	0.29	0/3431	0.57	0/4649
3	QH	0.29	0/3431	0.57	1/4649 (0.0%)
3	RF	0.30	0/3431	0.58	0/4649
3	RH	0.29	0/3431	0.57	0/4649
3	RJ	0.31	0/3431	0.57	1/4649 (0.0%)
3	SF	0.29	0/3431	0.59	1/4649 (0.0%)
3	SH	0.29	0/3431	0.58	0/4649
3	SJ	0.29	0/3431	0.58	0/4649
3	TF	0.29	0/3431	0.56	0/4649
3	TH	0.29	0/3431	0.57	1/4649 (0.0%)
3	TJ	0.29	0/3431	0.57	0/4649
3	UD	0.28	0/3431	0.58	1/4649 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	UF	0.29	0/3431	0.58	0/4649
3	UH	0.29	0/3431	0.56	0/4649
3	VD	0.30	0/3431	0.56	0/4649
3	VF	0.30	0/3431	0.59	0/4649
3	VH	0.30	0/3431	0.57	0/4649
3	WF	0.30	0/3431	0.58	0/4649
3	WH	0.29	0/3431	0.56	0/4649
4	B2	0.35	0/2053	0.61	1/2761 (0.0%)
4	B3	0.35	0/2850	0.62	0/3845
4	B7	0.33	0/3116	0.60	0/4198
4	B8	0.36	0/1475	0.65	0/1978
5	C2	0.33	0/1194	0.63	0/1609
5	C3	0.35	0/3011	0.63	0/4052
5	C4	0.39	0/674	0.76	2/904 (0.2%)
5	C7	0.36	0/2010	0.63	0/2708
5	C8	0.38	0/2561	0.66	0/3447
5	Cb	0.35	0/2143	0.62	0/2878
5	Cc	0.34	0/2188	0.60	0/2949
6	D2	0.34	0/596	0.59	0/802
6	D3	0.35	0/3270	0.59	0/4400
6	D4	0.34	0/1090	0.60	0/1460
6	D7	0.35	0/843	0.67	0/1129
6	D8	0.35	0/3234	0.61	1/4352 (0.0%)
6	D9	0.35	0/866	0.63	0/1166
7	E2	0.31	0/1613	0.66	0/2194
7	E3	0.41	0/540	0.74	2/736 (0.3%)
8	F2	0.33	0/2671	0.63	0/3591
8	F3	0.35	0/1956	0.66	0/2629
8	F6	0.31	0/2537	0.57	0/3406
8	F7	0.33	0/2021	0.65	0/2714
8	Fa	0.31	0/1763	0.62	0/2370
8	Fb	0.30	0/2669	0.58	0/3584
8	Fc	0.27	0/229	0.57	0/310
8	Fl	0.29	0/2751	0.61	0/3693
9	G1	0.31	0/4309	0.58	1/5839 (0.0%)
9	G2	0.30	0/4192	0.55	1/5678 (0.0%)
10	G5	0.32	0/6339	0.58	0/8570
11	H3	0.32	0/1219	0.70	1/1649 (0.1%)
11	H4	0.35	0/1154	0.66	0/1560
12	I2	0.41	0/306	0.64	0/413
12	I3	0.32	0/306	0.54	0/413
13	J2	0.31	0/1413	0.59	0/1923
13	J3	0.31	0/1413	0.60	0/1923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
14	K2	0.30	0/1749	0.63	0/2347
14	K3	0.30	0/3523	0.64	1/4741 (0.0%)
14	K4	0.28	0/1355	0.65	0/1833
15	L2	0.30	0/1970	0.60	1/2636 (0.0%)
15	L3	0.30	0/1970	0.60	0/2636
16	M2	0.33	0/525	0.67	1/708 (0.1%)
16	M3	0.28	0/525	0.56	0/708
17	N2	0.30	0/546	0.62	1/734 (0.1%)
17	N3	0.29	0/546	0.62	1/734 (0.1%)
18	O1	0.28	0/849	0.57	0/1160
18	O2	0.31	0/849	0.65	0/1160
19	P1	0.28	0/4793	0.58	0/6480
19	P2	0.30	0/4793	0.60	0/6480
20	Q1	0.29	0/1500	0.61	0/2007
20	Q2	0.29	0/1500	0.65	0/2007
21	R2	0.28	0/605	0.67	0/810
22	XC	0.29	0/1573	0.59	0/2122
22	XD	0.32	0/1573	0.60	0/2122
22	XE	0.31	0/1573	0.63	0/2122
23	XJ	0.30	0/1503	0.58	0/2028
23	XK	0.30	0/1503	0.58	0/2028
23	XL	0.30	0/1503	0.57	0/2028
24	YI	0.29	0/1393	0.65	1/1876 (0.1%)
24	YJ	0.29	0/1393	0.59	0/1876
24	YK	0.28	0/1393	0.58	0/1876
24	YL	0.28	0/1393	0.55	0/1876
24	YM	0.26	0/1393	0.56	0/1876
24	YN	0.29	0/1393	0.58	0/1876
All	All	0.31	10/548418 (0.0%)	0.59	110/742832 (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

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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

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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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	PG	32	PRO	CG-CD	-13.10	1.07	1.50
2	GE	224	TYR	CB-CG	-10.84	1.35	1.51
2	GE	224	TYR	CE1-CZ	-10.23	1.25	1.38
2	GE	224	TYR	CE2-CZ	8.96	1.50	1.38
2	DE	224	TYR	CD2-CE2	-7.18	1.28	1.39

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	PG	32	PRO	N-CD-CG	-17.36	77.15	103.20
3	CJ	15	GLN	CA-CB-CG	14.99	146.38	113.40
2	DE	224	TYR	CB-CG-CD2	-12.33	113.60	121.00
2	DE	224	TYR	CB-CG-CD1	11.86	128.11	121.00
2	PG	32	PRO	CA-CB-CG	-11.22	82.69	104.00

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 (i)

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	141	0
1	A3	1745	0	1736	89	0
2	AE	3418	0	3327	219	0
2	AG	3418	0	3328	227	0
2	AI	3418	0	3329	255	0
2	BE	3418	0	3327	174	0
2	BG	3418	0	3328	213	0
2	BI	3418	0	3328	189	0
2	CG	3418	0	3329	200	0
2	CI	3418	0	3329	205	0
2	DE	3418	0	3328	217	0
2	DG	3418	0	3329	199	0
2	EE	3418	0	3329	192	0
2	EG	3418	0	3329	199	0
2	FE	3418	0	3328	193	0
2	FG	3418	0	3329	189	0
2	GE	3418	0	3328	203	0
2	GG	3418	0	3328	200	0
2	GI	3418	0	3328	165	0
2	HE	3418	0	3327	197	0
2	HG	3418	0	3329	193	0
2	HI	3418	0	3329	164	0
2	IE	3418	0	3328	154	0
2	IG	3418	0	3328	179	0
2	II	3418	0	3328	165	0
2	JE	3418	0	3329	203	0
2	JG	3418	0	3327	175	0
2	KE	3418	0	3327	208	0
2	KG	3418	0	3328	191	0
2	KI	3418	0	3329	186	0
2	LE	3418	0	3331	190	0
2	LG	3418	0	3329	214	0
2	LI	3418	0	3328	191	0
2	ME	3418	0	3328	191	0
2	MG	3418	0	3328	242	0
2	MI	3418	0	3328	174	0
2	NE	3418	0	3328	235	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	NG	3418	0	3329	232	0
2	NI	3418	0	3328	210	0
2	OE	3418	0	3327	213	0
2	OG	3418	0	3327	228	0
2	OI	3418	0	3328	246	0
2	PE	3418	0	3327	218	0
2	PG	3418	0	3329	228	0
2	PI	3418	0	3328	233	0
2	QE	3418	0	3328	228	0
2	QG	3418	0	3329	229	0
2	QI	3418	0	3328	223	0
2	RE	3418	0	3329	225	0
2	RG	3418	0	3328	235	0
2	RI	3418	0	3327	262	0
2	SE	3418	0	3327	190	0
2	SG	3418	0	3328	260	0
2	SI	3418	0	3328	240	0
2	TG	3418	0	3328	214	0
2	TI	3418	0	3329	234	0
2	UE	3418	0	3327	230	0
2	UG	3418	0	3329	244	0
2	VE	3418	0	3327	234	0
2	VG	3418	0	3328	255	0
2	WE	3418	0	3329	255	0
2	WG	3418	0	3328	266	0
2	WI	3418	0	3329	264	0
3	AF	3356	0	3236	198	0
3	AH	3356	0	3235	213	0
3	BF	3356	0	3235	180	0
3	BH	3356	0	3235	198	0
3	CF	3356	0	3236	169	0
3	CH	3356	0	3237	192	0
3	CJ	3356	0	3237	168	0
3	DD	3356	0	3236	183	0
3	DF	3356	0	3236	194	0
3	DH	3356	0	3238	152	0
3	ED	3356	0	3237	176	0
3	EF	3356	0	3235	194	0
3	EH	3356	0	3237	167	0
3	FD	3356	0	3237	159	0
3	FF	3356	0	3235	167	0
3	FH	3356	0	3237	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	GD	3356	0	3237	178	0
3	GF	3356	0	3235	188	0
3	GH	3356	0	3235	177	0
3	HD	3356	0	3235	162	0
3	HF	3356	0	3235	178	0
3	HH	3356	0	3235	182	0
3	IF	3356	0	3237	191	0
3	IH	3356	0	3235	181	0
3	JD	3356	0	3235	173	0
3	JF	3356	0	3235	178	0
3	JH	3356	0	3237	160	0
3	KD	3356	0	3235	170	0
3	KF	3356	0	3236	163	0
3	KH	3356	0	3236	175	0
3	LD	3356	0	3233	175	0
3	LF	3356	0	3236	198	0
3	LH	3356	0	3235	187	0
3	MF	3356	0	3235	169	0
3	MH	3356	0	3235	230	0
3	ND	3356	0	3235	172	0
3	NF	3356	0	3236	209	0
3	NH	3356	0	3235	214	0
3	OD	3356	0	3235	171	0
3	OF	3356	0	3236	192	0
3	OH	3356	0	3234	242	0
3	PF	3356	0	3234	205	0
3	PH	3356	0	3236	216	0
3	QF	3356	0	3235	216	0
3	QH	3356	0	3235	215	0
3	RF	3356	0	3235	237	0
3	RH	3356	0	3235	238	0
3	RJ	3356	0	3237	208	0
3	SF	3356	0	3235	215	0
3	SH	3356	0	3235	231	0
3	SJ	3356	0	3237	209	0
3	TF	3356	0	3236	201	0
3	TH	3356	0	3236	191	0
3	TJ	3356	0	3238	179	0
3	UD	3356	0	3235	194	0
3	UF	3356	0	3235	217	0
3	UH	3356	0	3238	196	0
3	VD	3356	0	3234	222	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	VF	3356	0	3235	238	0
3	VH	3356	0	3236	207	0
3	WF	3356	0	3235	219	0
3	WH	3356	0	3235	202	0
4	B2	2036	0	2084	69	0
4	B3	2816	0	2822	136	0
4	B7	3082	0	3105	120	0
4	B8	1463	0	1499	90	0
5	C2	1175	0	1120	60	0
5	C3	2978	0	2969	161	0
5	C4	670	0	685	61	0
5	C7	1983	0	1923	82	0
5	C8	2534	0	2543	108	0
5	Cb	2125	0	2142	0	0
5	Cc	2159	0	2100	0	0
6	D2	583	0	539	18	0
6	D3	3225	0	3158	137	0
6	D4	1080	0	1095	51	0
6	D7	836	0	857	79	0
6	D8	3192	0	3146	145	0
6	D9	849	0	771	39	0
7	E2	1558	0	1502	82	0
7	E3	519	0	490	15	0
8	F2	2640	0	2658	126	0
8	F3	1927	0	1862	97	0
8	F6	2503	0	2456	98	0
8	F7	2003	0	2062	103	0
8	Fa	1746	0	1798	0	0
8	Fb	2634	0	2604	0	0
8	Fc	224	0	208	0	0
8	Fl	2721	0	2733	0	0
9	G1	4192	0	4130	182	0
9	G2	4081	0	4025	176	0
10	G5	6169	0	6044	330	0
11	H3	1185	0	1141	128	0
11	H4	1121	0	1073	157	0
12	I2	298	0	281	17	0
12	I3	298	0	281	15	0
13	J2	1378	0	1354	64	0
13	J3	1378	0	1354	54	0
14	K2	1722	0	1785	124	0
14	K3	3465	0	3572	221	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	K4	1327	0	1348	59	0
15	L2	1929	0	2013	150	0
15	L3	1929	0	2013	129	0
16	M2	510	0	492	41	0
16	M3	510	0	492	29	0
17	N2	535	0	512	39	0
17	N3	535	0	512	40	0
18	O1	825	0	817	39	0
18	O2	825	0	817	78	0
19	P1	4696	0	4674	277	0
19	P2	4696	0	4674	282	0
20	Q1	1473	0	1492	114	0
20	Q2	1473	0	1492	126	0
21	R2	597	0	589	45	0
22	XC	1540	0	1570	116	0
22	XD	1540	0	1570	106	0
22	XE	1540	0	1570	123	0
23	XJ	1469	0	1477	94	0
23	XK	1469	0	1477	99	0
23	XL	1469	0	1477	88	0
24	YI	1365	0	1356	107	0
24	YJ	1365	0	1356	76	0
24	YK	1365	0	1356	84	0
24	YL	1365	0	1356	73	0
24	YM	1365	0	1356	77	0
24	YN	1365	0	1356	89	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	11	0
25	BH	32	0	11	9	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

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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	10	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	9	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	7	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	3	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

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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	6	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	3	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	8	0
25	SG	32	0	12	9	0
25	SH	32	0	10	9	0
25	SI	32	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	SJ	32	0	11	7	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	28754	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 27.

The worst 5 of 28754 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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A2	351/418 (84%)	332 (95%)	18 (5%)	1 (0%)	41 76
1	A3	207/418 (50%)	198 (96%)	9 (4%)	0	100 100
2	AE	436/438 (100%)	404 (93%)	31 (7%)	1 (0%)	47 81
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%)	47 81
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%)	47 81
2	DE	436/438 (100%)	403 (92%)	32 (7%)	1 (0%)	47 81
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%)	47 81
2	FE	436/438 (100%)	403 (92%)	32 (7%)	1 (0%)	47 81
2	FG	436/438 (100%)	399 (92%)	35 (8%)	2 (0%)	29 68
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%)	47 81
2	HG	436/438 (100%)	404 (93%)	31 (7%)	1 (0%)	47 81
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	JE	436/438 (100%)	398 (91%)	37 (8%)	1 (0%)	47	81
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%)	47	81
2	KI	436/438 (100%)	400 (92%)	35 (8%)	1 (0%)	47	81
2	LE	436/438 (100%)	398 (91%)	37 (8%)	1 (0%)	47	81
2	LG	436/438 (100%)	396 (91%)	38 (9%)	2 (0%)	29	68
2	LI	436/438 (100%)	404 (93%)	31 (7%)	1 (0%)	47	81
2	ME	436/438 (100%)	404 (93%)	32 (7%)	0	100	100
2	MG	436/438 (100%)	395 (91%)	40 (9%)	1 (0%)	47	81
2	MI	436/438 (100%)	408 (94%)	27 (6%)	1 (0%)	47	81
2	NE	436/438 (100%)	400 (92%)	36 (8%)	0	100	100
2	NG	436/438 (100%)	412 (94%)	23 (5%)	1 (0%)	47	81
2	NI	436/438 (100%)	409 (94%)	27 (6%)	0	100	100
2	OE	436/438 (100%)	403 (92%)	32 (7%)	1 (0%)	47	81
2	OG	436/438 (100%)	405 (93%)	31 (7%)	0	100	100
2	OI	436/438 (100%)	407 (93%)	28 (6%)	1 (0%)	47	81
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%)	47	81
2	RG	436/438 (100%)	405 (93%)	31 (7%)	0	100	100
2	RI	436/438 (100%)	405 (93%)	30 (7%)	1 (0%)	47	81
2	SE	436/438 (100%)	409 (94%)	26 (6%)	1 (0%)	47	81
2	SG	436/438 (100%)	405 (93%)	30 (7%)	1 (0%)	47	81
2	SI	436/438 (100%)	405 (93%)	31 (7%)	0	100	100
2	TG	436/438 (100%)	411 (94%)	24 (6%)	1 (0%)	47	81
2	TI	436/438 (100%)	398 (91%)	37 (8%)	1 (0%)	47	81

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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%)	47	81
2	WI	436/438 (100%)	405 (93%)	31 (7%)	0	100	100
3	AF	425/427 (100%)	397 (93%)	26 (6%)	2 (0%)	29	68
3	AH	425/427 (100%)	394 (93%)	30 (7%)	1 (0%)	47	81
3	BF	425/427 (100%)	394 (93%)	29 (7%)	2 (0%)	29	68
3	BH	425/427 (100%)	392 (92%)	32 (8%)	1 (0%)	47	81
3	CF	425/427 (100%)	403 (95%)	21 (5%)	1 (0%)	47	81
3	CH	425/427 (100%)	400 (94%)	24 (6%)	1 (0%)	47	81
3	CJ	425/427 (100%)	402 (95%)	22 (5%)	1 (0%)	47	81
3	DD	425/427 (100%)	387 (91%)	37 (9%)	1 (0%)	47	81
3	DF	425/427 (100%)	389 (92%)	35 (8%)	1 (0%)	47	81
3	DH	425/427 (100%)	398 (94%)	25 (6%)	2 (0%)	29	68
3	ED	425/427 (100%)	389 (92%)	35 (8%)	1 (0%)	47	81
3	EF	425/427 (100%)	402 (95%)	22 (5%)	1 (0%)	47	81
3	EH	425/427 (100%)	402 (95%)	22 (5%)	1 (0%)	47	81
3	FD	425/427 (100%)	398 (94%)	26 (6%)	1 (0%)	47	81
3	FF	425/427 (100%)	394 (93%)	30 (7%)	1 (0%)	47	81
3	FH	425/427 (100%)	398 (94%)	25 (6%)	2 (0%)	29	68
3	GD	425/427 (100%)	402 (95%)	22 (5%)	1 (0%)	47	81
3	GF	425/427 (100%)	395 (93%)	29 (7%)	1 (0%)	47	81
3	GH	425/427 (100%)	400 (94%)	24 (6%)	1 (0%)	47	81
3	HD	425/427 (100%)	392 (92%)	32 (8%)	1 (0%)	47	81
3	HF	425/427 (100%)	389 (92%)	34 (8%)	2 (0%)	29	68
3	HH	425/427 (100%)	399 (94%)	25 (6%)	1 (0%)	47	81
3	IF	425/427 (100%)	401 (94%)	23 (5%)	1 (0%)	47	81
3	IH	425/427 (100%)	406 (96%)	18 (4%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	JD	425/427 (100%)	404 (95%)	20 (5%)	1 (0%)	47	81
3	JF	425/427 (100%)	394 (93%)	30 (7%)	1 (0%)	47	81
3	JH	425/427 (100%)	399 (94%)	25 (6%)	1 (0%)	47	81
3	KD	425/427 (100%)	395 (93%)	29 (7%)	1 (0%)	47	81
3	KF	425/427 (100%)	405 (95%)	19 (4%)	1 (0%)	47	81
3	KH	425/427 (100%)	396 (93%)	28 (7%)	1 (0%)	47	81
3	LD	425/427 (100%)	401 (94%)	23 (5%)	1 (0%)	47	81
3	LF	425/427 (100%)	393 (92%)	31 (7%)	1 (0%)	47	81
3	LH	425/427 (100%)	400 (94%)	24 (6%)	1 (0%)	47	81
3	MF	425/427 (100%)	398 (94%)	26 (6%)	1 (0%)	47	81
3	MH	425/427 (100%)	391 (92%)	34 (8%)	0	100	100
3	ND	425/427 (100%)	400 (94%)	24 (6%)	1 (0%)	47	81
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%)	47	81
3	OF	425/427 (100%)	396 (93%)	28 (7%)	1 (0%)	47	81
3	OH	425/427 (100%)	399 (94%)	25 (6%)	1 (0%)	47	81
3	PF	425/427 (100%)	400 (94%)	24 (6%)	1 (0%)	47	81
3	PH	425/427 (100%)	389 (92%)	35 (8%)	1 (0%)	47	81
3	QF	425/427 (100%)	394 (93%)	30 (7%)	1 (0%)	47	81
3	QH	425/427 (100%)	399 (94%)	25 (6%)	1 (0%)	47	81
3	RF	425/427 (100%)	399 (94%)	25 (6%)	1 (0%)	47	81
3	RH	425/427 (100%)	397 (93%)	26 (6%)	2 (0%)	29	68
3	RJ	425/427 (100%)	394 (93%)	30 (7%)	1 (0%)	47	81
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%)	47	81
3	TF	425/427 (100%)	402 (95%)	23 (5%)	0	100	100
3	TH	425/427 (100%)	405 (95%)	19 (4%)	1 (0%)	47	81
3	TJ	425/427 (100%)	393 (92%)	31 (7%)	1 (0%)	47	81
3	UD	425/427 (100%)	398 (94%)	26 (6%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	UF	425/427 (100%)	401 (94%)	22 (5%)	2 (0%)	29	68
3	UH	425/427 (100%)	395 (93%)	29 (7%)	1 (0%)	47	81
3	VD	425/427 (100%)	397 (93%)	27 (6%)	1 (0%)	47	81
3	VF	425/427 (100%)	405 (95%)	19 (4%)	1 (0%)	47	81
3	VH	425/427 (100%)	398 (94%)	26 (6%)	1 (0%)	47	81
3	WF	425/427 (100%)	397 (93%)	27 (6%)	1 (0%)	47	81
3	WH	425/427 (100%)	400 (94%)	24 (6%)	1 (0%)	47	81
4	B2	246/430 (57%)	233 (95%)	13 (5%)	0	100	100
4	B3	339/430 (79%)	317 (94%)	21 (6%)	1 (0%)	41	76
4	B7	372/430 (86%)	355 (95%)	14 (4%)	3 (1%)	19	60
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%)	41	76
6	D9	98/447 (22%)	89 (91%)	9 (9%)	0	100	100
7	E2	185/206 (90%)	140 (76%)	44 (24%)	1 (0%)	29	68
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%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	Fb	317/557 (57%)	307 (97%)	9 (3%)	1 (0%)	41 76
8	Fc	24/557 (4%)	24 (100%)	0	0	100 100
8	Fl	326/557 (58%)	312 (96%)	13 (4%)	1 (0%)	41 76
9	G1	506/648 (78%)	448 (88%)	56 (11%)	2 (0%)	34 72
9	G2	491/648 (76%)	428 (87%)	61 (12%)	2 (0%)	34 72
10	G5	745/750 (99%)	631 (85%)	107 (14%)	7 (1%)	17 56
11	H3	139/319 (44%)	99 (71%)	32 (23%)	8 (6%)	1 20
11	H4	131/319 (41%)	95 (72%)	26 (20%)	10 (8%)	1 15
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%)	25 65
13	J3	169/189 (89%)	132 (78%)	36 (21%)	1 (1%)	25 65
14	K2	205/499 (41%)	177 (86%)	21 (10%)	7 (3%)	3 29
14	K3	424/499 (85%)	358 (84%)	53 (12%)	13 (3%)	4 31
14	K4	163/499 (33%)	130 (80%)	28 (17%)	5 (3%)	4 31
15	L2	234/255 (92%)	193 (82%)	39 (17%)	2 (1%)	17 56
15	L3	234/255 (92%)	189 (81%)	44 (19%)	1 (0%)	34 72
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%)	15 54
19	P1	606/620 (98%)	563 (93%)	40 (7%)	3 (0%)	29 68
19	P2	606/620 (98%)	564 (93%)	39 (6%)	3 (0%)	29 68
20	Q1	176/1516 (12%)	143 (81%)	32 (18%)	1 (1%)	25 65
20	Q2	176/1516 (12%)	140 (80%)	34 (19%)	2 (1%)	14 52
21	R2	67/283 (24%)	58 (87%)	8 (12%)	1 (2%)	10 46
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

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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%)	25	65
24	YJ	166/168 (99%)	152 (92%)	13 (8%)	1 (1%)	25	65
24	YK	166/168 (99%)	148 (89%)	18 (11%)	0	100	100
24	YL	166/168 (99%)	148 (89%)	16 (10%)	2 (1%)	13	50
24	YM	166/168 (99%)	150 (90%)	14 (8%)	2 (1%)	13	50
24	YN	166/168 (99%)	144 (87%)	20 (12%)	2 (1%)	13	50
All	All	67499/80058 (84%)	62373 (92%)	4946 (7%)	180 (0%)	44	76

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A2	326/380 (86%)	323 (99%)	3 (1%)	78	87
1	A3	200/380 (53%)	194 (97%)	6 (3%)	41	63
2	AE	366/366 (100%)	364 (100%)	2 (0%)	88	93
2	AG	366/366 (100%)	360 (98%)	6 (2%)	62	79
2	AI	366/366 (100%)	363 (99%)	3 (1%)	81	89
2	BE	366/366 (100%)	363 (99%)	3 (1%)	81	89
2	BG	366/366 (100%)	358 (98%)	8 (2%)	52	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BI	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	CG	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	CI	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	DE	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	DG	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	EE	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	EG	366/366 (100%)	360 (98%)	6 (2%)	62	79
2	FE	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	FG	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	GE	366/366 (100%)	360 (98%)	6 (2%)	62	79
2	GG	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	GI	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	HE	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	HG	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	HI	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	IE	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	IG	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	II	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	JE	366/366 (100%)	360 (98%)	6 (2%)	62	79
2	JG	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	KE	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	KG	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	KI	366/366 (100%)	363 (99%)	3 (1%)	81	89
2	LE	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	LG	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	LI	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	ME	366/366 (100%)	363 (99%)	3 (1%)	81	89
2	MG	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	MI	366/366 (100%)	364 (100%)	2 (0%)	88	93
2	NE	366/366 (100%)	360 (98%)	6 (2%)	62	79
2	NG	366/366 (100%)	360 (98%)	6 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	NI	366/366 (100%)	360 (98%)	6 (2%)	62	79
2	OE	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	OG	366/366 (100%)	360 (98%)	6 (2%)	62	79
2	OI	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	PE	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	PG	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	PI	366/366 (100%)	363 (99%)	3 (1%)	81	89
2	QE	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	QG	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	QI	366/366 (100%)	363 (99%)	3 (1%)	81	89
2	RE	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	RG	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	RI	366/366 (100%)	359 (98%)	7 (2%)	57	75
2	SE	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	SG	366/366 (100%)	363 (99%)	3 (1%)	81	89
2	SI	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	TG	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	TI	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	UE	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	UG	366/366 (100%)	360 (98%)	6 (2%)	62	79
2	VE	366/366 (100%)	361 (99%)	5 (1%)	67	81
2	VG	366/366 (100%)	360 (98%)	6 (2%)	62	79
2	WE	366/366 (100%)	362 (99%)	4 (1%)	73	85
2	WG	366/366 (100%)	363 (99%)	3 (1%)	81	89
2	WI	366/366 (100%)	360 (98%)	6 (2%)	62	79
3	AF	367/367 (100%)	366 (100%)	1 (0%)	92	95
3	AH	367/367 (100%)	367 (100%)	0	100	100
3	BF	367/367 (100%)	365 (100%)	2 (0%)	88	93
3	BH	367/367 (100%)	366 (100%)	1 (0%)	92	95
3	CF	367/367 (100%)	364 (99%)	3 (1%)	81	89
3	CH	367/367 (100%)	365 (100%)	2 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	CJ	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	DD	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	DF	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	DH	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	ED	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	EF	367/367 (100%)	367 (100%)	0	100 100
3	EH	367/367 (100%)	366 (100%)	1 (0%)	92 95
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%)	364 (99%)	3 (1%)	81 89
3	GF	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	GH	367/367 (100%)	367 (100%)	0	100 100
3	HD	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	HF	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	HH	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	IF	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	IH	367/367 (100%)	367 (100%)	0	100 100
3	JD	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	JF	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	JH	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	KD	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	KF	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	KH	367/367 (100%)	367 (100%)	0	100 100
3	LD	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	LF	367/367 (100%)	363 (99%)	4 (1%)	73 85
3	LH	367/367 (100%)	364 (99%)	3 (1%)	81 89
3	MF	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	MH	367/367 (100%)	363 (99%)	4 (1%)	73 85
3	ND	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	NF	367/367 (100%)	364 (99%)	3 (1%)	81 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	NH	367/367 (100%)	364 (99%)	3 (1%)	81 89
3	OD	367/367 (100%)	367 (100%)	0	100 100
3	OF	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	OH	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	PF	367/367 (100%)	364 (99%)	3 (1%)	81 89
3	PH	367/367 (100%)	364 (99%)	3 (1%)	81 89
3	QF	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	QH	367/367 (100%)	364 (99%)	3 (1%)	81 89
3	RF	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	RH	367/367 (100%)	364 (99%)	3 (1%)	81 89
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%)	365 (100%)	2 (0%)	88 93
3	SJ	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	TF	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	TH	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	TJ	367/367 (100%)	364 (99%)	3 (1%)	81 89
3	UD	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	UF	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	UH	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	VD	367/367 (100%)	365 (100%)	2 (0%)	88 93
3	VF	367/367 (100%)	367 (100%)	0	100 100
3	VH	367/367 (100%)	366 (100%)	1 (0%)	92 95
3	WF	367/367 (100%)	364 (99%)	3 (1%)	81 89
3	WH	367/367 (100%)	365 (100%)	2 (0%)	88 93
4	B2	225/395 (57%)	224 (100%)	1 (0%)	91 94
4	B3	315/395 (80%)	315 (100%)	0	100 100
4	B7	343/395 (87%)	337 (98%)	6 (2%)	60 78
4	B8	163/395 (41%)	162 (99%)	1 (1%)	86 92
5	C2	132/445 (30%)	131 (99%)	1 (1%)	81 89
5	C3	331/445 (74%)	330 (100%)	1 (0%)	92 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C4	76/445 (17%)	76 (100%)	0	100	100
5	C7	219/445 (49%)	217 (99%)	2 (1%)	78	87
5	C8	282/445 (63%)	279 (99%)	3 (1%)	73	85
5	Cb	236/445 (53%)	235 (100%)	1 (0%)	91	94
5	Cc	238/445 (54%)	236 (99%)	2 (1%)	81	89
6	D2	56/402 (14%)	56 (100%)	0	100	100
6	D3	354/402 (88%)	352 (99%)	2 (1%)	86	92
6	D4	121/402 (30%)	120 (99%)	1 (1%)	81	89
6	D7	92/402 (23%)	90 (98%)	2 (2%)	52	71
6	D8	354/402 (88%)	352 (99%)	2 (1%)	86	92
6	D9	92/402 (23%)	91 (99%)	1 (1%)	73	85
7	E2	159/174 (91%)	156 (98%)	3 (2%)	57	75
7	E3	50/174 (29%)	50 (100%)	0	100	100
8	F2	298/487 (61%)	296 (99%)	2 (1%)	84	90
8	F3	214/487 (44%)	211 (99%)	3 (1%)	67	81
8	F6	280/487 (58%)	278 (99%)	2 (1%)	84	90
8	F7	228/487 (47%)	227 (100%)	1 (0%)	91	94
8	Fa	199/487 (41%)	197 (99%)	2 (1%)	76	86
8	Fb	295/487 (61%)	291 (99%)	4 (1%)	67	81
8	Fc	23/487 (5%)	23 (100%)	0	100	100
8	Fl	305/487 (63%)	302 (99%)	3 (1%)	76	86
9	G1	465/589 (79%)	464 (100%)	1 (0%)	93	96
9	G2	452/589 (77%)	448 (99%)	4 (1%)	78	87
10	G5	681/683 (100%)	677 (99%)	4 (1%)	86	92
11	H3	125/279 (45%)	121 (97%)	4 (3%)	39	62
11	H4	118/279 (42%)	108 (92%)	10 (8%)	10	36
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%)	152 (99%)	1 (1%)	84	90
13	J3	153/169 (90%)	152 (99%)	1 (1%)	84	90
14	K2	191/434 (44%)	190 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	K3	375/434 (86%)	370 (99%)	5 (1%)	69	82
14	K4	136/434 (31%)	134 (98%)	2 (2%)	65	80
15	L2	216/235 (92%)	211 (98%)	5 (2%)	50	70
15	L3	216/235 (92%)	213 (99%)	3 (1%)	67	81
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%)	87 (99%)	1 (1%)	73	85
18	O2	88/165 (53%)	85 (97%)	3 (3%)	37	61
19	P1	511/522 (98%)	508 (99%)	3 (1%)	86	92
19	P2	511/522 (98%)	506 (99%)	5 (1%)	76	86
20	Q1	162/1391 (12%)	161 (99%)	1 (1%)	86	92
20	Q2	162/1391 (12%)	158 (98%)	4 (2%)	47	68
21	R2	61/250 (24%)	60 (98%)	1 (2%)	62	79
22	XC	173/180 (96%)	171 (99%)	2 (1%)	71	84
22	XD	173/180 (96%)	170 (98%)	3 (2%)	60	78
22	XE	173/180 (96%)	172 (99%)	1 (1%)	86	92
23	XJ	161/215 (75%)	158 (98%)	3 (2%)	57	75
23	XK	161/215 (75%)	159 (99%)	2 (1%)	71	84
23	XL	161/215 (75%)	159 (99%)	2 (1%)	71	84
24	YI	157/157 (100%)	156 (99%)	1 (1%)	86	92
24	YJ	157/157 (100%)	153 (98%)	4 (2%)	47	68
24	YK	157/157 (100%)	156 (99%)	1 (1%)	86	92
24	YL	157/157 (100%)	154 (98%)	3 (2%)	57	75
24	YM	157/157 (100%)	155 (99%)	2 (1%)	69	82
24	YN	157/157 (100%)	154 (98%)	3 (2%)	57	75
All	All	58384/69159 (84%)	57865 (99%)	519 (1%)	79	87

5 of 519 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	VE	124	LYS

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Mol	Chain	Res	Type
2	WE	264	ARG
2	VE	84	ARG
2	HI	214	ARG
2	HG	339	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 464 such sidechains are listed below:

Mol	Chain	Res	Type
2	LE	380	ASN
2	WI	342	GLN
3	OH	423	GLN
3	WH	37	HIS
2	UG	228	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	SG	501	3,2	26,34,34	1.04	1 (3%)	32,54,54	1.87	6 (18%)
25	GTP	KF	501	3	26,34,34	1.19	2 (7%)	32,54,54	1.47	6 (18%)
25	GTP	SI	501	3,2	26,34,34	1.03	1 (3%)	32,54,54	1.50	6 (18%)
25	GTP	AF	501	3	26,34,34	1.28	2 (7%)	32,54,54	1.63	5 (15%)
25	GTP	LG	501	3,2	26,34,34	1.13	2 (7%)	32,54,54	1.59	8 (25%)
25	GTP	SH	501	3	26,34,34	1.18	2 (7%)	32,54,54	1.48	7 (21%)
25	GTP	CI	501	2	26,34,34	1.22	2 (7%)	32,54,54	1.70	8 (25%)
25	GTP	OD	501	3	26,34,34	1.14	2 (7%)	32,54,54	1.53	8 (25%)
25	GTP	EF	501	3	26,34,34	1.20	2 (7%)	32,54,54	1.57	6 (18%)
25	GTP	II	501	3,2	26,34,34	1.05	1 (3%)	32,54,54	1.53	6 (18%)
25	GTP	BF	501	3	26,34,34	1.18	2 (7%)	32,54,54	1.36	5 (15%)
25	GTP	SJ	501	3	26,34,34	1.16	2 (7%)	32,54,54	1.42	7 (21%)
25	GTP	LE	501	3,2	26,34,34	1.39	4 (15%)	32,54,54	1.72	7 (21%)
25	GTP	JH	501	3	26,34,34	1.20	2 (7%)	32,54,54	1.68	6 (18%)
25	GTP	NH	501	3	26,34,34	1.25	2 (7%)	32,54,54	1.54	6 (18%)
25	GTP	NE	501	3,2	26,34,34	1.04	1 (3%)	32,54,54	1.55	6 (18%)
25	GTP	GE	501	2	26,34,34	1.82	4 (15%)	32,54,54	1.90	7 (21%)
25	GTP	WG	501	3,2	26,34,34	1.01	1 (3%)	32,54,54	1.54	7 (21%)
25	GTP	GF	501	3	26,34,34	1.23	2 (7%)	32,54,54	1.53	8 (25%)
25	GTP	AE	501	2	26,34,34	0.99	1 (3%)	32,54,54	1.72	8 (25%)
25	GTP	VE	501	3,2	26,34,34	1.03	1 (3%)	32,54,54	1.53	8 (25%)
25	GTP	KI	501	3,2	26,34,34	1.13	2 (7%)	32,54,54	1.67	7 (21%)
25	GTP	LF	501	3	26,34,34	1.20	2 (7%)	32,54,54	1.63	7 (21%)
25	GTP	WE	501	2	26,34,34	1.13	1 (3%)	32,54,54	1.43	6 (18%)
25	GTP	DF	501	3	26,34,34	1.23	2 (7%)	32,54,54	1.48	6 (18%)
25	GTP	IG	501	3,2	26,34,34	1.15	1 (3%)	32,54,54	1.50	5 (15%)
25	GTP	TI	501	3,2	26,34,34	1.04	2 (7%)	32,54,54	1.53	7 (21%)
25	GTP	RF	501	3	26,34,34	1.19	2 (7%)	32,54,54	1.42	7 (21%)
25	GTP	QG	501	3,2	26,34,34	1.01	2 (7%)	32,54,54	1.57	6 (18%)
25	GTP	NF	501	3	26,34,34	1.24	2 (7%)	32,54,54	1.84	7 (21%)
25	GTP	CG	501	3,2	26,34,34	1.09	2 (7%)	32,54,54	2.02	7 (21%)
25	GTP	QE	501	2	26,34,34	1.00	1 (3%)	32,54,54	1.82	8 (25%)
25	GTP	WH	501	3	26,34,34	1.17	2 (7%)	32,54,54	1.44	7 (21%)
25	GTP	KH	501	3	26,34,34	1.18	2 (7%)	32,54,54	1.50	8 (25%)
25	GTP	HI	501	3,2	26,34,34	1.10	1 (3%)	32,54,54	3.38	11 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	GTP	JE	501	3,2	26,34,34	1.07	1 (3%)	32,54,54	1.46	8 (25%)
25	GTP	RE	501	2	26,34,34	1.08	2 (7%)	32,54,54	1.69	6 (18%)
25	GTP	OH	501	3	26,34,34	1.15	2 (7%)	32,54,54	1.46	7 (21%)
25	GTP	FF	501	3	26,34,34	1.19	2 (7%)	32,54,54	1.71	9 (28%)
25	GTP	DD	501	3	26,34,34	1.33	2 (7%)	32,54,54	1.66	7 (21%)
25	GTP	EE	501	2	26,34,34	1.23	3 (11%)	32,54,54	1.18	3 (9%)
25	GTP	GD	501	3	26,34,34	1.21	2 (7%)	32,54,54	1.55	5 (15%)
25	GTP	LH	501	3	26,34,34	1.20	2 (7%)	32,54,54	1.56	7 (21%)
25	GTP	SF	501	3	26,34,34	1.25	2 (7%)	32,54,54	1.55	6 (18%)
25	GTP	HG	501	3,2	26,34,34	1.51	4 (15%)	32,54,54	1.83	9 (28%)
25	GTP	ND	501	3	26,34,34	1.61	3 (11%)	32,54,54	1.96	7 (21%)
25	GTP	WF	501	3	26,34,34	1.25	2 (7%)	32,54,54	1.66	9 (28%)
25	GTP	VH	501	3	26,34,34	1.16	2 (7%)	32,54,54	1.51	7 (21%)
25	GTP	UD	501	3	26,34,34	1.11	2 (7%)	32,54,54	1.47	7 (21%)
25	GTP	EG	501	3,2	26,34,34	1.38	3 (11%)	32,54,54	1.96	6 (18%)
25	GTP	NG	501	3,2	26,34,34	1.03	2 (7%)	32,54,54	1.77	7 (21%)
25	GTP	UG	501	3,2	26,34,34	1.07	1 (3%)	32,54,54	1.59	6 (18%)
25	GTP	PF	501	3	26,34,34	1.21	2 (7%)	32,54,54	1.48	8 (25%)
25	GTP	UH	501	3	26,34,34	1.16	2 (7%)	32,54,54	1.48	6 (18%)
25	GTP	OE	501	3,2	26,34,34	1.04	2 (7%)	32,54,54	1.55	7 (21%)
25	GTP	RH	501	3	26,34,34	1.16	2 (7%)	32,54,54	1.54	8 (25%)
25	GTP	JD	501	3	26,34,34	2.08	5 (19%)	32,54,54	2.35	7 (21%)
25	GTP	CH	501	3	26,34,34	1.18	2 (7%)	32,54,54	1.60	7 (21%)
25	GTP	RI	501	3,2	26,34,34	1.13	2 (7%)	32,54,54	1.45	6 (18%)
25	GTP	PE	501	2	26,34,34	1.13	2 (7%)	32,54,54	1.55	10 (31%)
25	GTP	TJ	501	3	26,34,34	1.14	2 (7%)	32,54,54	1.43	7 (21%)
25	GTP	FH	501	3	26,34,34	1.27	2 (7%)	32,54,54	1.55	8 (25%)
25	GTP	TG	501	3,2	26,34,34	1.07	1 (3%)	32,54,54	1.51	7 (21%)
25	GTP	MG	501	3,2	26,34,34	1.11	1 (3%)	32,54,54	1.68	8 (25%)
25	GTP	VF	501	3	26,34,34	1.19	2 (7%)	32,54,54	1.43	7 (21%)
25	GTP	QF	501	3	26,34,34	1.10	2 (7%)	32,54,54	1.56	7 (21%)
25	GTP	IH	501	3	26,34,34	1.18	2 (7%)	32,54,54	1.54	7 (21%)
25	GTP	DH	501	3	26,34,34	1.23	2 (7%)	32,54,54	1.75	8 (25%)
25	GTP	LD	501	3	26,34,34	1.16	2 (7%)	32,54,54	1.37	6 (18%)
25	GTP	KD	501	3	26,34,34	1.18	2 (7%)	32,54,54	1.60	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	GTP	FE	501	2	26,34,34	1.14	2 (7%)	32,54,54	1.90	9 (28%)
25	GTP	PG	501	3,2	26,34,34	1.02	2 (7%)	32,54,54	1.49	6 (18%)
25	GTP	VG	501	3,2	26,34,34	1.00	1 (3%)	32,54,54	1.40	6 (18%)
25	GTP	RJ	501	3	26,34,34	1.16	2 (7%)	32,54,54	1.54	8 (25%)
25	GTP	BH	501	3	26,34,34	1.21	2 (7%)	32,54,54	1.47	7 (21%)
25	GTP	ME	501	2	26,34,34	1.07	1 (3%)	32,54,54	1.35	6 (18%)
25	GTP	NI	501	3,2	26,34,34	1.09	1 (3%)	32,54,54	1.64	7 (21%)
25	GTP	SE	501	2	26,34,34	0.95	2 (7%)	32,54,54	1.47	6 (18%)
25	GTP	EH	501	3	26,34,34	1.19	2 (7%)	32,54,54	1.50	8 (25%)
25	GTP	MI	501	3,2	26,34,34	1.08	1 (3%)	32,54,54	1.58	7 (21%)
25	GTP	IE	501	2	26,34,34	0.97	1 (3%)	32,54,54	1.70	7 (21%)
25	GTP	TF	501	3	26,34,34	1.15	2 (7%)	32,54,54	1.45	7 (21%)
25	GTP	MF	501	3	26,34,34	1.25	2 (7%)	32,54,54	1.65	8 (25%)
25	GTP	BE	501	2	26,34,34	1.21	2 (7%)	32,54,54	1.63	7 (21%)
25	GTP	JG	501	3,2	26,34,34	0.96	1 (3%)	32,54,54	1.59	7 (21%)
25	GTP	AI	501	3,2	26,34,34	1.13	1 (3%)	32,54,54	1.60	6 (18%)
25	GTP	IF	501	3	26,34,34	1.22	2 (7%)	32,54,54	1.57	9 (28%)
25	GTP	UF	501	3	26,34,34	1.17	2 (7%)	32,54,54	1.44	6 (18%)
25	GTP	GH	502	3,2	26,34,34	1.11	2 (7%)	32,54,54	1.64	7 (21%)
25	GTP	KE	501	3,2	26,34,34	1.07	1 (3%)	32,54,54	1.53	7 (21%)
25	GTP	JF	501	3	26,34,34	1.19	2 (7%)	32,54,54	1.54	7 (21%)
25	GTP	LI	501	3,2	26,34,34	1.16	3 (11%)	32,54,54	1.63	8 (25%)
25	GTP	RG	501	3,2	26,34,34	0.96	2 (7%)	32,54,54	1.64	6 (18%)
25	GTP	QH	501	3	26,34,34	1.17	2 (7%)	32,54,54	1.40	7 (21%)
25	GTP	OF	501	3	26,34,34	1.28	2 (7%)	32,54,54	1.66	9 (28%)
25	GTP	KG	501	3,2	26,34,34	1.17	3 (11%)	32,54,54	1.99	6 (18%)
25	GTP	MH	501	3	26,34,34	1.50	2 (7%)	32,54,54	2.21	9 (28%)
25	GTP	TH	501	3	26,34,34	1.16	2 (7%)	32,54,54	1.45	7 (21%)
25	GTP	VD	501	3	26,34,34	1.16	2 (7%)	32,54,54	1.46	7 (21%)
25	GTP	PI	501	3,2	26,34,34	1.13	2 (7%)	32,54,54	1.74	8 (25%)
25	GTP	HH	501	3	26,34,34	1.19	2 (7%)	32,54,54	1.58	8 (25%)
25	GTP	CJ	501	3	26,34,34	1.76	3 (11%)	32,54,54	1.89	6 (18%)
25	GTP	PH	501	3	26,34,34	1.14	2 (7%)	32,54,54	1.41	7 (21%)
25	GTP	WI	501	3,2	26,34,34	1.08	1 (3%)	32,54,54	1.62	6 (18%)
25	GTP	UE	501	3,2	26,34,34	1.06	2 (7%)	32,54,54	1.52	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	GTP	AH	501	3	26,34,34	1.19	2 (7%)	32,54,54	1.49	4 (12%)
25	GTP	ED	501	3	26,34,34	1.80	3 (11%)	32,54,54	1.93	8 (25%)
25	GTP	AG	501	3,2	26,34,34	1.10	2 (7%)	32,54,54	1.49	8 (25%)
25	GTP	HE	501	3,2	26,34,34	1.18	2 (7%)	32,54,54	1.60	7 (21%)
25	GTP	OI	501	3,2	26,34,34	1.07	1 (3%)	32,54,54	1.45	6 (18%)
25	GTP	GH	501	3	26,34,34	1.19	2 (7%)	32,54,54	1.44	7 (21%)
25	GTP	HF	501	3	26,34,34	1.52	4 (15%)	32,54,54	1.85	8 (25%)
25	GTP	BI	501	3,2	26,34,34	1.02	1 (3%)	32,54,54	1.40	7 (21%)
25	GTP	HD	501	3	26,34,34	1.16	2 (7%)	32,54,54	1.45	6 (18%)
25	GTP	BG	501	3,2	26,34,34	1.13	2 (7%)	32,54,54	1.73	9 (28%)
25	GTP	OG	501	3,2	26,34,34	1.01	1 (3%)	32,54,54	1.47	6 (18%)
25	GTP	QI	501	3,2	26,34,34	1.04	1 (3%)	32,54,54	1.57	8 (25%)
25	GTP	FD	501	3	26,34,34	1.16	2 (7%)	32,54,54	1.41	7 (21%)
25	GTP	GG	501	3,2	26,34,34	0.93	1 (3%)	32,54,54	1.87	9 (28%)
25	GTP	FF	502	3,2	26,34,34	1.26	1 (3%)	32,54,54	1.62	5 (15%)
25	GTP	CF	501	3	26,34,34	1.20	2 (7%)	32,54,54	1.43	8 (25%)
25	GTP	DG	501	3,2	26,34,34	1.23	2 (7%)	32,54,54	1.25	3 (9%)
25	GTP	DE	501	3,2	26,34,34	1.23	2 (7%)	32,54,54	2.10	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GTP	SG	501	3,2	-	6/18/38/38	0/3/3/3
25	GTP	KF	501	3	-	9/18/38/38	0/3/3/3
25	GTP	SI	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	AF	501	3	-	6/18/38/38	0/3/3/3
25	GTP	LG	501	3,2	-	6/18/38/38	0/3/3/3
25	GTP	SH	501	3	-	6/18/38/38	0/3/3/3
25	GTP	CI	501	2	-	6/18/38/38	0/3/3/3
25	GTP	OD	501	3	-	5/18/38/38	0/3/3/3
25	GTP	EF	501	3	-	6/18/38/38	0/3/3/3
25	GTP	II	501	3,2	-	10/18/38/38	0/3/3/3
25	GTP	BF	501	3	-	10/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GTP	SJ	501	3	-	1/18/38/38	0/3/3/3
25	GTP	LE	501	3,2	-	8/18/38/38	0/3/3/3
25	GTP	JH	501	3	-	0/18/38/38	0/3/3/3
25	GTP	NH	501	3	-	5/18/38/38	0/3/3/3
25	GTP	NE	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	GE	501	2	-	6/18/38/38	0/3/3/3
25	GTP	WG	501	3,2	-	6/18/38/38	0/3/3/3
25	GTP	GF	501	3	-	7/18/38/38	0/3/3/3
25	GTP	AE	501	2	-	5/18/38/38	0/3/3/3
25	GTP	VE	501	3,2	-	4/18/38/38	0/3/3/3
25	GTP	KI	501	3,2	-	4/18/38/38	0/3/3/3
25	GTP	LF	501	3	-	4/18/38/38	0/3/3/3
25	GTP	WE	501	2	-	6/18/38/38	0/3/3/3
25	GTP	DF	501	3	-	6/18/38/38	0/3/3/3
25	GTP	IG	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	TI	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	RF	501	3	-	5/18/38/38	0/3/3/3
25	GTP	QG	501	3,2	-	7/18/38/38	0/3/3/3
25	GTP	NF	501	3	-	4/18/38/38	0/3/3/3
25	GTP	CG	501	3,2	-	8/18/38/38	0/3/3/3
25	GTP	QE	501	2	-	4/18/38/38	0/3/3/3
25	GTP	WH	501	3	-	6/18/38/38	0/3/3/3
25	GTP	KH	501	3	-	10/18/38/38	0/3/3/3
25	GTP	HI	501	3,2	-	4/18/38/38	0/3/3/3
25	GTP	JE	501	3,2	-	6/18/38/38	0/3/3/3
25	GTP	RE	501	2	-	6/18/38/38	0/3/3/3
25	GTP	OH	501	3	-	5/18/38/38	0/3/3/3
25	GTP	FF	501	3	-	2/18/38/38	0/3/3/3
25	GTP	DD	501	3	-	6/18/38/38	0/3/3/3
25	GTP	EE	501	2	-	9/18/38/38	0/3/3/3
25	GTP	GD	501	3	-	5/18/38/38	0/3/3/3
25	GTP	LH	501	3	-	3/18/38/38	0/3/3/3
25	GTP	SF	501	3	-	4/18/38/38	0/3/3/3
25	GTP	HG	501	3,2	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GTP	ND	501	3	-	8/18/38/38	0/3/3/3
25	GTP	WF	501	3	-	0/18/38/38	0/3/3/3
25	GTP	VH	501	3	-	3/18/38/38	0/3/3/3
25	GTP	UD	501	3	-	5/18/38/38	0/3/3/3
25	GTP	EG	501	3,2	-	6/18/38/38	0/3/3/3
25	GTP	NG	501	3,2	-	6/18/38/38	0/3/3/3
25	GTP	UG	501	3,2	-	7/18/38/38	0/3/3/3
25	GTP	PF	501	3	-	0/18/38/38	0/3/3/3
25	GTP	UH	501	3	-	6/18/38/38	0/3/3/3
25	GTP	OE	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	RH	501	3	-	4/18/38/38	0/3/3/3
25	GTP	JD	501	3	-	10/18/38/38	0/3/3/3
25	GTP	CH	501	3	-	7/18/38/38	0/3/3/3
25	GTP	RI	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	PE	501	2	-	4/18/38/38	0/3/3/3
25	GTP	TJ	501	3	-	2/18/38/38	0/3/3/3
25	GTP	FH	501	3	-	8/18/38/38	0/3/3/3
25	GTP	TG	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	MG	501	3,2	-	8/18/38/38	0/3/3/3
25	GTP	VF	501	3	-	7/18/38/38	0/3/3/3
25	GTP	QF	501	3	-	4/18/38/38	0/3/3/3
25	GTP	IH	501	3	-	6/18/38/38	0/3/3/3
25	GTP	DH	501	3	-	0/18/38/38	0/3/3/3
25	GTP	LD	501	3	-	2/18/38/38	0/3/3/3
25	GTP	KD	501	3	-	1/18/38/38	0/3/3/3
25	GTP	FE	501	2	-	8/18/38/38	0/3/3/3
25	GTP	PG	501	3,2	-	7/18/38/38	0/3/3/3
25	GTP	VG	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	RJ	501	3	-	4/18/38/38	0/3/3/3
25	GTP	BH	501	3	-	8/18/38/38	0/3/3/3
25	GTP	ME	501	2	-	9/18/38/38	0/3/3/3
25	GTP	NI	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	SE	501	2	-	4/18/38/38	0/3/3/3
25	GTP	EH	501	3	-	10/18/38/38	0/3/3/3
25	GTP	MI	501	3,2	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GTP	IE	501	2	-	7/18/38/38	0/3/3/3
25	GTP	TF	501	3	-	3/18/38/38	0/3/3/3
25	GTP	MF	501	3	-	7/18/38/38	0/3/3/3
25	GTP	BE	501	2	-	2/18/38/38	0/3/3/3
25	GTP	JG	501	3,2	-	10/18/38/38	0/3/3/3
25	GTP	AI	501	3,2	-	7/18/38/38	0/3/3/3
25	GTP	IF	501	3	-	3/18/38/38	0/3/3/3
25	GTP	UF	501	3	-	5/18/38/38	0/3/3/3
25	GTP	GH	502	3,2	-	9/18/38/38	0/3/3/3
25	GTP	KE	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	JF	501	3	-	10/18/38/38	0/3/3/3
25	GTP	LI	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	RG	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	QH	501	3	-	8/18/38/38	0/3/3/3
25	GTP	OF	501	3	-	5/18/38/38	0/3/3/3
25	GTP	KG	501	3,2	-	9/18/38/38	0/3/3/3
25	GTP	MH	501	3	-	4/18/38/38	0/3/3/3
25	GTP	TH	501	3	-	6/18/38/38	0/3/3/3
25	GTP	VD	501	3	-	5/18/38/38	0/3/3/3
25	GTP	PI	501	3,2	-	6/18/38/38	0/3/3/3
25	GTP	HH	501	3	-	7/18/38/38	0/3/3/3
25	GTP	CJ	501	3	-	4/18/38/38	0/3/3/3
25	GTP	PH	501	3	-	2/18/38/38	0/3/3/3
25	GTP	WI	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	UE	501	3,2	-	4/18/38/38	0/3/3/3
25	GTP	AH	501	3	-	8/18/38/38	0/3/3/3
25	GTP	ED	501	3	-	2/18/38/38	0/3/3/3
25	GTP	AG	501	3,2	-	6/18/38/38	0/3/3/3
25	GTP	HE	501	3,2	-	3/18/38/38	0/3/3/3
25	GTP	OI	501	3,2	-	6/18/38/38	0/3/3/3
25	GTP	GH	501	3	-	6/18/38/38	0/3/3/3
25	GTP	HF	501	3	-	2/18/38/38	0/3/3/3
25	GTP	BI	501	3,2	-	6/18/38/38	0/3/3/3
25	GTP	HD	501	3	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GTP	BG	501	3,2	-	5/18/38/38	0/3/3/3
25	GTP	OG	501	3,2	-	6/18/38/38	0/3/3/3
25	GTP	QI	501	3,2	-	6/18/38/38	0/3/3/3
25	GTP	FD	501	3	-	3/18/38/38	0/3/3/3
25	GTP	GG	501	3,2	-	7/18/38/38	0/3/3/3
25	GTP	FF	502	3,2	-	9/18/38/38	0/3/3/3
25	GTP	CF	501	3	-	4/18/38/38	0/3/3/3
25	GTP	DG	501	3,2	-	2/18/38/38	0/3/3/3
25	GTP	DE	501	3,2	-	3/18/38/38	0/3/3/3

The worst 5 of 234 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	JD	501	GTP	C2-N2	7.05	1.50	1.34
25	GE	501	GTP	C5-C6	-6.51	1.34	1.47
25	ED	501	GTP	C2-N3	5.74	1.47	1.33
25	HG	501	GTP	C5-C6	-5.40	1.36	1.47
25	ND	501	GTP	C2-N3	5.20	1.45	1.33

The worst 5 of 860 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	HI	501	GTP	O3G-PG-O3B	-7.88	78.20	104.64
25	HI	501	GTP	O3G-PG-O2G	-7.61	78.56	107.64
25	HI	501	GTP	O3G-PG-O1G	7.40	139.64	110.68
25	JD	501	GTP	C5-C6-N1	6.85	126.05	113.95
25	CG	501	GTP	O6-C6-N1	-6.76	112.67	120.65

There are no chirality outliers.

5 of 665 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	AF	501	GTP	C5'-O5'-PA-O3A
25	AG	501	GTP	C3'-C4'-C5'-O5'
25	AI	501	GTP	O4'-C4'-C5'-O5'
25	AI	501	GTP	C3'-C4'-C5'-O5'
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	SG	501	GTP	9	0
25	KF	501	GTP	9	0
25	SI	501	GTP	5	0
25	AF	501	GTP	5	0
25	LG	501	GTP	5	0
25	SH	501	GTP	9	0
25	CI	501	GTP	5	0
25	OD	501	GTP	7	0
25	EF	501	GTP	7	0
25	II	501	GTP	7	0
25	BF	501	GTP	9	0
25	SJ	501	GTP	7	0
25	LE	501	GTP	9	0
25	JH	501	GTP	5	0
25	NH	501	GTP	7	0
25	NE	501	GTP	5	0
25	GE	501	GTP	7	0
25	WG	501	GTP	9	0
25	GF	501	GTP	6	0
25	AE	501	GTP	3	0
25	VE	501	GTP	4	0
25	KI	501	GTP	5	0
25	LF	501	GTP	3	0
25	WE	501	GTP	7	0
25	DF	501	GTP	8	0
25	IG	501	GTP	3	0
25	TI	501	GTP	8	0
25	RF	501	GTP	11	0
25	QG	501	GTP	4	0
25	NF	501	GTP	4	0
25	CG	501	GTP	6	0
25	QE	501	GTP	9	0
25	WH	501	GTP	9	0
25	KH	501	GTP	5	0
25	HI	501	GTP	9	0
25	JE	501	GTP	12	0
25	RE	501	GTP	3	0
25	OH	501	GTP	7	0
25	FF	501	GTP	3	0
25	DD	501	GTP	2	0
25	EE	501	GTP	10	0
25	GD	501	GTP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	LH	501	GTP	6	0
25	SF	501	GTP	8	0
25	HG	501	GTP	5	0
25	ND	501	GTP	6	0
25	WF	501	GTP	6	0
25	VH	501	GTP	7	0
25	UD	501	GTP	6	0
25	EG	501	GTP	13	0
25	NG	501	GTP	5	0
25	UG	501	GTP	5	0
25	PF	501	GTP	7	0
25	UH	501	GTP	8	0
25	OE	501	GTP	7	0
25	RH	501	GTP	9	0
25	JD	501	GTP	4	0
25	CH	501	GTP	4	0
25	RI	501	GTP	6	0
25	PE	501	GTP	10	0
25	TJ	501	GTP	6	0
25	FH	501	GTP	4	0
25	TG	501	GTP	7	0
25	MG	501	GTP	11	0
25	VF	501	GTP	8	0
25	QF	501	GTP	6	0
25	IH	501	GTP	9	0
25	DH	501	GTP	6	0
25	LD	501	GTP	6	0
25	KD	501	GTP	5	0
25	FE	501	GTP	9	0
25	PG	501	GTP	4	0
25	VG	501	GTP	2	0
25	RJ	501	GTP	10	0
25	BH	501	GTP	9	0
25	ME	501	GTP	5	0
25	NI	501	GTP	5	0
25	SE	501	GTP	4	0
25	EH	501	GTP	6	0
25	MI	501	GTP	4	0
25	IE	501	GTP	3	0
25	TF	501	GTP	7	0
25	MF	501	GTP	10	0
25	BE	501	GTP	4	0

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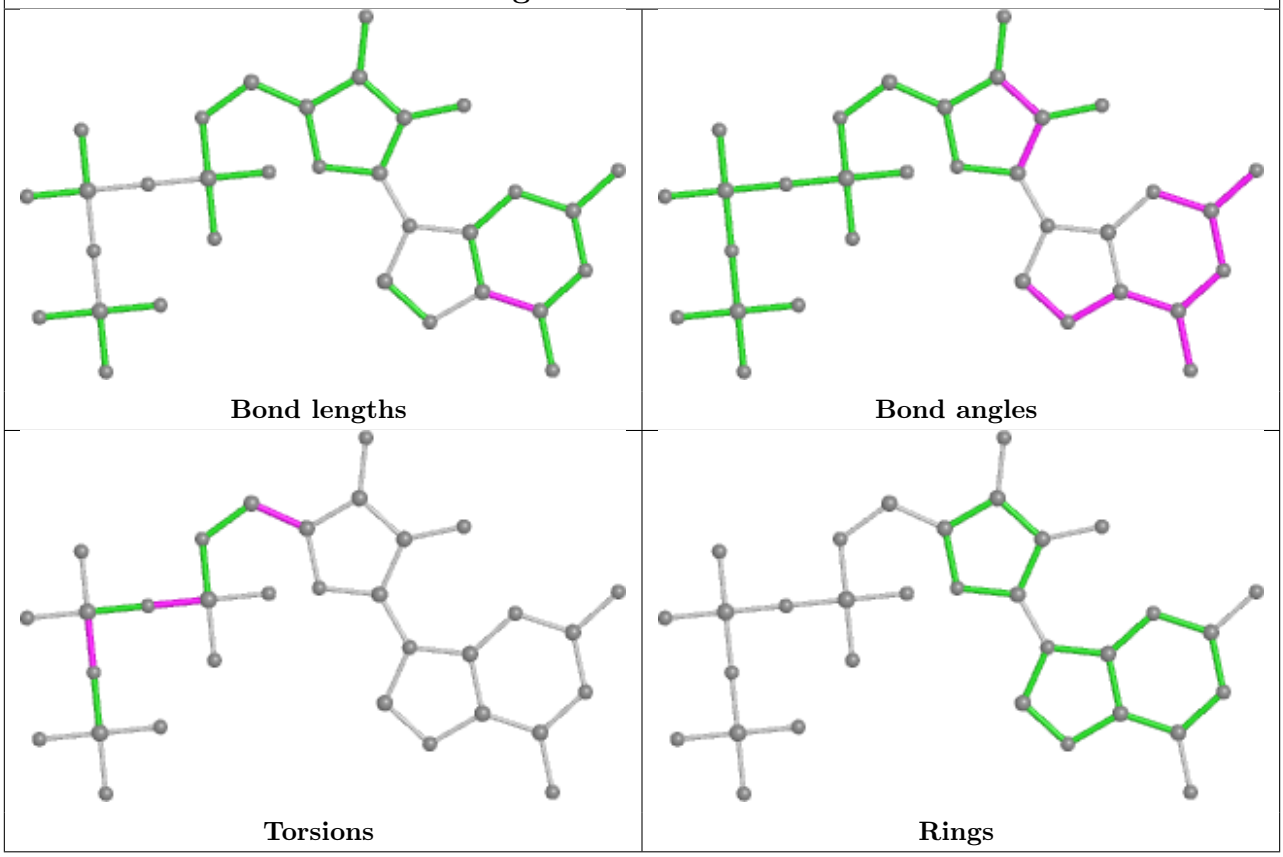
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	JG	501	GTP	3	0
25	AI	501	GTP	6	0
25	IF	501	GTP	8	0
25	UF	501	GTP	9	0
25	GH	502	GTP	5	0
25	KE	501	GTP	6	0
25	JF	501	GTP	9	0
25	LI	501	GTP	7	0
25	RG	501	GTP	5	0
25	QH	501	GTP	11	0
25	OF	501	GTP	10	0
25	KG	501	GTP	5	0
25	MH	501	GTP	3	0
25	TH	501	GTP	7	0
25	VD	501	GTP	5	0
25	PI	501	GTP	11	0
25	HH	501	GTP	4	0
25	CJ	501	GTP	4	0
25	PH	501	GTP	7	0
25	WI	501	GTP	5	0
25	UE	501	GTP	5	0
25	AH	501	GTP	8	0
25	ED	501	GTP	5	0
25	AG	501	GTP	4	0
25	HE	501	GTP	4	0
25	OI	501	GTP	6	0
25	GH	501	GTP	7	0
25	HF	501	GTP	3	0
25	BI	501	GTP	8	0
25	HD	501	GTP	10	0
25	BG	501	GTP	11	0
25	OG	501	GTP	7	0
25	QI	501	GTP	9	0
25	FD	501	GTP	9	0
25	GG	501	GTP	6	0
25	FF	502	GTP	10	0
25	CF	501	GTP	6	0
25	DG	501	GTP	9	0
25	DE	501	GTP	11	0

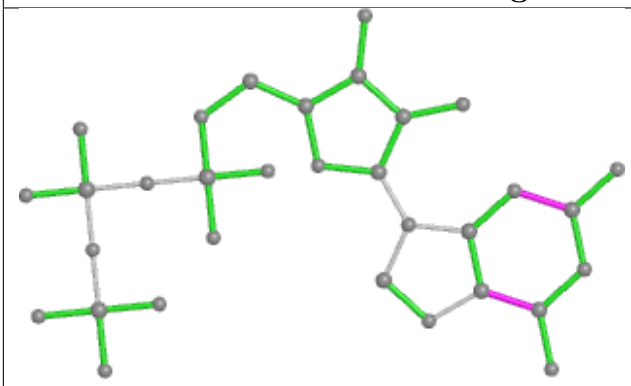
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

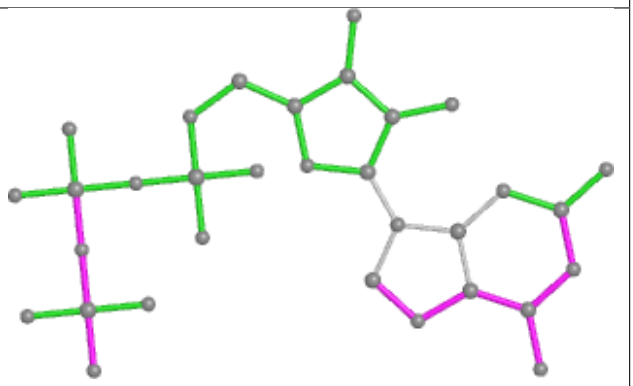
Ligand GTP SG 501



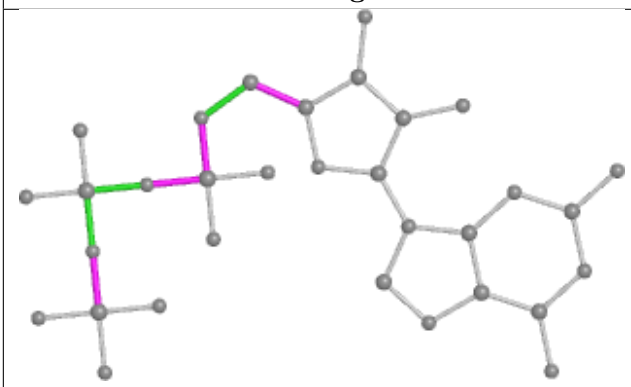
Ligand GTP KF 501



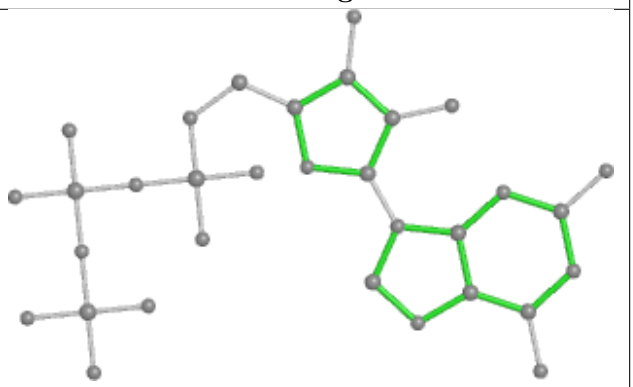
Bond lengths



Bond angles

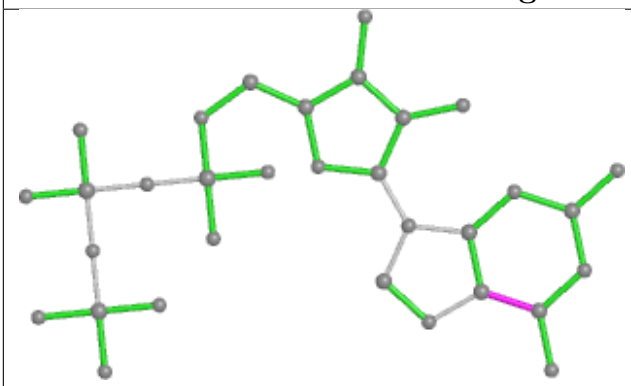


Torsions

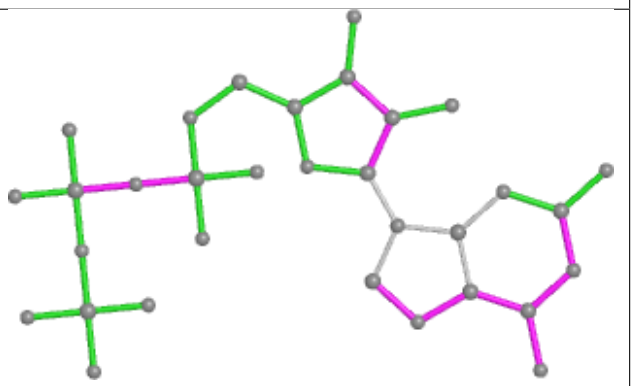


Rings

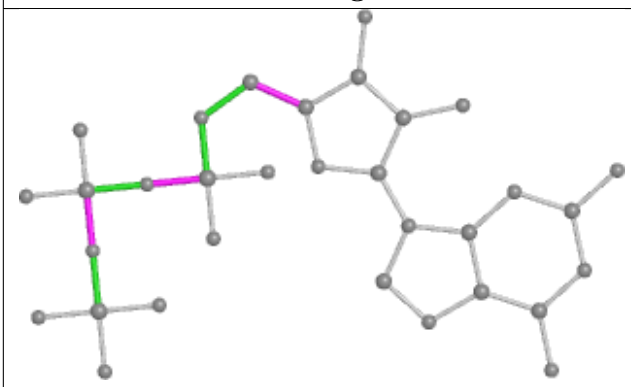
Ligand GTP SI 501



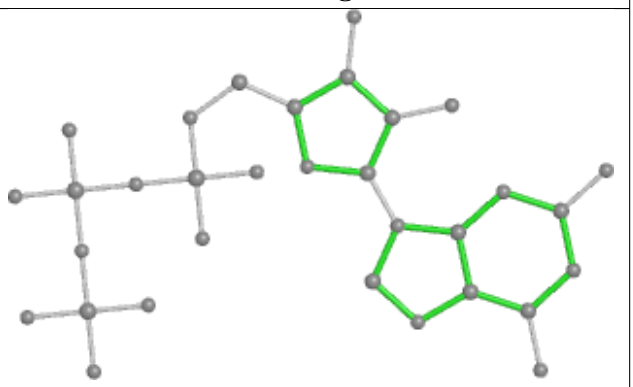
Bond lengths



Bond angles

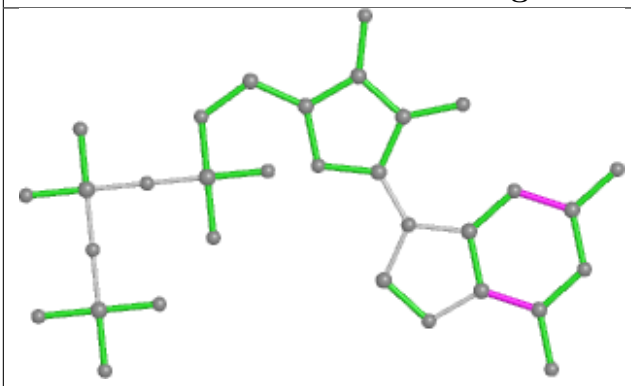


Torsions



Rings

Ligand GTP AF 501



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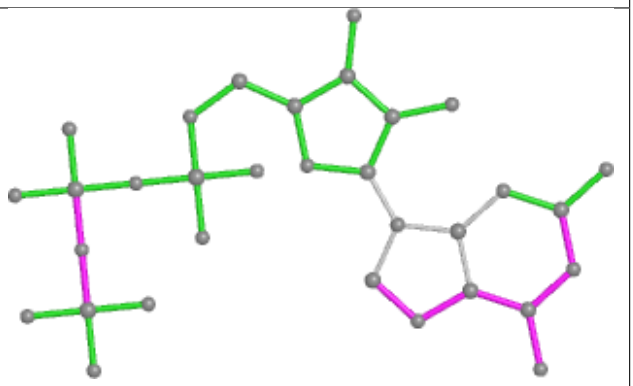
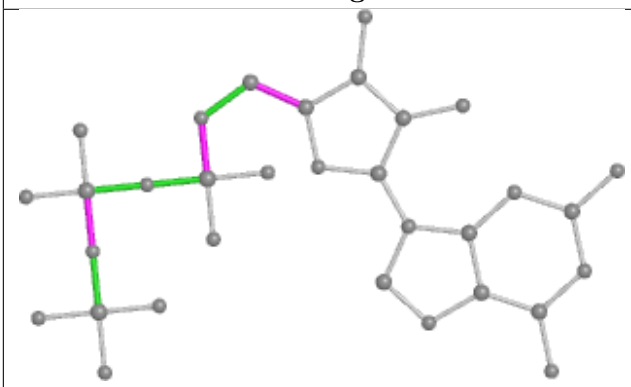


Bond angles



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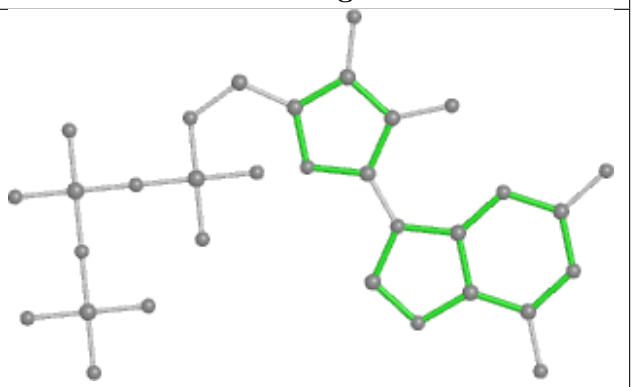
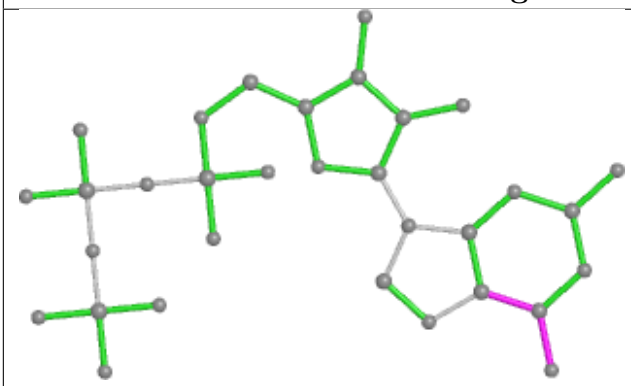


Rings

Ligand GTP LG 501



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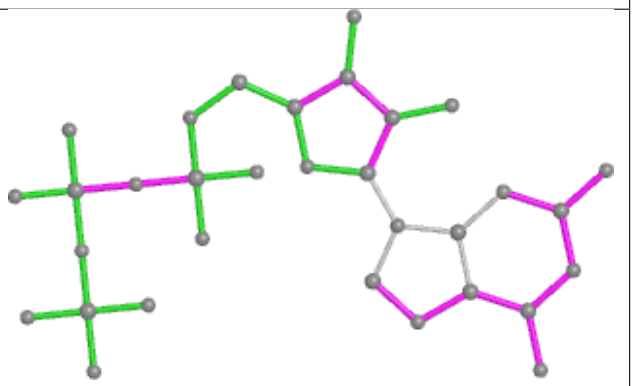
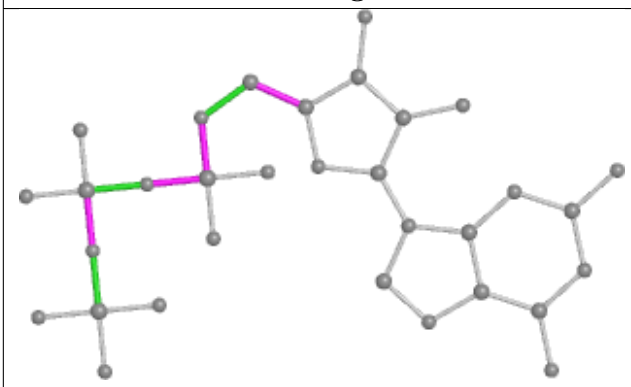


Bond angles



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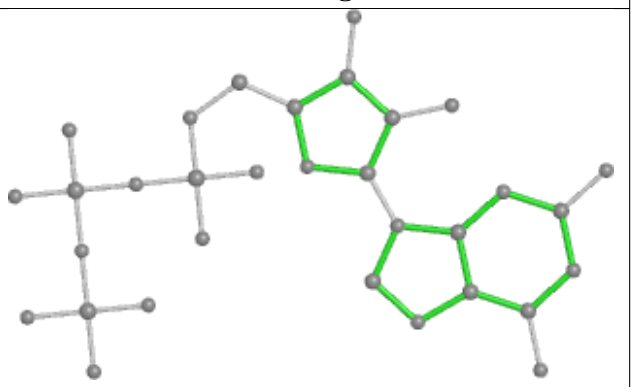
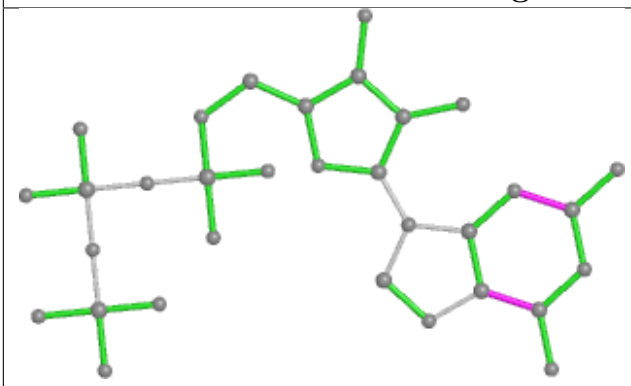


Rings

Ligand GTP SH 501



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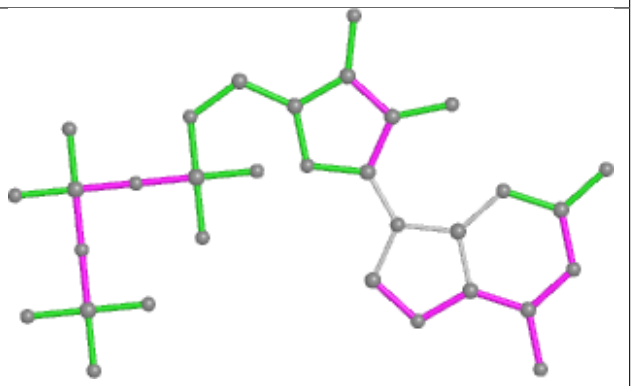
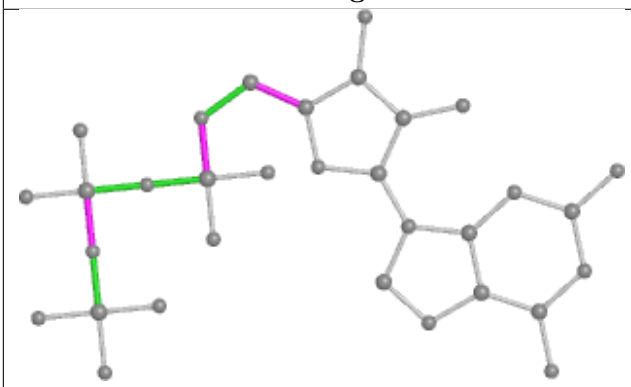
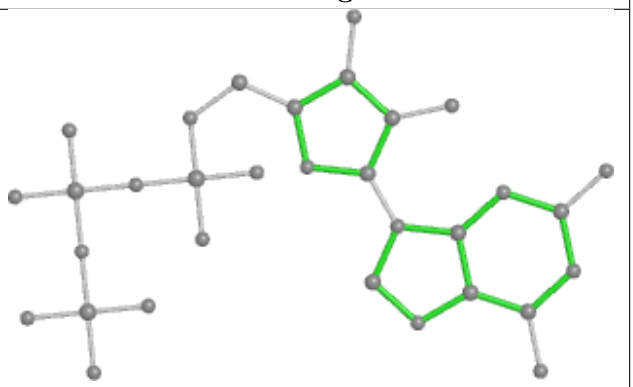


Bond angles

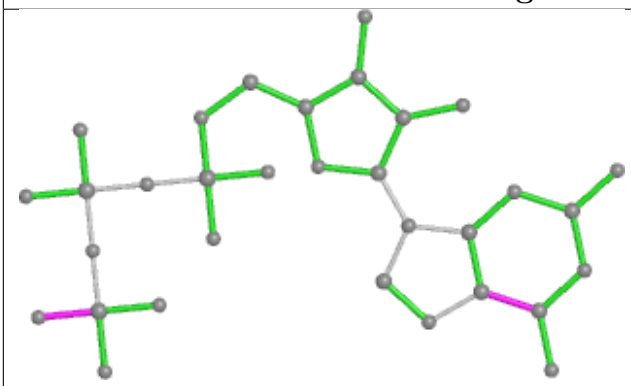


Torsions



Rings

Ligand GTP CI 501



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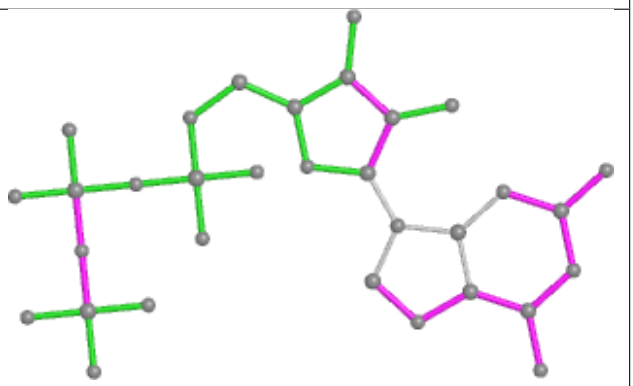
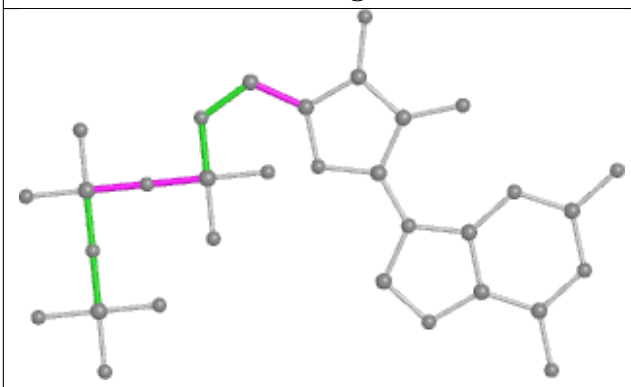


Bond angles



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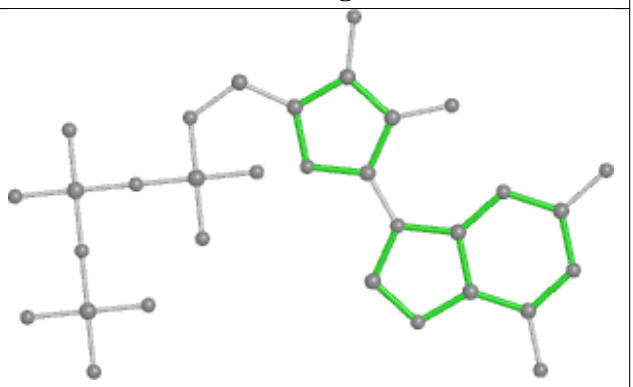
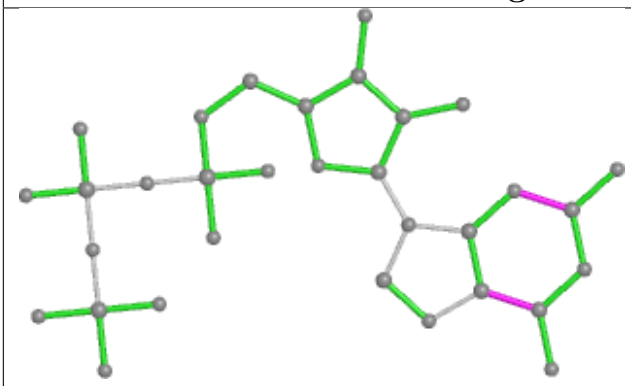
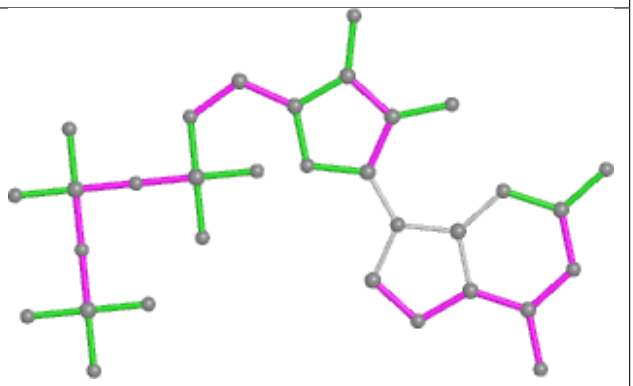


Rings

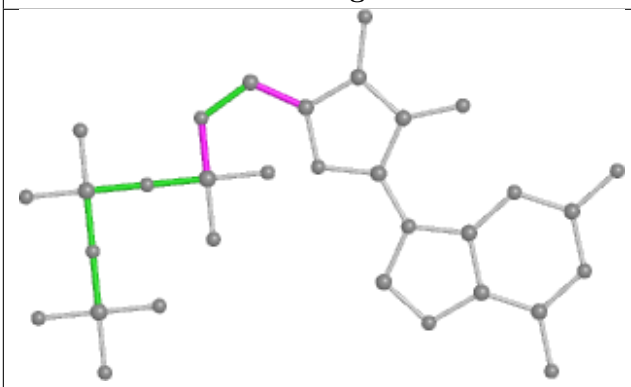
Ligand GTP OD 501



Bond lengths



Bond angles



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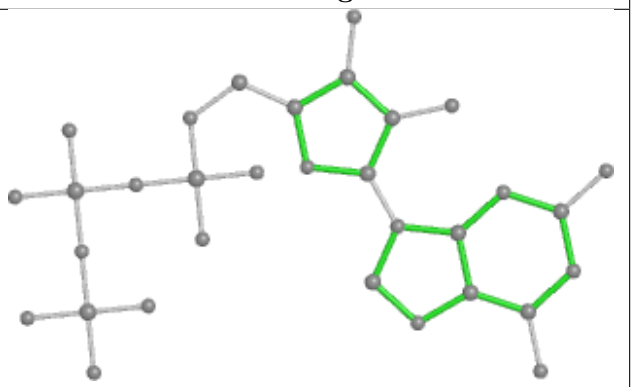
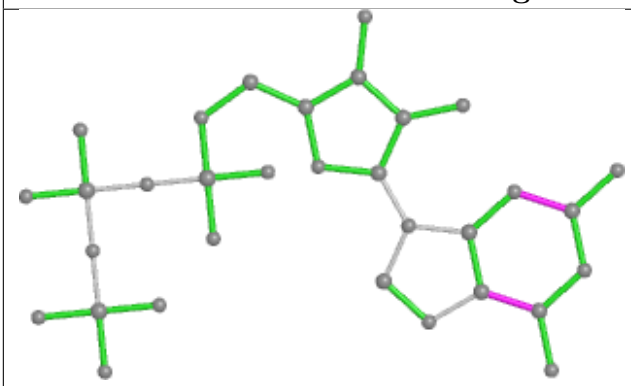


Rings

Ligand GTP EF 501



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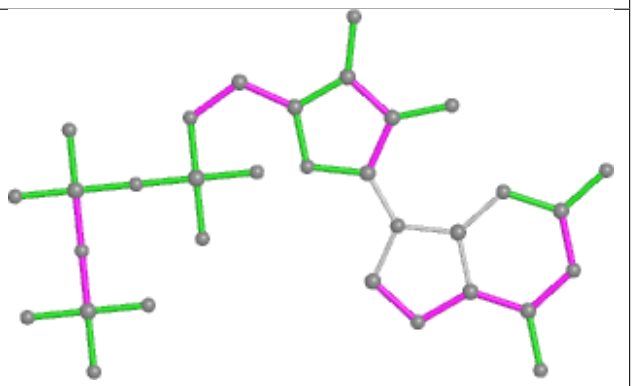
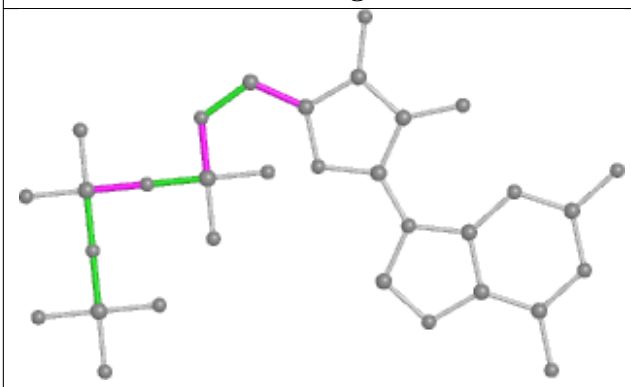


Bond angles



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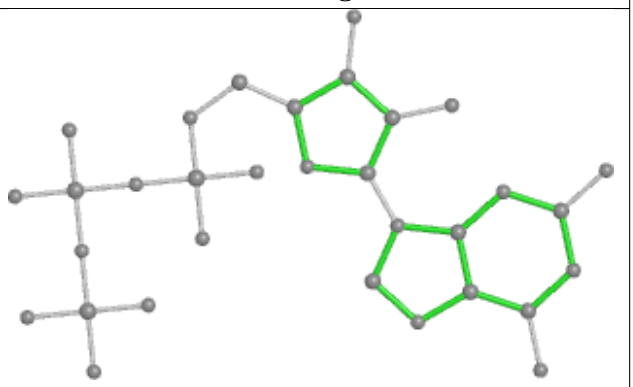
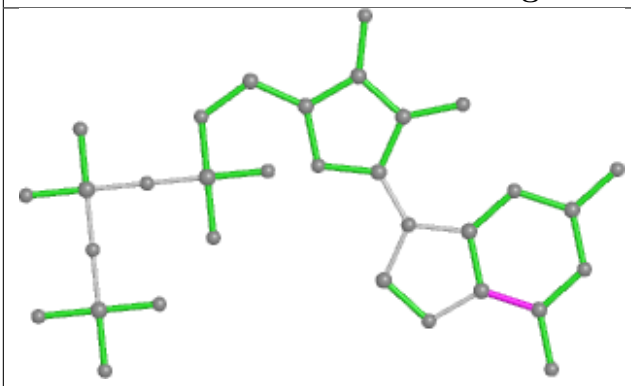
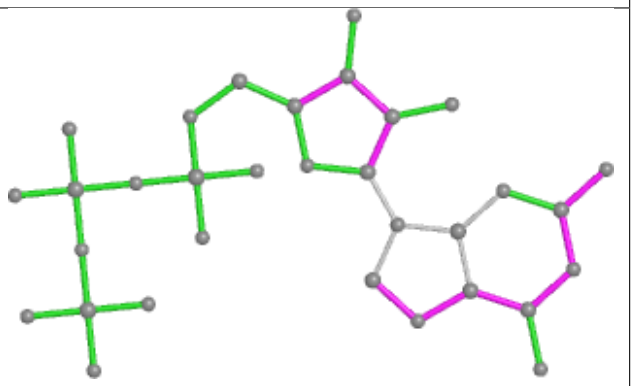


Rings

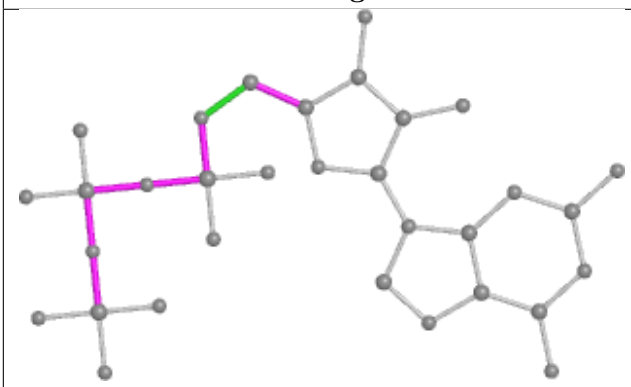
Ligand GTP II 501



Bond lengths



Bond angles



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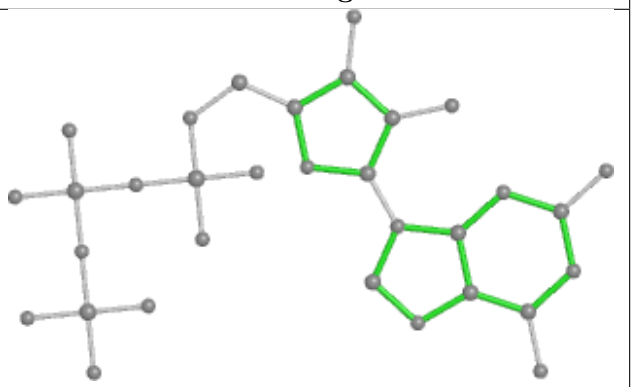
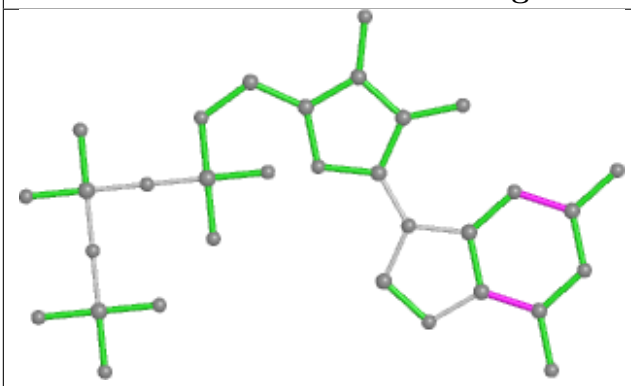


Rings

Ligand GTP BF 501



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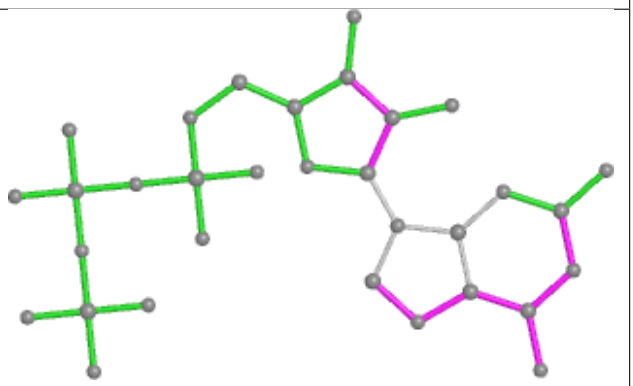
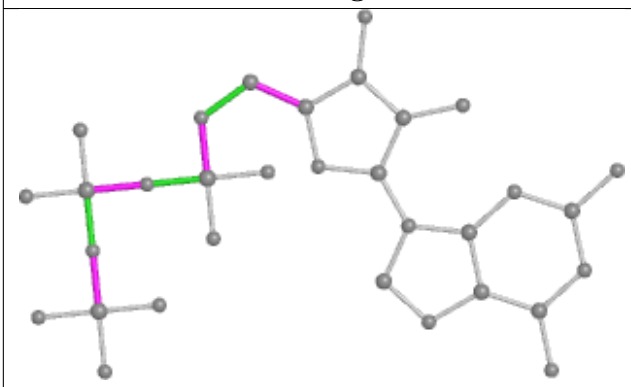
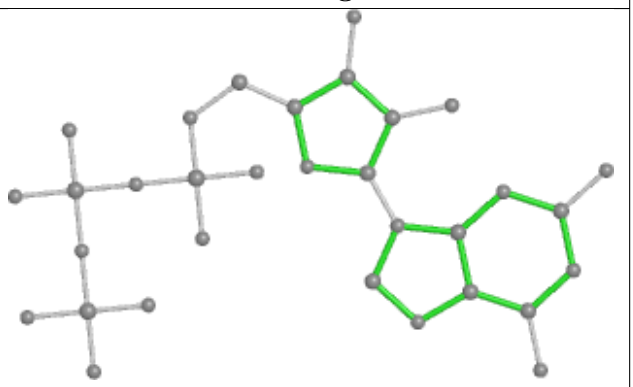


Bond angles

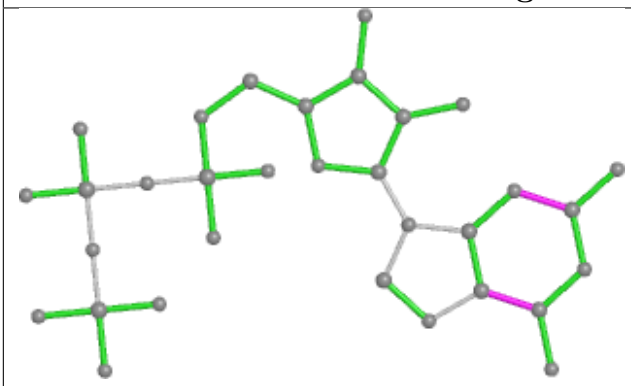


Torsions



Rings

Ligand GTP SJ 501



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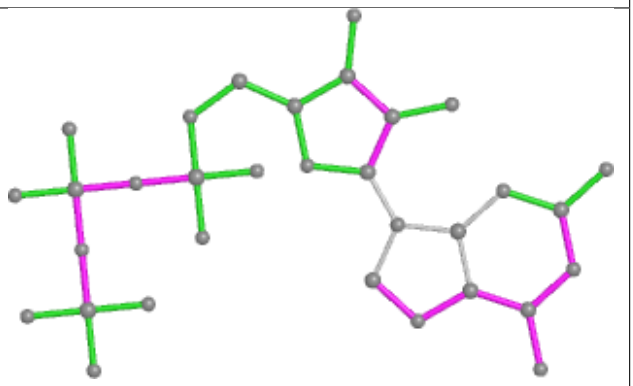
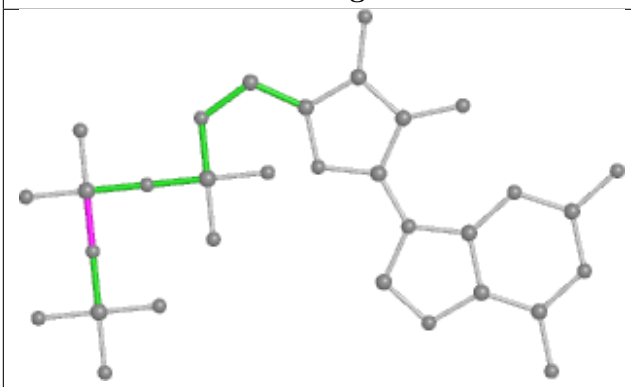
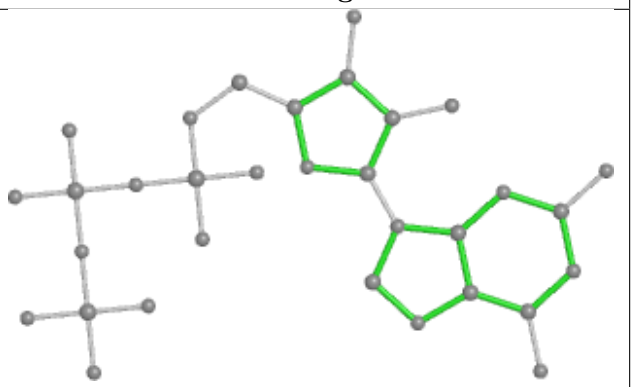


Bond angles

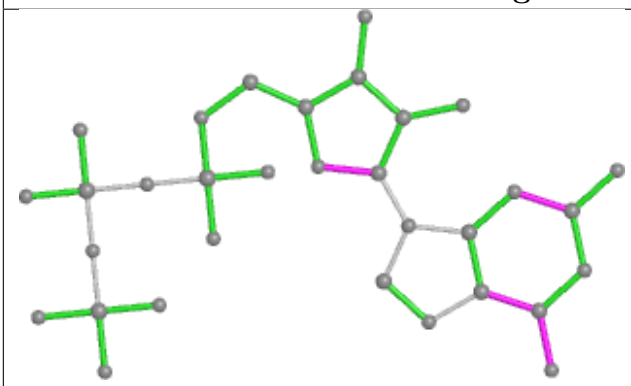


Torsions

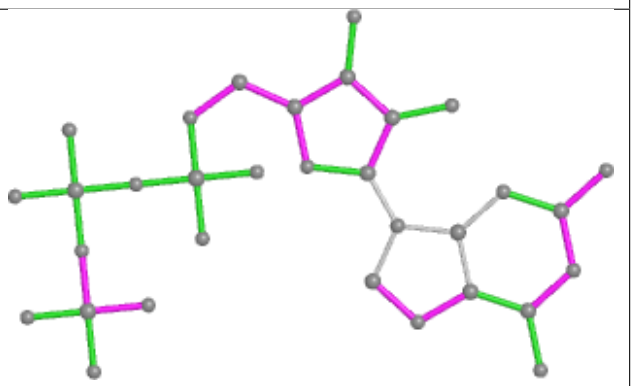


Rings

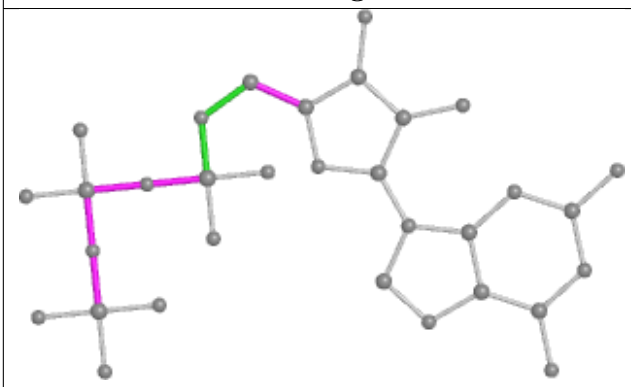
Ligand GTP LE 501



Bond lengths



Bond angles



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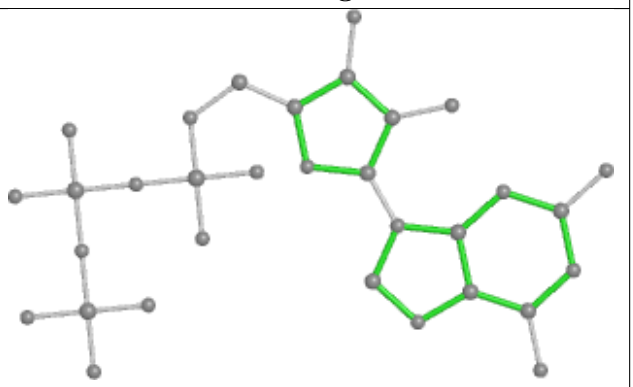
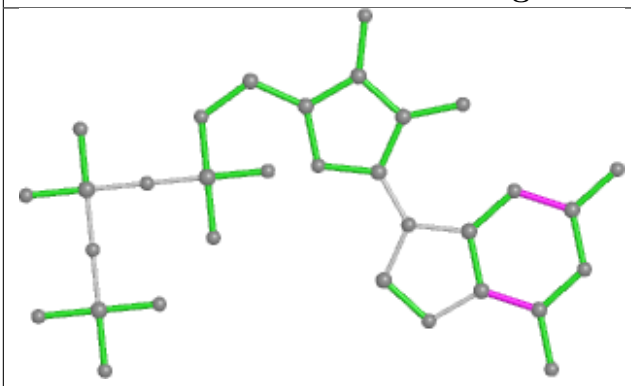


Rings

Ligand GTP JH 501



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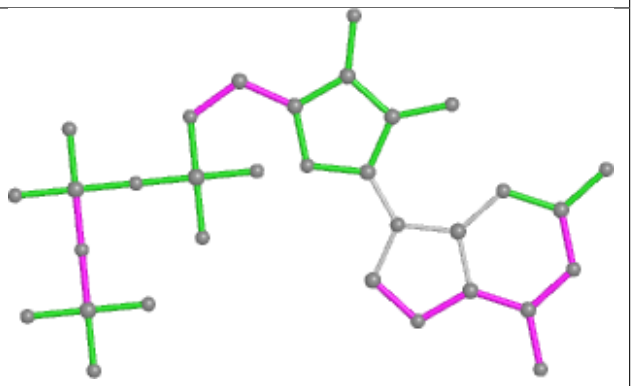
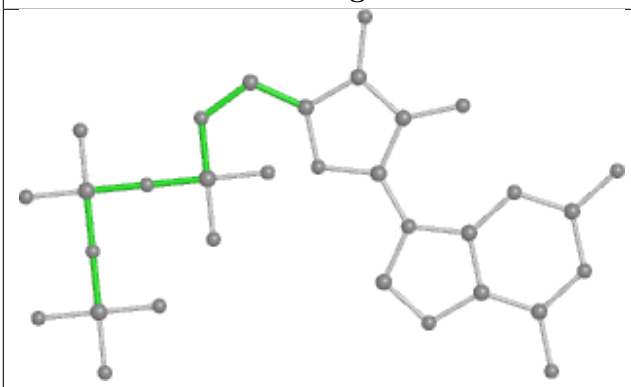


Bond angles



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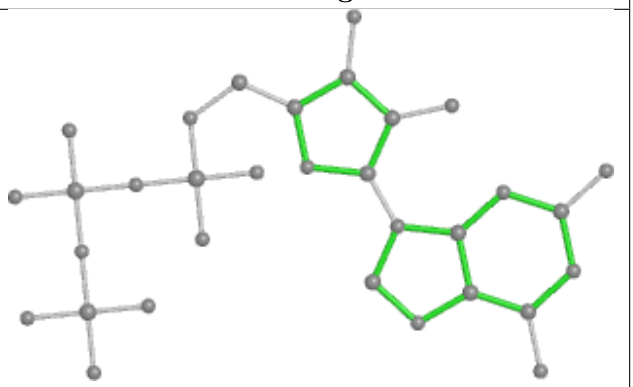
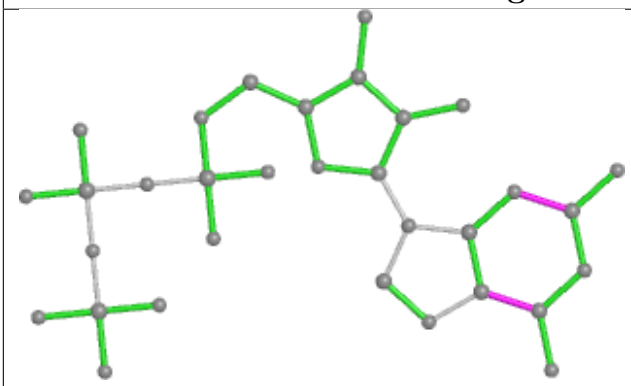
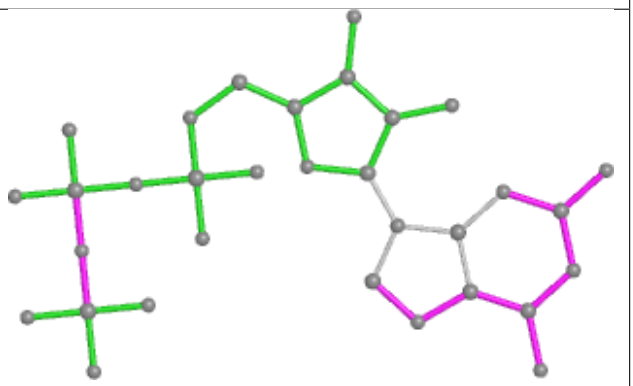


Rings

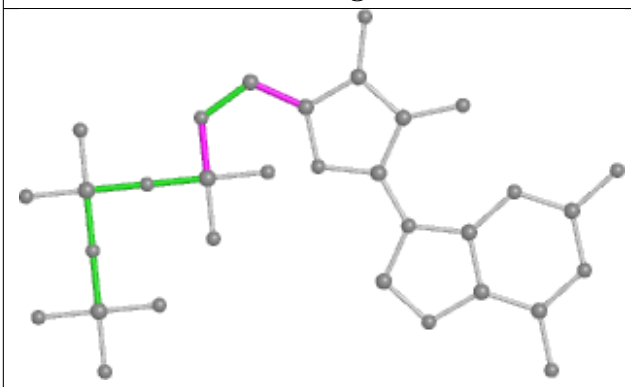
Ligand GTP NH 501



Bond lengths



Bond angles



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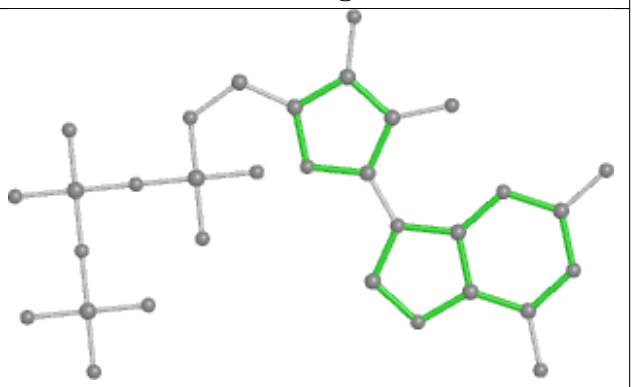
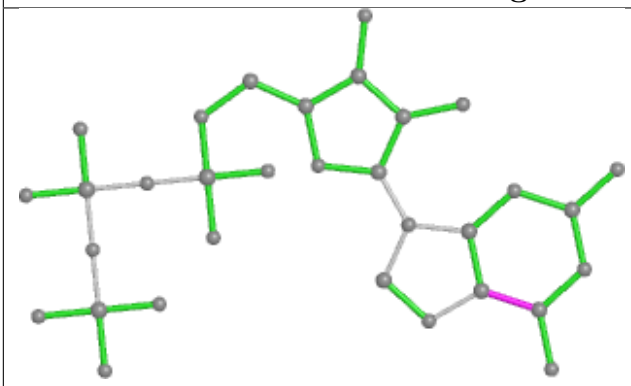
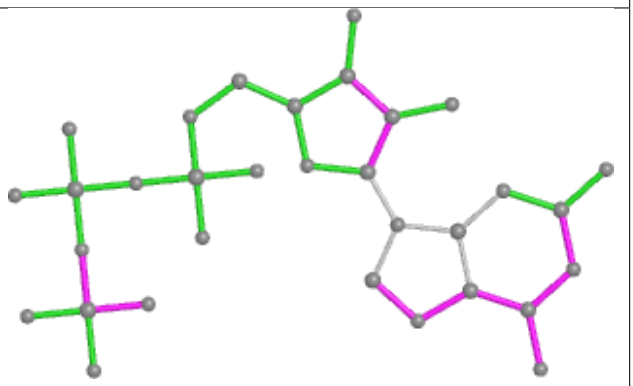


Rings

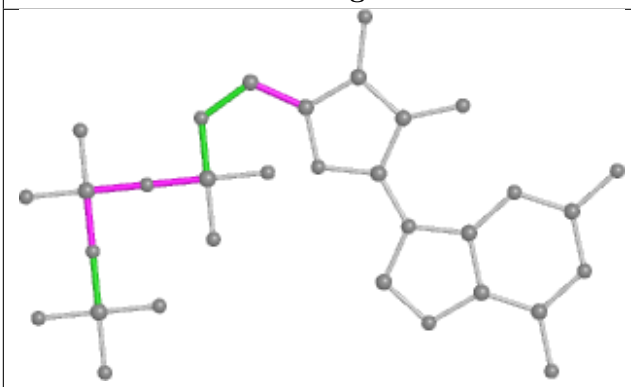
Ligand GTP NE 501



Bond lengths



Bond angles



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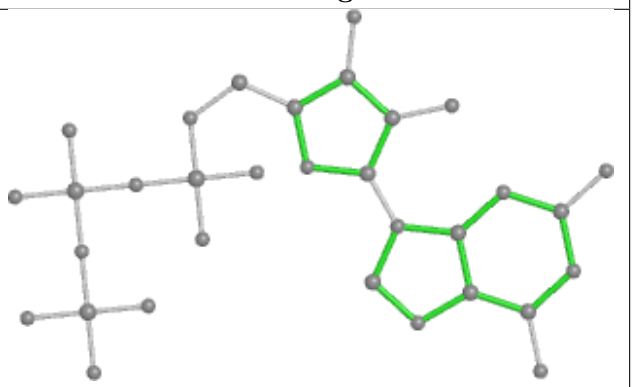
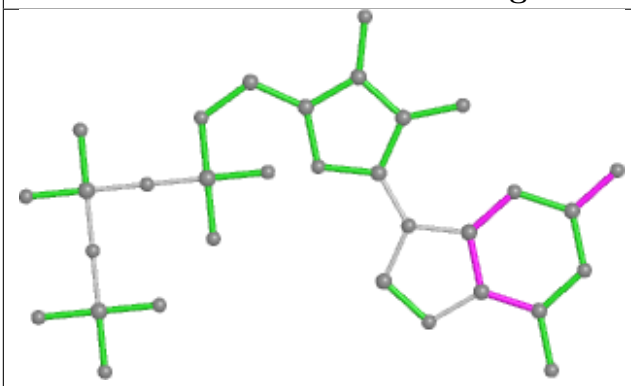
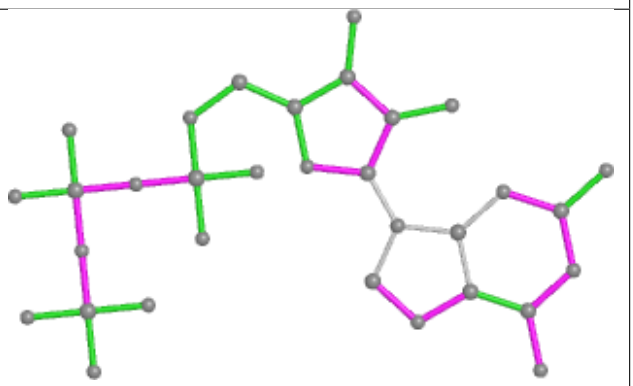


Rings

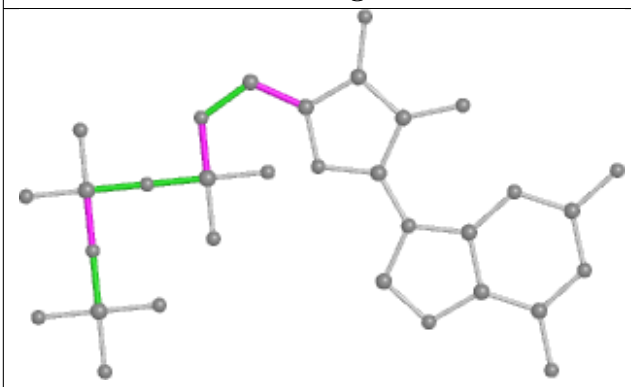
Ligand GTP GE 501



Bond lengths



Bond angles



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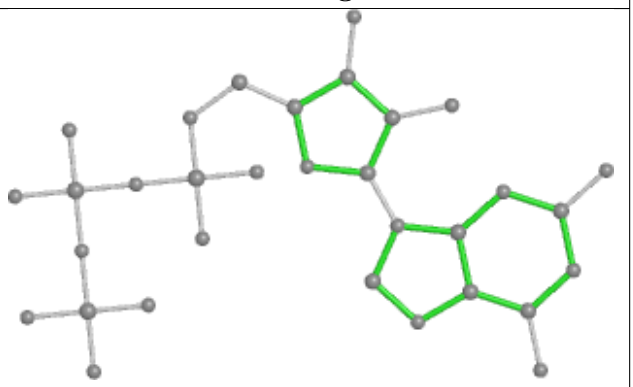
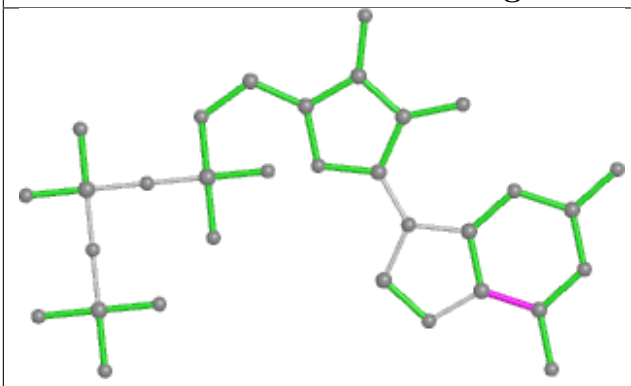
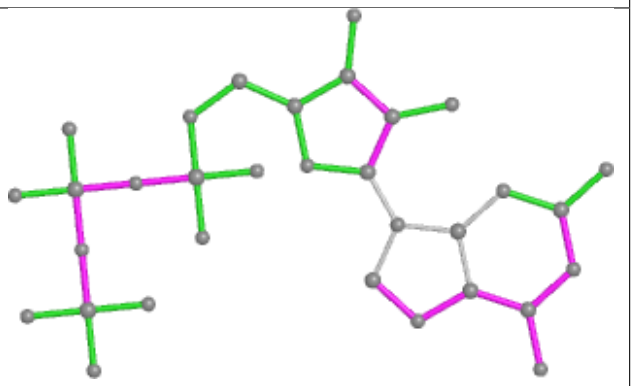


Rings

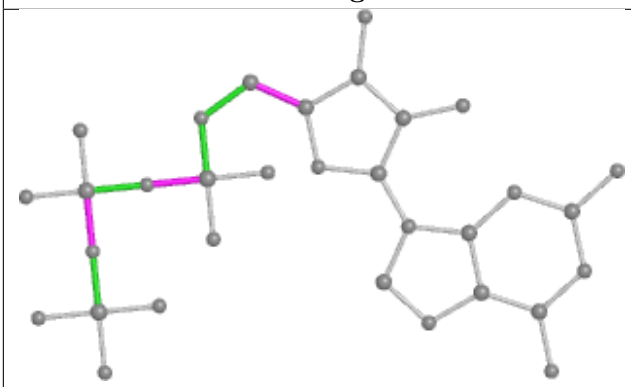
Ligand GTP WG 501



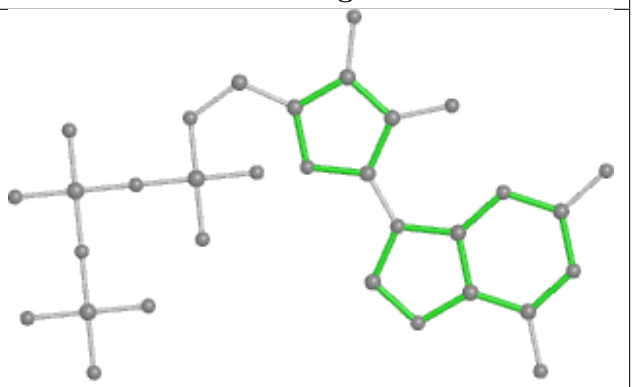
Bond lengths



Bond angles

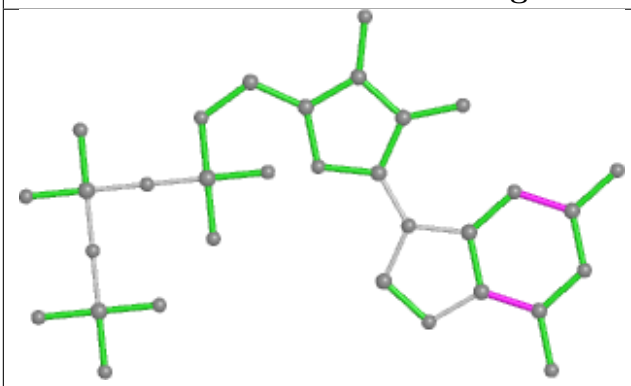


Torsions



Rings

Ligand GTP GF 501



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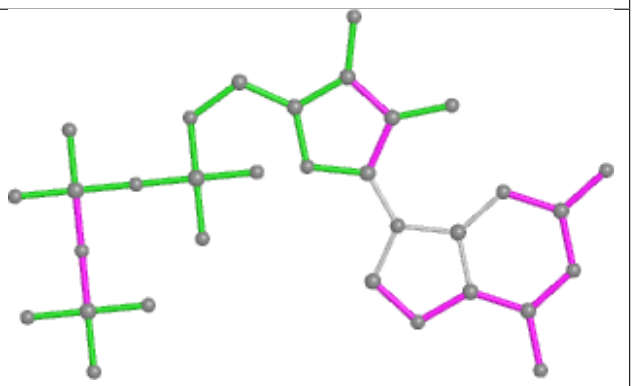
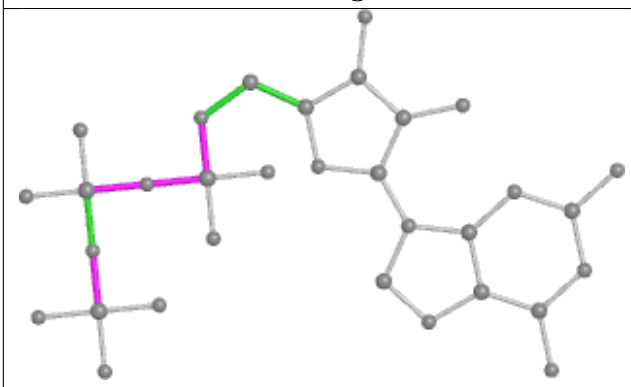


Bond angles



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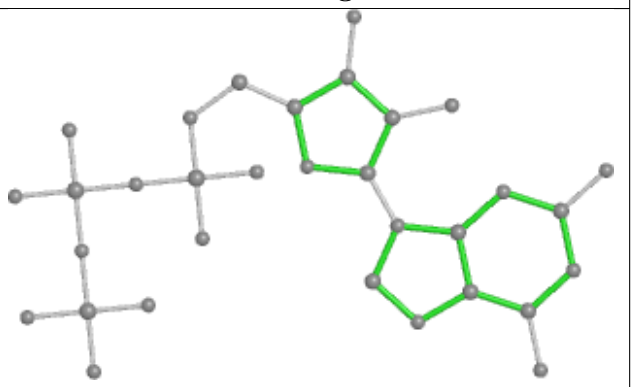
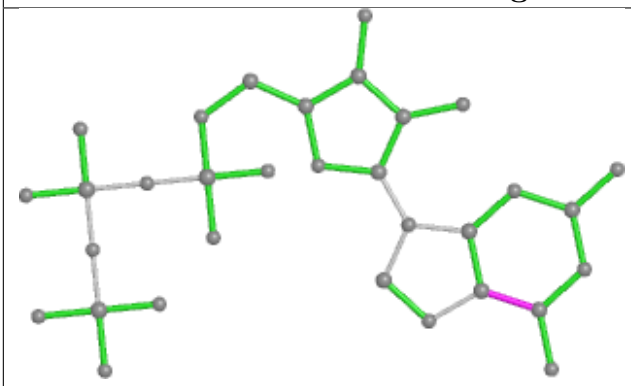


Rings

Ligand GTP AE 501



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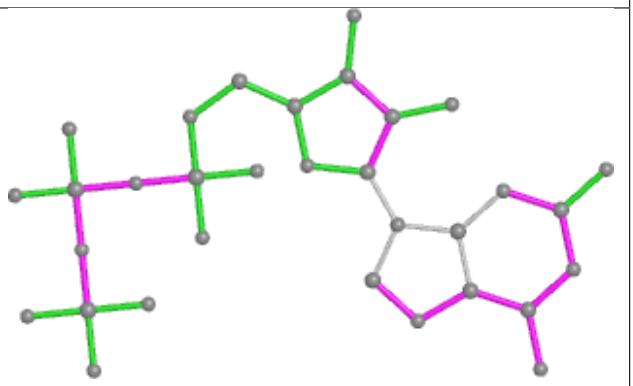
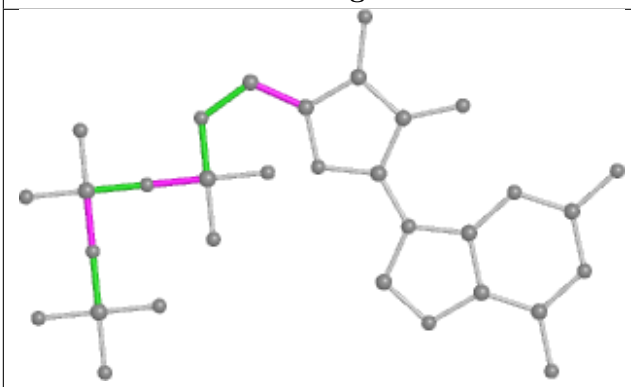
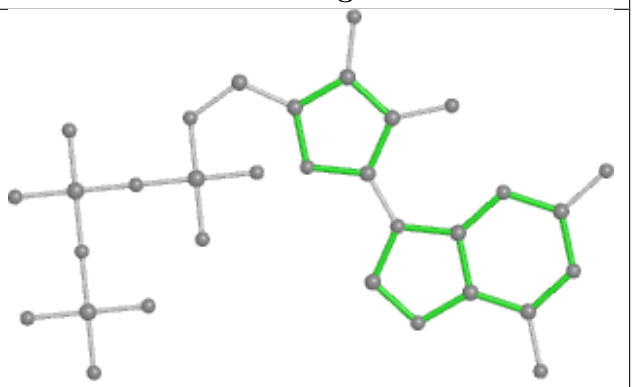


Bond angles

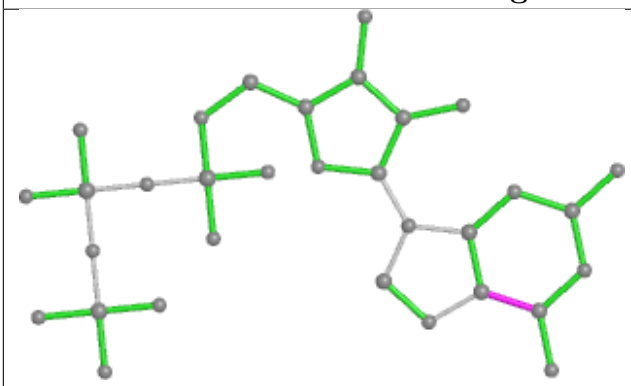


Torsions



Rings

Ligand GTP VE 501



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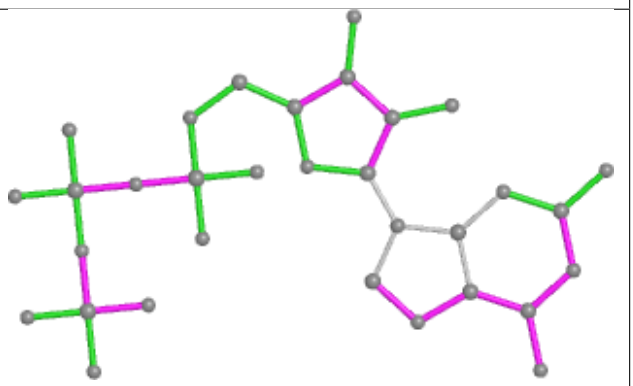
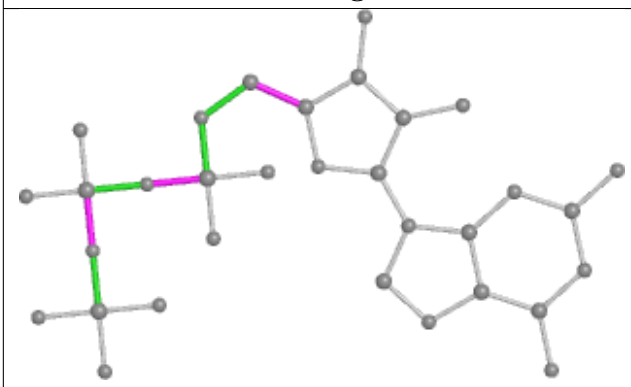
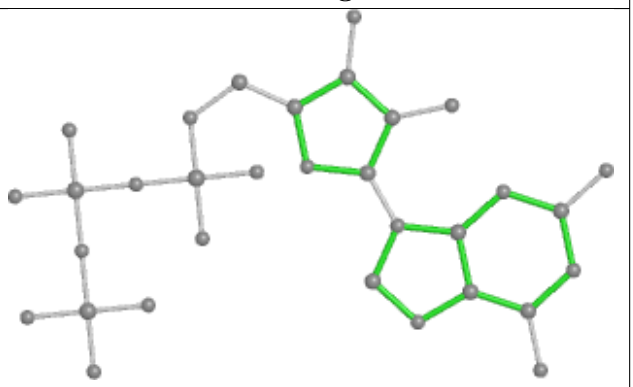


Bond angles

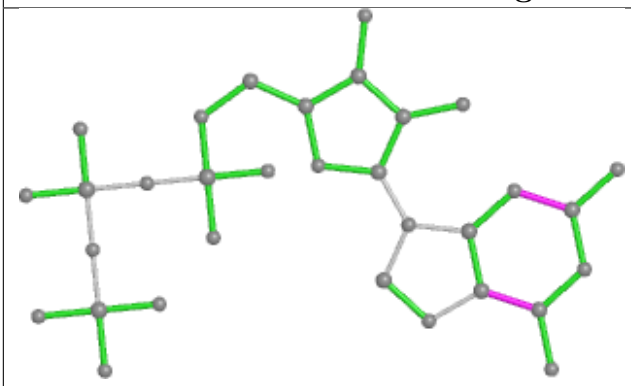


Torsions



Rings

Ligand GTP KI 501



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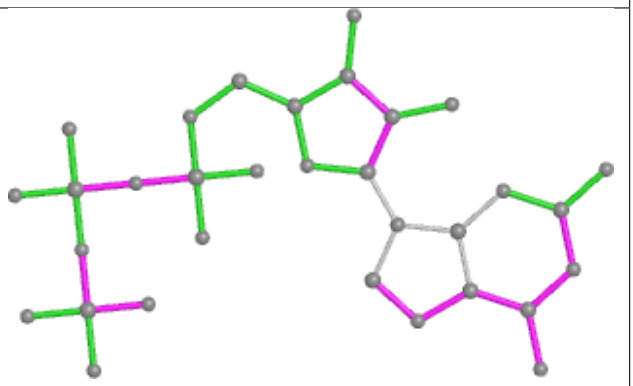
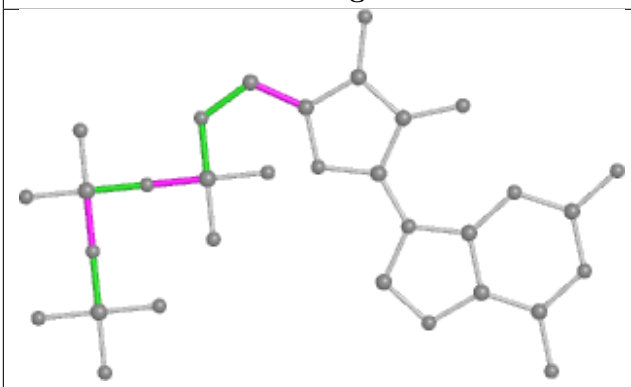
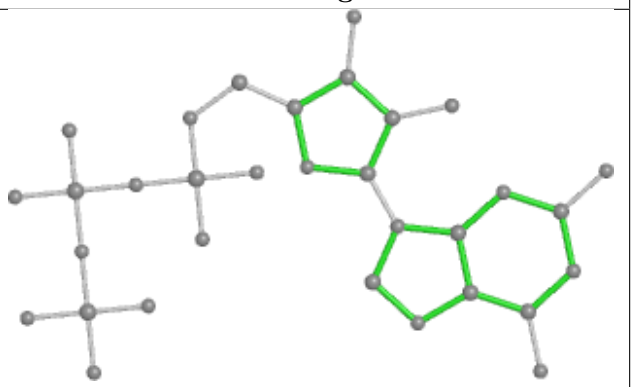


Bond angles

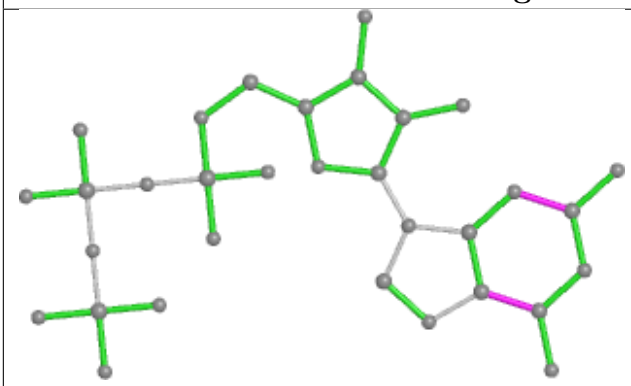


Torsions

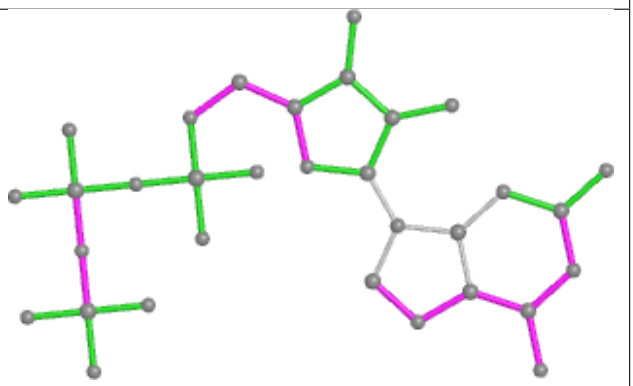


Rings

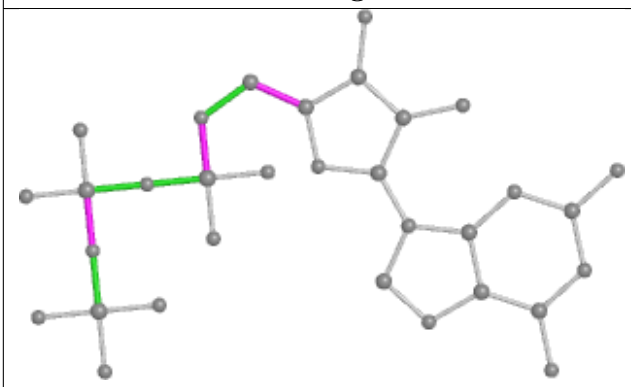
Ligand GTP LF 501



Bond lengths



Bond angles



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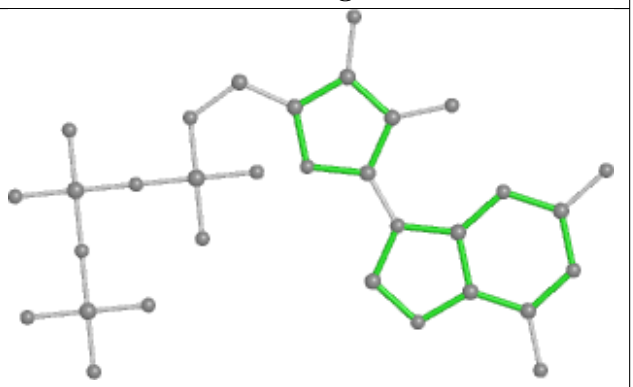
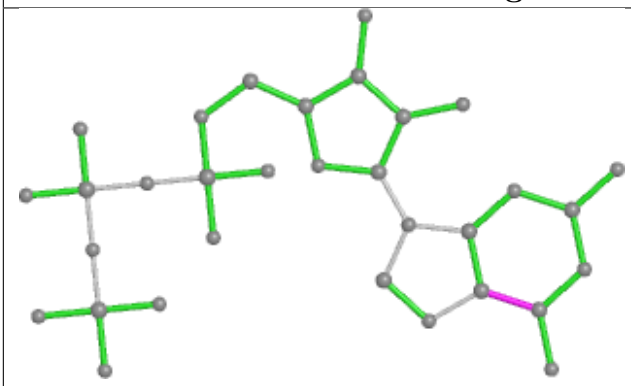
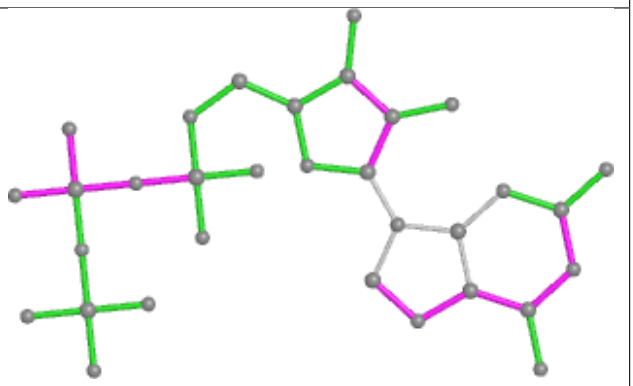


Rings

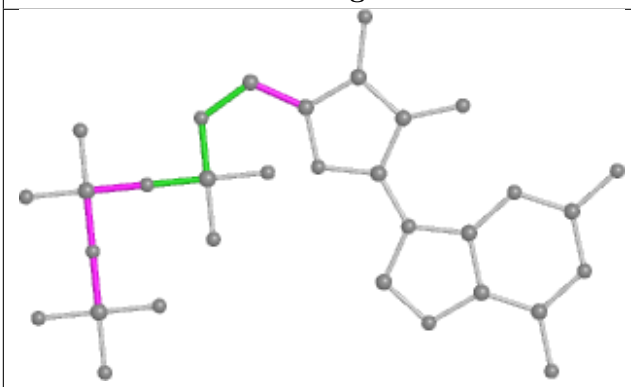
Ligand GTP WE 501



Bond lengths



Bond angles



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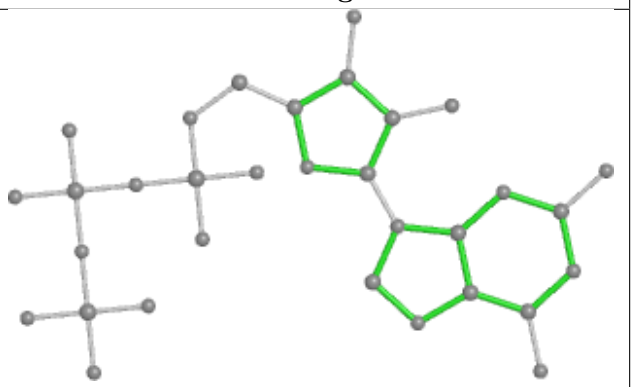
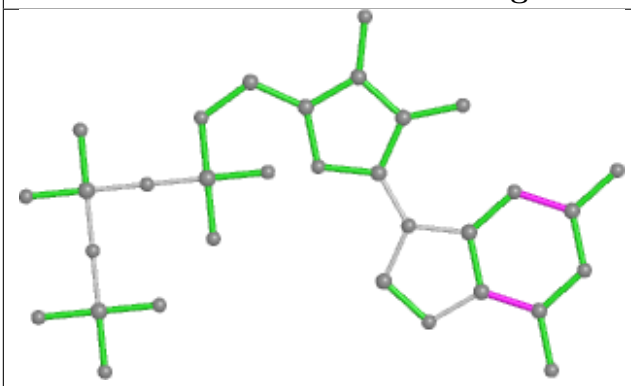
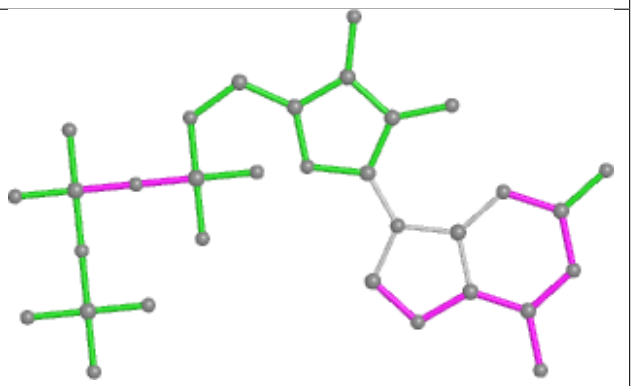


Rings

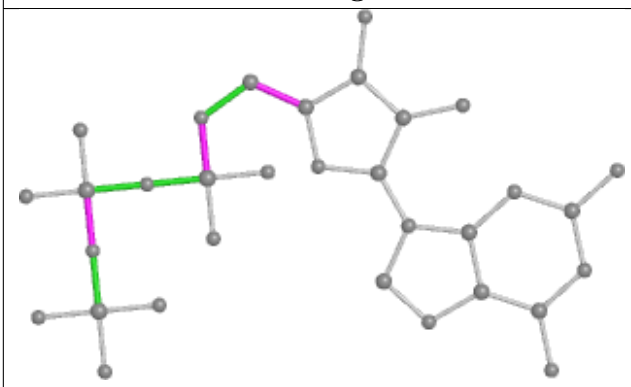
Ligand GTP DF 501



Bond lengths



Bond angles



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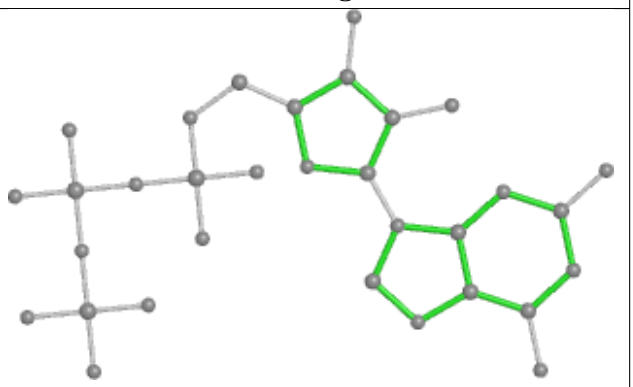
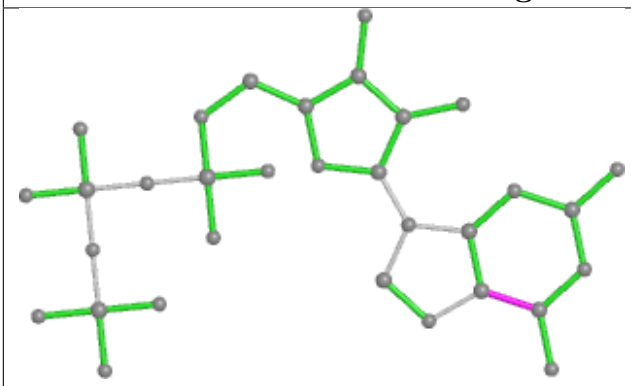


Rings

Ligand GTP IG 501



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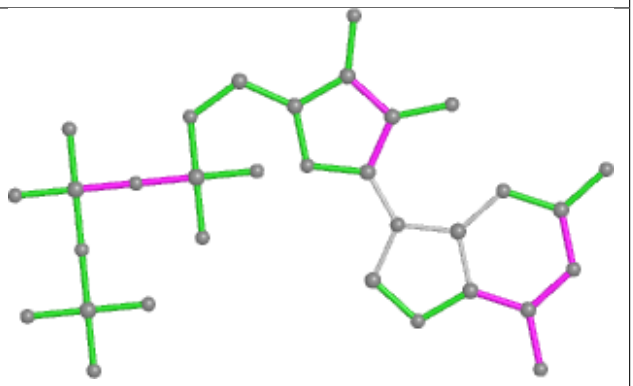
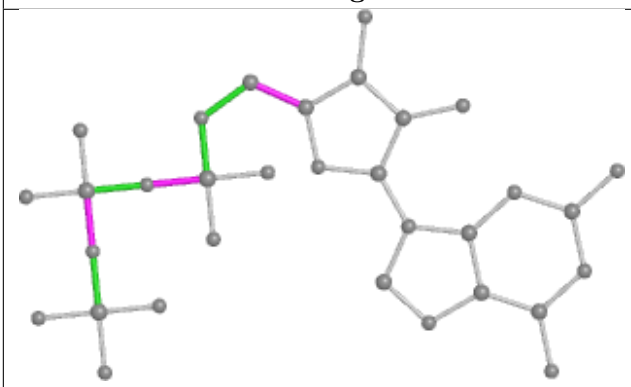
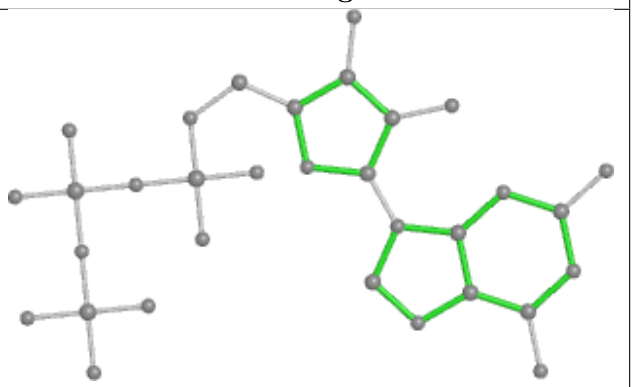


Bond angles

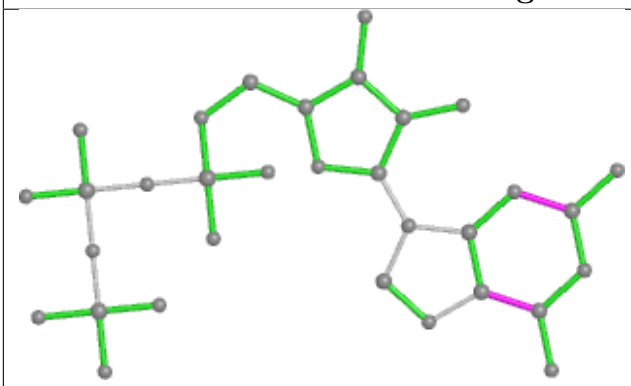


Torsions

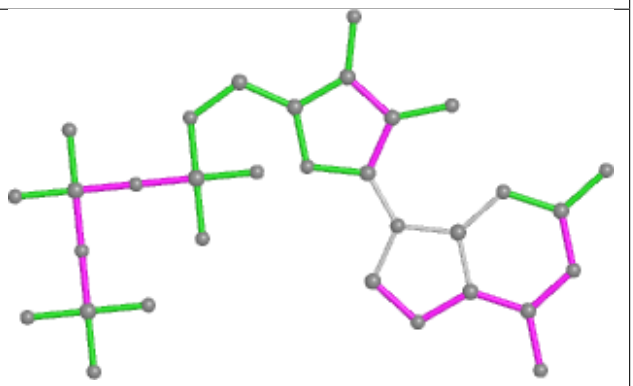


Rings

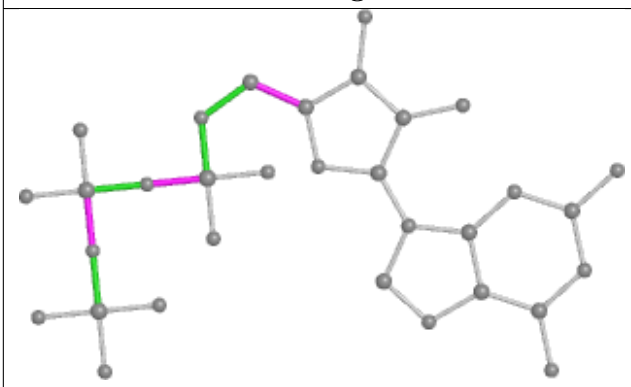
Ligand GTP TI 501



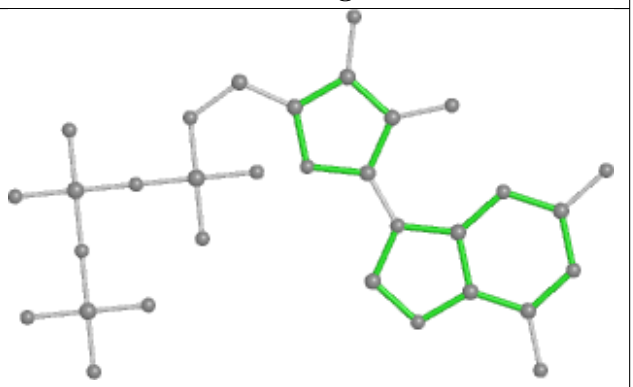
Bond lengths



Bond angles

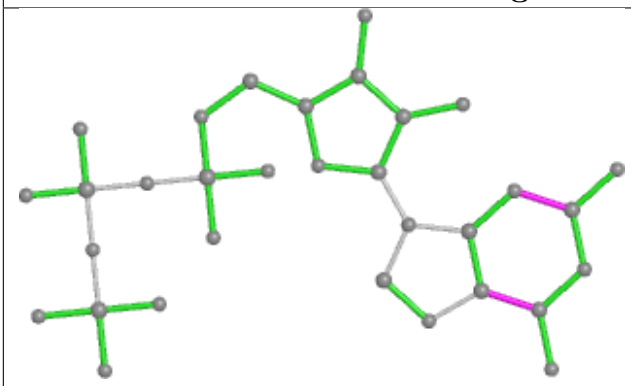


Torsions

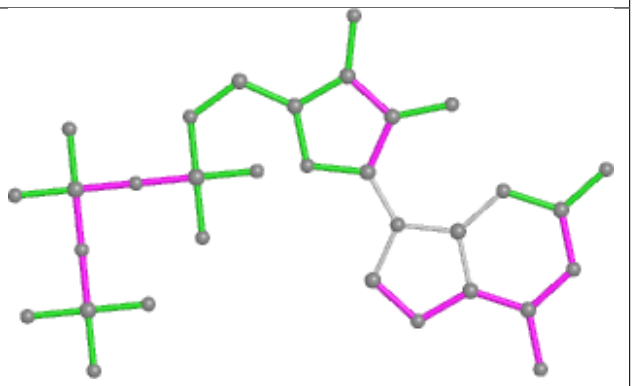


Rings

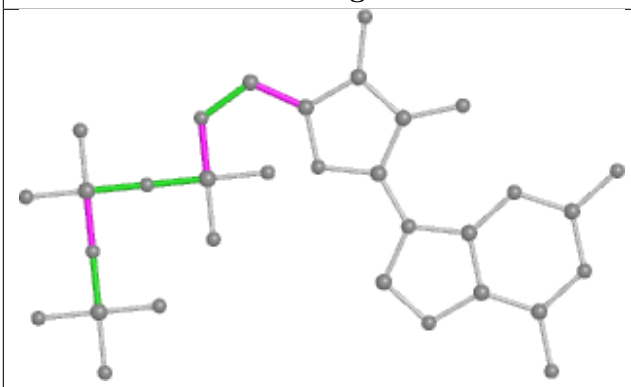
Ligand GTP RF 501



Bond lengths



Bond angles



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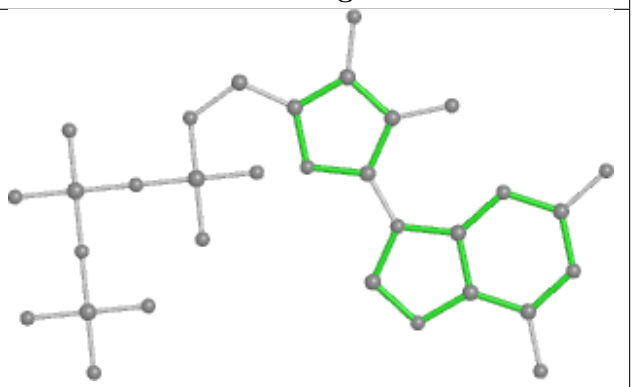
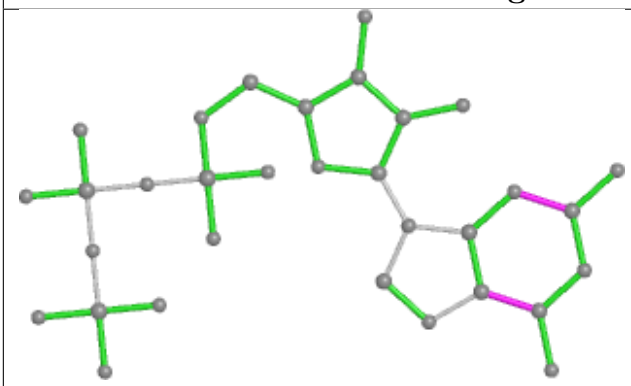


Rings

Ligand GTP QG 501



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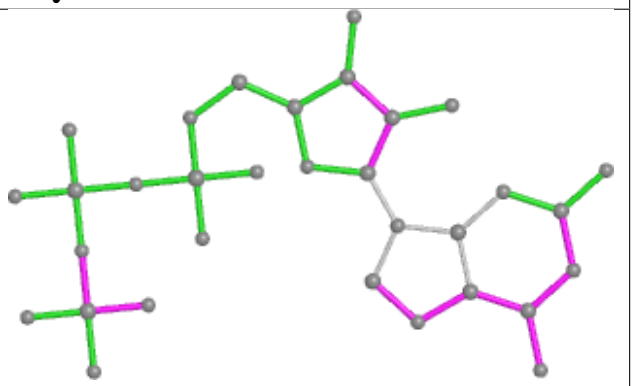
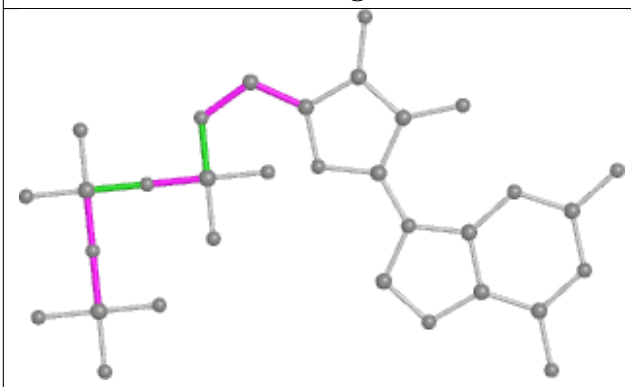


Bond angles



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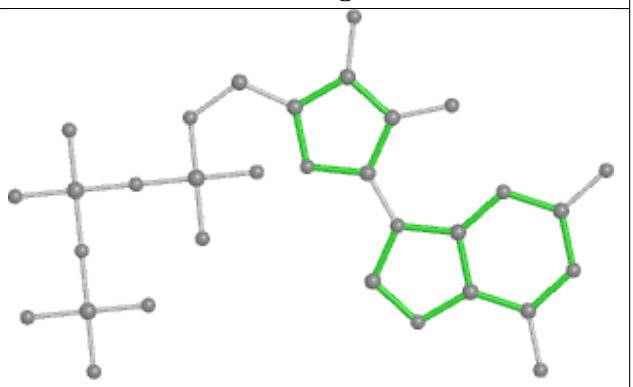
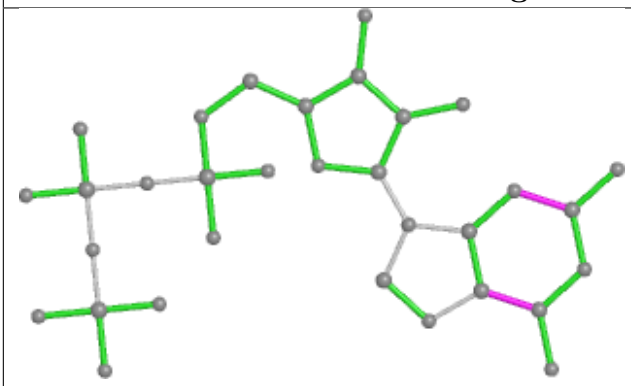


Rings

Ligand GTP NF 501



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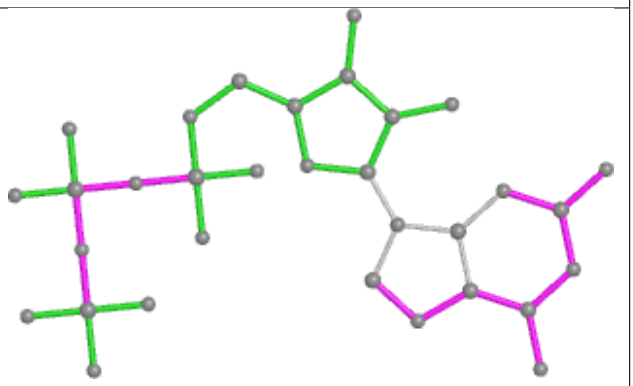

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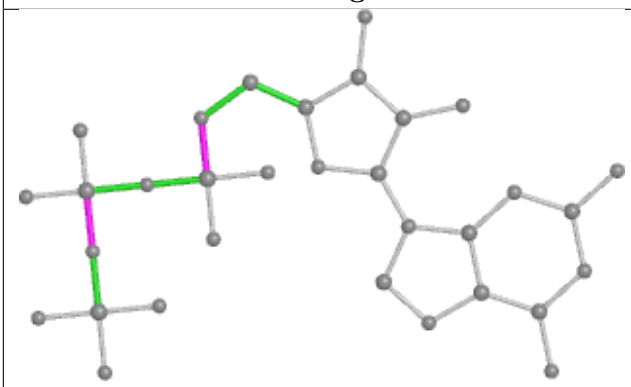

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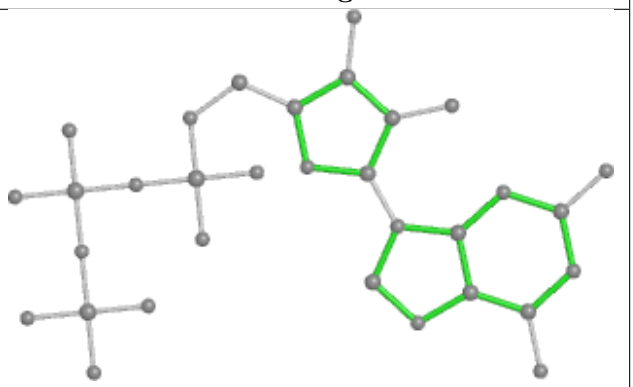
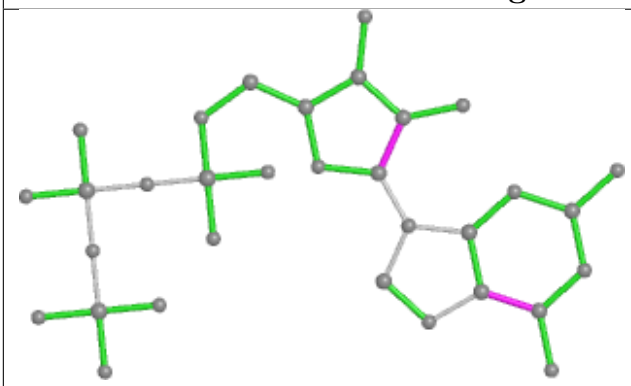


Rings

Ligand GTP CG 501



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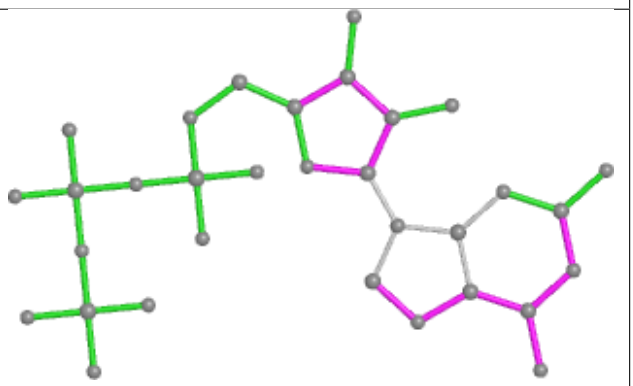
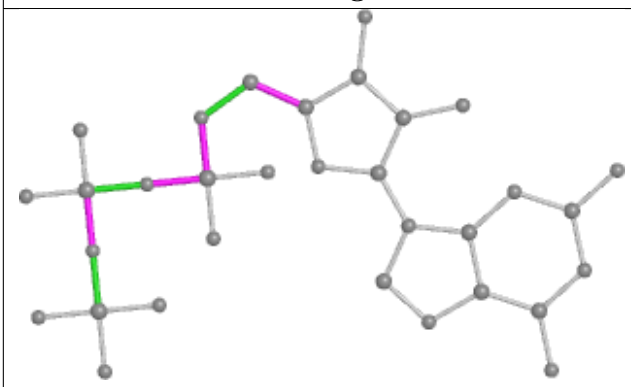
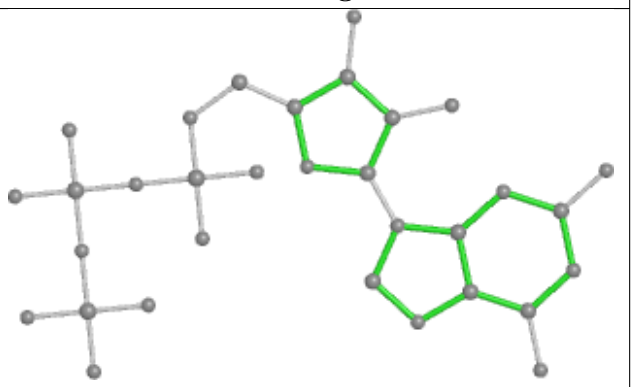


Bond angles

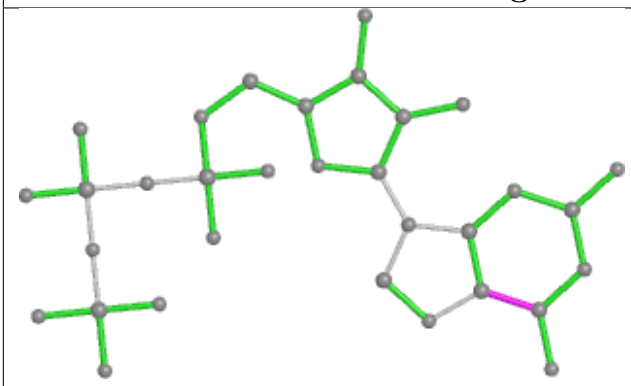


Torsions

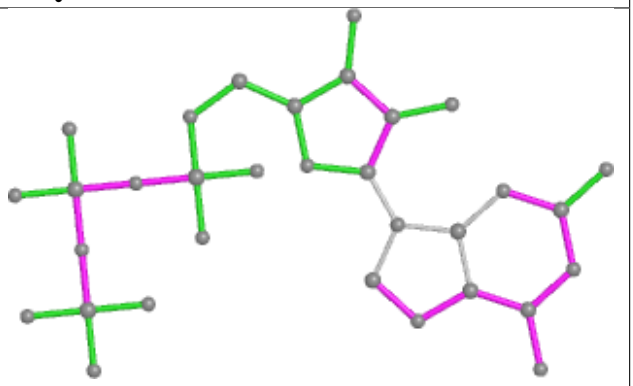


Rings

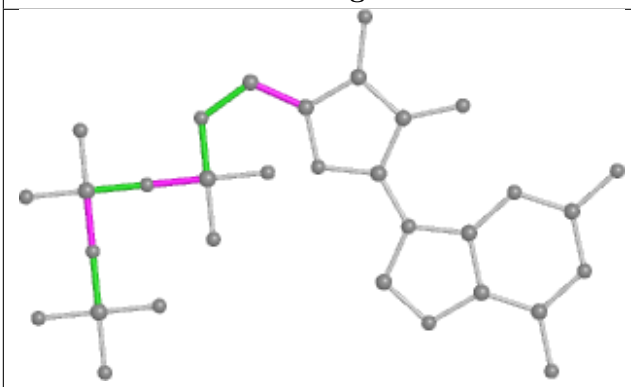
Ligand GTP QE 501



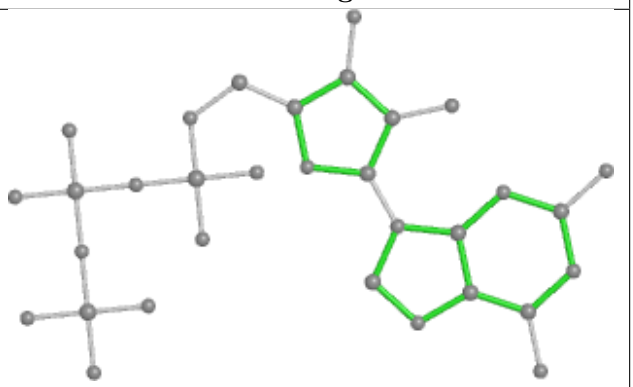
Bond lengths



Bond angles

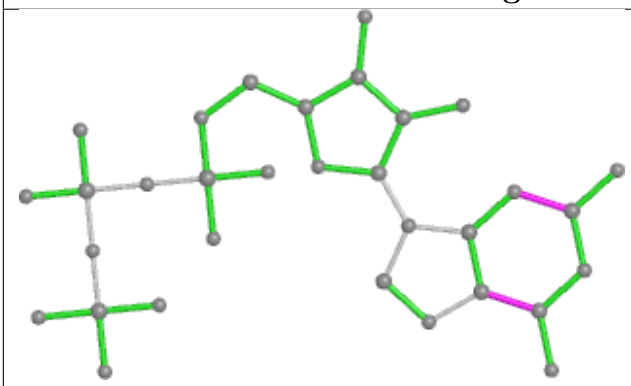


Torsions

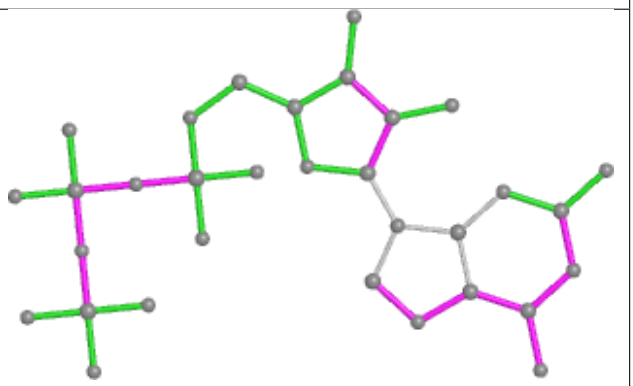


Rings

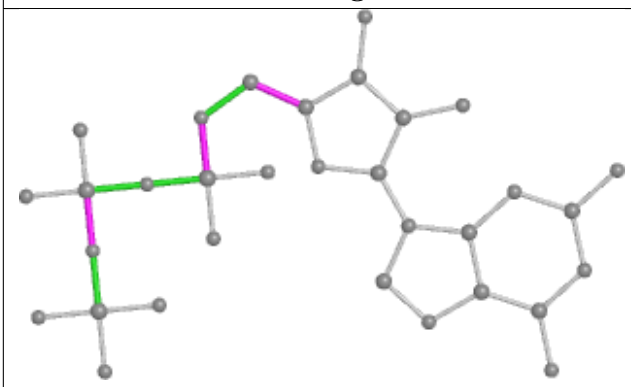
Ligand GTP WH 501



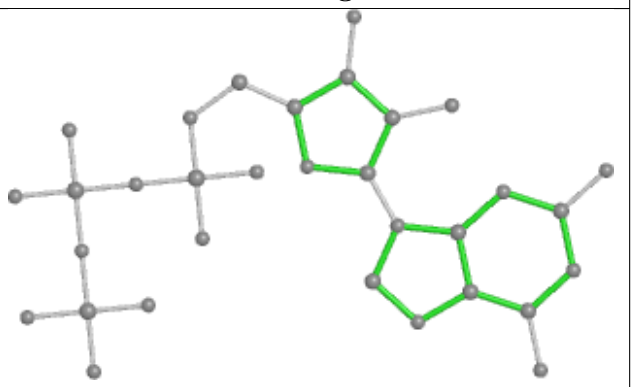
Bond lengths



Bond angles

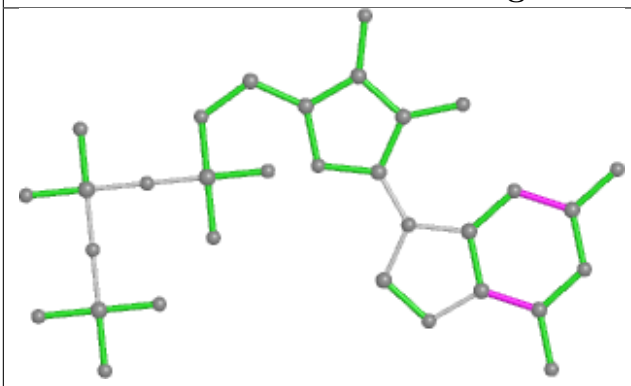


Torsions



Rings

Ligand GTP KH 501



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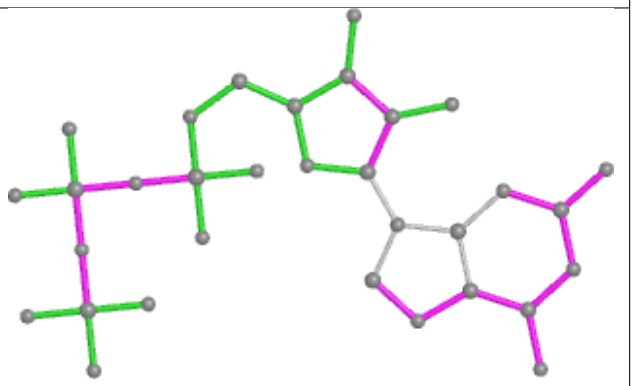
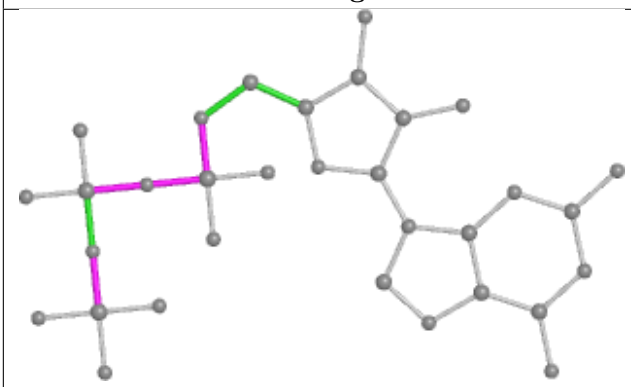


Bond angles



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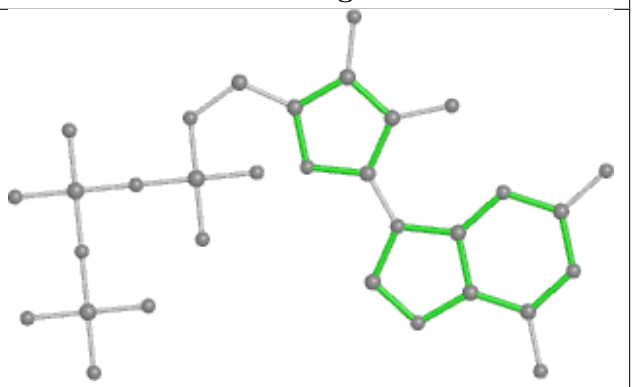
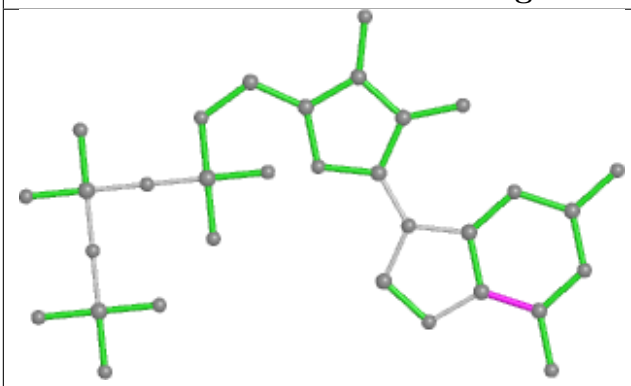


Rings

Ligand GTP HI 501



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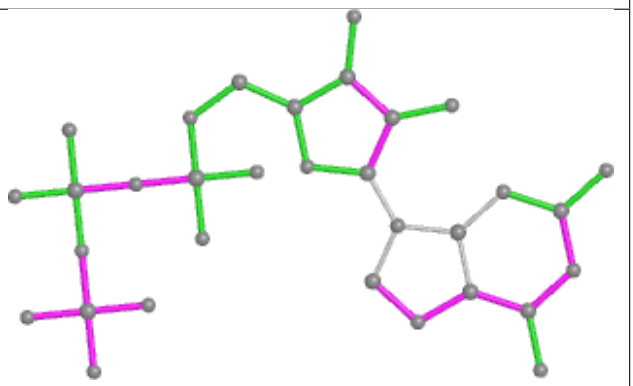
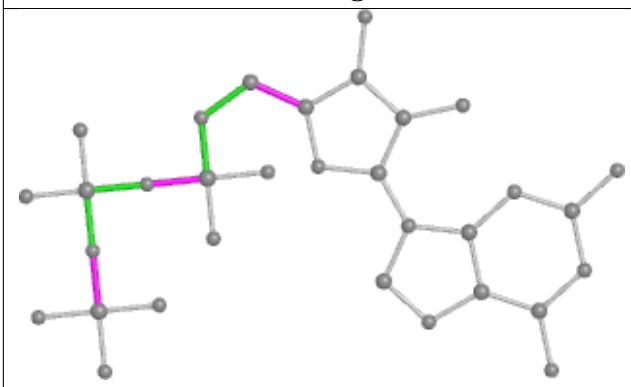


Bond angles



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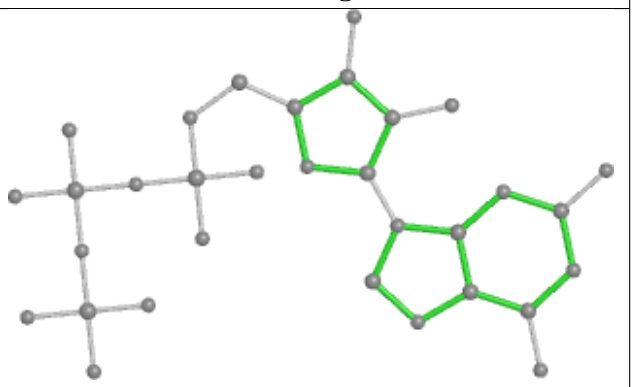
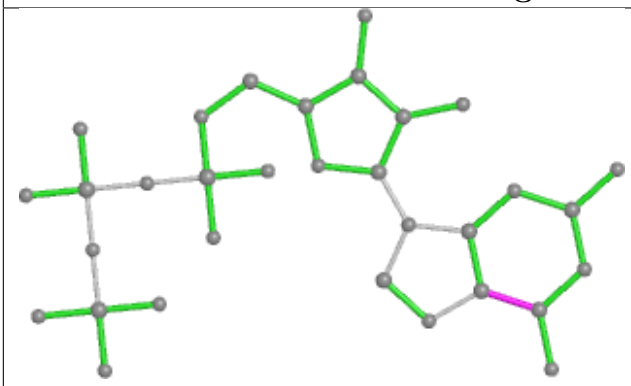


Rings

Ligand GTP JE 501



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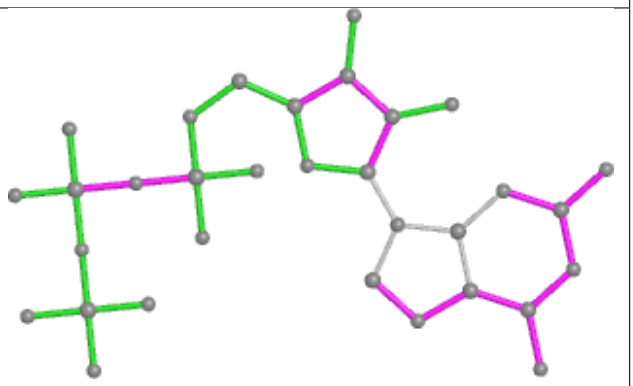
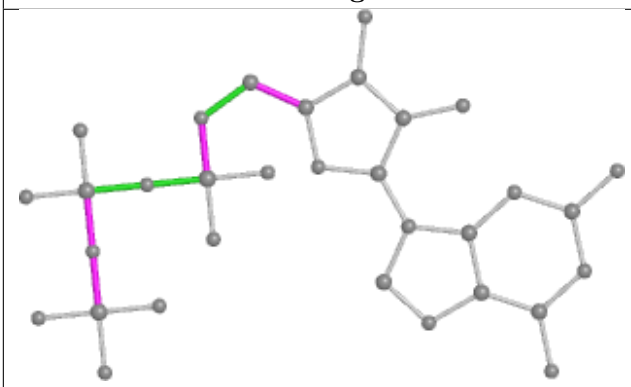


Bond angles



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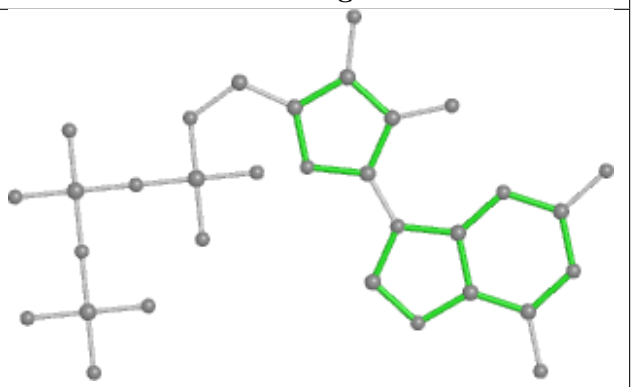
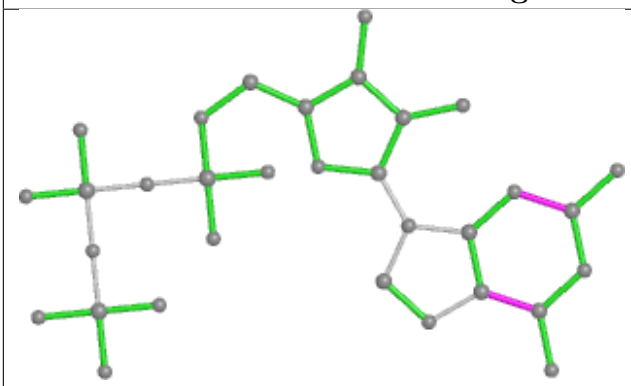


Rings

Ligand GTP RE 501



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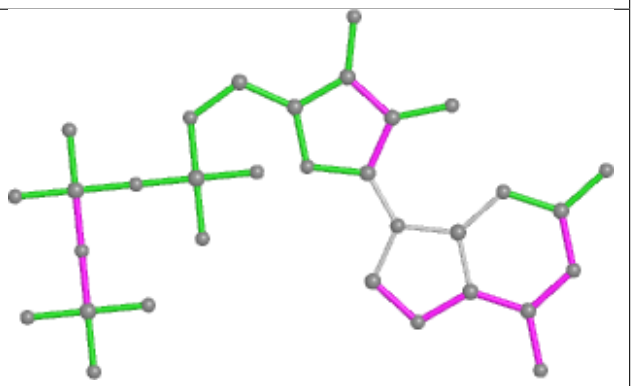
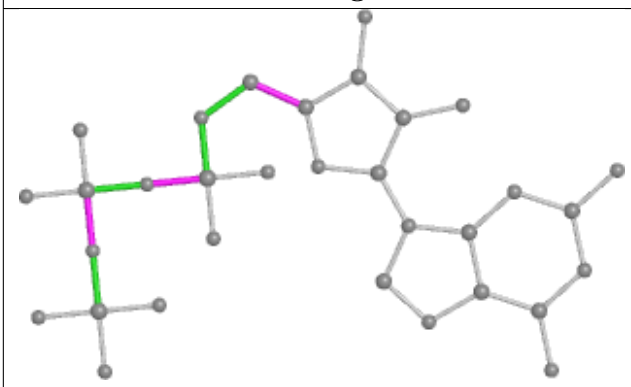


Bond angles



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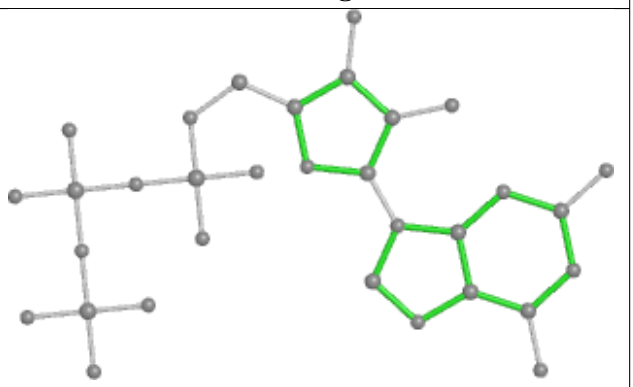
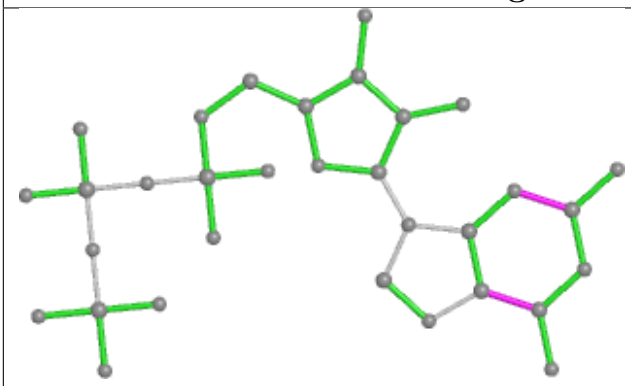


Rings

Ligand GTP OH 501



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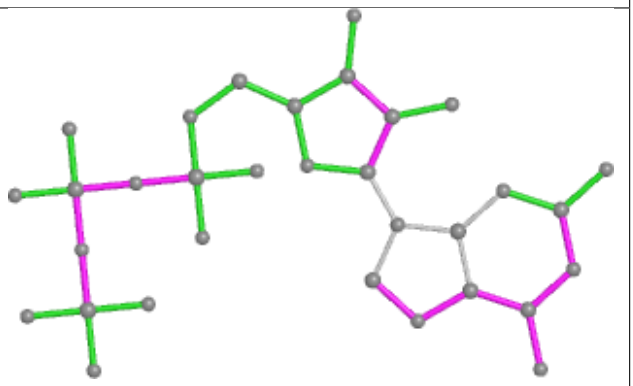
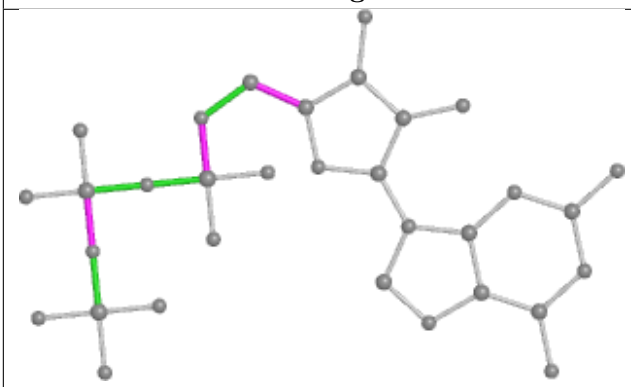


Bond angles



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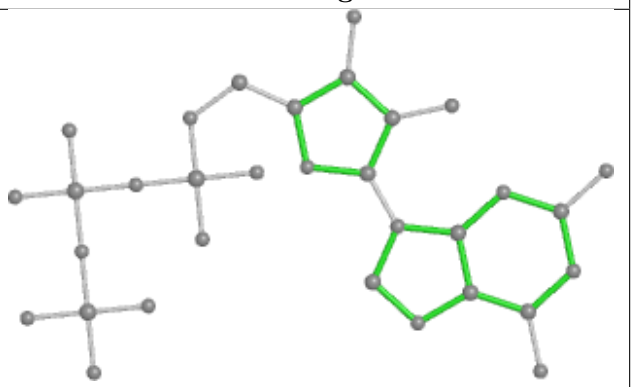
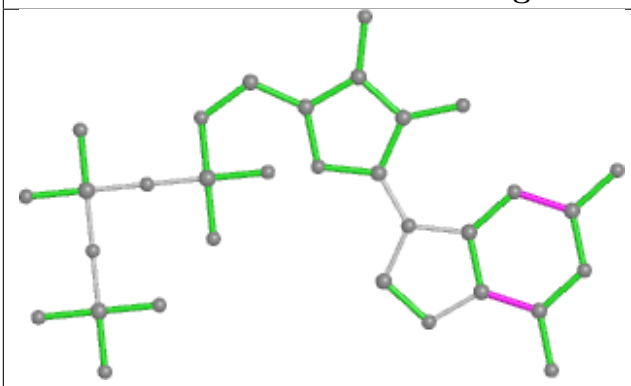


Rings

Ligand GTP FF 501



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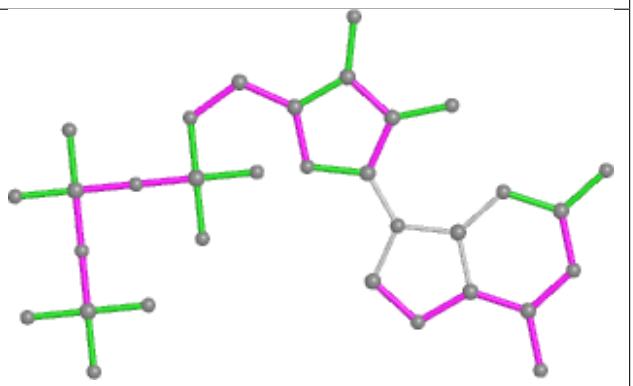
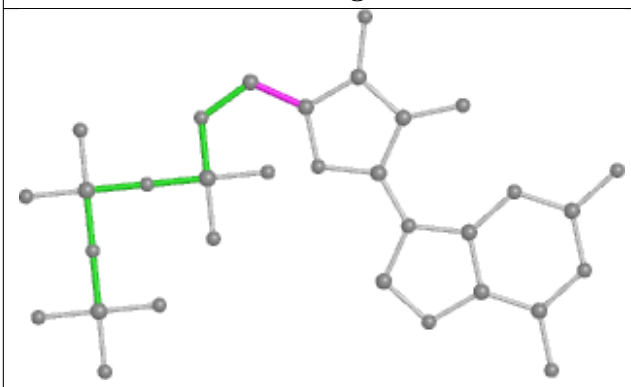


Bond angles



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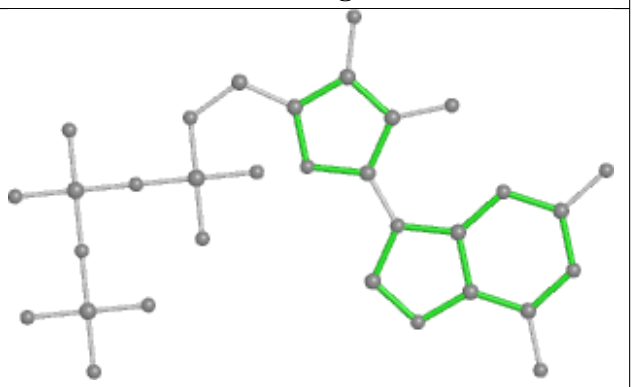
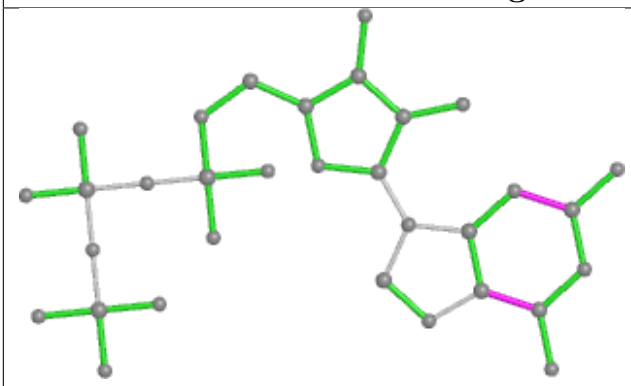


Rings

Ligand GTP DD 501



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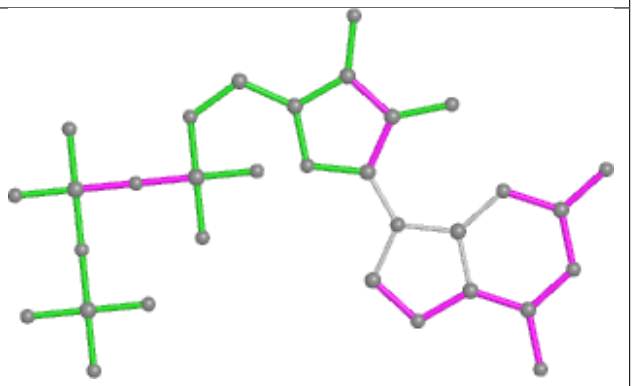
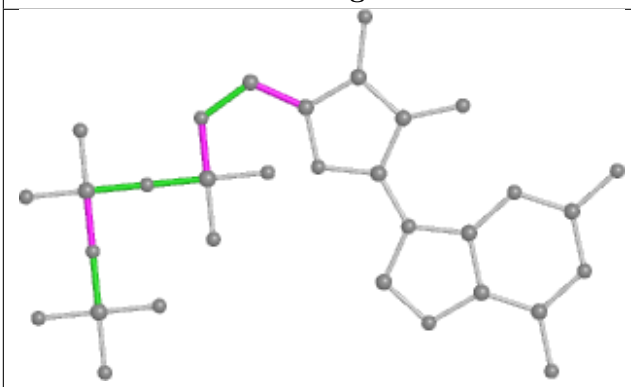


Bond angles



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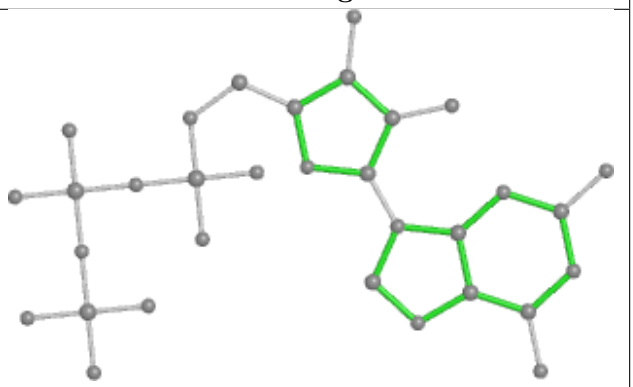
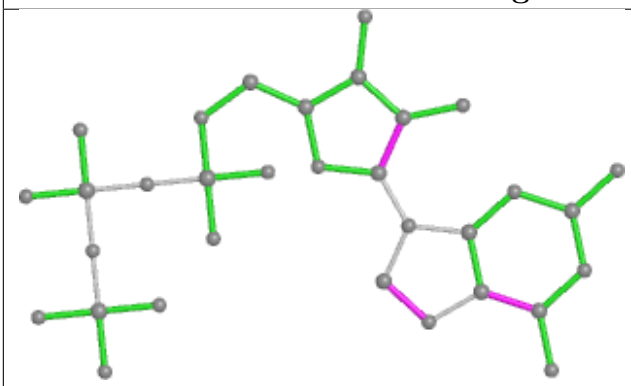


Rings

Ligand GTP EE 501



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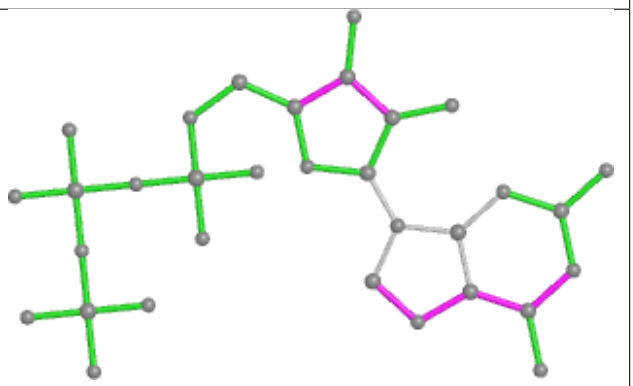
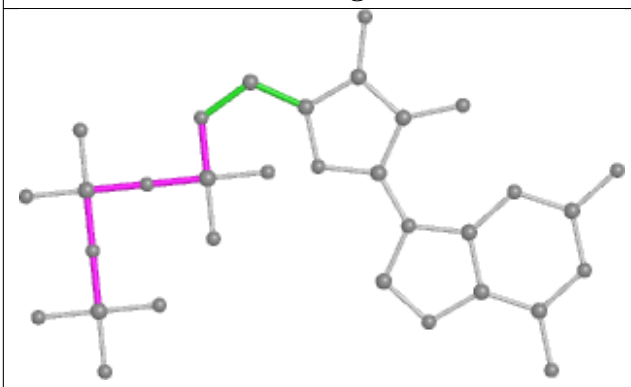
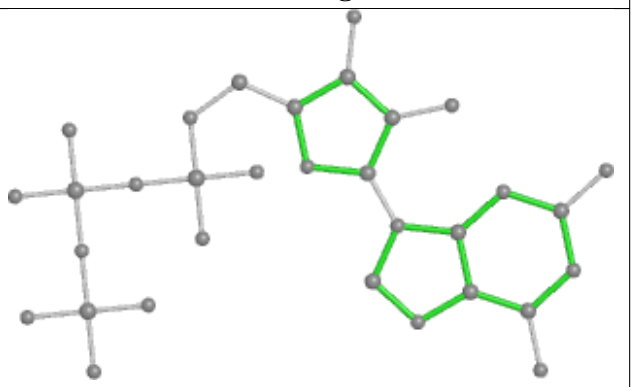


Bond angles

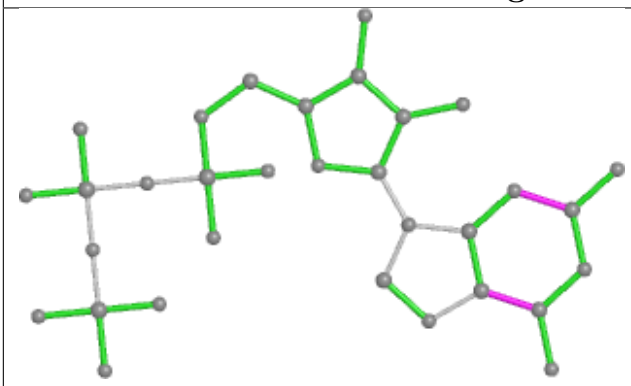


Torsions

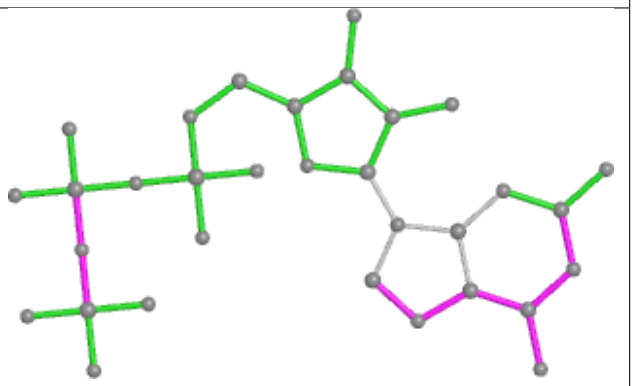


Rings

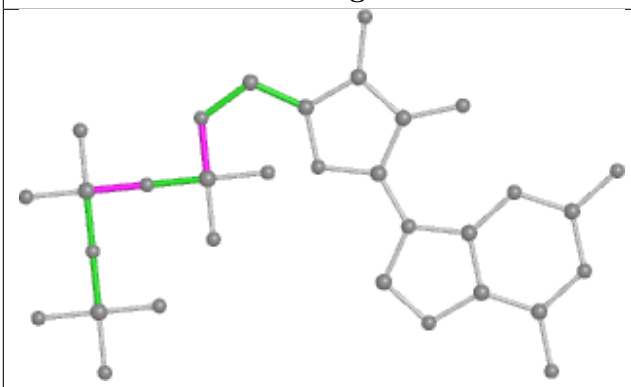
Ligand GTP GD 501



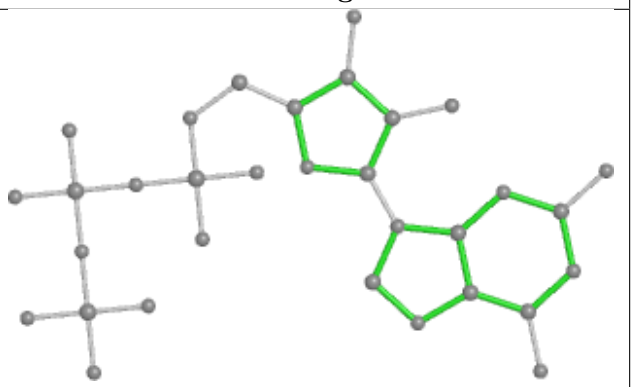
Bond lengths



Bond angles

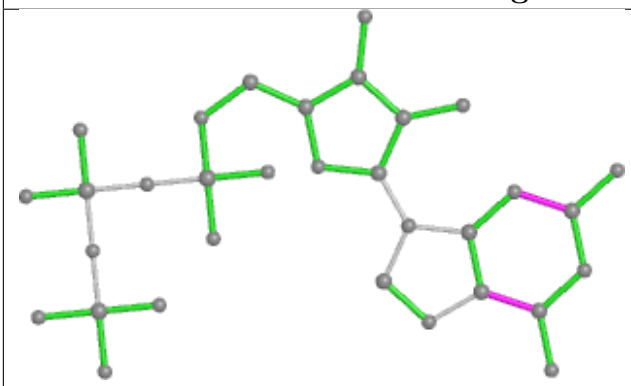


Torsions

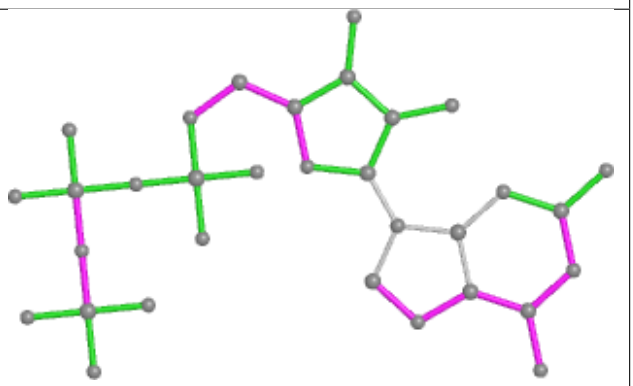


Rings

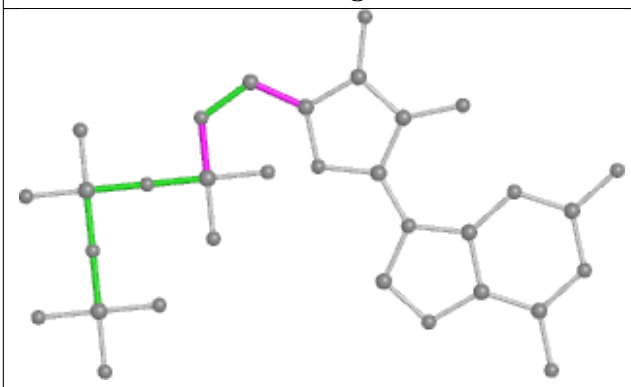
Ligand GTP LH 501



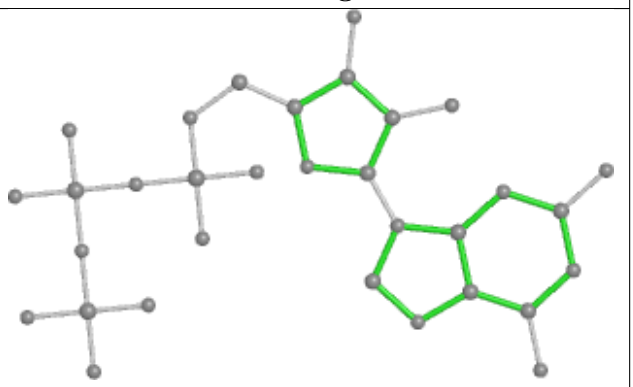
Bond lengths



Bond angles

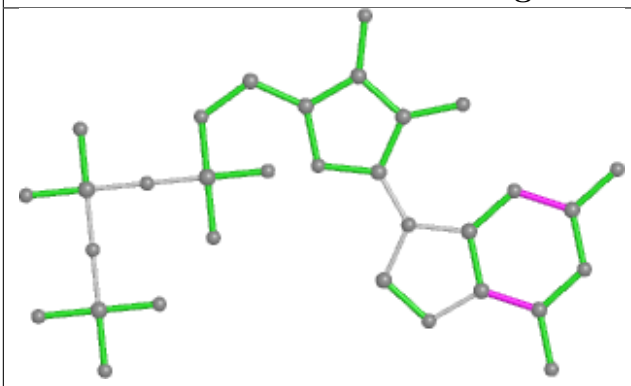


Torsions



Rings

Ligand GTP SF 501



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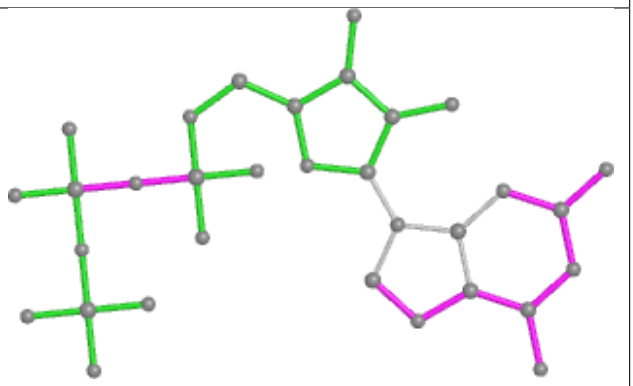
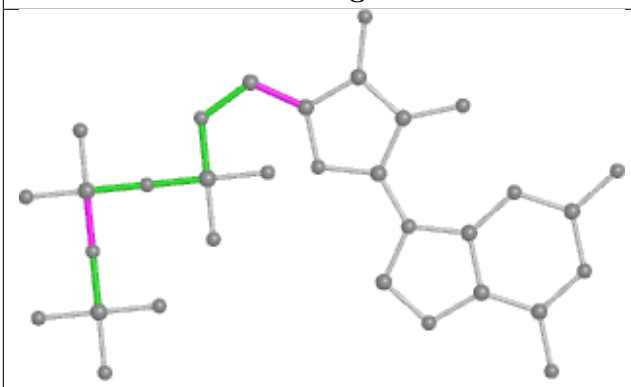


Bond angles



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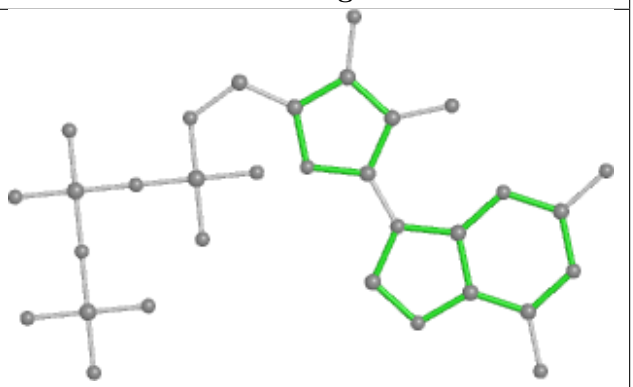
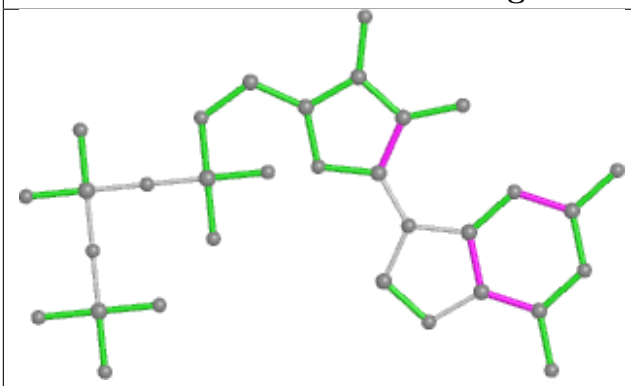


Rings

Ligand GTP HG 501



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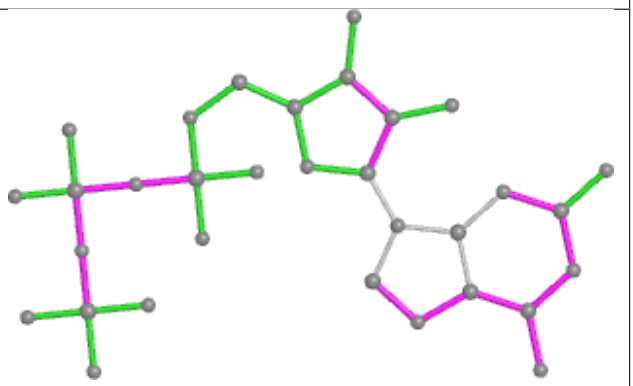
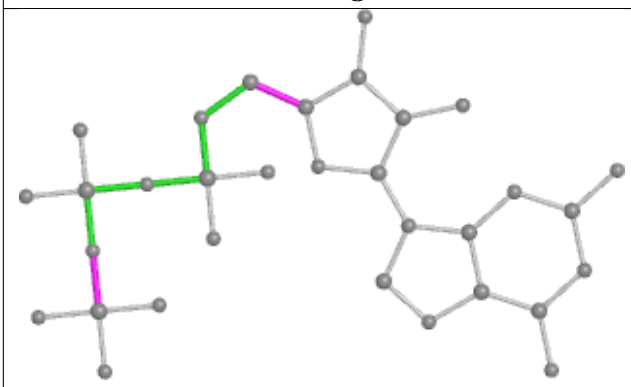


Bond angles



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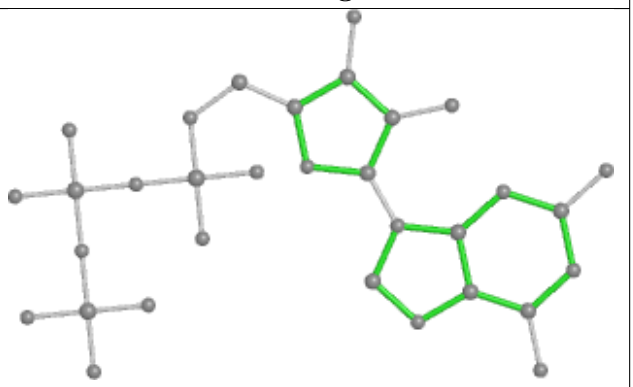
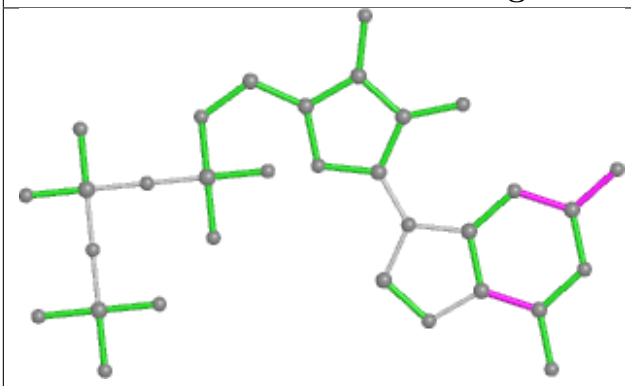
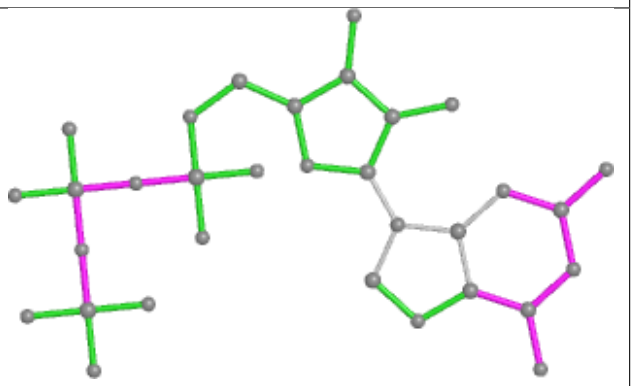


Rings

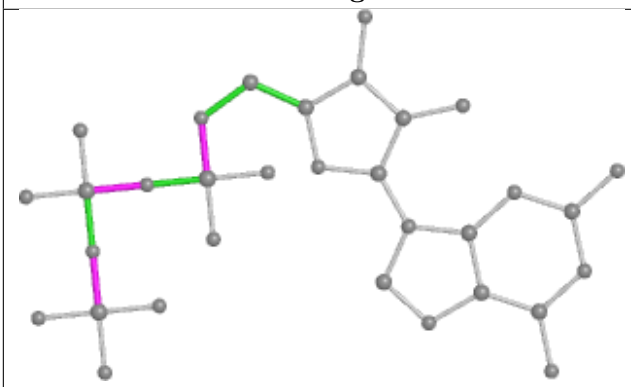
Ligand GTP ND 501



Bond lengths



Bond angles



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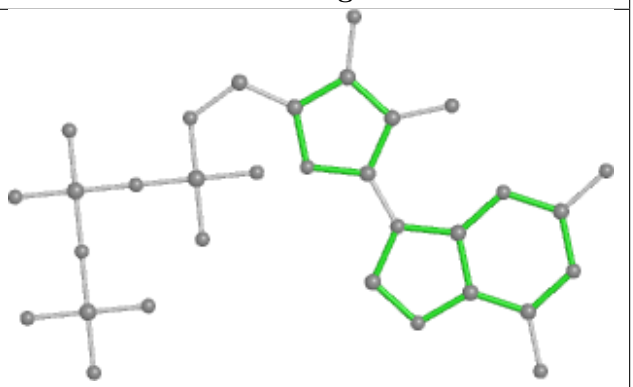
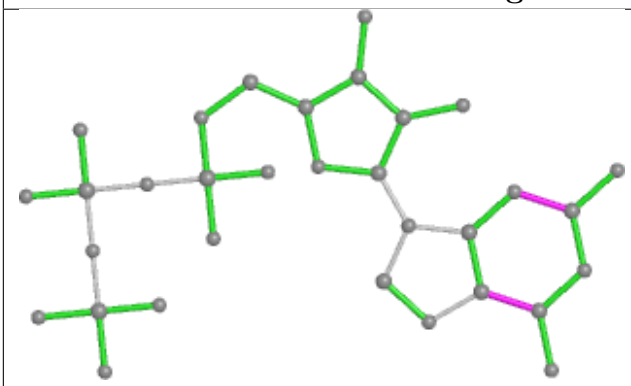


Rings

Ligand GTP WF 501



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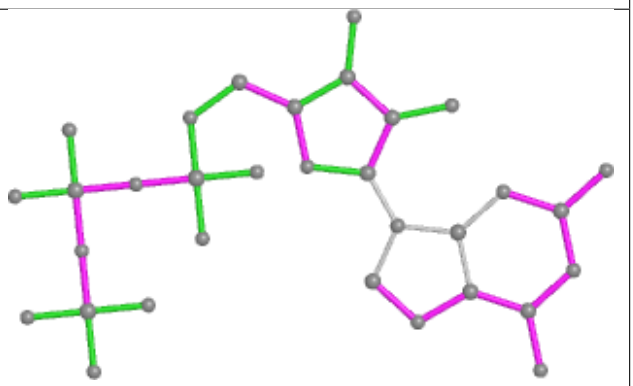
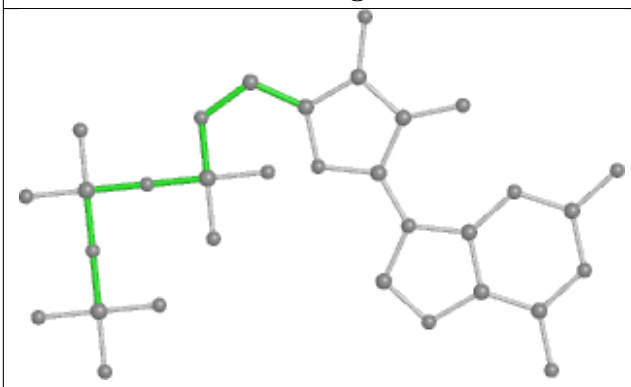


Bond angles



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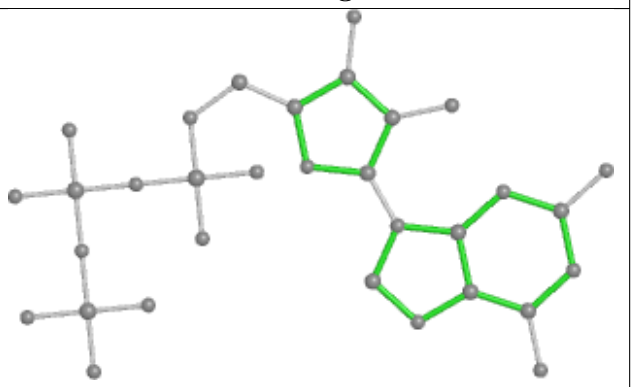
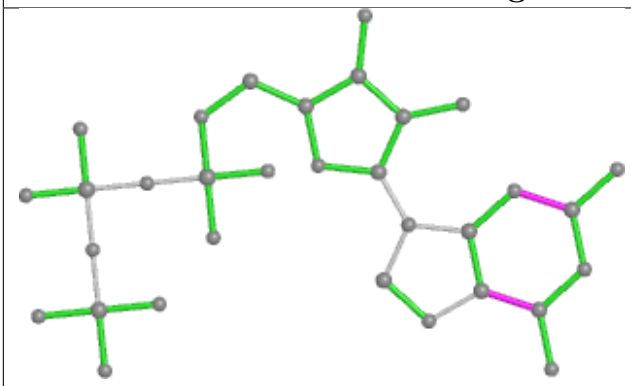
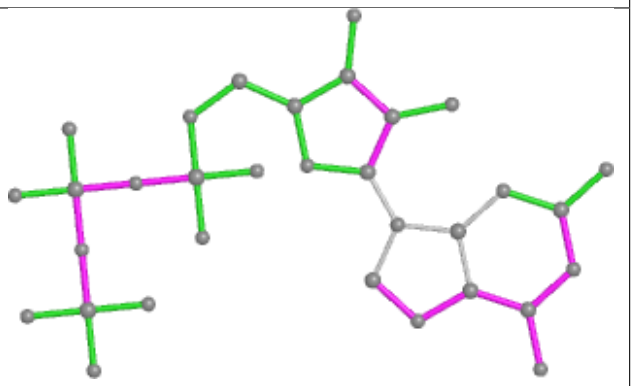


Rings

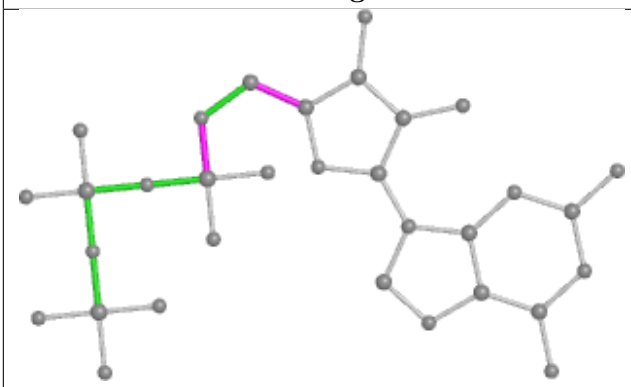
Ligand GTP VH 501



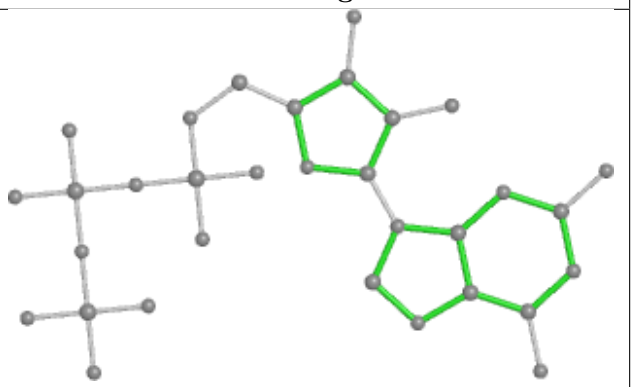
Bond lengths



Bond angles

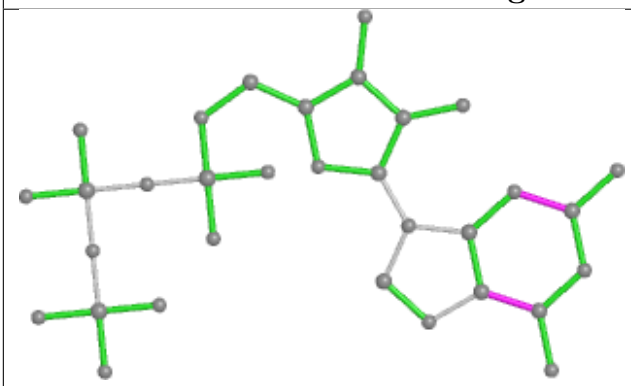


Torsions



Rings

Ligand GTP UD 501



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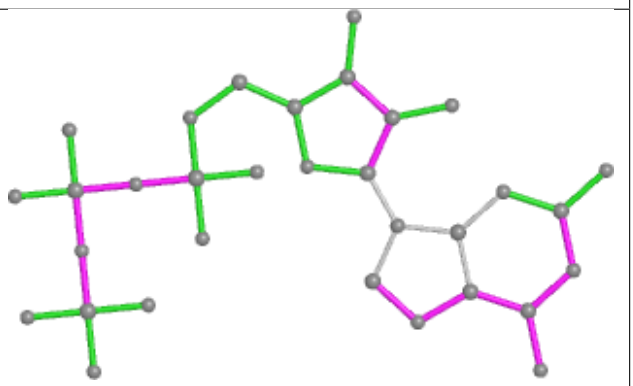
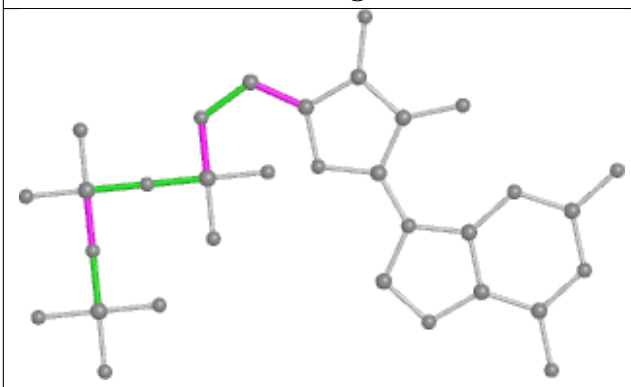


Bond angles



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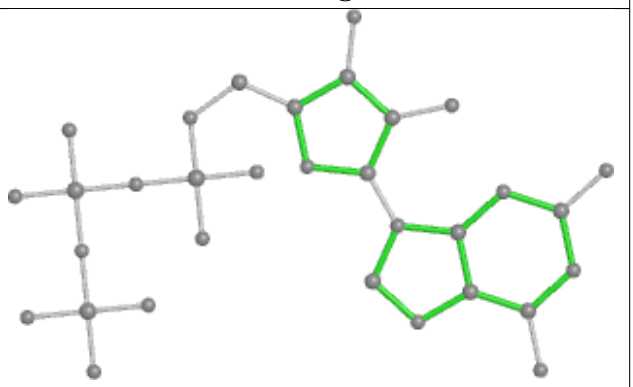
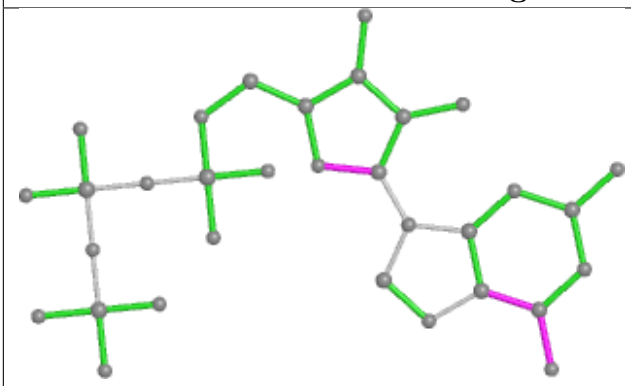


Rings

Ligand GTP EG 501



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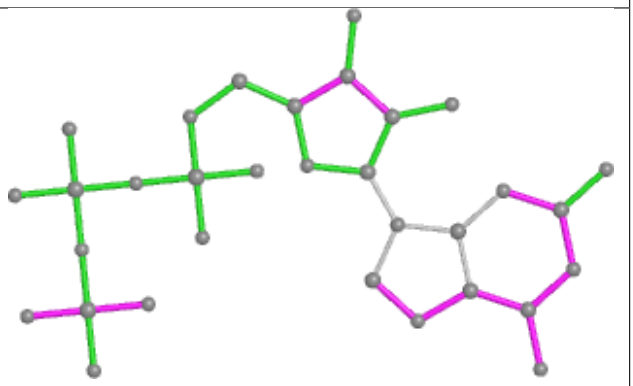
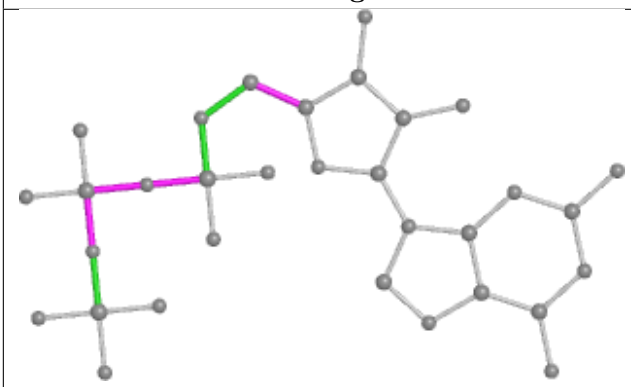


Bond angles



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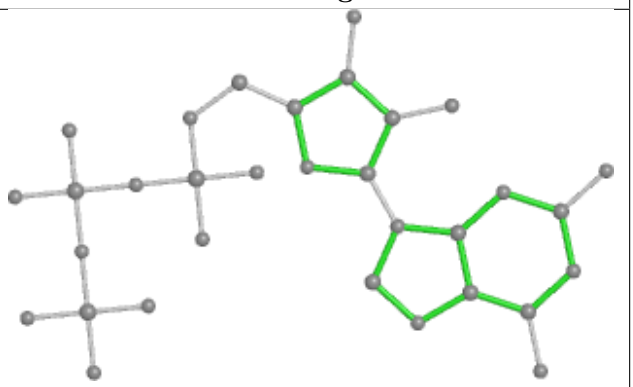
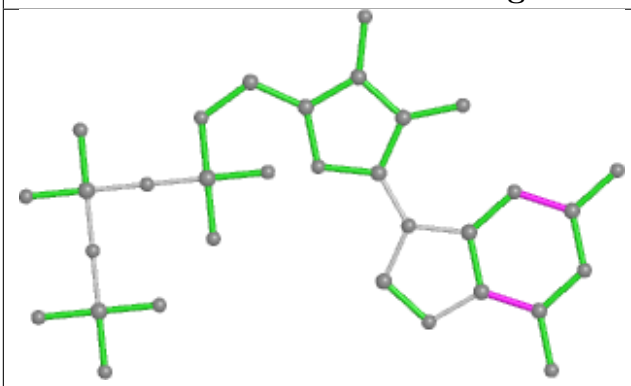


Rings

Ligand GTP NG 501



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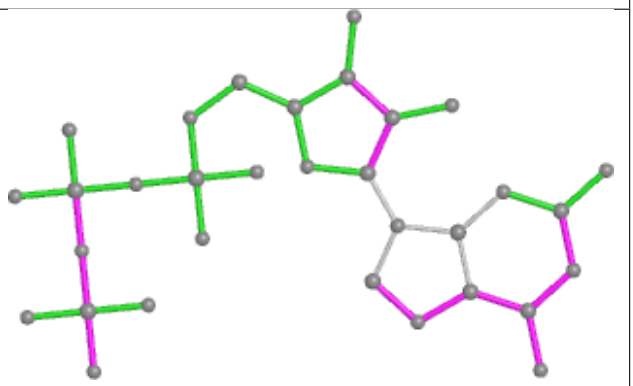
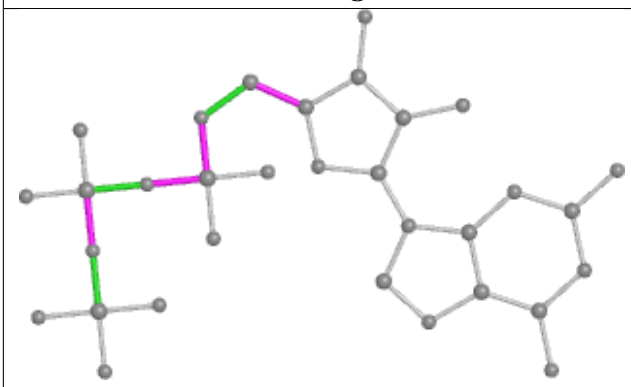


Bond angles



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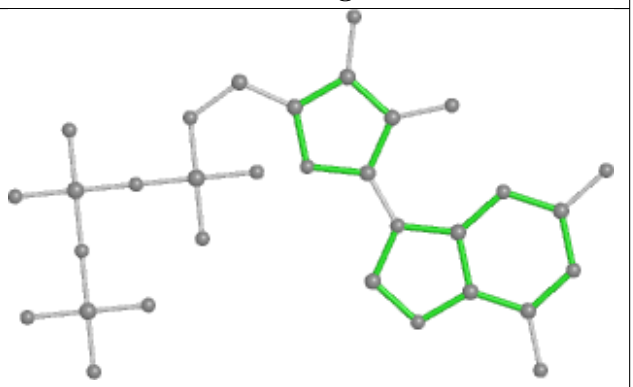
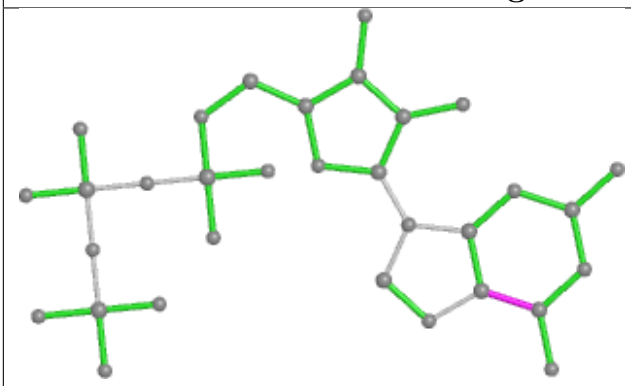


Rings

Ligand GTP UG 501



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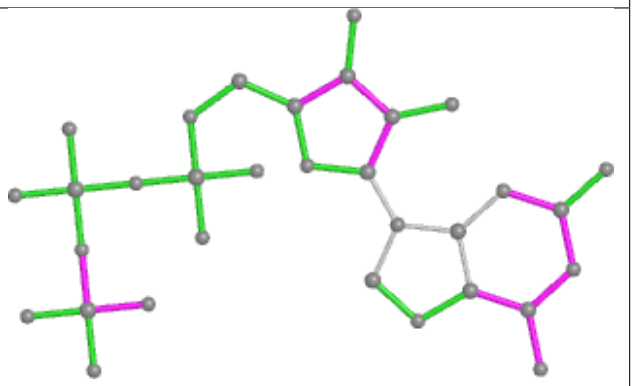
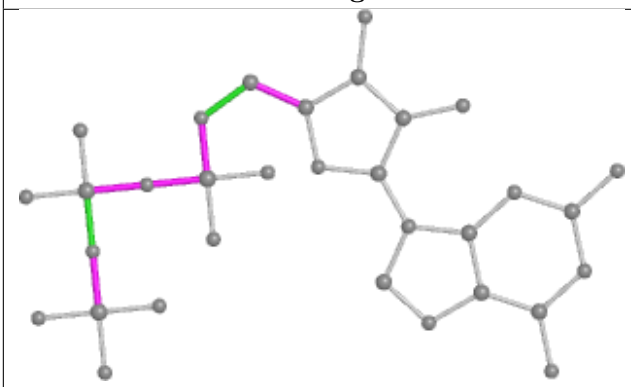


Bond angles



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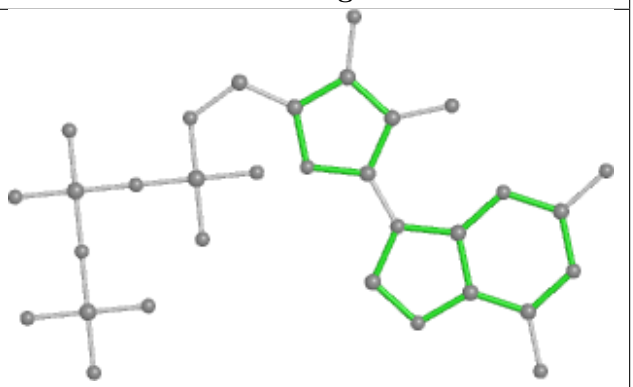
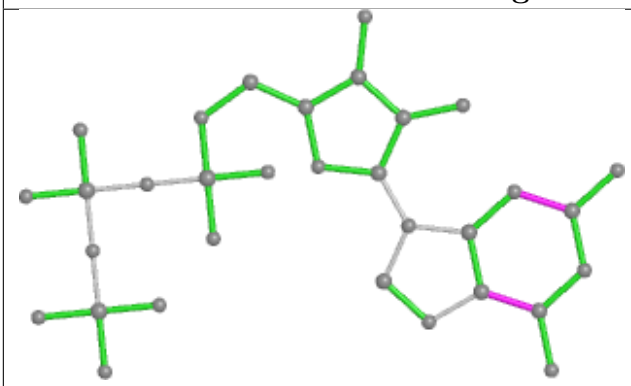


Rings

Ligand GTP PF 501



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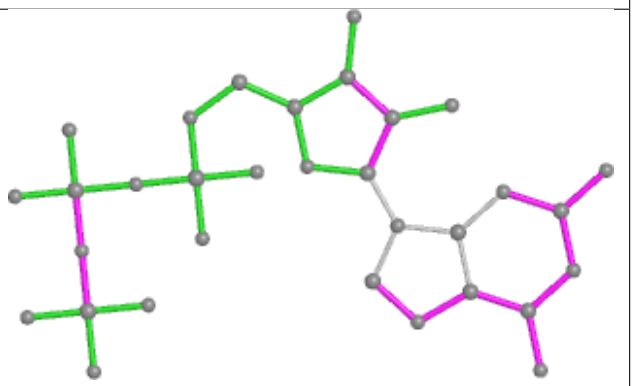
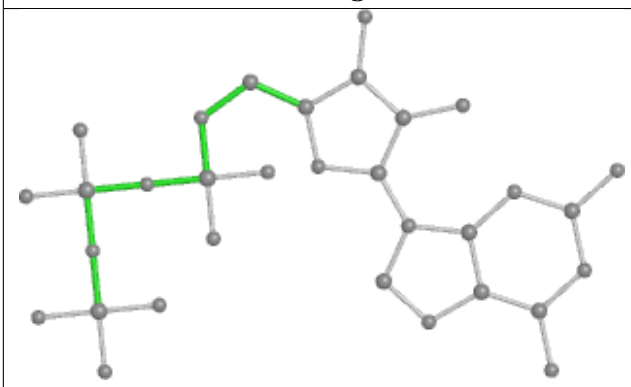


Bond angles



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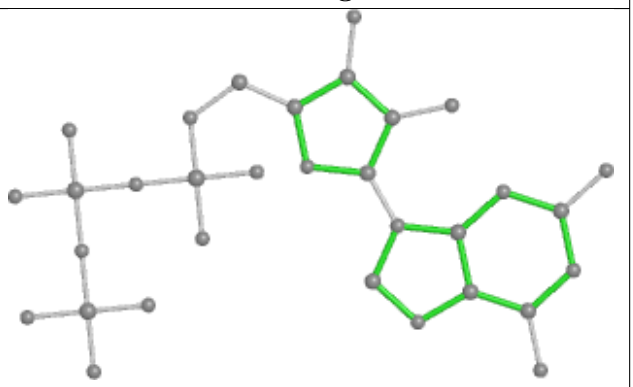
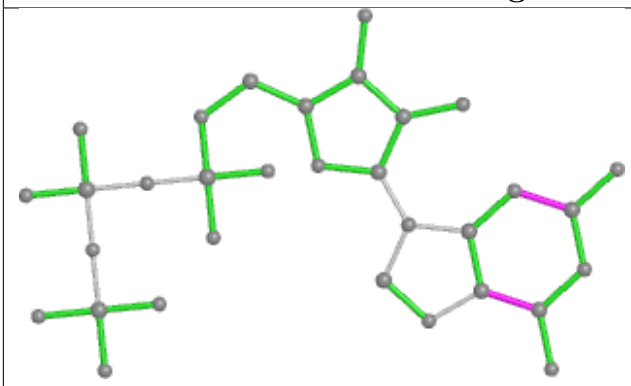


Rings

Ligand GTP UH 501



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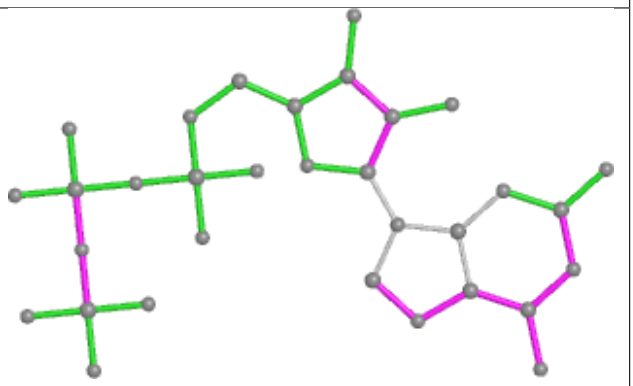
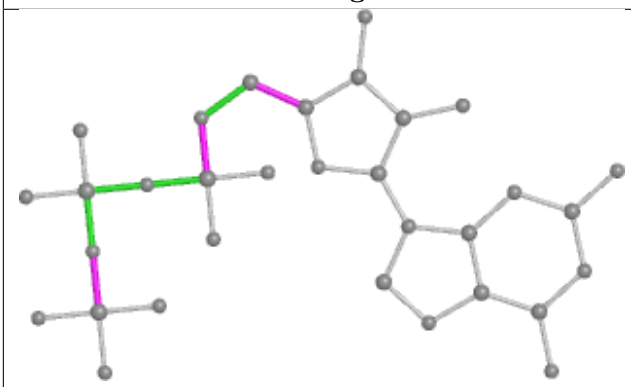


Bond angles



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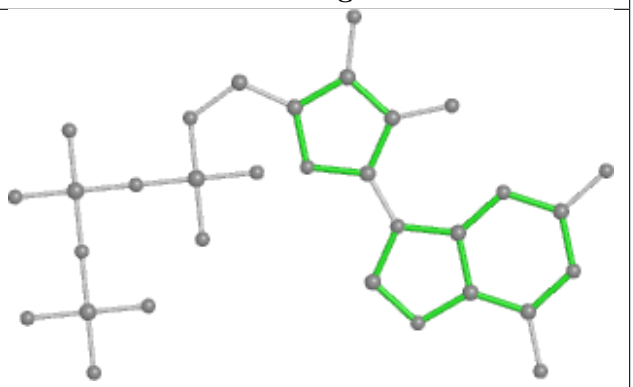
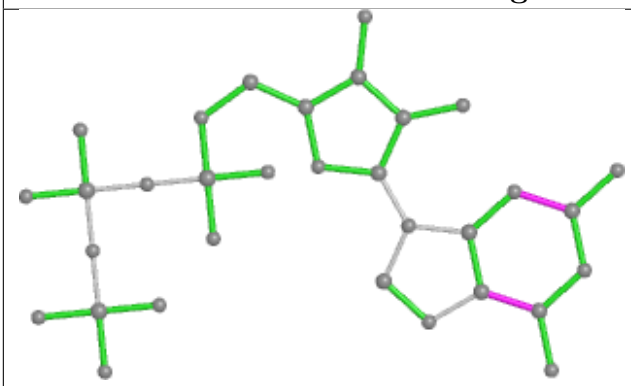


Rings

Ligand GTP OE 501



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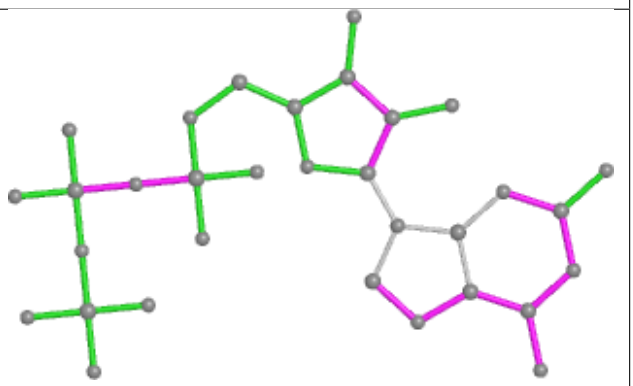
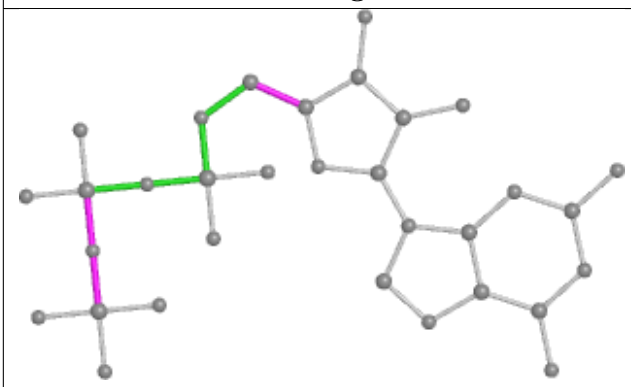


Bond angles



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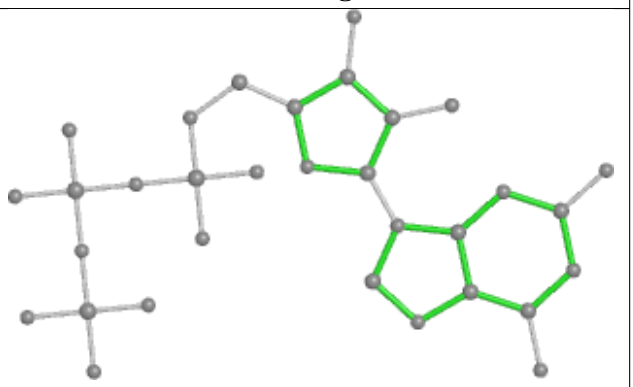
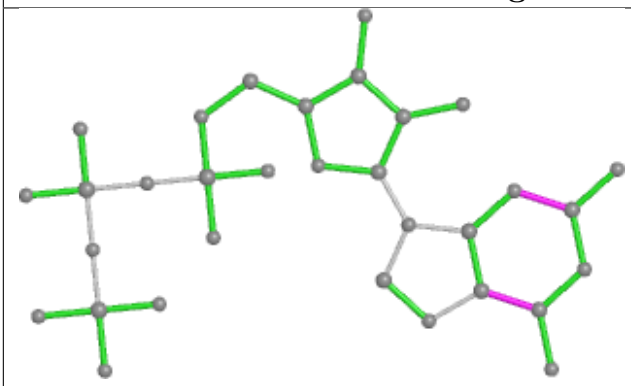


Rings

Ligand GTP RH 501



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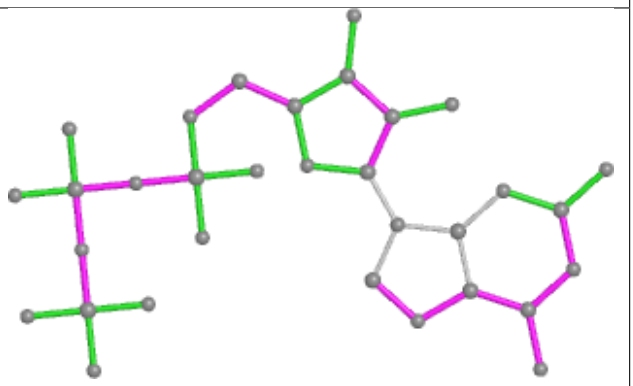
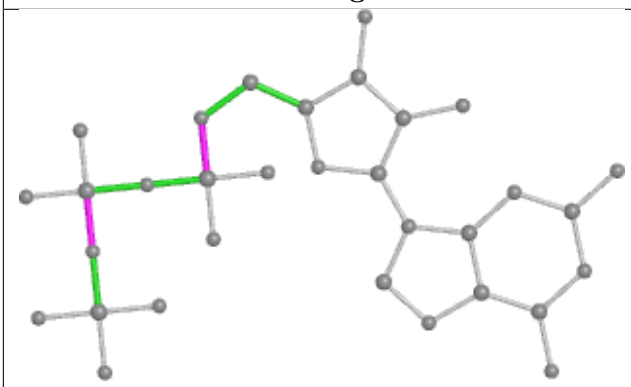
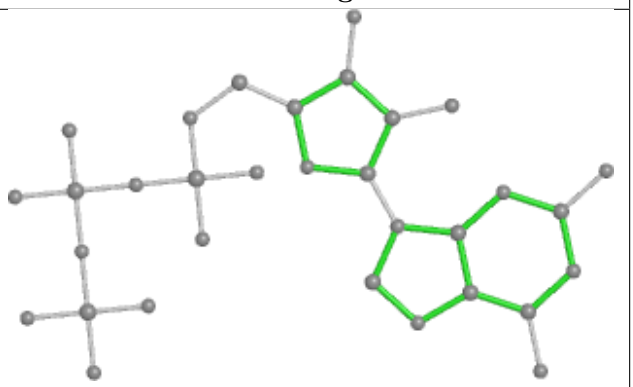


Bond angles

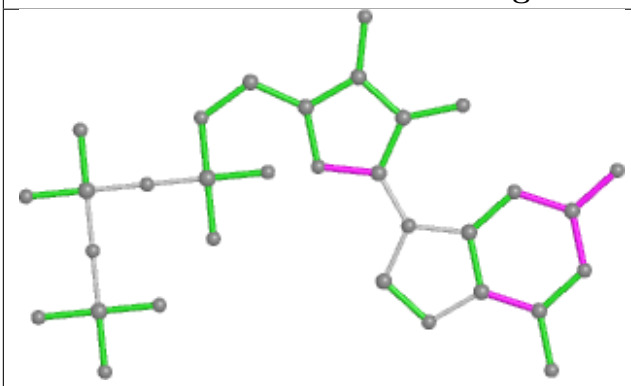


Torsions



Rings

Ligand GTP JD 501



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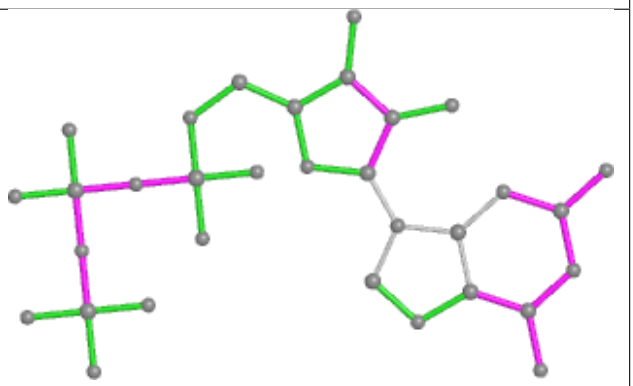
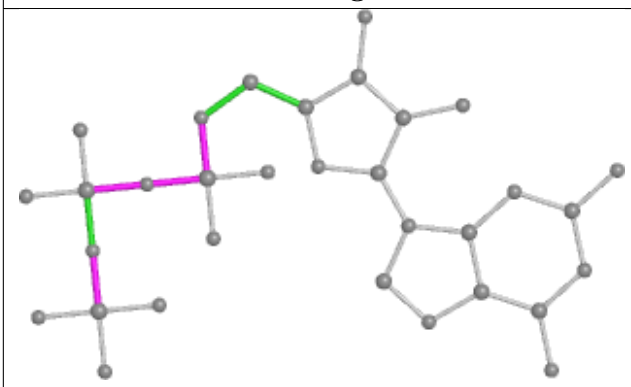


Bond angles



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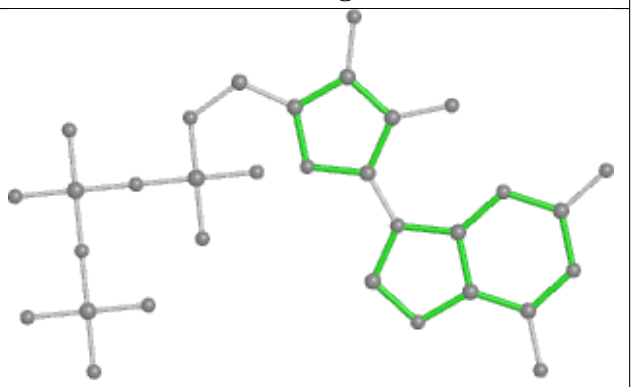
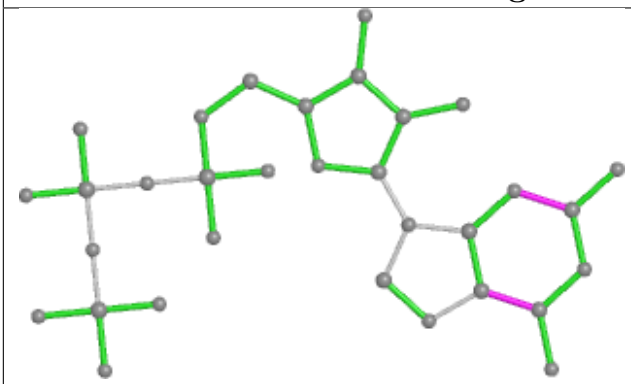
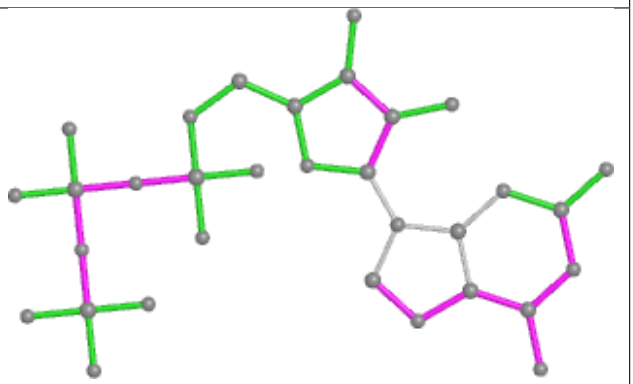


Rings

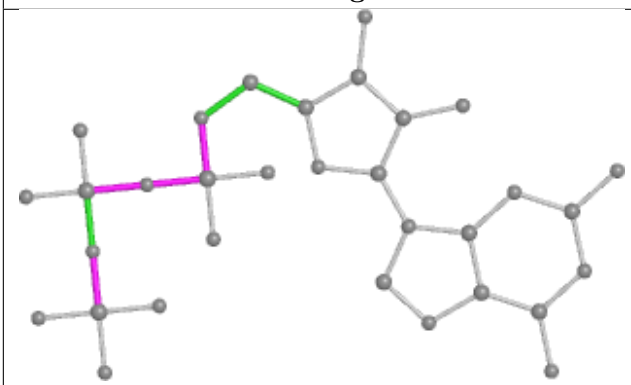
Ligand GTP CH 501



Bond lengths



Bond angles



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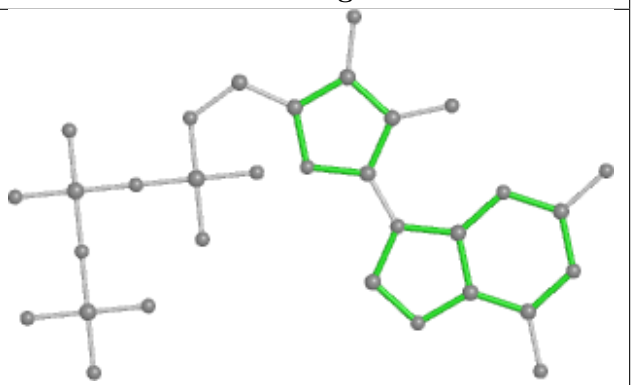
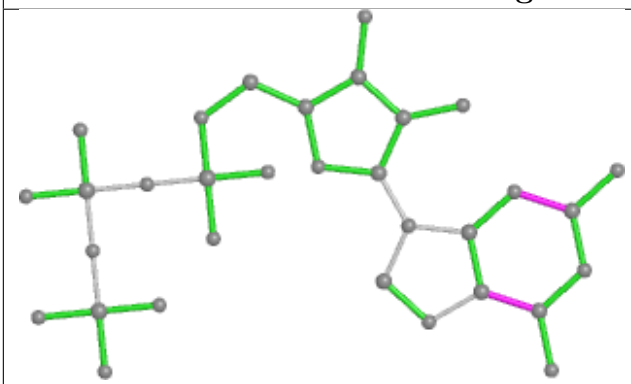


Rings

Ligand GTP RI 501



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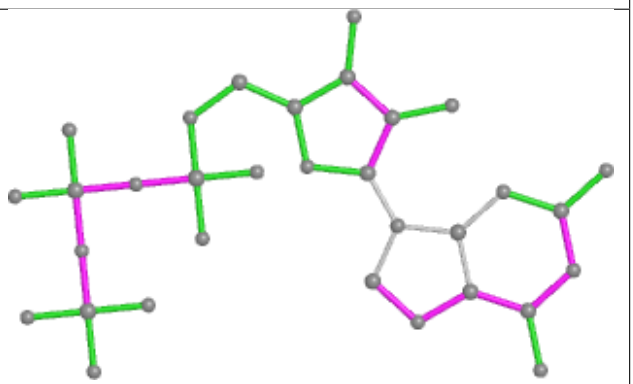
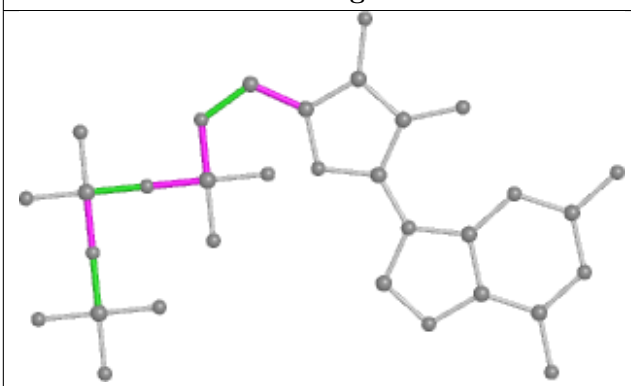


Bond angles



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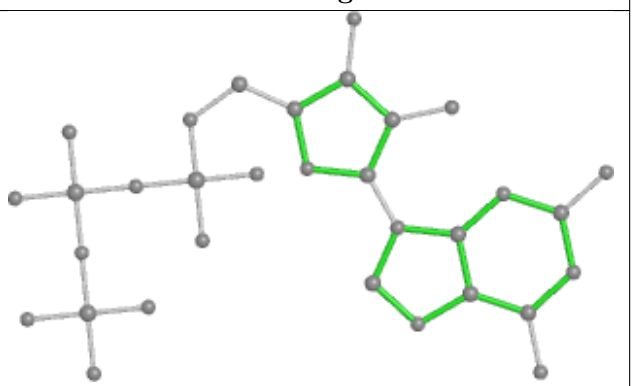
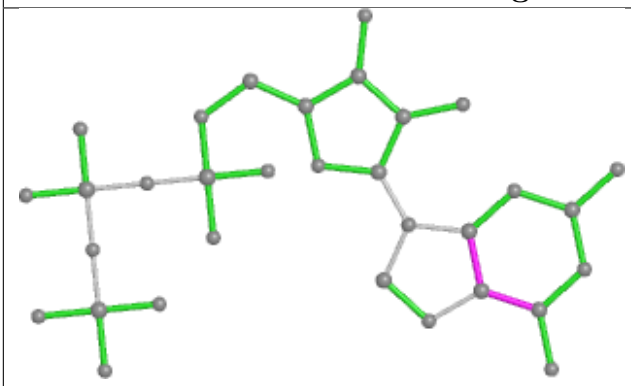


Rings

Ligand GTP PE 501



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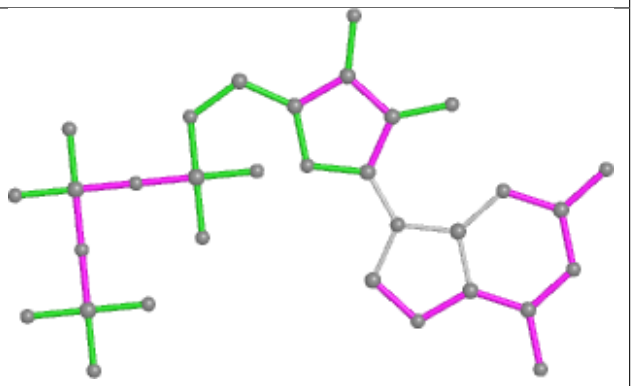
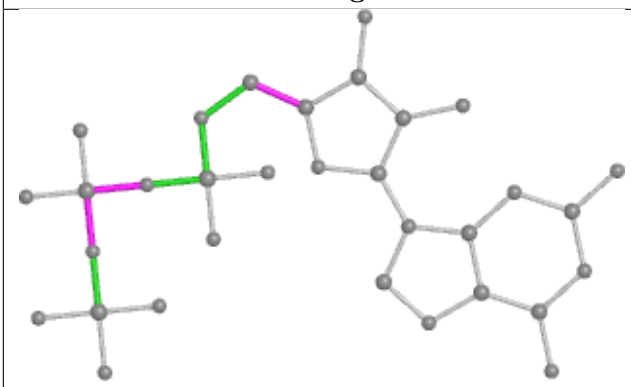


Bond angles



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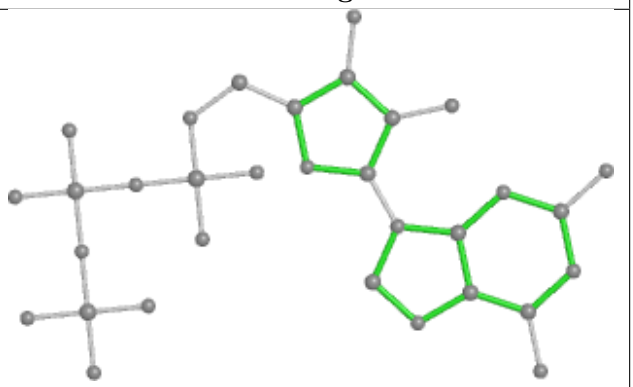
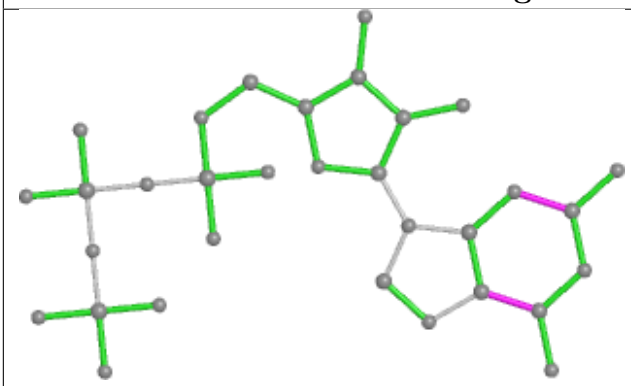


Rings

Ligand GTP TJ 501



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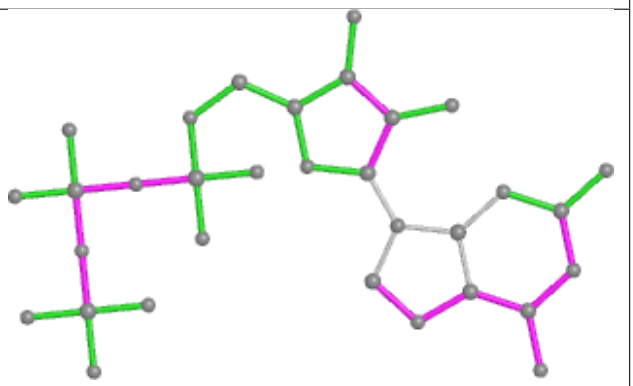
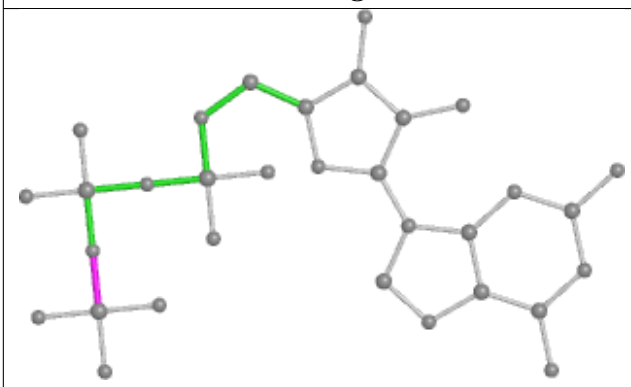


Bond angles



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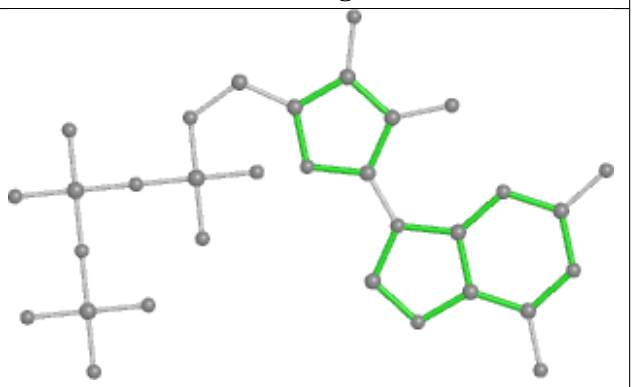
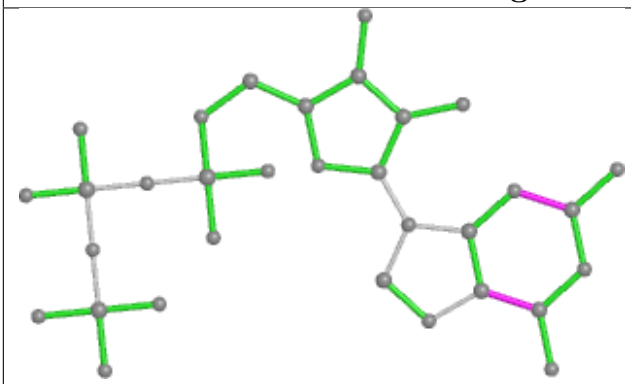
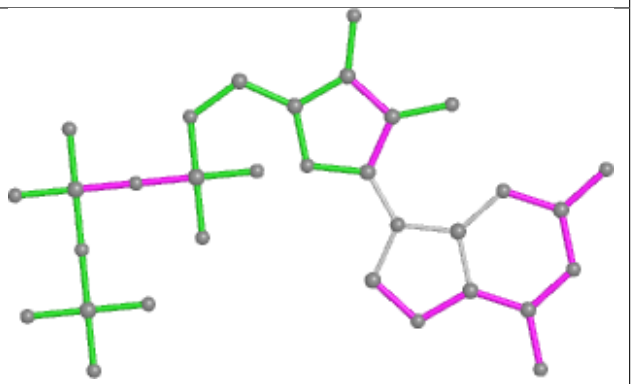


Rings

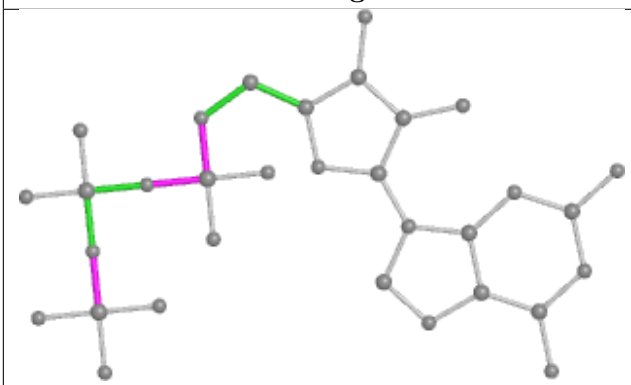
Ligand GTP FH 501



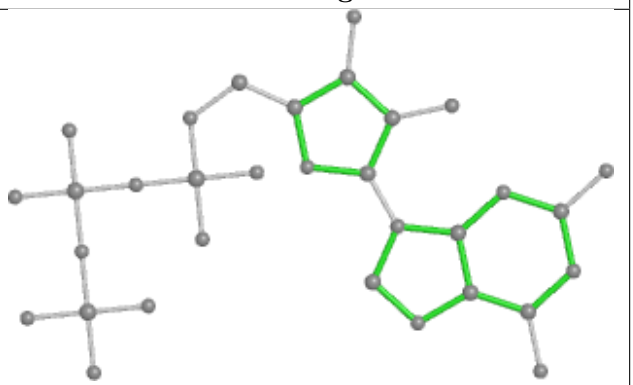
Bond lengths



Bond angles

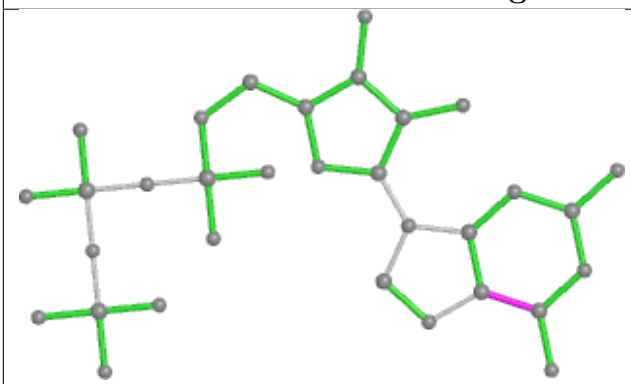


Torsions

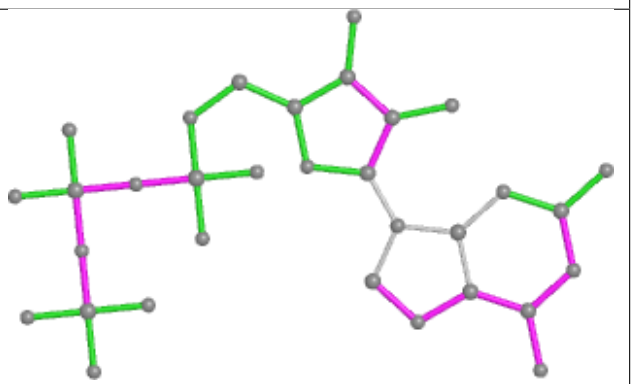


Rings

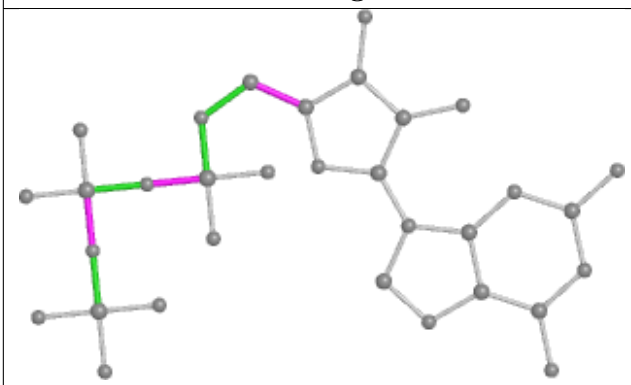
Ligand GTP TG 501



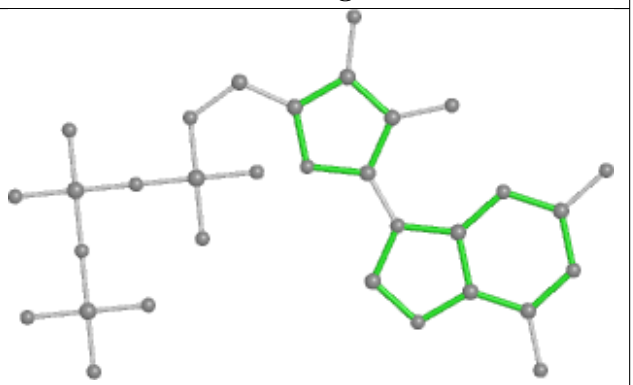
Bond lengths



Bond angles

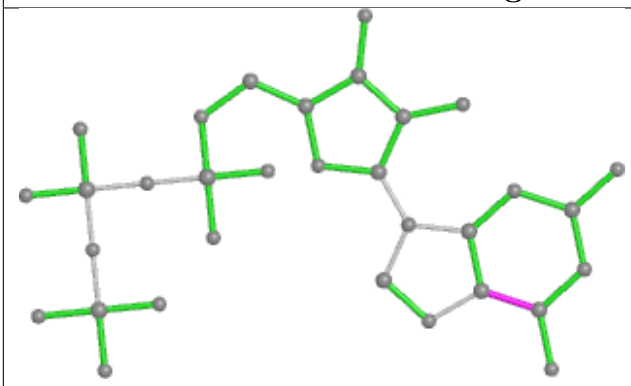


Torsions



Rings

Ligand GTP MG 501



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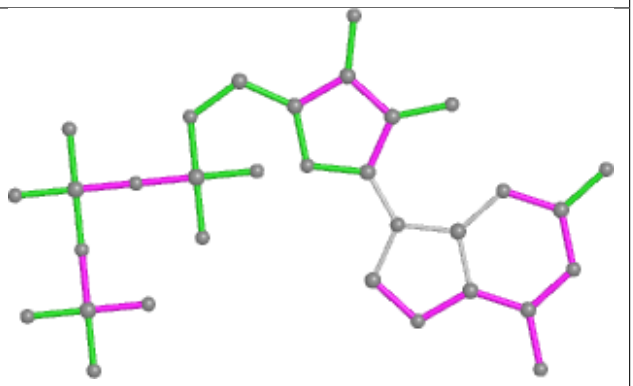

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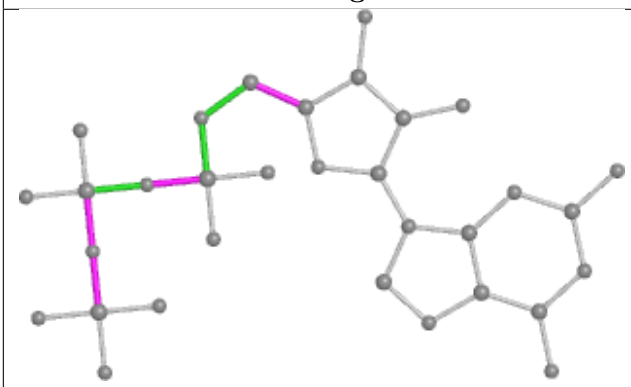

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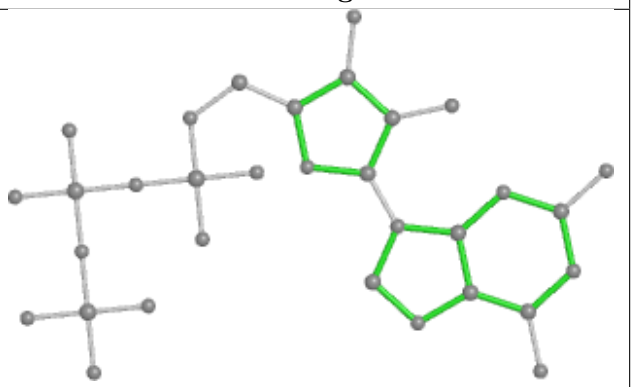
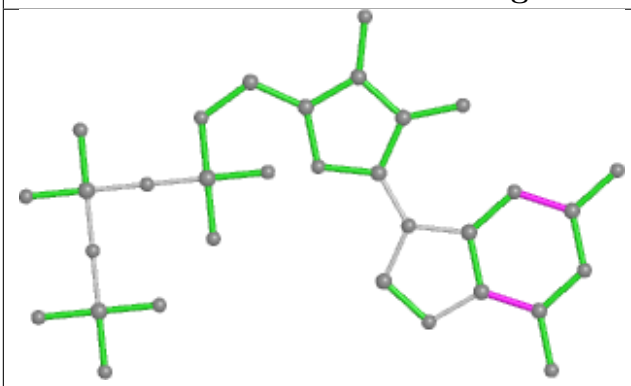


Rings

Ligand GTP VF 501



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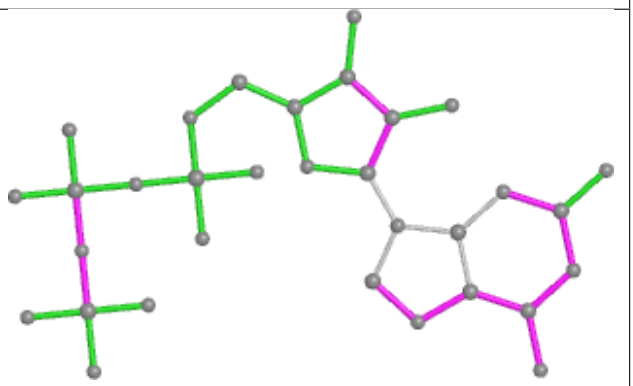
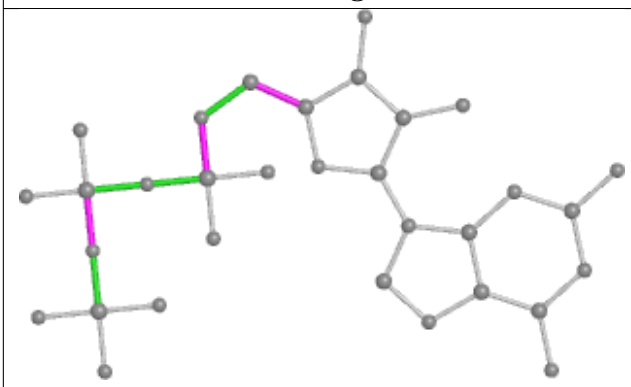
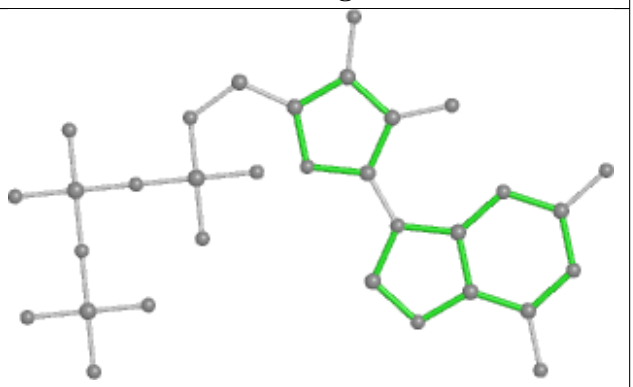


Bond angles

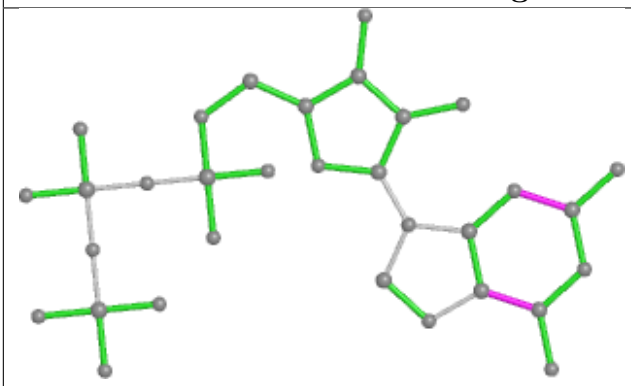


Torsions



Rings

Ligand GTP QF 501



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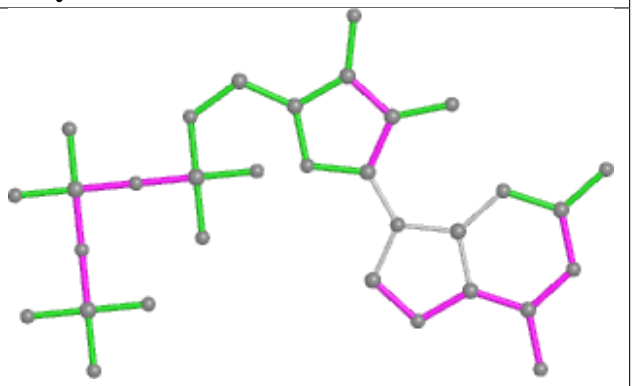
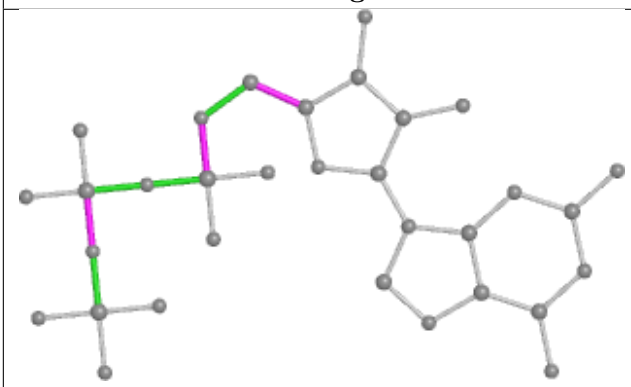
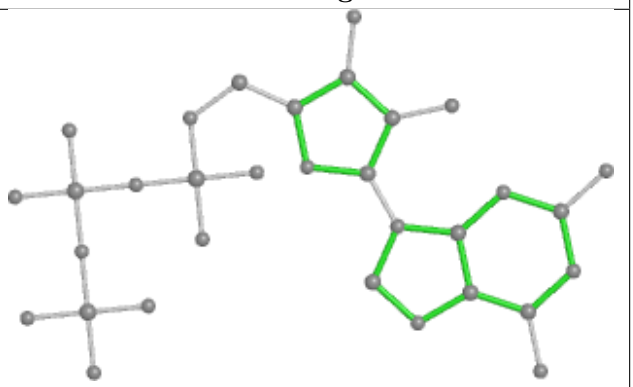


Bond angles

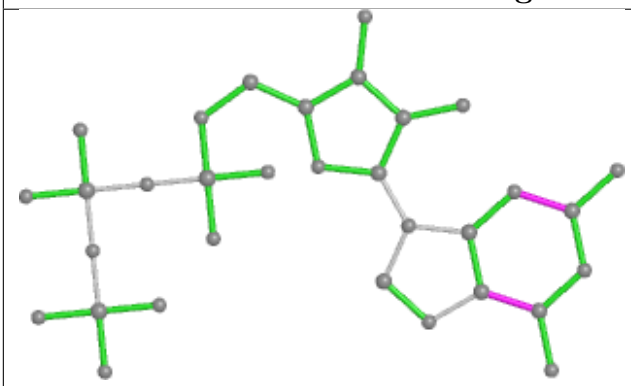


Torsions



Rings

Ligand GTP IH 501



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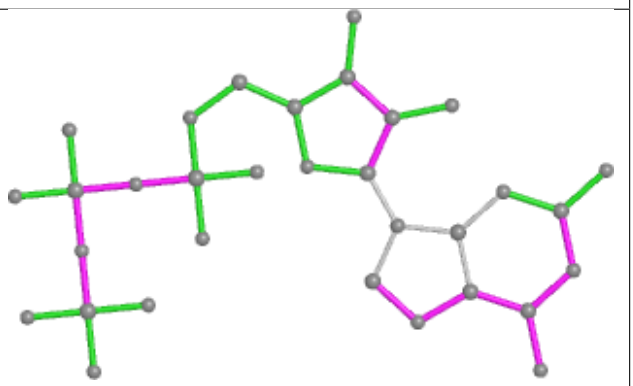
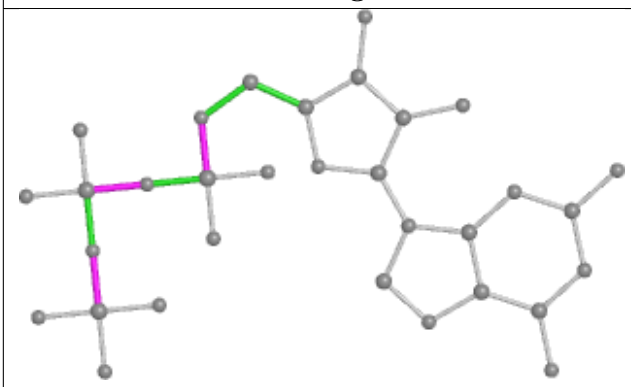
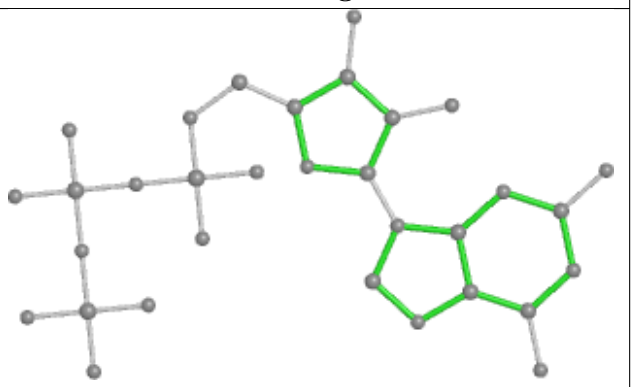


Bond angles

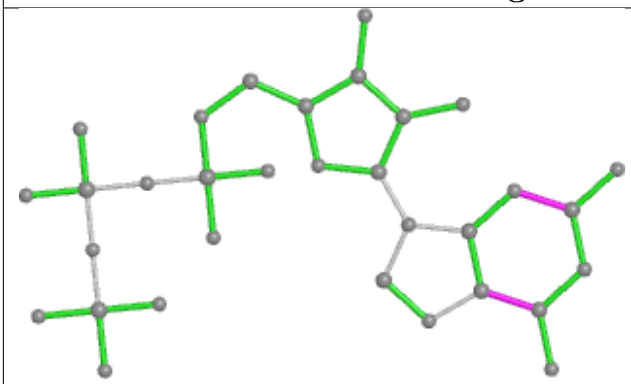


Torsions

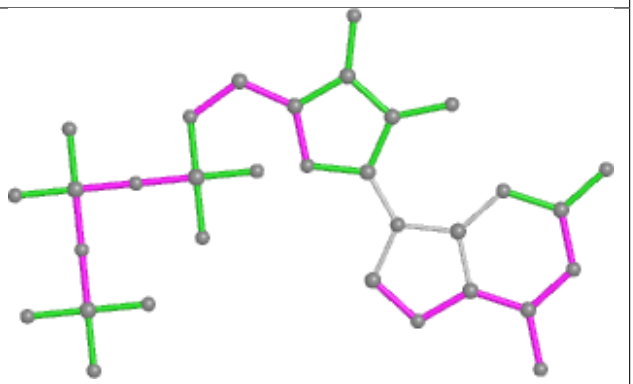


Rings

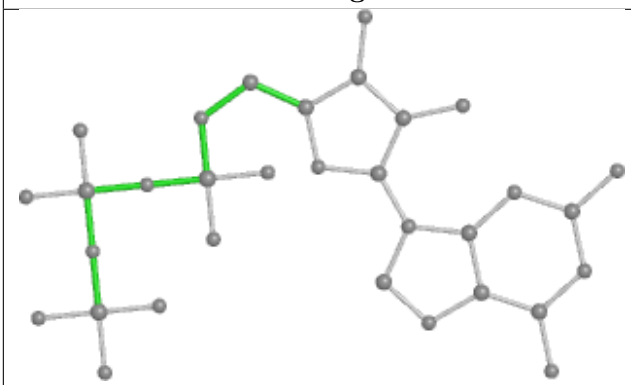
Ligand GTP DH 501



Bond lengths



Bond angles



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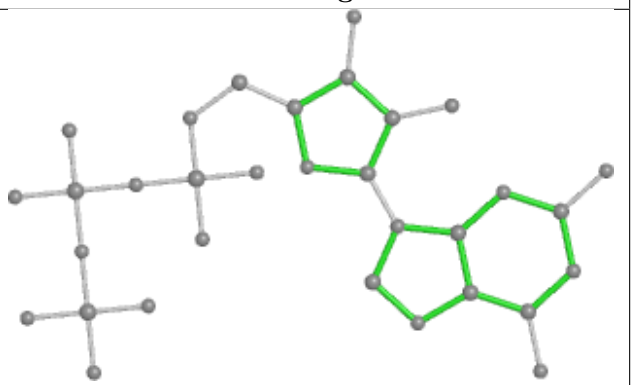
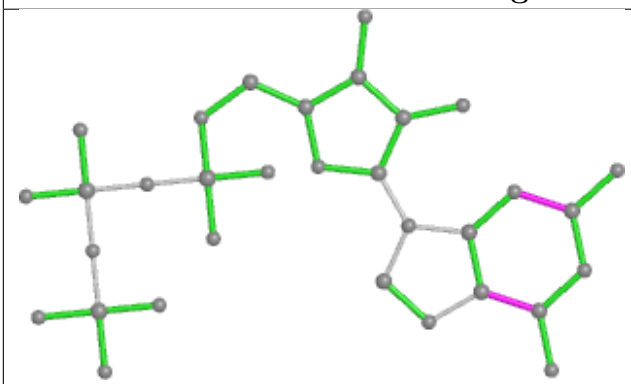


Rings

Ligand GTP LD 501



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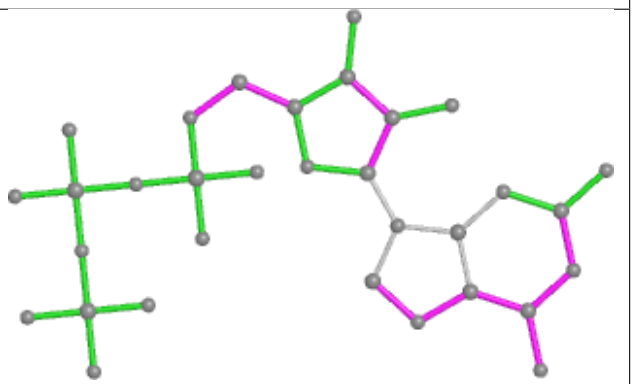
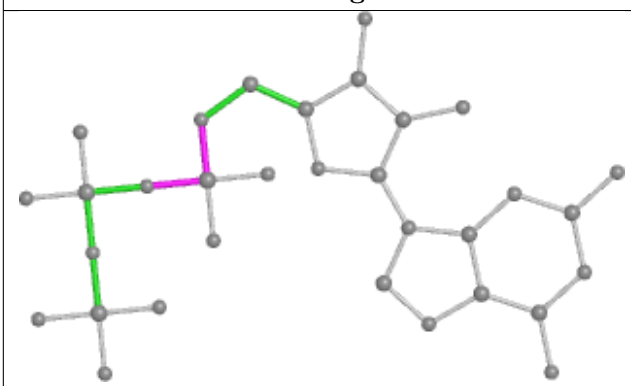


Bond angles



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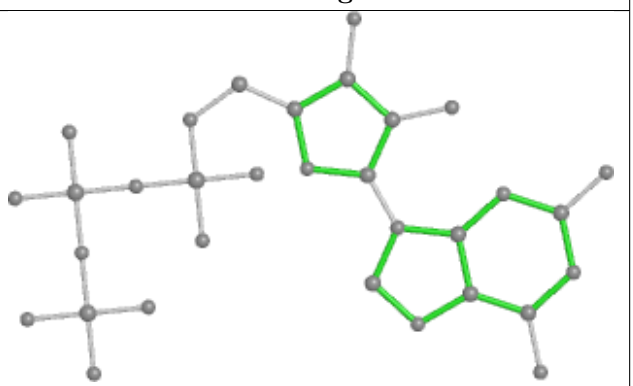
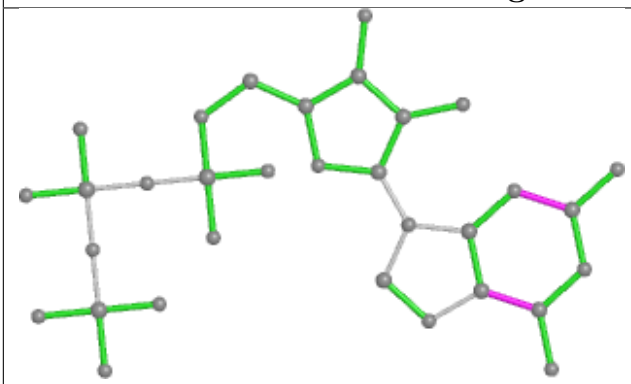
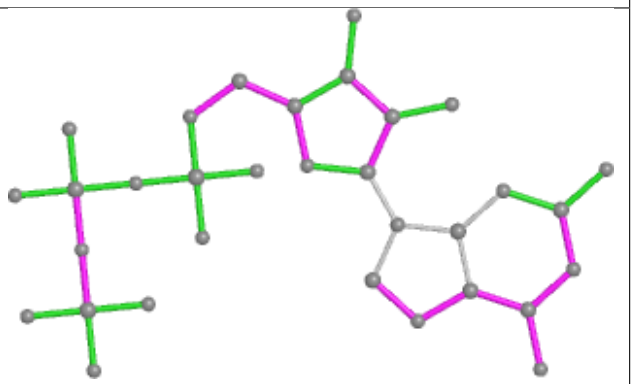


Rings

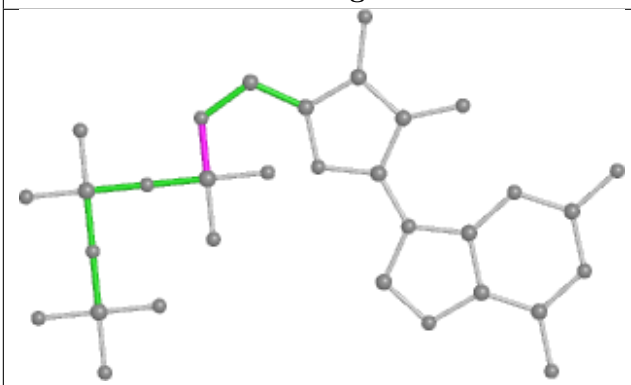
Ligand GTP KD 501



Bond lengths



Bond angles



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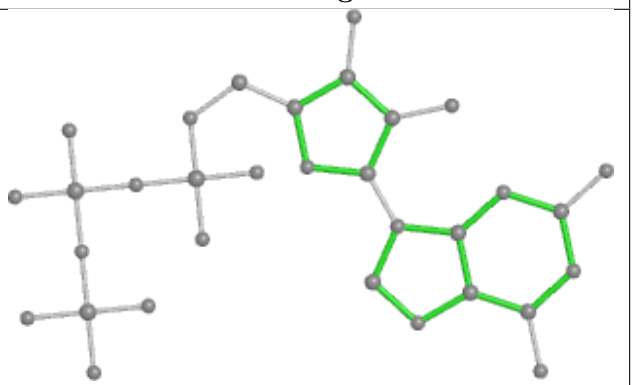
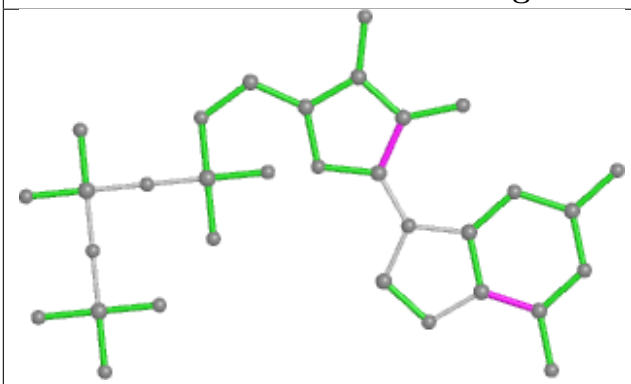


Rings

Ligand GTP FE 501



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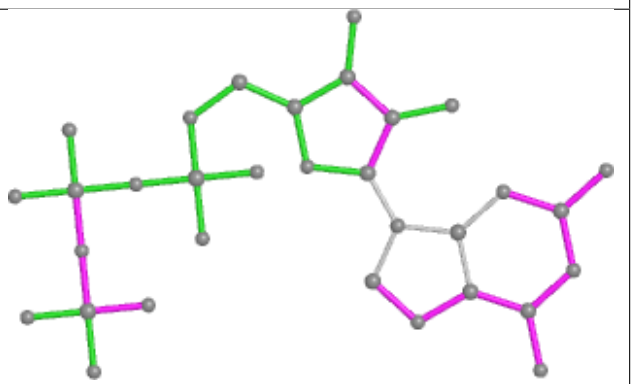
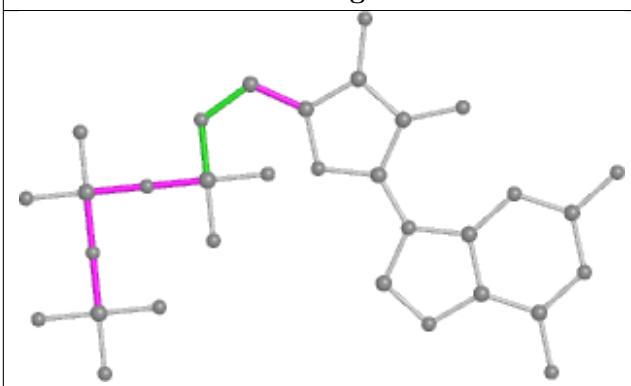


Bond angles



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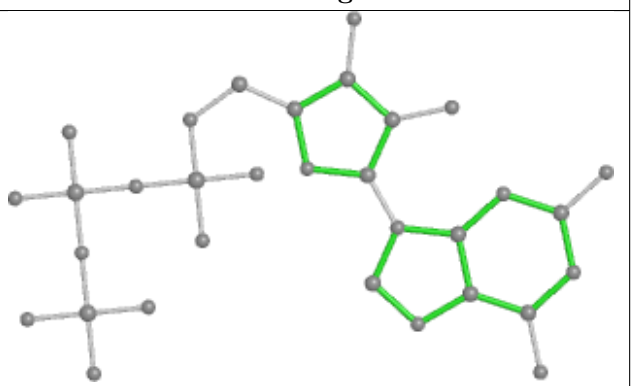
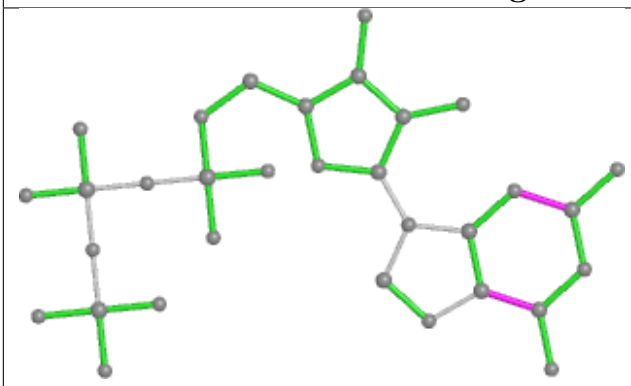
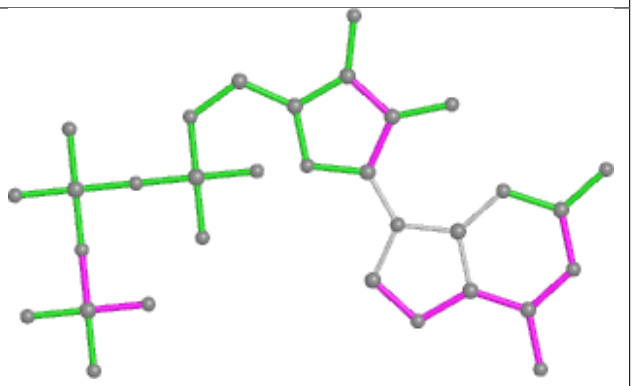


Rings

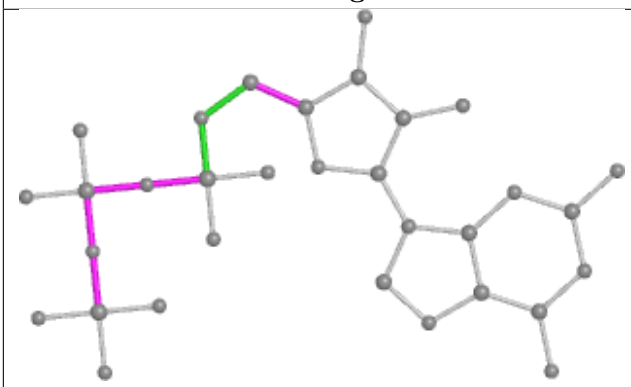
Ligand GTP PG 501



Bond lengths



Bond angles



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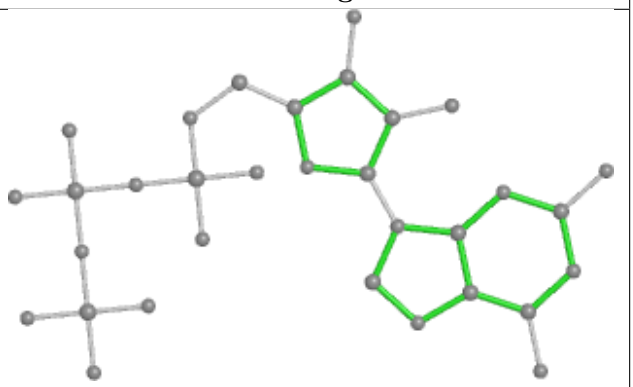
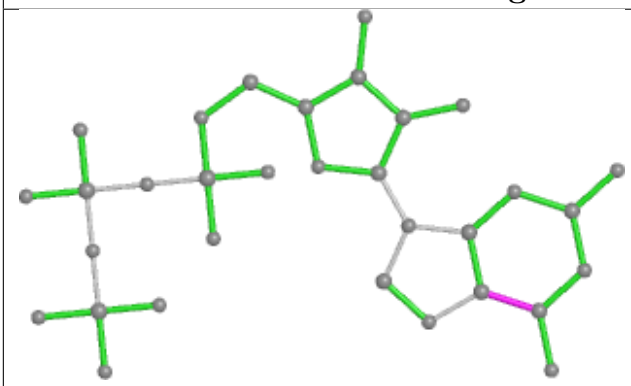
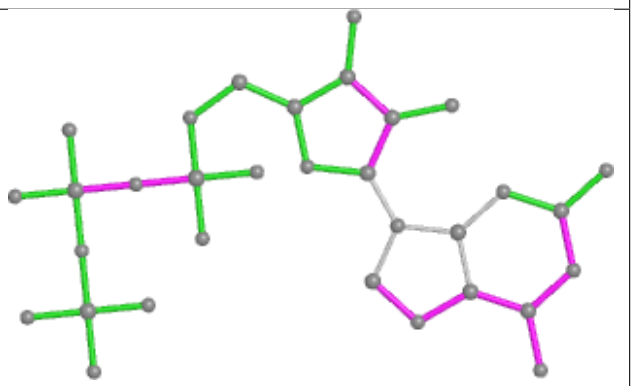


Rings

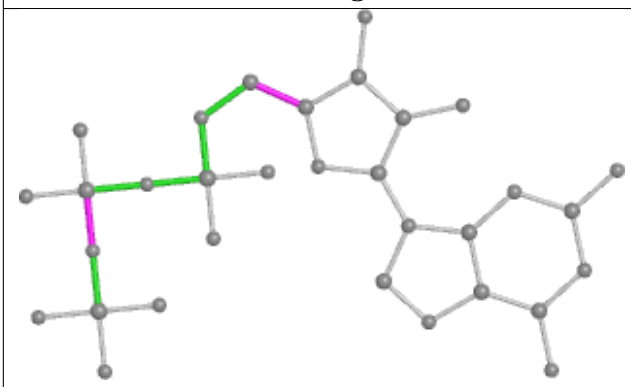
Ligand GTP VG 501



Bond lengths



Bond angles



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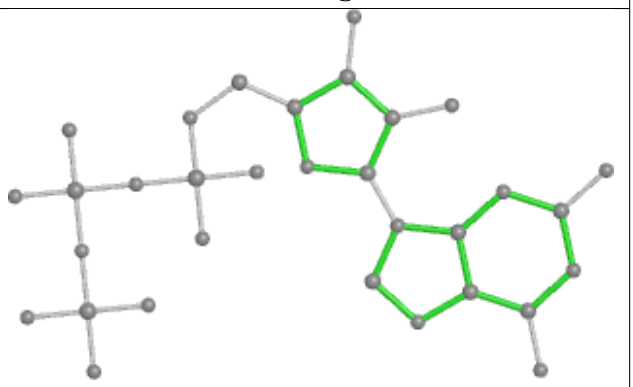
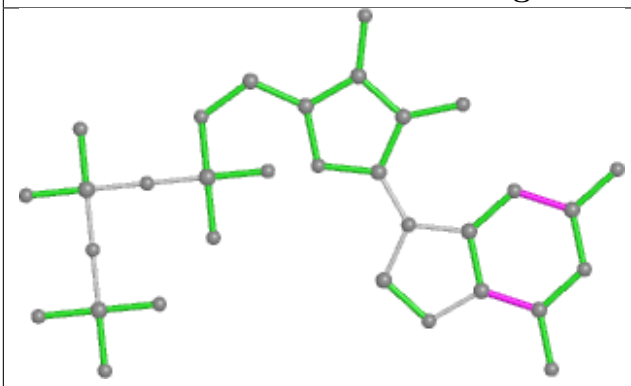


Rings

Ligand GTP RJ 501



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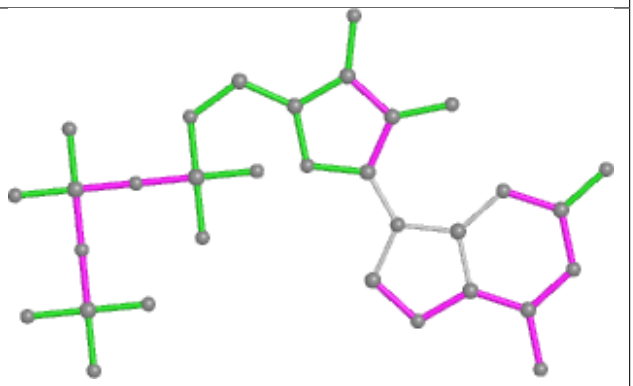
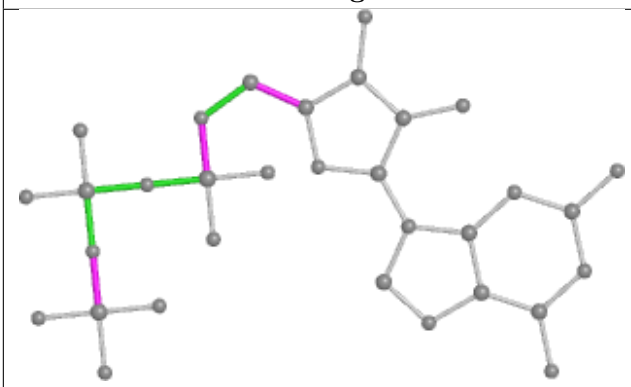


Bond angles



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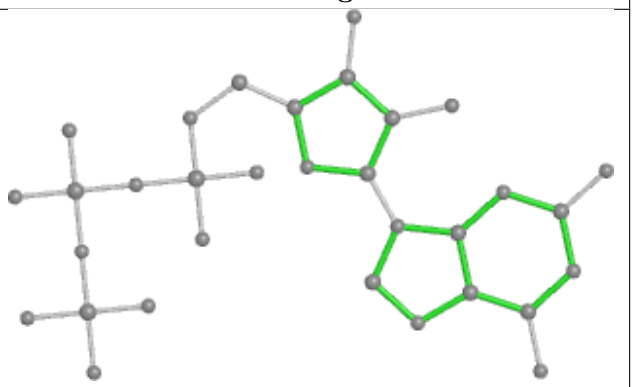
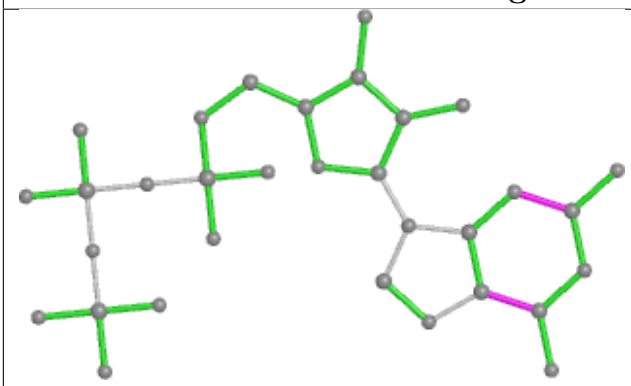
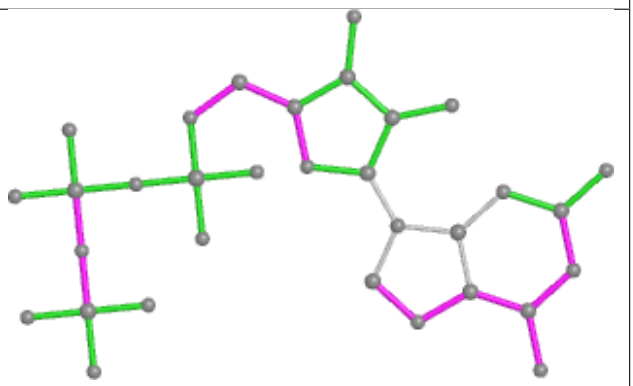


Rings

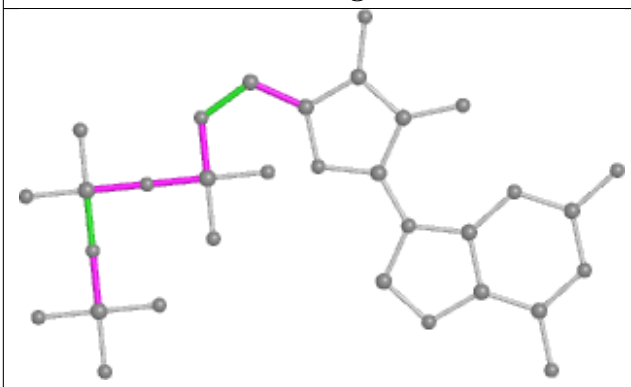
Ligand GTP BH 501



Bond lengths



Bond angles



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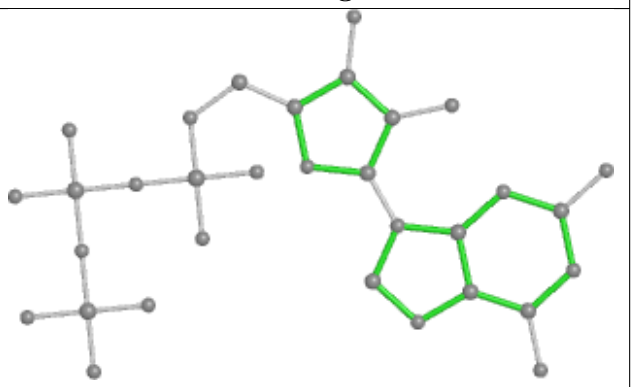
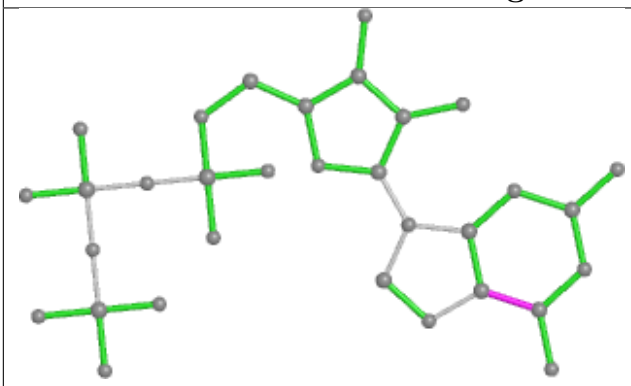
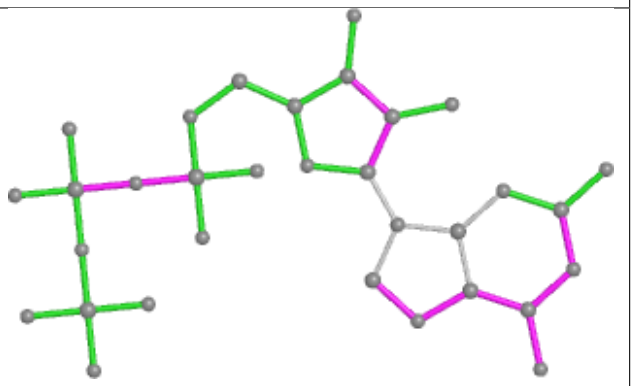


Rings

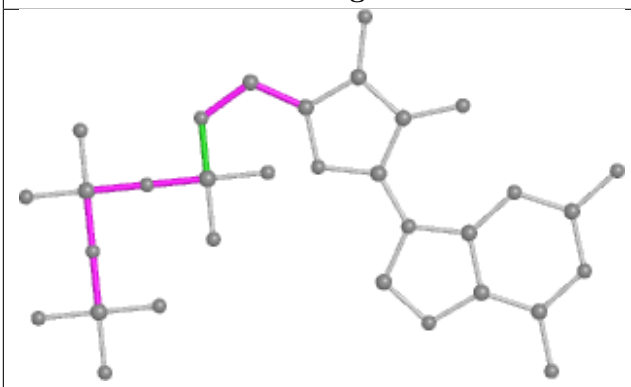
Ligand GTP ME 501



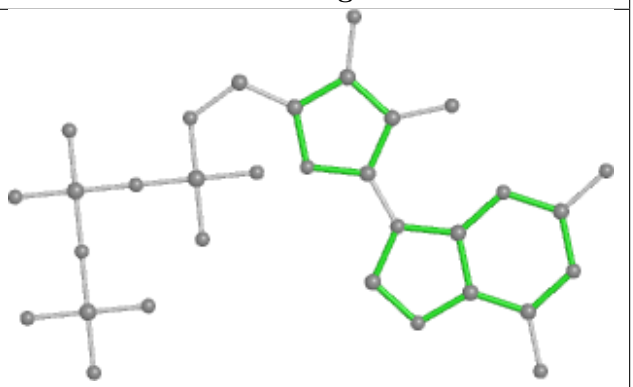
Bond lengths



Bond angles

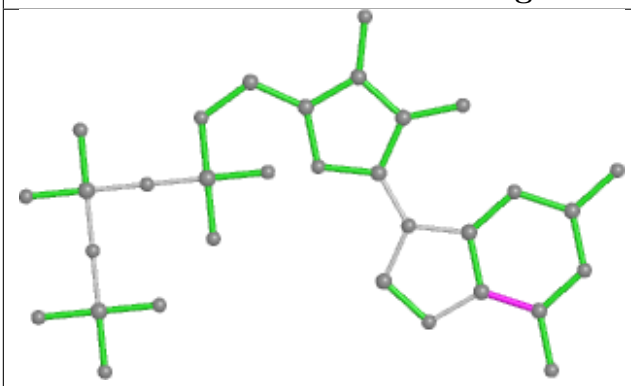


Torsions

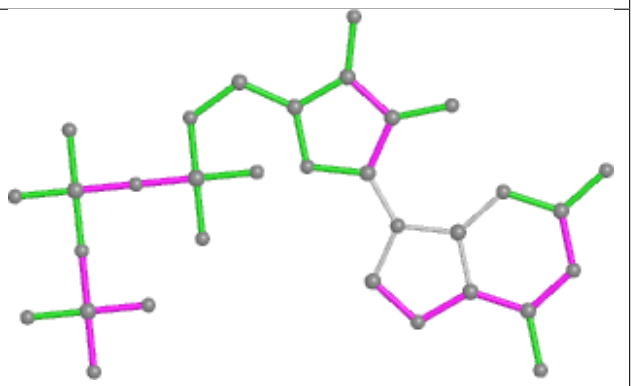


Rings

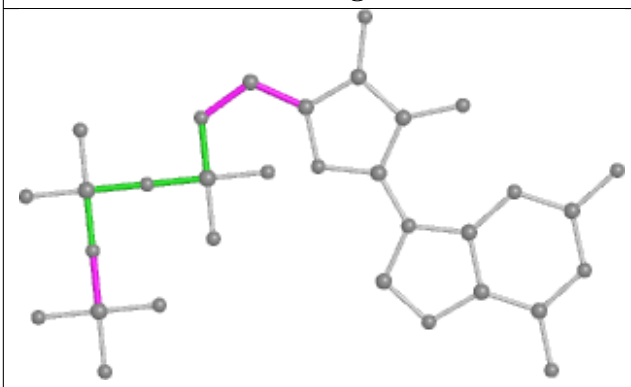
Ligand GTP NI 501



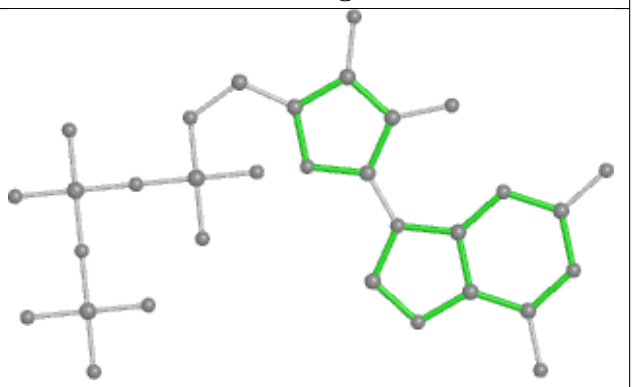
Bond lengths



Bond angles

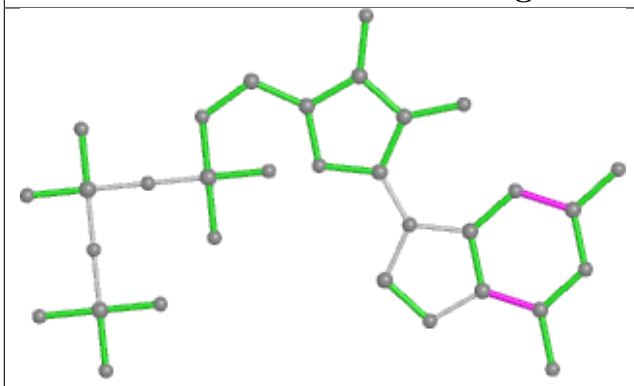


Torsions

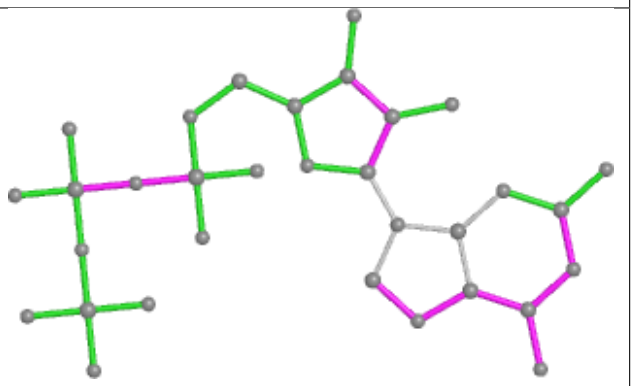


Rings

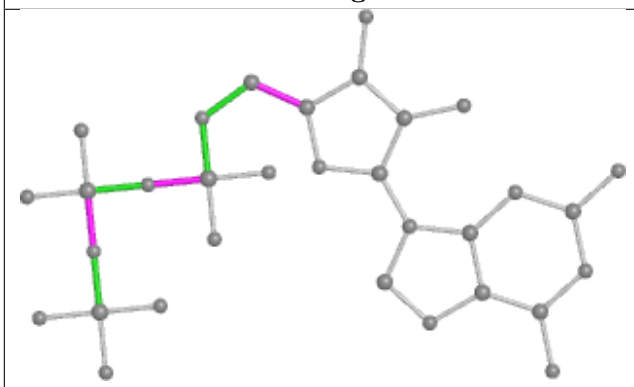
Ligand GTP SE 501



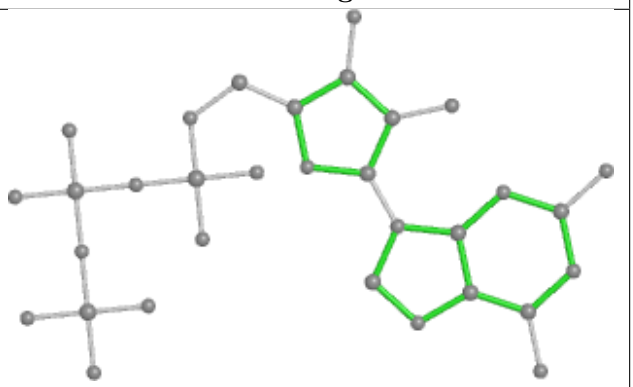
Bond lengths



Bond angles

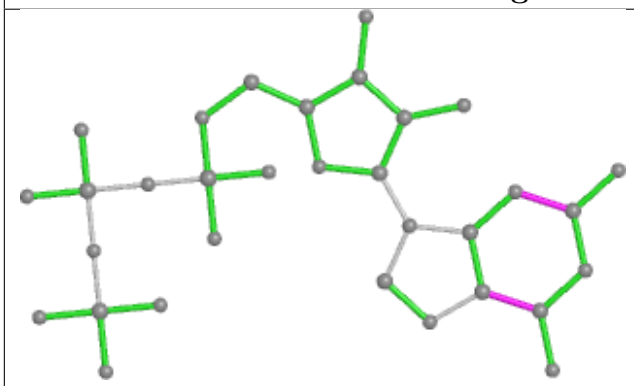


Torsions



Rings

Ligand GTP EH 501



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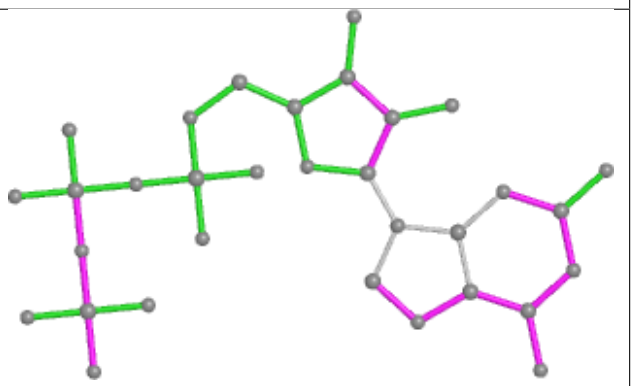
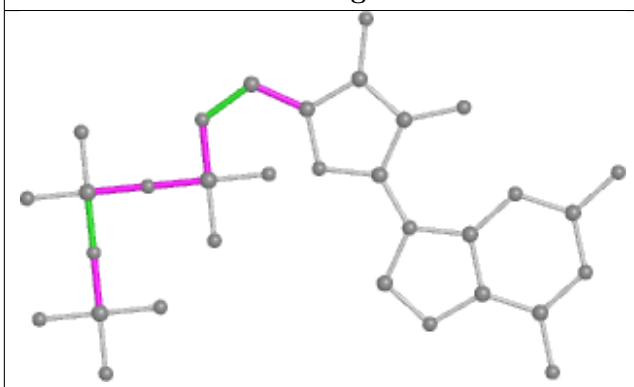


Bond angles



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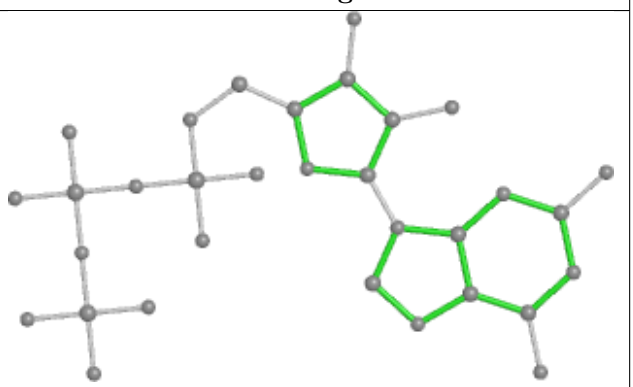
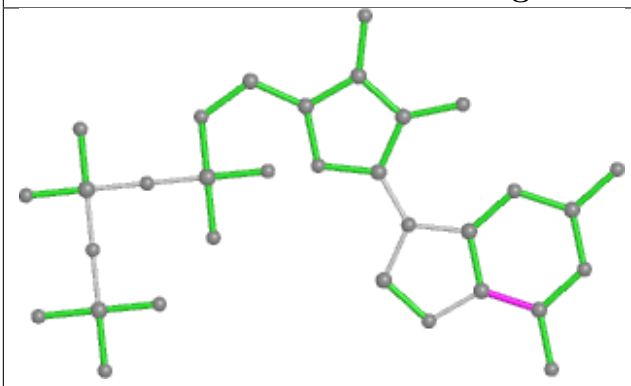


Rings

Ligand GTP MI 501



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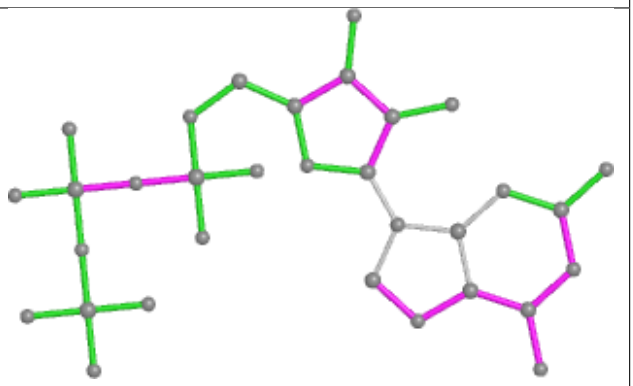
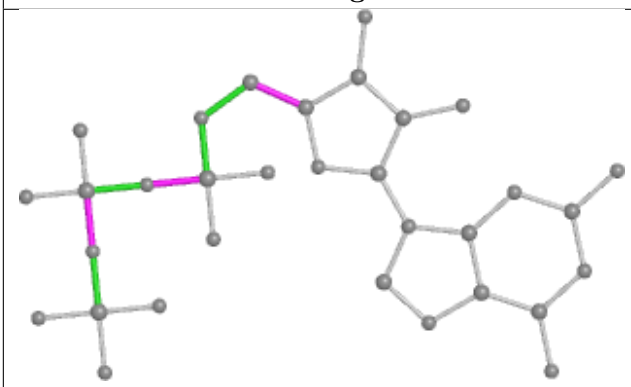
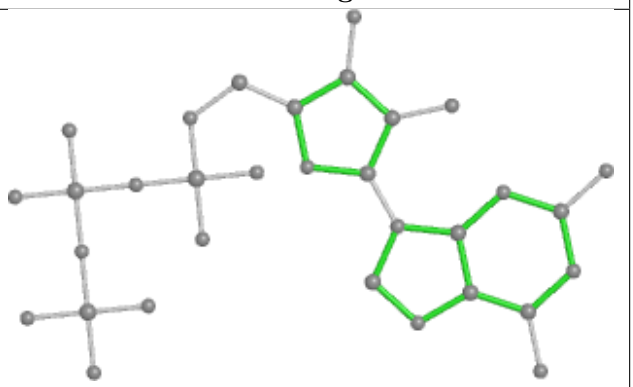


Bond angles

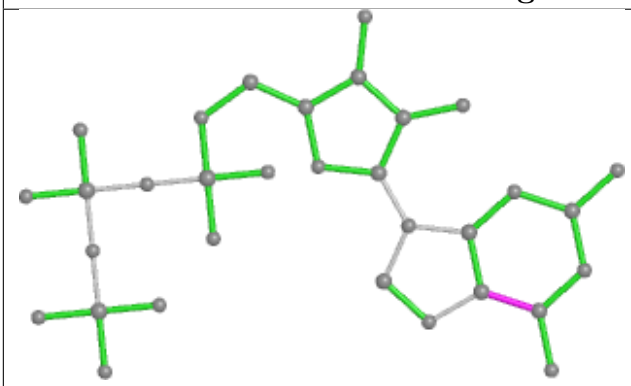


Torsions



Rings

Ligand GTP IE 501



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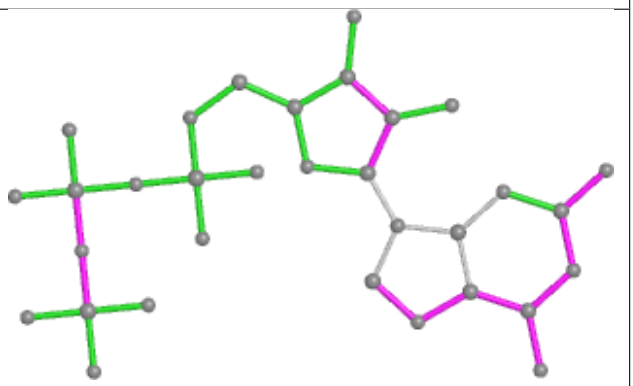
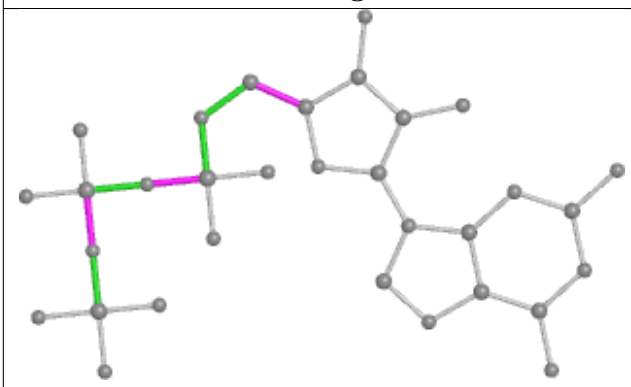


Bond angles



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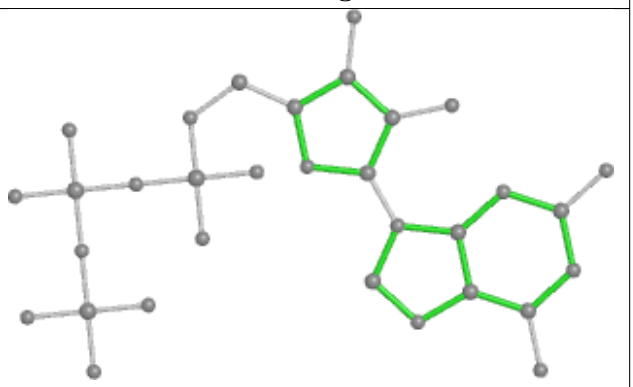
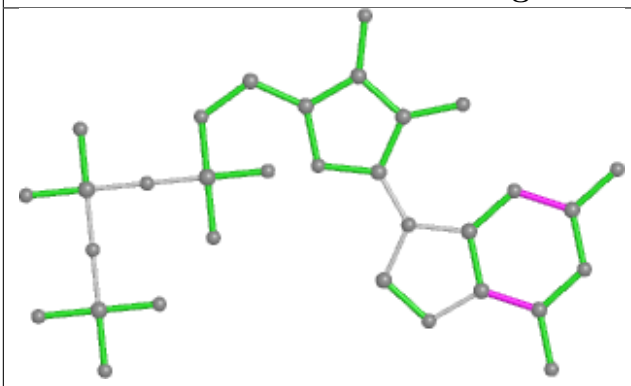


Rings

Ligand GTP TF 501



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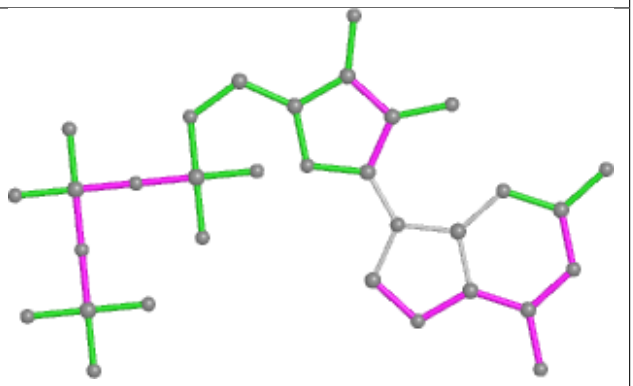
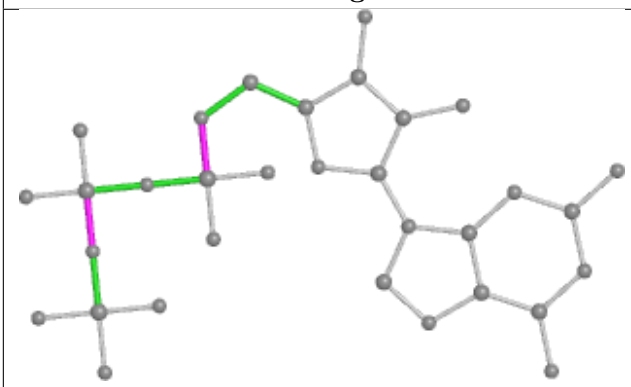
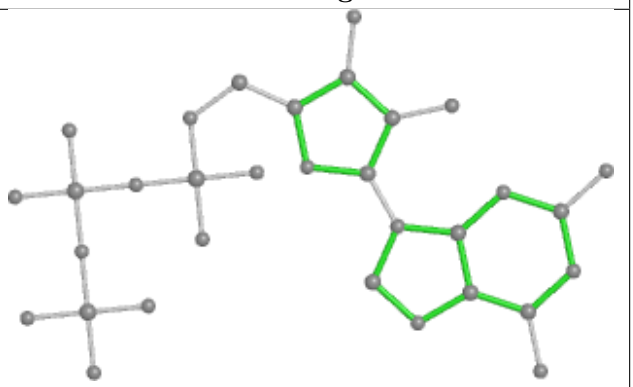


Bond angles

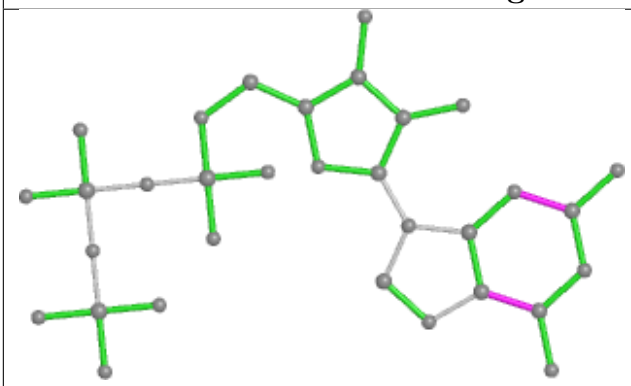


Torsions



Rings

Ligand GTP MF 501



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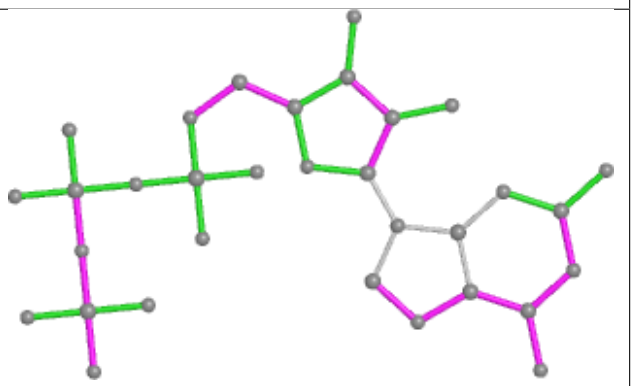

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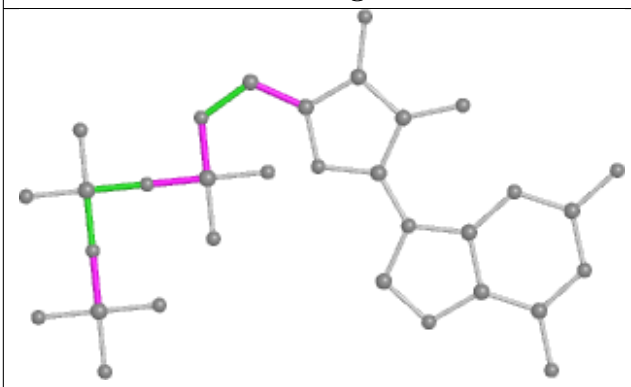

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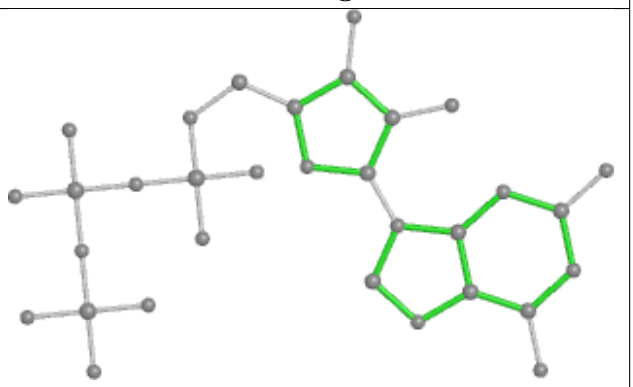
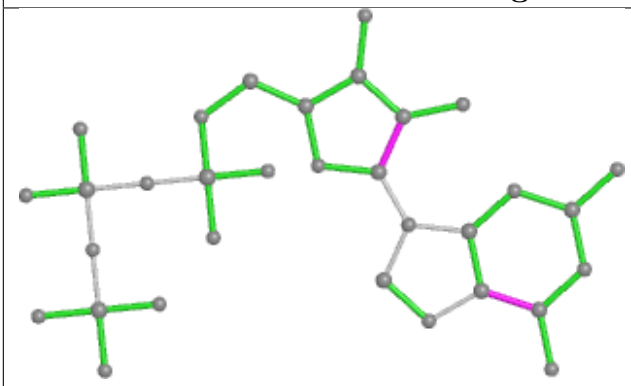


Rings

Ligand GTP BE 501



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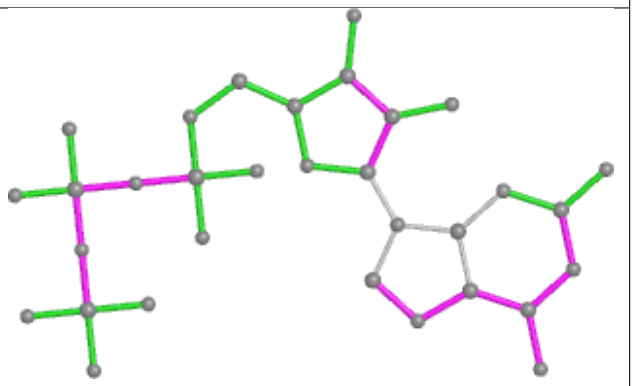
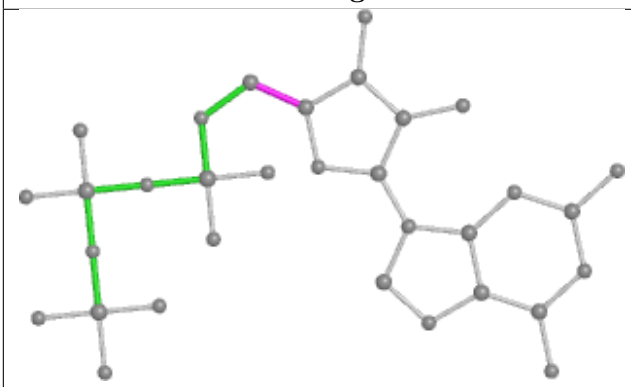


Bond angles



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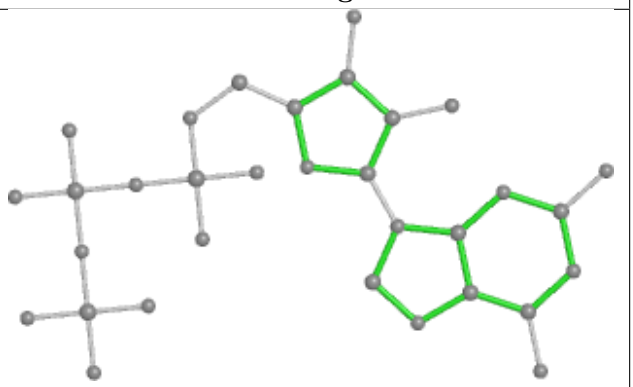
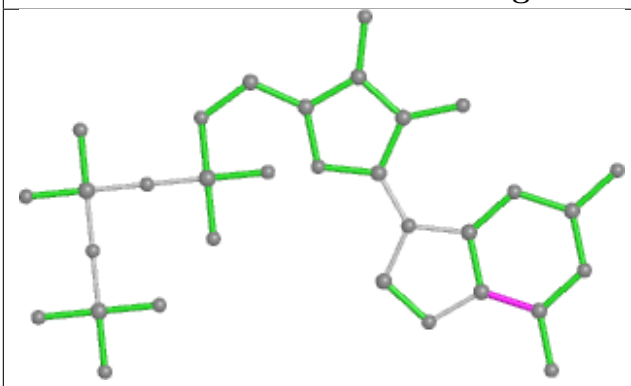
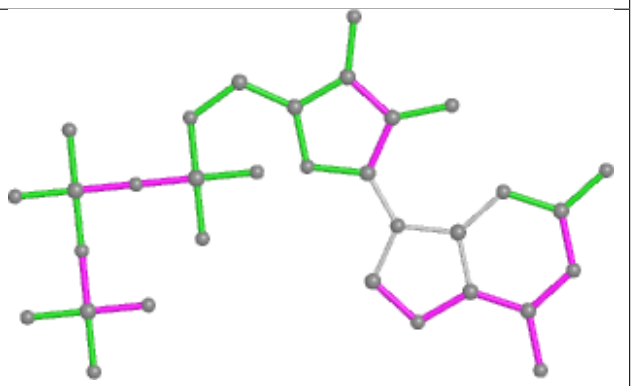


Rings

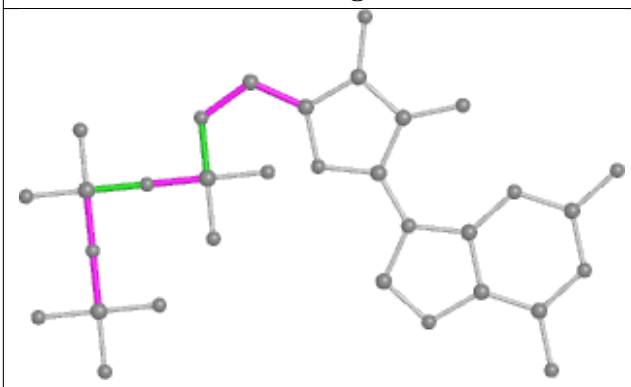
Ligand GTP JG 501



Bond lengths



Bond angles



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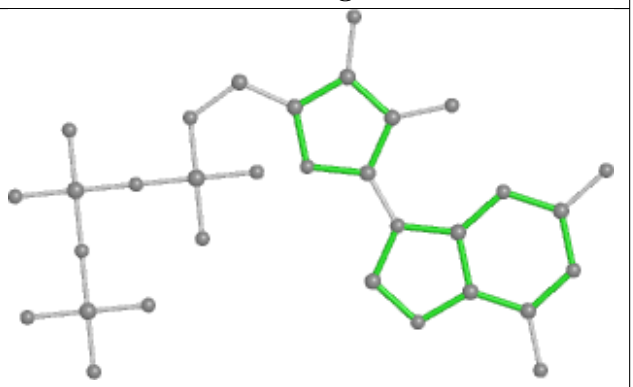
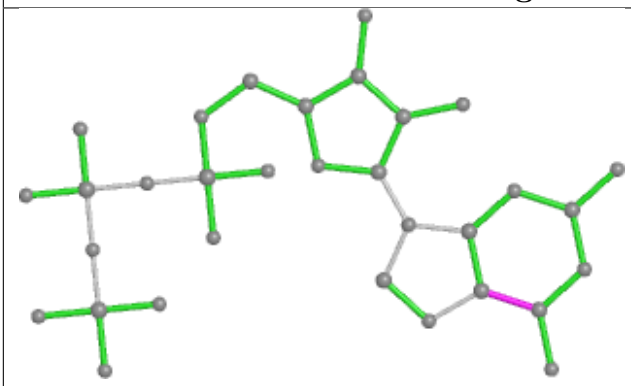


Rings

Ligand GTP AI 501



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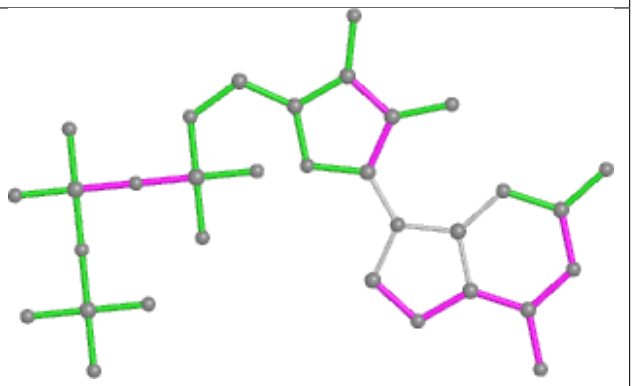
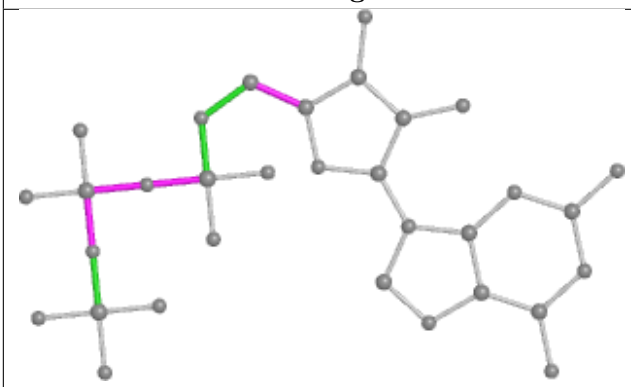


Bond angles



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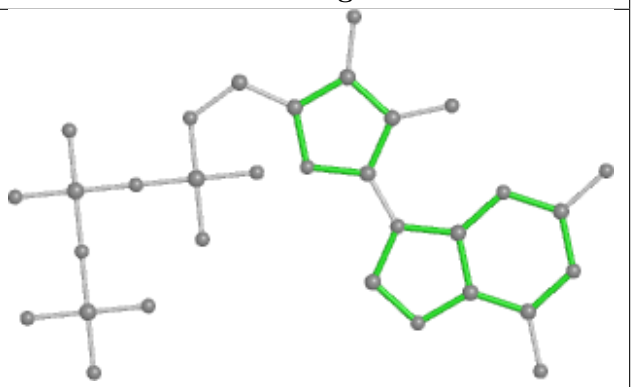
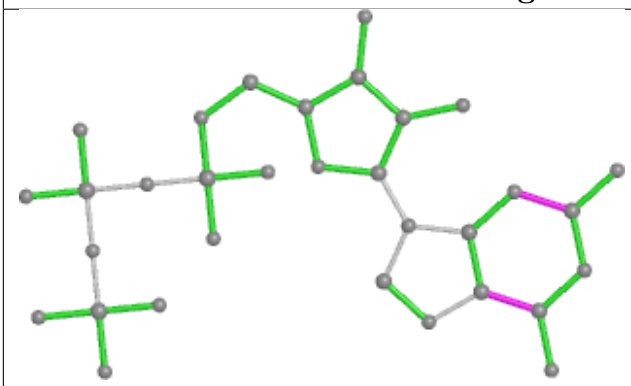
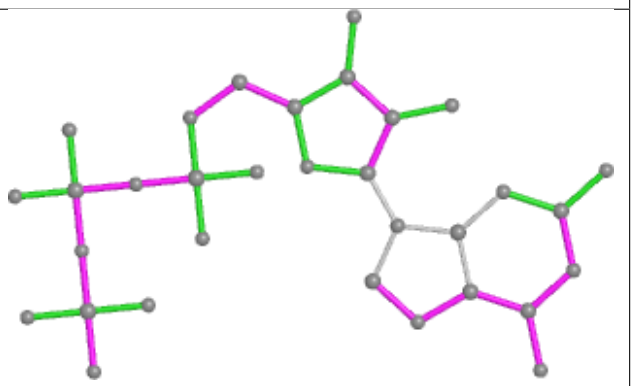


Rings

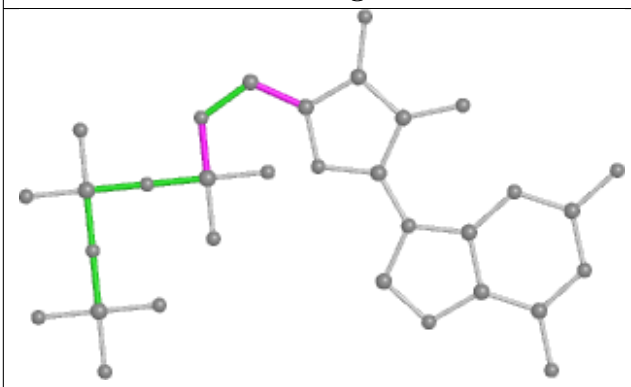
Ligand GTP IF 501



Bond lengths



Bond angles



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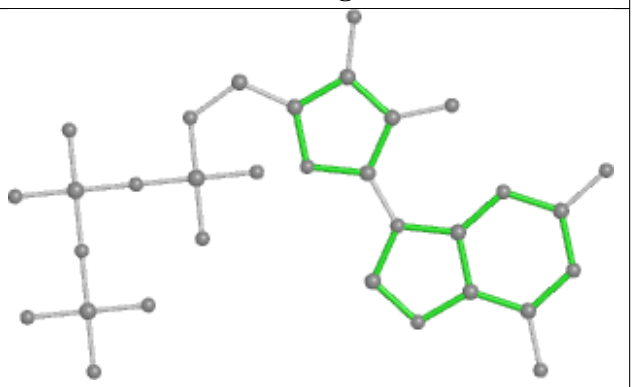
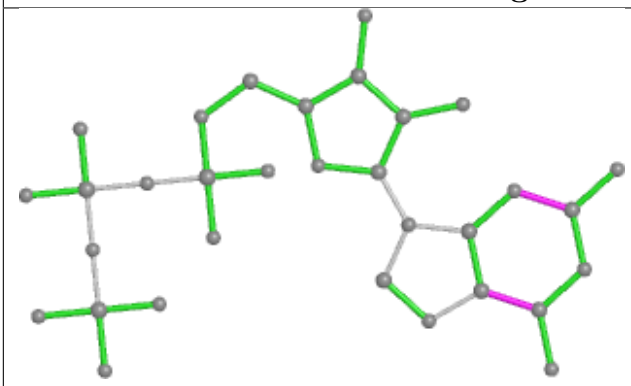
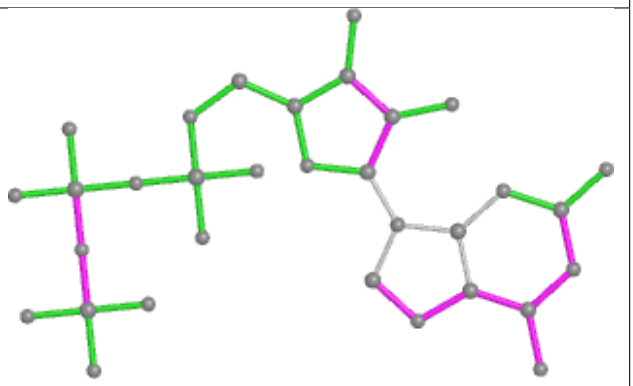


Rings

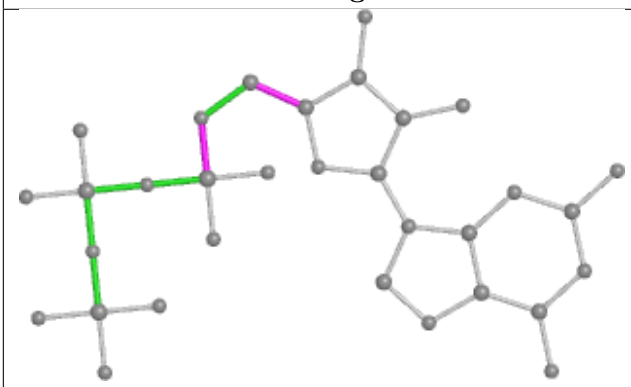
Ligand GTP UF 501



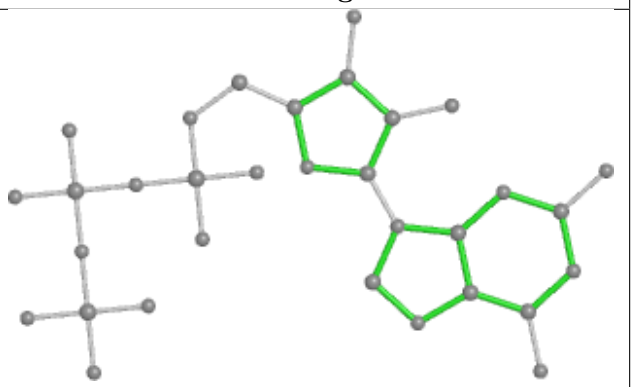
Bond lengths



Bond angles

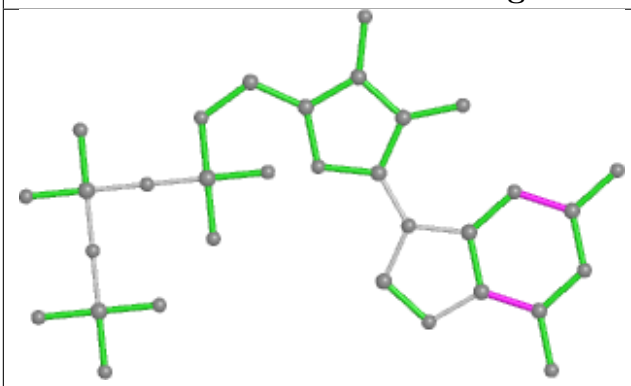


Torsions



Rings

Ligand GTP GH 502



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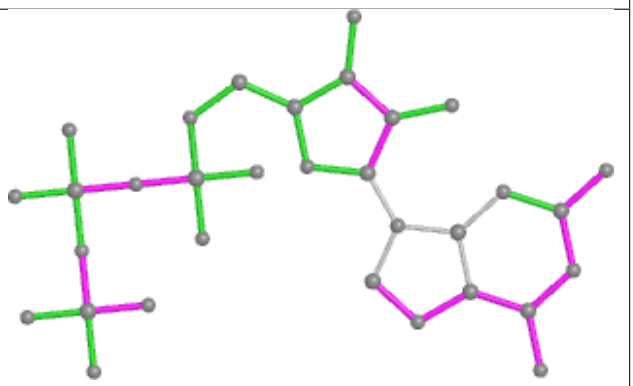
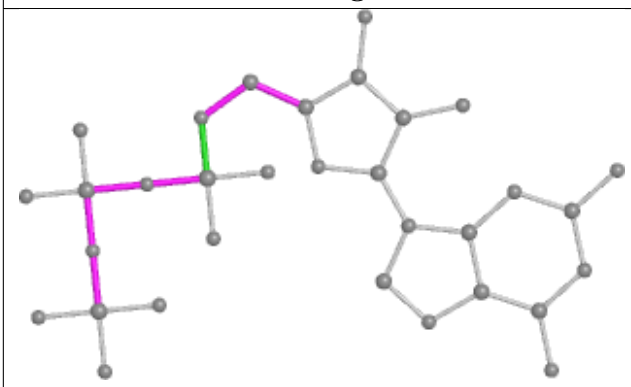


Bond angles



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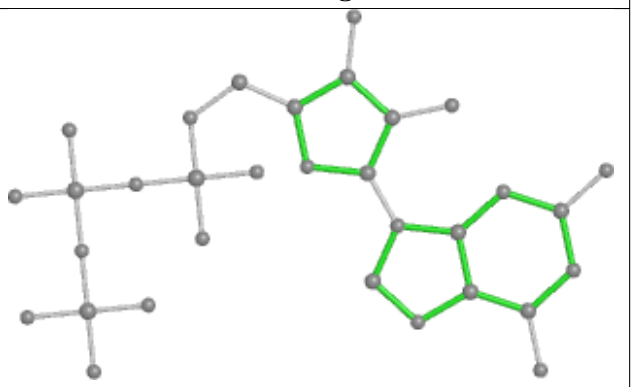
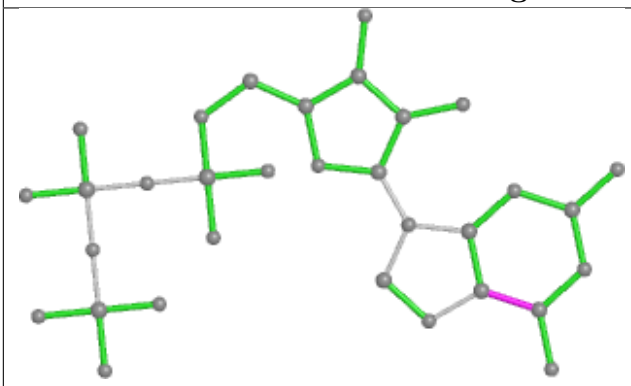


Rings

Ligand GTP KE 501



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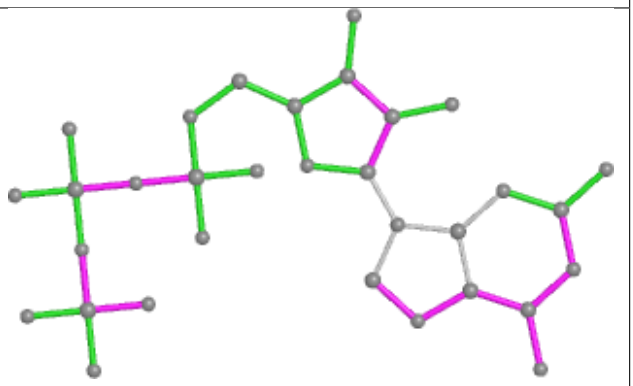
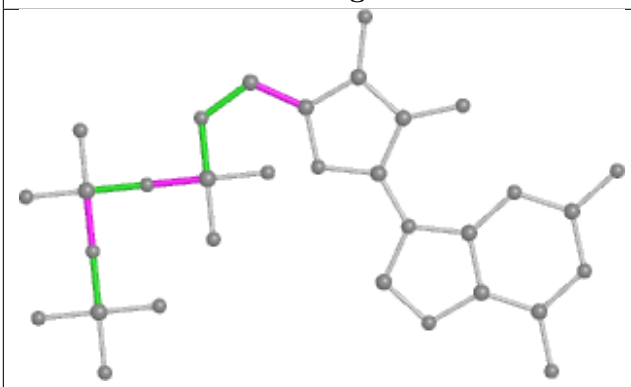


Bond angles



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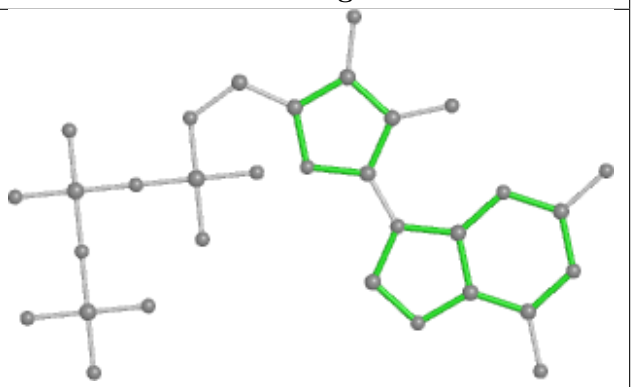
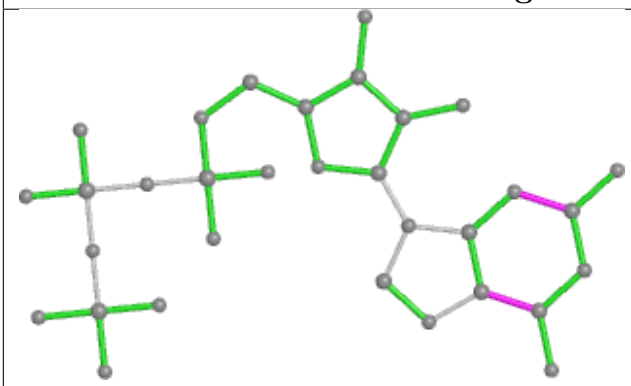
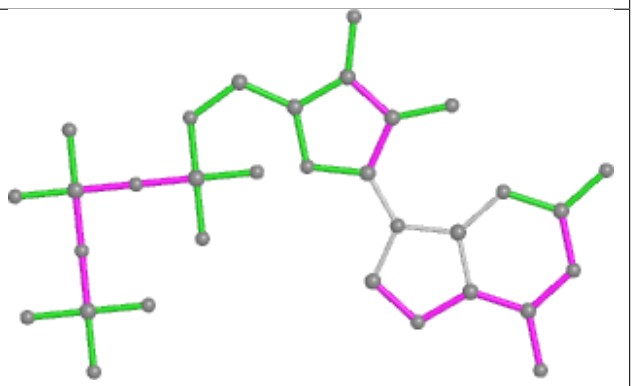


Rings

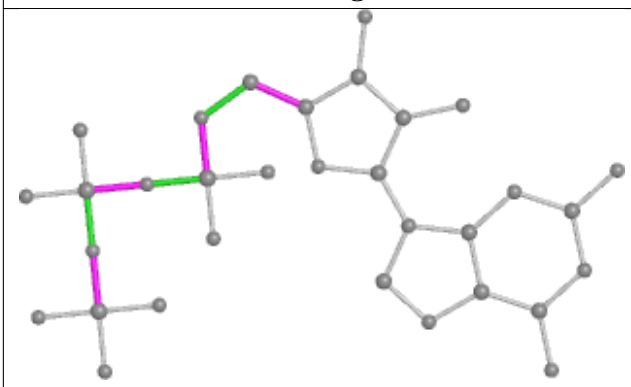
Ligand GTP JF 501



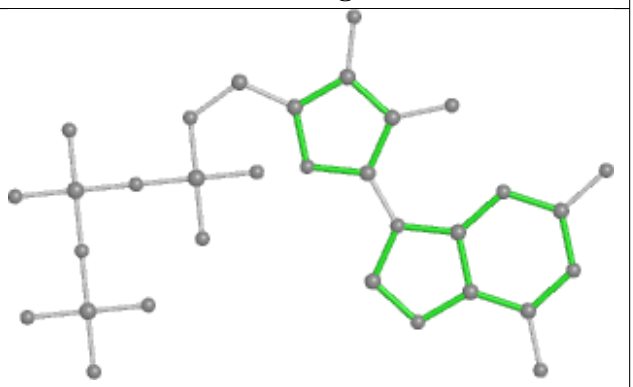
Bond lengths



Bond angles

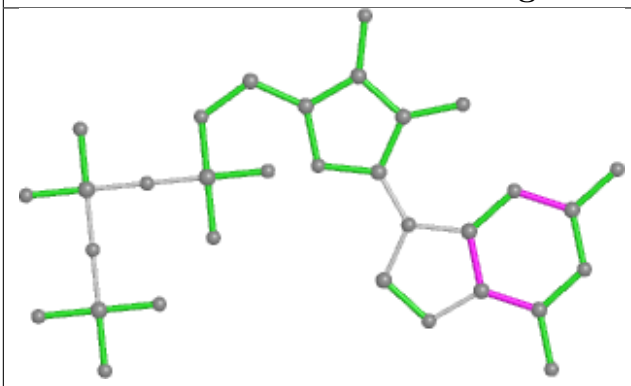


Torsions

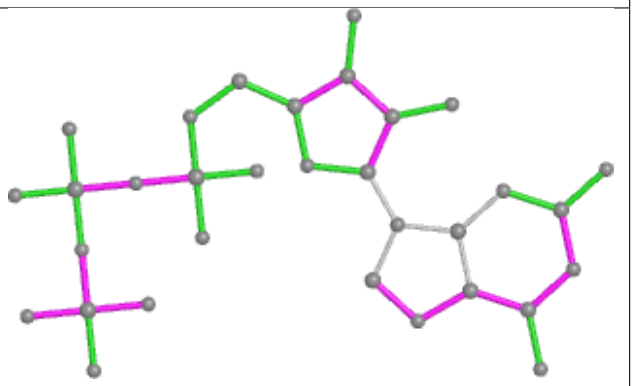


Rings

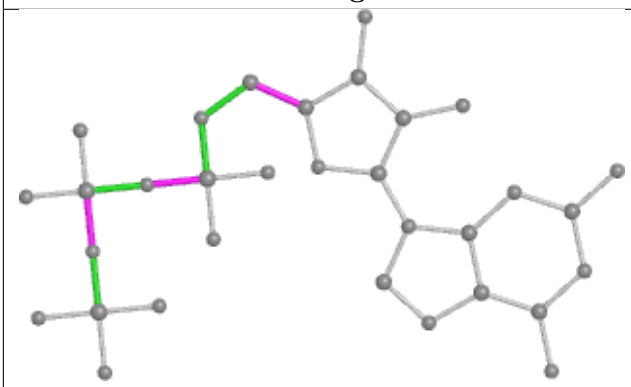
Ligand GTP LI 501



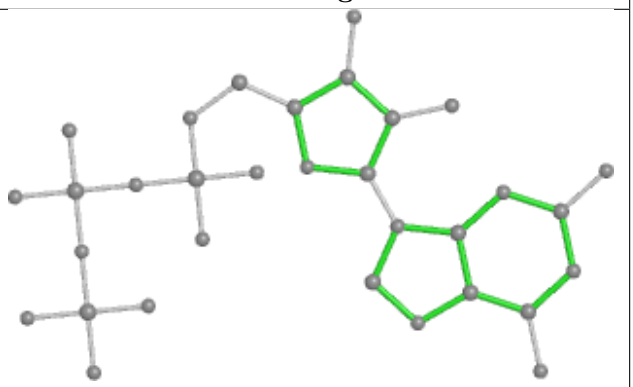
Bond lengths



Bond angles

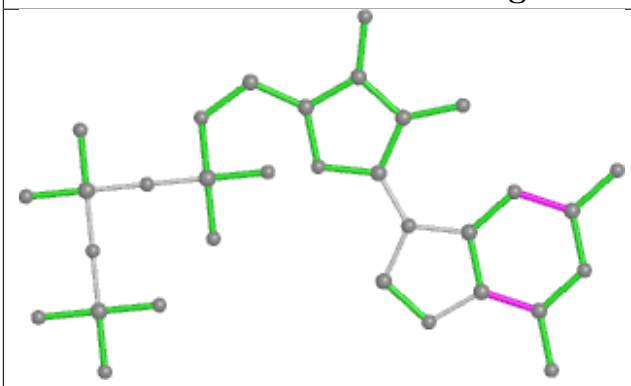


Torsions

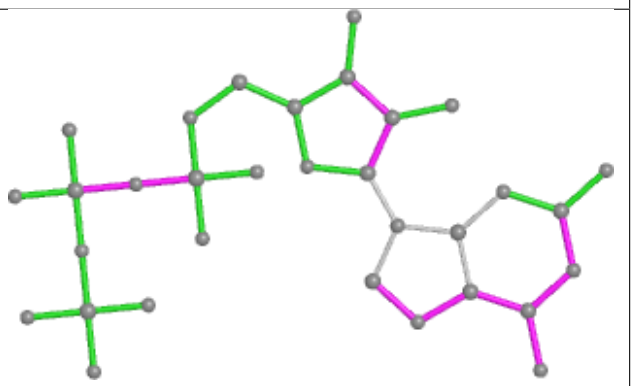


Rings

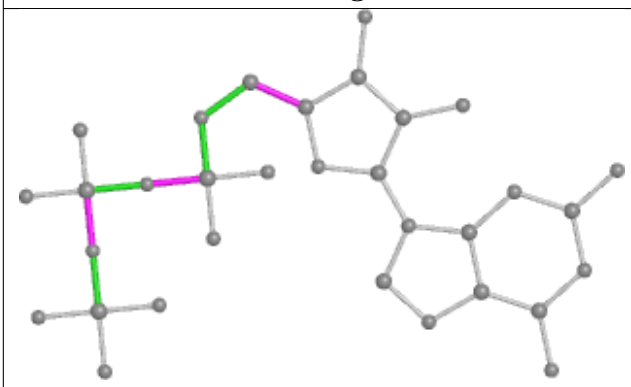
Ligand GTP RG 501



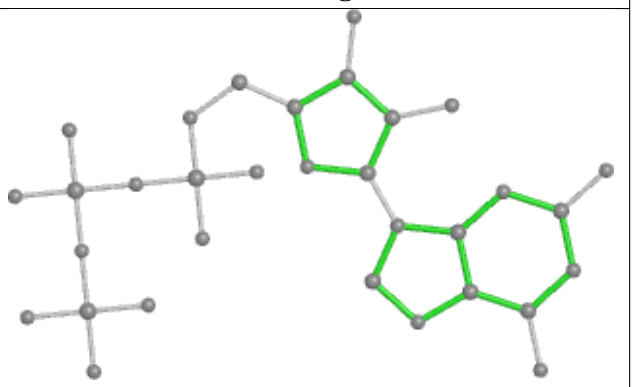
Bond lengths



Bond angles

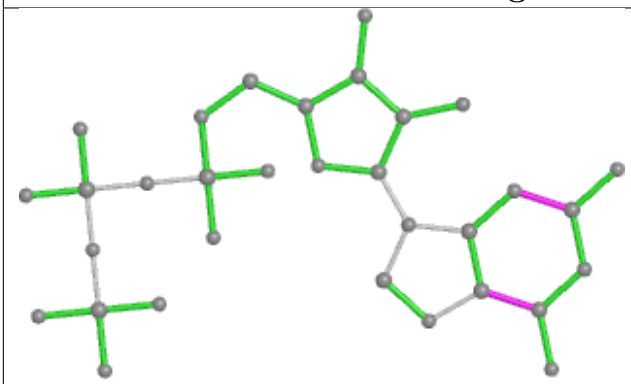


Torsions



Rings

Ligand GTP QH 501



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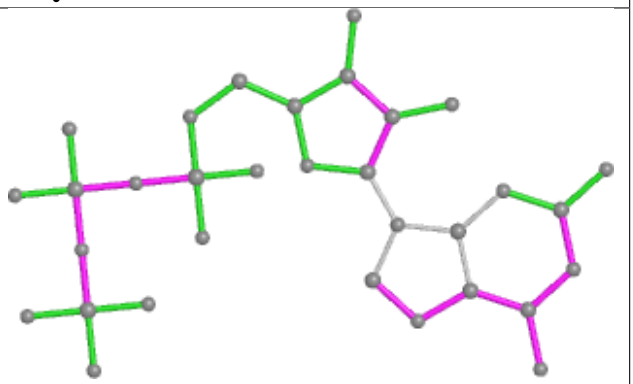

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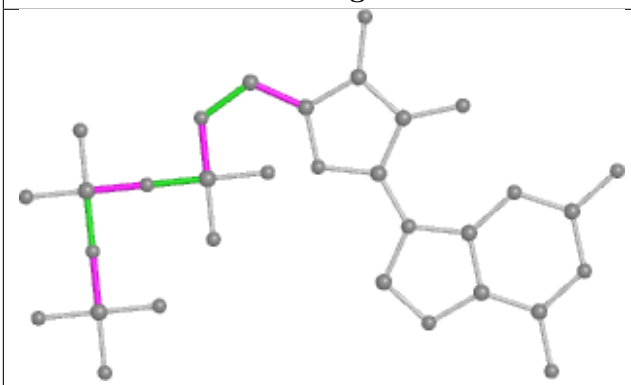

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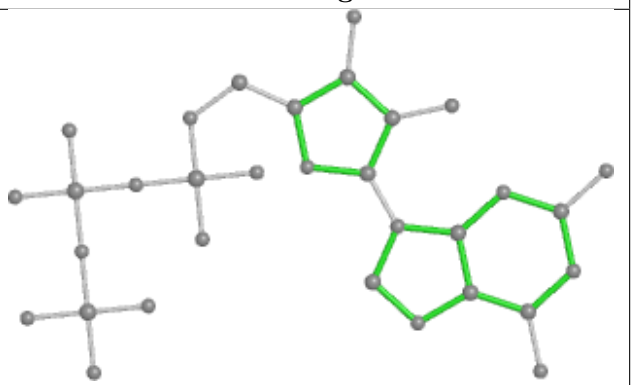
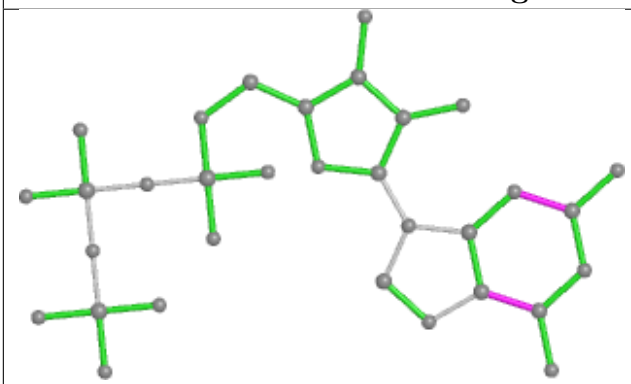


Rings

Ligand GTP OF 501



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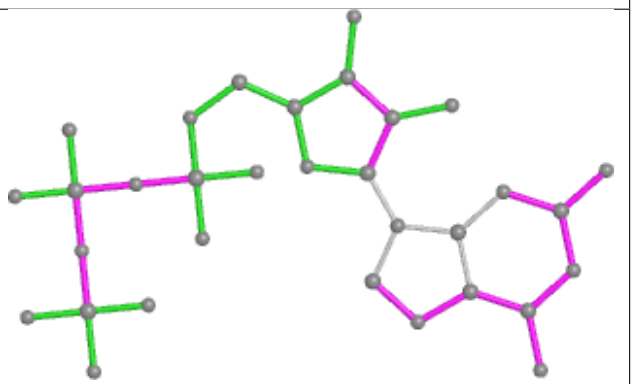
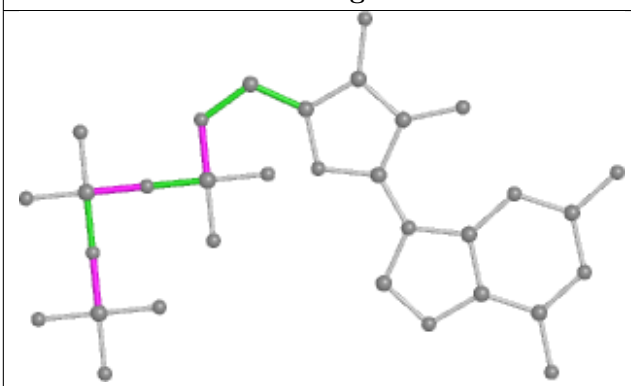


Bond angles



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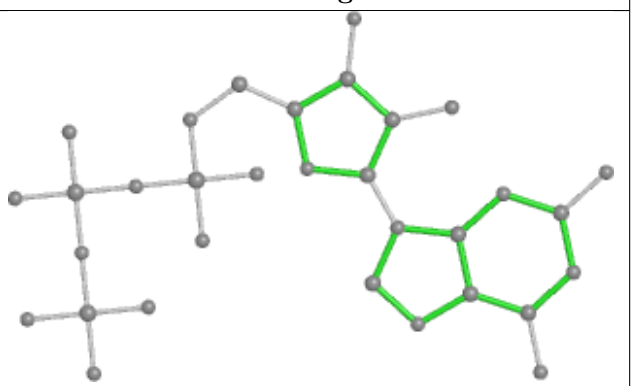
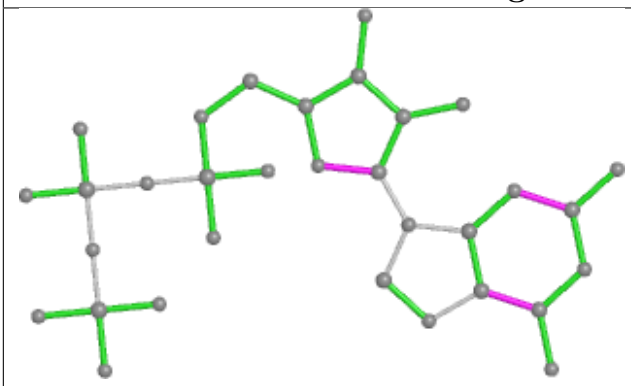
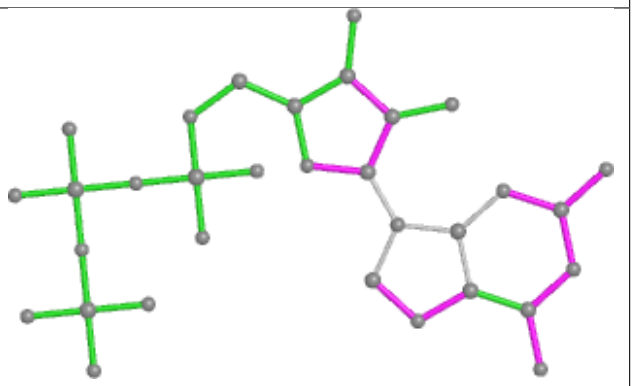


Rings

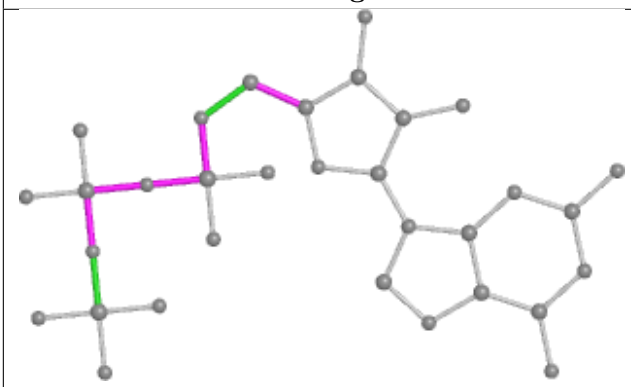
Ligand GTP KG 501



Bond lengths



Bond angles



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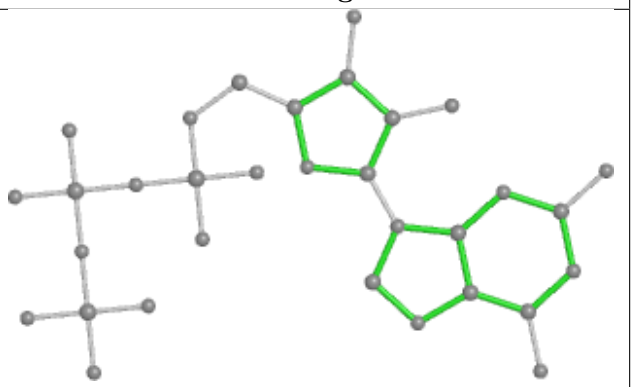
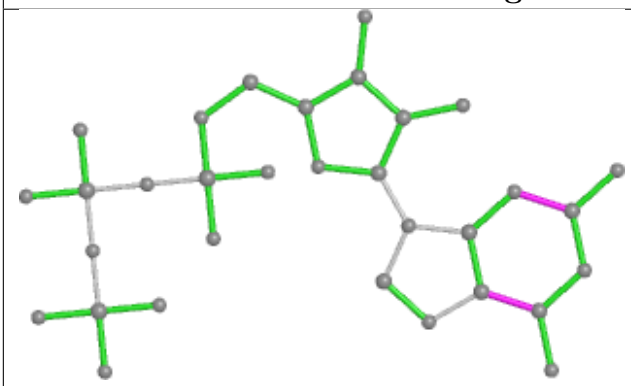


Rings

Ligand GTP MH 501



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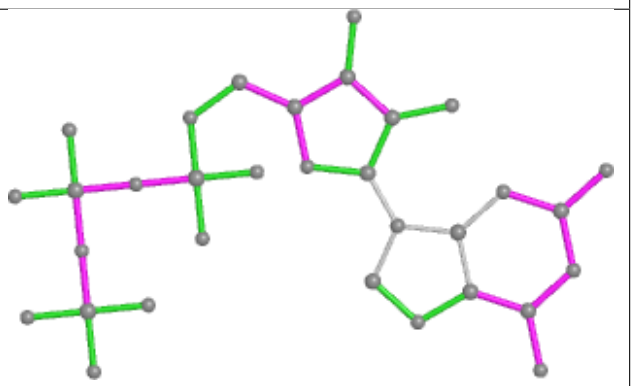
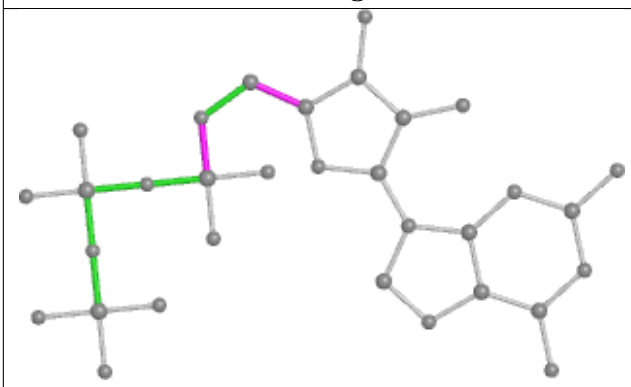


Bond angles



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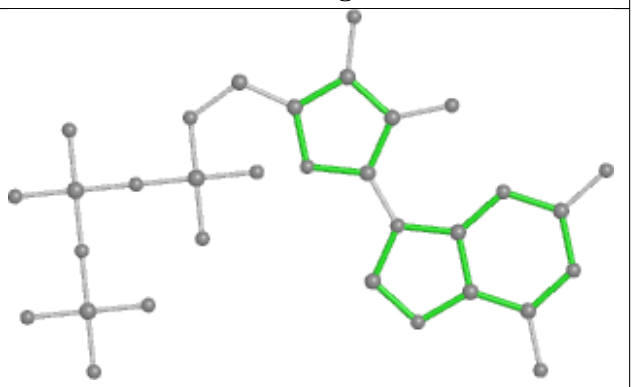
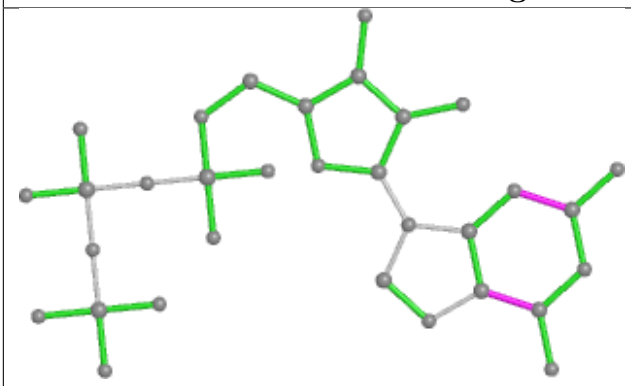
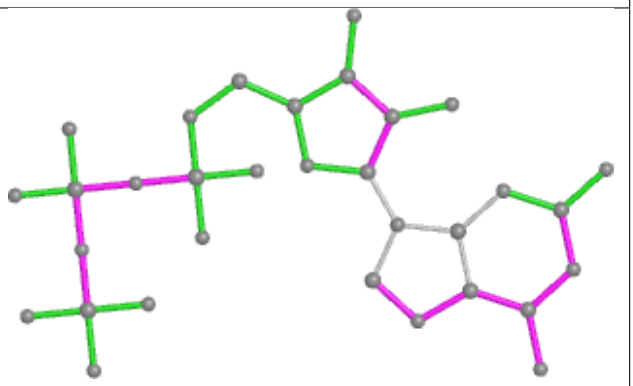


Rings

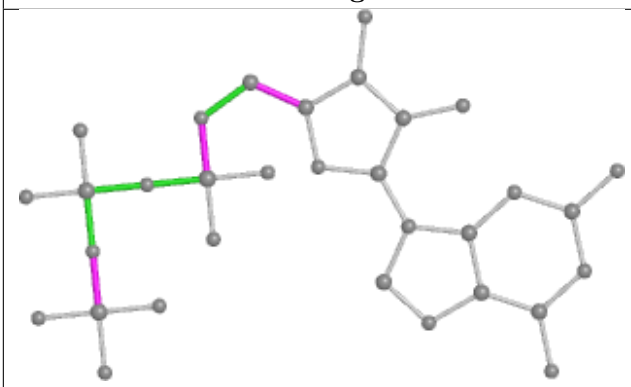
Ligand GTP TH 501



Bond lengths



Bond angles



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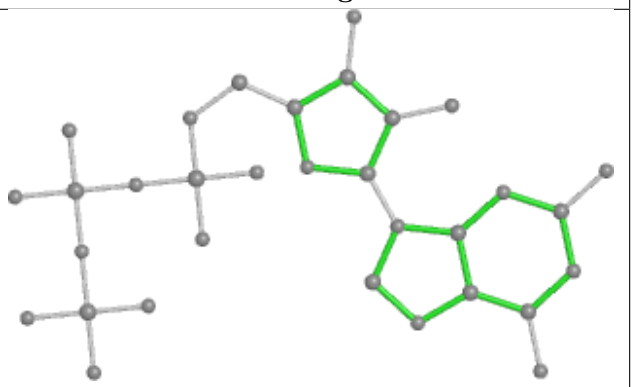
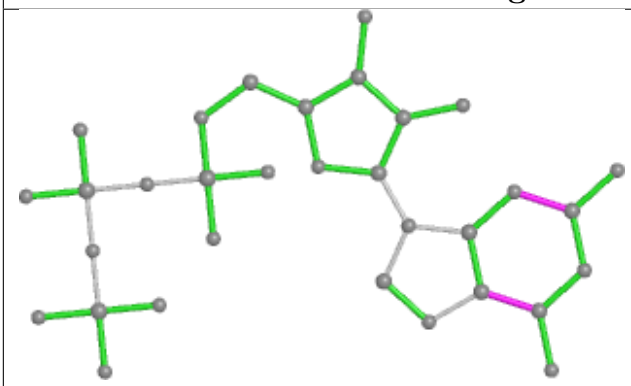


Rings

Ligand GTP VD 501



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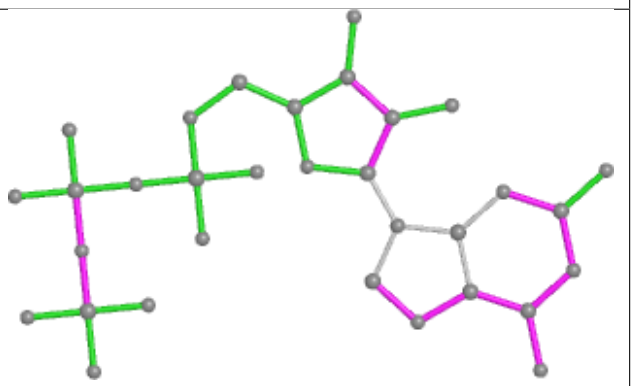
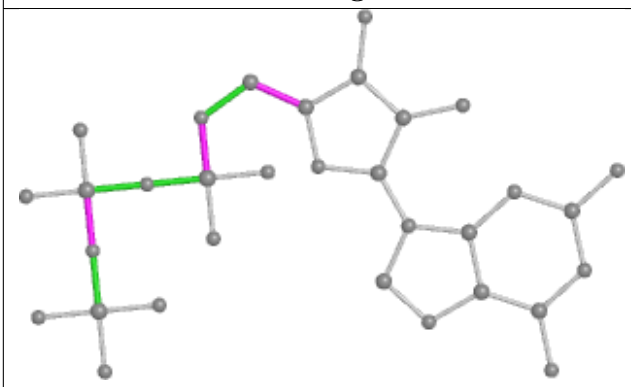


Bond angles



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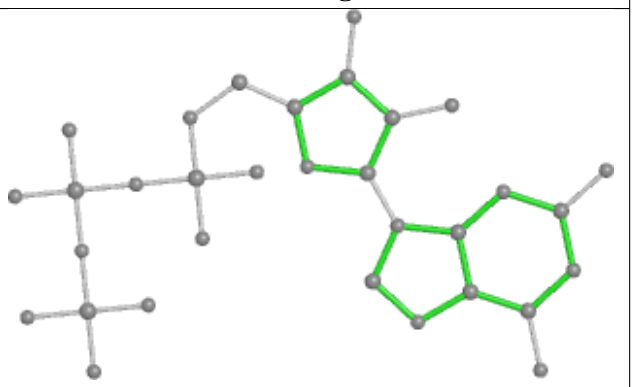
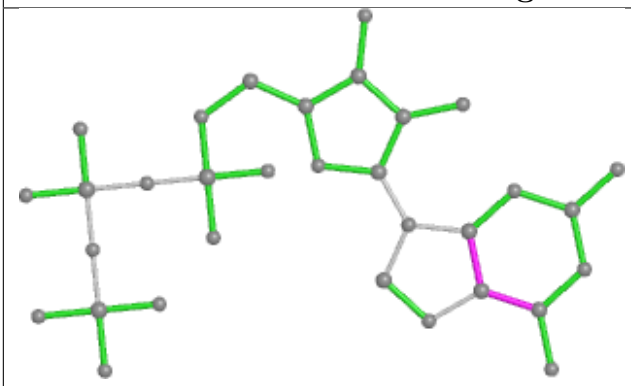
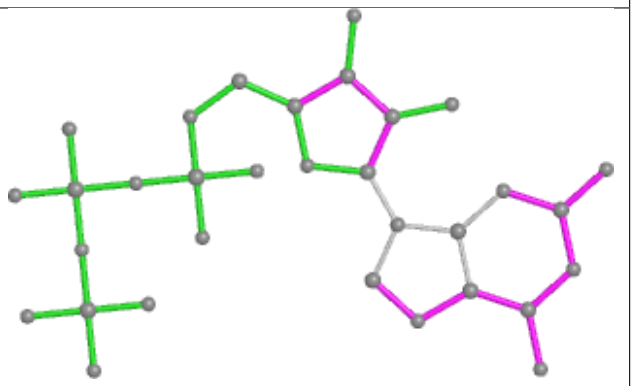


Rings

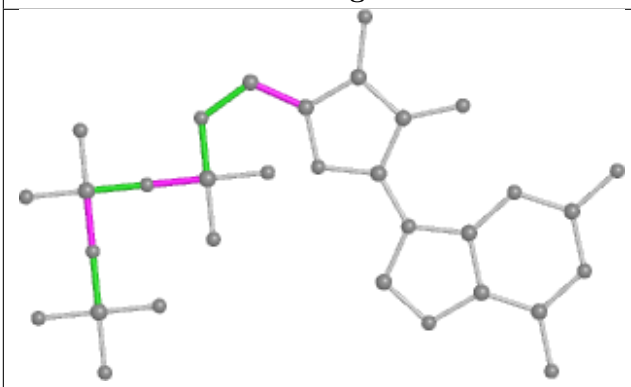
Ligand GTP PI 501



Bond lengths



Bond angles



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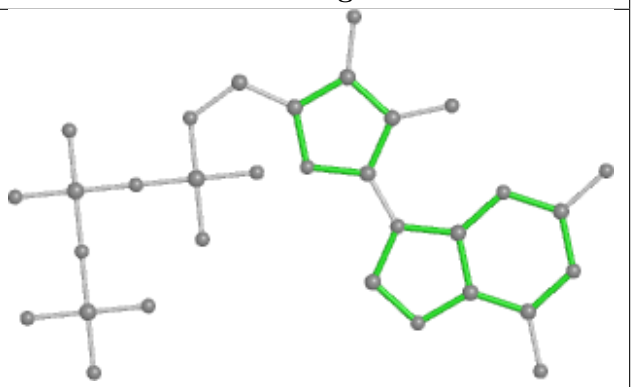
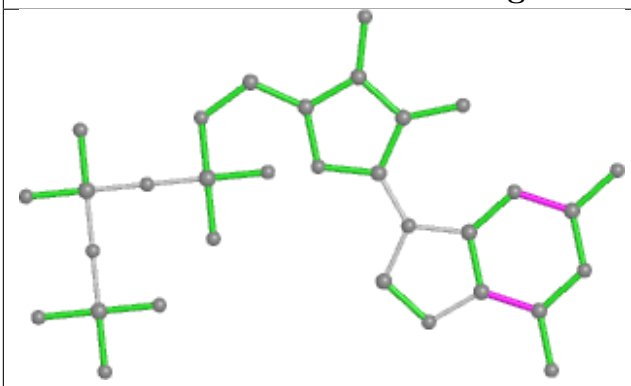


Rings

Ligand GTP HH 501



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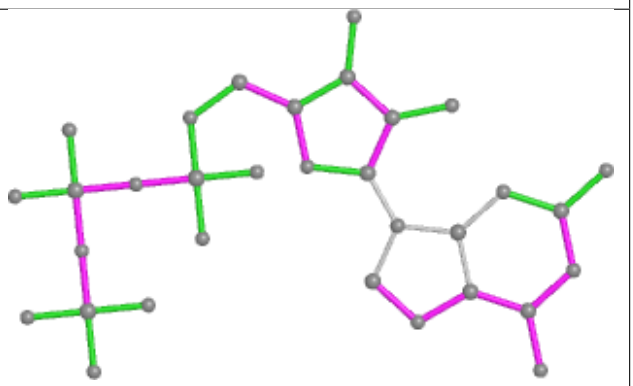
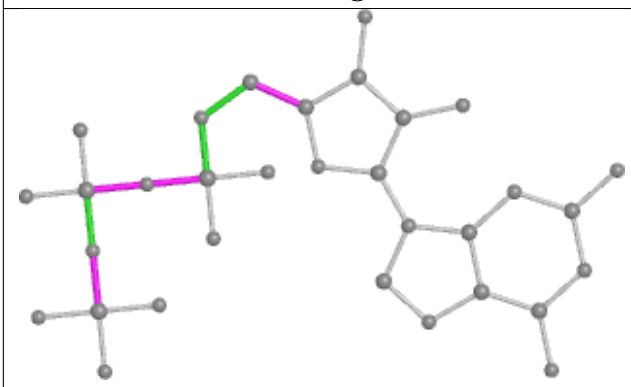
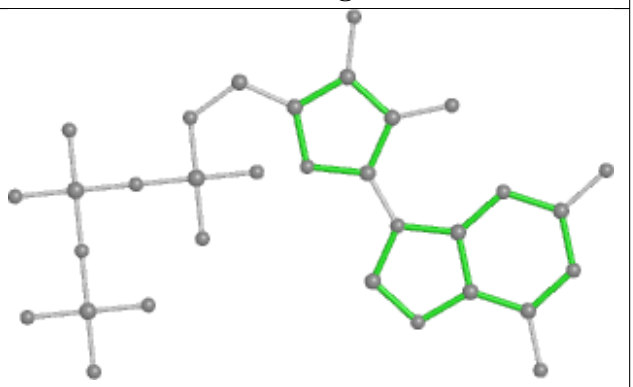


Bond angles

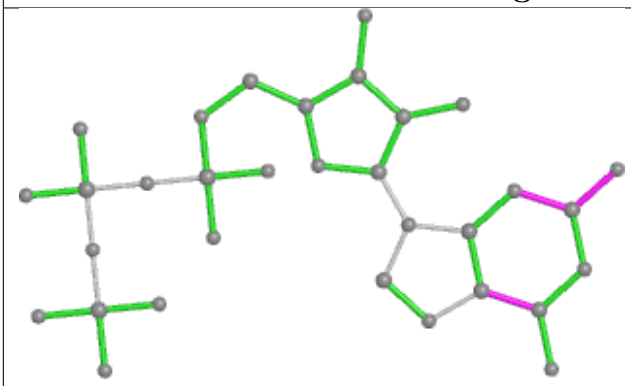


Torsions



Rings

Ligand GTP CJ 501



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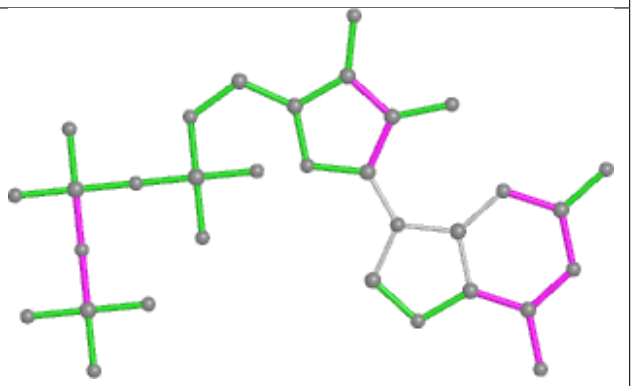
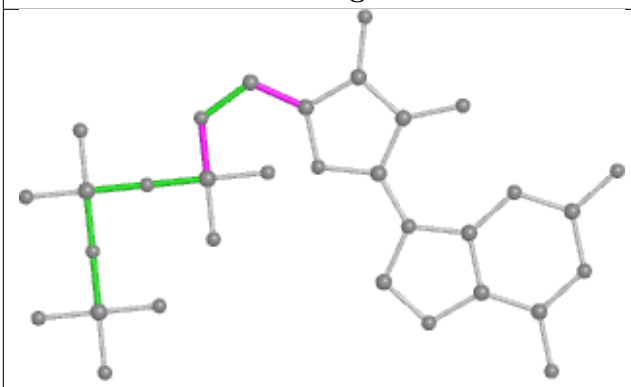


Bond angles



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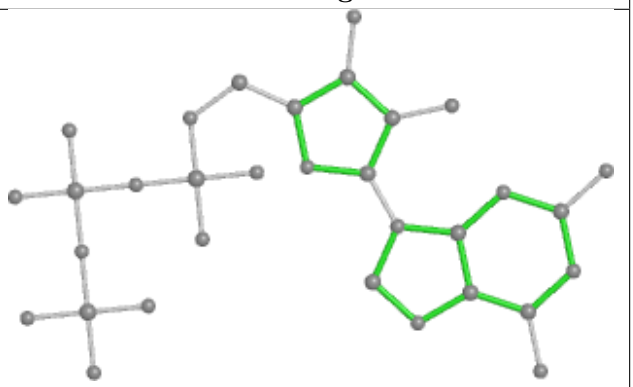
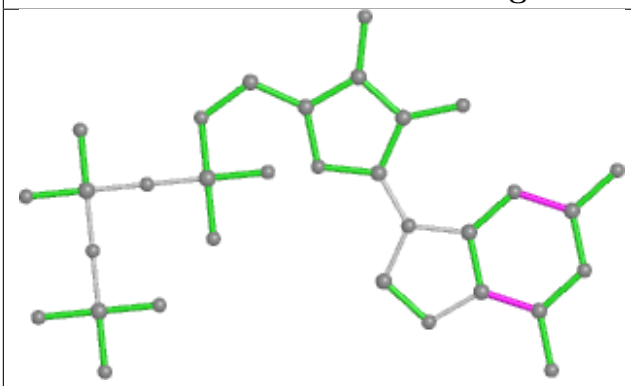
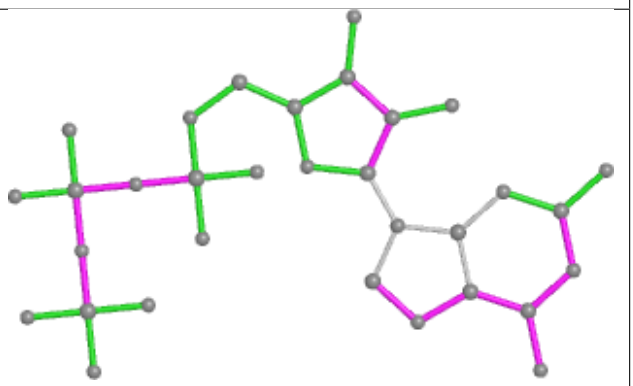


Rings

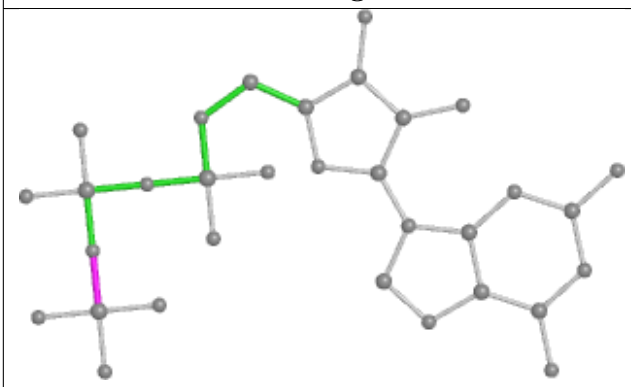
Ligand GTP PH 501



Bond lengths



Bond angles



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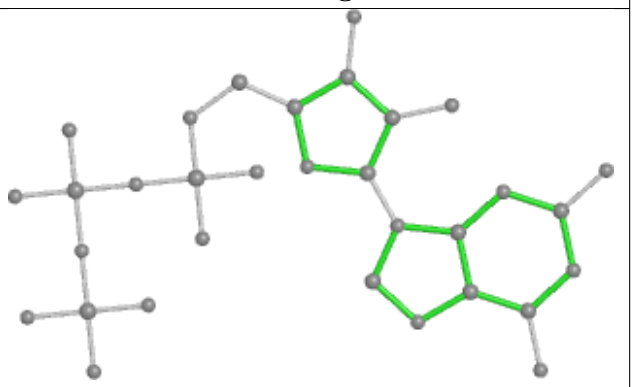
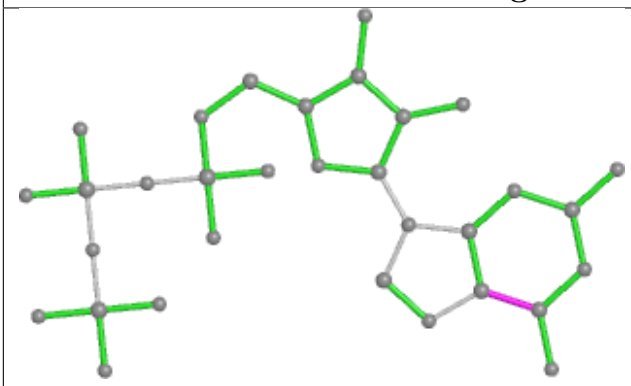


Rings

Ligand GTP WI 501



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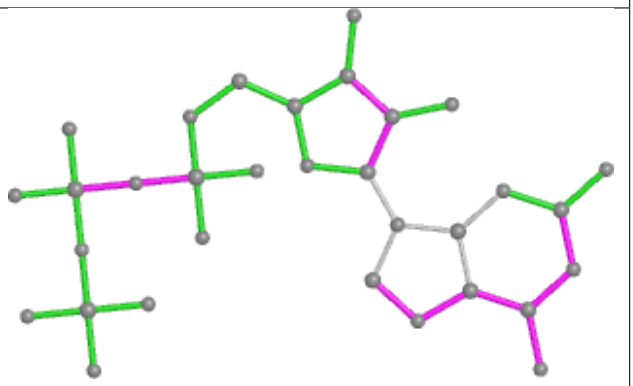
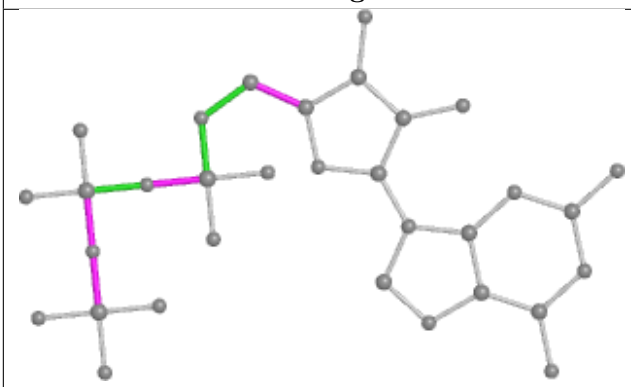


Bond angles



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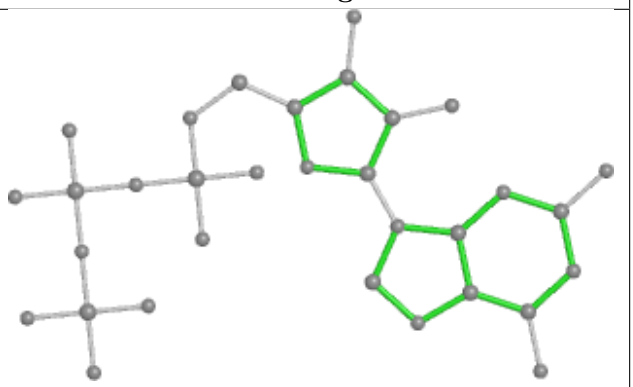
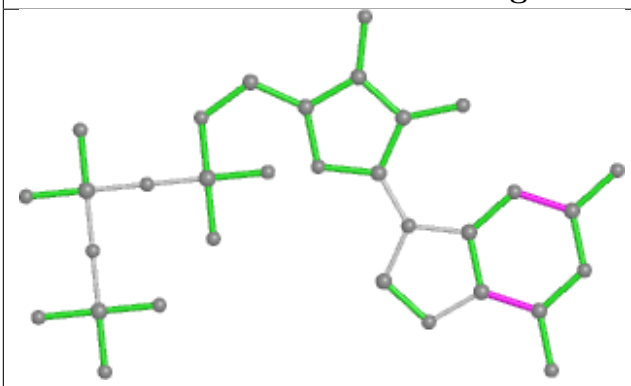


Rings

Ligand GTP UE 501



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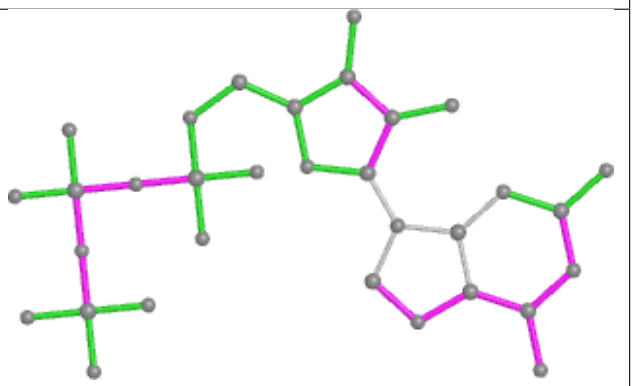
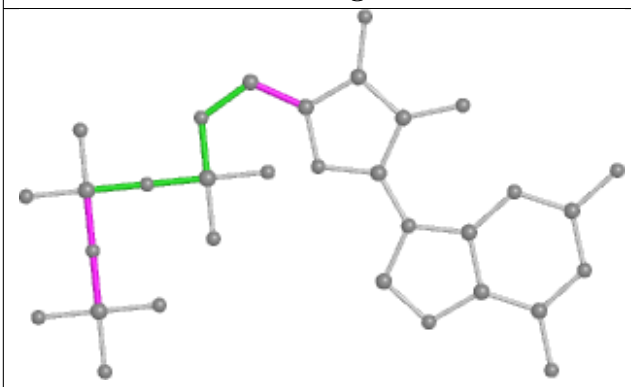


Bond angles



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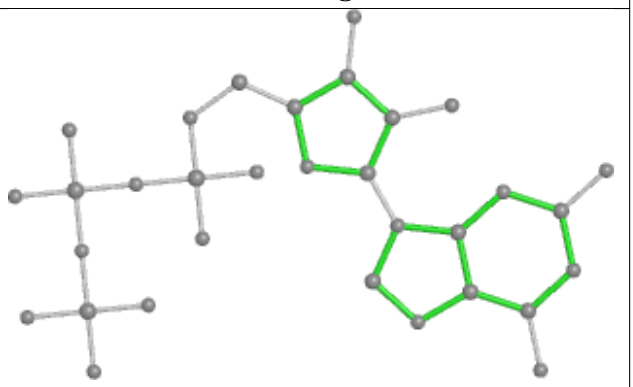
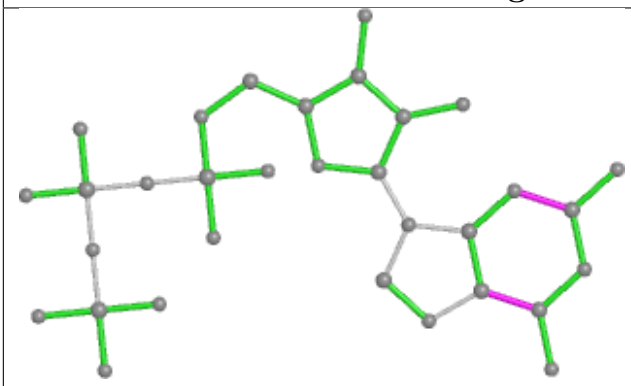
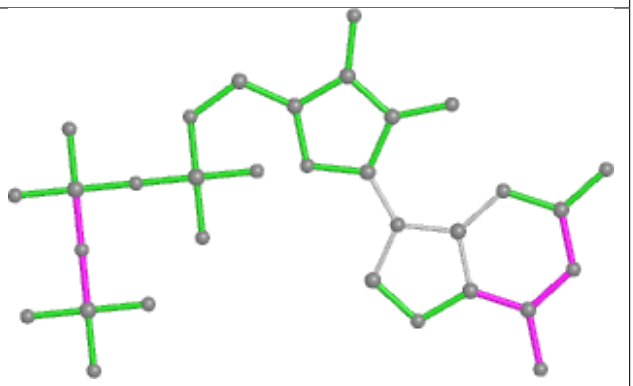


Rings

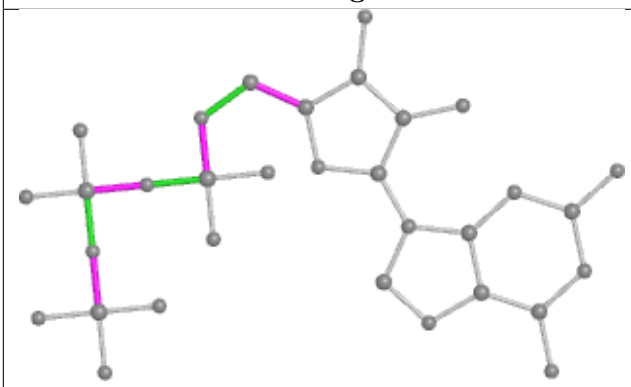
Ligand GTP AH 501



Bond lengths



Bond angles



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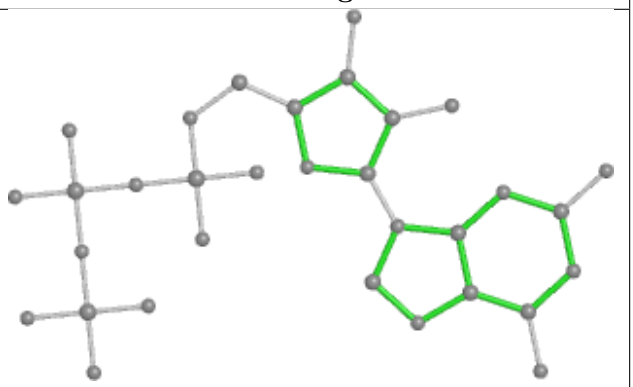
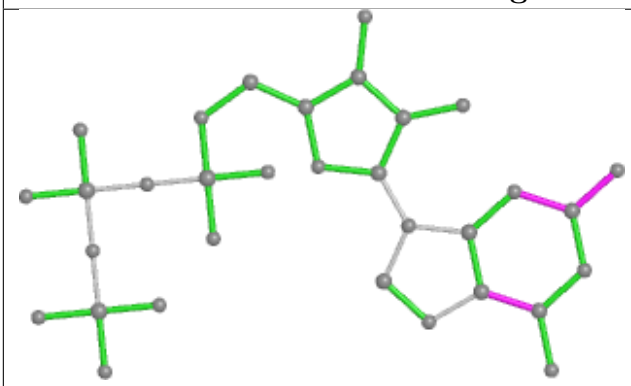


Rings

Ligand GTP ED 501



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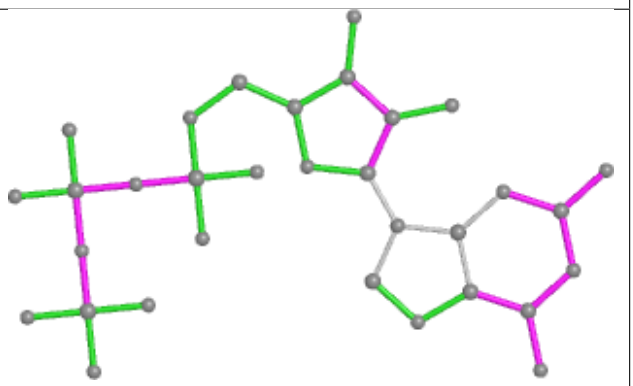
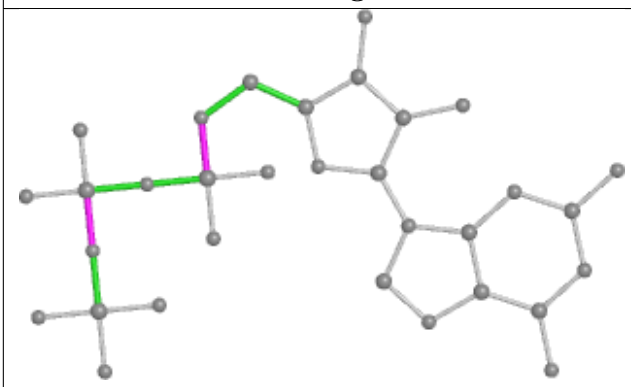


Bond angles



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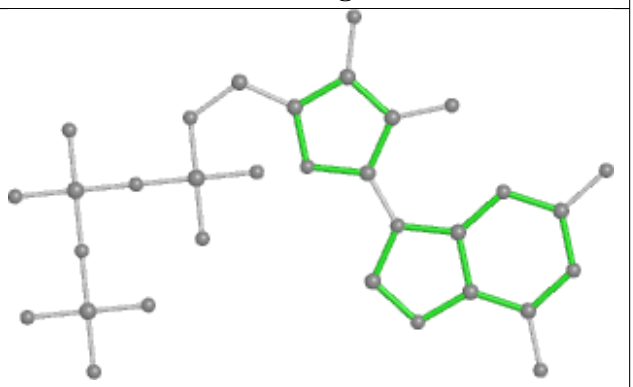
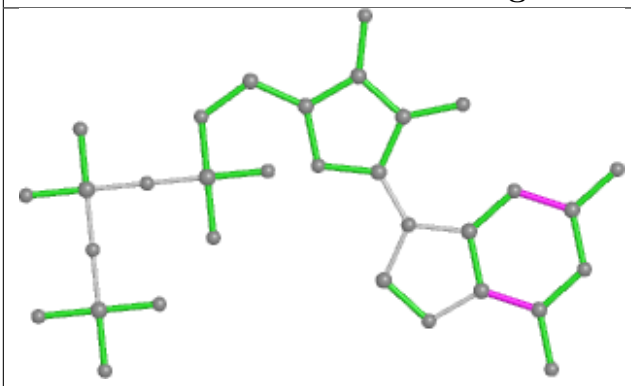
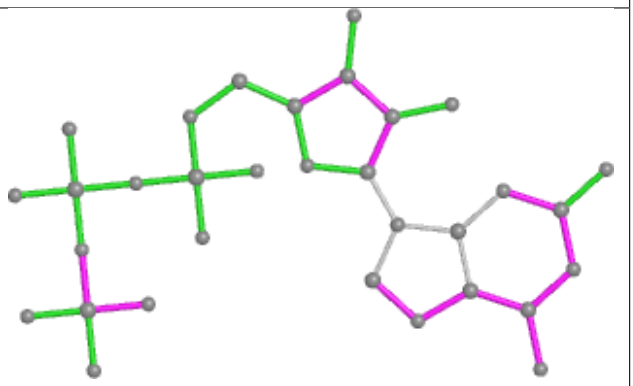


Rings

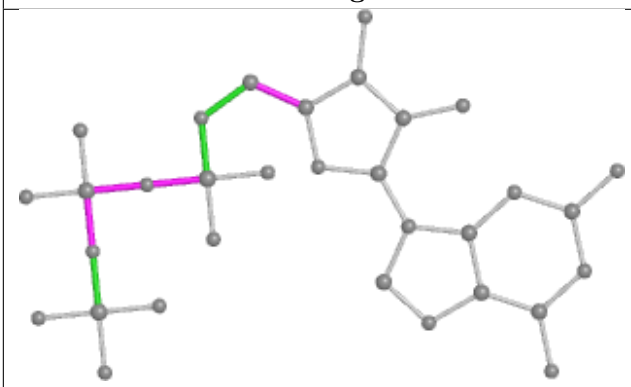
Ligand GTP AG 501



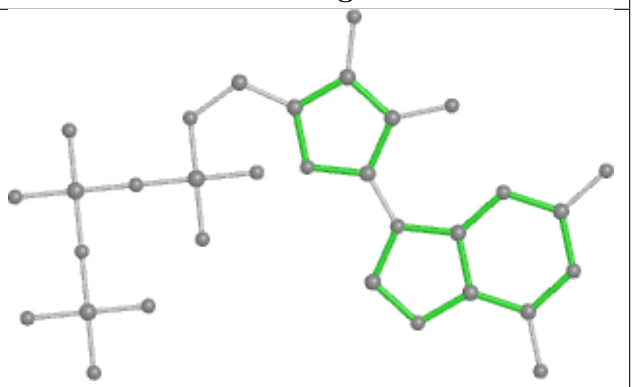
Bond lengths



Bond angles

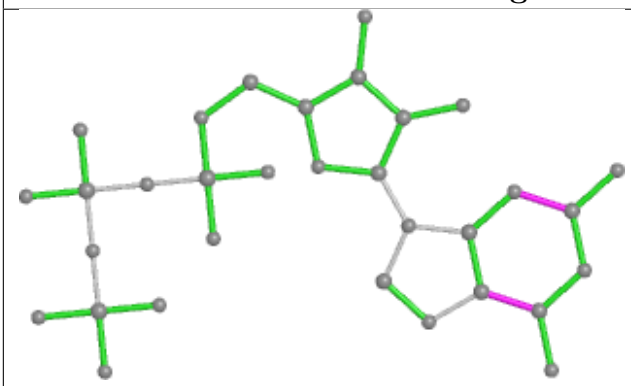


Torsions



Rings

Ligand GTP HE 501



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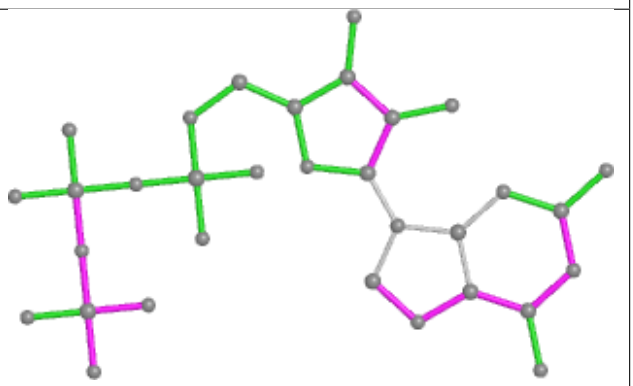
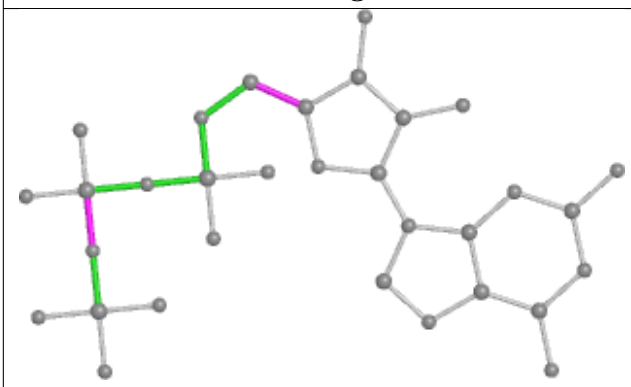


Bond angles



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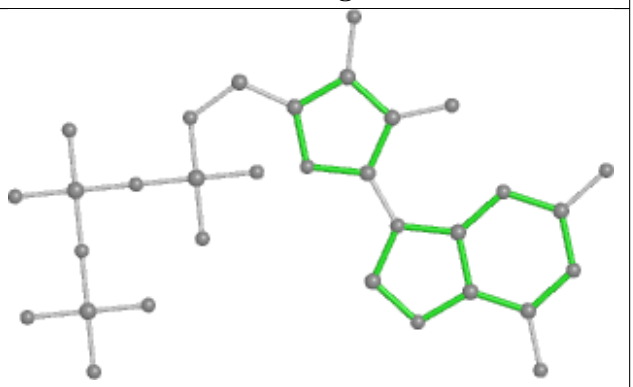
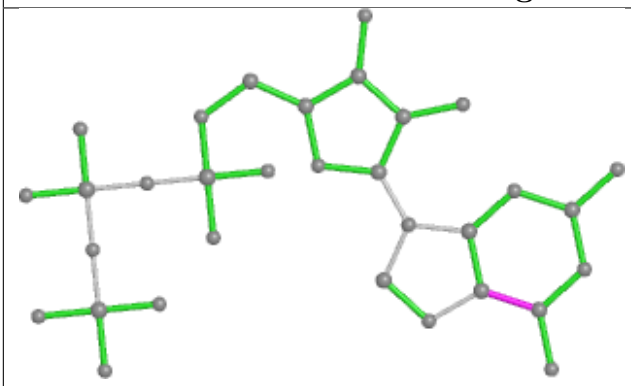


Rings

Ligand GTP OI 501



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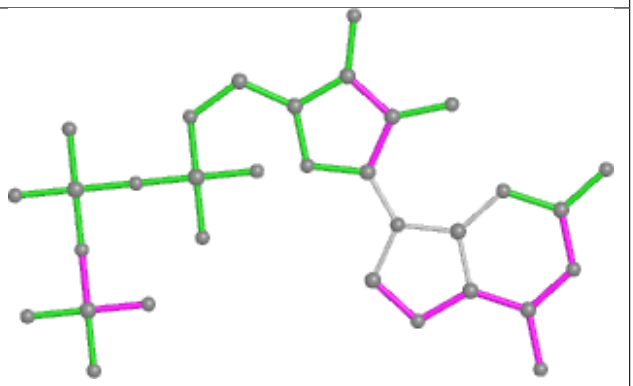
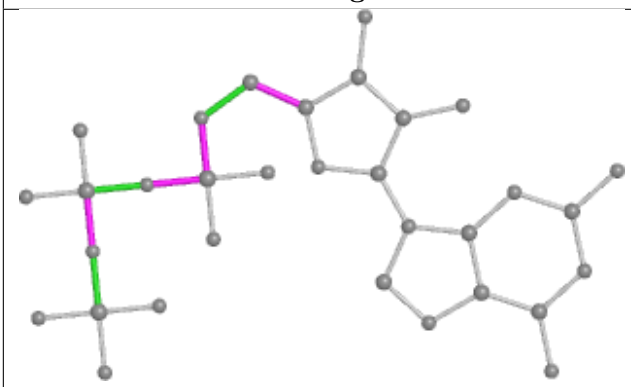
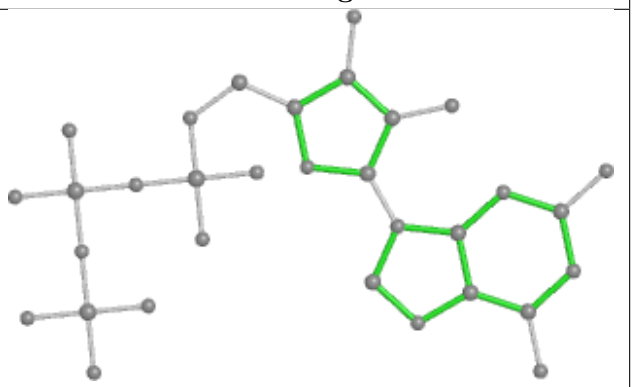


Bond angles

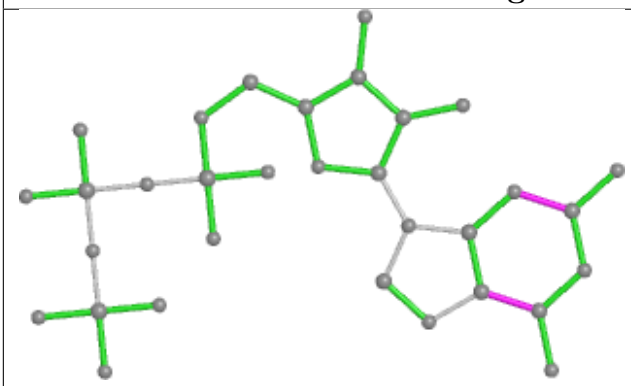


Torsions



Rings

Ligand GTP GH 501



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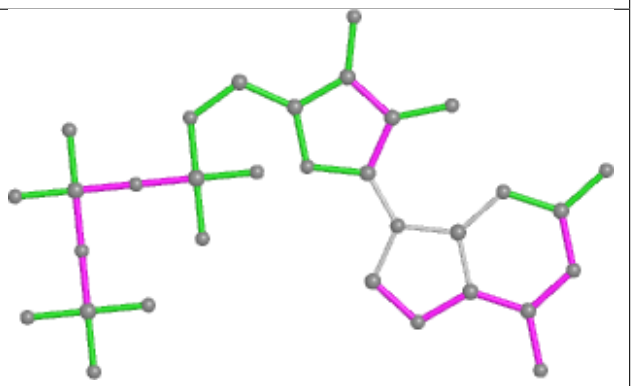
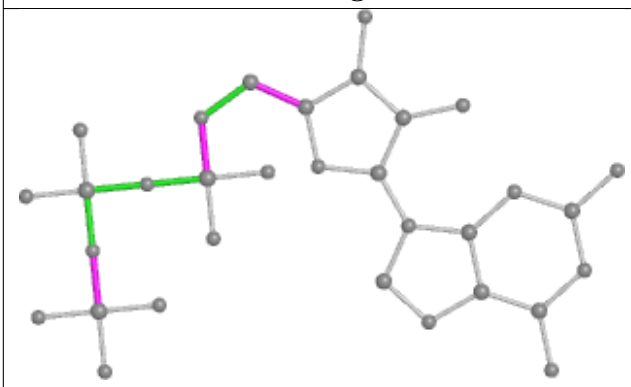
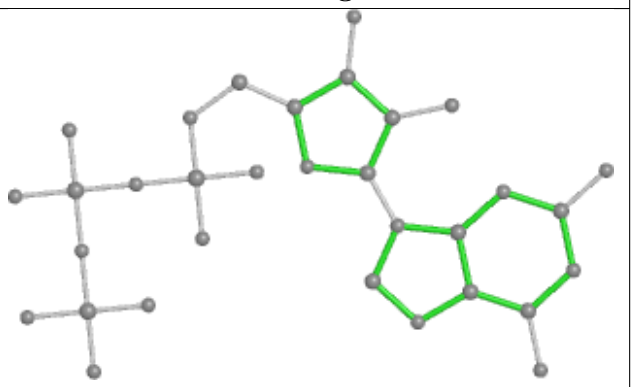


Bond angles

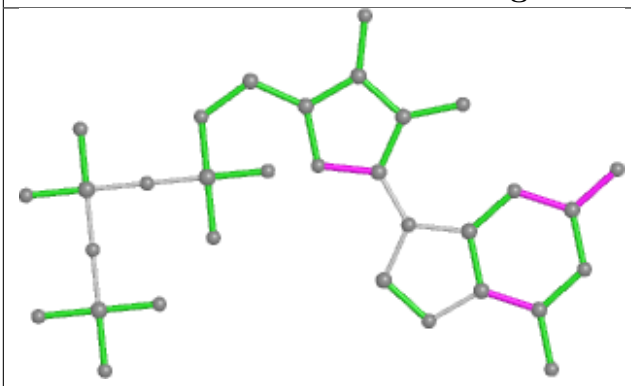


Torsions

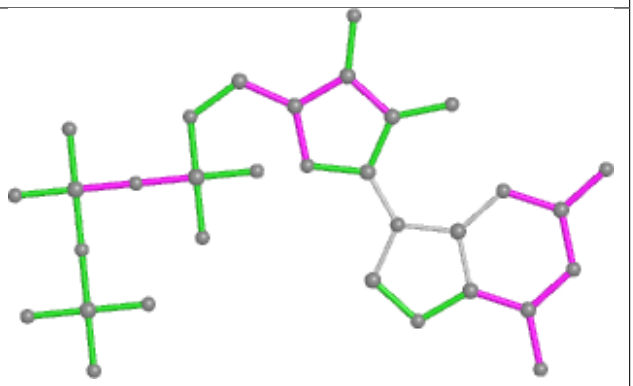


Rings

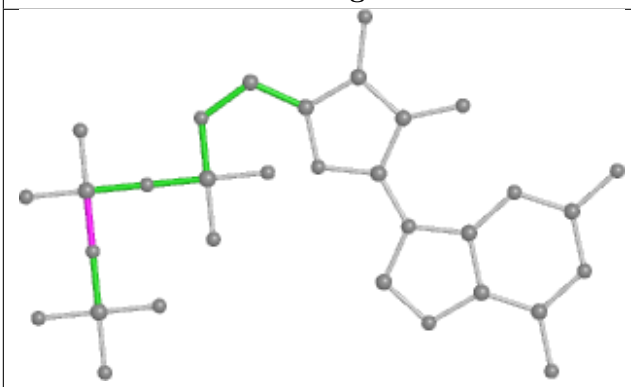
Ligand GTP HF 501



Bond lengths



Bond angles



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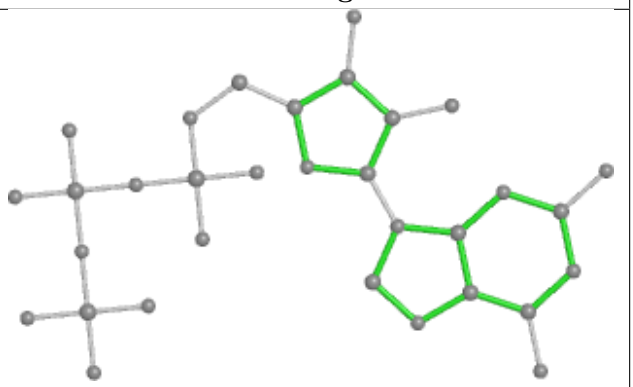
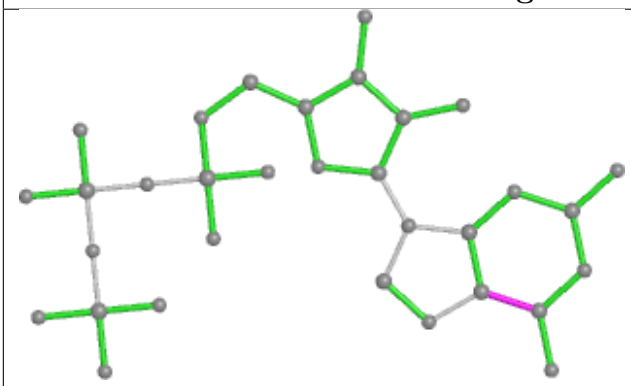


Rings

Ligand GTP BI 501



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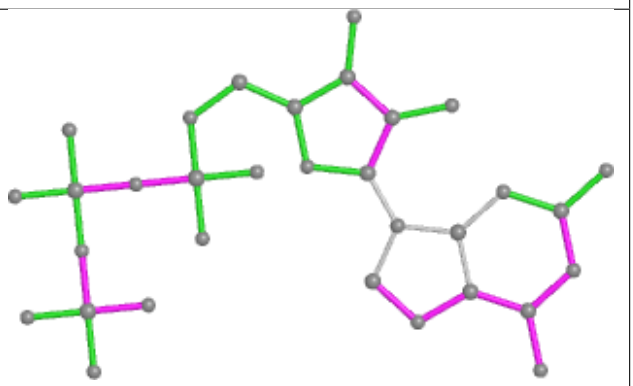
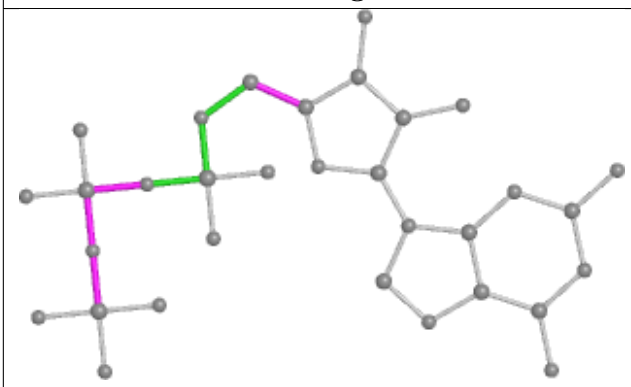


Bond angles



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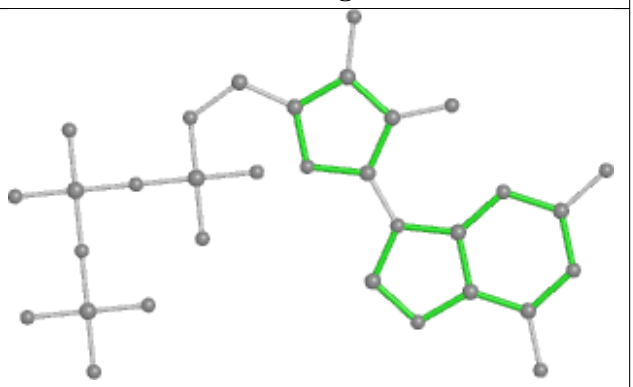
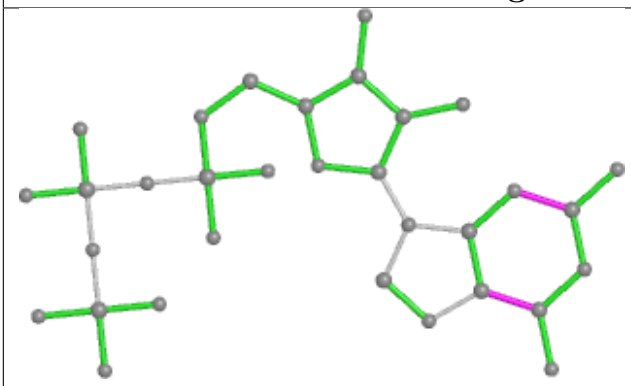


Rings

Ligand GTP HD 501



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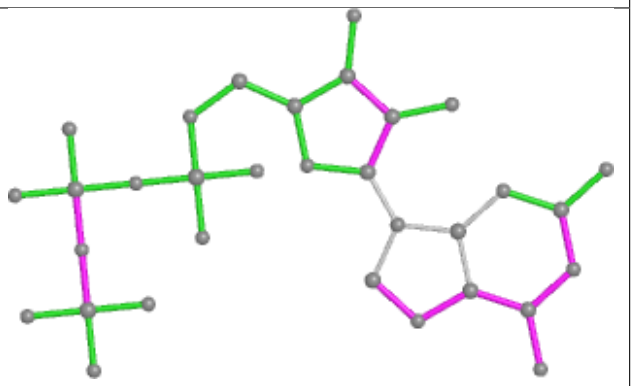
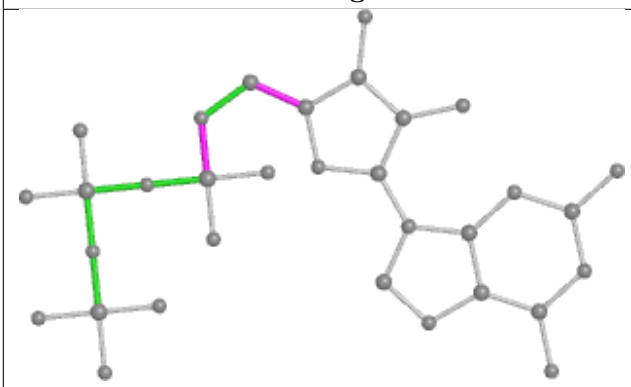
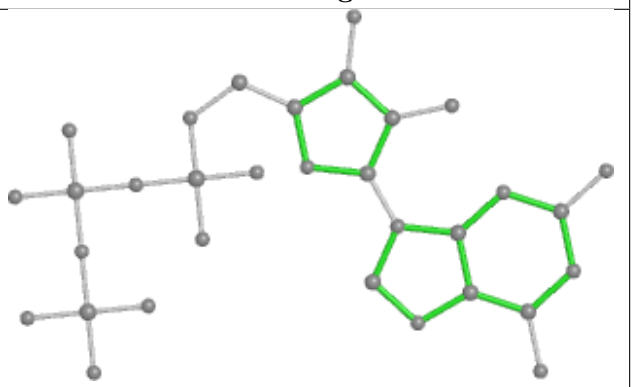


Bond angles

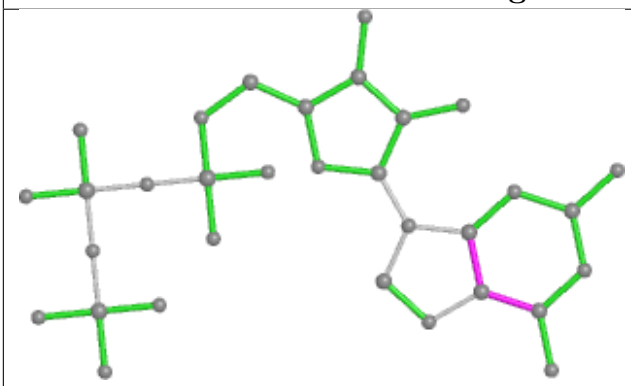


Torsions

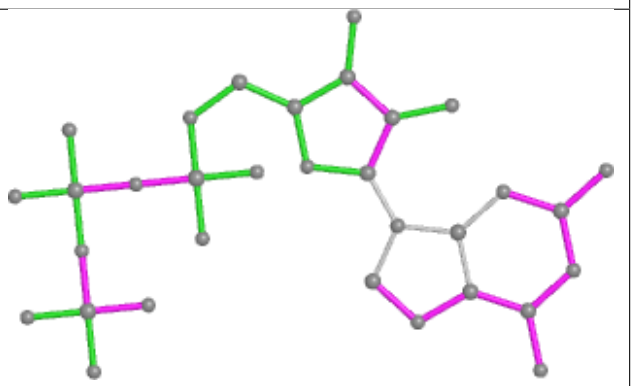


Rings

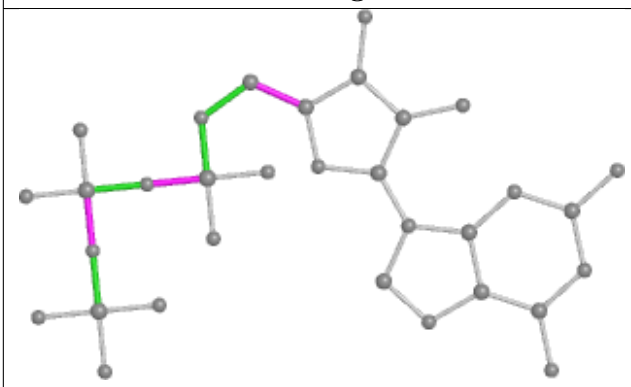
Ligand GTP BG 501



Bond lengths



Bond angles



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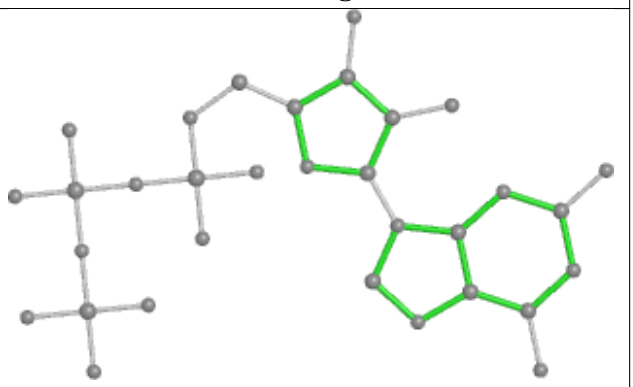
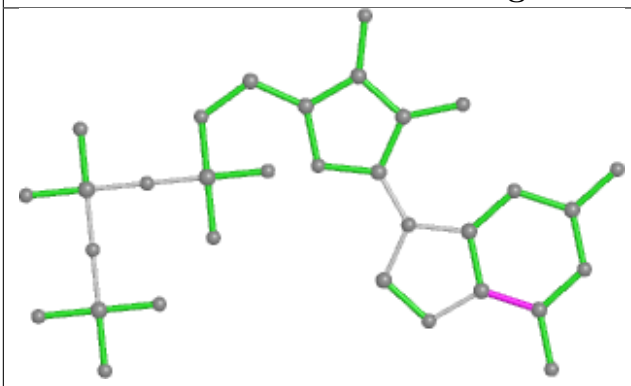


Rings

Ligand GTP OG 501



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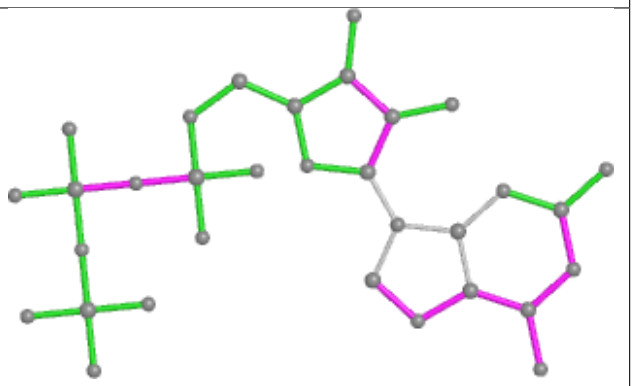
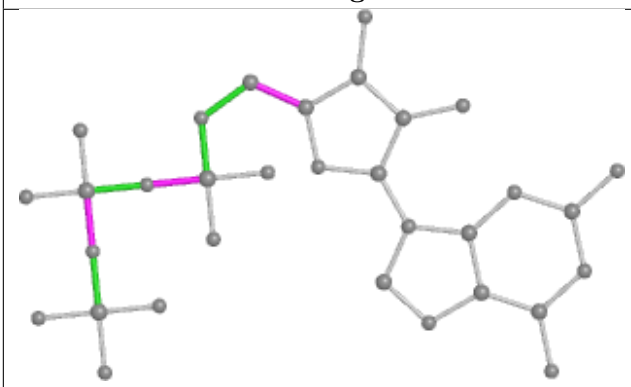
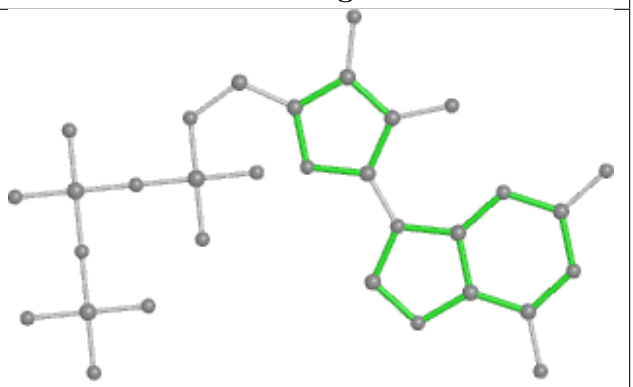


Bond angles

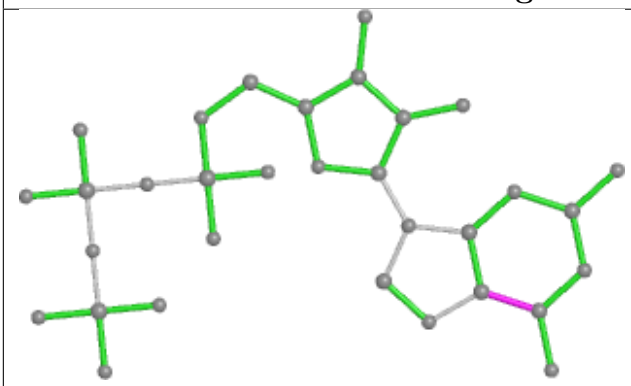


Torsions

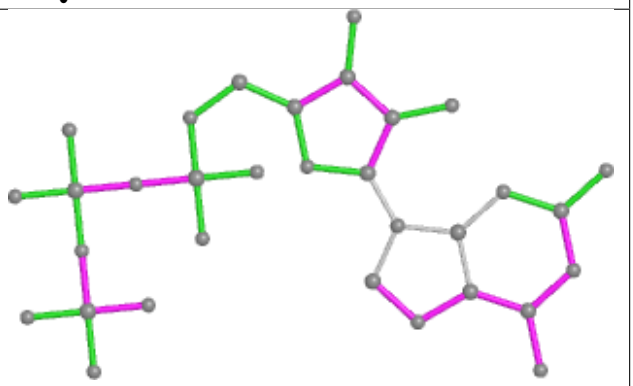


Rings

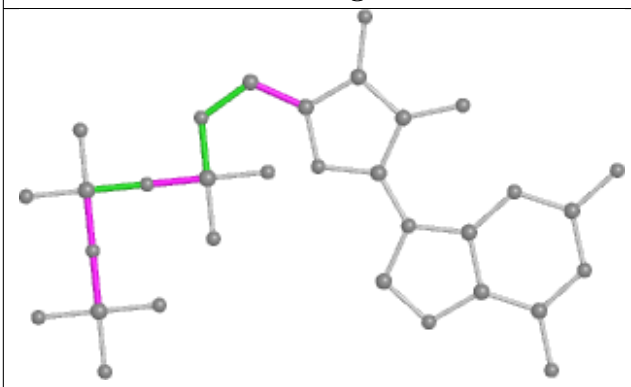
Ligand GTP QI 501



Bond lengths



Bond angles



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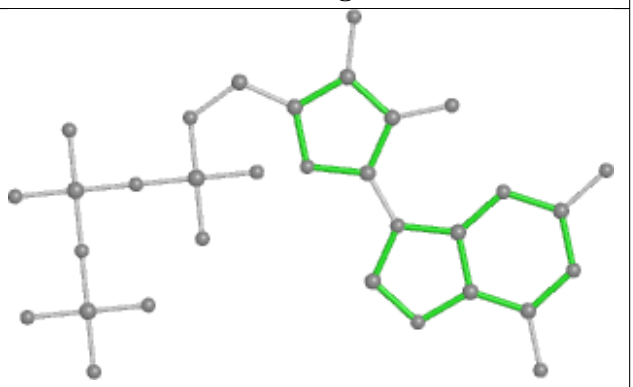
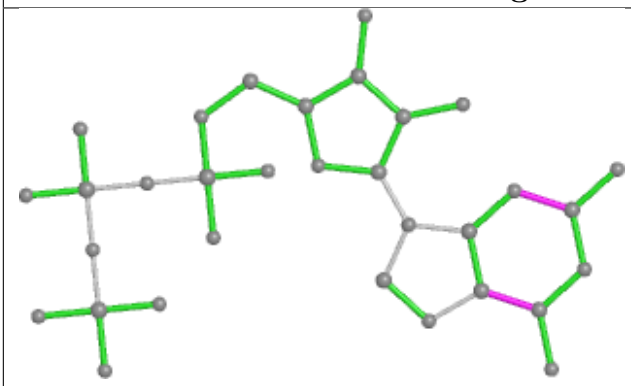
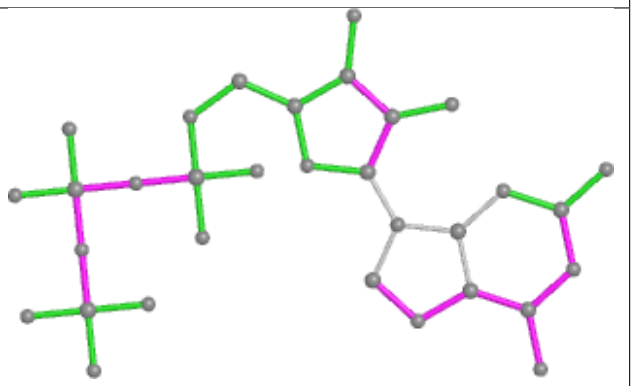


Rings

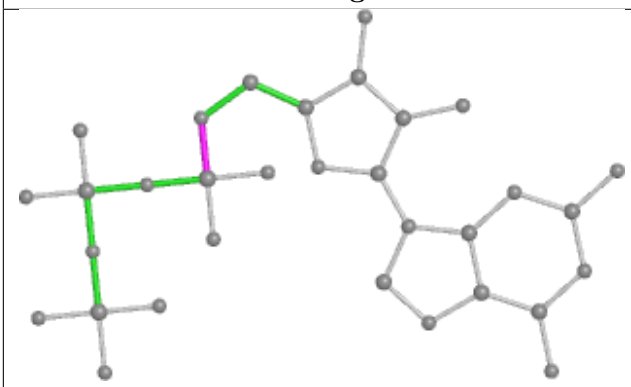
Ligand GTP FD 501



Bond lengths



Bond angles



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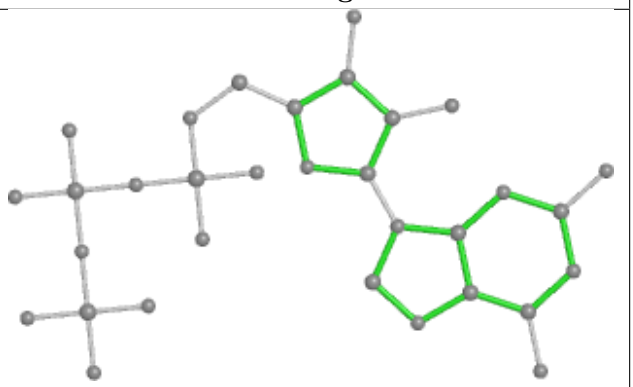
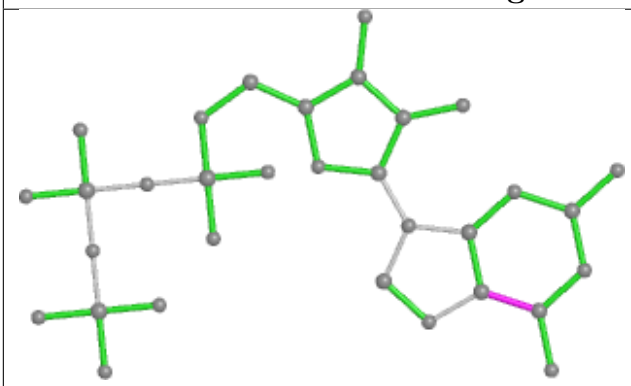
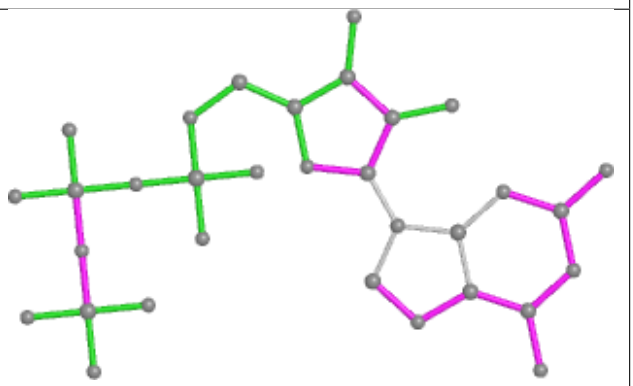


Rings

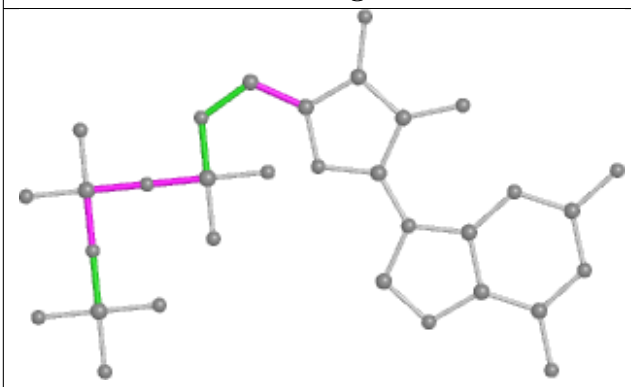
Ligand GTP GG 501



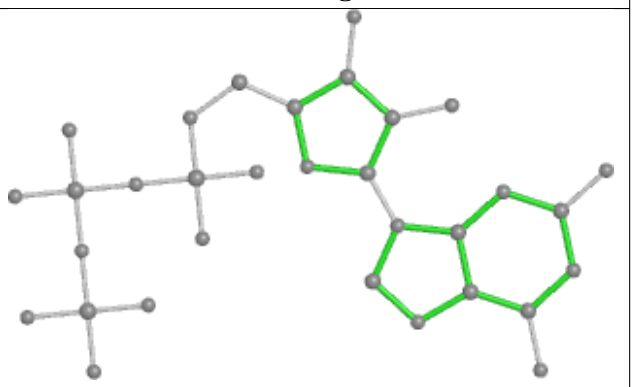
Bond lengths



Bond angles

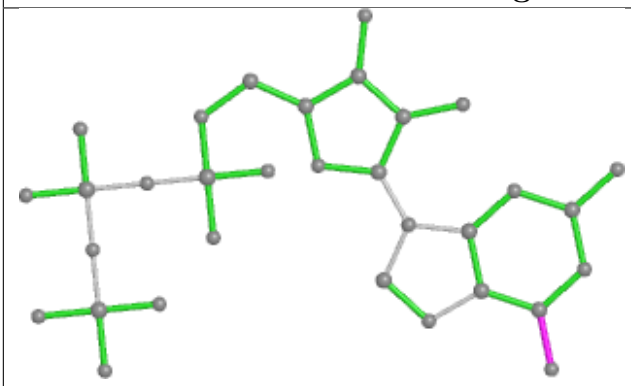


Torsions

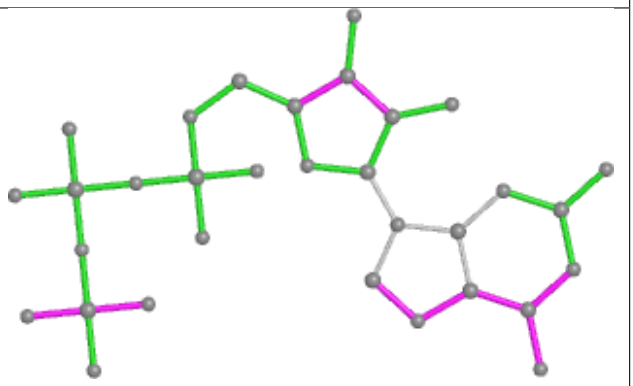


Rings

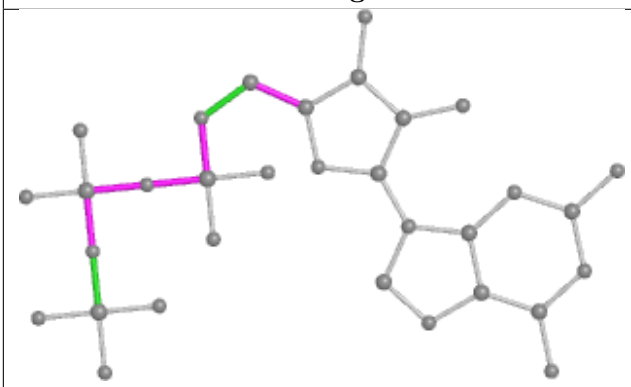
Ligand GTP FF 502



Bond lengths



Bond angles



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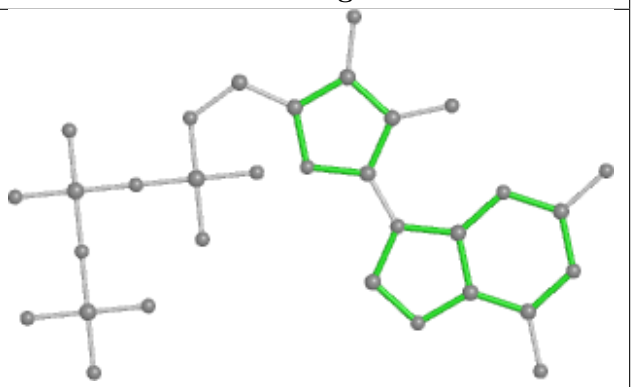
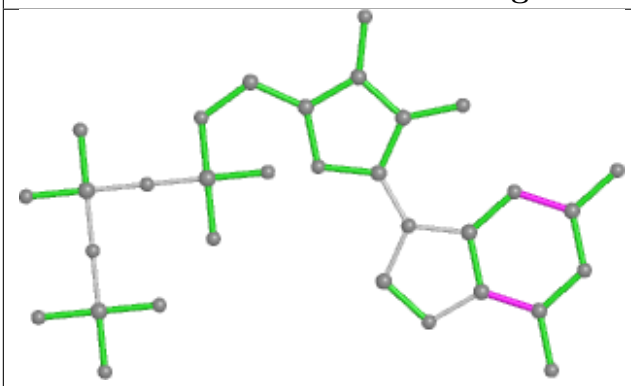
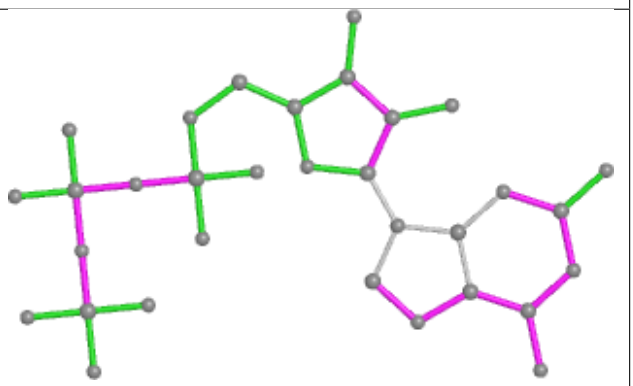


Rings

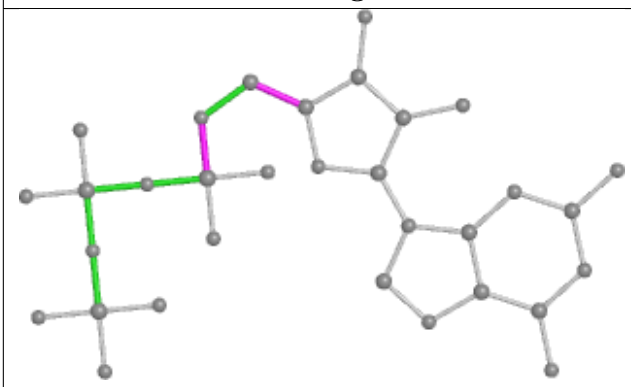
Ligand GTP CF 501



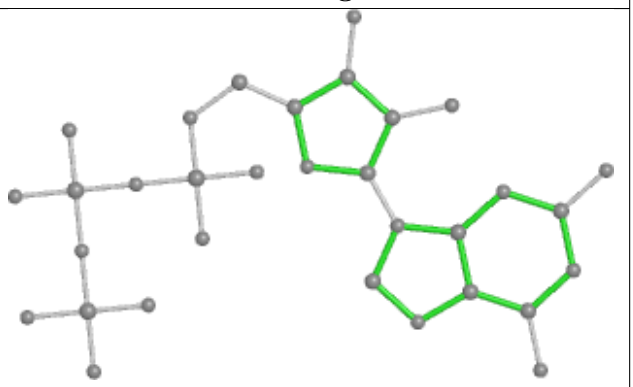
Bond lengths



Bond angles

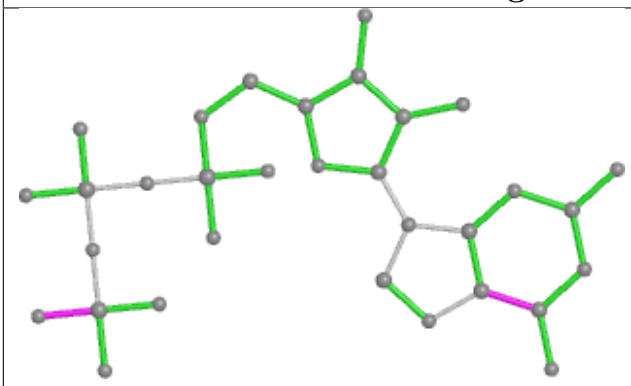


Torsions

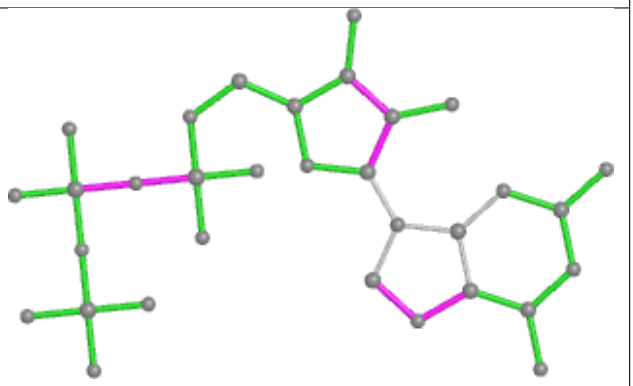


Rings

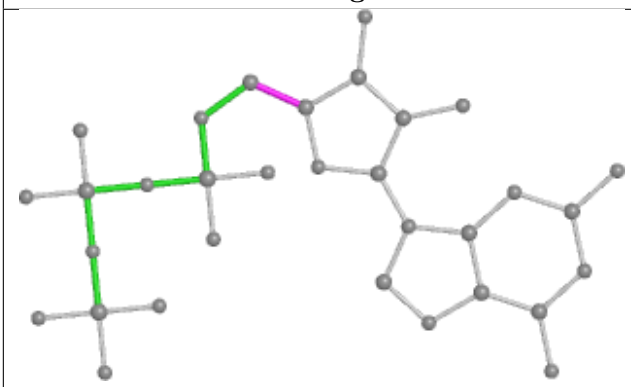
Ligand GTP DG 501



Bond lengths



Bond angles



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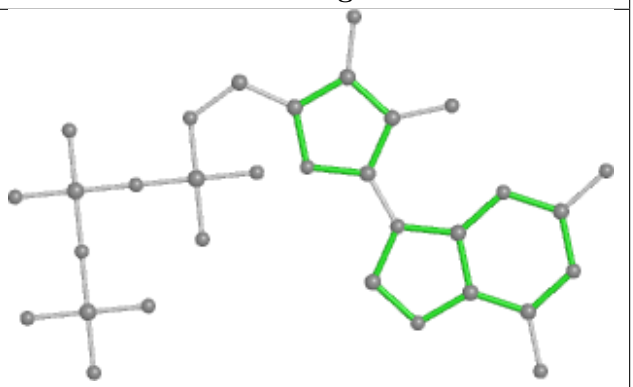
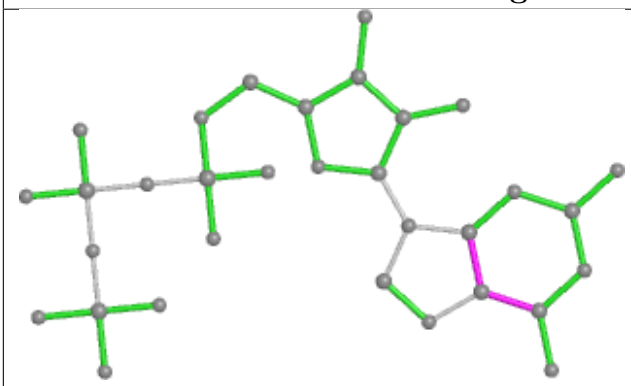
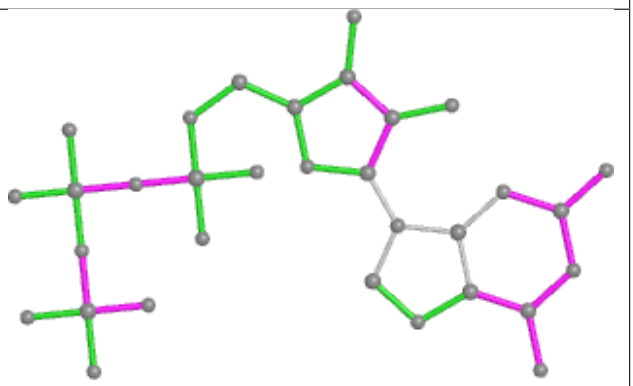


Rings

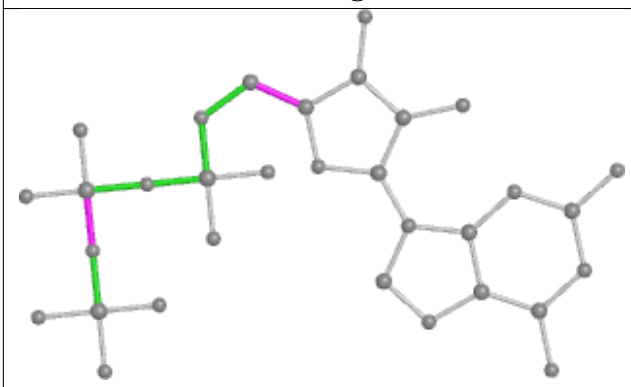
Ligand GTP DE 501



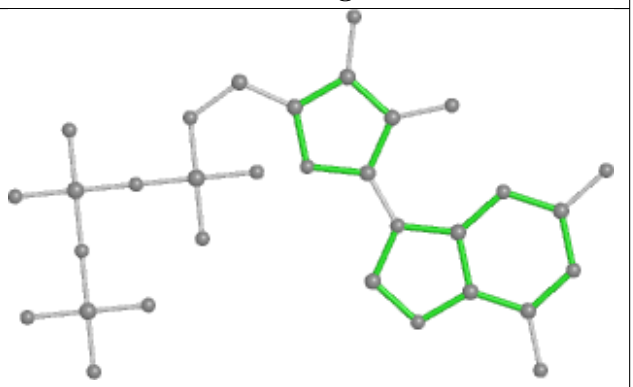
Bond lengths



Bond angles



Torsions



Rings

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.

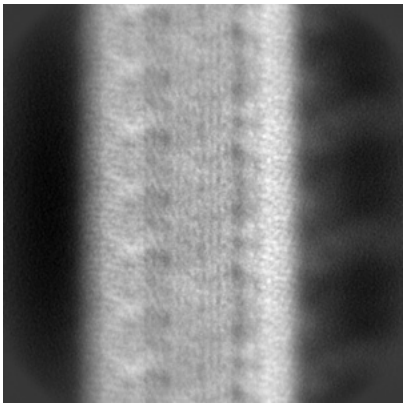
6 Map visualisation

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.

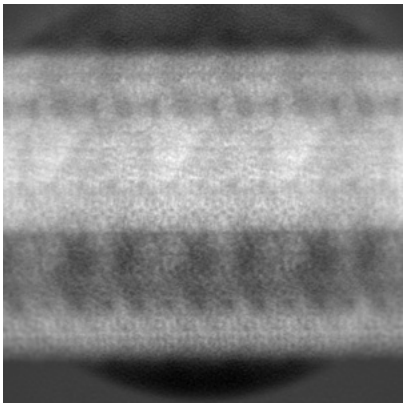
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

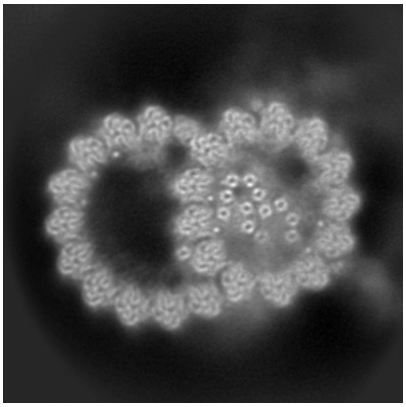
6.1.1 Primary map



X



Y

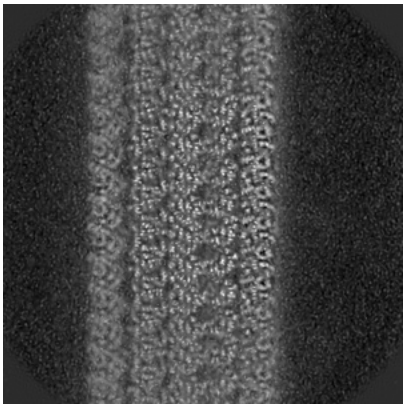


Z

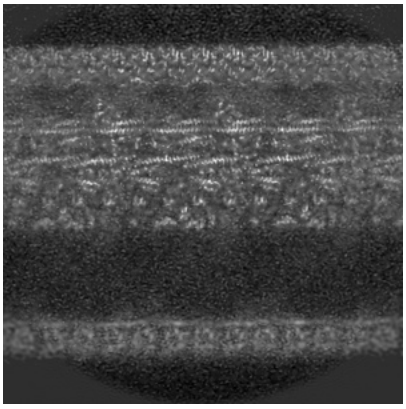
The images above show the map projected in three orthogonal directions.

6.2 Central slices

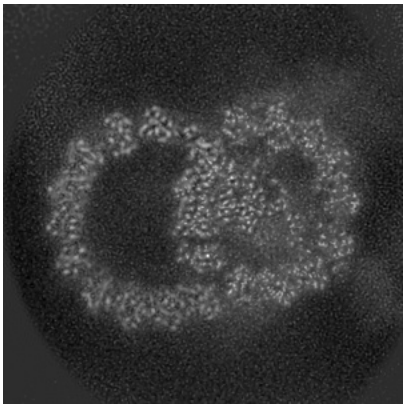
6.2.1 Primary map



X Index: 160



Y Index: 160

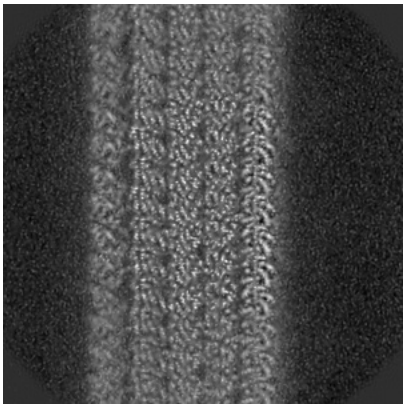


Z Index: 160

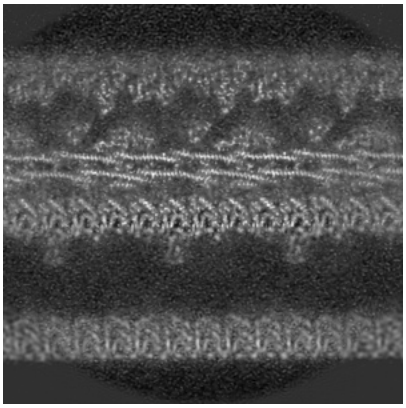
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

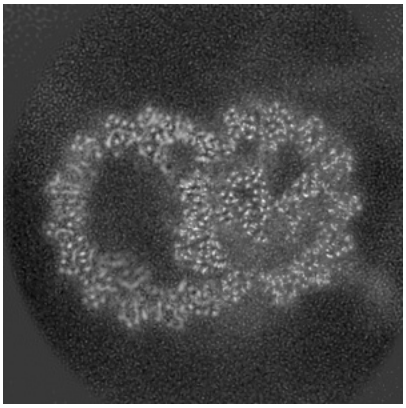
6.3.1 Primary map



X Index: 158



Y Index: 175

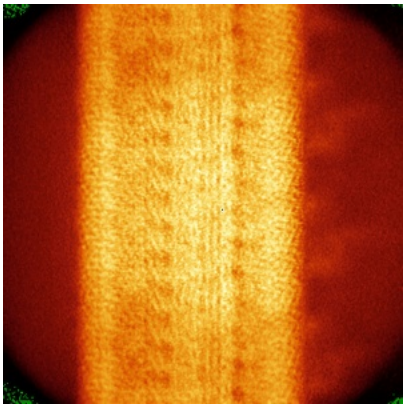


Z Index: 178

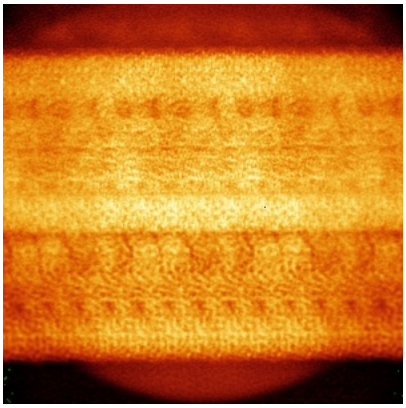
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

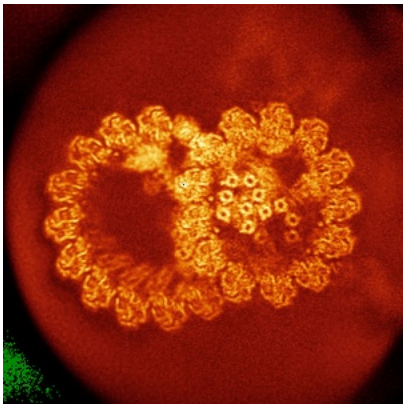
6.4.1 Primary map



X



Y

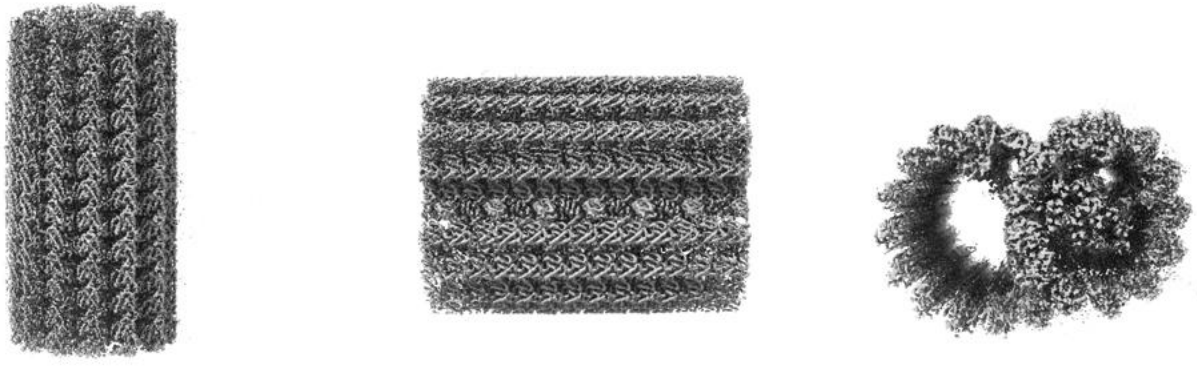


Z

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



X Y Z

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.

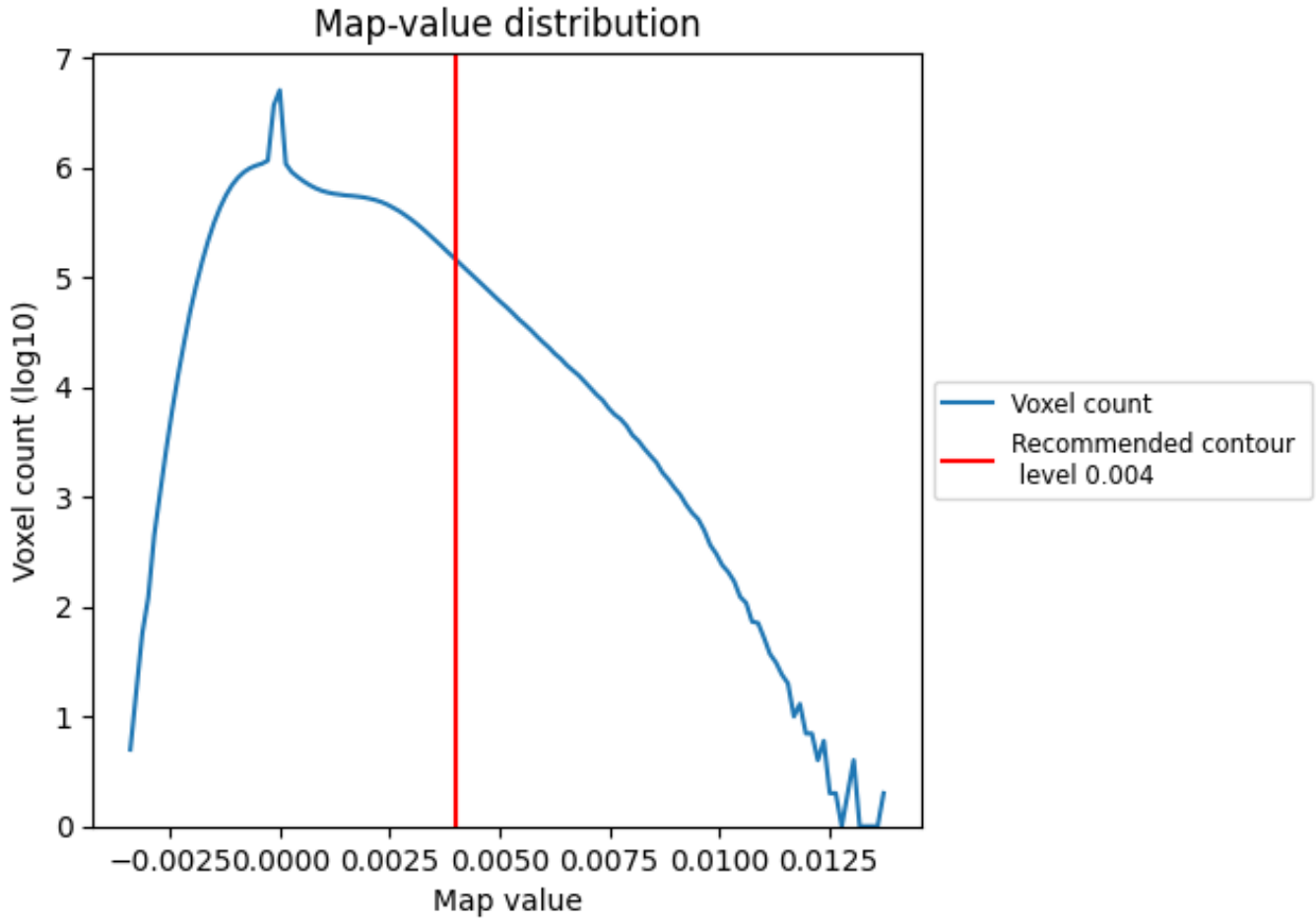
6.6 Mask visualisation (i)

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

7 Map analysis

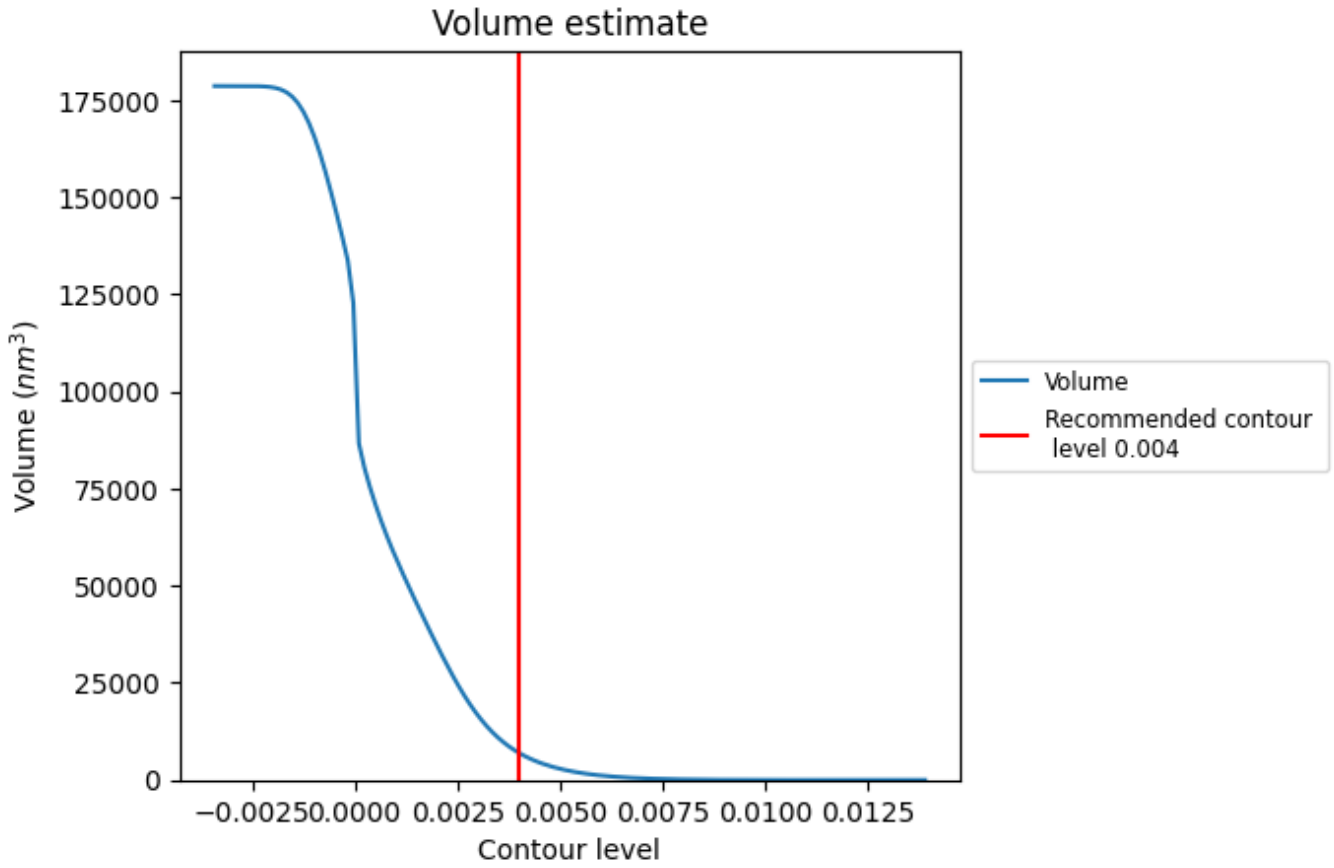
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

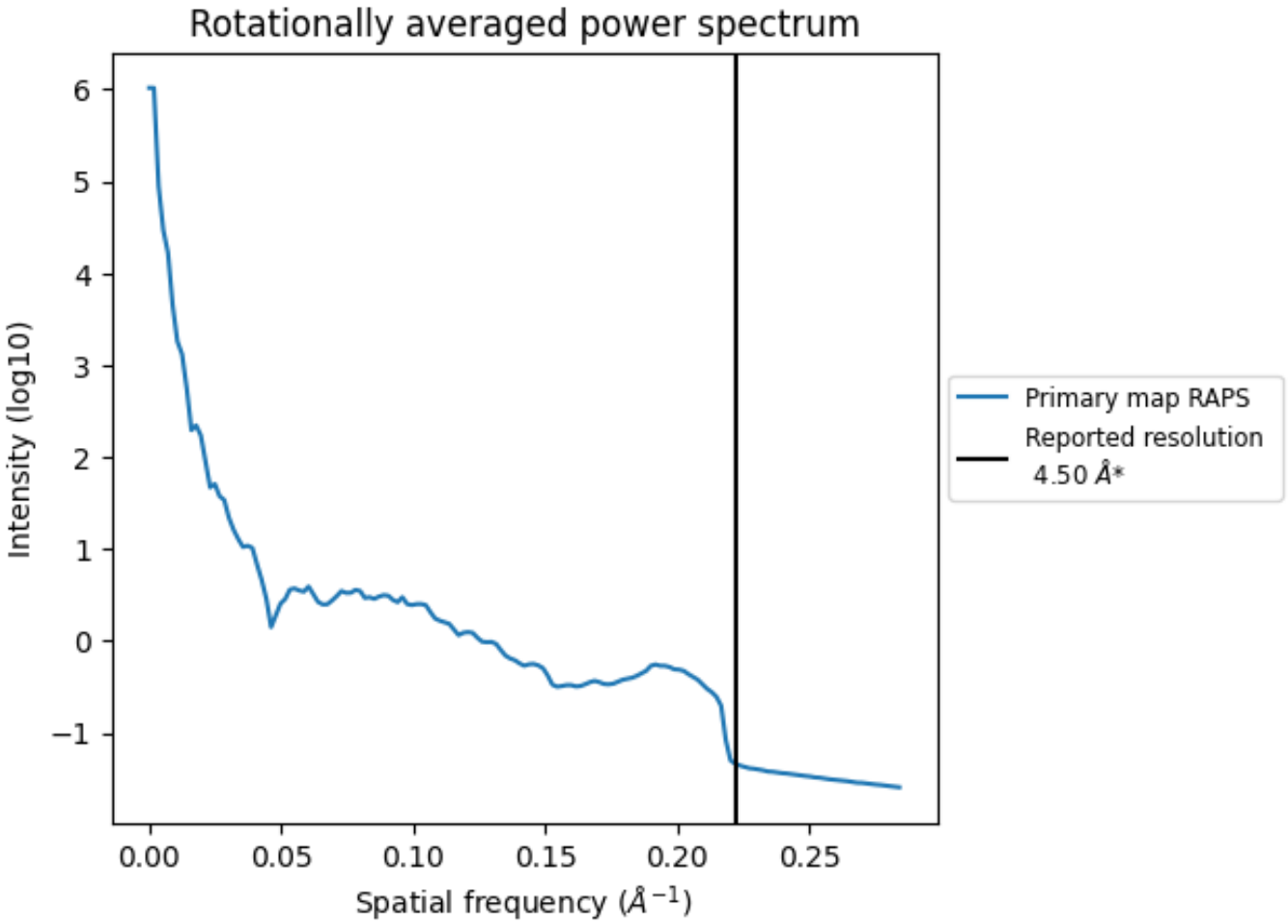
7.2 Volume estimate



The volume at the recommended contour level is 6982 nm^3; 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}

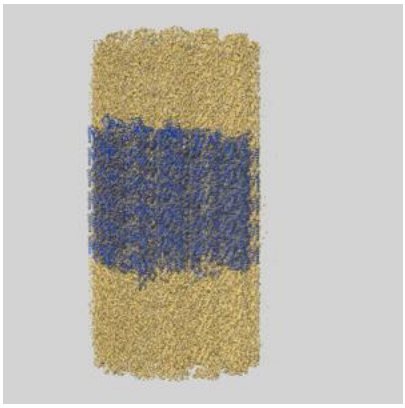
8 Fourier-Shell correlation

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

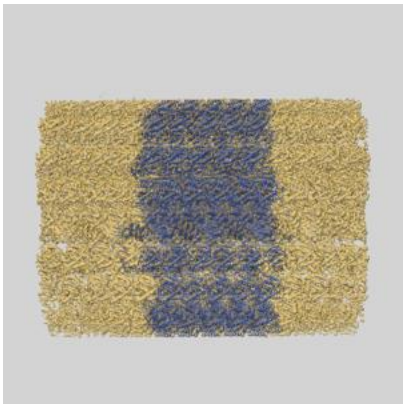
9 Map-model fit

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.

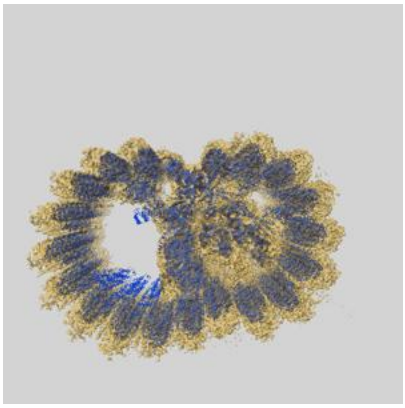
9.1 Map-model overlay



X



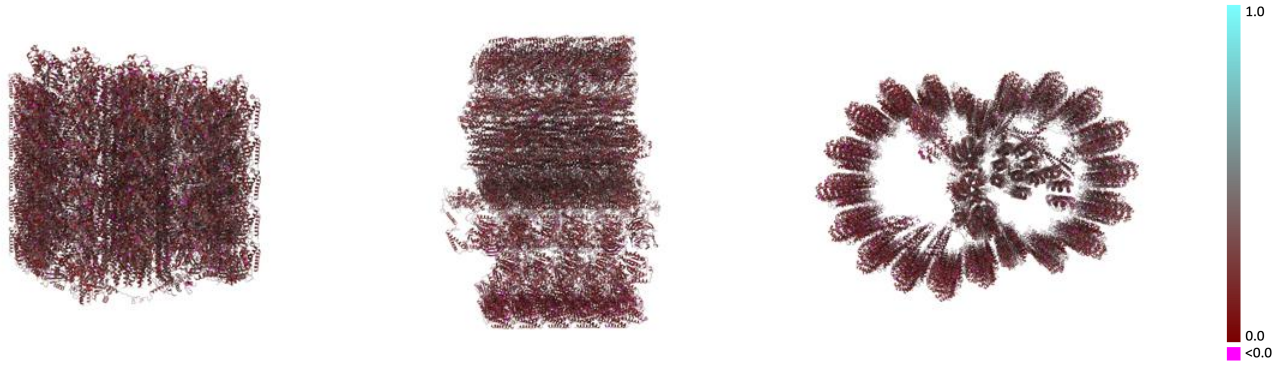
Y



Z

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.

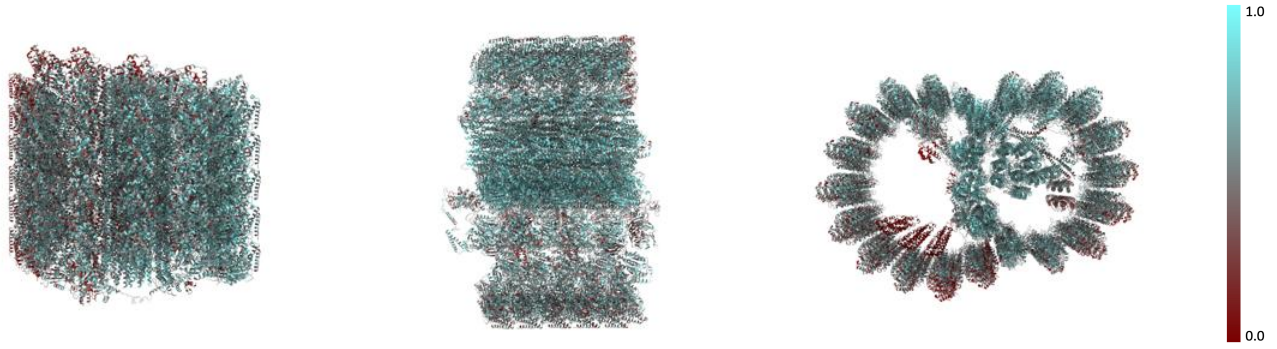
9.2 Q-score mapped to coordinate model



X Y Z

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.

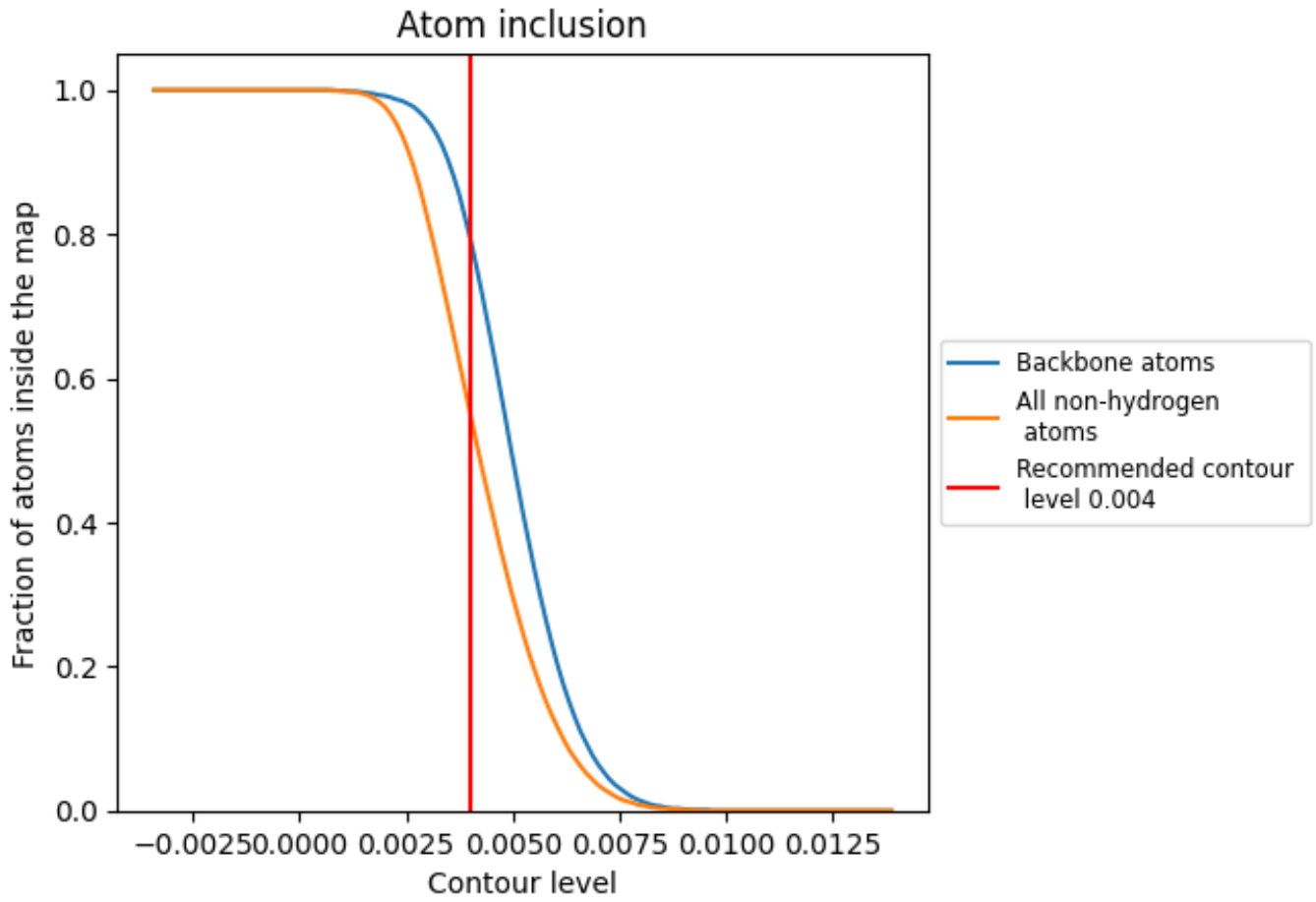
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

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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
Fl	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

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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

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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

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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