wwPDB EM Validation Summary Report (i)

Mar 15, 2026 – 06:46 PM EDT

PDB ID	:	8G2Z / pdb_00008g2z
EMDB ID	:	EMD-29685
Title	:	48-nm doublet microtubule from Tetrahymena thermophila strain CU428
Authors	:	Black, C.S.; Kubo, S.; Yang, S.K.; Bui, K.H.
Deposited on	:	2023-02-06
Resolution	:	4.10 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 (i) 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 (i)) were used in the production of this report:

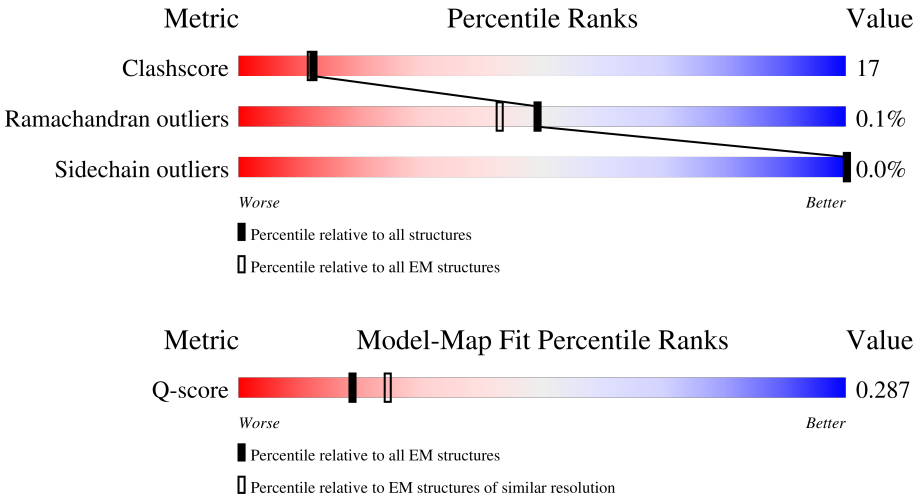
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	0A	236	13% 39% 23% • 36%
1	1A	236	13% 40% 23% • 36%
1	2A	236	9% 39% 24% • 36%
1	3A	236	11% 39% 24% • 36%

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Mol	Chain	Length	Quality of chain
2	0B	329	5% 61% 35%
3	0C	156	8% 30% 29% 39%
3	1C	156	8% 32% 27% 39%
4	0D	225	33% 46% 40% 10%
4	1D	225	23% 48% 37% 10%
4	2D	225	23% 48% 37% 10%
5	0E	191	42% 51% 47%
5	1E	191	38% 48% 50%
5	2E	191	28% 49% 49%
5	3E	191	64% 53% 45%
6	0F	219	7% 42% 50% 6%
7	0G	183	23% 45% 43% 8%
7	1G	183	17% 39% 33% 26%
8	0H	447	16% 14% 13% 73%
8	1H	447	47% 48% 46% 5%
9	0N	492	8% 33% 24% 43%
9	1N	492	5% 61% 33% 6%
9	2N	492	11% 35% 22% 43%
10	0Q	195	8% 55% 41% 5%
10	1Q	195	6% 50% 46% 5%
10	2Q	195	6% 54% 41% 5%
10	3Q	195	5% 51% 44% 5%
10	4Q	195	7% 52% 44% 5%
10	5Q	195	7% 55% 40% 5%
10	6Q	195	13% 54% 42% 5%

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Mol	Chain	Length	Quality of chain
11	0S	319	49% 56% 34% 10%
11	1S	319	6% 49% 41% 10%
11	2S	319	7% 55% 34% 10%
11	3S	319	57% 33% 10%
12	0T	298	45% 57% 31% 12%
12	1T	298	6% 57% 38%
12	2T	298	5% 51% 44%
12	3T	298	7% 50% 46%
13	0U	656	14% 49% 43% 7%
13	1U	656	6% 54% 38% 7%
13	2U	656	5% 52% 41% 7%
13	3U	656	14% 50% 42% 7%
14	0V	269	45% 59% 19% 21%
14	1V	269	24% 64% 32%
14	2V	269	24% 51% 45%
14	3V	269	29% 63% 34%
15	0X	142	11% 41% 35% 23%
15	1X	142	63% 35%
15	2X	142	65% 33%
15	3X	142	13% 65% 34%
15	4X	142	10% 53% 46%
16	1B	498	12% 65% 34%
16	2B	498	9% 38% 21% 41%
16	3B	498	12% 35% 24% 41%
17	1F	173	12% 44% 31% 21%

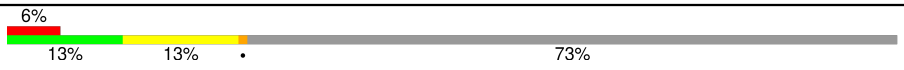
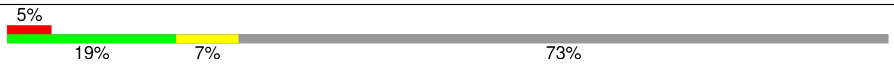
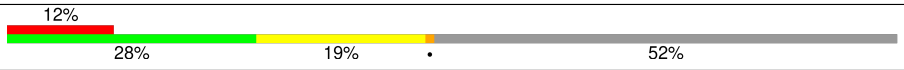
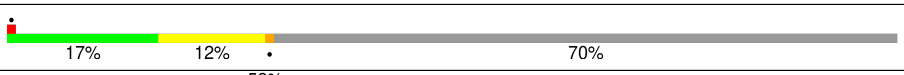
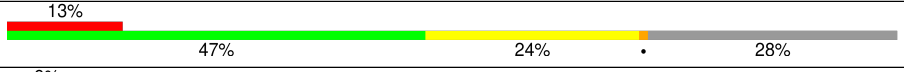
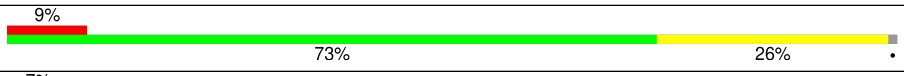
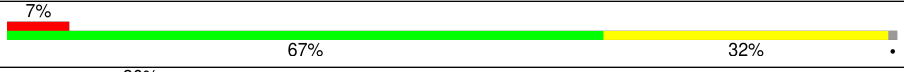
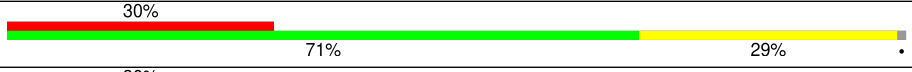
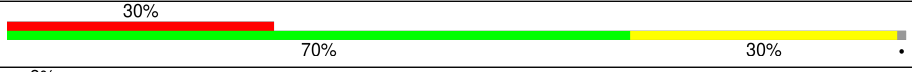
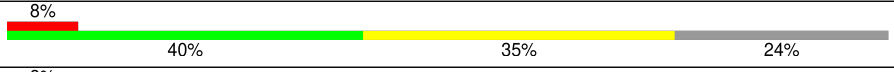
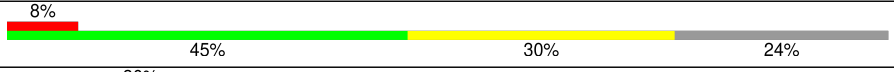
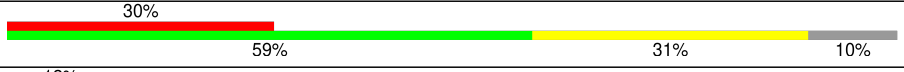
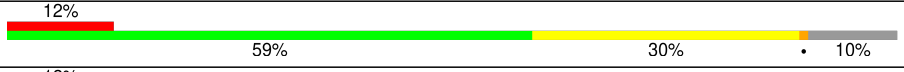
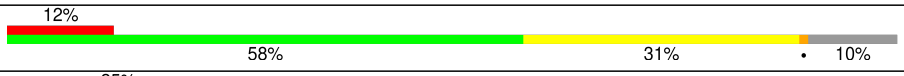
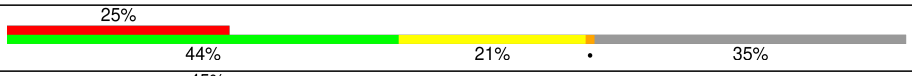
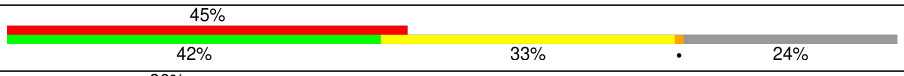
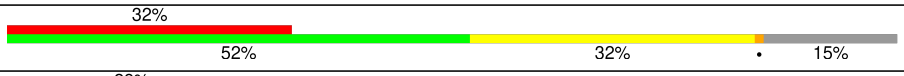
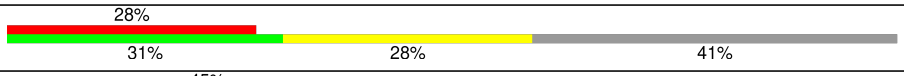
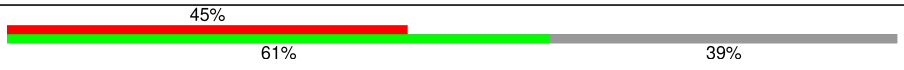
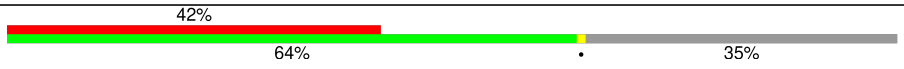
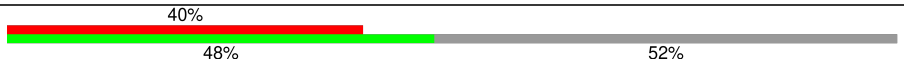
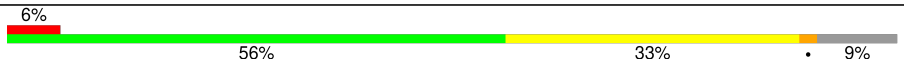
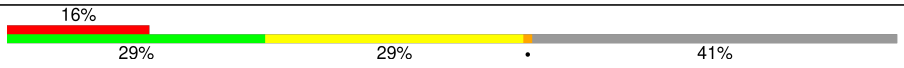
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Mol	Chain	Length	Quality of chain
18	1I	263	6% 41% 29% 29%
19	1J	422	16% 49% 38% 12%
20	1K	489	18% 33% 24% 43%
20	2K	489	22% 33% 26% 41%
21	1L	940	20% 52% 35% 13%
21	2L	940	32% 42% 23% 34%
21	3L	940	15% 12% 9% 79%
22	1M	372	6% 65% 34%
22	2M	372	66% 33%
23	1O	494	28% 24% 24% 51%
23	2O	494	38% 30% 45% 25%
23	3O	494	32% 33% 23% 44%
24	1P	507	32% 38% 32% 30%
24	2P	507	15% 21% 16% 63%
25	1R	516	9% 68% 30%
25	2R	516	8% 65% 34%
25	3R	516	7% 66% 32%
26	1W	280	10% 54% 26% 20%
26	2W	280	18% 19% 22% 59%
27	2C	300	26% 59% 40%
27	3C	300	17% 61% 38%
27	4C	300	17% 59% 40%
28	2F	96	10% 54% 36% 9%
29	2G	99	7% 64% 35%
30	2H	229	5% 14% 12% 73%

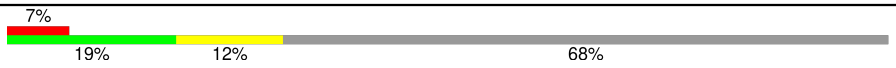
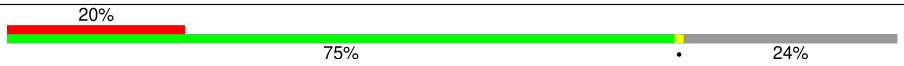
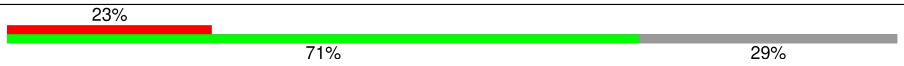
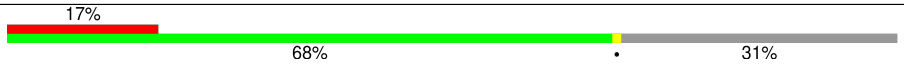
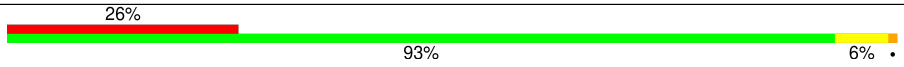
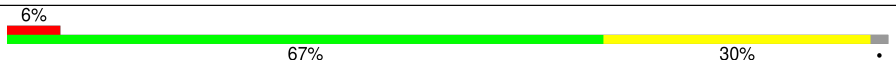
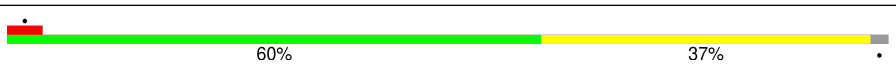
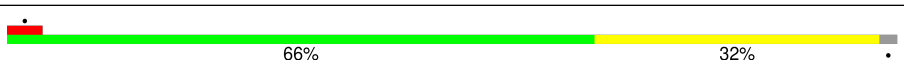
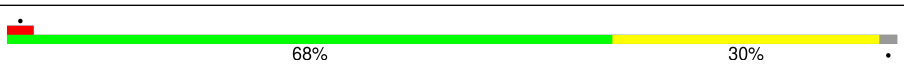
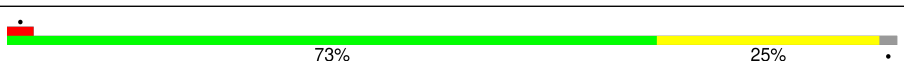
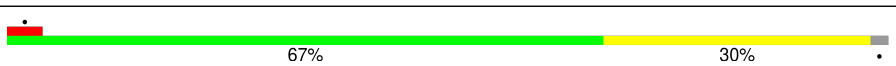
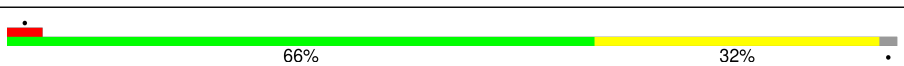
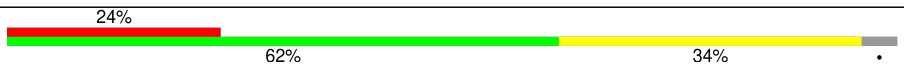
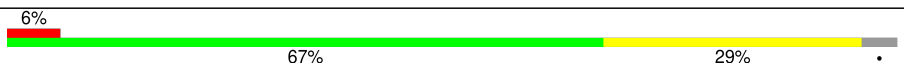
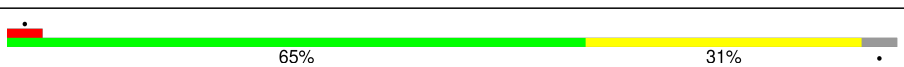
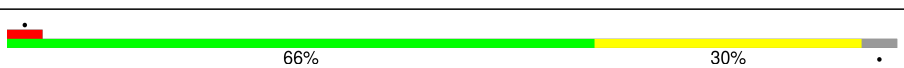
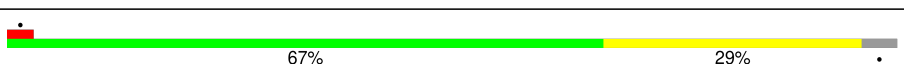
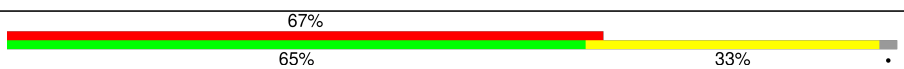
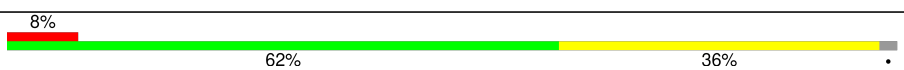
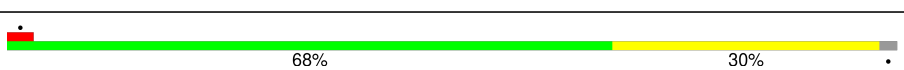
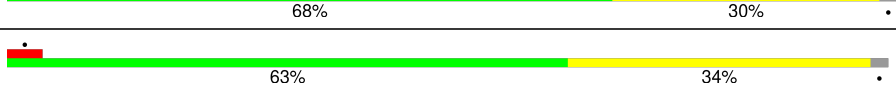
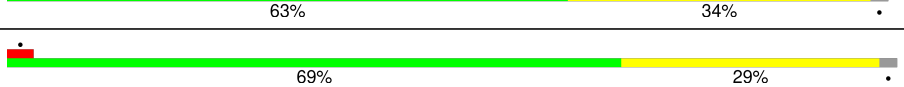
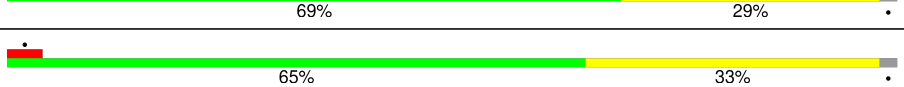
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Mol	Chain	Length	Quality of chain
30	3H	229	
30	4H	229	
31	2I	293	
31	3I	293	
32	3D	237	
33	4F	276	
34	4R	613	
34	5R	613	
34	6R	613	
34	7R	613	
35	4S	249	
35	5S	249	
36	5A	175	
36	5B	175	
36	5C	175	
36	5D	175	
37	5E	247	
37	5F	247	
37	5G	247	
37	5H	247	
38	5I	168	
38	5J	168	
38	5K	168	
39	6F	145	
40	6G	364	

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Mol	Chain	Length	Quality of chain
41	6H	518	
42	8L	507	
42	8N	507	
43	8P	529	
44	8R	361	
45	AA	449	
45	AC	449	
45	AE	449	
45	AG	449	
45	AI	449	
45	AK	449	
45	AM	449	
45	BA	449	
45	BC	449	
45	BE	449	
45	BG	449	
45	BI	449	
45	BK	449	
45	BM	449	
45	CA	449	
45	CC	449	
45	CE	449	
45	CG	449	
45	CI	449	
45	CK	449	

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Mol	Chain	Length	Quality of chain
45	CM	449	21% 69% 29%
45	DA	449	94% 74% 23%
45	DC	449	7% 59% 38%
45	DE	449	65% 32%
45	DG	449	5% 64% 33%
45	DI	449	64% 33%
45	DK	449	64% 33%
45	DM	449	22% 60% 37%
45	EA	449	98% 78% 20%
45	EC	449	17% 58% 40%
45	EE	449	5% 63% 35%
45	EG	449	5% 64% 34%
45	EI	449	6% 66% 32%
45	EK	449	5% 68% 29%
45	EM	449	26% 61% 36%
45	FA	449	18% 64% 31%
45	FC	449	67% 29%
45	FE	449	69% 28%
45	FG	449	6% 71% 27%
45	FI	449	68% 29%
45	FK	449	12% 62% 34%
45	FM	449	96% 73% 22%
45	GA	449	21% 61% 34%
45	GC	449	69% 27%
45	GE	449	62% 34%

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Mol	Chain	Length	Quality of chain
45	GG	449	6% 67% 29%
45	GI	449	68% 27%
45	GK	449	62% 35%
45	GM	449	96% 75% 20%
45	HA	449	19% 66% 30%
45	HC	449	65% 31%
45	HE	449	64% 32%
45	HG	449	5% 70% 26%
45	HI	449	67% 29%
45	HK	449	63% 33%
45	HM	449	89% 72% 24%
45	IA	449	10% 61% 35%
45	IC	449	62% 36%
45	IE	449	63% 33%
45	IG	449	5% 62% 35%
45	II	449	67% 30%
45	IK	449	63% 33%
45	IM	449	31% 59% 37%
45	JA	449	63% 33%
45	JC	449	66% 31%
45	JE	449	70% 27%
45	JG	449	63% 35%
45	JI	449	65% 32%
45	JK	449	62% 35%
45	JM	449	69% 64% 32%

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Mol	Chain	Length	Quality of chain
45	KA	449	63% 33%
45	KC	449	66% 30%
45	KE	449	65% 31%
45	KG	449	65% 32%
45	KI	449	69% 29%
45	KK	449	65% 33%
45	KM	449	17% 63% 33%
45	LA	449	68% 29%
45	LC	449	72% 26%
45	LE	449	71% 26%
45	LG	449	70% 28%
45	LI	449	65% 31%
45	LK	449	67% 31%
45	LM	449	66% 31%
45	MA	449	6% 65% 32%
45	MC	449	63% 33%
45	ME	449	68% 28%
45	MG	449	5% 66% 31%
45	MI	449	6% 70% 28%
45	MK	449	5% 66% 31%
45	MM	449	7% 69% 28%
45	NA	449	12% 56% 42%
45	NC	449	6% 64% 32%
45	NE	449	6% 67% 31%
45	NG	449	5% 61% 35%

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Mol	Chain	Length	Quality of chain
45	NI	449	7% 63% 35%
45	NK	449	5% 60% 36%
45	NM	449	44% 61% 36%
45	OA	449	16% 53% 43%
45	OC	449	59% 37%
45	OE	449	5% 62% 34%
45	OG	449	64% 33%
45	OI	449	6% 64% 33%
45	OK	449	60% 37%
45	OM	449	47% 66% 31%
45	PA	449	40% 56% 39%
45	PC	449	7% 61% 35%
45	PE	449	5% 58% 37%
45	PG	449	5% 58% 37%
45	PI	449	64% 32%
45	PK	449	6% 63% 32%
45	PM	449	59% 66% 29%
45	QA	449	72% 65% 31%
45	QC	449	10% 59% 37%
45	QE	449	60% 36%
45	QG	449	7% 53% 43%
45	QI	449	7% 60% 36%
45	QK	449	6% 61% 35%
45	QM	449	73% 65% 31%
45	RA	449	88% 72% 24%

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Mol	Chain	Length	Quality of chain
45	RC	449	12% 60% 36%
45	RE	449	9% 61% 35%
45	RG	449	9% 60% 36%
45	RI	449	7% 65% 31%
45	RK	449	8% 62% 34%
45	RM	449	67% 65% 31%
45	SA	449	95% 76% 20%
45	SC	449	11% 59% 37%
45	SE	449	7% 59% 37%
45	SG	449	6% 59% 37%
45	SI	449	8% 63% 33%
45	SK	449	6% 57% 39%
45	SM	449	50% 64% 32%
45	TA	449	96% 73% 22%
45	TC	449	17% 55% 41%
45	TE	449	9% 60% 36%
45	TG	449	10% 63% 33%
45	TI	449	10% 66% 30%
45	TK	449	9% 63% 33%
45	TM	449	36% 58% 37%
45	UA	449	94% 75% 21%
45	UC	449	16% 57% 39%
45	UE	449	8% 61% 35%
45	UG	449	10% 65% 31%
45	UI	449	12% 67% 29%

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Mol	Chain	Length	Quality of chain
45	UK	449	10% 63% 33%
45	UM	449	20% 57% 39%
45	VA	449	7% 54% 43%
45	VC	449	7% 65% 33%
45	VE	449	61% 36%
45	VG	449	6% 59% 39%
45	VI	449	5% 61% 35%
45	VK	449	7% 59% 39%
45	VM	449	96% 75% 21%
45	WA	449	5% 59% 37%
45	WC	449	5% 59% 39%
45	WE	449	61% 35%
45	WG	449	5% 61% 37%
45	WI	449	63% 33%
45	WK	449	6% 59% 39%
45	WM	449	70% 69% 27%
46	AB	443	32% 62% 35%
46	AD	443	62% 35%
46	AF	443	63% 34%
46	AH	443	63% 34%
46	AJ	443	68% 29%
46	AL	443	63% 34%
46	AN	443	63% 34%
46	BB	443	89% 70% 27%
46	BD	443	7% 60% 37%

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Mol	Chain	Length	Quality of chain
46	BF	443	5% 63% 34%
46	BH	443	6% 60% 36%
46	BJ	443	67% 30%
46	BL	443	5% 59% 38%
46	BN	443	6% 59% 38%
46	CB	443	13% 56% 42%
46	CD	443	5% 66% 31%
46	CF	443	6% 60% 37%
46	CH	443	60% 37%
46	CJ	443	65% 33%
46	CL	443	8% 60% 37%
46	CN	443	96% 70% 27%
46	DB	443	37% 61% 36%
46	DD	443	62% 35%
46	DF	443	69% 28%
46	DH	443	65% 33%
46	DJ	443	5% 61% 36%
46	DL	443	7% 55% 42%
46	DN	443	94% 75% 22%
46	EB	443	68% 60% 37%
46	ED	443	6% 63% 34%
46	EF	443	5% 58% 39%
46	EH	443	7% 60% 37%
46	EJ	443	5% 62% 35%
46	EL	443	9% 54% 43%

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Mol	Chain	Length	Quality of chain
46	EN	443	93% 67% 30%
46	FB	443	80% 64% 33%
46	FD	443	5% 60% 37%
46	FF	443	62% 35%
46	FH	443	63% 35%
46	FJ	443	66% 31%
46	FL	443	62% 35%
46	FN	443	77% 65% 33%
46	GB	443	90% 70% 28%
46	GD	443	6% 60% 37%
46	GF	443	5% 64% 33%
46	GH	443	65% 33%
46	GJ	443	68% 29%
46	GL	443	66% 31%
46	GN	443	41% 62% 35%
46	HB	443	83% 67% 30%
46	HD	443	62% 35%
46	HF	443	65% 32%
46	HH	443	64% 33%
46	HJ	443	64% 33%
46	HL	443	6% 67% 30%
46	HN	443	17% 59% 38%
46	IB	443	67% 64% 33%
46	ID	443	63% 34%
46	IF	443	72% 25%

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Mol	Chain	Length	Quality of chain
46	IH	443	62% 35%
46	IJ	443	64% 33%
46	IL	443	61% 36%
46	IN	443	5% 58% 39%
46	JB	443	6% 63% 34%
46	JD	443	71% 26%
46	JF	443	68% 29%
46	JH	443	67% 30%
46	JJ	443	66% 31%
46	JL	443	64% 33%
46	JN	443	6% 60% 37%
46	KB	443	5% 64% 33%
46	KD	443	65% 32%
46	KF	443	65% 31%
46	KH	443	70% 27%
46	KJ	443	66% 31%
46	KL	443	65% 32%
46	KN	443	63% 34%
46	LB	443	64% 33%
46	LD	443	68% 29%
46	LF	443	70% 28%
46	LH	443	67% 30%
46	LJ	443	66% 31%
46	LL	443	65% 32%
46	LN	443	67% 30%

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Mol	Chain	Length	Quality of chain
46	MB	443	5% 63% 34%
46	MD	443	64% 33%
46	MF	443	69% 28%
46	MH	443	69% 28%
46	MJ	443	60% 37%
46	ML	443	70% 27%
46	MN	443	67% 30%
46	NB	443	30% 56% 39% 5%
46	ND	443	8% 60% 37%
46	NF	443	65% 31% 5%
46	NH	443	7% 60% 36%
46	NJ	443	5% 61% 34% 5%
46	NL	443	6% 60% 37%
46	NN	443	8% 63% 33% 5%
46	OB	443	67% 59% 37%
46	OD	443	8% 59% 38%
46	OF	443	5% 65% 32%
46	OH	443	5% 65% 32%
46	OJ	443	7% 62% 35%
46	OL	443	5% 65% 32%
46	ON	443	9% 60% 37%
46	PB	443	89% 71% 26%
46	PD	443	15% 55% 42%
46	PF	443	7% 63% 34%
46	PH	443	8% 60% 37%

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Mol	Chain	Length	Quality of chain
46	PJ	443	7% 61% 36%
46	PL	443	7% 59% 38%
46	PN	443	12% 54% 42%
46	QB	443	21% 54% 43%
46	QD	443	9% 63% 33%
46	QF	443	7% 62% 35%
46	QH	443	7% 57% 40%
46	QJ	443	7% 63% 34%
46	QL	443	13% 54% 43%
46	QN	443	97% 76% 21%
46	RB	443	29% 55% 42%
46	RD	443	9% 58% 39%
46	RF	443	8% 58% 39%
46	RH	443	7% 58% 40%
46	RJ	443	8% 59% 38%
46	RL	443	14% 54% 43%
46	RN	443	97% 77% 20%
46	SB	443	41% 56% 41%
46	SD	443	7% 57% 40%
46	SF	443	7% 58% 39%
46	SH	443	8% 60% 37%
46	SJ	443	8% 60% 37%
46	SL	443	11% 55% 42%
46	SN	443	97% 73% 24%
46	TB	443	62% 58% 39%

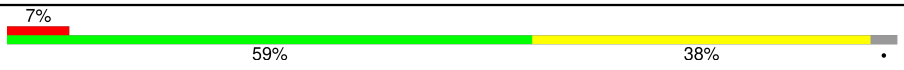
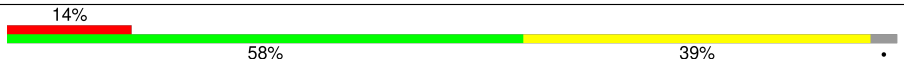
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Mol	Chain	Length	Quality of chain
46	TD	443	10% 62% 35%
46	TF	443	8% 55% 42%
46	TH	443	12% 58% 39%
46	TJ	443	10% 58% 39%
46	TL	443	12% 53% 44%
46	TN	443	94% 72% 26%
46	UB	443	54% 56% 41%
46	UD	443	11% 61% 36%
46	UF	443	9% 57% 40%
46	UH	443	12% 58% 39%
46	UJ	443	10% 55% 42%
46	UL	443	12% 49% 48%
46	UN	443	76% 58% 39%
46	VB	443	37% 54% 43%
46	VD	443	5% 60% 37%
46	VF	443	60% 37%
46	VH	443	5% 56% 41%
46	VJ	443	5% 59% 38%
46	VL	443	5% 55% 42%
46	VN	443	40% 53% 44%
46	WB	443	31% 59% 38%
46	WD	443	5% 58% 39%
46	WF	443	5% 58% 39%
46	WH	443	6% 60% 37%
46	WJ	443	5% 60% 37%

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Mol	Chain	Length	Quality of chain
46	WL	443	
46	WN	443	

2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 1325153 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 RIB27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0A	152	Total	C	N	O	S	0	0
			1229	776	224	228	1		
1	1A	152	Total	C	N	O	S	0	0
			1229	776	224	228	1		
1	2A	152	Total	C	N	O	S	0	0
			1229	776	224	228	1		
1	3A	152	Total	C	N	O	S	0	0
			1229	776	224	228	1		

- Molecule 2 is a protein called RIB38.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0B	321	Total	C	N	O	S	0	0
			2615	1634	472	502	7		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0B	10	THR	SER	conflict	UNP Q23JL9
0B	11	ALA	THR	conflict	UNP Q23JL9
0B	12	LEU	ALA	conflict	UNP Q23JL9
0B	13	MET	LEU	conflict	UNP Q23JL9
0B	36	SER	THR	conflict	UNP Q23JL9

- Molecule 3 is a protein called CFAM166B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0C	95	Total	C	N	O	S	0	0
			747	471	131	143	2		
3	1C	95	Total	C	N	O	S	0	0
			747	471	131	143	2		

- Molecule 4 is a protein called CFAM166A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	0D	202	Total	C	N	O	S	1	0
			1619	1018	292	307	2		
4	1D	202	Total	C	N	O	S	1	0
			1619	1018	292	307	2		
4	2D	202	Total	C	N	O	S	1	0
			1619	1018	292	307	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0D	86	ALA	THR	conflict	UNP Q238X3
0D	87	GLU	GLN	conflict	UNP Q238X3
1D	86	ALA	THR	conflict	UNP Q238X3
1D	87	GLU	GLN	conflict	UNP Q238X3
2D	86	ALA	THR	conflict	UNP Q238X3
2D	87	GLU	GLN	conflict	UNP Q238X3

- Molecule 5 is a protein called RIB22.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	0E	189	Total	C	N	O	S	0	0
			1557	978	280	294	5		
5	1E	189	Total	C	N	O	S	0	0
			1557	978	280	294	5		
5	2E	189	Total	C	N	O	S	0	0
			1557	978	280	294	5		
5	3E	189	Total	C	N	O	S	0	0
			1557	978	280	294	5		

- Molecule 6 is a protein called CFAM166C.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	0F	206	Total	C	N	O	S	0	0
			1665	1048	300	314	3		

- Molecule 7 is a protein called CFAP107.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	0G	168	Total	C	N	O	S	0	0
			1378	871	237	265	5		
7	1G	135	Total	C	N	O	S	0	0
			1109	702	190	214	3		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0G	127	ALA	LEU	conflict	UNP Q237T1
0G	128	LEU	SER	conflict	UNP Q237T1
0G	129	SER	ALA	conflict	UNP Q237T1
0G	130	ALA	SER	conflict	UNP Q237T1
0G	131	SER	ALA	conflict	UNP Q237T1
0G	140	PHE	TYR	conflict	UNP Q237T1
1G	127	ALA	LEU	conflict	UNP Q237T1
1G	128	LEU	SER	conflict	UNP Q237T1
1G	129	SER	ALA	conflict	UNP Q237T1
1G	130	ALA	SER	conflict	UNP Q237T1
1G	131	SER	ALA	conflict	UNP Q237T1
1G	140	PHE	TYR	conflict	UNP Q237T1

- Molecule 8 is a protein called CFAP127.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	0H	120	Total	C	N	O	S	0	0
			1046	654	189	198	5		
8	1H	425	Total	C	N	O	S	0	0
			3706	2281	691	720	14		

- Molecule 9 is a protein called CFAP161A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	0N	280	Total	C	N	O	S	0	0
			2305	1455	396	441	13		
9	1N	463	Total	C	N	O	S	0	0
			3805	2414	653	723	15		
9	2N	280	Total	C	N	O	S	0	0
			2305	1455	396	441	13		

- Molecule 10 is a protein called CFAP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	0Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
10	1Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
10	2Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	3Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
10	4Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
10	5Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
10	6Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		

- Molecule 11 is a protein called Parkin co-regulated protein PACRGA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	0S	288	Total	C	N	O	S	0	0
			2310	1485	397	422	6		
11	1S	288	Total	C	N	O	S	0	0
			2310	1485	397	422	6		
11	2S	288	Total	C	N	O	S	0	0
			2310	1485	397	422	6		
11	3S	288	Total	C	N	O	S	0	0
			2310	1485	397	422	6		

- Molecule 12 is a protein called IJ34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	0T	261	Total	C	N	O	S	0	0
			2124	1351	373	391	9		
12	1T	285	Total	C	N	O	S	0	0
			2321	1471	411	430	9		
12	2T	285	Total	C	N	O	S	0	0
			2321	1471	411	430	9		
12	3T	285	Total	C	N	O	S	0	0
			2321	1471	411	430	9		

- Molecule 13 is a protein called CFAP52A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	0U	607	Total	C	N	O	S	0	0
			4774	3025	819	906	24		
13	1U	607	Total	C	N	O	S	0	0
			4774	3025	819	906	24		
13	2U	607	Total	C	N	O	S	0	0
			4774	3025	819	906	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	3U	607	Total	C	N	O	S	0	0
			4774	3025	819	906	24		

- Molecule 14 is a protein called DNA polymerase delta C4-type zinc-finger protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	0V	212	Total	C	N	O	S	0	0
			1750	1095	317	332	6		
14	1V	263	Total	C	N	O	S	0	0
			2168	1359	388	412	9		
14	2V	263	Total	C	N	O	S	0	0
			2168	1359	388	412	9		
14	3V	263	Total	C	N	O	S	0	0
			2168	1359	388	412	9		

- Molecule 15 is a protein called RIB43A protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	0X	110	Total	C	N	O	S	0	0
			935	570	175	185	5		
15	1X	141	Total	C	N	O	S	0	0
			1202	732	227	237	6		
15	2X	141	Total	C	N	O	S	0	0
			1202	732	227	237	6		
15	3X	141	Total	C	N	O	S	0	0
			1202	732	227	237	6		
15	4X	141	Total	C	N	O	S	0	0
			1202	732	227	237	6		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0X	13	SER	PRO	conflict	UNP A4VDZ5
0X	14	ASP	HIS	conflict	UNP A4VDZ5
1X	13	SER	PRO	conflict	UNP A4VDZ5
1X	14	ASP	HIS	conflict	UNP A4VDZ5
2X	13	SER	PRO	conflict	UNP A4VDZ5
2X	14	ASP	HIS	conflict	UNP A4VDZ5
3X	13	SER	PRO	conflict	UNP A4VDZ5
3X	14	ASP	HIS	conflict	UNP A4VDZ5
4X	13	SER	PRO	conflict	UNP A4VDZ5
4X	14	ASP	HIS	conflict	UNP A4VDZ5

- Molecule 16 is a protein called RIB57.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1B	498	Total	C	N	O	S	0	0
			4066	2598	692	768	8		
16	2B	295	Total	C	N	O	S	0	0
			2439	1553	416	464	6		
16	3B	295	Total	C	N	O	S	0	0
			2437	1552	416	463	6		

- Molecule 17 is a protein called CFAP182A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1F	136	Total	C	N	O	S	0	0
			1093	696	184	208	5		

- Molecule 18 is a protein called CFAP143.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1I	188	Total	C	N	O	S	0	0
			1546	951	285	306	4		

- Molecule 19 is a protein called CFAP21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1J	370	Total	C	N	O	S	0	0
			3025	1901	533	580	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1J	322	ASP	ASN	conflict	UNP I7MLS4

- Molecule 20 is a protein called CFAP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1K	277	Total	C	N	O	S	0	0
			2425	1500	452	466	7		
20	2K	288	Total	C	N	O	S	0	0
			2506	1547	460	492	7		

- Molecule 21 is a protein called CFAP115.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1L	820	Total	C	N	O	S	0	0
			6842	4358	1186	1280	18		
21	2L	616	Total	C	N	O	S	0	0
			5151	3286	896	957	12		
21	3L	200	Total	C	N	O	S	0	0
			1660	1053	284	317	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1L	863	GLU	GLY	conflict	UNP Q23KF9
1L	864	ALA	GLU	conflict	UNP Q23KF9
2L	863	GLU	GLY	conflict	UNP Q23KF9
2L	864	ALA	GLU	conflict	UNP Q23KF9
3L	863	GLU	GLY	conflict	UNP Q23KF9
3L	864	ALA	GLU	conflict	UNP Q23KF9

- Molecule 22 is a protein called Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1M	369	Total	C	N	O	S	0	0
			2978	1910	501	552	15		
22	2M	369	Total	C	N	O	S	0	0
			2978	1910	501	552	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1O	241	Total	C	N	O	S	0	0
			2032	1266	359	395	12		
23	2O	370	Total	C	N	O	S	0	0
			3173	1948	595	617	13		
23	3O	279	Total	C	N	O	S	0	0
			2397	1471	456	466	4		

- Molecule 24 is a protein called CFAP210.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1P	355	Total	C	N	O	S	0	0
			3060	1889	575	588	8		
24	2P	190	Total	C	N	O	S	0	0
			1633	1005	309	313	6		

- Molecule 25 is a protein called RIB72B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1R	508	Total	C	N	O	S	0	0
			4244	2744	711	777	12		
25	2R	508	Total	C	N	O	S	0	0
			4244	2744	711	777	12		
25	3R	508	Total	C	N	O	S	0	0
			4244	2744	711	777	12		

- Molecule 26 is a protein called Protofilament ribbon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1W	224	Total	C	N	O	S	0	0
			1924	1167	380	368	9		
26	2W	116	Total	C	N	O	S	0	0
			990	611	189	184	6		

- Molecule 27 is a protein called RIB35.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2C	300	Total	C	N	O	S	0	0
			2467	1581	417	464	5		
27	3C	300	Total	C	N	O	S	0	0
			2467	1581	417	464	5		
27	4C	300	Total	C	N	O	S	0	0
			2467	1581	417	464	5		

- Molecule 28 is a protein called CFAP182B.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2F	87	Total	C	N	O	S	0	0
			746	469	136	137	4		

- Molecule 29 is a protein called Flagellar FliJ protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2G	99	Total	C	N	O	S	0	0
			848	536	153	155	4		

- Molecule 30 is a protein called RIB27B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	2H	61	Total	C	N	O	S	0	0
			501	313	92	94	2		
30	3H	61	Total	C	N	O	S	0	0
			501	313	92	94	2		
30	4H	61	Total	C	N	O	S	0	0
			501	313	92	94	2		

- Molecule 31 is a protein called STPG2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2I	142	Total	C	N	O	S	0	0
			1150	736	204	209	1		
31	3I	87	Total	C	N	O	S	0	0
			712	451	130	127	4		

- Molecule 32 is a protein called RIB26.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	3D	237	Total	C	N	O	S	0	0
			1835	1174	310	340	11		

- Molecule 33 is a protein called CFAP129.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	4F	200	Total	C	N	O	S	0	0
			1618	1022	286	308	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4F	70	VAL	ASP	conflict	UNP I7M9I4

- Molecule 34 is a protein called Flagellar microtubule protofilament ribbon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	4R	609	Total	C	N	O	S	0	0
			5070	3267	847	932	24		
34	5R	609	Total	C	N	O	S	0	0
			5070	3267	847	932	24		
34	6R	609	Total	C	N	O	S	0	0
			5070	3267	847	932	24		
34	7R	609	Total	C	N	O	S	0	0
			5070	3267	847	932	24		

- Molecule 35 is a protein called Parkin co-regulated protein PACRGB.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4S	188	Total	C	N	O	S	0	0
			1537	999	251	279	8		
35	5S	188	Total	C	N	O	S	0	0
			1537	999	251	279	8		

- Molecule 36 is a protein called OJ2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	5A	157	Total	C	N	O	S	0	0
			1261	795	234	229	3		
36	5B	157	Total	C	N	O	S	0	0
			1261	795	234	229	3		
36	5C	157	Total	C	N	O	S	0	0
			1261	795	234	229	3		
36	5D	114	Total	C	N	O	S	0	0
			908	571	165	169	3		

- Molecule 37 is a protein called CFAP77A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	5E	188	Total	C	N	O	S	0	0
			1566	992	281	288	5		
37	5F	210	Total	C	N	O	S	0	0
			1750	1107	316	322	5		
37	5G	210	Total	C	N	O	S	0	0
			1750	1107	316	322	5		
37	5H	146	Total	C	N	O	S	0	0
			1210	764	217	225	4		

- Molecule 38 is a protein called OJ3.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	5I	103	Total	C	N	O	0	0
			515	309	103	103		
38	5J	109	Total	C	N	O	0	0
			545	327	109	109		
38	5K	80	Total	C	N	O	0	0
			400	240	80	80		

- Molecule 39 is a protein called SB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	6F	132	Total	C	N	O	S	0	0
			1140	718	197	221	4		

- Molecule 40 is a protein called STPG1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	6G	216	Total	C	N	O	S	0	0
			1769	1128	303	333	5		

- Molecule 41 is a protein called Nebulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	6H	165	Total	C	N	O	S	0	0
			1362	857	234	266	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6H	186	HIS	GLN	conflict	UNP Q231B6
6H	198	HIS	MET	conflict	UNP Q231B6

- Molecule 42 is a protein called B5B6_fMIP.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	8L	385	Total	C	N	O	0	0
			1925	1155	385	385		
42	8N	358	Total	C	N	O	0	0
			1790	1074	358	358		

- Molecule 43 is a protein called CFAP112A.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	8P	363	Total	C	N	O	0	0
			1815	1089	363	363		

- Molecule 44 is a protein called B2B3_fMIP.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	8R	361	Total	C	N	O	0	0
			2020	1269	361	390		

- Molecule 45 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	AC	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	AE	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	AG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	AI	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	AK	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	AM	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	BA	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	BC	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	BE	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	BG	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	BI	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	BK	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	BM	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	CA	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	CC	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	CG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	CI	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	CK	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	CM	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	DA	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	DE	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	DG	436	Total	C	N	O	S	0	0
			3389	2143	576	648	22		
45	DI	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	DK	436	Total	C	N	O	S	0	0
			3389	2143	576	648	22		
45	DM	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	EA	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	EC	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	EE	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	EG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	EI	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	EK	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	EM	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	FA	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	FC	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	FE	434	Total	C	N	O	S	0	0
			3376	2135	573	646	22		
45	FG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	FI	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	FK	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	FM	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	GA	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	GC	431	Total	C	N	O	S	0	0
			3358	2126	570	640	22		
45	GE	431	Total	C	N	O	S	0	0
			3358	2126	570	640	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	GG	431	Total	C	N	O	S	0	0
			3358	2126	570	640	22		
45	GI	431	Total	C	N	O	S	0	0
			3358	2126	570	640	22		
45	GK	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	GM	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	HA	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	HC	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	HE	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	HG	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	HI	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	HK	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	HM	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	IA	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	IC	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	IE	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	IG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	II	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	IK	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	IM	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	JA	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	JC	434	Total	C	N	O	S	0	0
			3376	2135	573	646	22		
45	JE	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	JG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	JI	439	Total	C	N	O	S	0	0
			3404	2151	579	652	22		
45	JK	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	JM	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	KA	434	Total	C	N	O	S	0	0
			3376	2135	573	646	22		
45	KC	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	KE	435	Total	C	N	O	S	0	0
			3385	2141	575	647	22		
45	KG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	KI	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	KK	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	KM	434	Total	C	N	O	S	0	0
			3376	2135	573	646	22		
45	LA	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	LC	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	LE	438	Total	C	N	O	S	0	0
			3400	2149	578	651	22		
45	LG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	LI	434	Total	C	N	O	S	0	0
			3381	2139	574	646	22		
45	LK	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	LM	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	MA	436	Total	C	N	O	S	0	0
			3392	2145	576	649	22		
45	MC	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	ME	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	MG	437	Total	C	N	O	S	0	0
			3400	2151	577	650	22		
45	MI	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	MK	436	Total	C	N	O	S	0	0
			3384	2139	575	648	22		
45	MM	436	Total	C	N	O	S	0	0
			3392	2145	576	649	22		
45	NA	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	NC	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	NE	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	NG	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	NI	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	NK	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	NM	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	OA	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	OC	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	OE	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	OG	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	OI	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	OK	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	OM	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	PA	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	PC	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	PE	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	PG	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	PI	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	PK	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	PM	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	QA	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	QC	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	QE	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	QG	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	QI	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	QK	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	QM	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	RA	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	RC	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	RE	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	RG	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	RI	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	RK	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	RM	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	SA	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	SC	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	SE	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	SG	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	SI	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	SK	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	SM	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	TA	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	TC	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	TE	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	TG	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	TI	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	TK	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	TM	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
45	UA	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	UC	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	UE	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	UG	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	UI	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	UK	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	UM	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	VA	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	VC	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	VE	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	VG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	VI	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	VK	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	VM	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	WA	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	WC	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	WE	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	WG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	WI	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	WK	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	WM	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	CE	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
45	DC	436	Total	C	N	O	S	0	0
			3389	2143	576	648	22		

- Molecule 46 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	AD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	AF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	AH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	AJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	AL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	AN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	CB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	CD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	CF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	CH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	CJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	CL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	CN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	DB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	DD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	DF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	DH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	DJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	DL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	DN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	EB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	ED	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	EF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	EH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	EJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	EL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	EN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	FB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	FD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	FF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	FH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	FJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	FL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	FN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	GB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	GD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	GF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	GH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	GJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	GL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	GN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	HB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	HD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	HF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	HH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	HJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	HL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	HN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	IB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	ID	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	IF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	IH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	IJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	IL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	IN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	JB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	JD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	JF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	JH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	JJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	JL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	JN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	KB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	KD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	KF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	KH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	KJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	KL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	KN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	LB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	LD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	LF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	LH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	LJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	LL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	LN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	MB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	MD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	MF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	MH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	MJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	ML	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	MN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	NB	423	Total	C	N	O	S	0	0
			3304	2079	562	635	28		
46	ND	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	NF	423	Total	C	N	O	S	0	0
			3304	2079	562	635	28		
46	NH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	NJ	423	Total	C	N	O	S	0	0
			3304	2079	562	635	28		
46	NL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	NN	423	Total	C	N	O	S	0	0
			3304	2079	562	635	28		
46	OB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	OD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	OF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	OH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	OJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	OL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	ON	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	PB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	PD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	PF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	PH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	PJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	PL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	PN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	QB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	QD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	QF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	QH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	QJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	QL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	QN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	RB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	RD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	RF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	RH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	RJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	RL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	RN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	SB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	SD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	SF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	SH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	SJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	SL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

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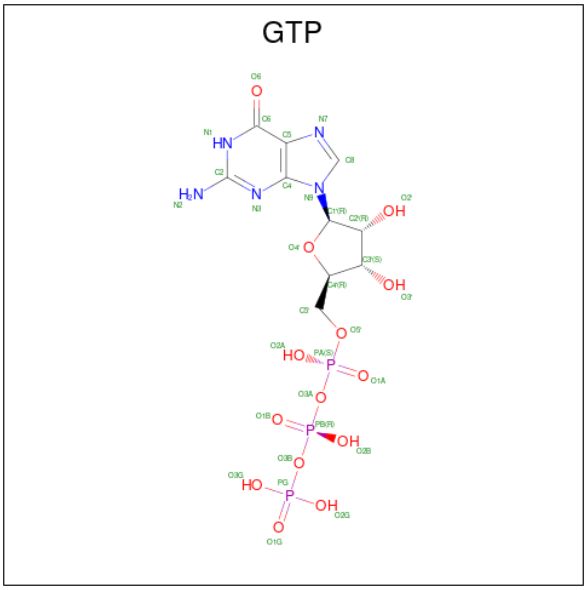
Mol	Chain	Residues	Atoms					AltConf	Trace
46	SN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	TB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	TD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	TF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	TH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	TJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	TL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	TN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	UB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	UD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	UF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	UH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	UJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	UL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	UN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	VN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

- Molecule 47 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
47	AA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	AC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
47	AG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	AI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	AK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	AM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	CA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	CC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	CG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	CI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	CK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	CM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	DA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	DE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	DG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	DI	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
47	DK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	DM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	EA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	EC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	EE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	EG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	EI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	EK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	EM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	FA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	FC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	FE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	FG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	FI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	FK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	FM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	GA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	GC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	GE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	GG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	GI	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
47	GK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	GM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	HA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	HC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	HE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	HG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	HI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	HK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	HM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	IA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	IC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	IE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	IG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	II	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	IK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	IM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	JA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	JC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	JE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	JG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	JI	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
47	JK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	JM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	KA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	KC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	KE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	KG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	KI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	KK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	KM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	LA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	LC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	LE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	LG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	LI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	LK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	LM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	MA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	MC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	ME	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	MG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	MI	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
47	MK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	MM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	NA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	NC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	NE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	NG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	NI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	NK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	NM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	OA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	OC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	OF	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	OG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	OI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	OK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	OM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	PA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	PD	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	PE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	PG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	PI	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
47	PK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	PM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	QA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	QC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	QE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	QG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	QI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	QK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	QM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	RA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	RC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	RE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	RG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	RI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	RK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	RM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	SA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	SC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	SE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	SG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	SI	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
47	SK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	SM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	TA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	TC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	TE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	TG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	TI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	TK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	TM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	UA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	UC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	UE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	UG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	UI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	UK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	UM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	VA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	VC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	VE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	VG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	VI	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
47	VK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	VM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	WA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	WC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	WE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	WG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	WI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	WK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	WM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	CE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	DC	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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Mol	Chain	Residues	Atoms	AltConf
48	BC	1	Total Mg 1 1	0
48	BE	1	Total Mg 1 1	0
48	BG	1	Total Mg 1 1	0
48	BI	1	Total Mg 1 1	0
48	BK	1	Total Mg 1 1	0
48	BM	1	Total Mg 1 1	0
48	CA	1	Total Mg 1 1	0
48	CC	1	Total Mg 1 1	0
48	CG	1	Total Mg 1 1	0
48	CI	1	Total Mg 1 1	0
48	CK	1	Total Mg 1 1	0
48	CM	1	Total Mg 1 1	0
48	DA	1	Total Mg 1 1	0
48	DE	1	Total Mg 1 1	0
48	DG	1	Total Mg 1 1	0
48	DI	1	Total Mg 1 1	0
48	DK	1	Total Mg 1 1	0
48	DM	1	Total Mg 1 1	0
48	EA	1	Total Mg 1 1	0
48	EC	1	Total Mg 1 1	0
48	EE	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
48	EG	1	Total Mg 1 1	0
48	EI	1	Total Mg 1 1	0
48	EK	1	Total Mg 1 1	0
48	EM	1	Total Mg 1 1	0
48	FA	1	Total Mg 1 1	0
48	FC	1	Total Mg 1 1	0
48	FE	1	Total Mg 1 1	0
48	FG	1	Total Mg 1 1	0
48	FI	1	Total Mg 1 1	0
48	FL	1	Total Mg 1 1	0
48	FM	1	Total Mg 1 1	0
48	GB	1	Total Mg 1 1	0
48	GC	1	Total Mg 1 1	0
48	GE	1	Total Mg 1 1	0
48	GG	1	Total Mg 1 1	0
48	GI	1	Total Mg 1 1	0
48	GL	1	Total Mg 1 1	0
48	GN	1	Total Mg 1 1	0
48	HA	1	Total Mg 1 1	0
48	HC	1	Total Mg 1 1	0
48	HE	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
48	HG	1	Total Mg 1 1	0
48	HI	1	Total Mg 1 1	0
48	HK	1	Total Mg 1 1	0
48	HM	1	Total Mg 1 1	0
48	IA	1	Total Mg 1 1	0
48	IC	1	Total Mg 1 1	0
48	IE	1	Total Mg 1 1	0
48	IG	1	Total Mg 1 1	0
48	II	1	Total Mg 1 1	0
48	IK	1	Total Mg 1 1	0
48	IM	1	Total Mg 1 1	0
48	JA	1	Total Mg 1 1	0
48	JC	1	Total Mg 1 1	0
48	JE	1	Total Mg 1 1	0
48	JG	1	Total Mg 1 1	0
48	JI	1	Total Mg 1 1	0
48	JK	1	Total Mg 1 1	0
48	JM	1	Total Mg 1 1	0
48	KA	1	Total Mg 1 1	0
48	KC	1	Total Mg 1 1	0
48	KE	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
48	KG	1	Total Mg 1 1	0
48	KI	1	Total Mg 1 1	0
48	KK	1	Total Mg 1 1	0
48	KM	1	Total Mg 1 1	0
48	LA	1	Total Mg 1 1	0
48	LC	1	Total Mg 1 1	0
48	LE	1	Total Mg 1 1	0
48	LG	1	Total Mg 1 1	0
48	LI	1	Total Mg 1 1	0
48	LK	1	Total Mg 1 1	0
48	LM	1	Total Mg 1 1	0
48	MA	1	Total Mg 1 1	0
48	MC	1	Total Mg 1 1	0
48	ME	1	Total Mg 1 1	0
48	MG	1	Total Mg 1 1	0
48	MI	1	Total Mg 1 1	0
48	MK	1	Total Mg 1 1	0
48	MM	1	Total Mg 1 1	0
48	NA	1	Total Mg 1 1	0
48	ND	1	Total Mg 1 1	0
48	NE	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
48	NG	1	Total Mg 1 1	0
48	NI	1	Total Mg 1 1	0
48	NK	1	Total Mg 1 1	0
48	NM	1	Total Mg 1 1	0
48	OA	1	Total Mg 1 1	0
48	OC	1	Total Mg 1 1	0
48	OE	1	Total Mg 1 1	0
48	OG	1	Total Mg 1 1	0
48	OI	1	Total Mg 1 1	0
48	OK	1	Total Mg 1 1	0
48	OM	1	Total Mg 1 1	0
48	PA	1	Total Mg 1 1	0
48	PC	1	Total Mg 1 1	0
48	PE	1	Total Mg 1 1	0
48	PG	1	Total Mg 1 1	0
48	PI	1	Total Mg 1 1	0
48	PK	1	Total Mg 1 1	0
48	PN	1	Total Mg 1 1	0
48	QA	1	Total Mg 1 1	0
48	QC	1	Total Mg 1 1	0
48	QE	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
48	QG	1	Total Mg 1 1	0
48	QI	1	Total Mg 1 1	0
48	QK	1	Total Mg 1 1	0
48	QM	1	Total Mg 1 1	0
48	RA	1	Total Mg 1 1	0
48	RC	1	Total Mg 1 1	0
48	RD	1	Total Mg 1 1	0
48	RG	1	Total Mg 1 1	0
48	RI	1	Total Mg 1 1	0
48	RK	1	Total Mg 1 1	0
48	RM	1	Total Mg 1 1	0
48	SA	1	Total Mg 1 1	0
48	SC	1	Total Mg 1 1	0
48	SE	1	Total Mg 1 1	0
48	SG	1	Total Mg 1 1	0
48	SI	1	Total Mg 1 1	0
48	SK	1	Total Mg 1 1	0
48	SM	1	Total Mg 1 1	0
48	TA	1	Total Mg 1 1	0
48	TB	1	Total Mg 1 1	0
48	TE	1	Total Mg 1 1	0

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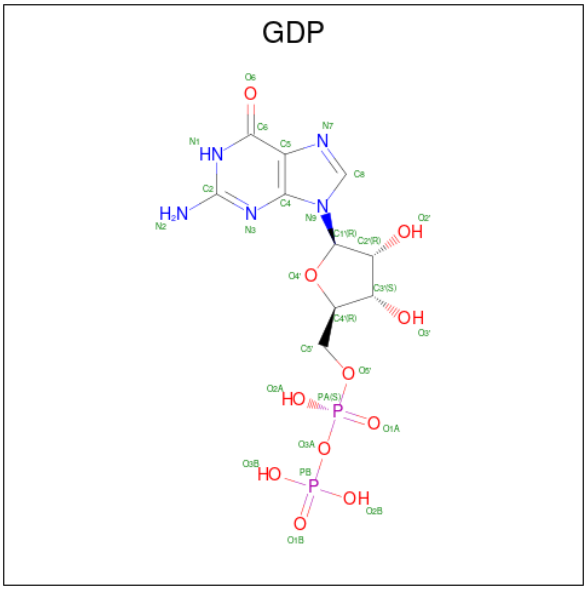
Mol	Chain	Residues	Atoms	AltConf
48	TF	1	Total Mg 1 1	0
48	TI	1	Total Mg 1 1	0
48	TK	1	Total Mg 1 1	0
48	TL	1	Total Mg 1 1	0
48	UA	1	Total Mg 1 1	0
48	UC	1	Total Mg 1 1	0
48	UE	1	Total Mg 1 1	0
48	UG	1	Total Mg 1 1	0
48	UI	1	Total Mg 1 1	0
48	UK	1	Total Mg 1 1	0
48	UM	1	Total Mg 1 1	0
48	VA	1	Total Mg 1 1	0
48	VC	1	Total Mg 1 1	0
48	VE	1	Total Mg 1 1	0
48	VG	1	Total Mg 1 1	0
48	VI	1	Total Mg 1 1	0
48	VK	1	Total Mg 1 1	0
48	VM	1	Total Mg 1 1	0
48	WA	1	Total Mg 1 1	0
48	WC	1	Total Mg 1 1	0
48	WE	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
48	WG	1	Total Mg 1 1	0
48	WI	1	Total Mg 1 1	0
48	WK	1	Total Mg 1 1	0
48	WM	1	Total Mg 1 1	0
48	CE	1	Total Mg 1 1	0
48	DC	1	Total Mg 1 1	0

- Molecule 49 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
49	AB	1	Total C N O P 28 10 5 11 2	0
49	AD	1	Total C N O P 28 10 5 11 2	0
49	AF	1	Total C N O P 28 10 5 11 2	0
49	AH	1	Total C N O P 28 10 5 11 2	0
49	AJ	1	Total C N O P 28 10 5 11 2	0

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Mol	Chain	Residues	Atoms					AltConf
49	AL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	AN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	BB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	BD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	BF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	BH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	BJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	BL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	BN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	CB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	CF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	CH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	CJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	CL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	CN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	DB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	DD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	DF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	DH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	DJ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
49	DL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	DN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	EB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	ED	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	EF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	EH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	EJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	EL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	EN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	FB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	FD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	FF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	FH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	FJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	FL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	FN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	GB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	GD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	GF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	GH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	GJ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
49	GL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	GN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	HB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	HD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	HF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	HH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	HJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	HL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	HN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	IB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	ID	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	IF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	IH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	IJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	IL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	IN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	JB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	JD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	JF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	JH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	JJ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
49	JL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	JN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	KB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	KD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	KF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	KH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	KJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	KL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	KN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	LB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	LD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	LF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	LH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	LJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	LL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	LN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	MB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	MD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	MF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	MH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	MJ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
49	ML	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	MN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	NB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	ND	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	NF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	NH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	NJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	NL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	NN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	OB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	OD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	OF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	OH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	OJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	OL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	ON	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	PB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	PD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	PF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	PH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	PJ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
49	PL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	PN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	QB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	QD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	QF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	QH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	QJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	QL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	QN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	RB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	RD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	RF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	RH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	RJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	RL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	RN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	SB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	SD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	SF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	SH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	SJ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
49	SL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	SN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	TB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	TD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	TF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	TH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	TJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	TL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	TN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VJ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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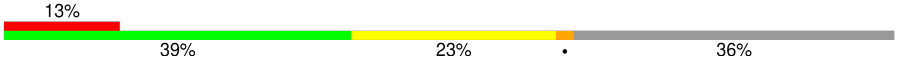
Mol	Chain	Residues	Atoms					AltConf
49	VL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WN	1	Total	C	N	O	P	0
			28	10	5	11	2	

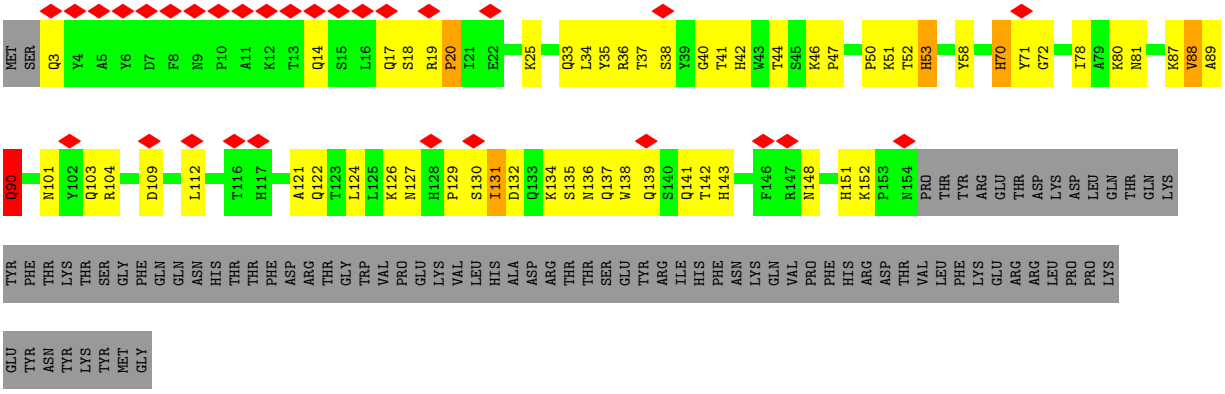
3 Residue-property plots

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

- Molecule 1: RIB27A

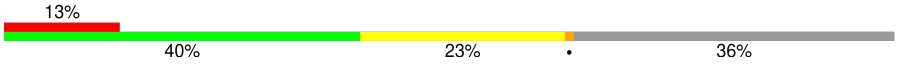
Chain 0A:

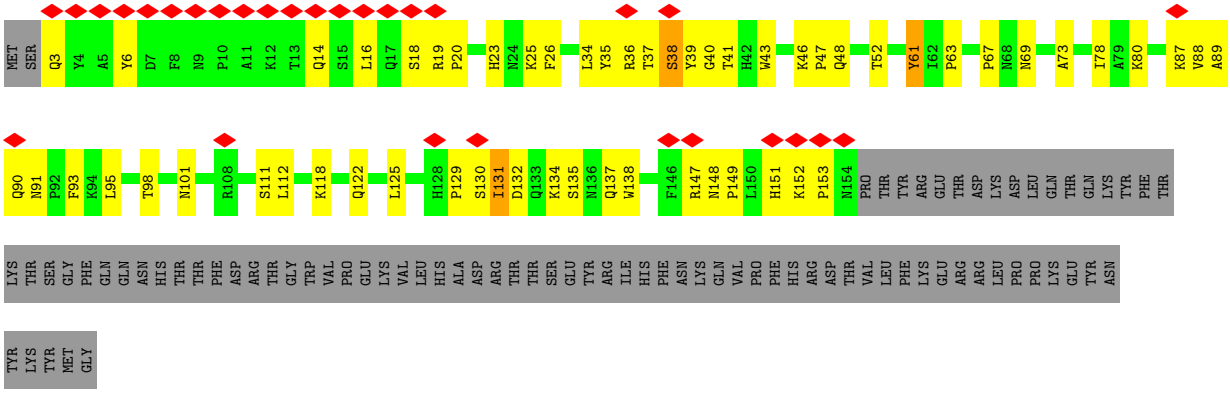




- Molecule 1: RIB27A

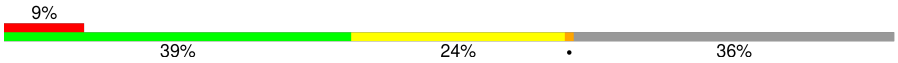
Chain 1A:

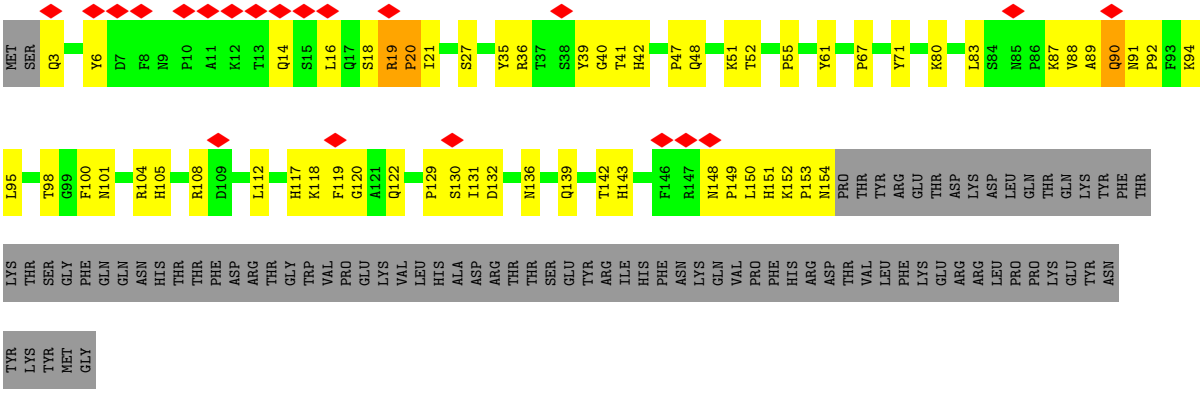




- Molecule 1: RIB27A

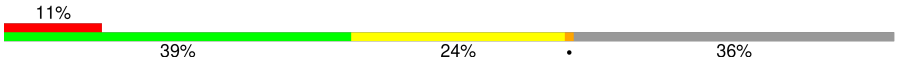
Chain 2A:

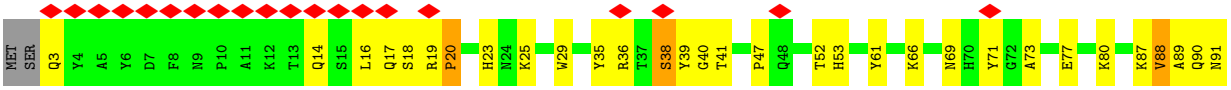




• Molecule 1: RIB27A

Chain 3A:







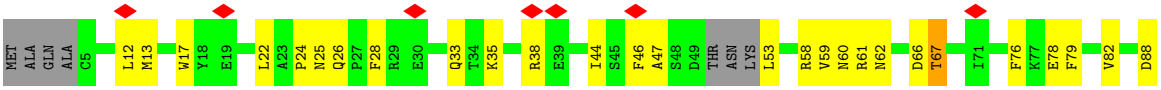


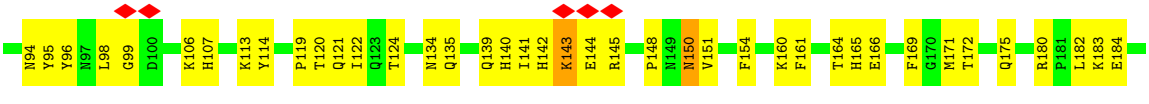


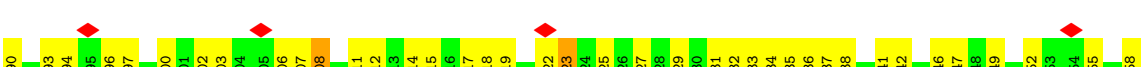
• Molecule 2: RIB38

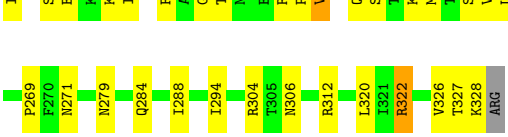
Chain 0B:





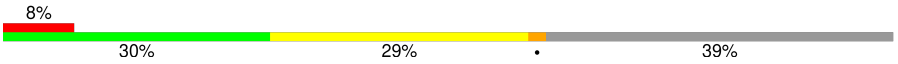


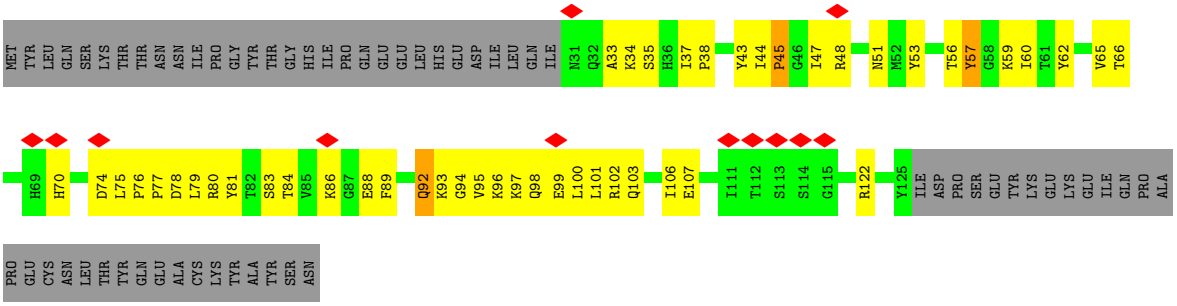




• Molecule 3: CFAM166B

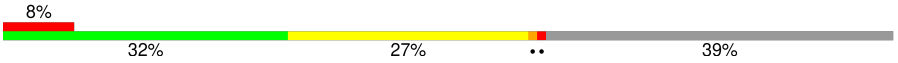
Chain 0C:

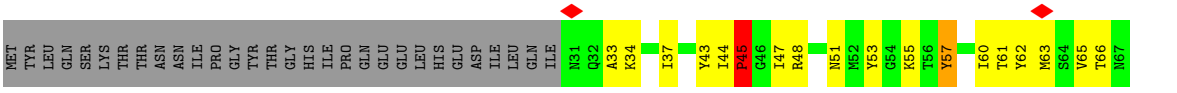


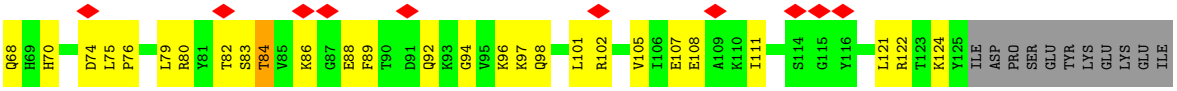


• Molecule 3: CFAM166B

Chain 1C:





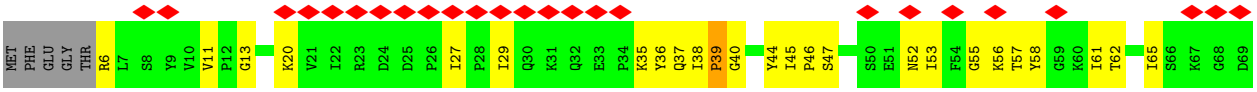


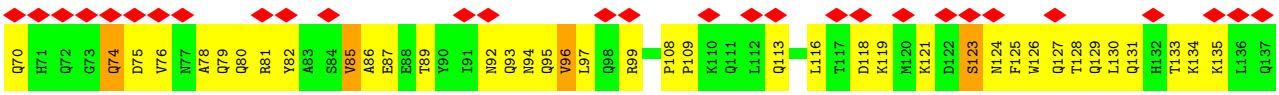


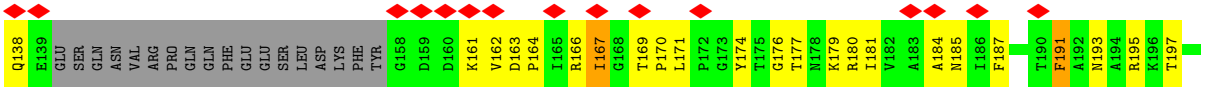
• Molecule 4: CFAM166A

Chain 0D:







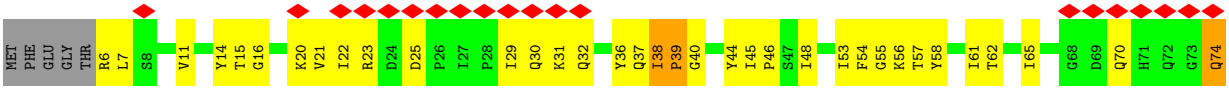


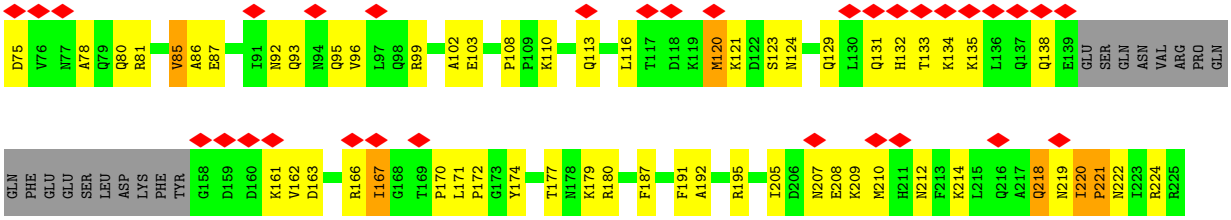


• Molecule 4: CFAM166A

Chain 1D:



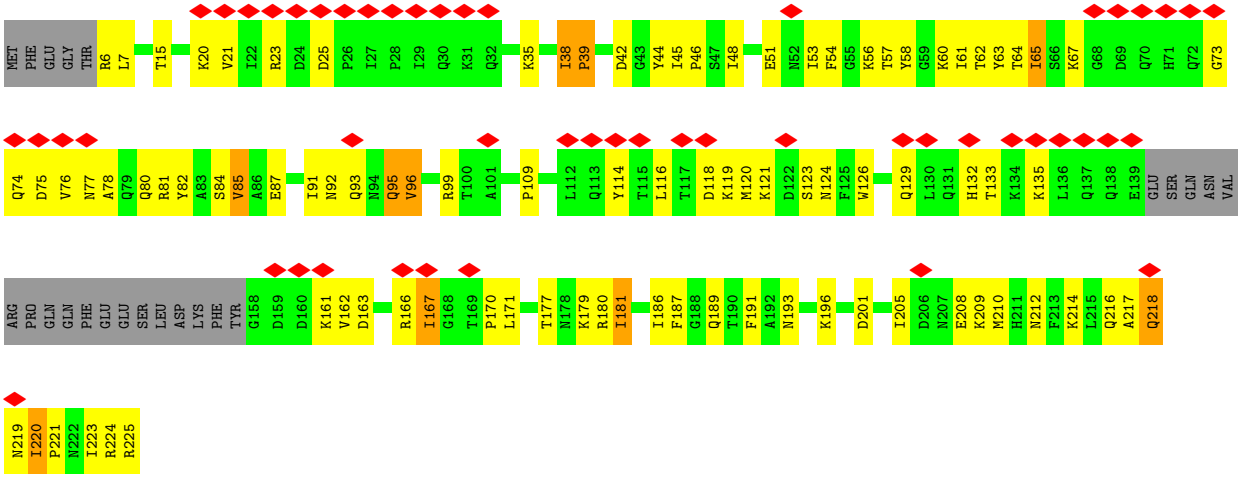




• Molecule 4: CFAM166A

Chain 2D:

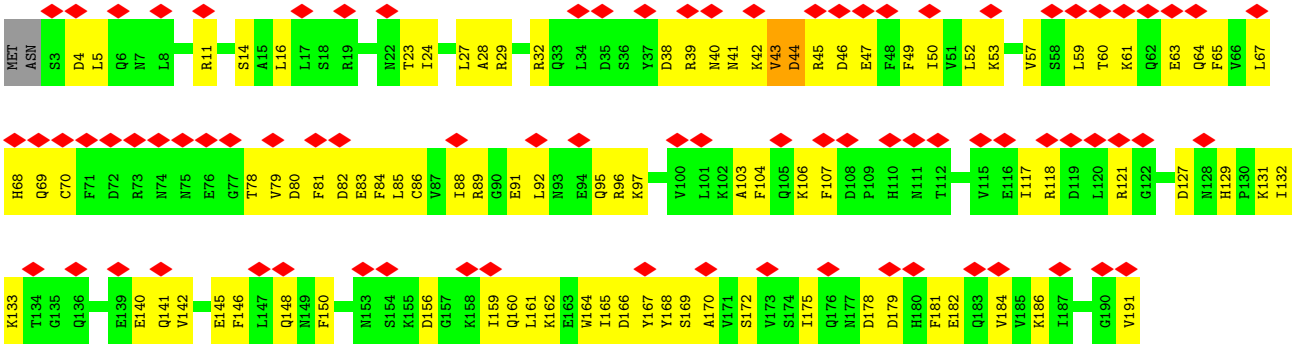




• Molecule 5: RIB22

Chain 0E:

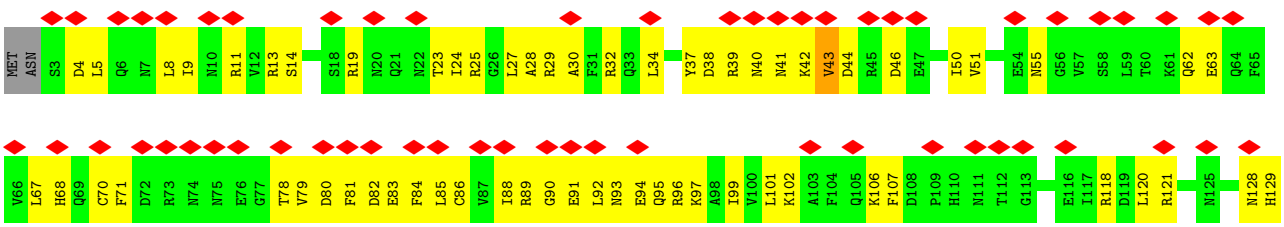


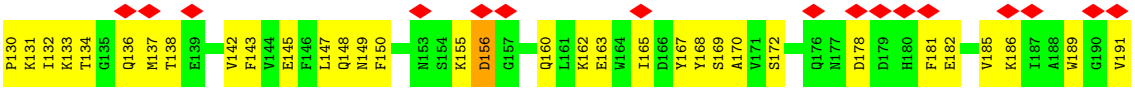


• Molecule 5: RIB22

Chain 1E:



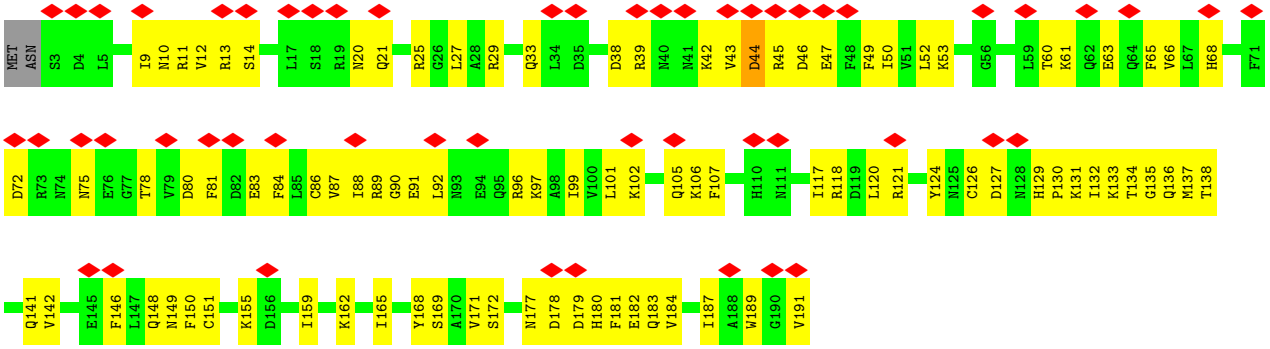




- Molecule 5: RIB22

Chain 2E:

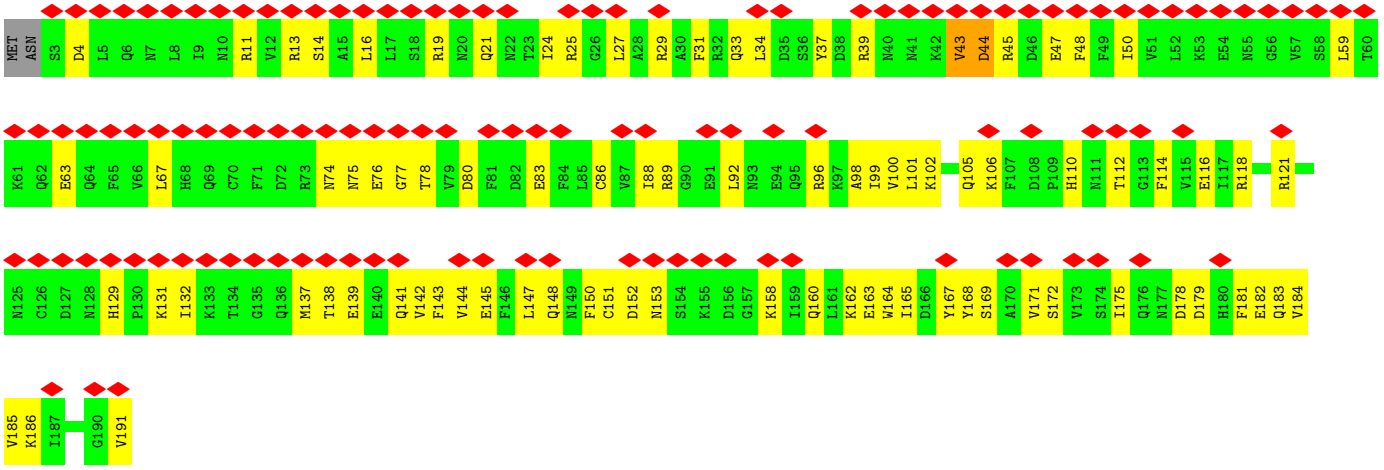




- Molecule 5: RIB22

Chain 3E:

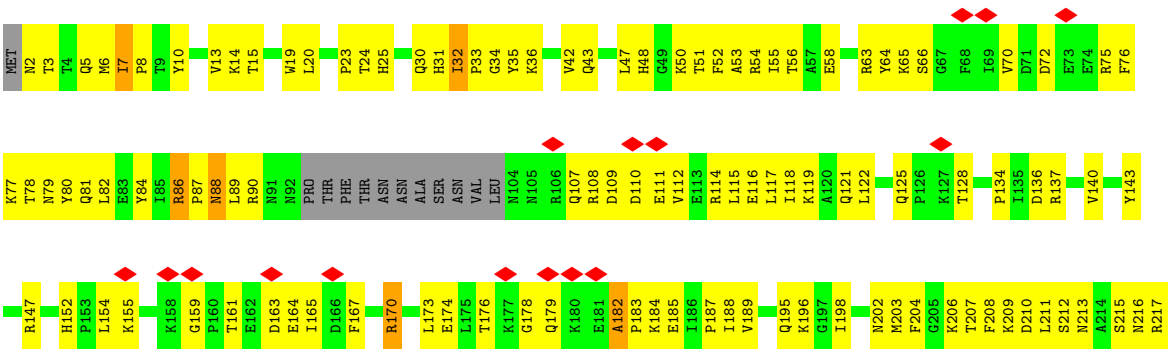




- Molecule 6: CFAM166C

Chain 0F:

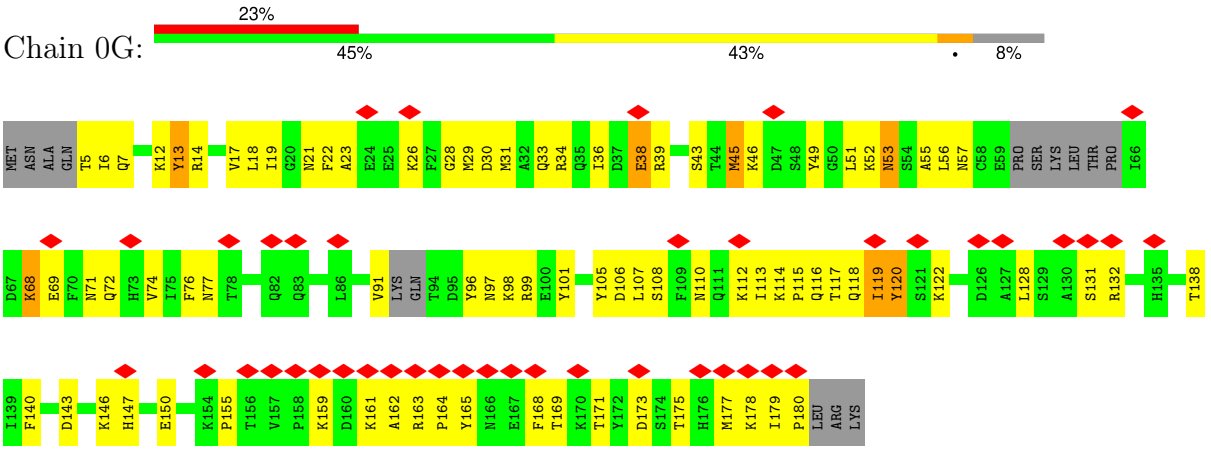






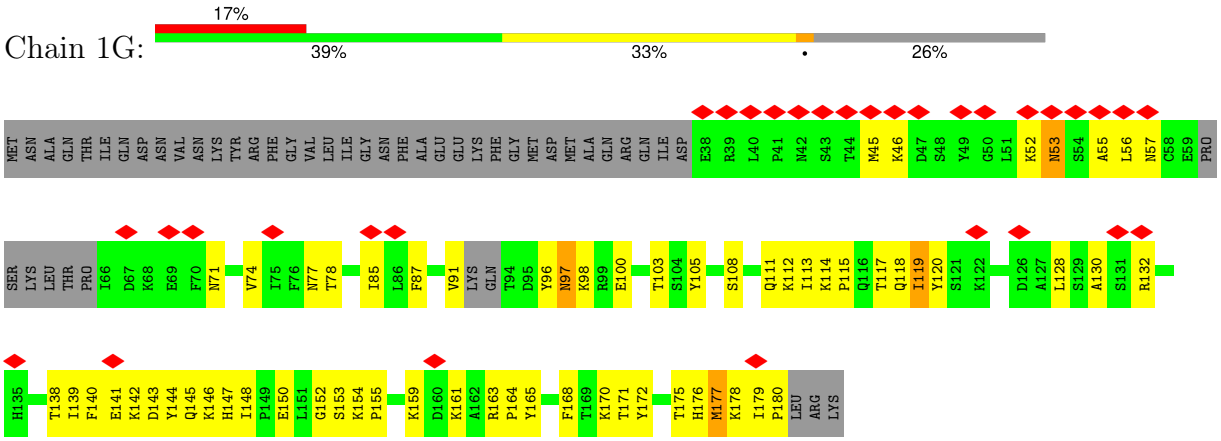
• Molecule 7: CFAP107

Chain 0G:



• Molecule 7: CFAP107

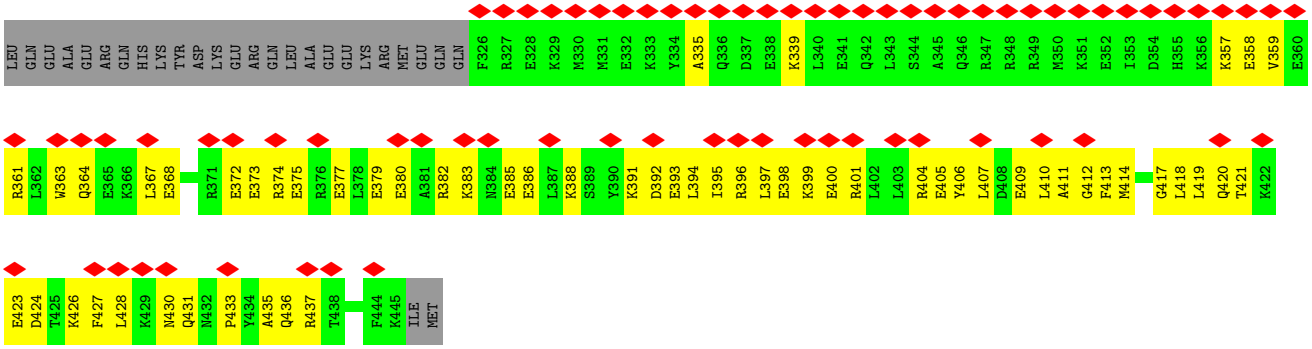
Chain 1G:

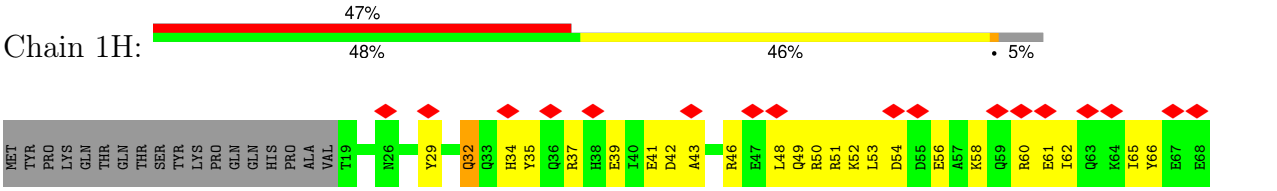


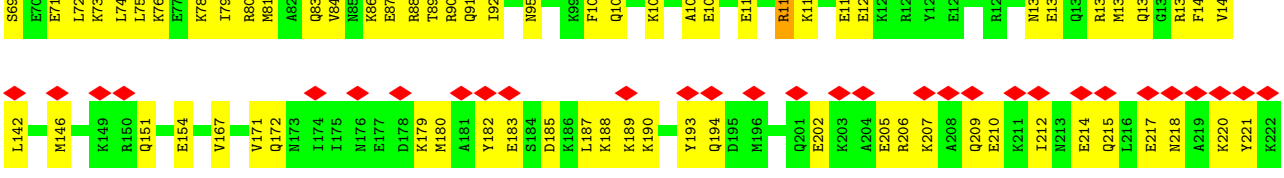
• Molecule 8: CFAP127

Chain 0H:



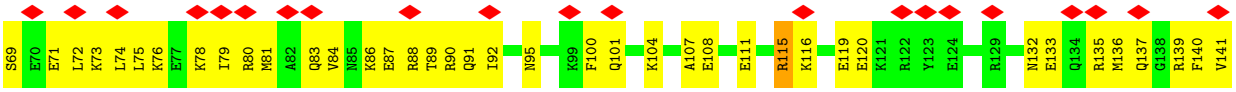


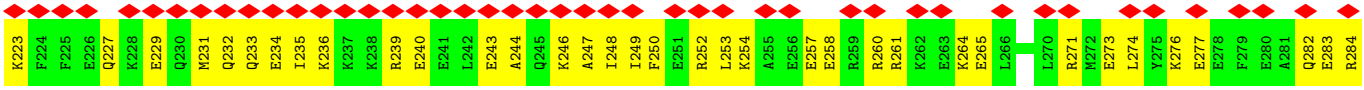


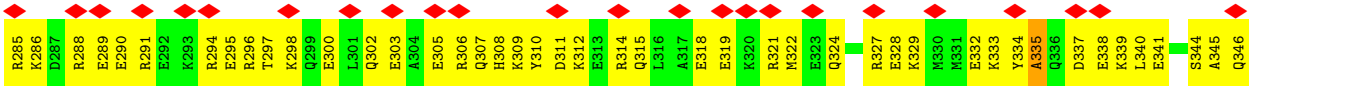


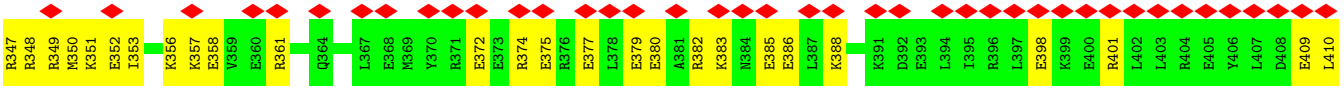
• Molecule 8: CFAP127

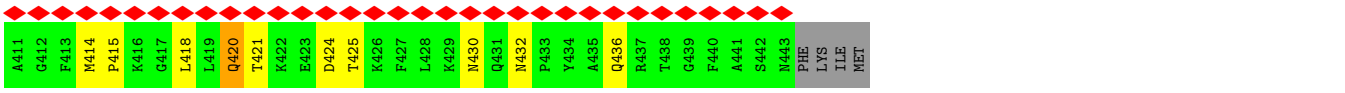
Chain 1H:







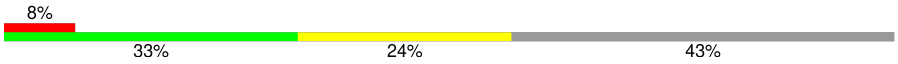


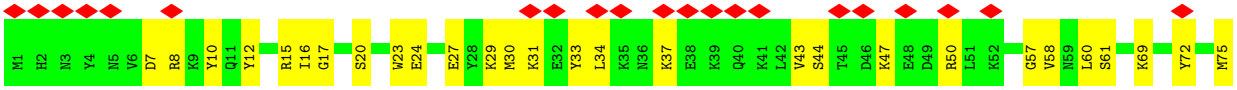


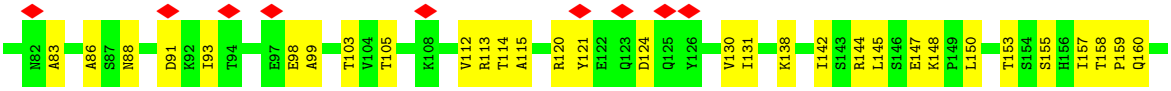


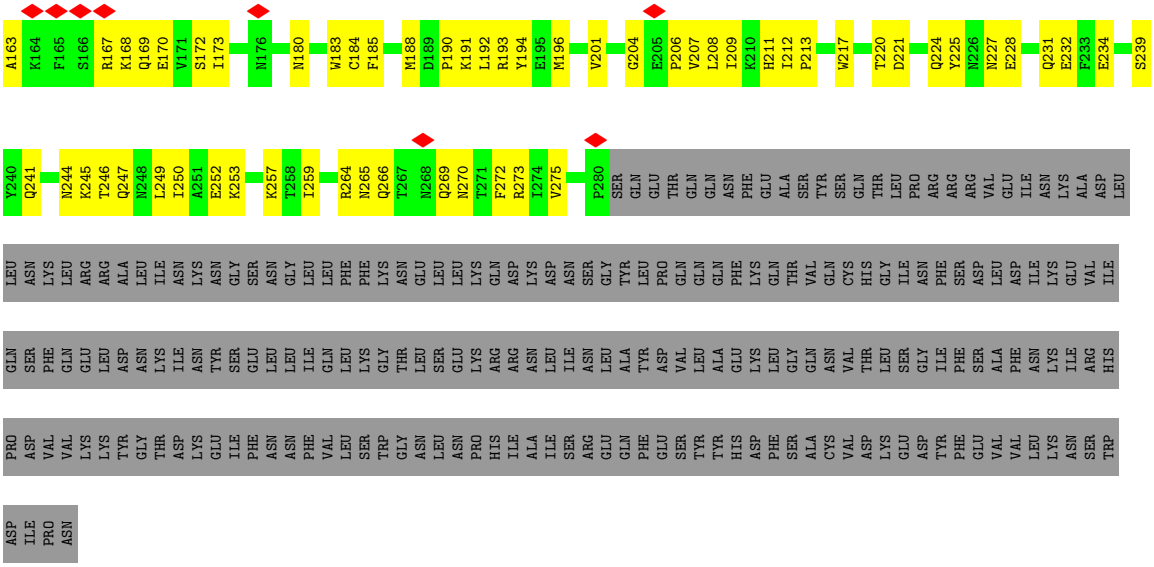
• Molecule 9: CFAP161A

Chain 0N:





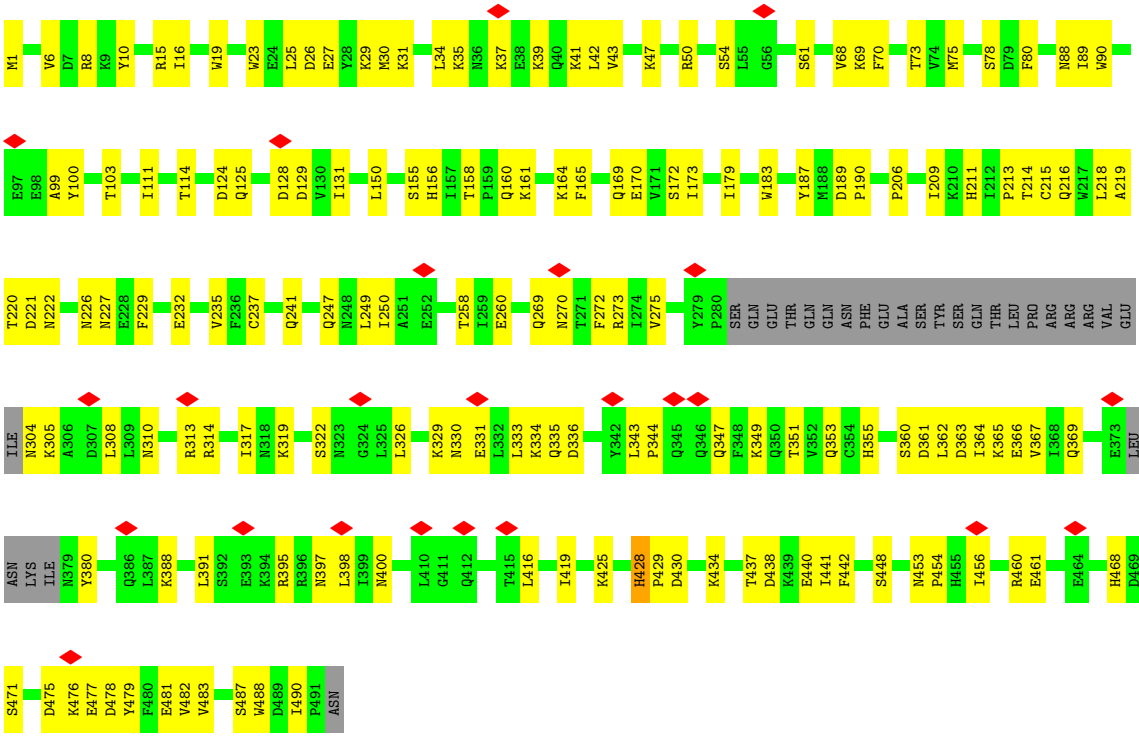




• Molecule 9: CFAP161A

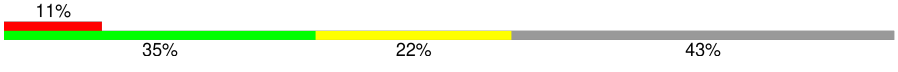
Chain 1N:

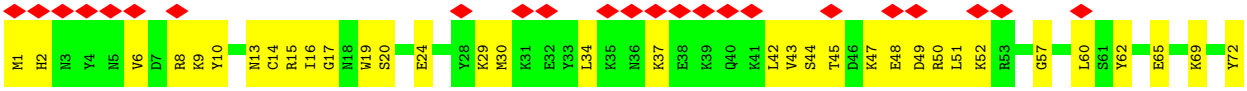


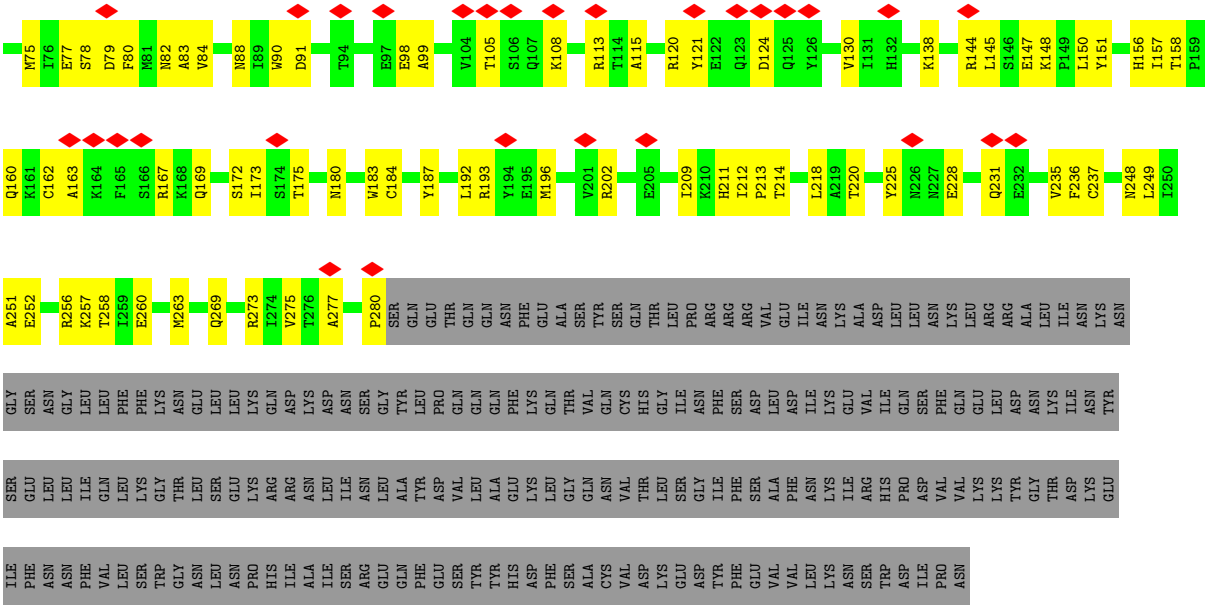


• Molecule 9: CFAP161A

Chain 2N:



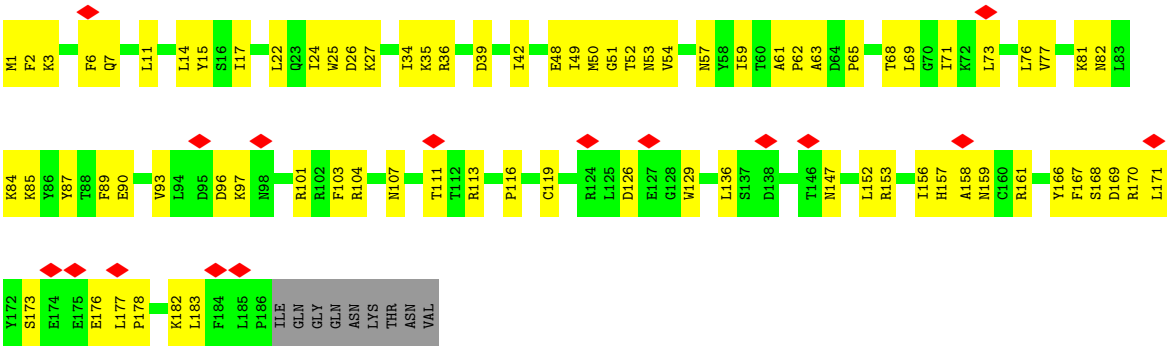




- Molecule 10: CFAP20

Chain 0Q:

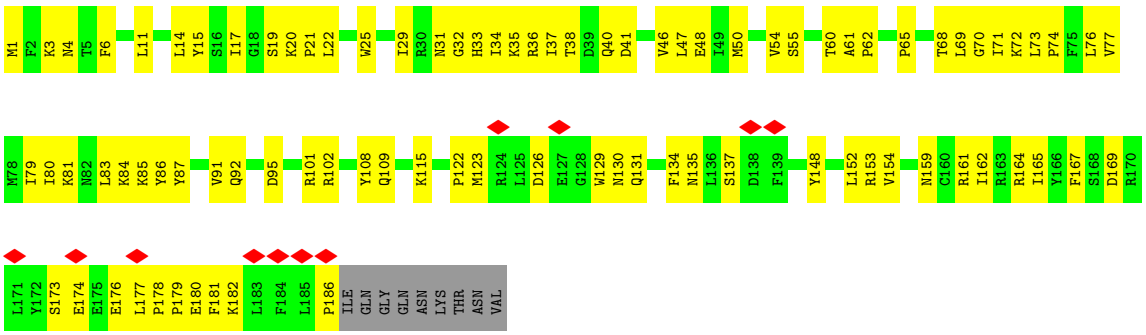




- Molecule 10: CFAP20

Chain 1Q:

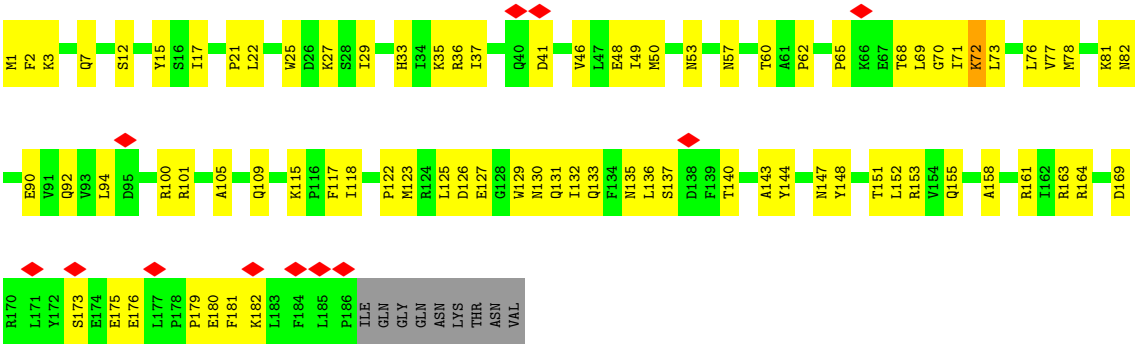




- Molecule 10: CFAP20

Chain 2Q:

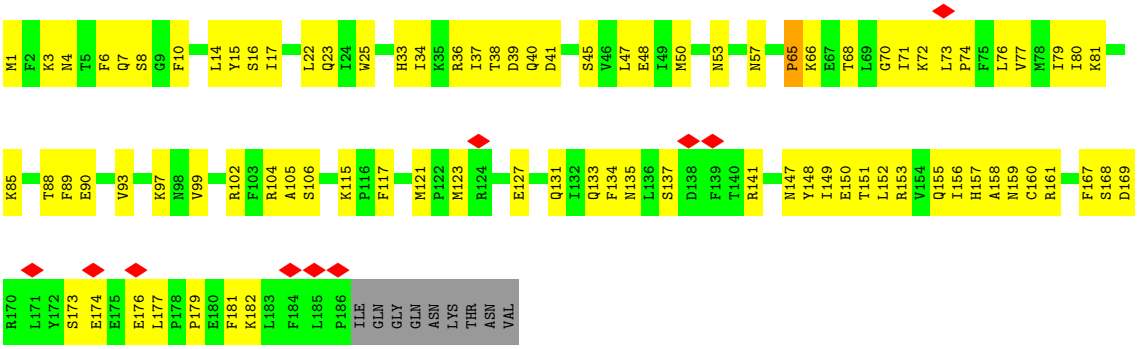




• Molecule 10: CFAP20

Chain 3Q:

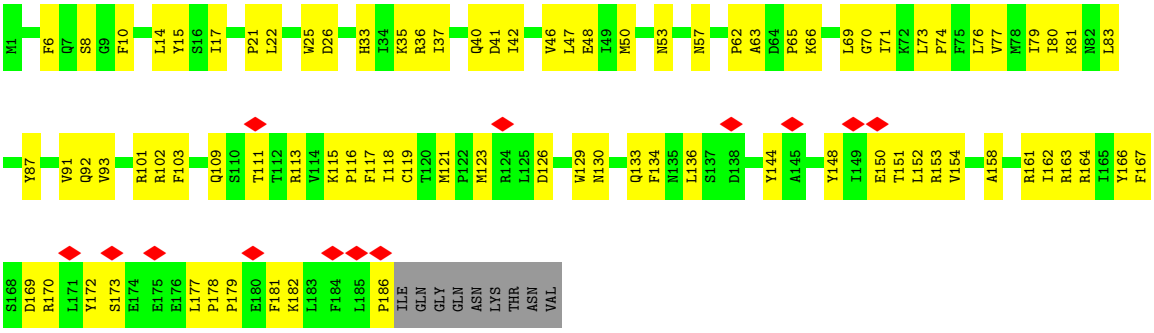




• Molecule 10: CFAP20

Chain 4Q:

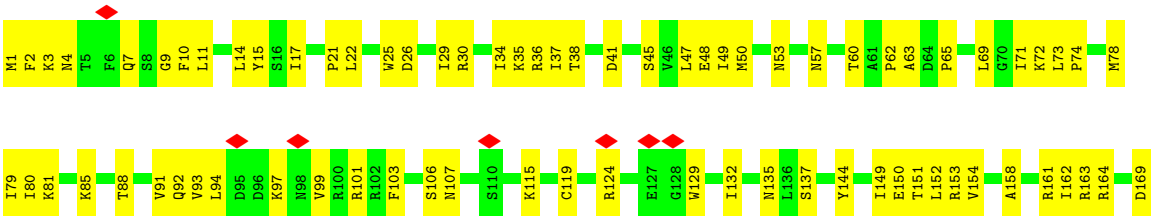


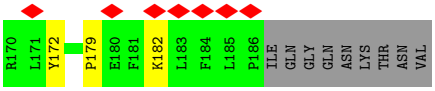


• Molecule 10: CFAP20

Chain 5Q:



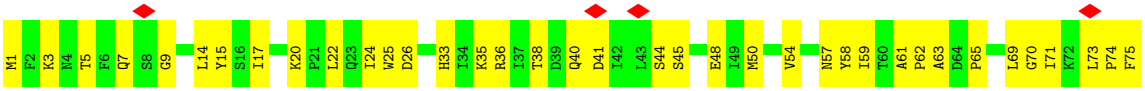


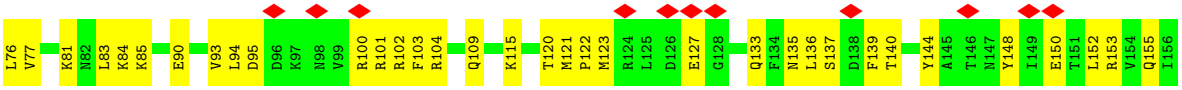


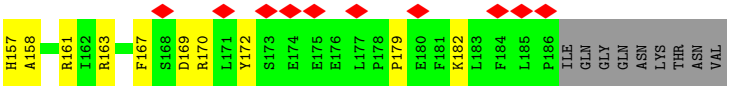
• Molecule 10: CFAP20

Chain 6Q:





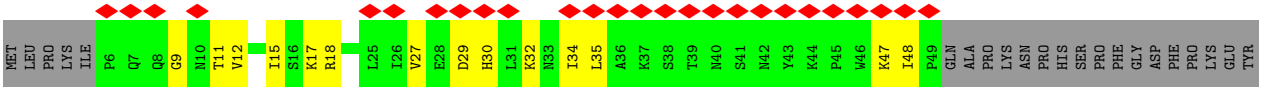


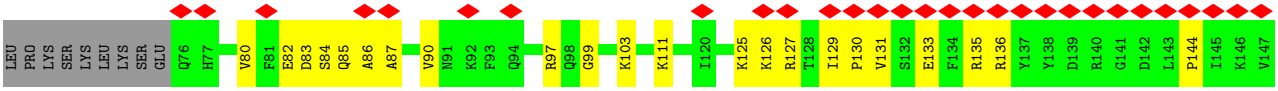


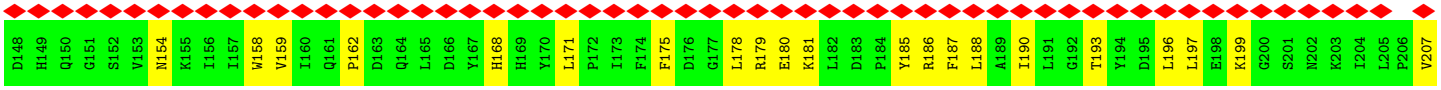
• Molecule 11: Parkin co-regulated protein PACRGA

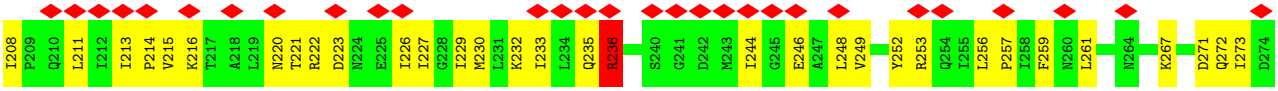
Chain 0S:

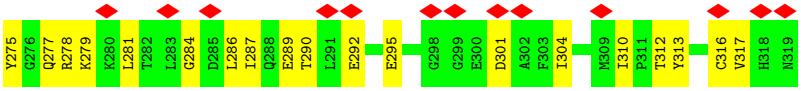








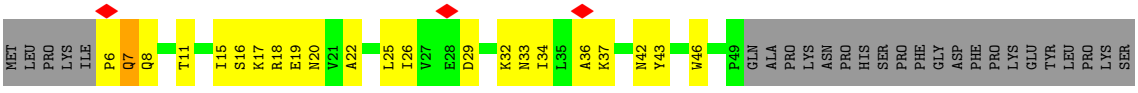


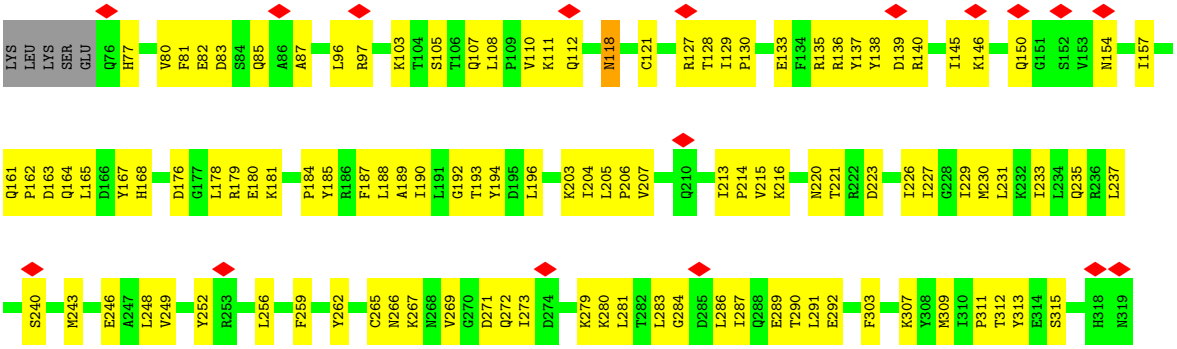


• Molecule 11: Parkin co-regulated protein PACRGA

Chain 1S:



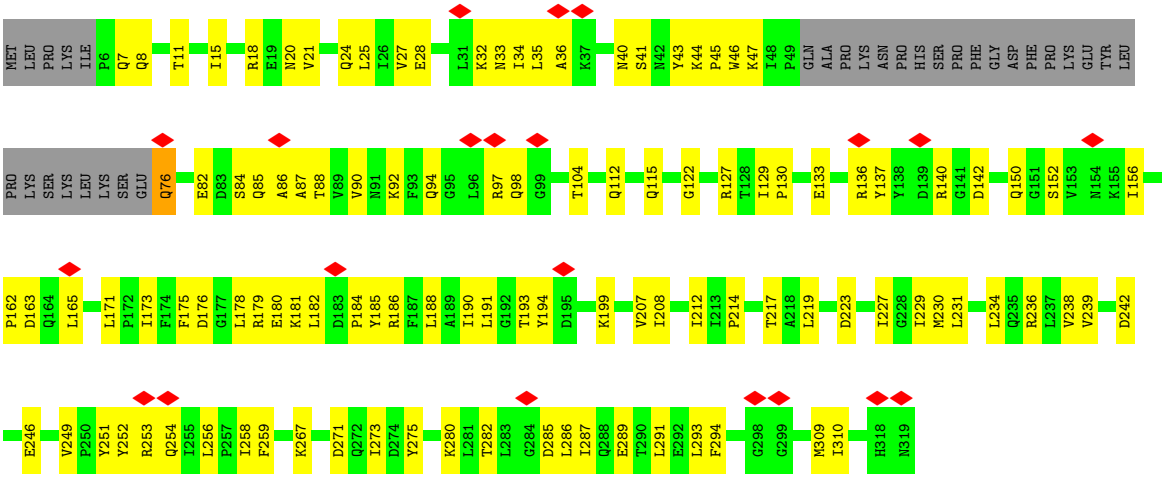




• Molecule 11: Parkin co-regulated protein PACRGA

Chain 2S:

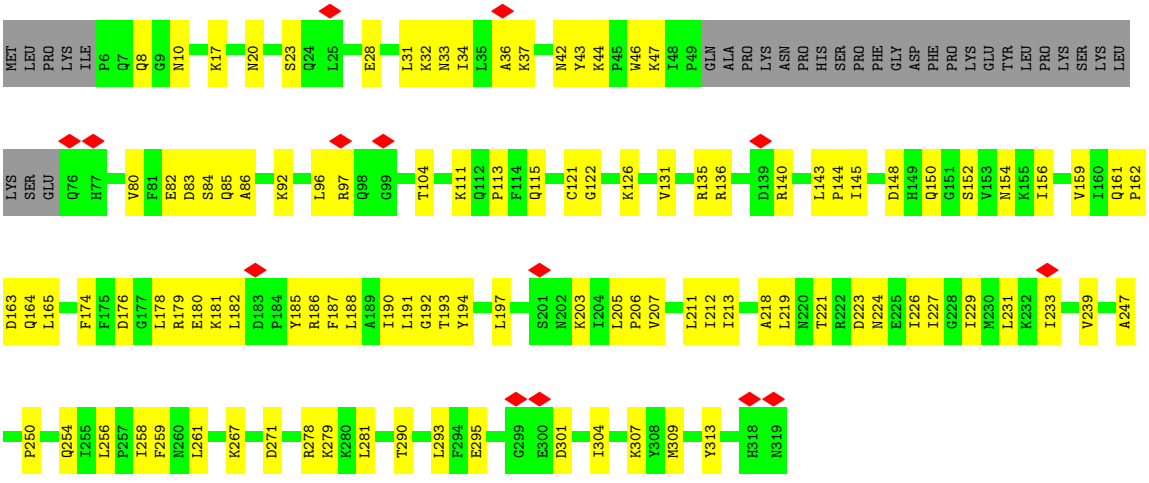




• Molecule 11: Parkin co-regulated protein PACRGA

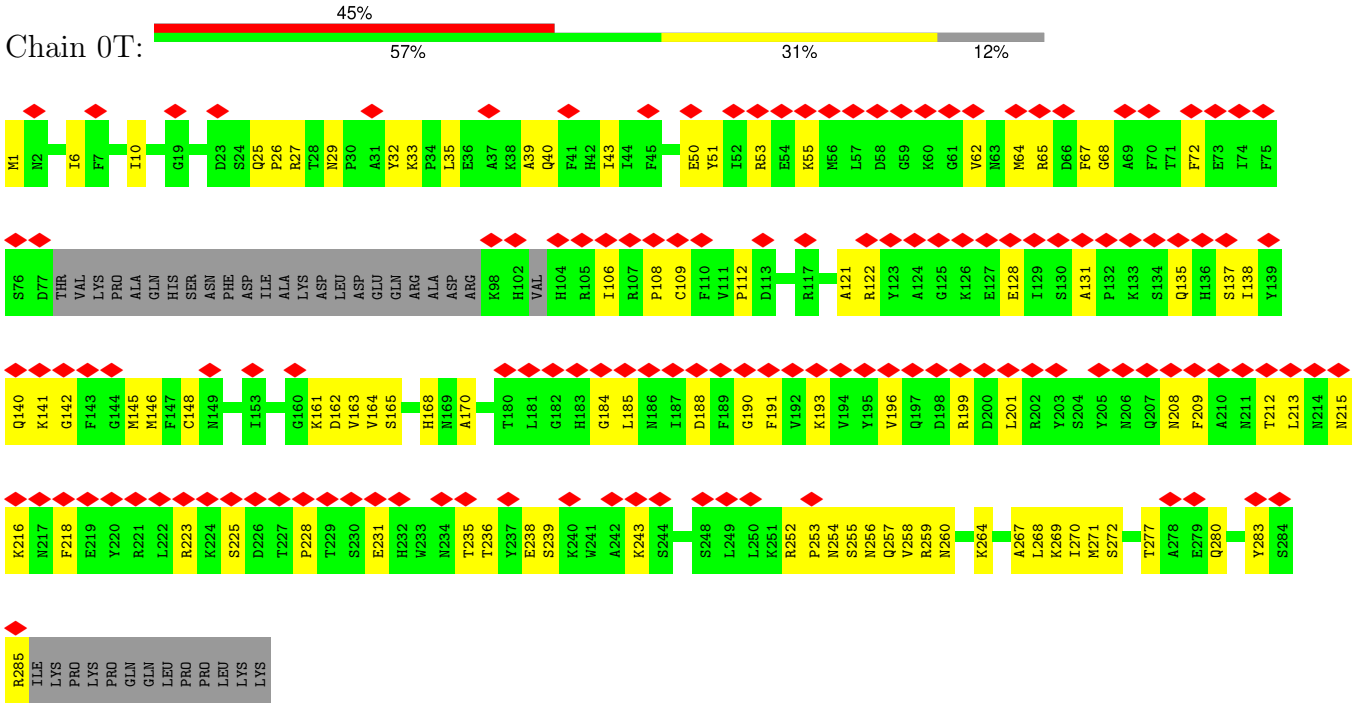
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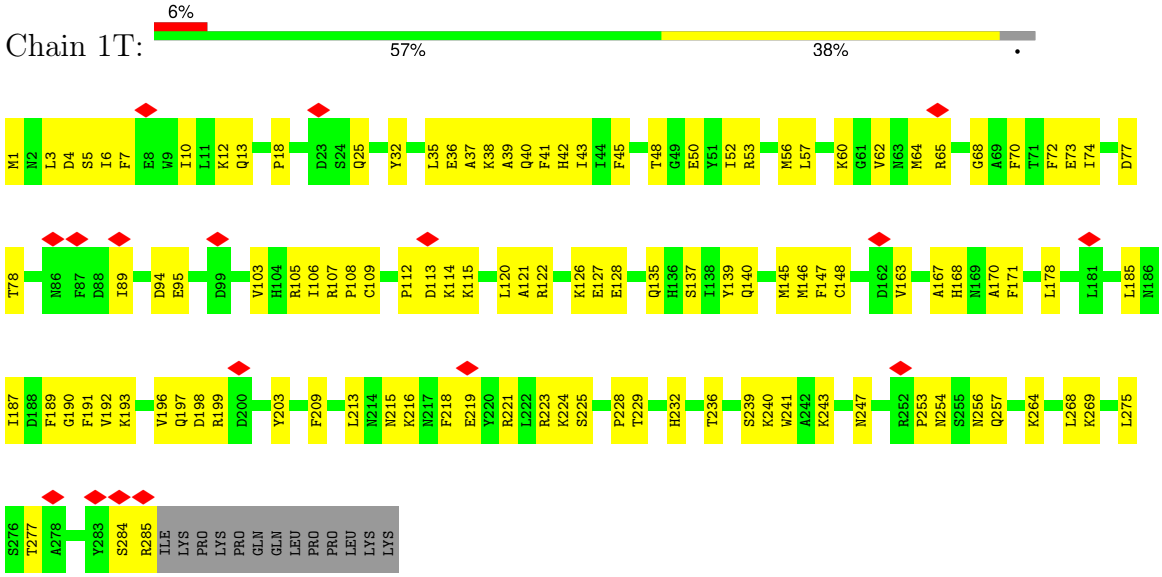
• Molecule 12: IJ34

Chain 0T:



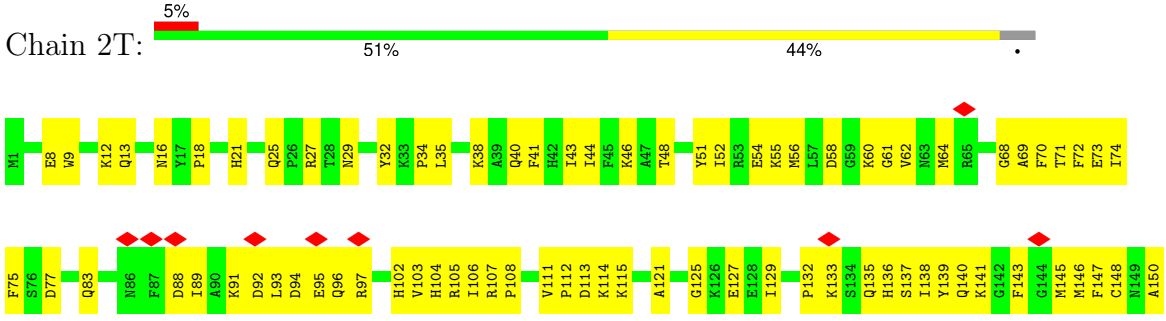
• Molecule 12: IJ34

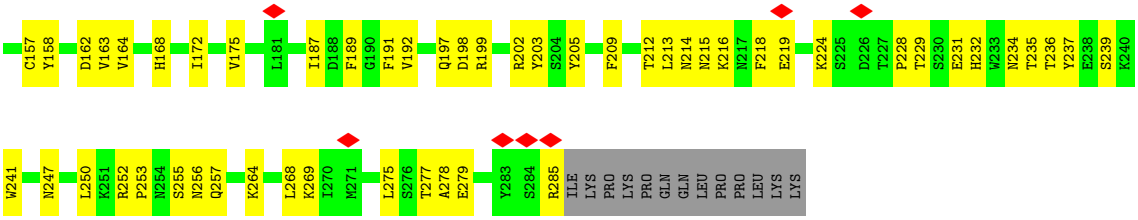
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• Molecule 12: IJ34

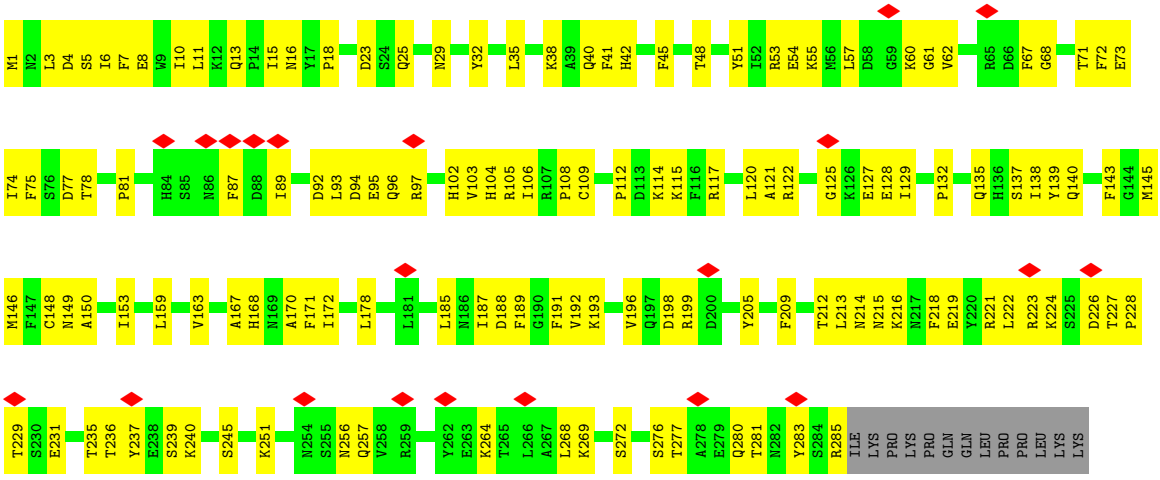
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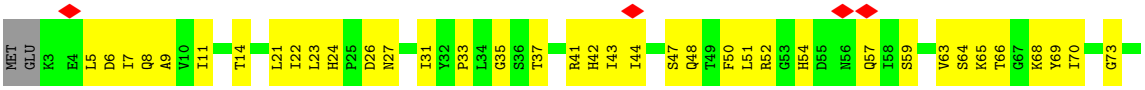
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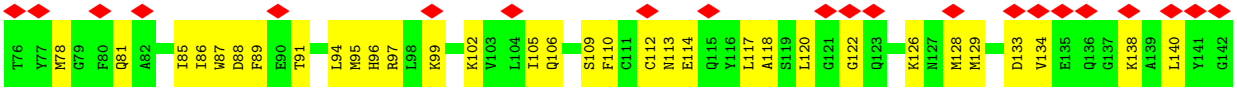


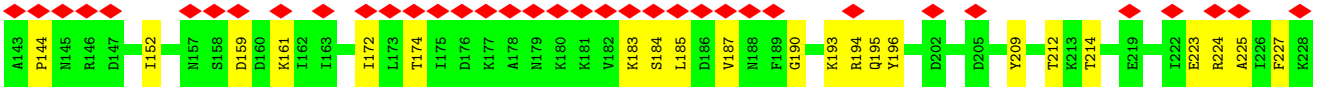


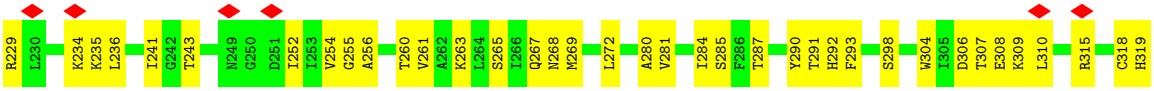
• Molecule 13: CFAP52A

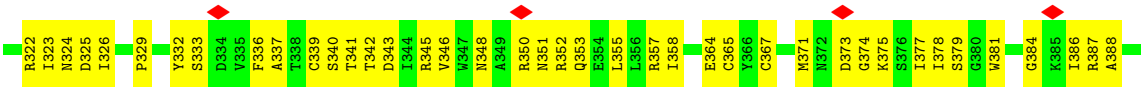




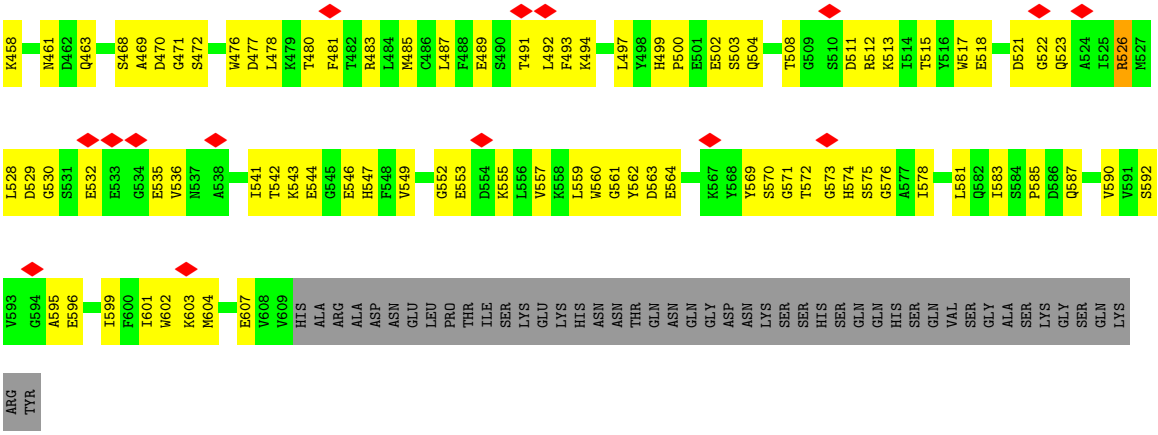








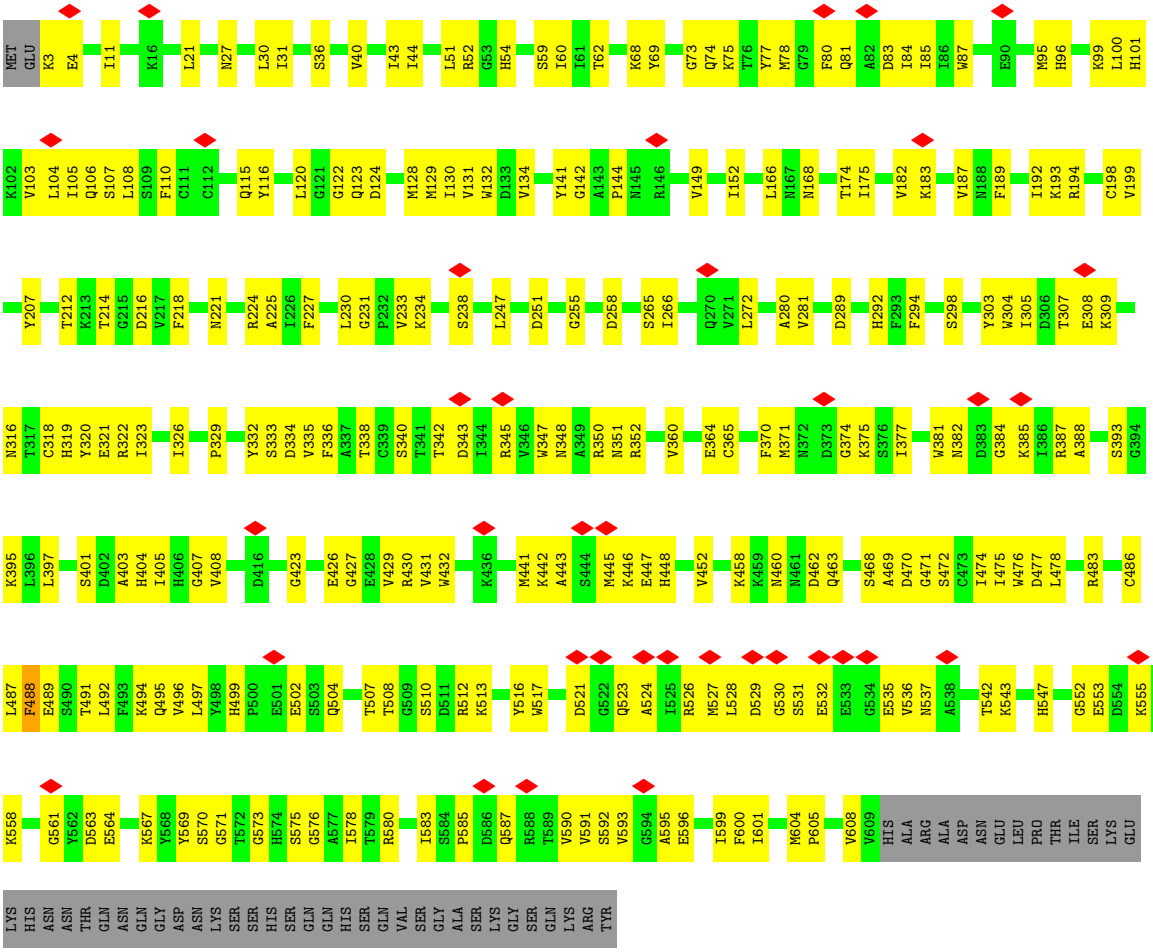




• Molecule 13: CFAP52A

Chain 1U:

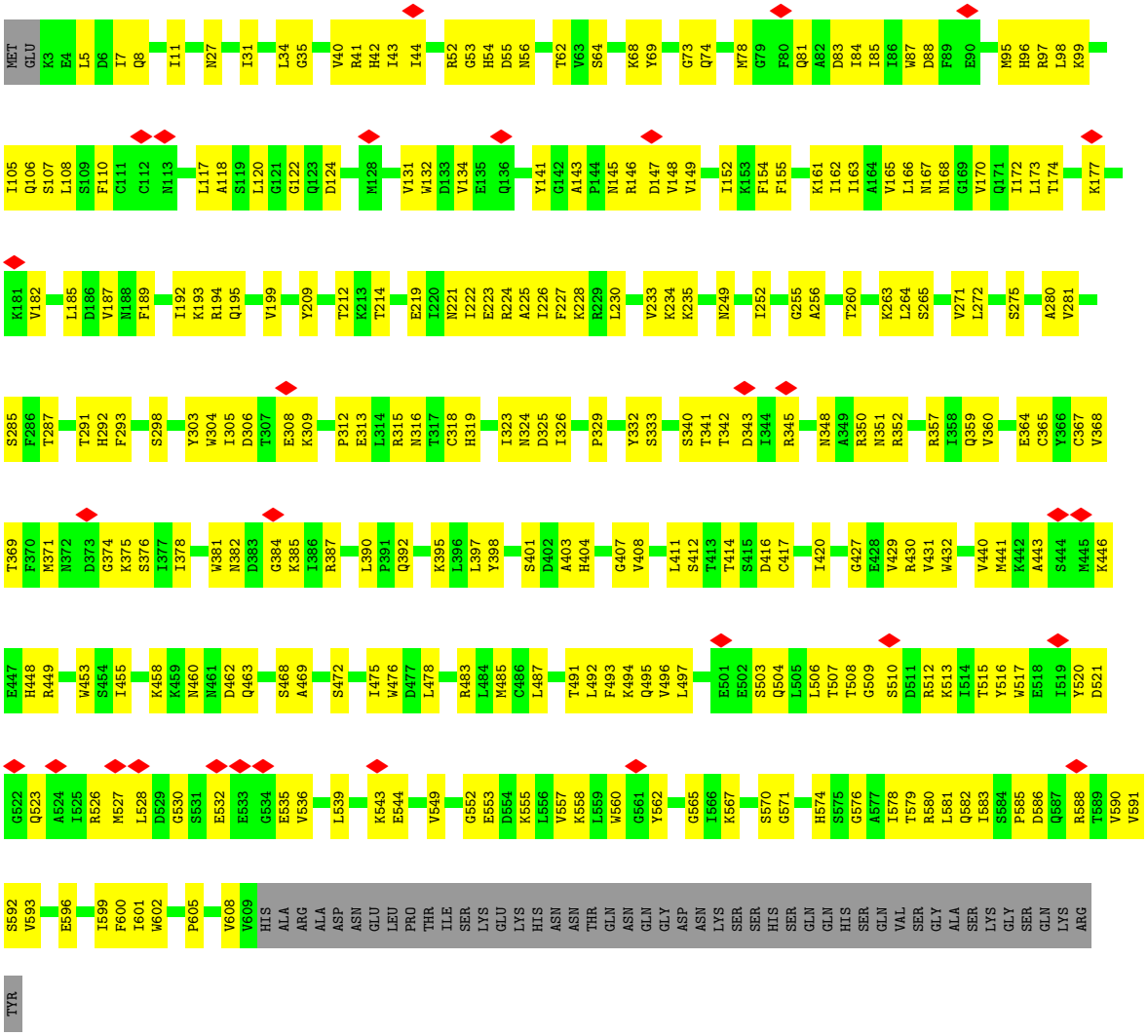




• Molecule 13: CFAP52A

Chain 2U:

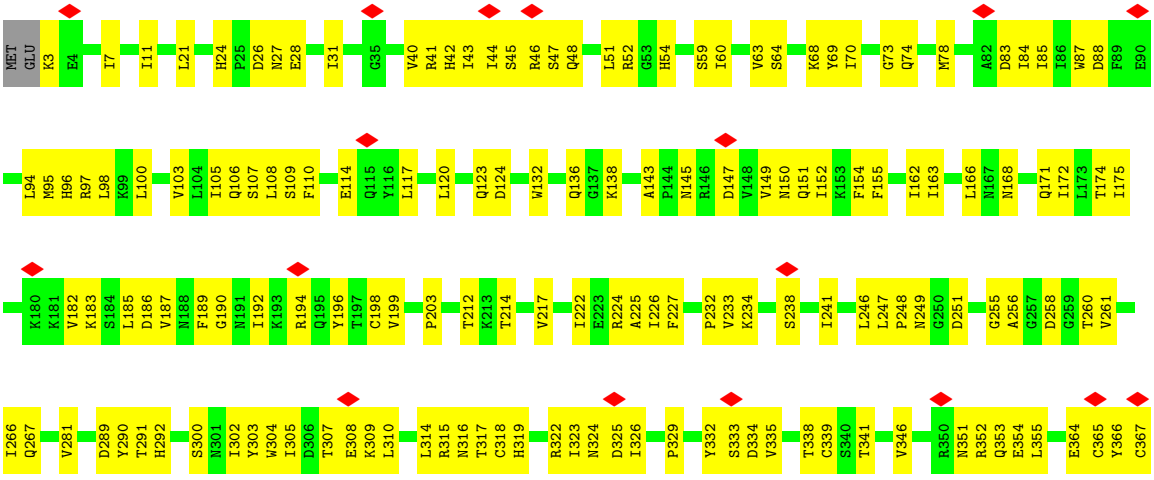


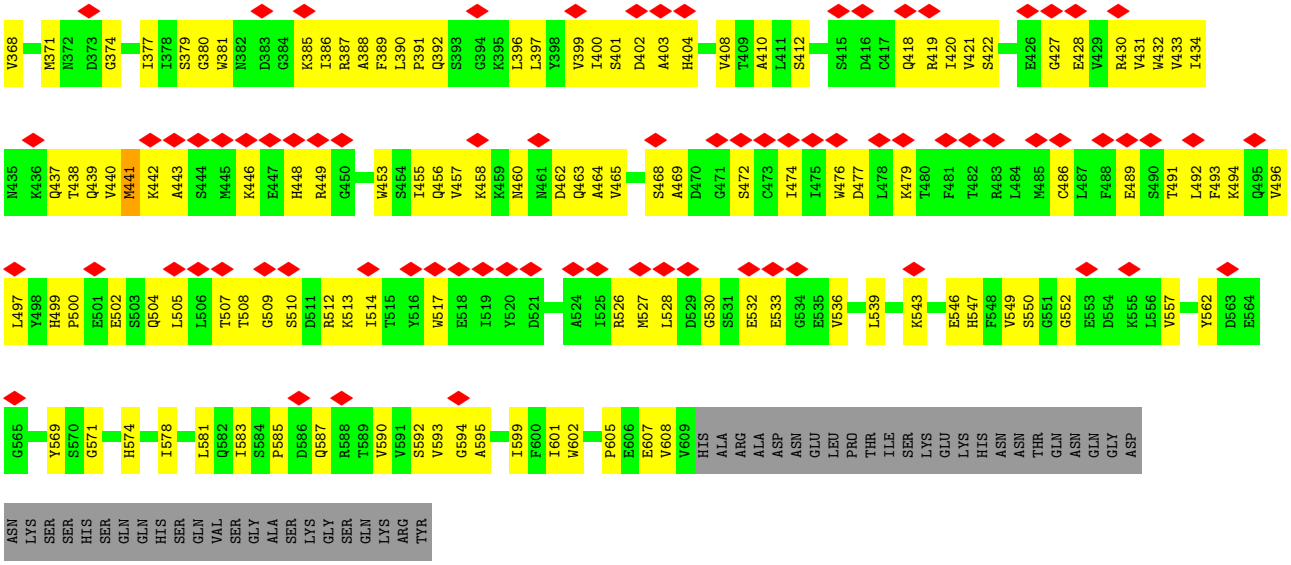


• Molecule 13: CFAP52A

Chain 3U:



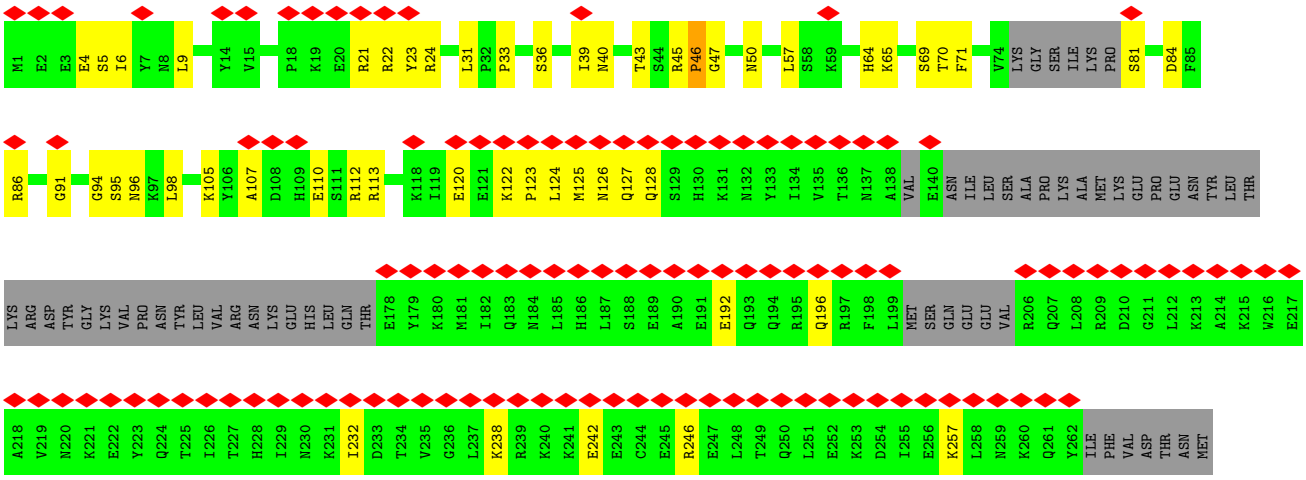




• Molecule 14: DNA polymerase delta C4-type zinc-finger protein

Chain 0V:

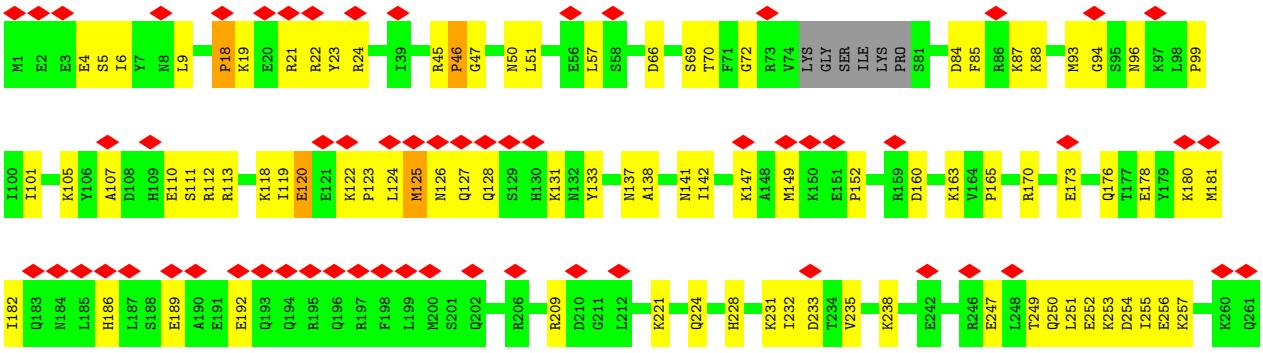


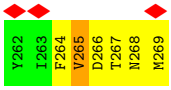


• Molecule 14: DNA polymerase delta C4-type zinc-finger protein

Chain 1V:



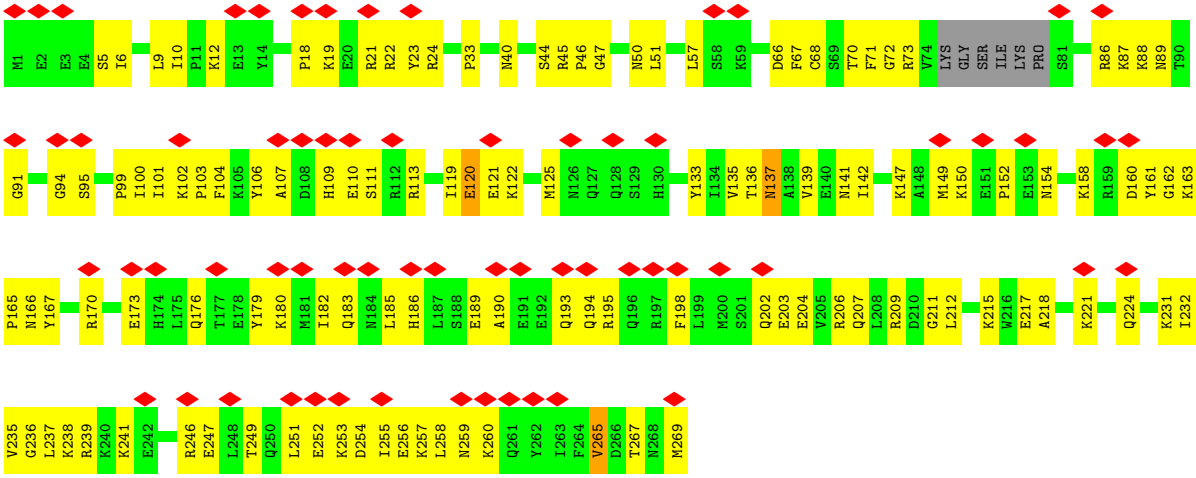




• Molecule 14: DNA polymerase delta C4-type zinc-finger protein

Chain 2V:

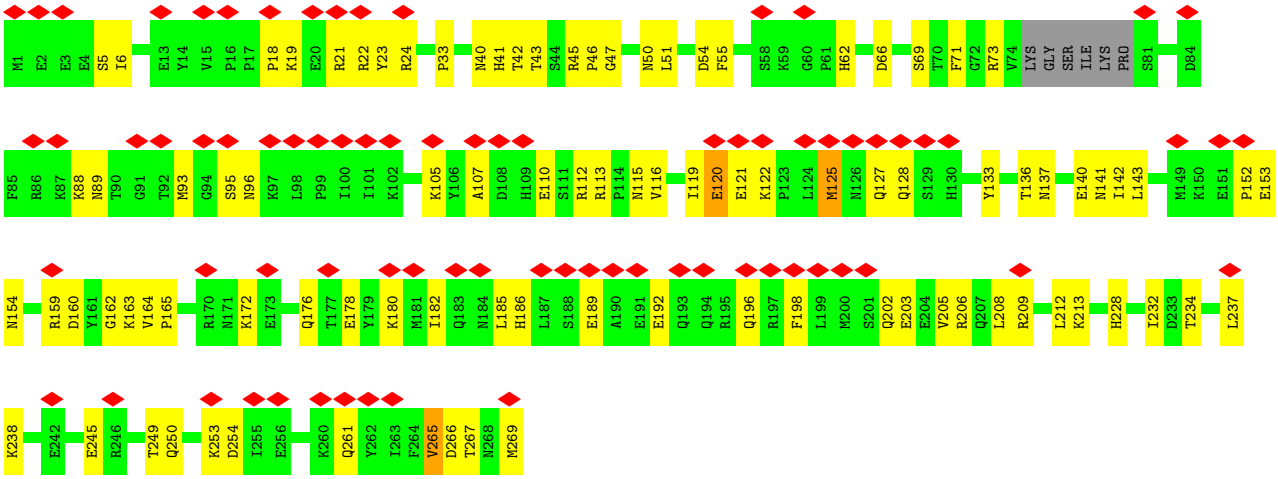




• Molecule 14: DNA polymerase delta C4-type zinc-finger protein

Chain 3V:

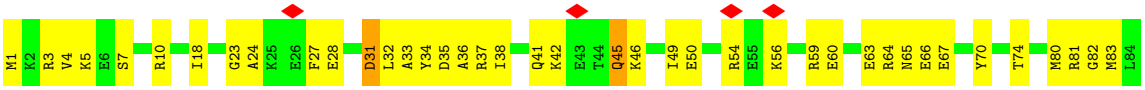


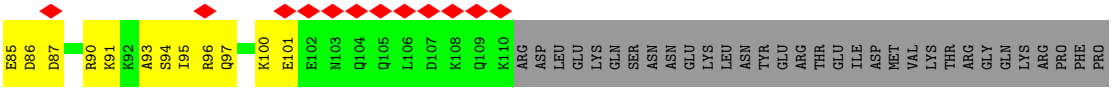


• Molecule 15: RIB43A protein

Chain 0X:



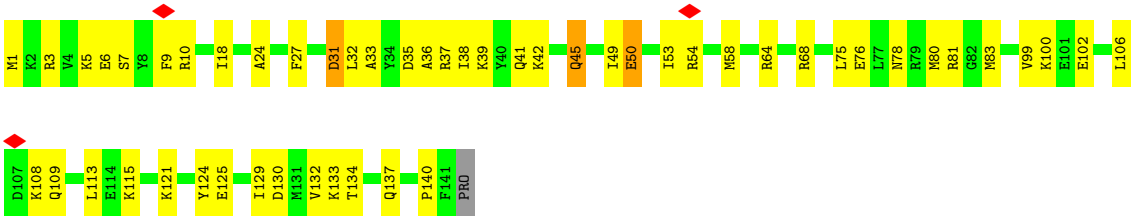




• Molecule 15: RIB43A protein

Chain 1X:

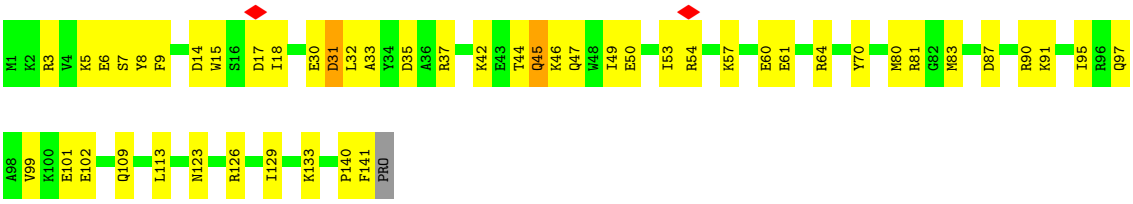




• Molecule 15: RIB43A protein

Chain 2X:

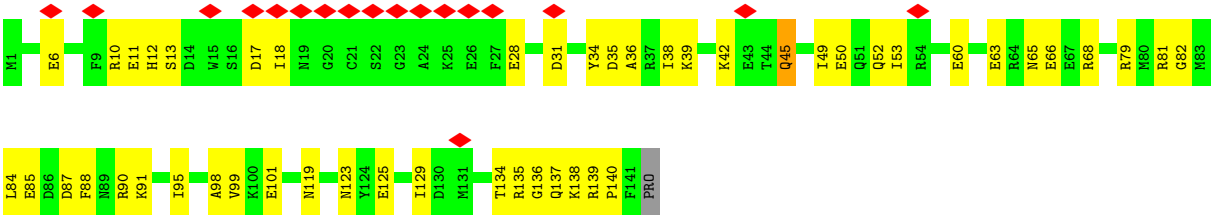




• Molecule 15: RIB43A protein

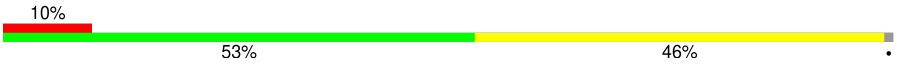
Chain 3X:

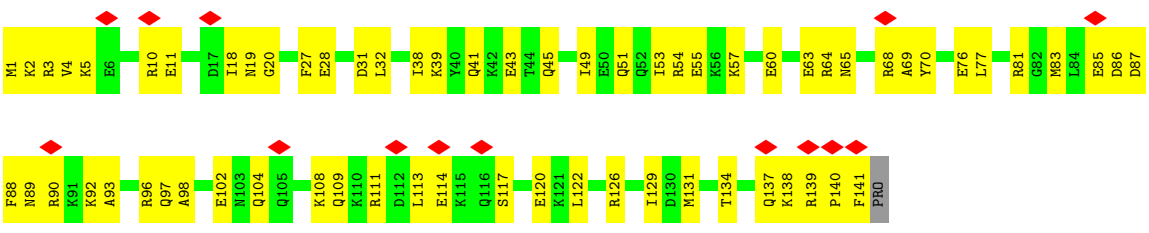




• Molecule 15: RIB43A protein

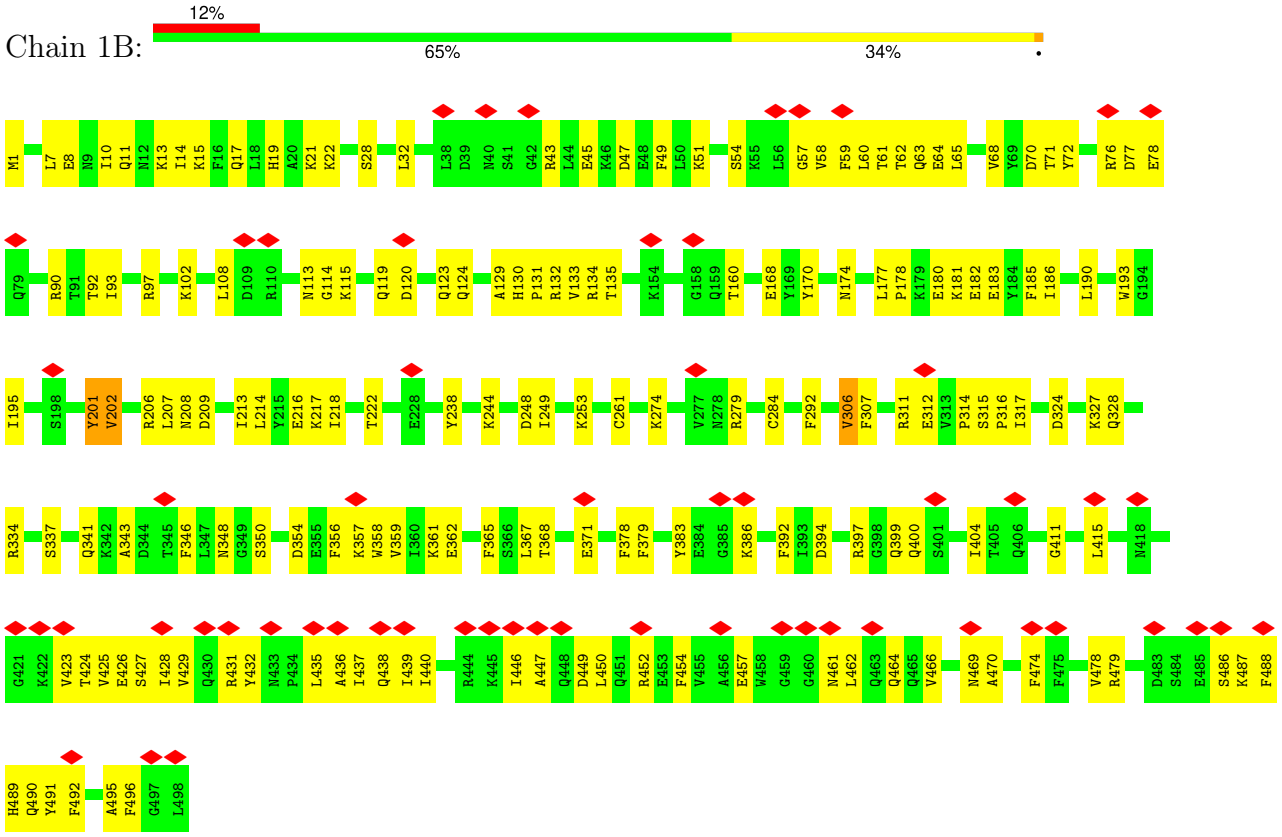
Chain 4X:





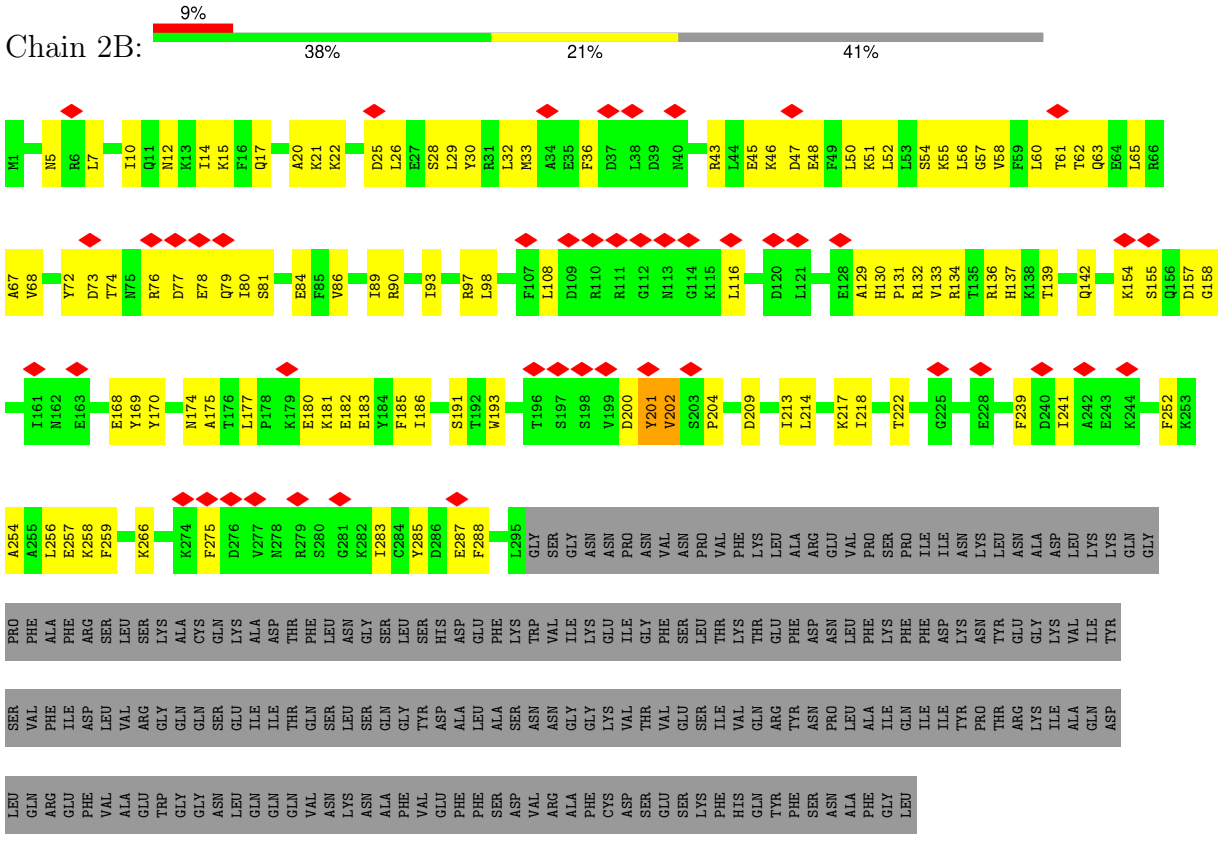
• Molecule 16: RIB57

Chain 1B:



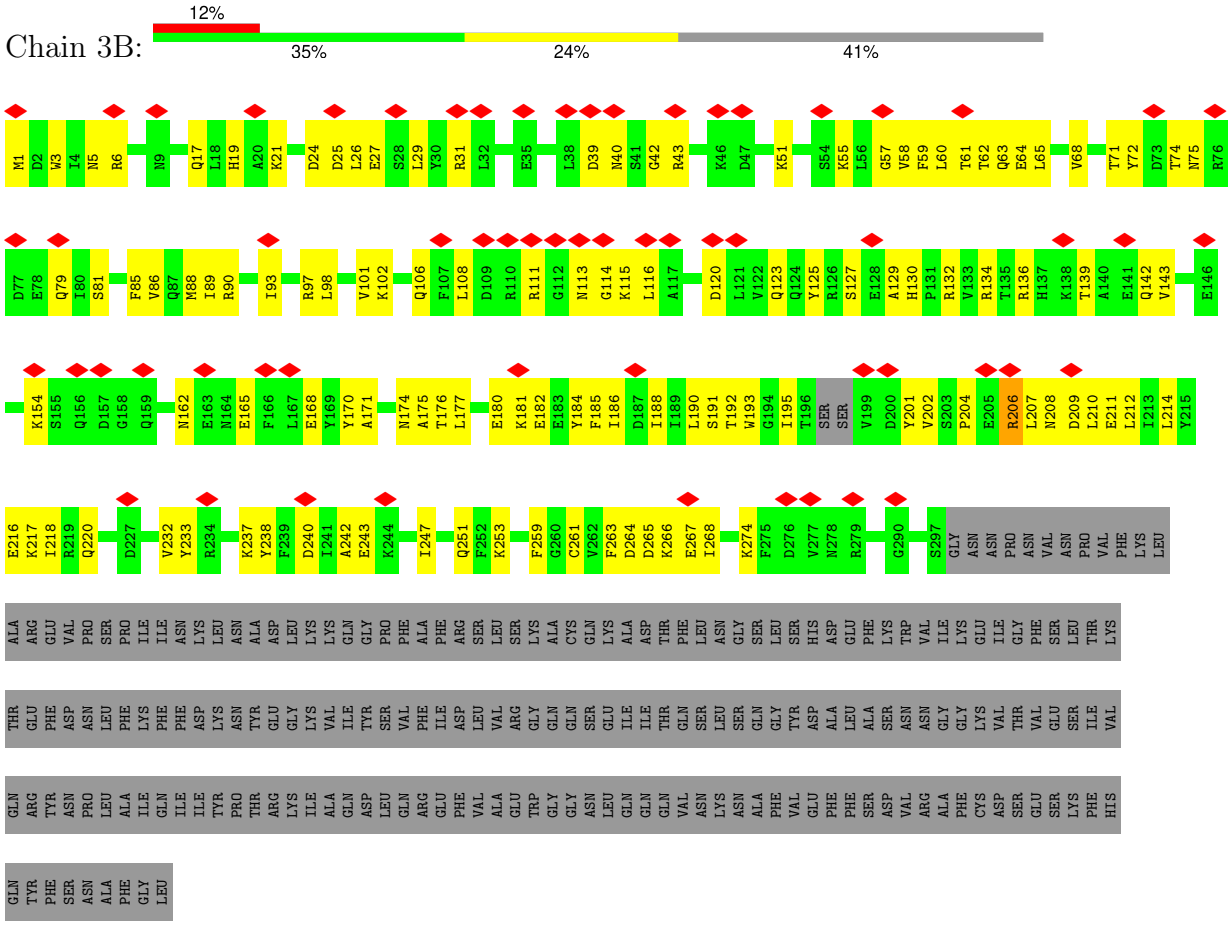
• Molecule 16: RIB57

Chain 2B:



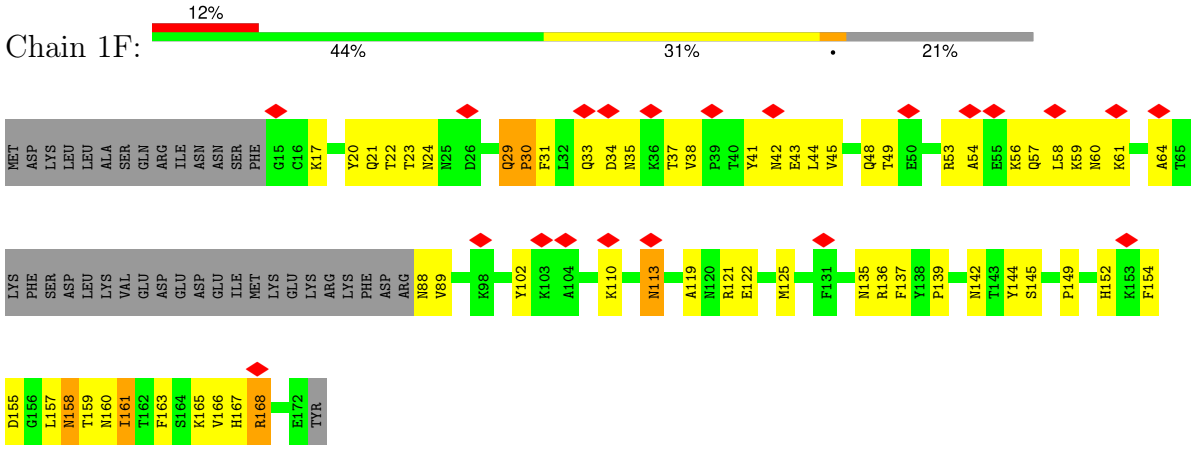
• Molecule 16: RIB57

Chain 3B:



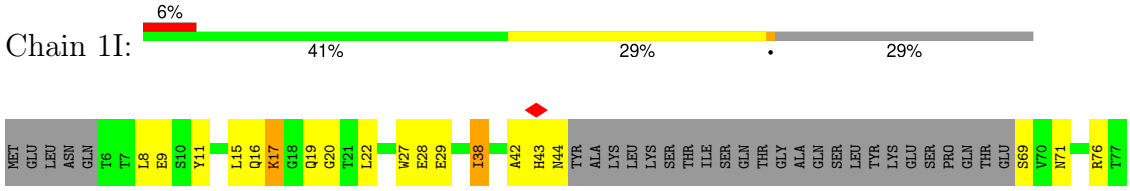
• Molecule 17: CFAP182A

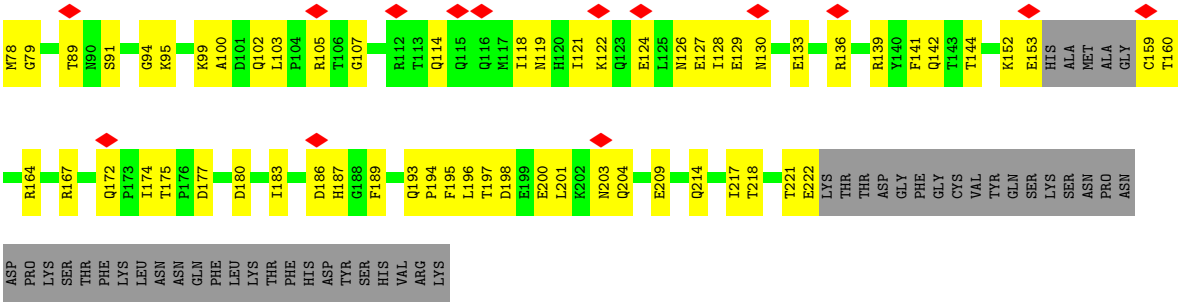
Chain 1F:



• Molecule 18: CFAP143

Chain 1I:

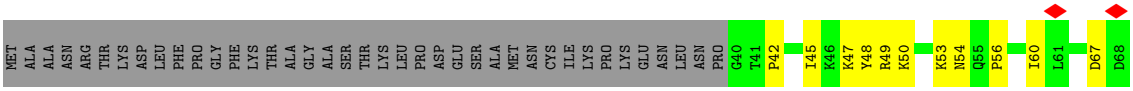




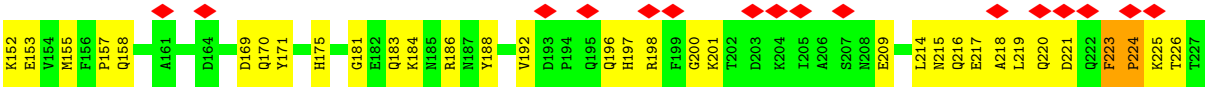
• Molecule 19: CFAP21A

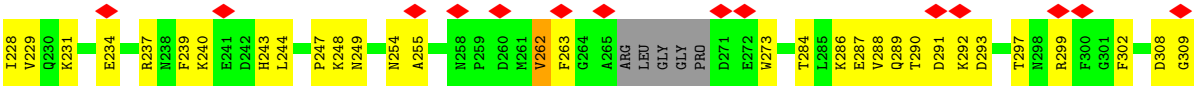
Chain 1J:

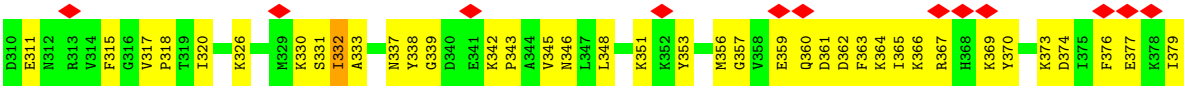


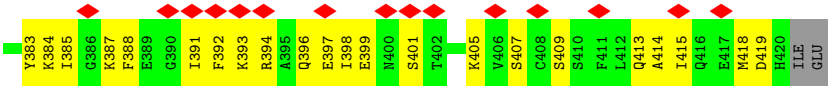






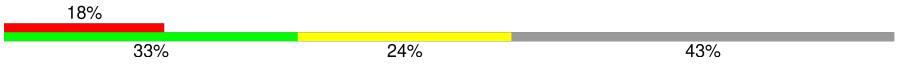


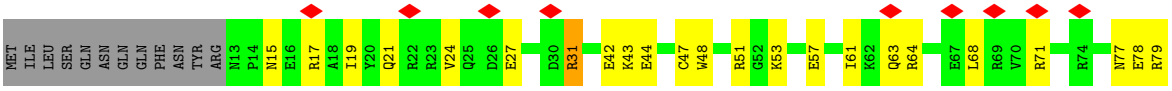


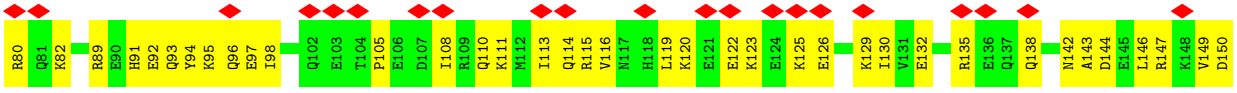


• Molecule 20: CFAP53

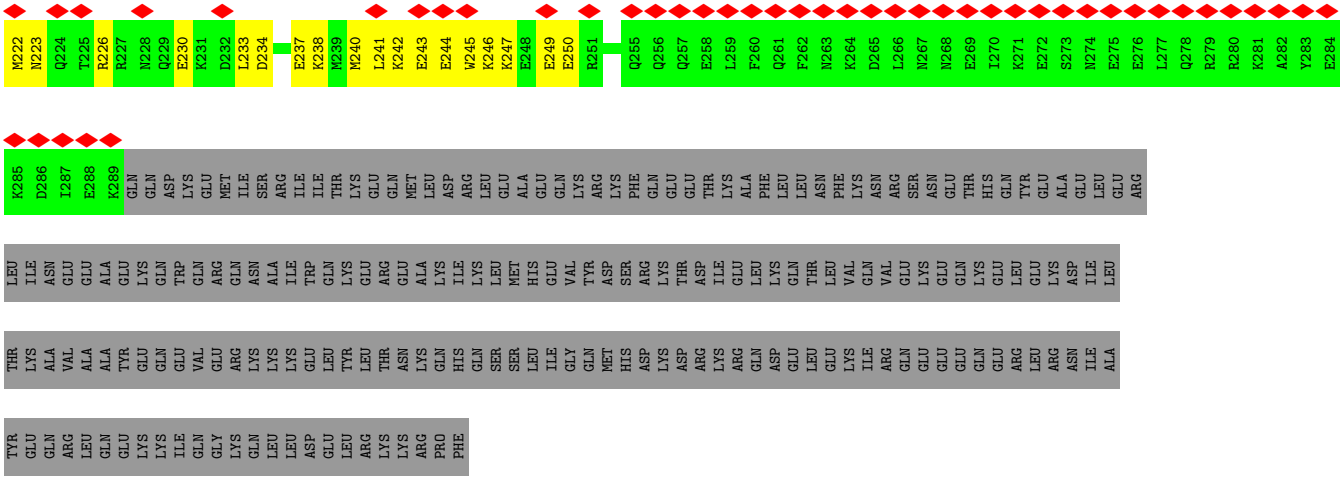
Chain 1K:





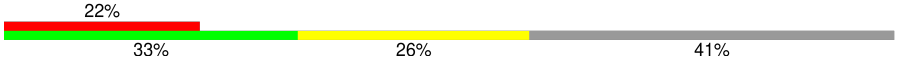


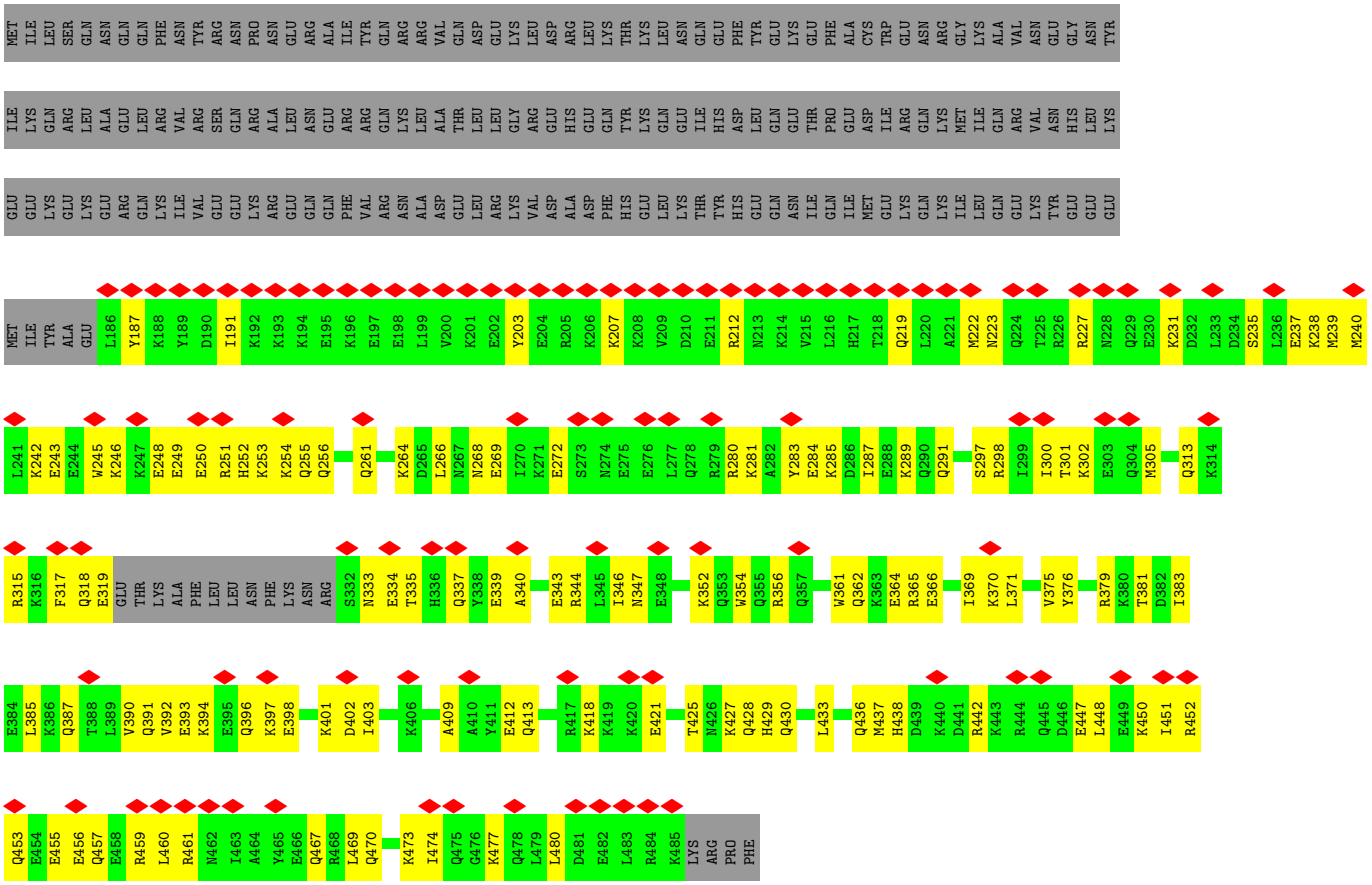




• Molecule 20: CFAP53

Chain 2K:

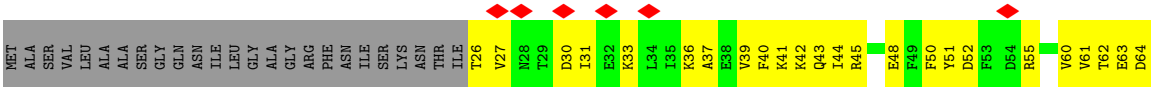


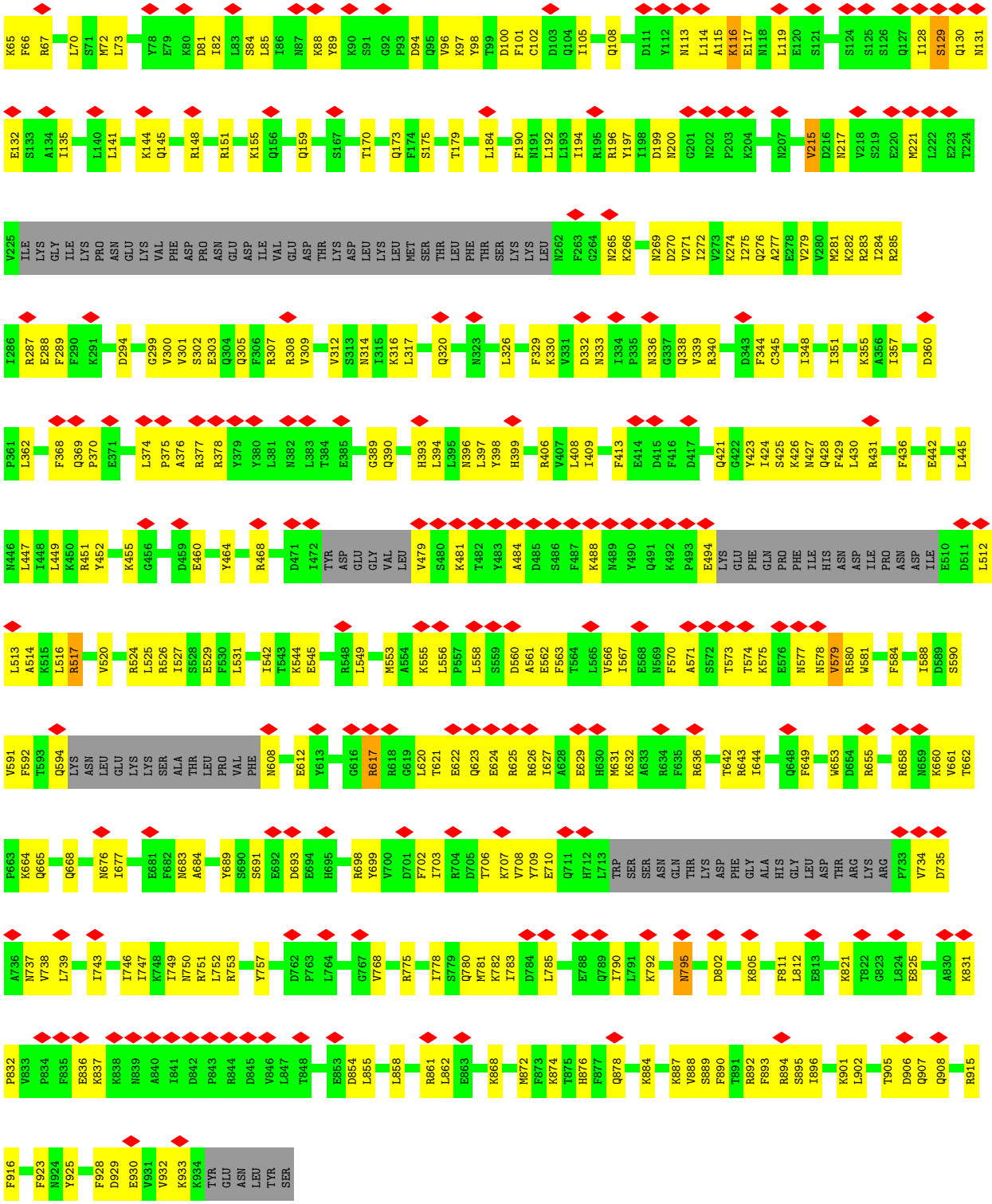


• Molecule 21: CFAP115

Chain 1L:

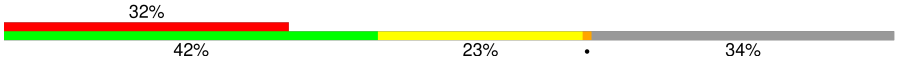


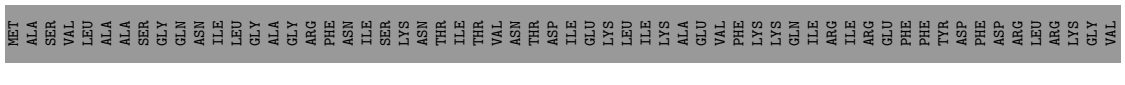


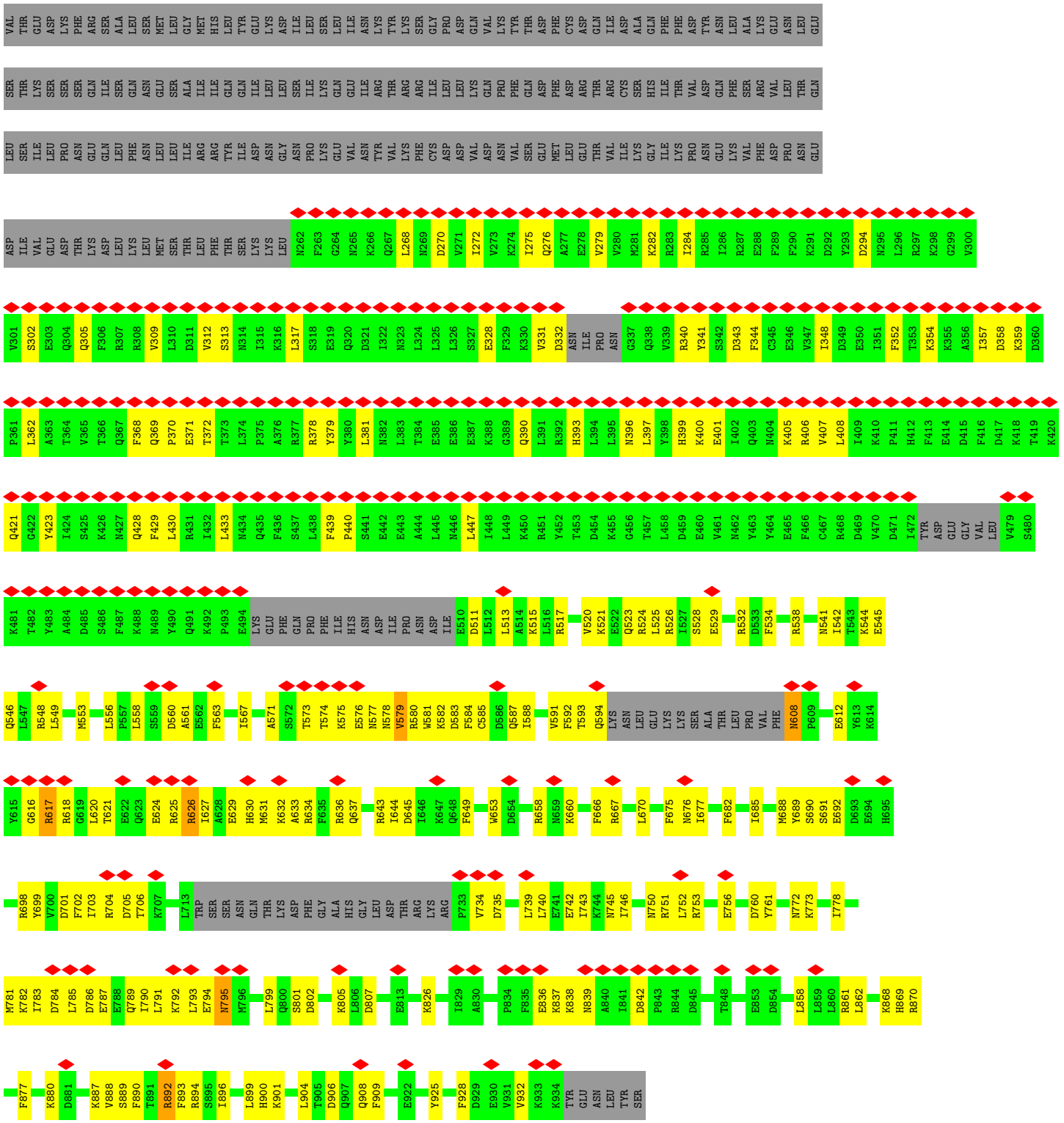


• Molecule 21: CFAP115

Chain 2L:



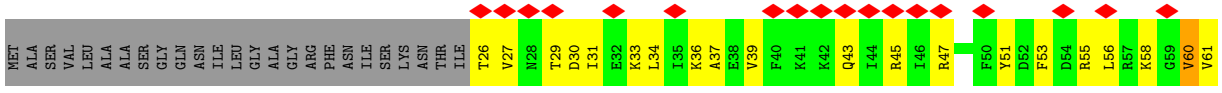


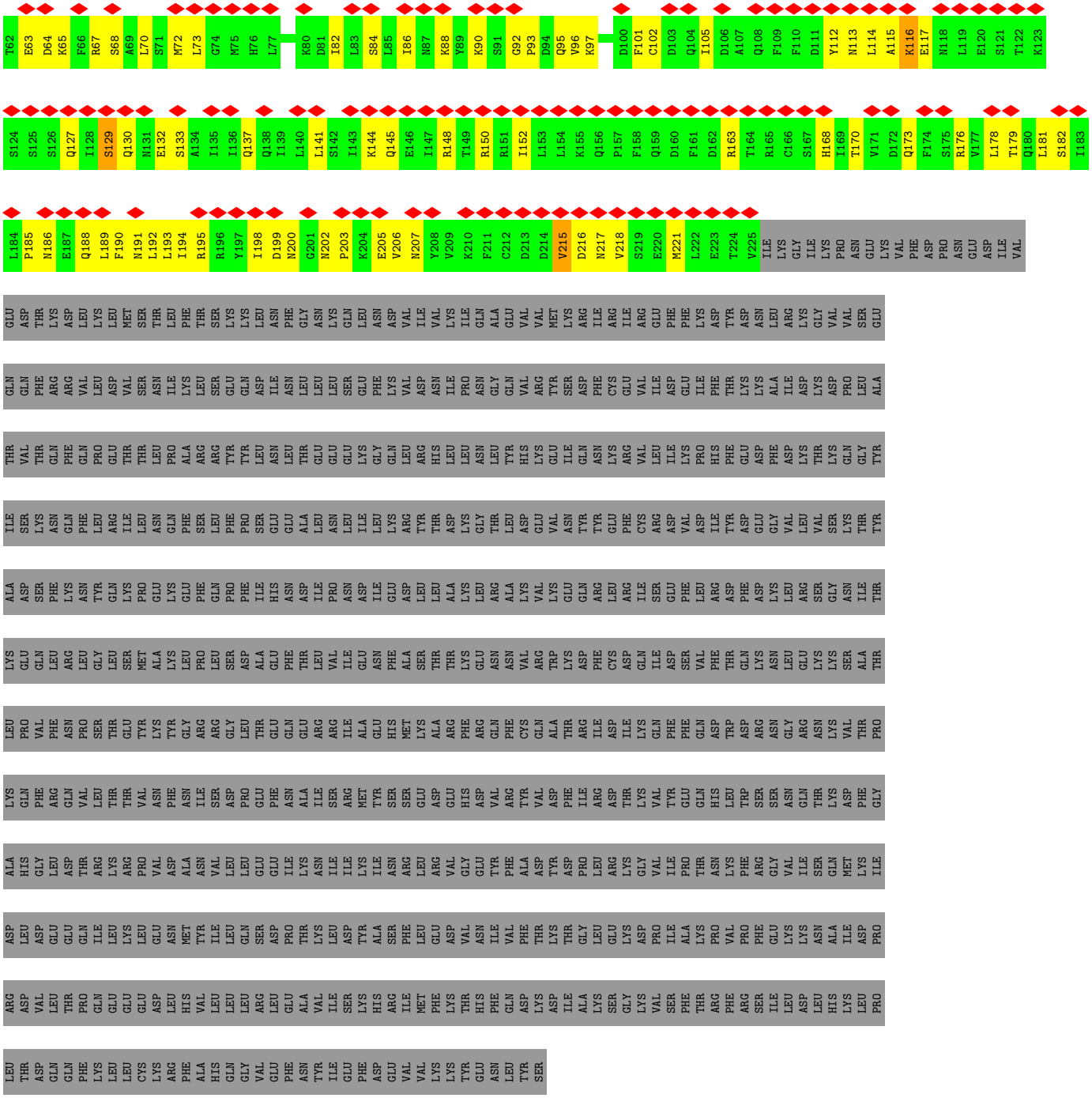


• Molecule 21: CFAP115

Chain 3L:





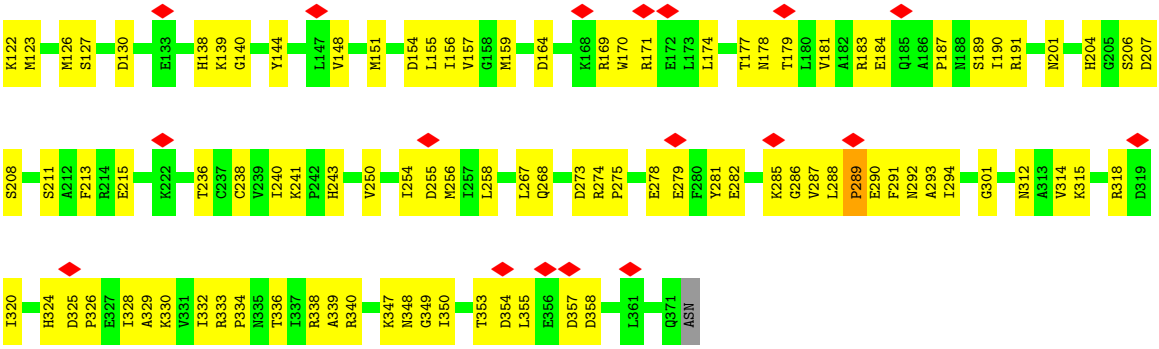


• Molecule 22: Nucleoside diphosphate kinase

Chain 1M:



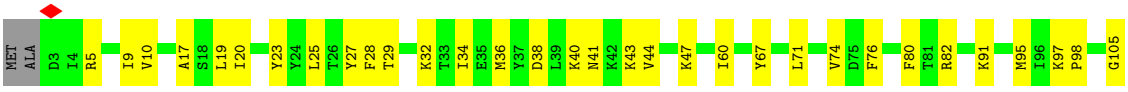




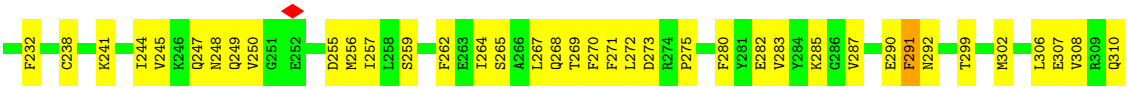
• Molecule 22: Nucleoside diphosphate kinase

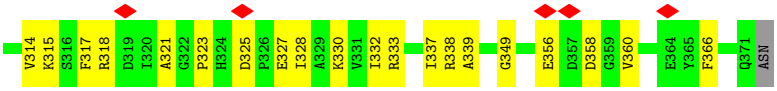
Chain 2M:







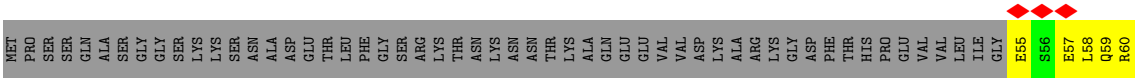


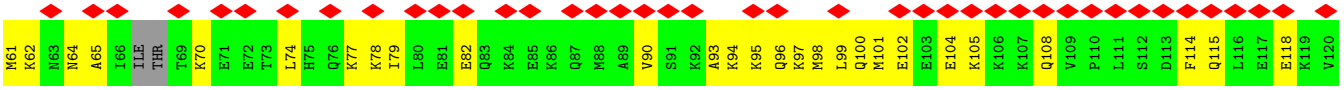


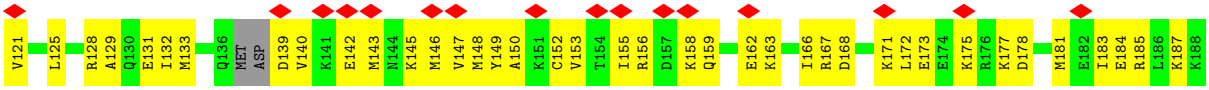
• Molecule 23: Cilia- and flagella-associated protein 45

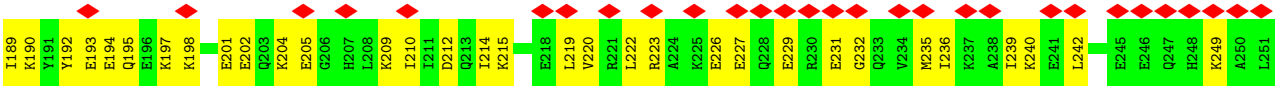
Chain 1O:

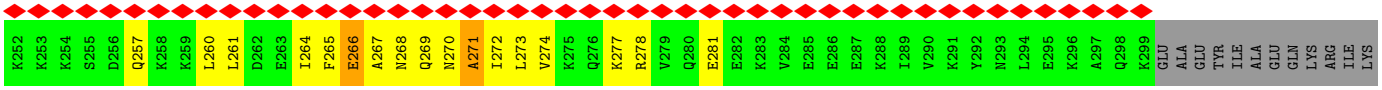


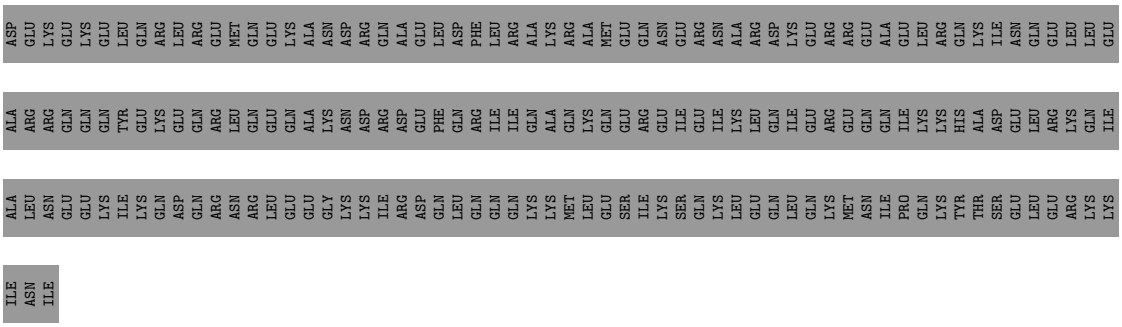






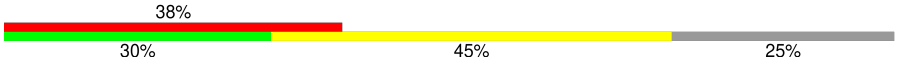


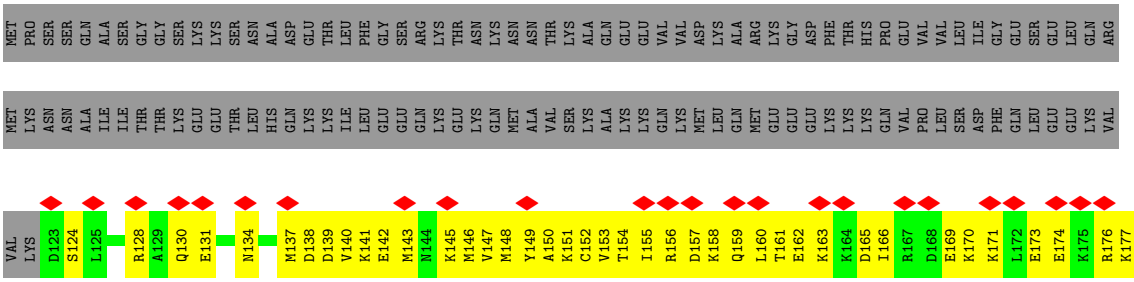




• Molecule 23: Cilia- and flagella-associated protein 45

Chain 2O:



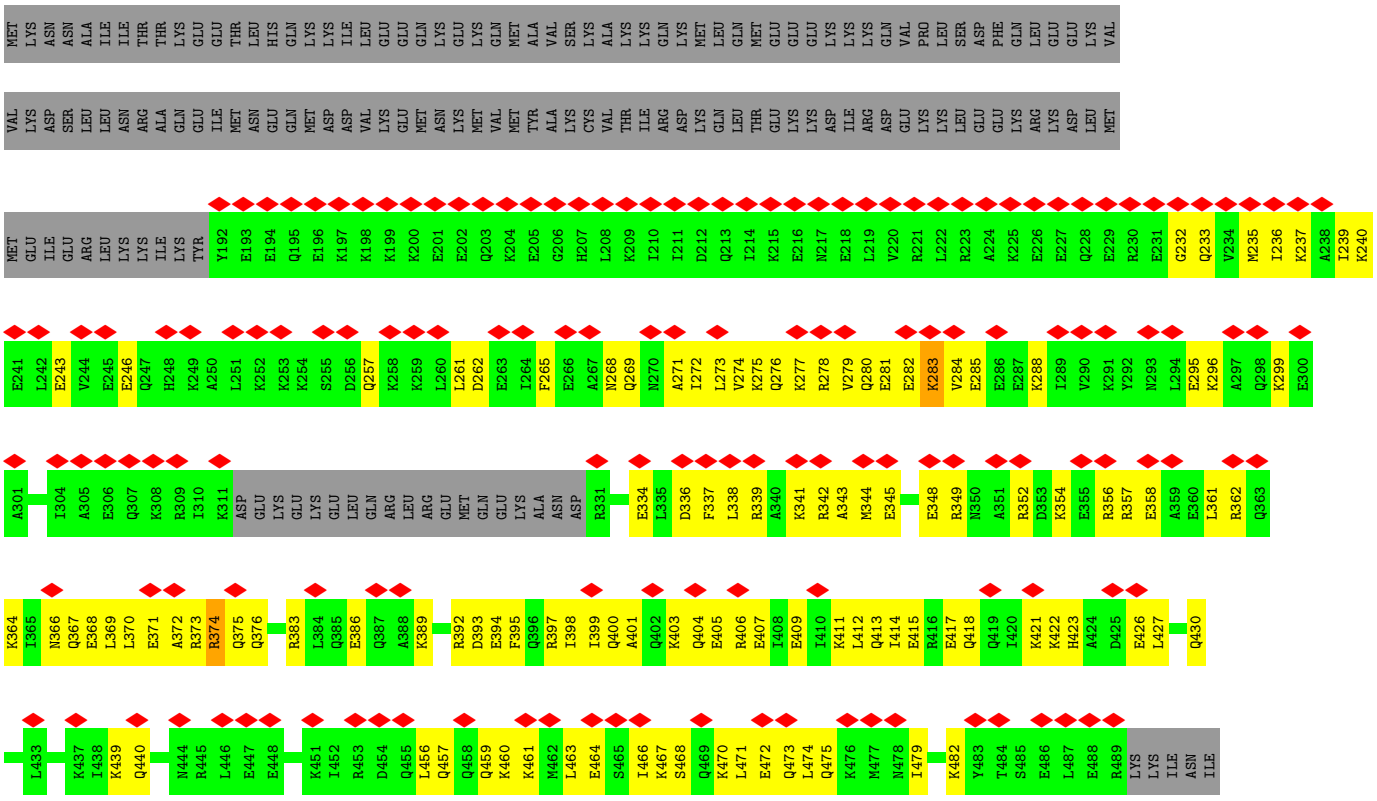


• Molecule 23: Cilia- and flagella-associated protein 45

Chain 3O:

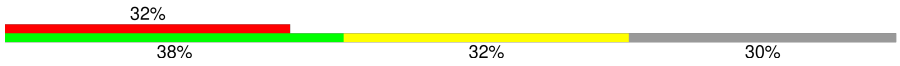


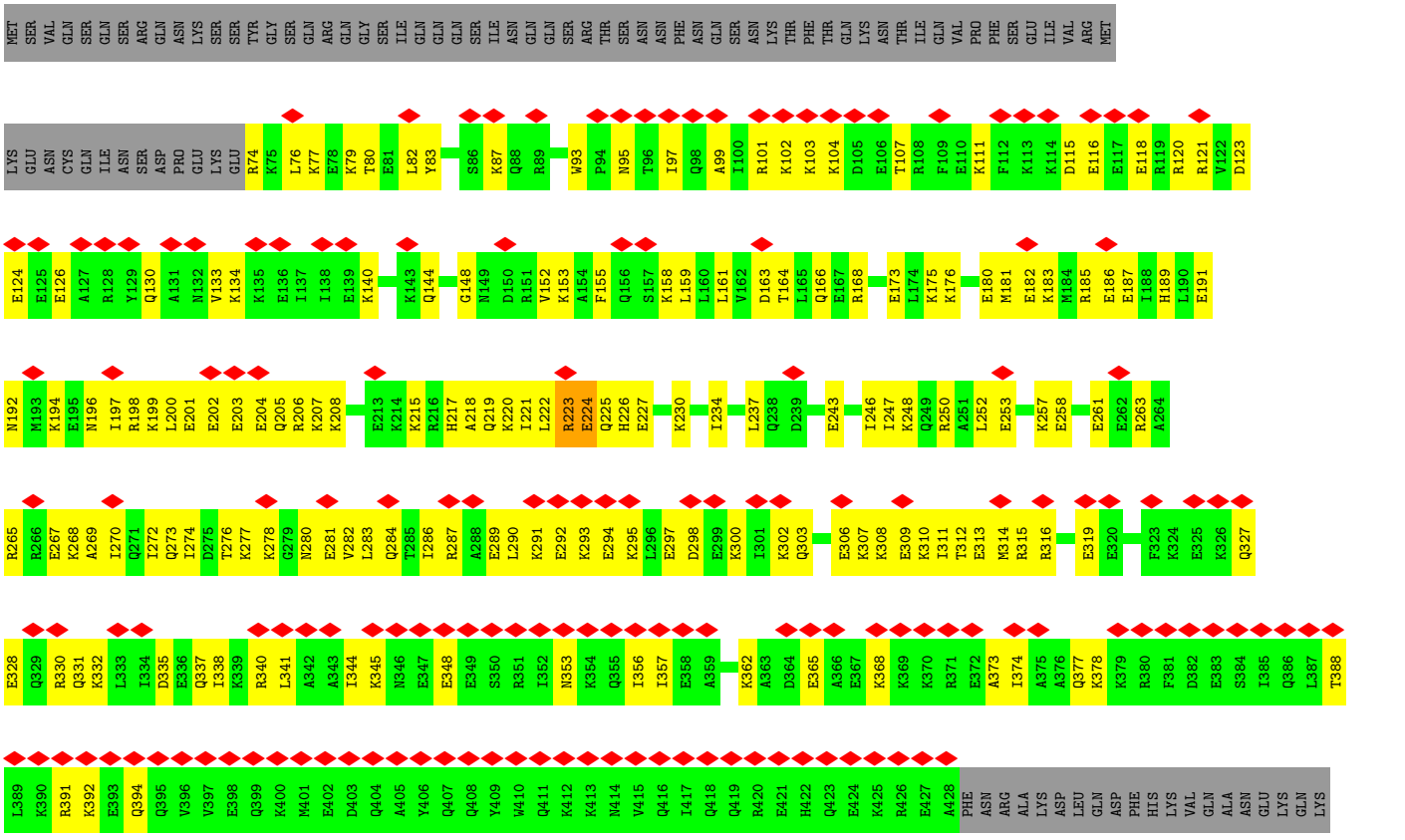




• Molecule 24: CFAP210

Chain 1P:



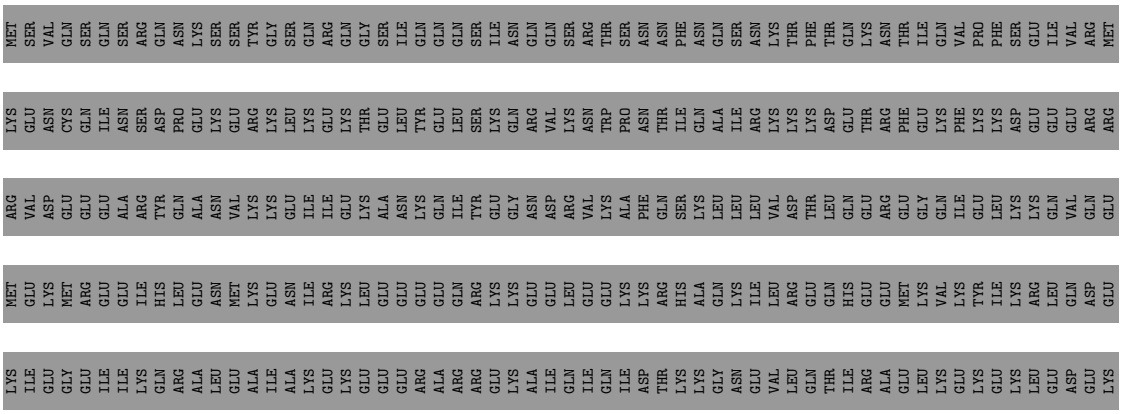


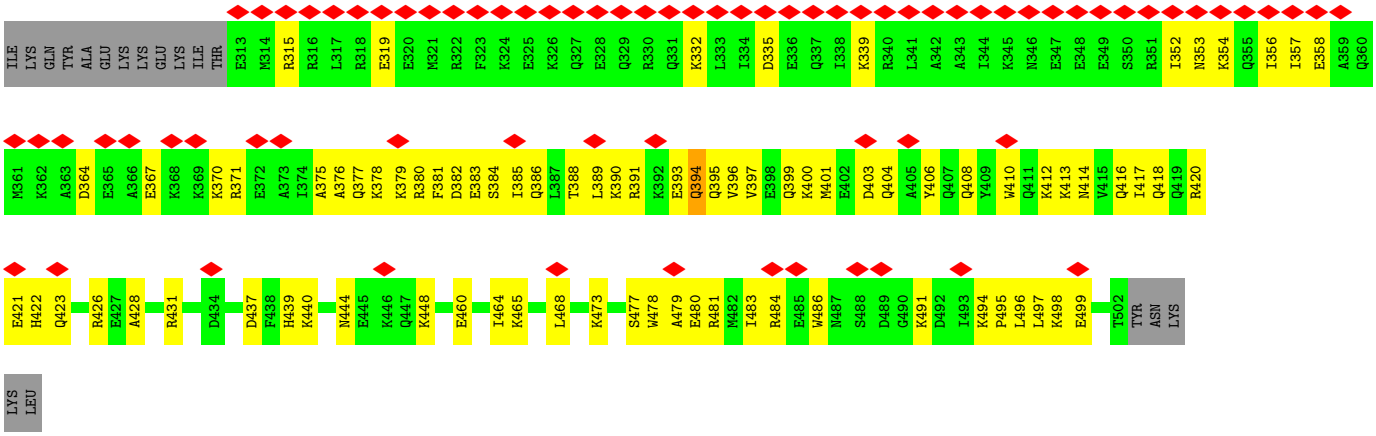


• Molecule 24: CFAP210

Chain 2P:



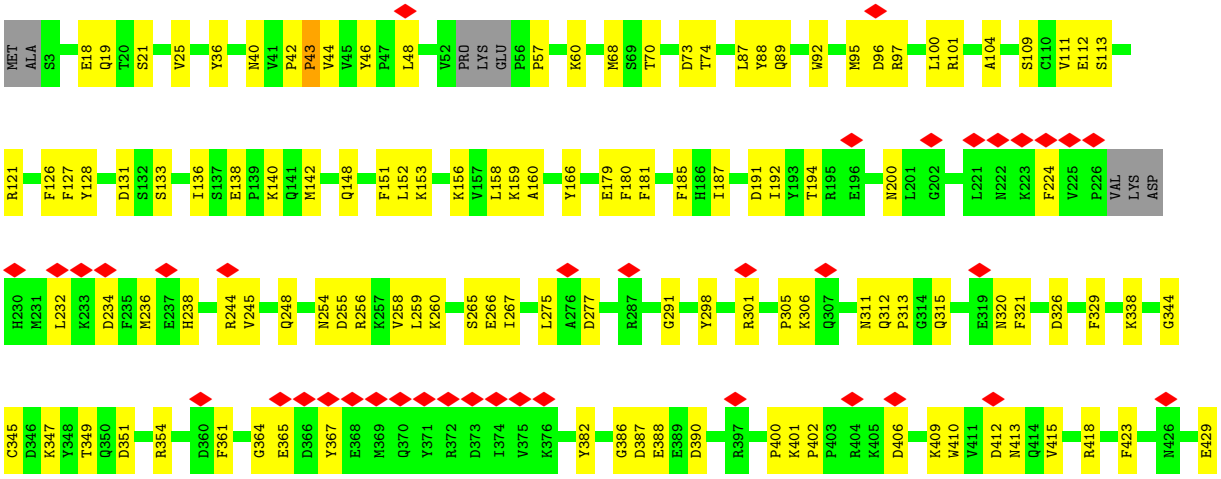


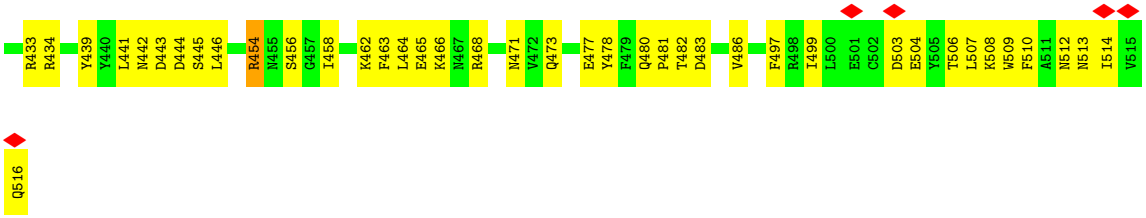


• Molecule 25: RIB72B

Chain 1R:



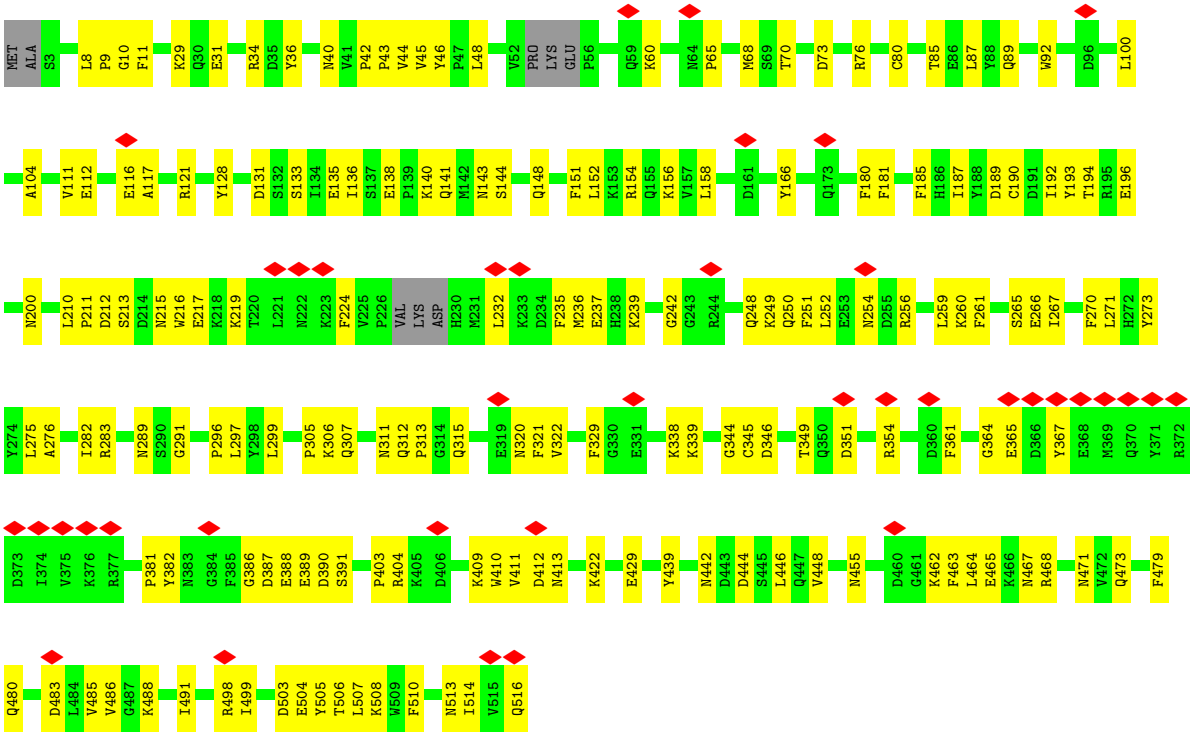




• Molecule 25: RIB72B

Chain 2R:

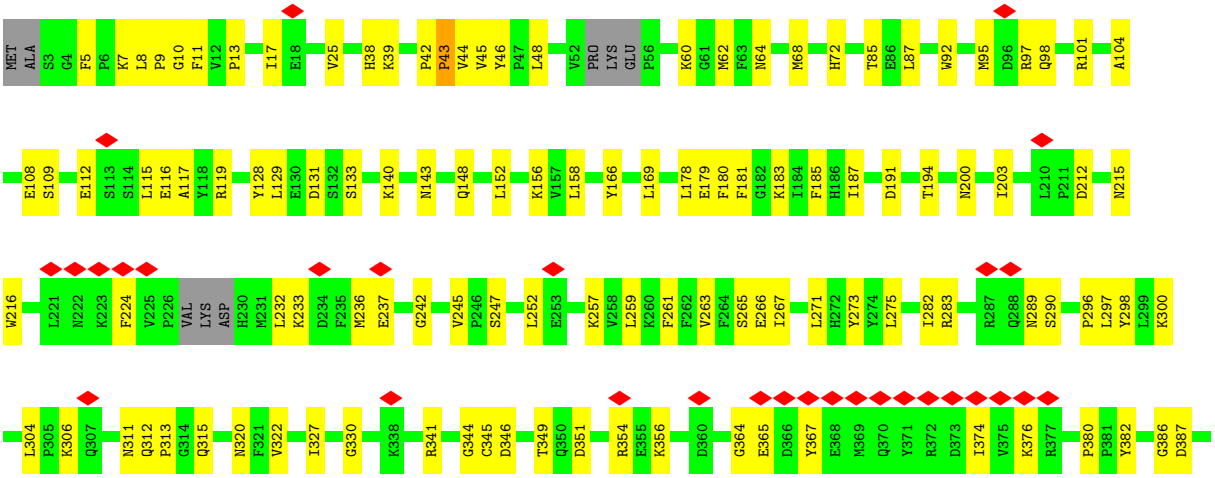


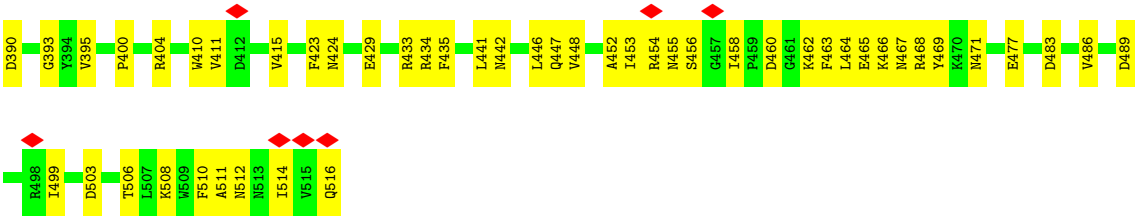


• Molecule 25: RIB72B

Chain 3R:



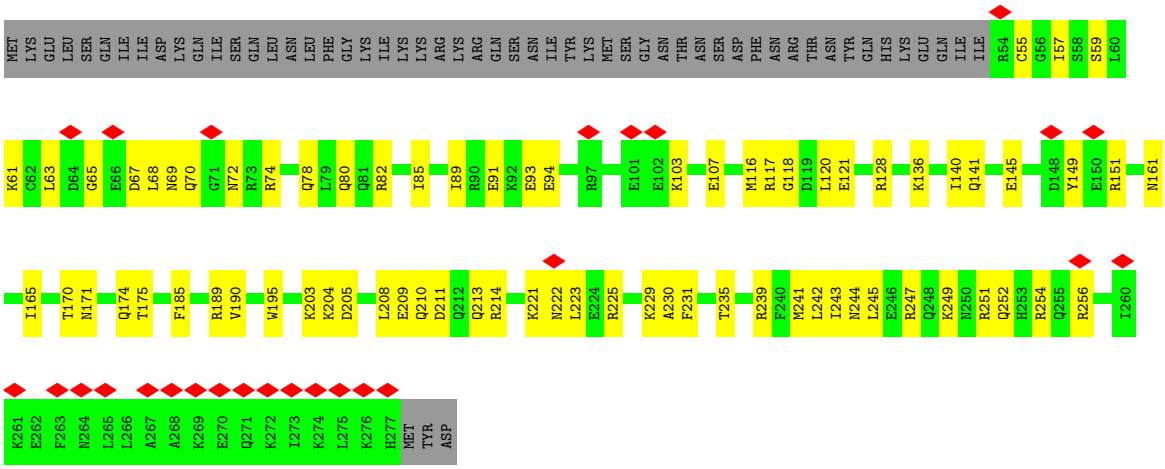




• Molecule 26: Protofilament ribbon protein

Chain 1W:

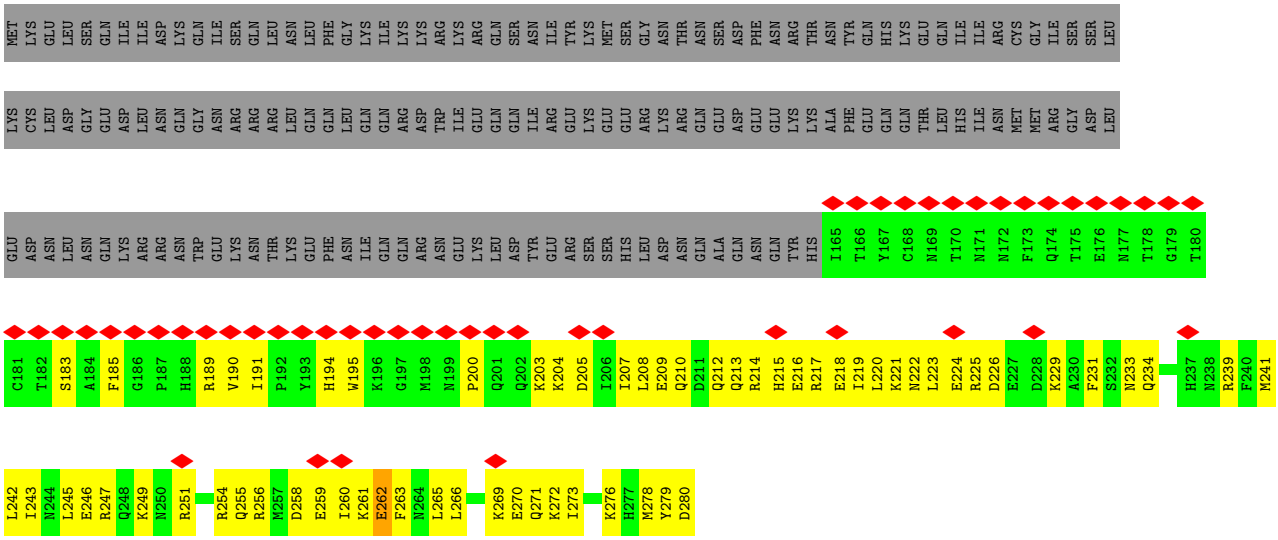




• Molecule 26: Protofilament ribbon protein

Chain 2W:

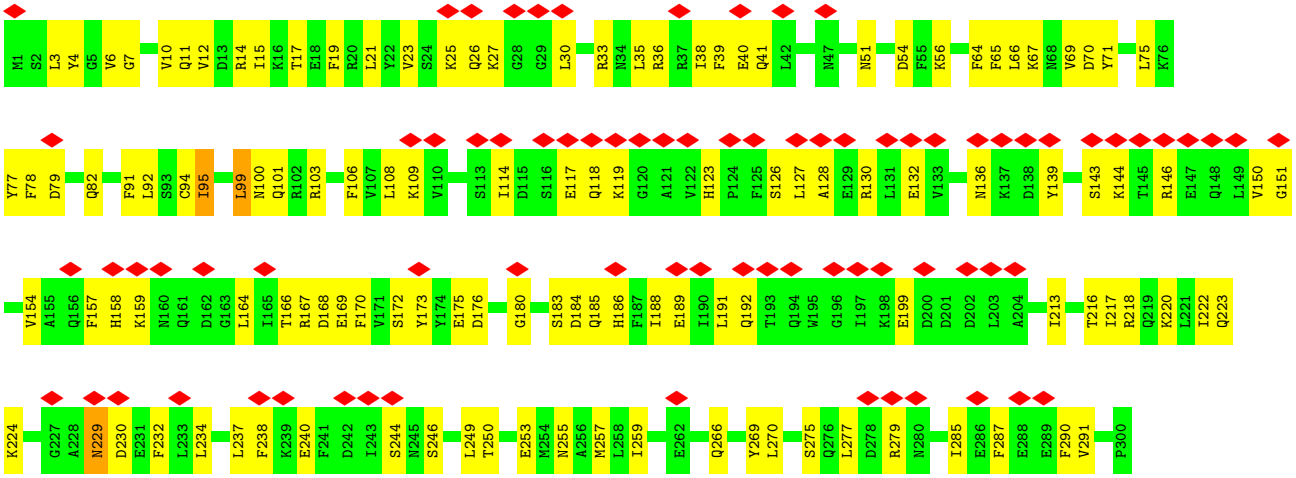




• Molecule 27: RIB35

Chain 2C:

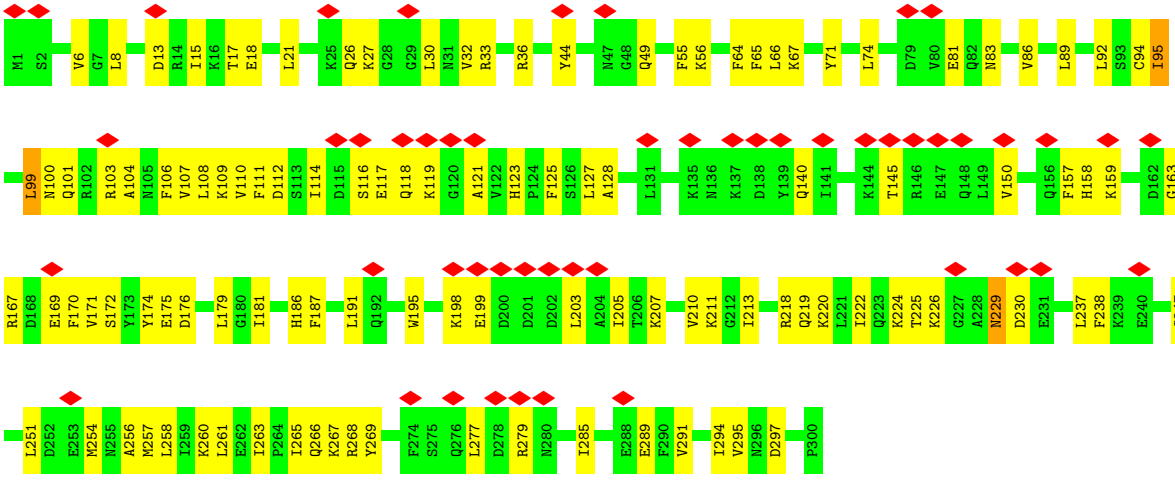




- Molecule 27: RIB35

Chain 3C:

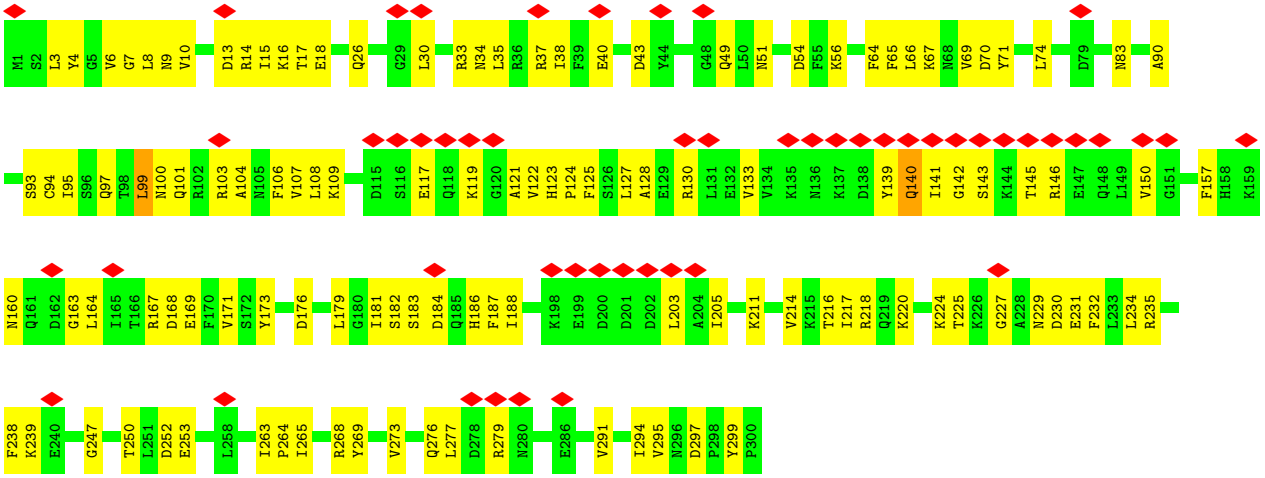




- Molecule 27: RIB35

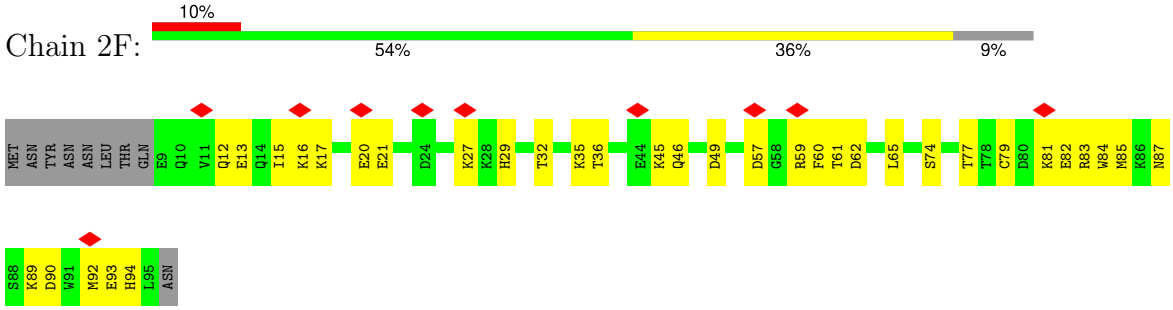
Chain 4C:





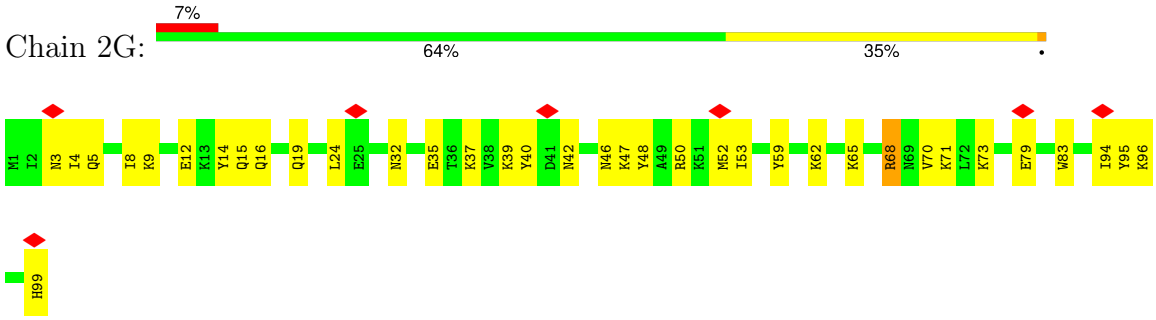
• Molecule 28: CFAP182B

Chain 2F:



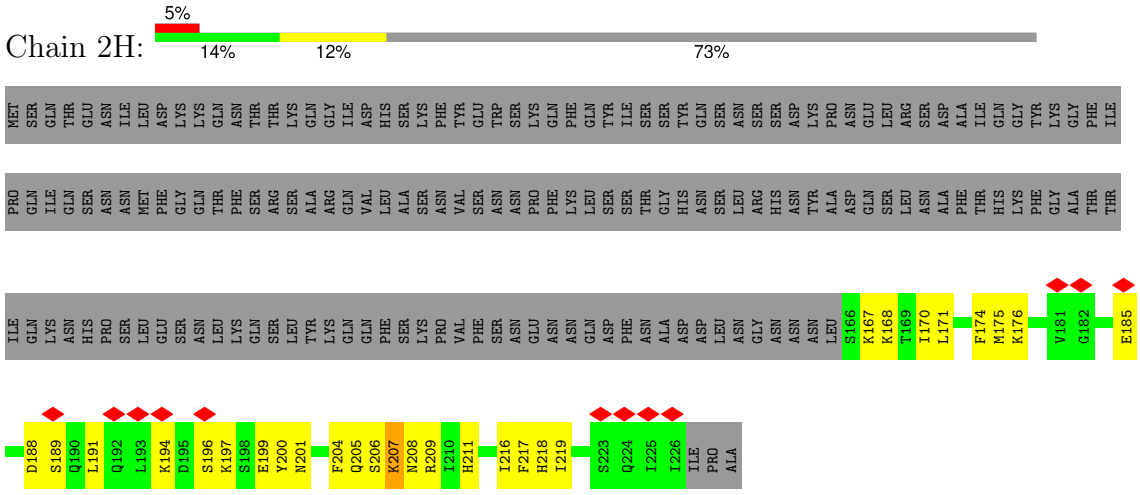
• Molecule 29: Flagellar FliJ protein

Chain 2G:



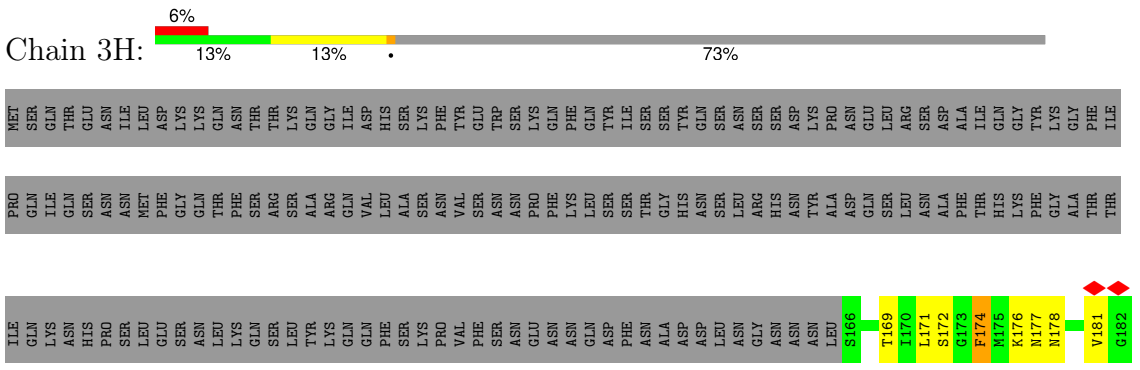
• Molecule 30: RIB27B

Chain 2H:



• Molecule 30: RIB27B

Chain 3H:

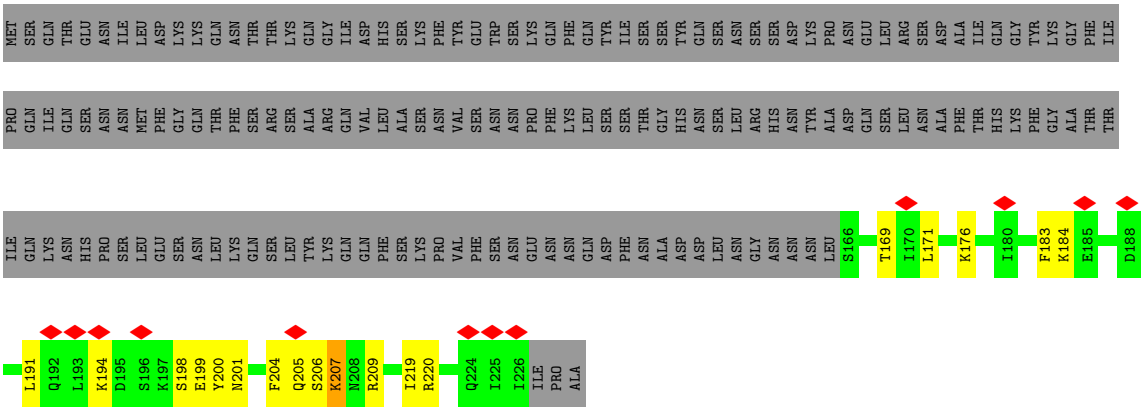




• Molecule 30: RIB27B

Chain 4H:

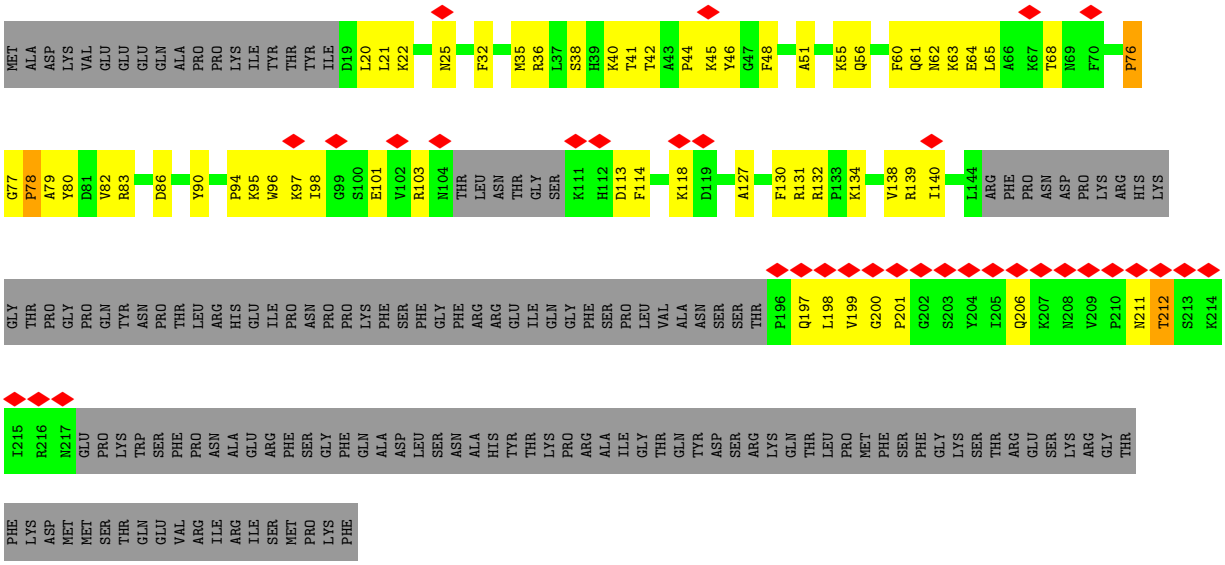




• Molecule 31: STPG2

Chain 2I:

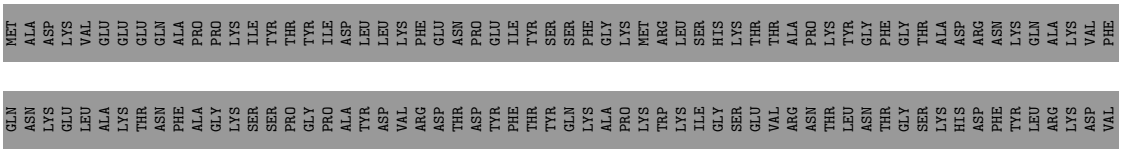


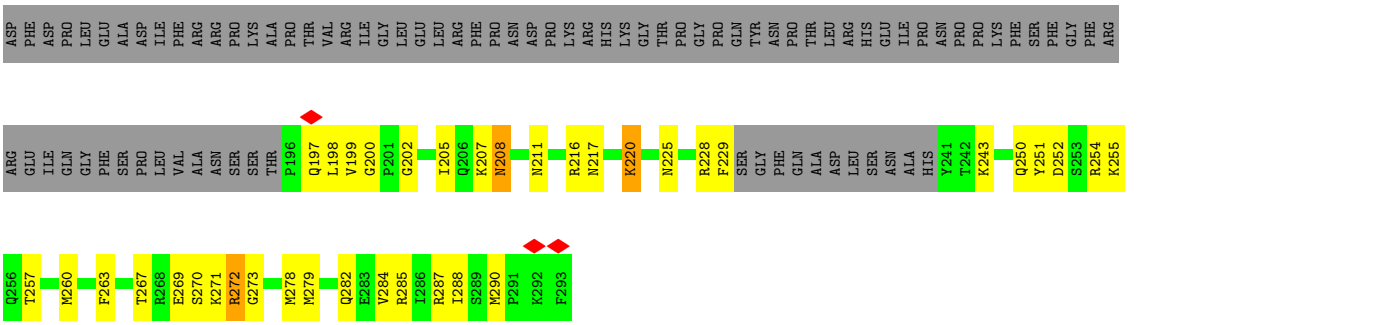


• Molecule 31: STPG2

Chain 3I:



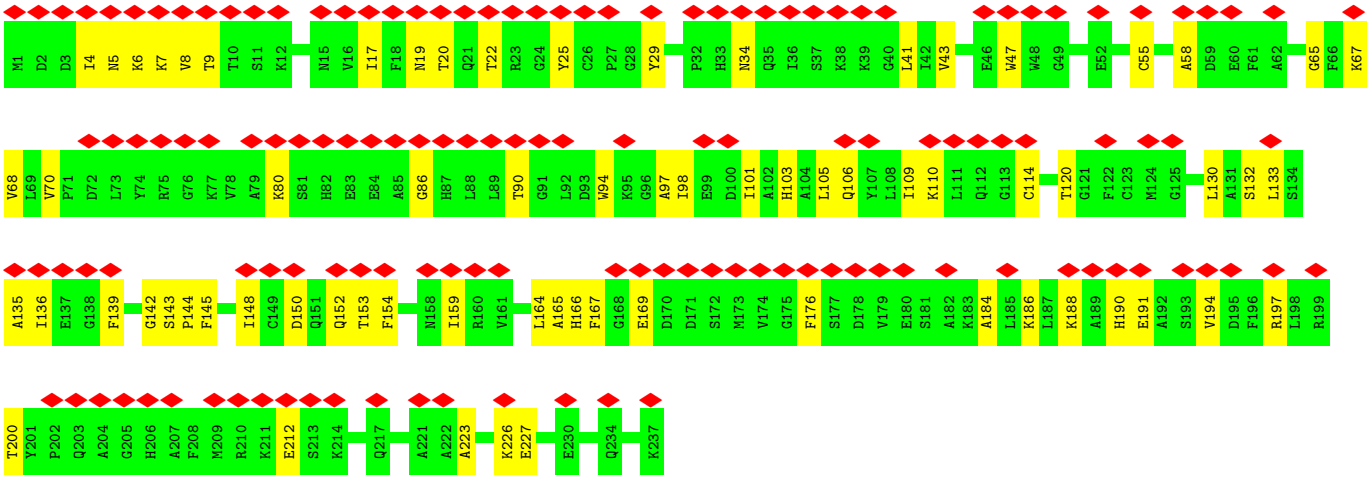




• Molecule 32: RIB26

Chain 3D:

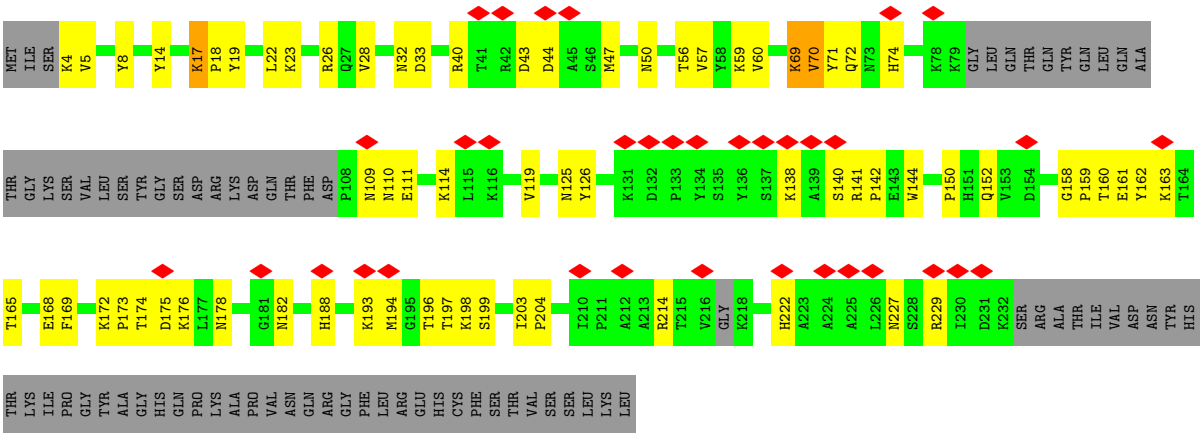




• Molecule 33: CFAP129

Chain 4F:

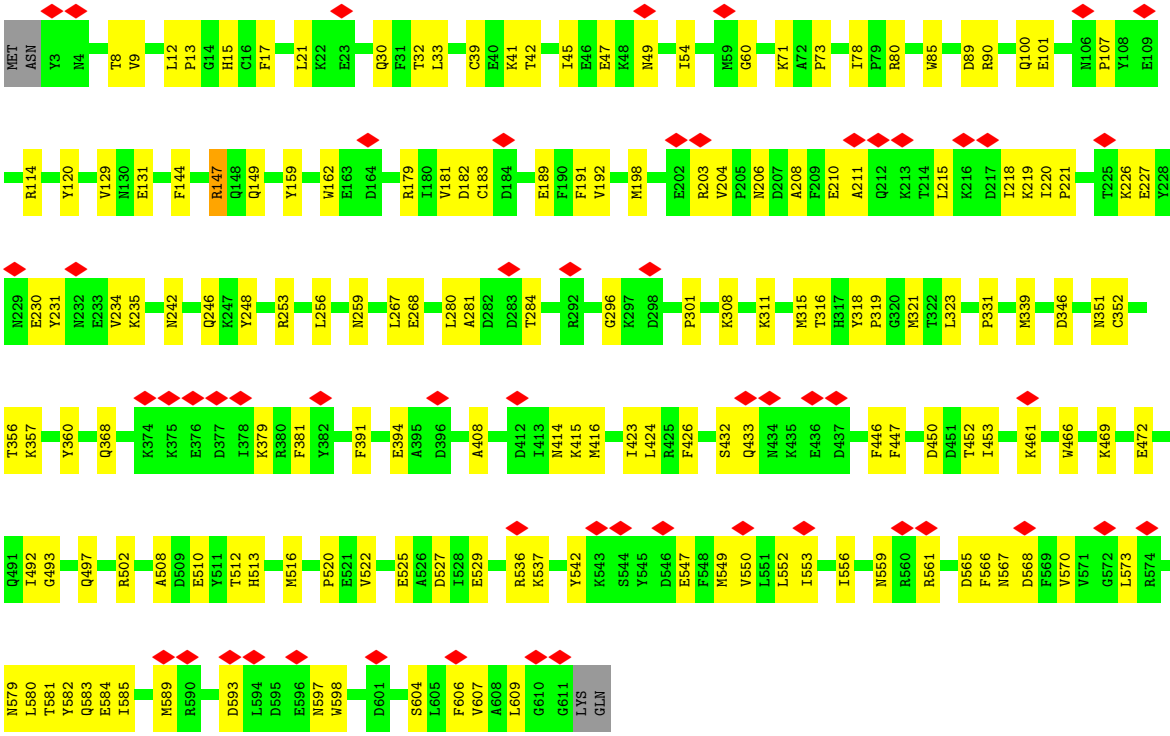




• Molecule 34: Flagellar microtubule protofilament ribbon protein

Chain 4R:

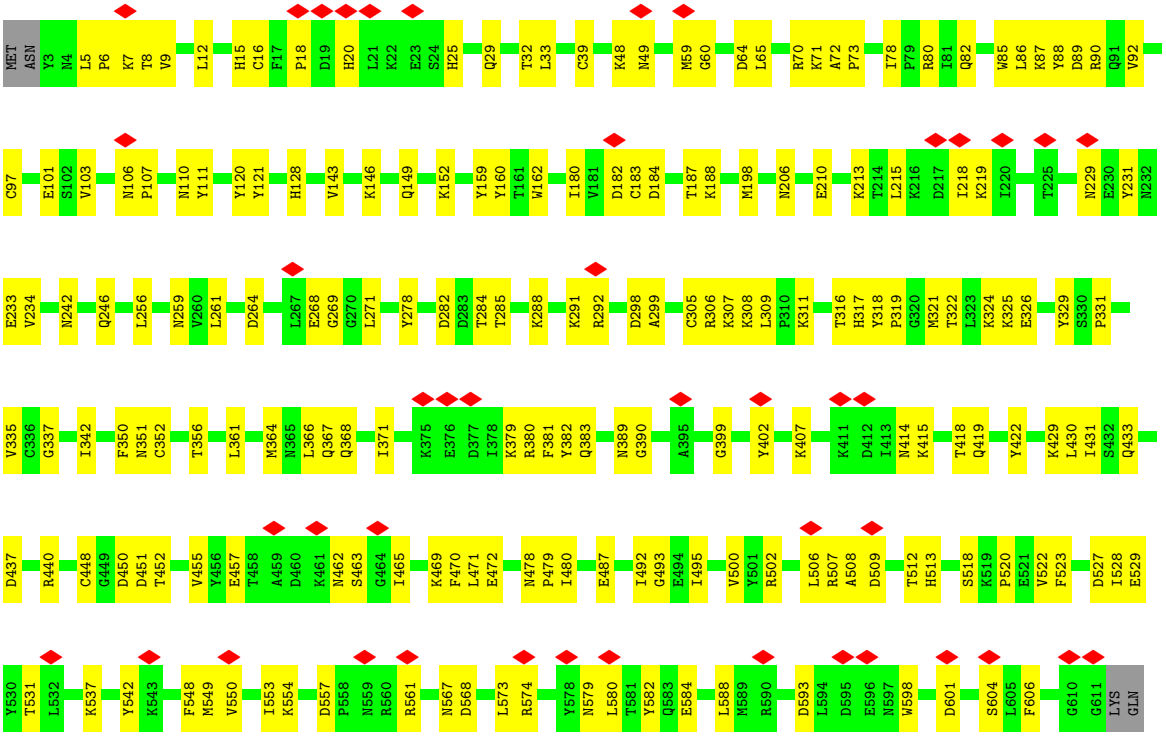




• Molecule 34: Flagellar microtubule protofilament ribbon protein

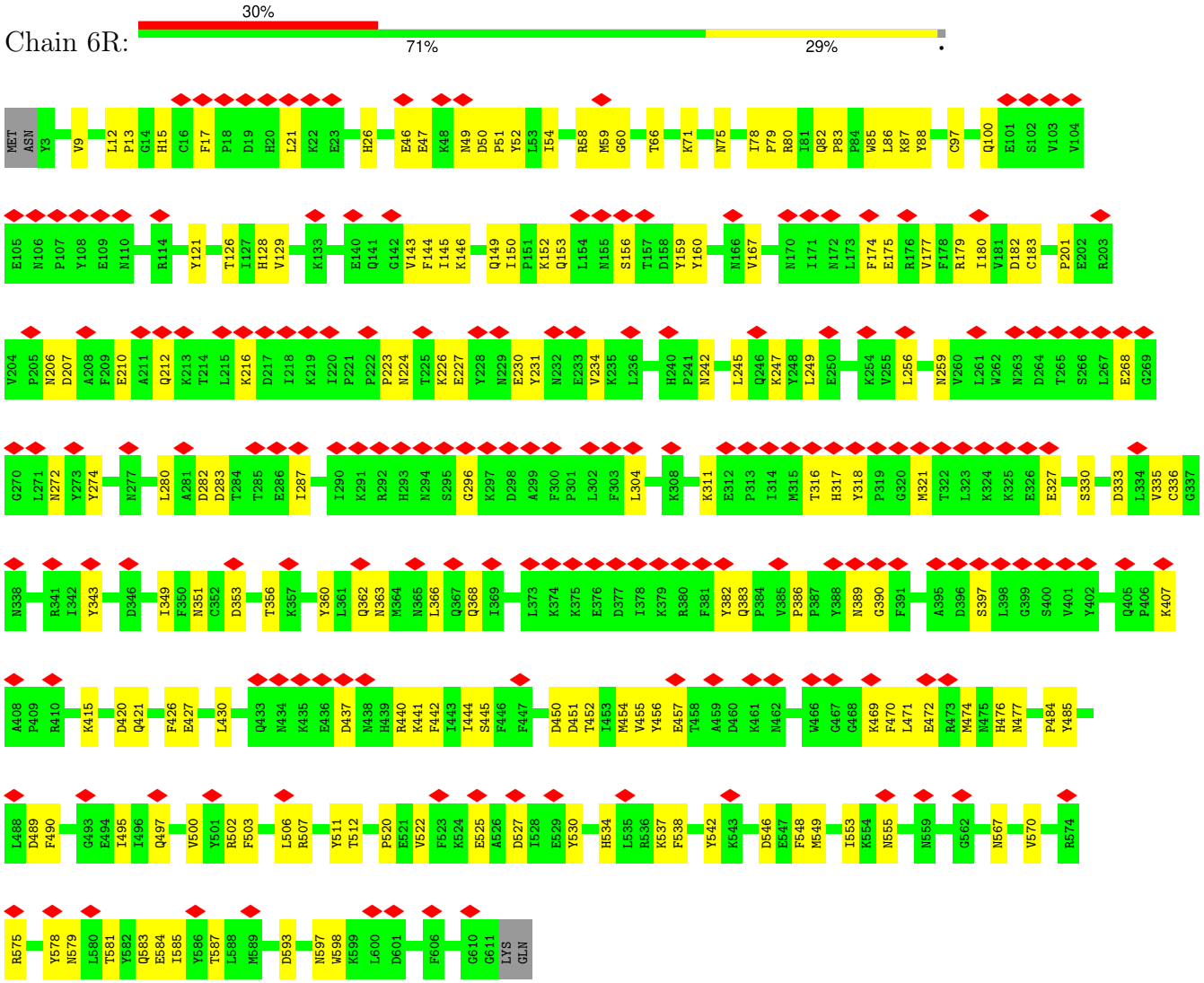
Chain 5R:





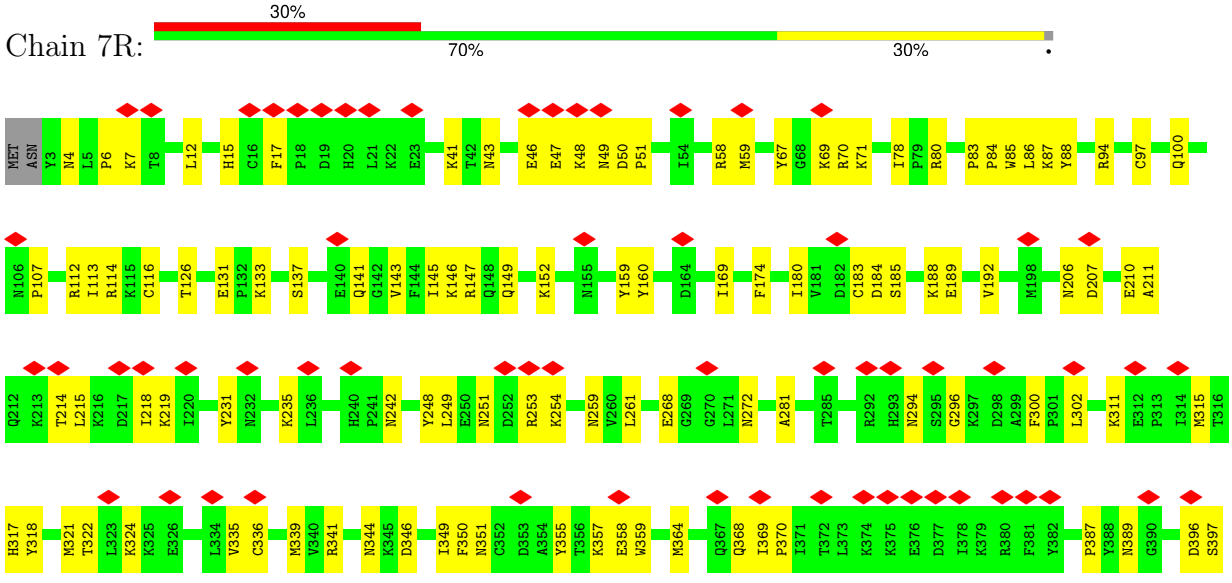
• Molecule 34: Flagellar microtubule protofilament ribbon protein

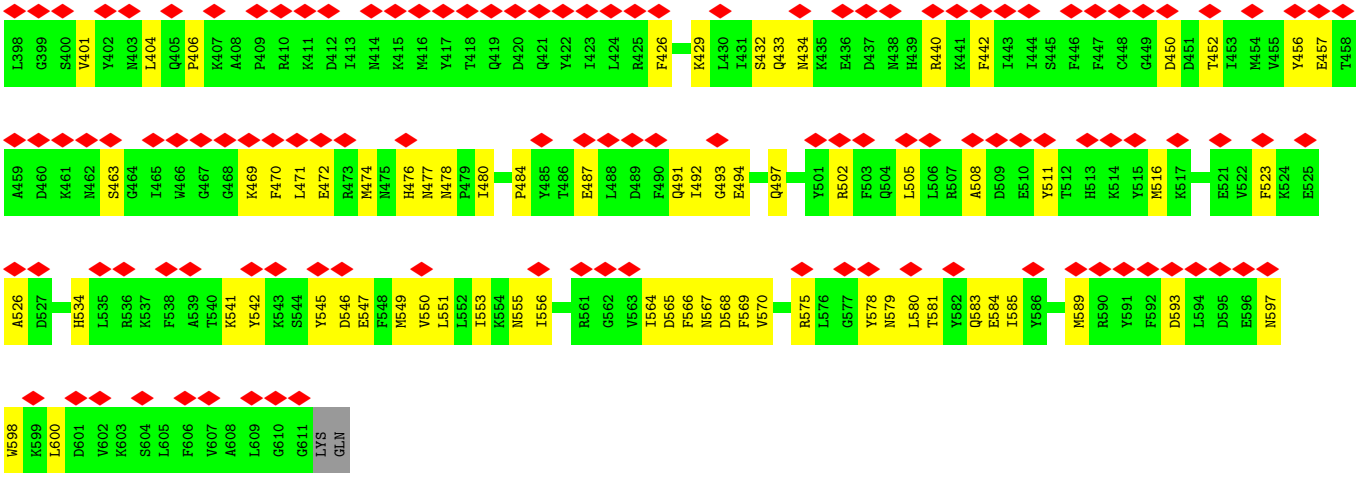
Chain 6R:



• Molecule 34: Flagellar microtubule protofilament ribbon protein

Chain 7R:

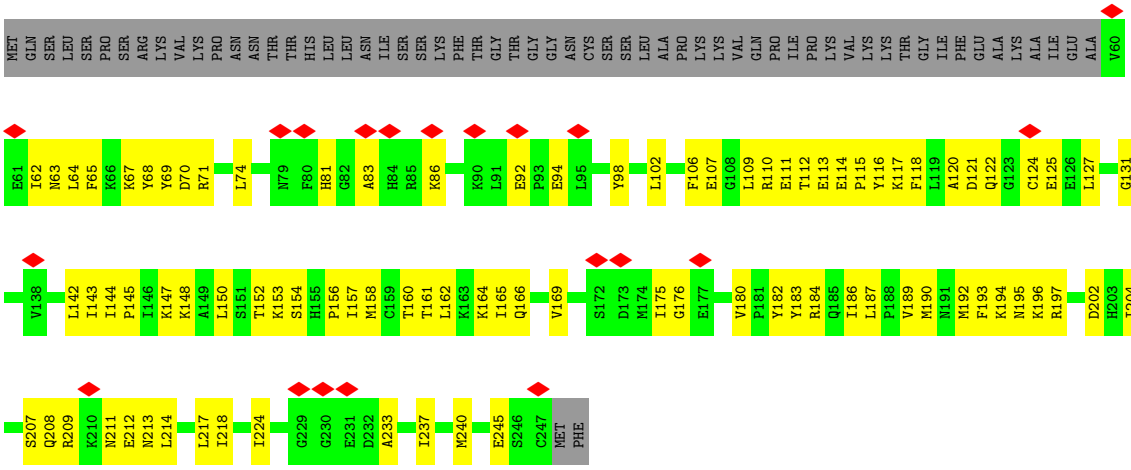




• Molecule 35: Parkin co-regulated protein PACRGB

Chain 4S:

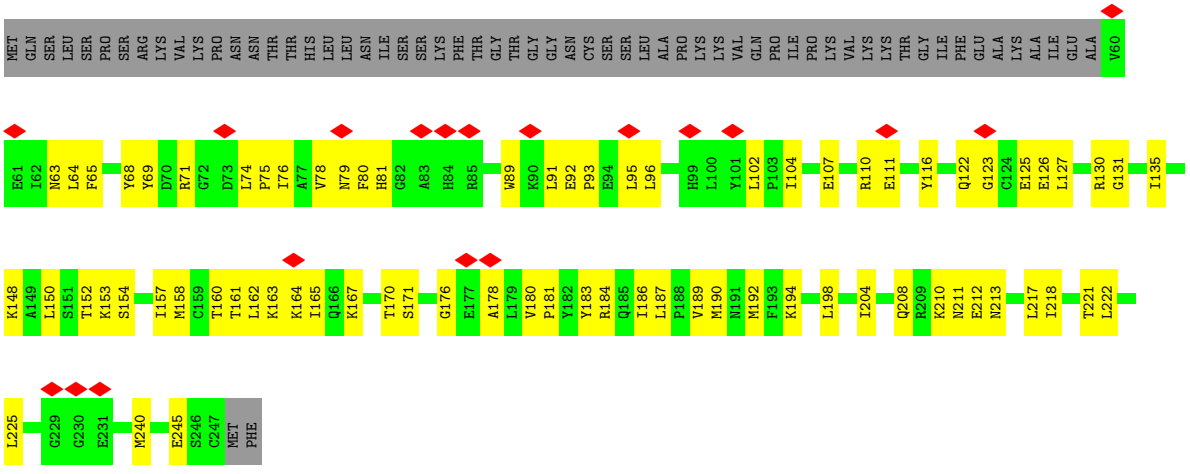




• Molecule 35: Parkin co-regulated protein PACRGB

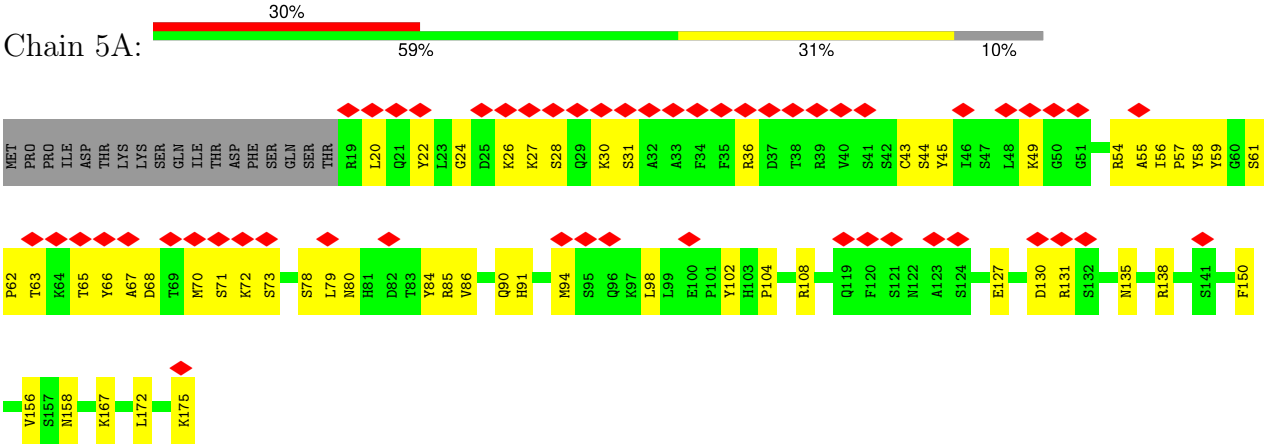
Chain 5S:





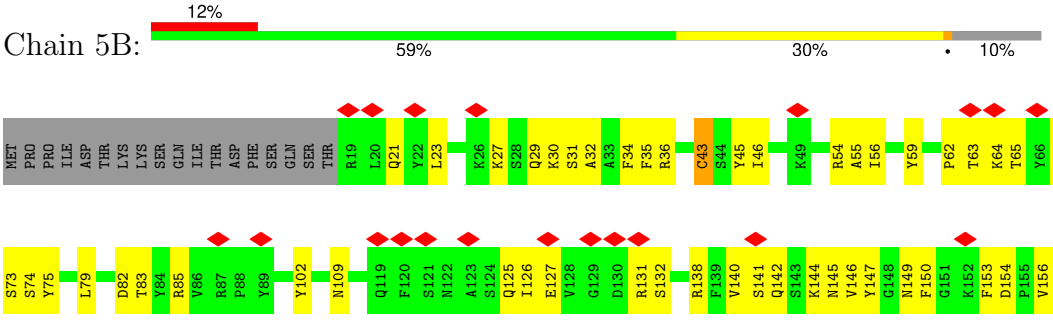
- Molecule 36: OJ2

Chain 5A:



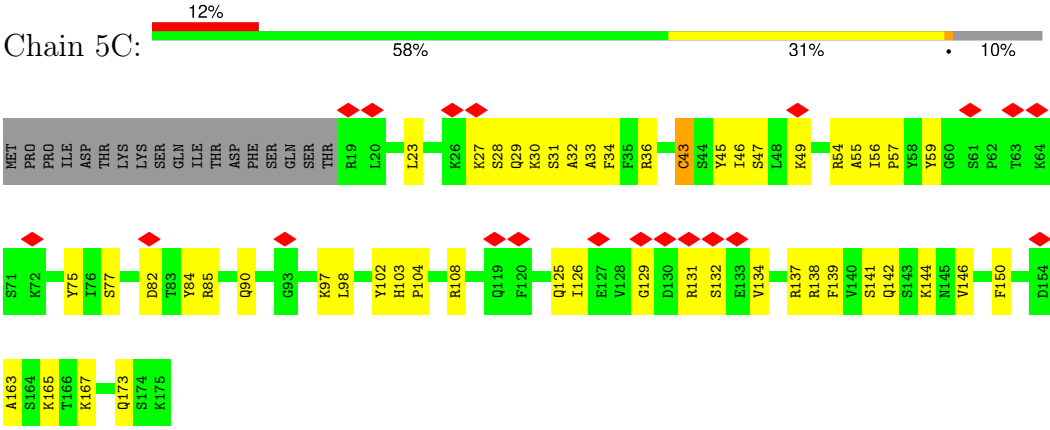
- Molecule 36: OJ2

Chain 5B:



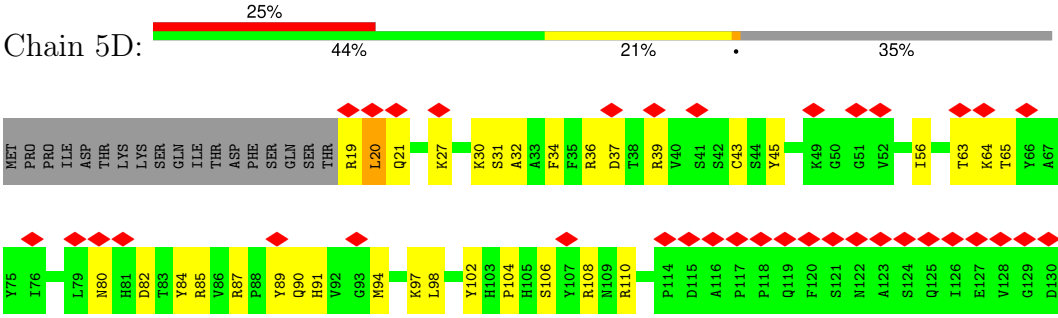
- Molecule 36: OJ2

Chain 5C:



- Molecule 36: OJ2

Chain 5D:

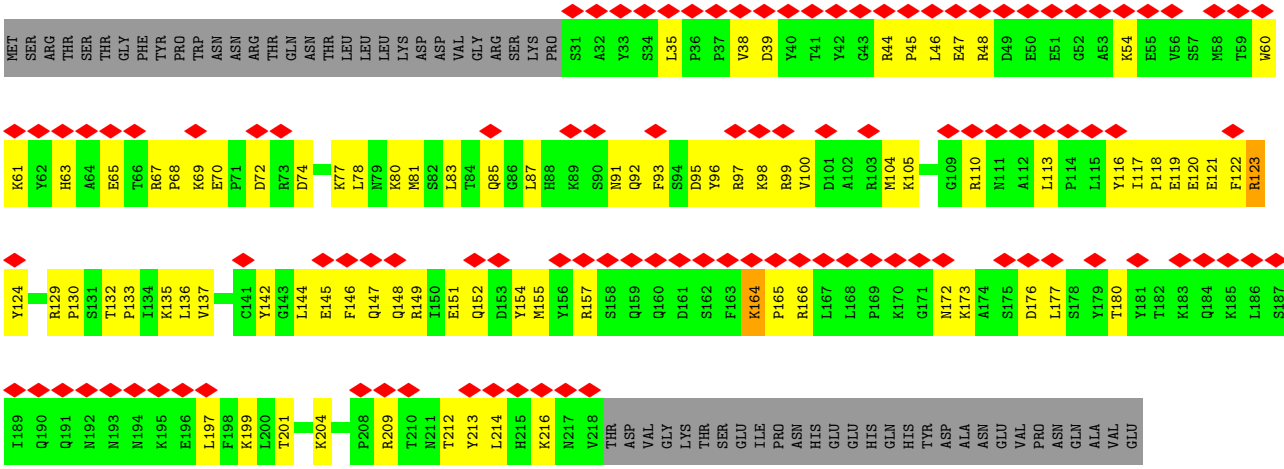




• Molecule 37: CFAP77A

Chain 5E:

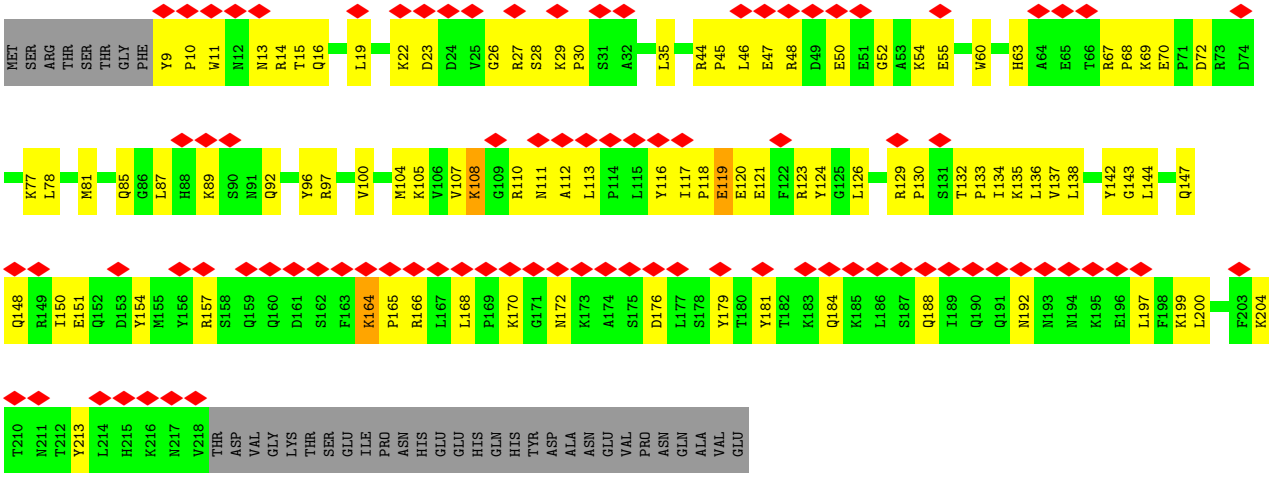




• Molecule 37: CFAP77A

Chain 5F:

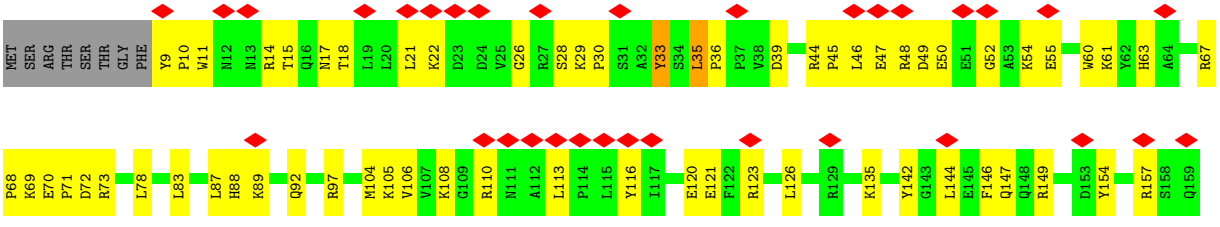


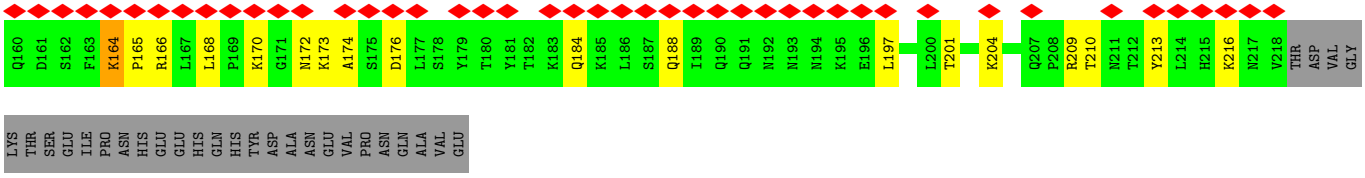


• Molecule 37: CFAP77A

Chain 5G:

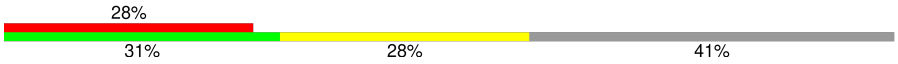


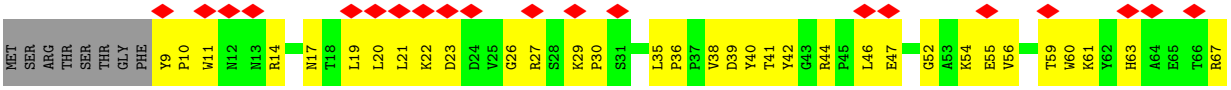


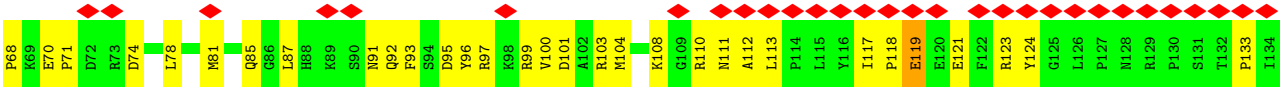


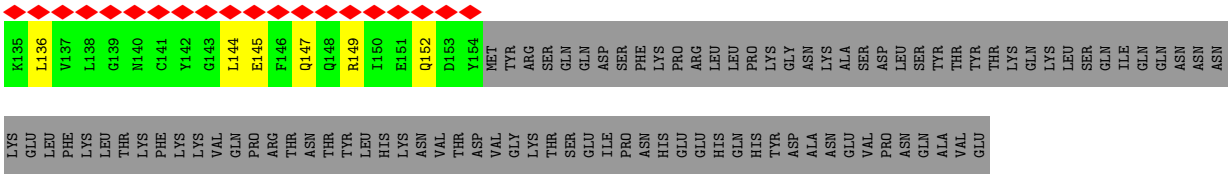
• Molecule 37: CFAP77A

Chain 5H:





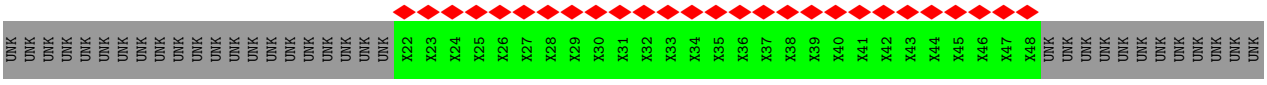


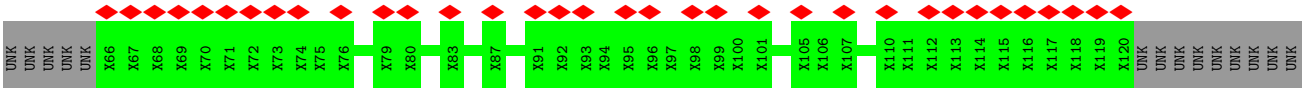


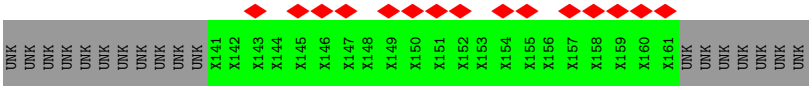
• Molecule 38: OJ3

Chain 5I:





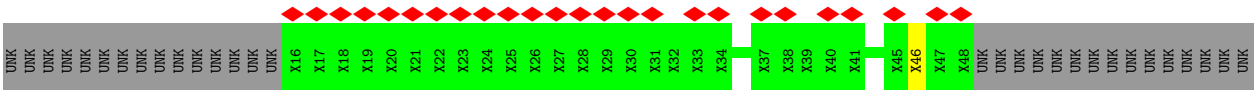


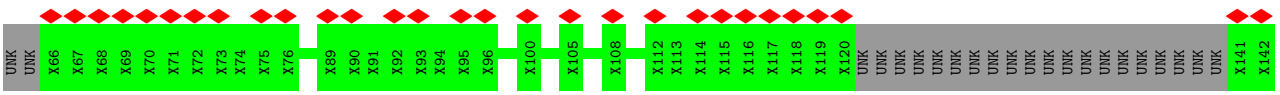


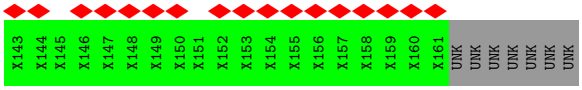
• Molecule 38: OJ3

Chain 5J:





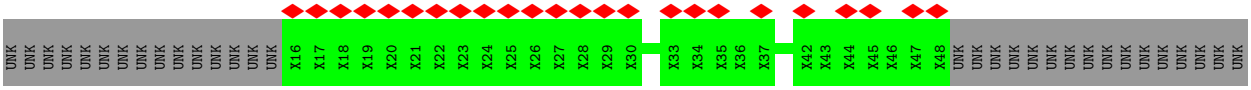


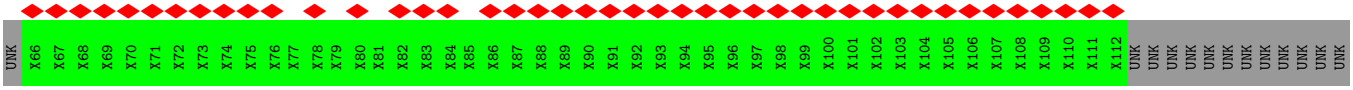


• Molecule 38: OJ3

Chain 5K:





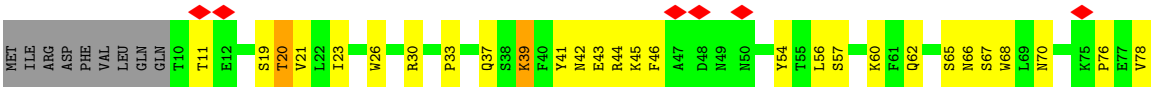




• Molecule 39: SB1

Chain 6F:





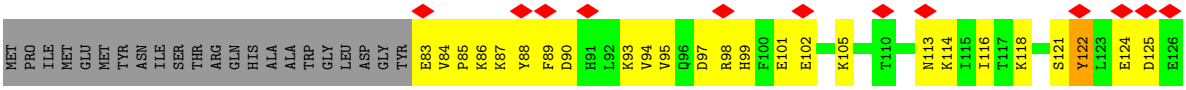


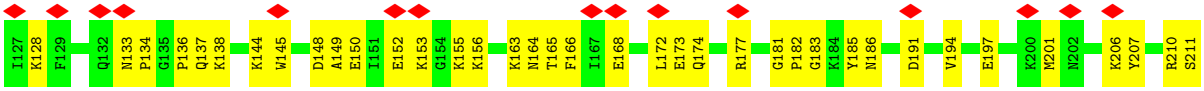
• Molecule 40: STPG1A

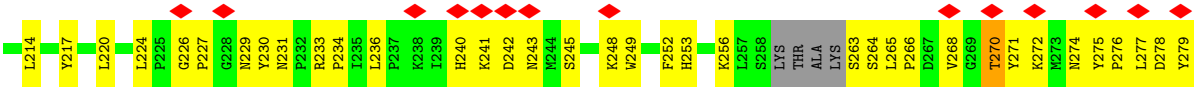
Chain 6G:











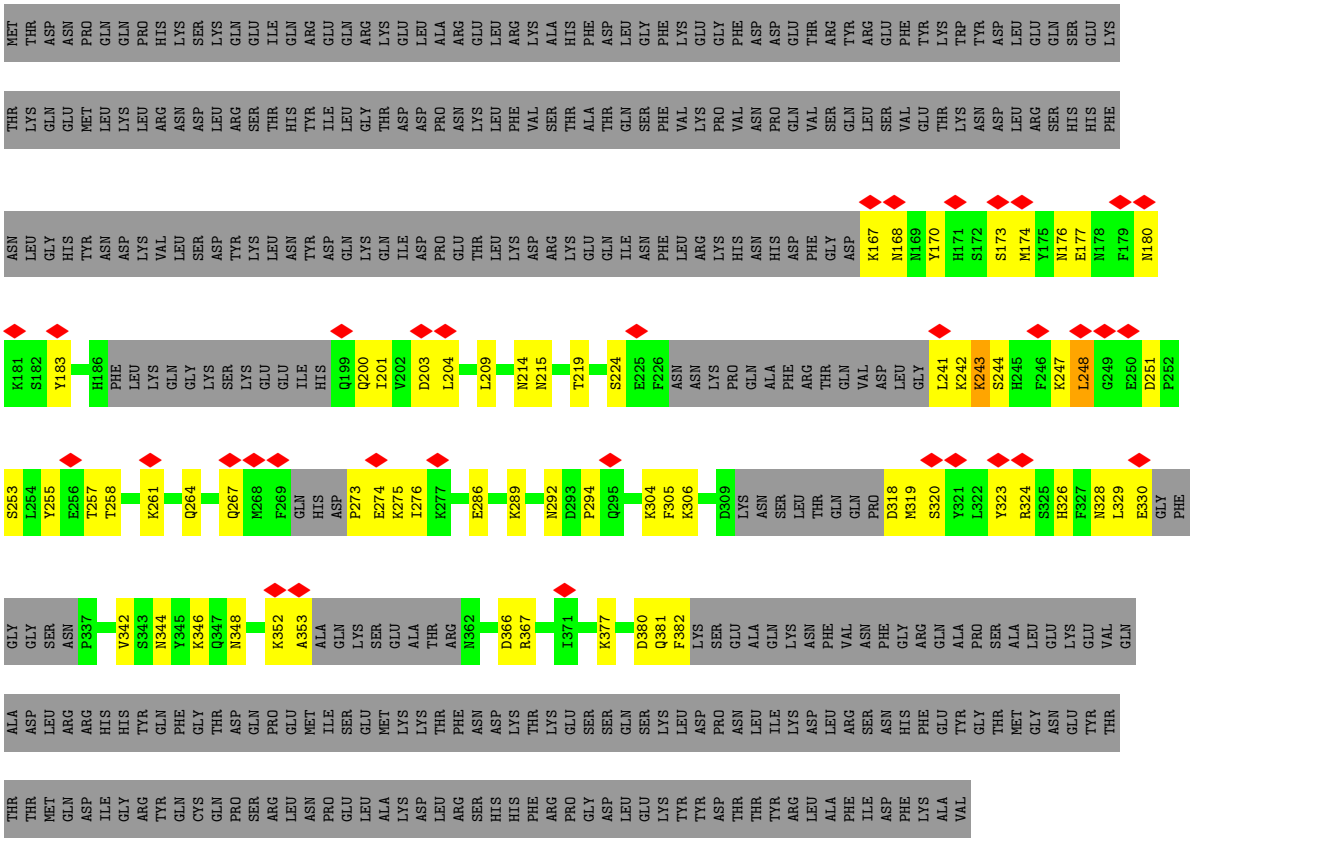




• Molecule 41: Nebulin

Chain 6H:

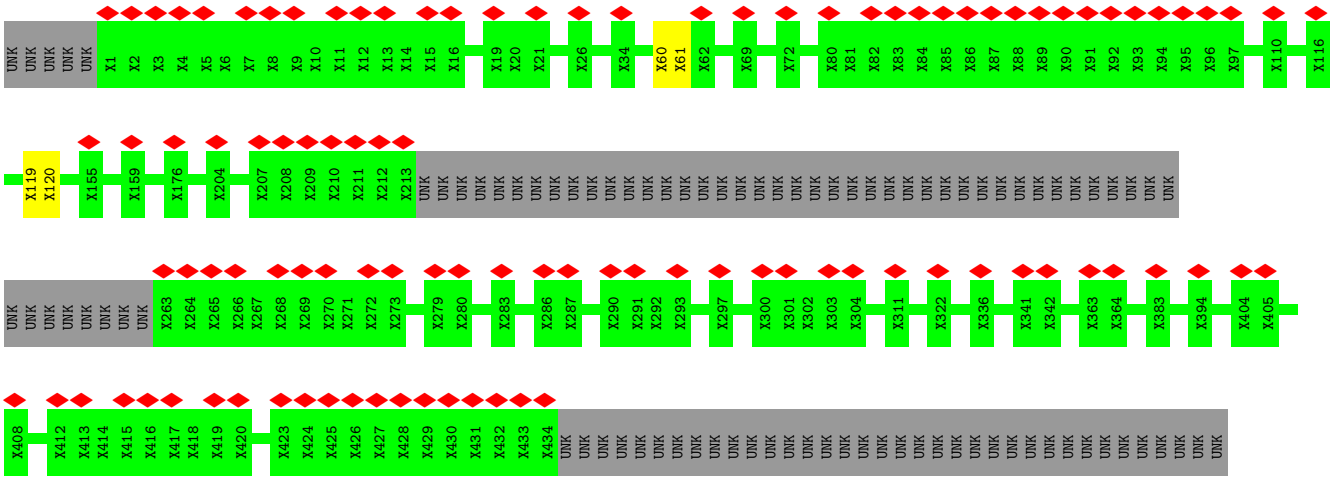




• Molecule 42: B5B6_fMIP

Chain 8L:



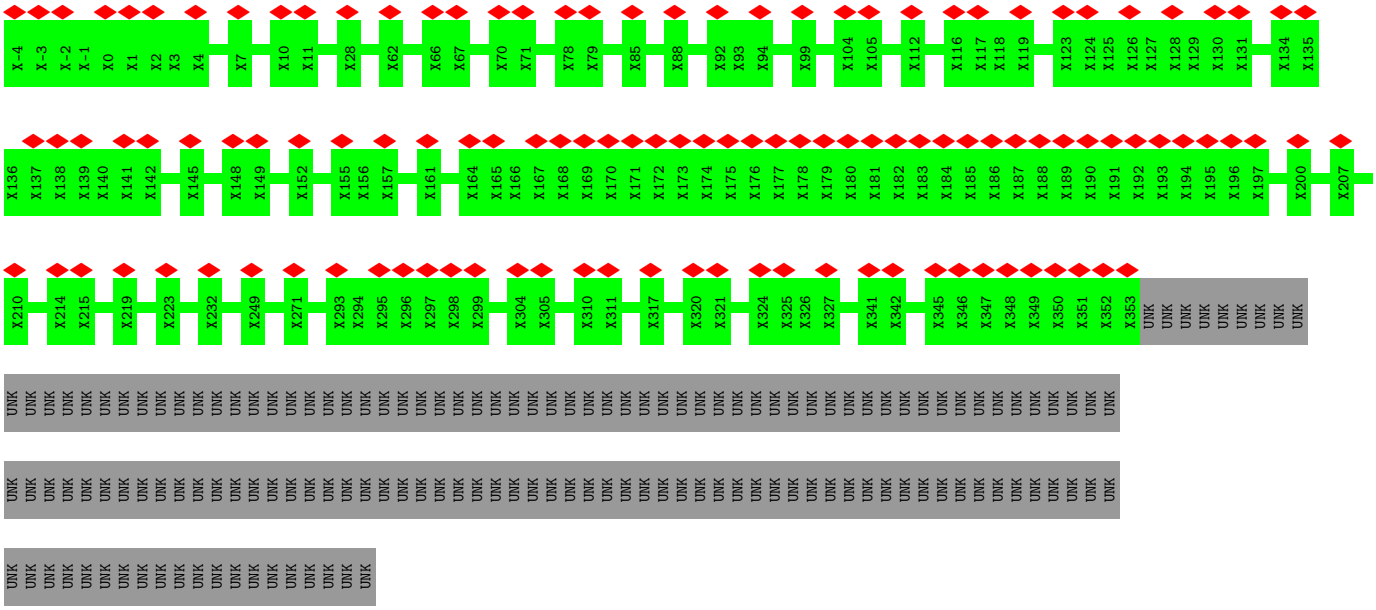




- Molecule 42: B5B6_fMIP

Chain 8N:

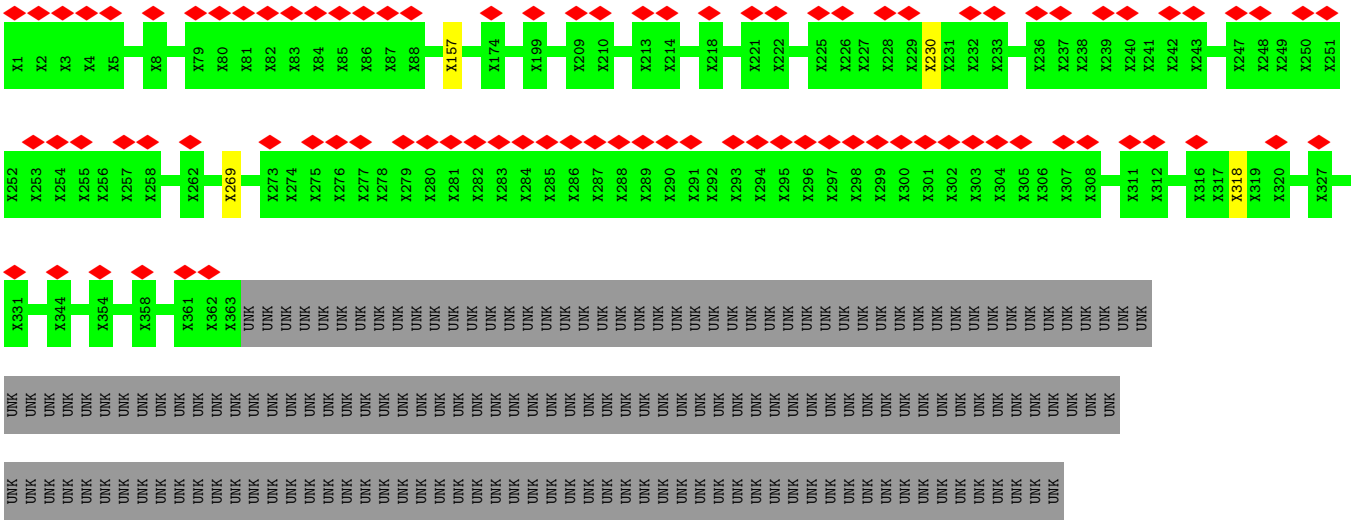




- Molecule 43: CFAP112A

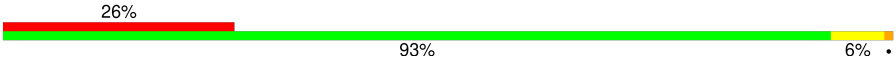
Chain 8P:

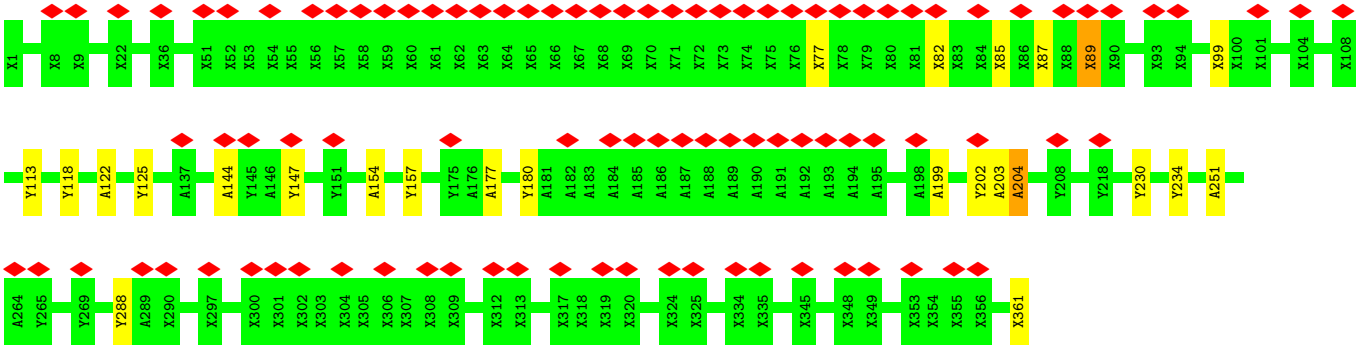




- Molecule 44: B2B3_fMIP

Chain 8R:

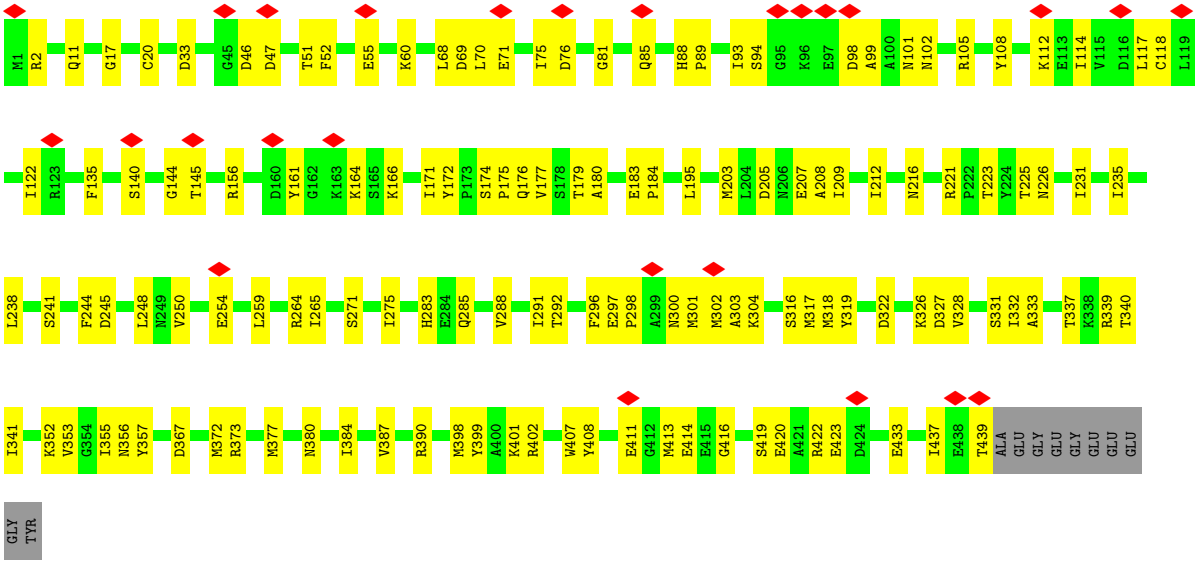




• Molecule 45: Tubulin alpha chain

Chain AA:

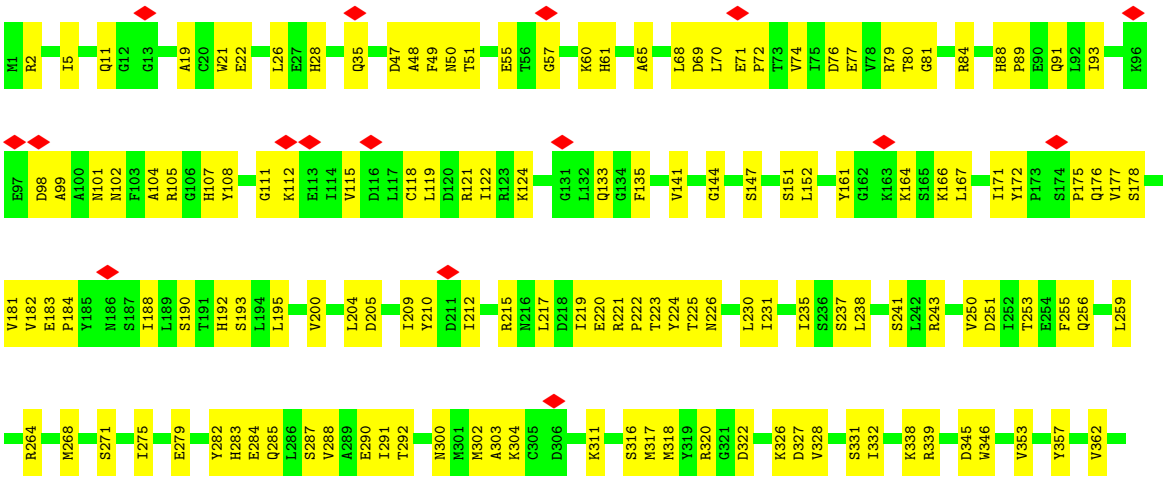




• Molecule 45: Tubulin alpha chain

Chain AC:



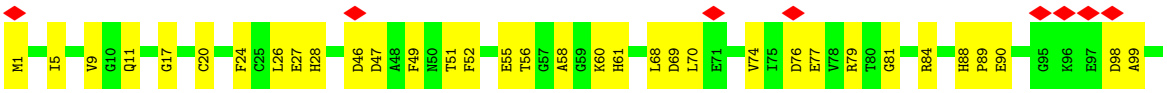


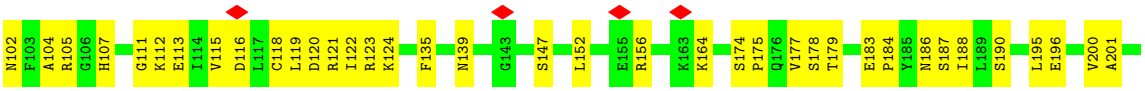


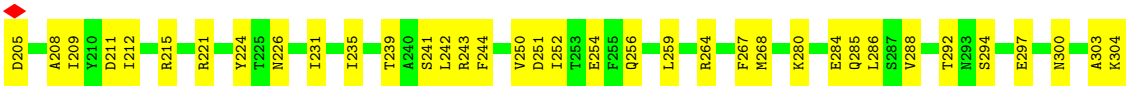
• Molecule 45: Tubulin alpha chain

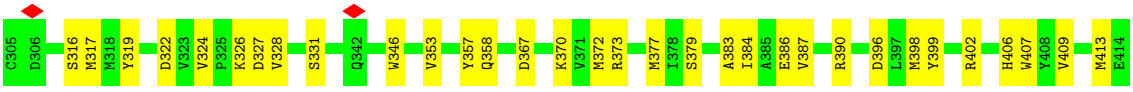
Chain AE:

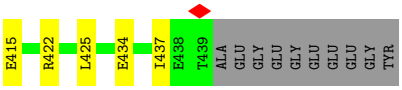








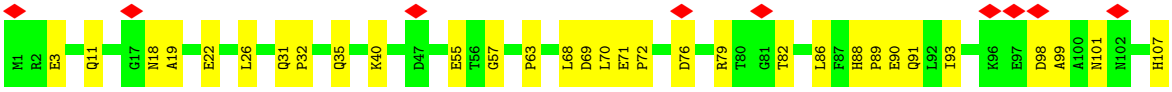




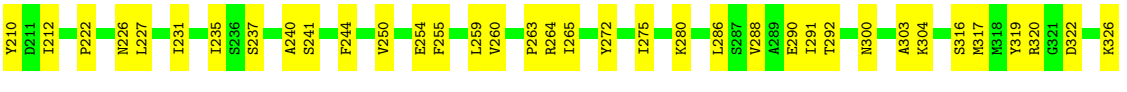
• Molecule 45: Tubulin alpha chain

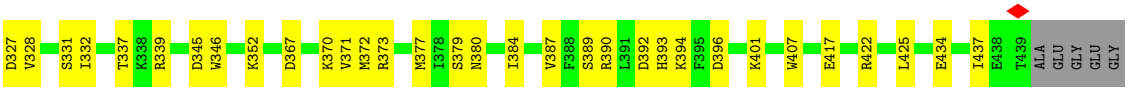
Chain AG:









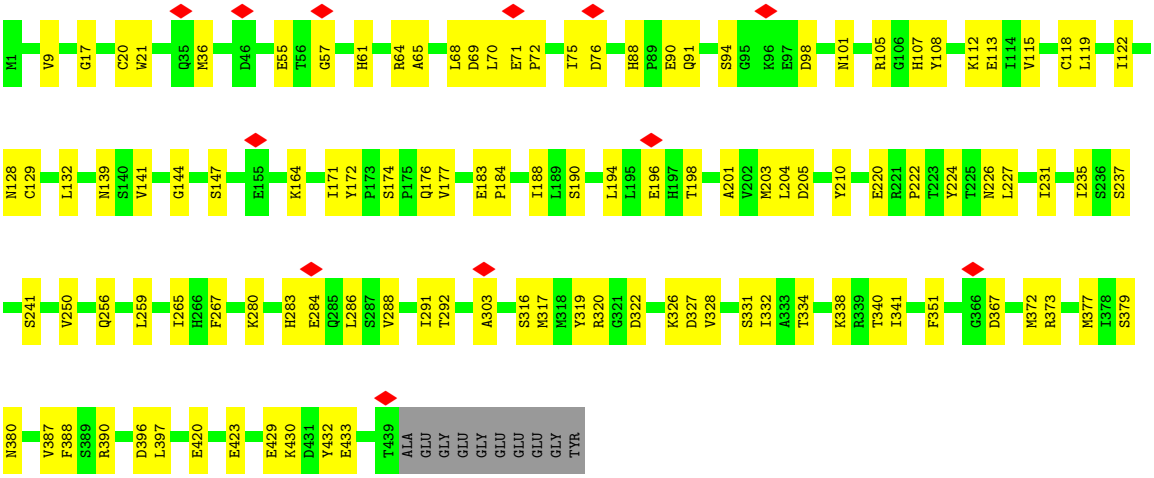




• Molecule 45: Tubulin alpha chain

Chain AI:

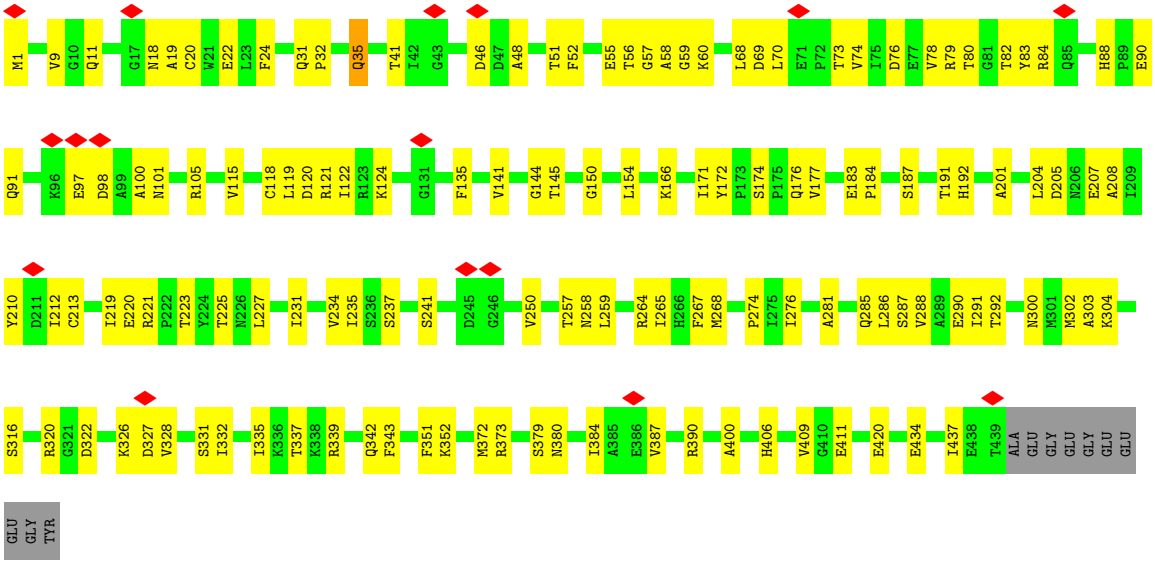




• Molecule 45: Tubulin alpha chain

Chain AK:

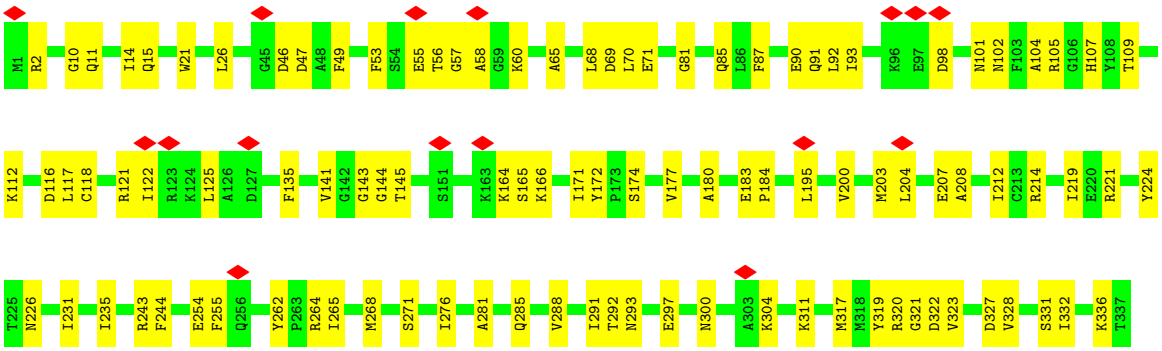


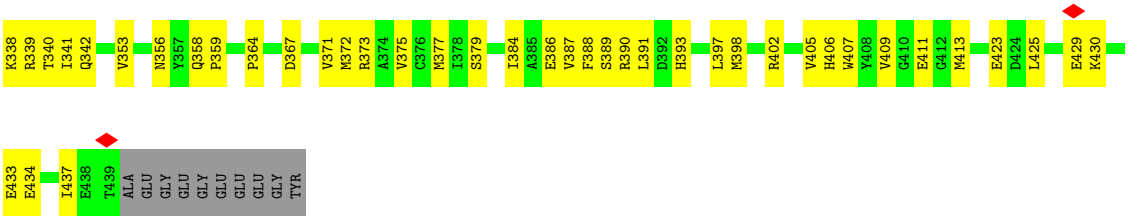


• Molecule 45: Tubulin alpha chain

Chain AM:



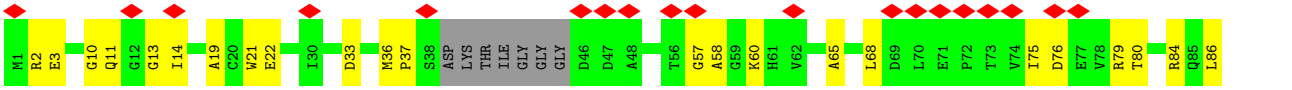


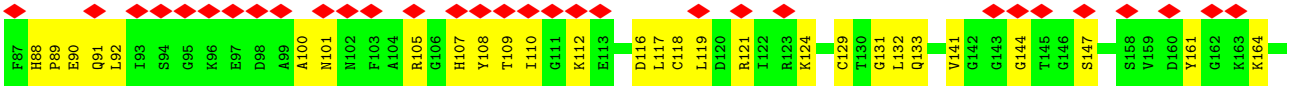


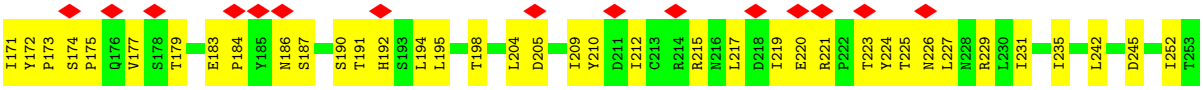
• Molecule 45: Tubulin alpha chain

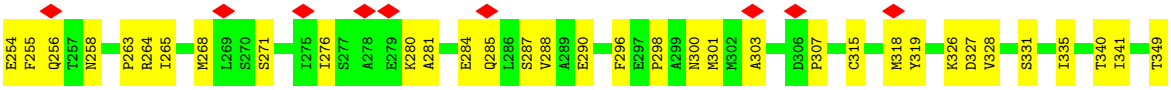
Chain BA:

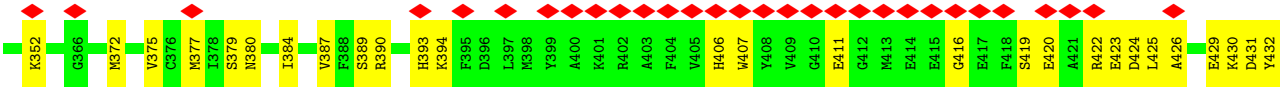


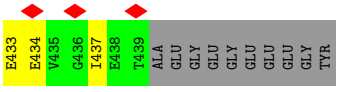








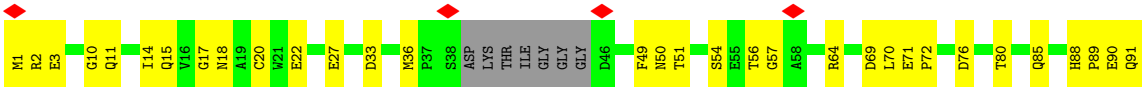




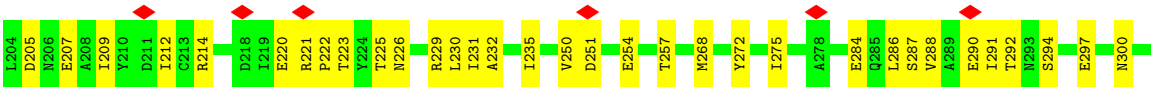
• Molecule 45: Tubulin alpha chain

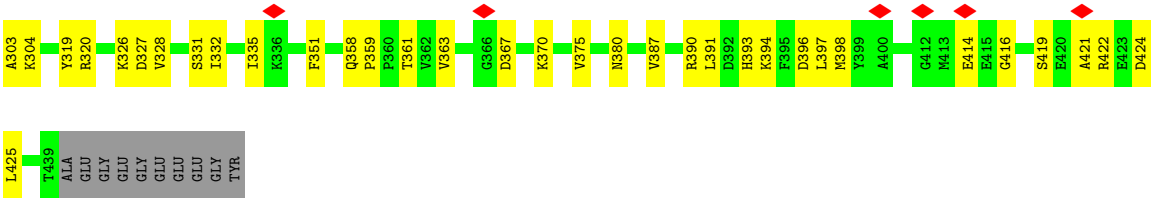
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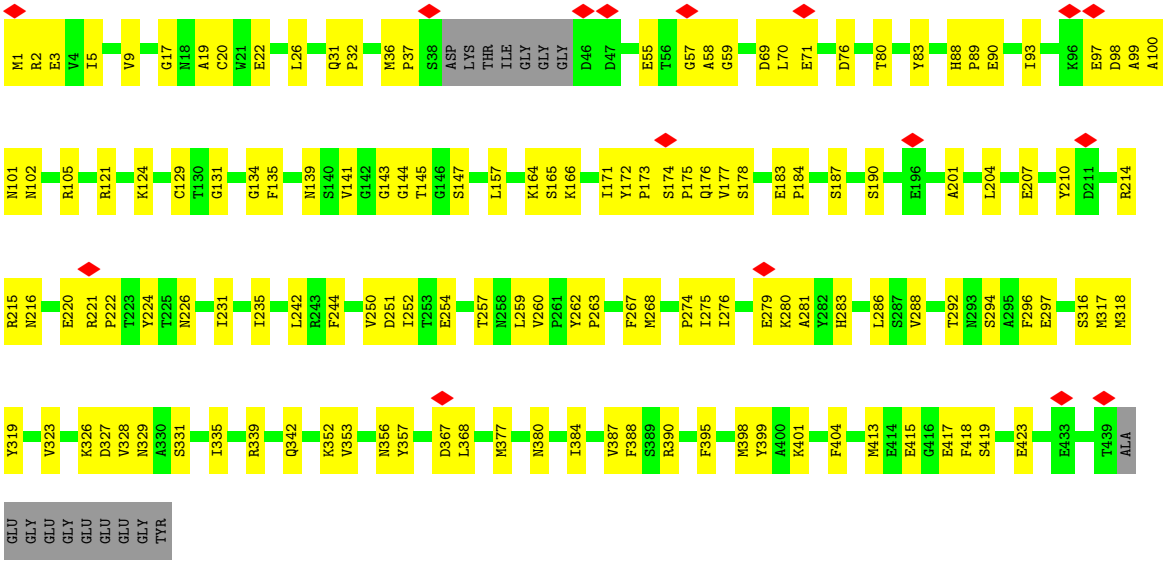




• Molecule 45: Tubulin alpha chain

Chain BE:

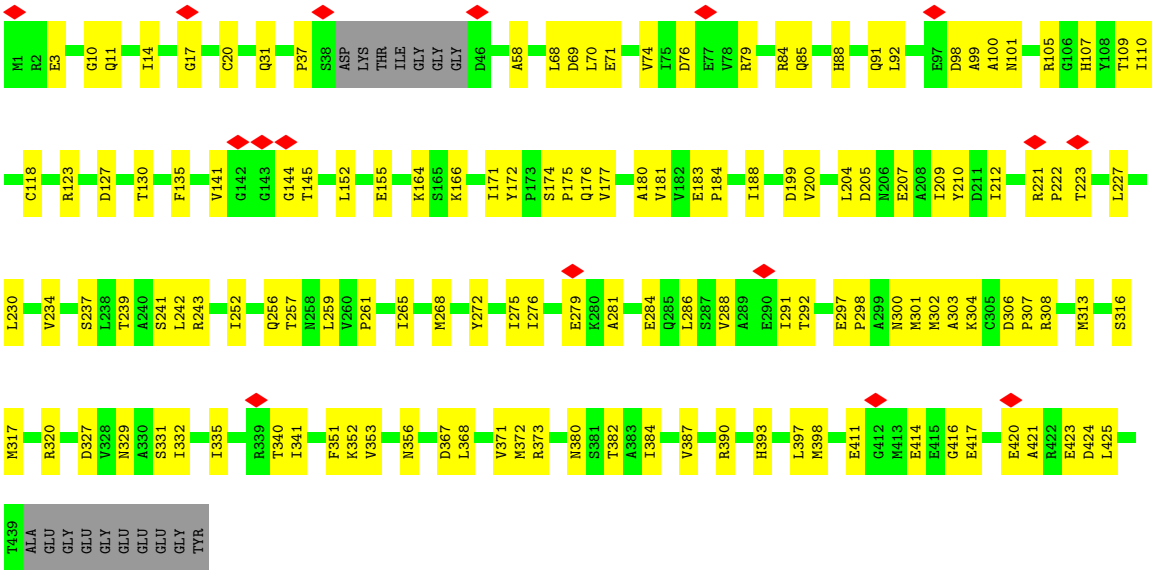




• Molecule 45: Tubulin alpha chain

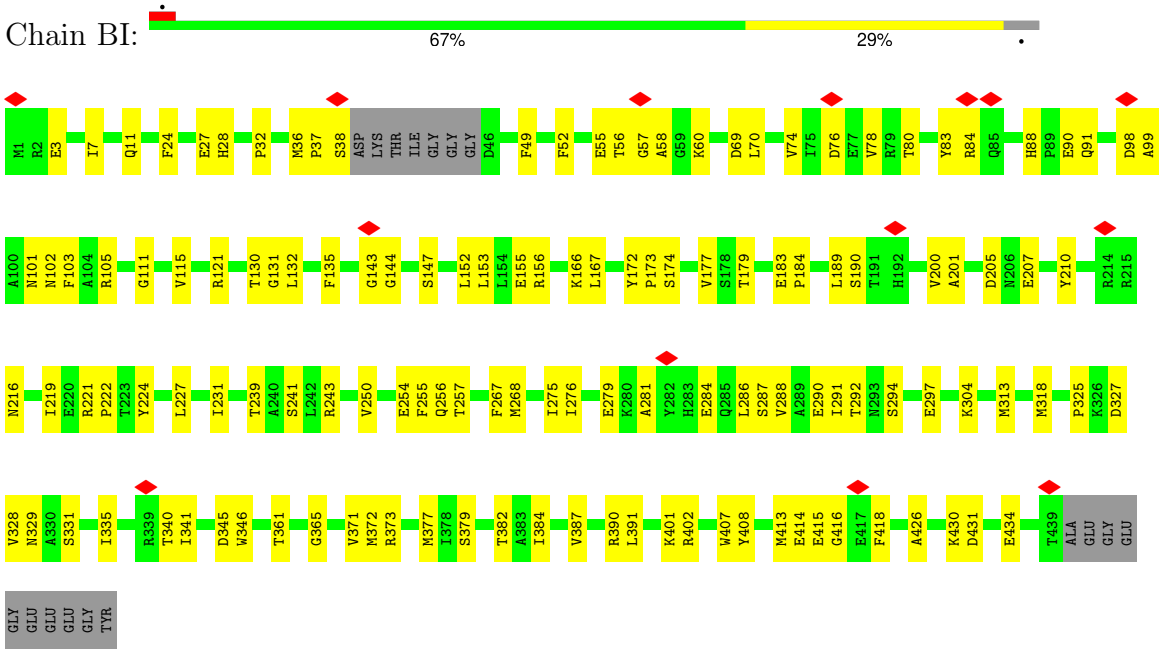
Chain BG:





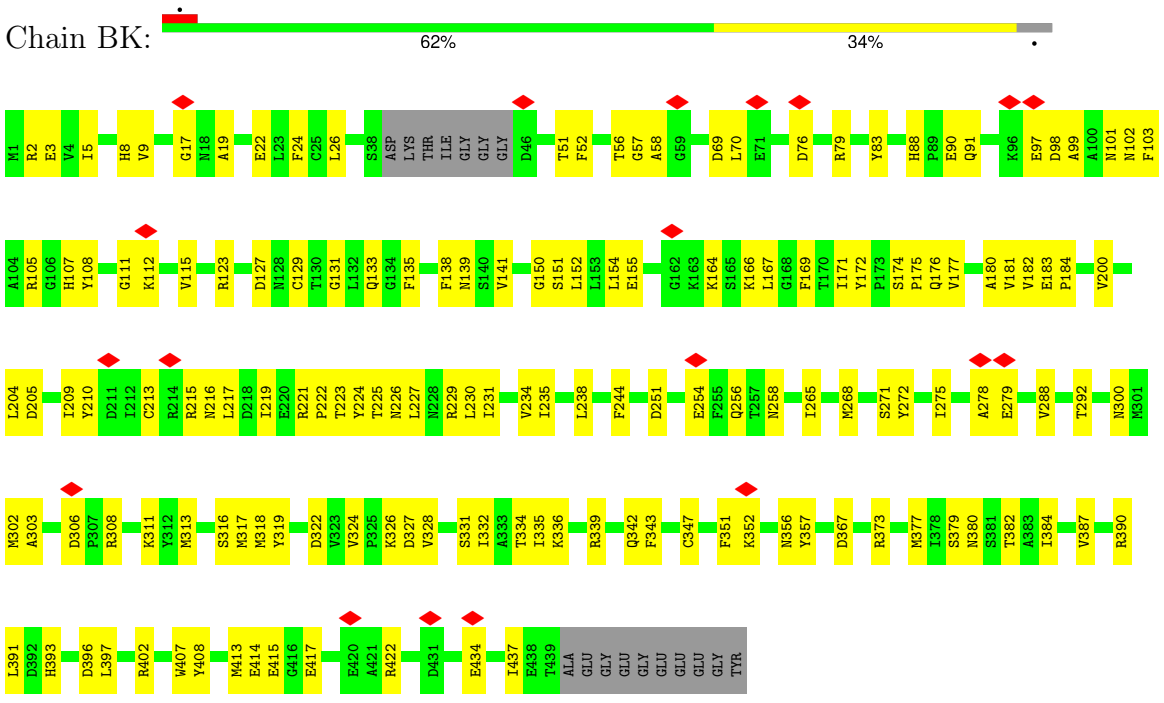
• Molecule 45: Tubulin alpha chain

Chain BI:



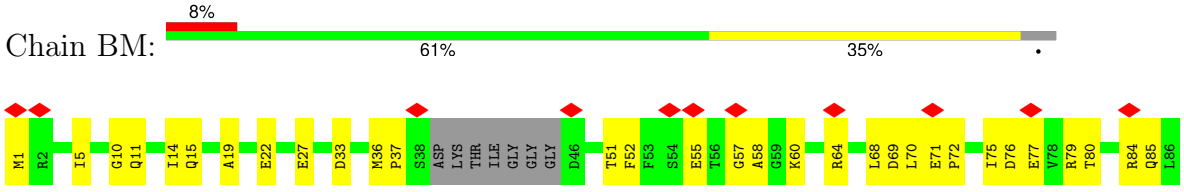
• Molecule 45: Tubulin alpha chain

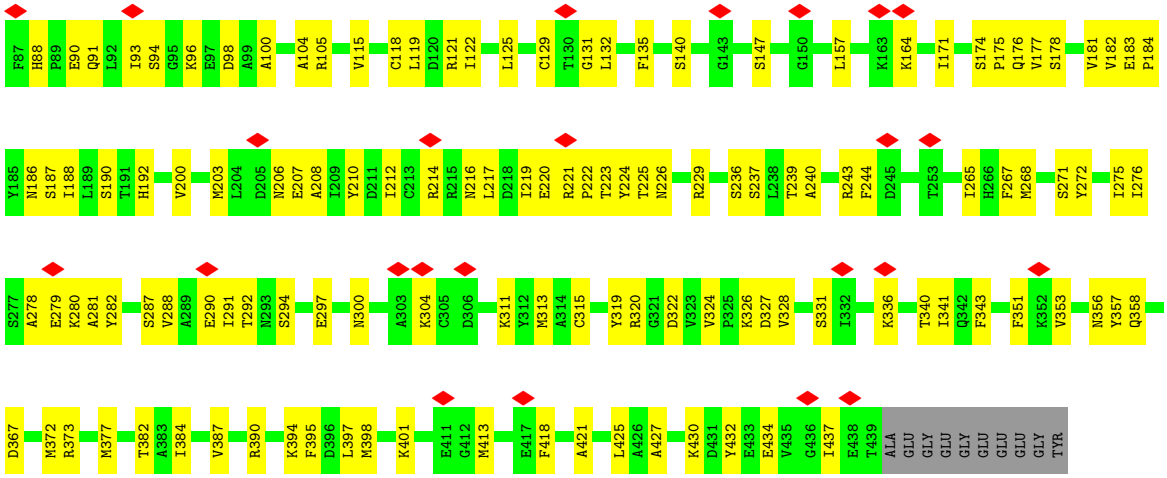
Chain BK:



• Molecule 45: Tubulin alpha chain

Chain BM:

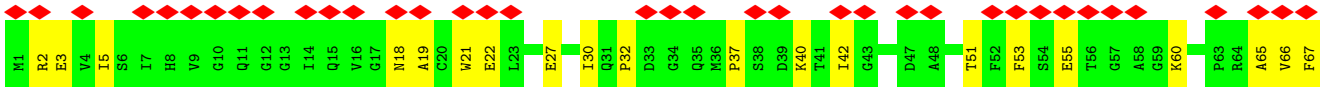


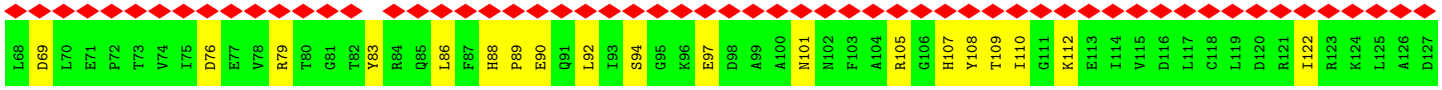


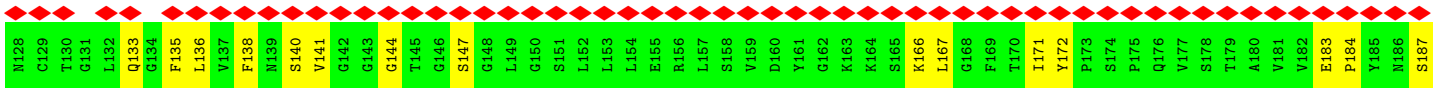
• Molecule 45: Tubulin alpha chain

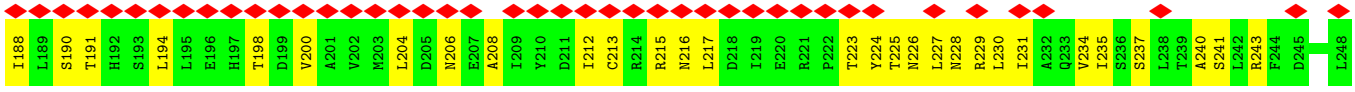
Chain CA:

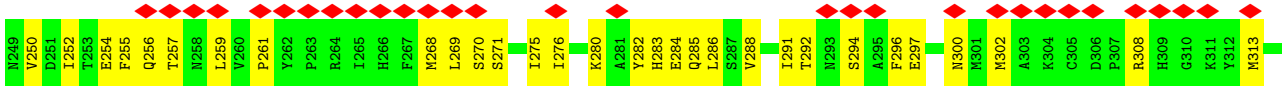


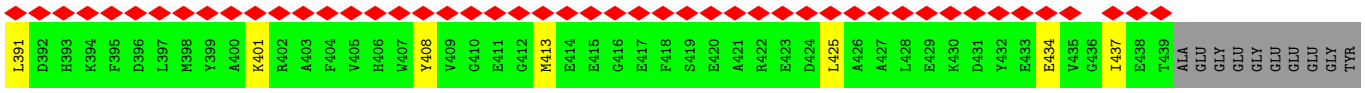








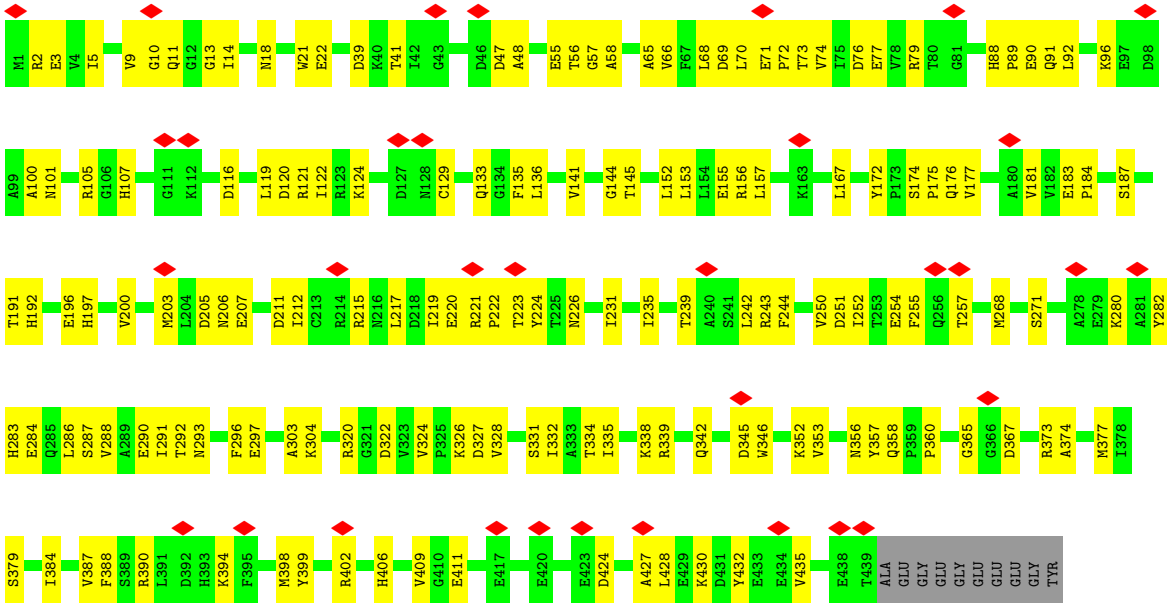




• Molecule 45: Tubulin alpha chain

Chain CC:

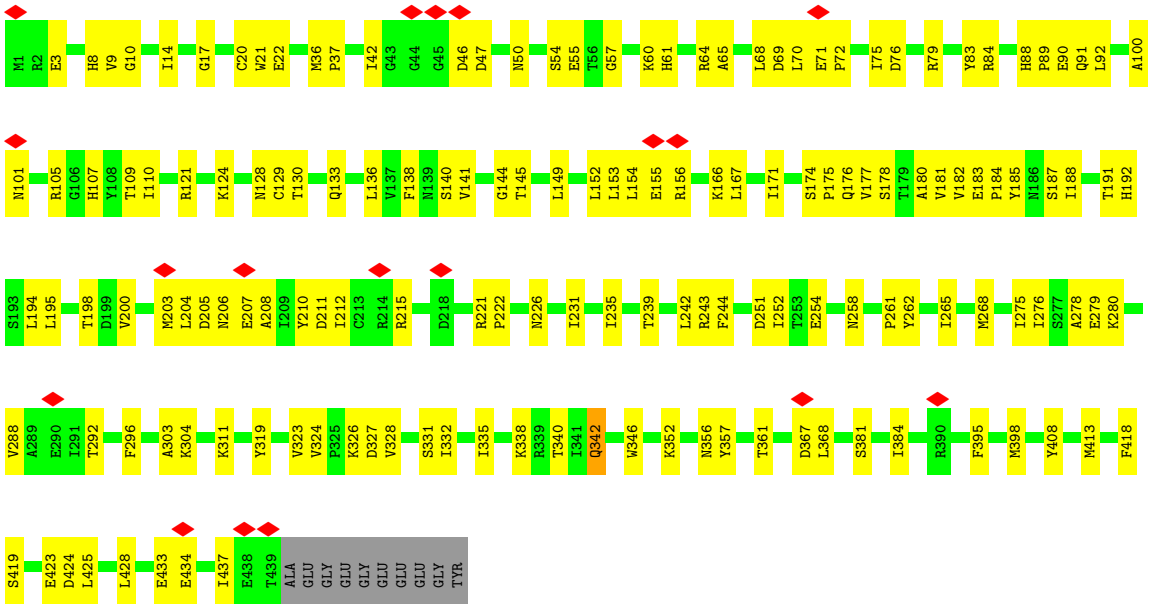




• Molecule 45: Tubulin alpha chain

Chain CG:



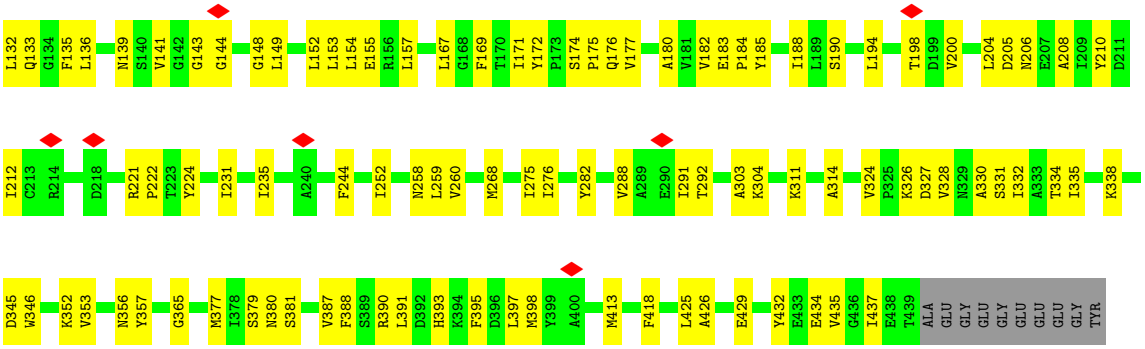


• Molecule 45: Tubulin alpha chain

Chain CI:



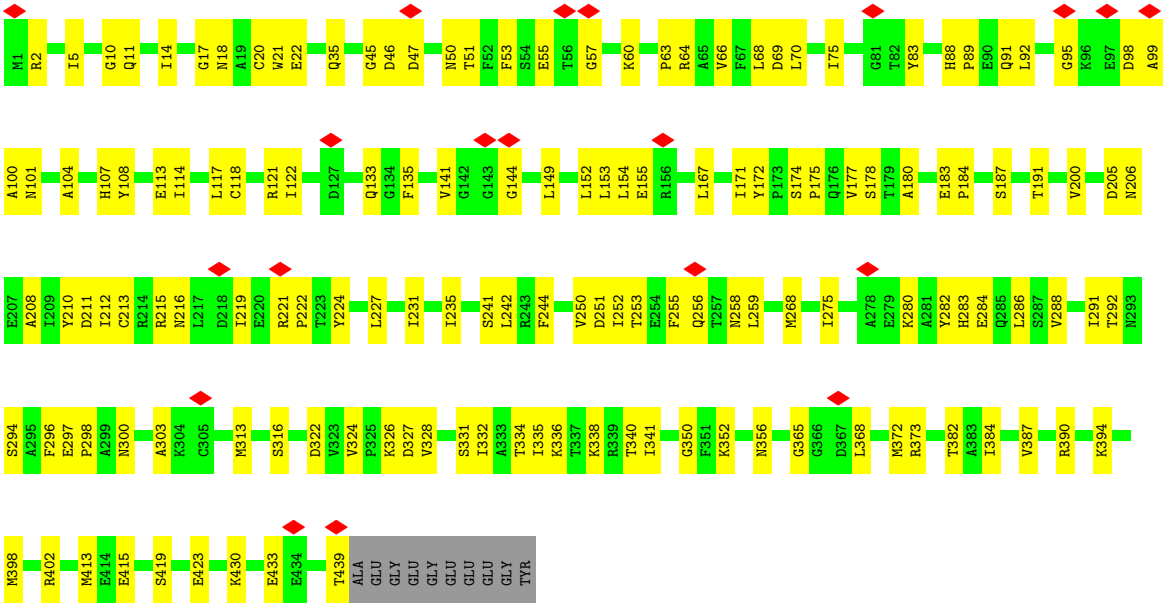




• Molecule 45: Tubulin alpha chain

Chain CK:

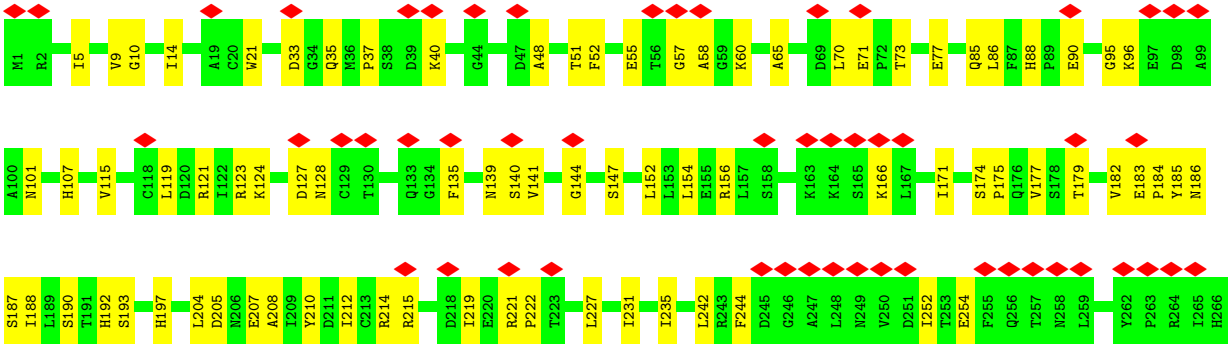


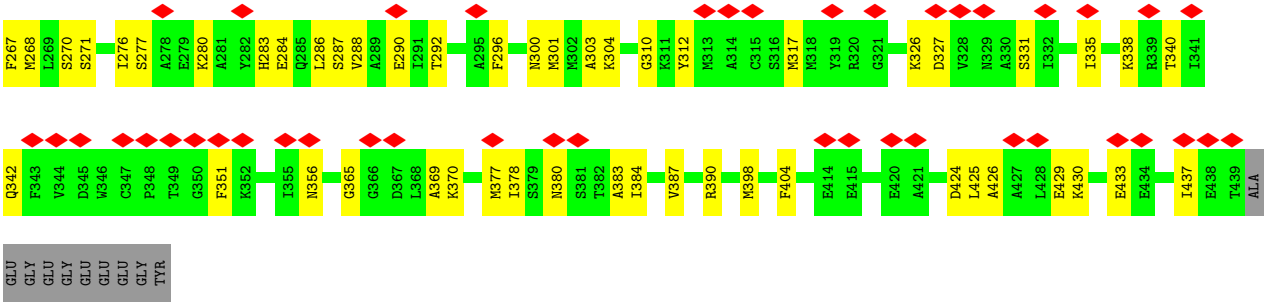


• Molecule 45: Tubulin alpha chain

Chain CM:

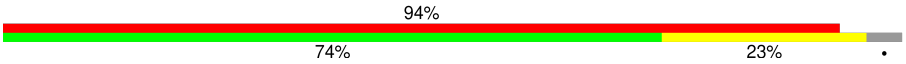


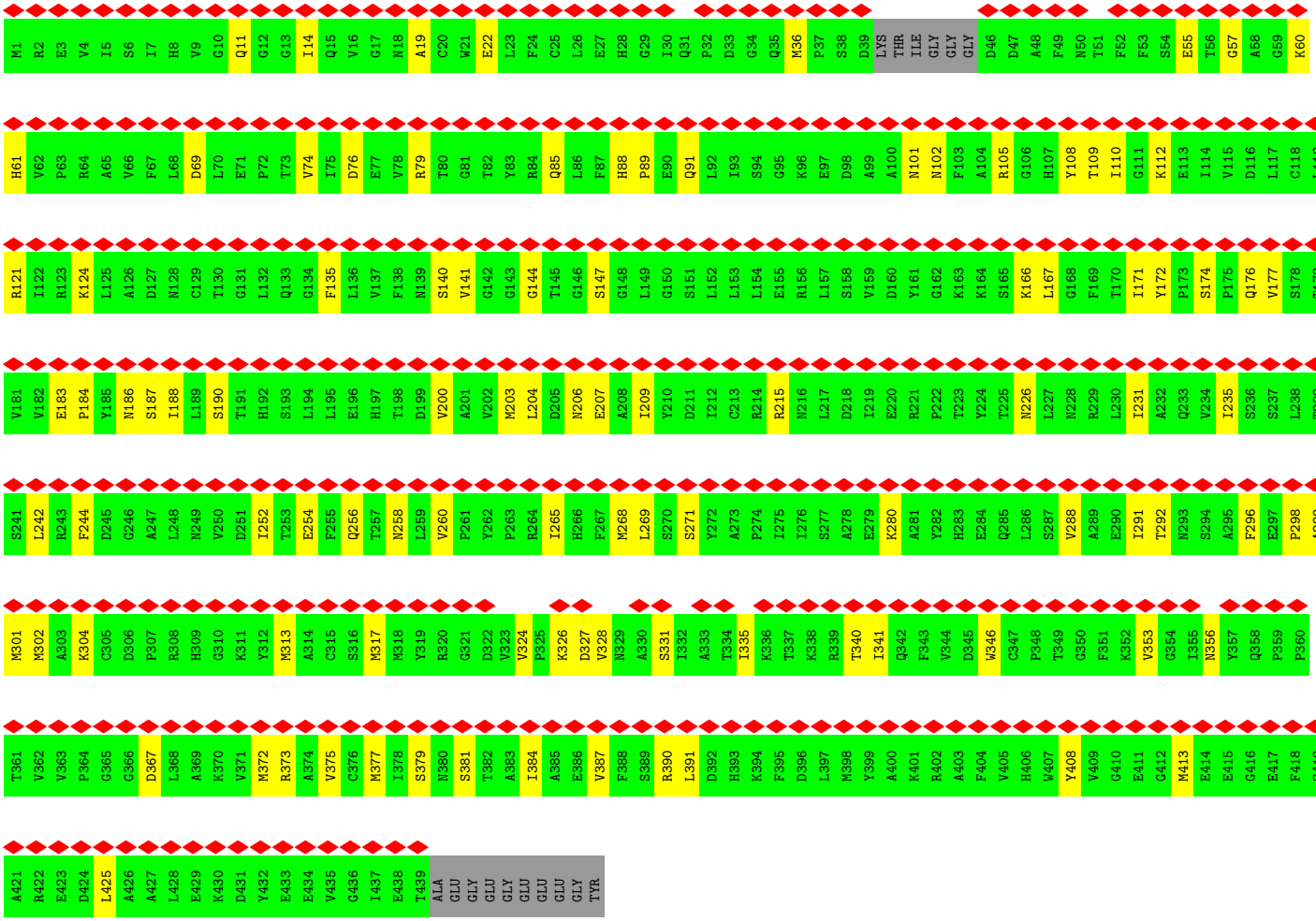




• Molecule 45: Tubulin alpha chain

Chain DA:

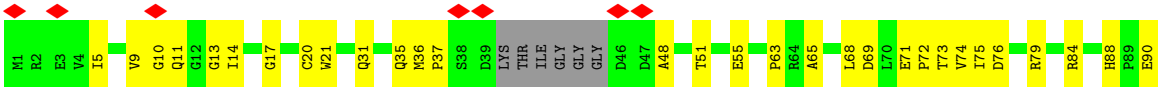


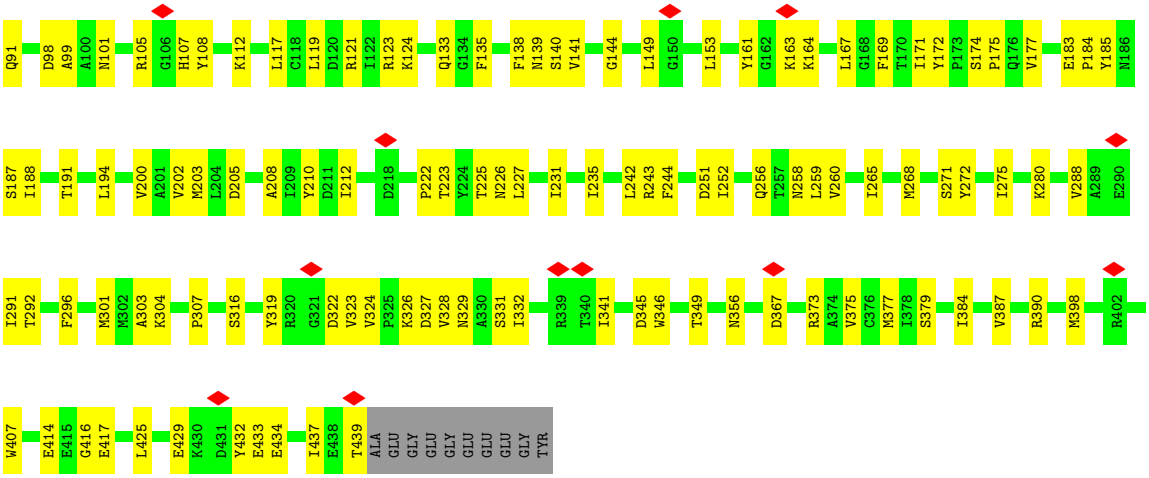


• Molecule 45: Tubulin alpha chain

Chain DE:



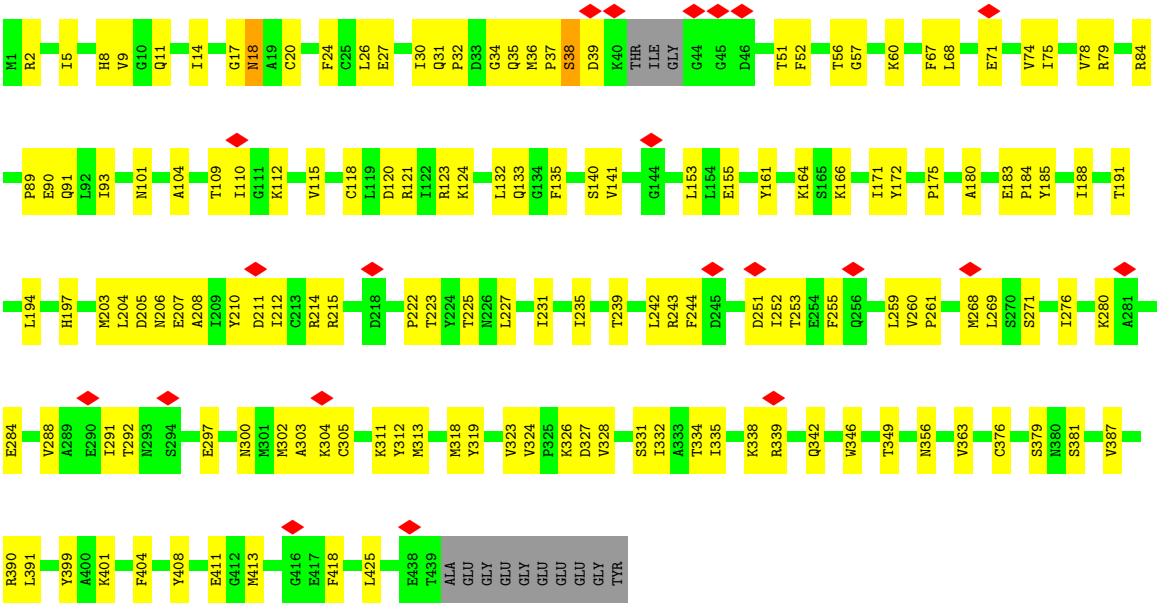




• Molecule 45: Tubulin alpha chain

Chain DG:

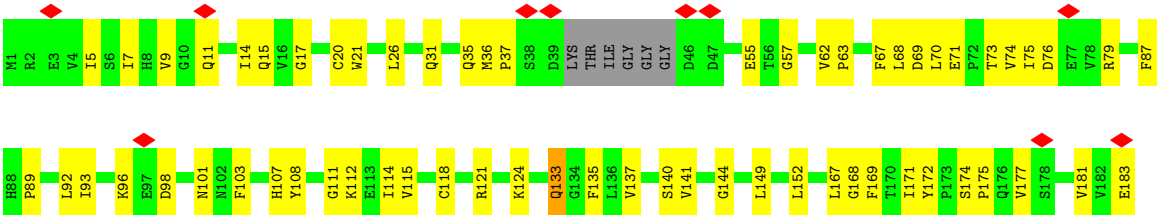


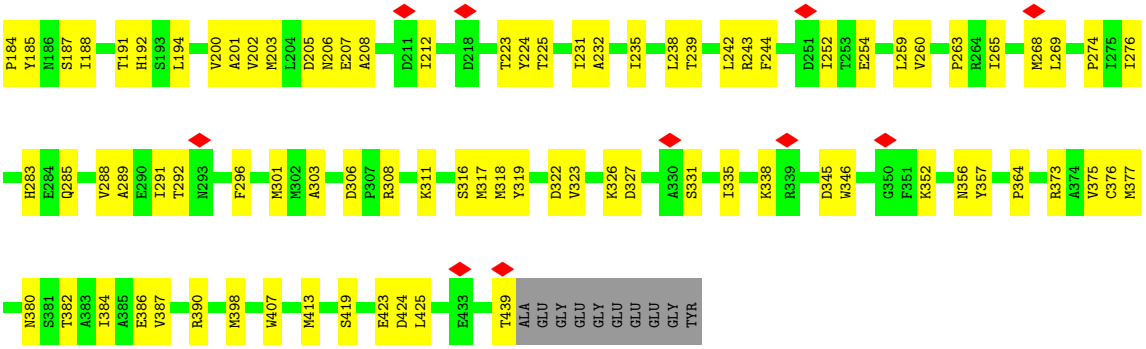


• Molecule 45: Tubulin alpha chain

Chain DI:



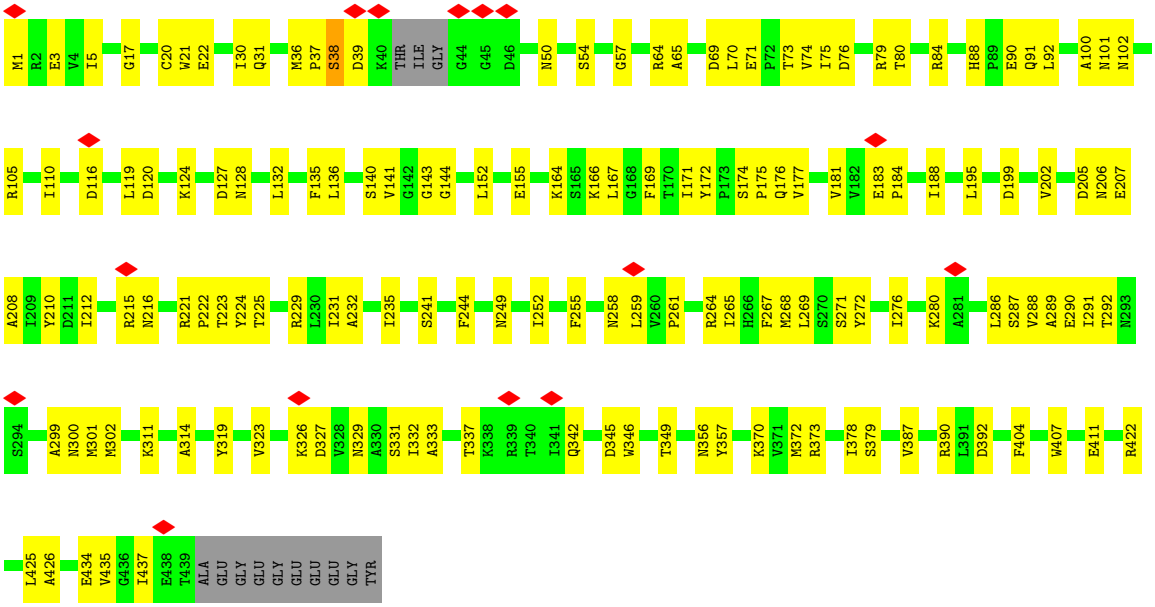




• Molecule 45: Tubulin alpha chain

Chain DK:

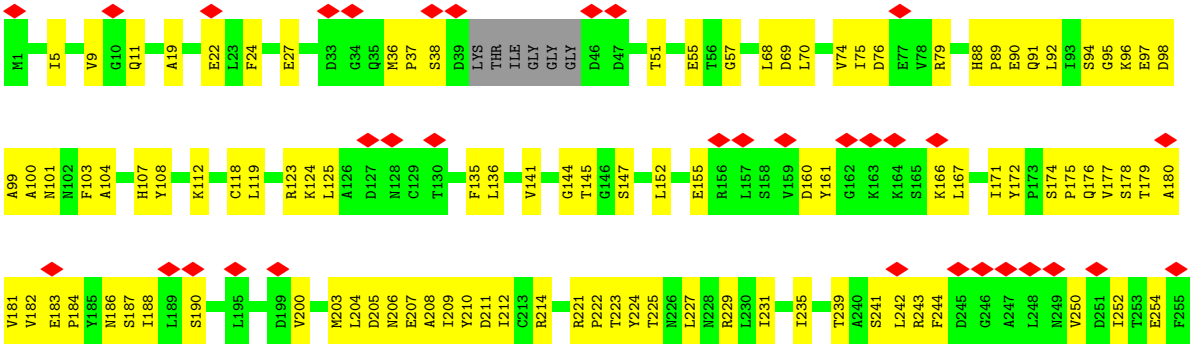


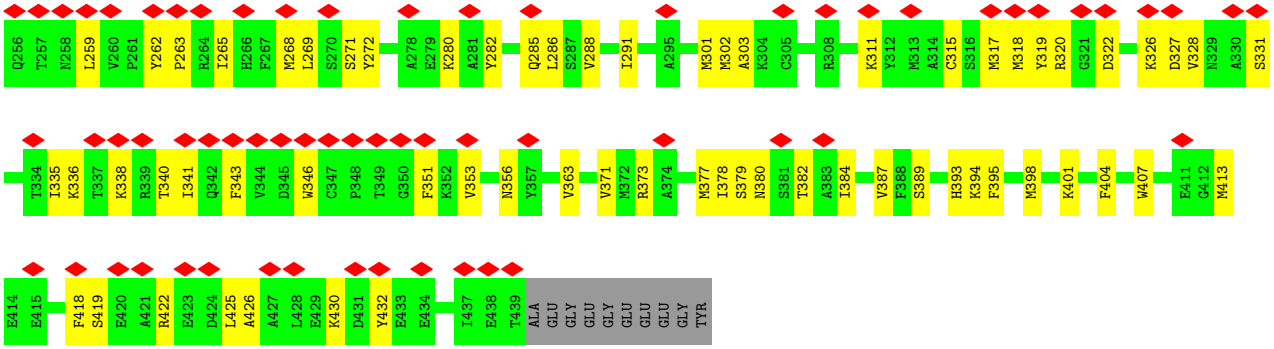


• Molecule 45: Tubulin alpha chain

Chain DM:

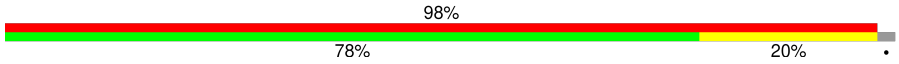


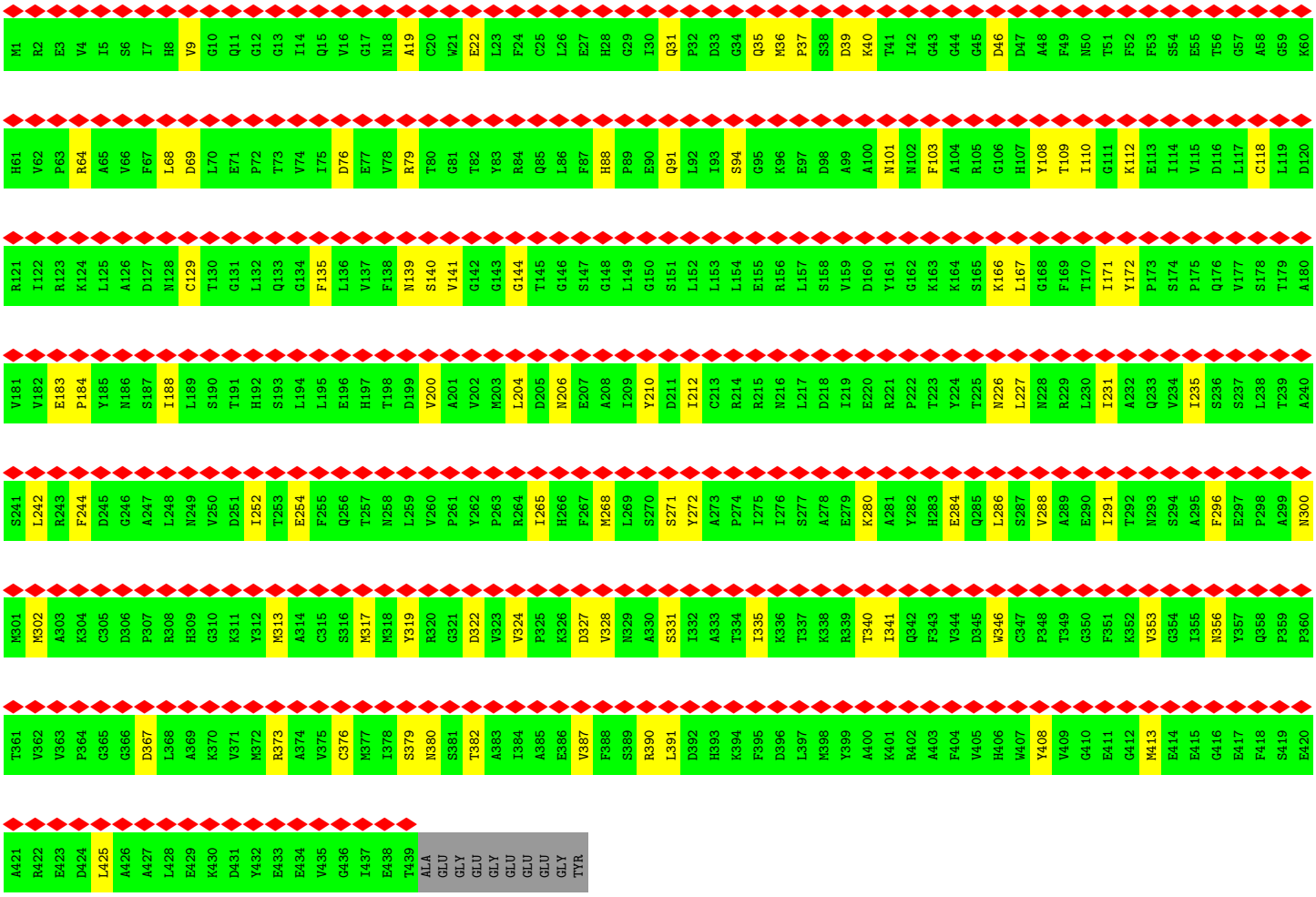




• Molecule 45: Tubulin alpha chain

Chain EA:

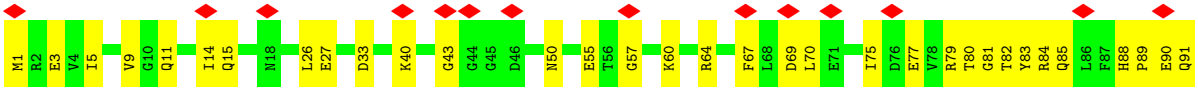


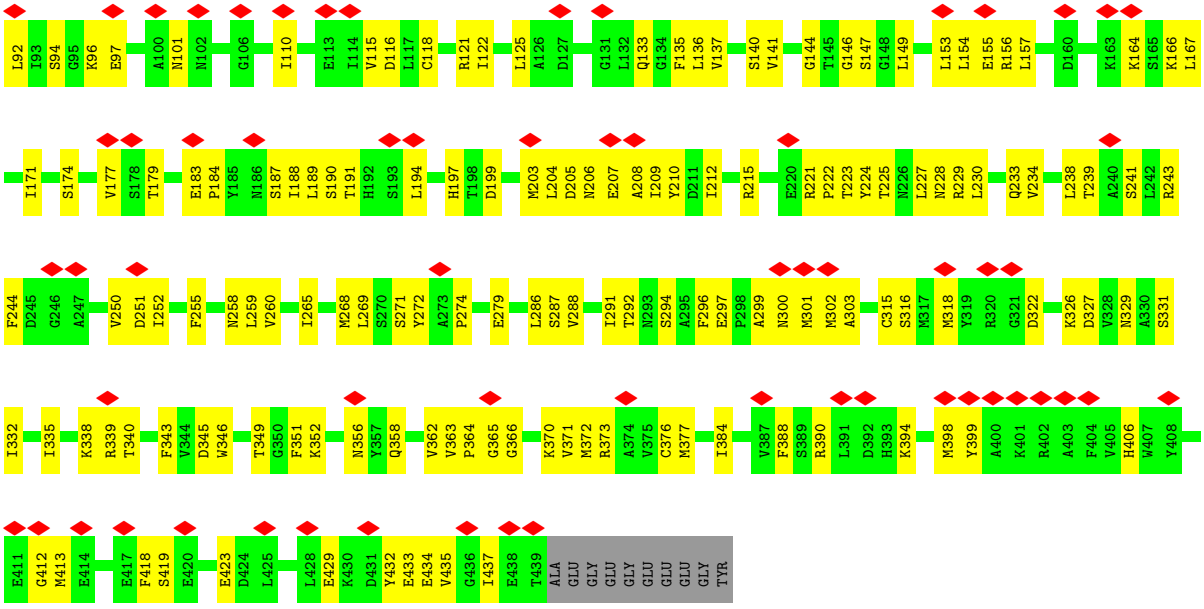


• Molecule 45: Tubulin alpha chain

Chain EC:



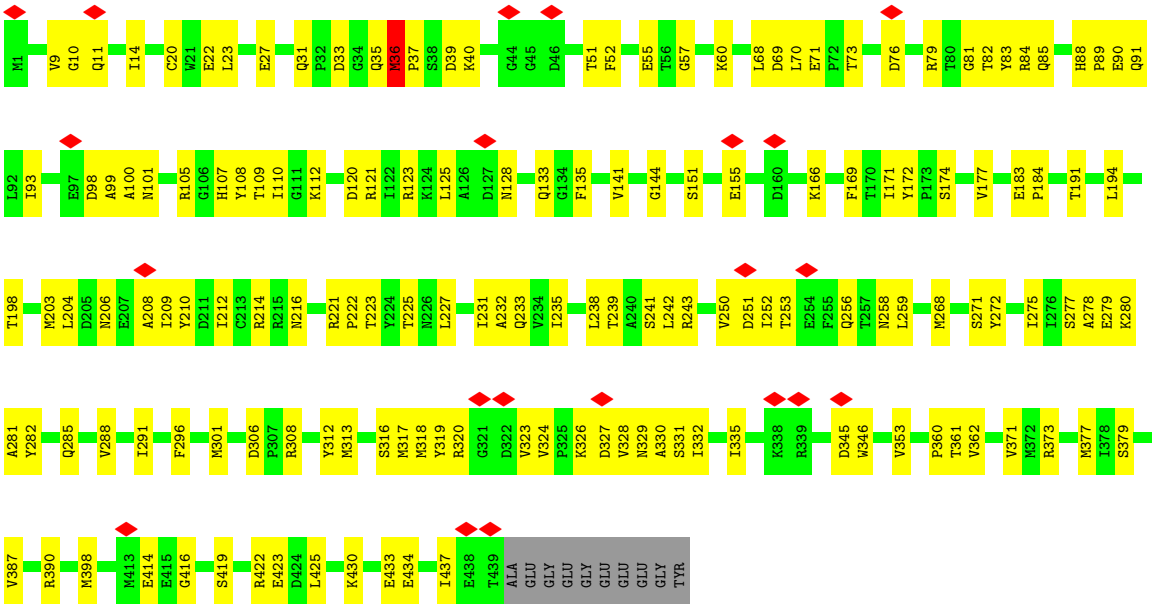




• Molecule 45: Tubulin alpha chain

Chain EE:

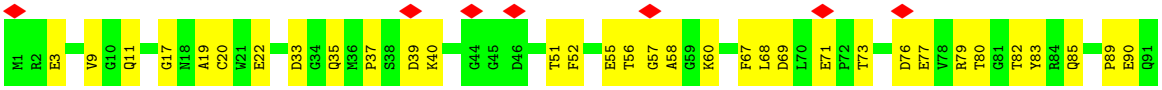


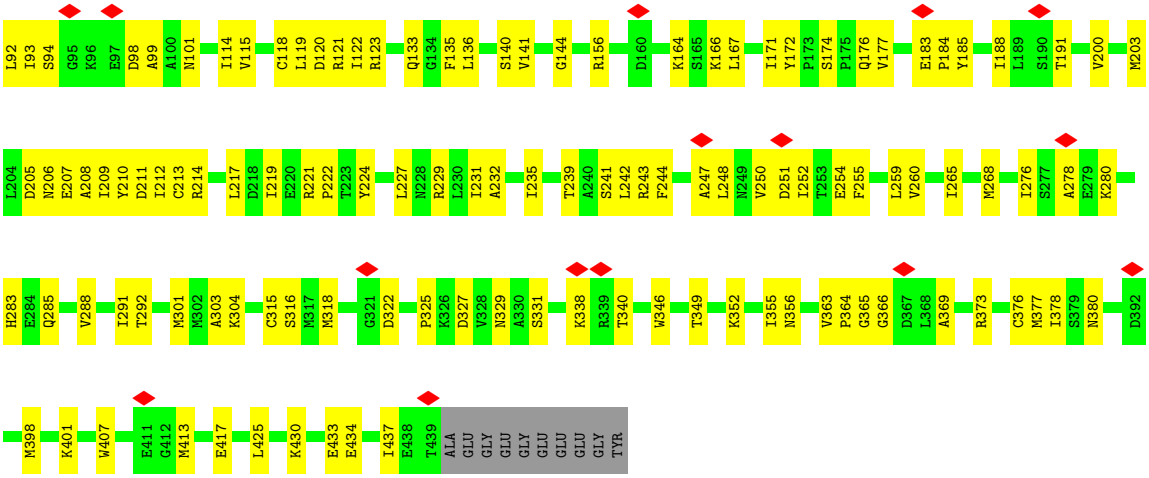


• Molecule 45: Tubulin alpha chain

Chain EG:



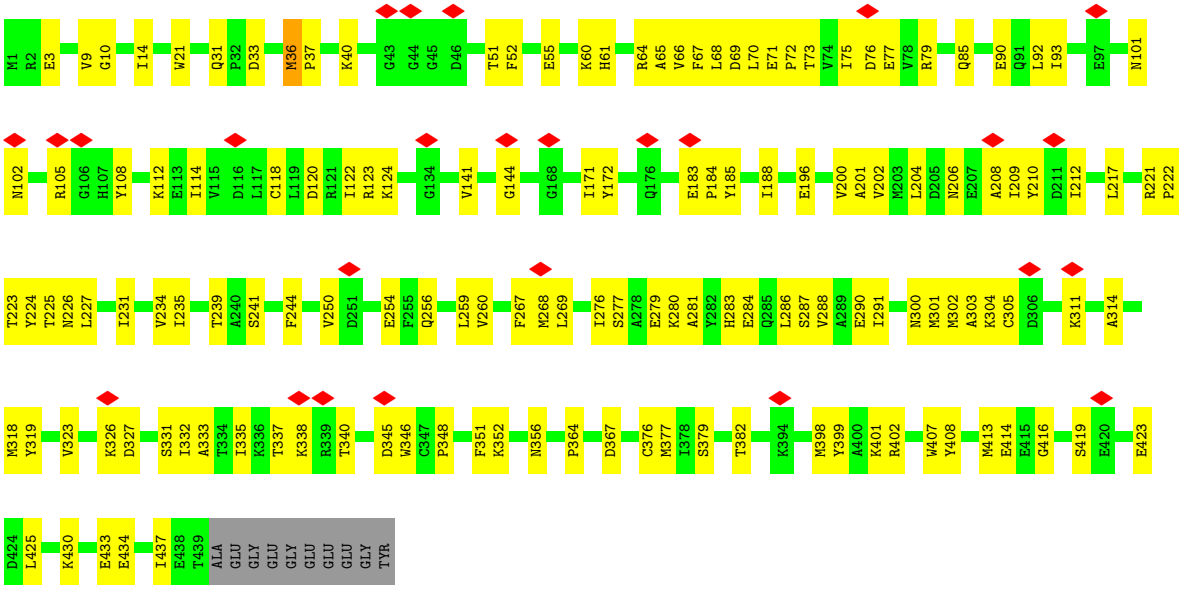




• Molecule 45: Tubulin alpha chain

Chain EI:

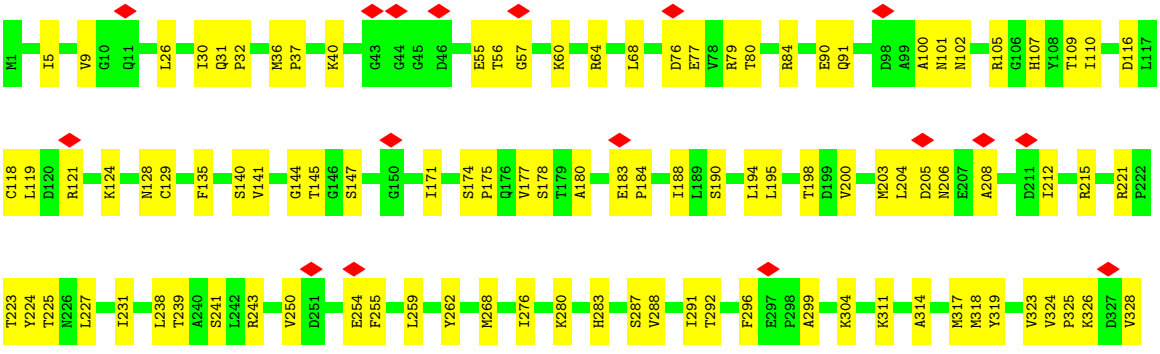


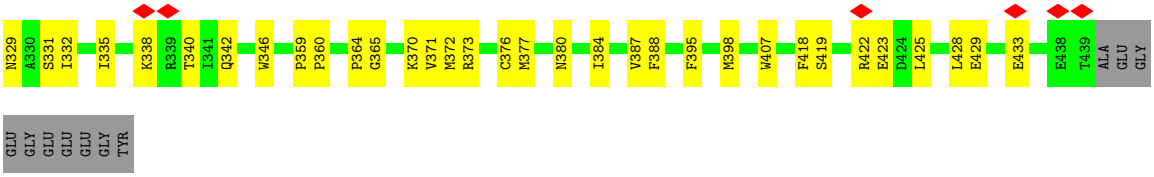


• Molecule 45: Tubulin alpha chain

Chain EK:



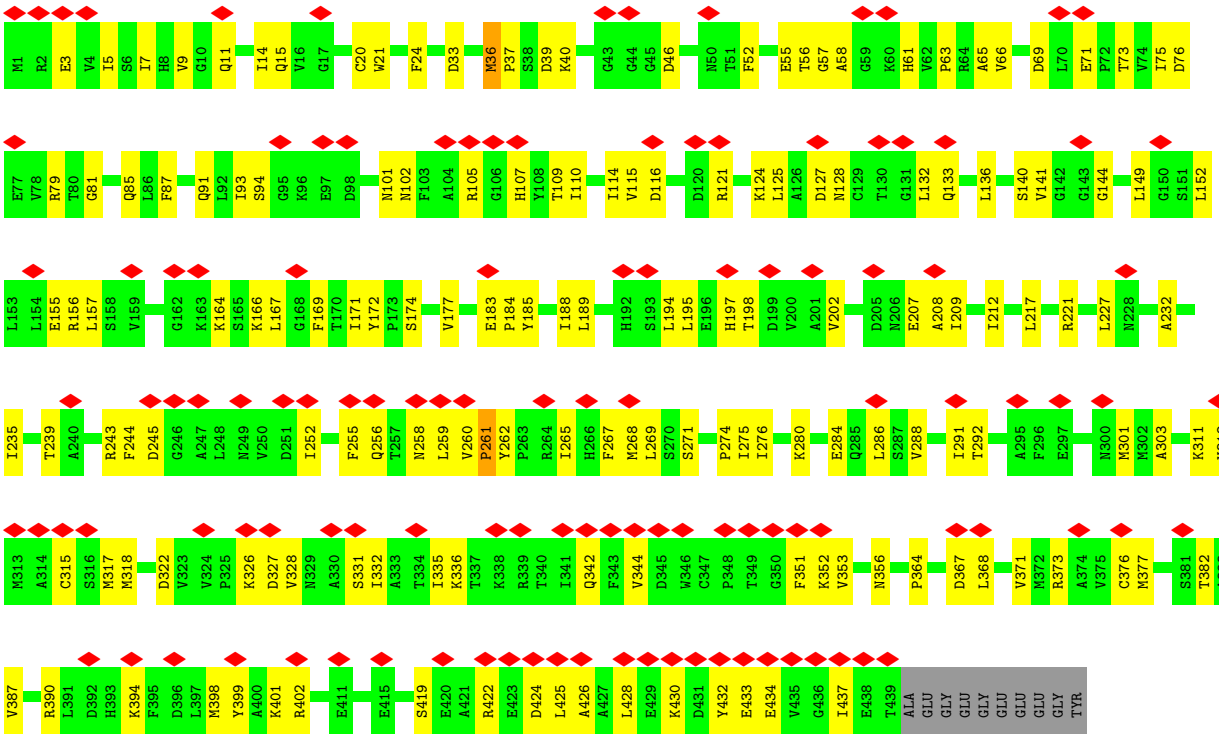




• Molecule 45: Tubulin alpha chain

Chain EM:

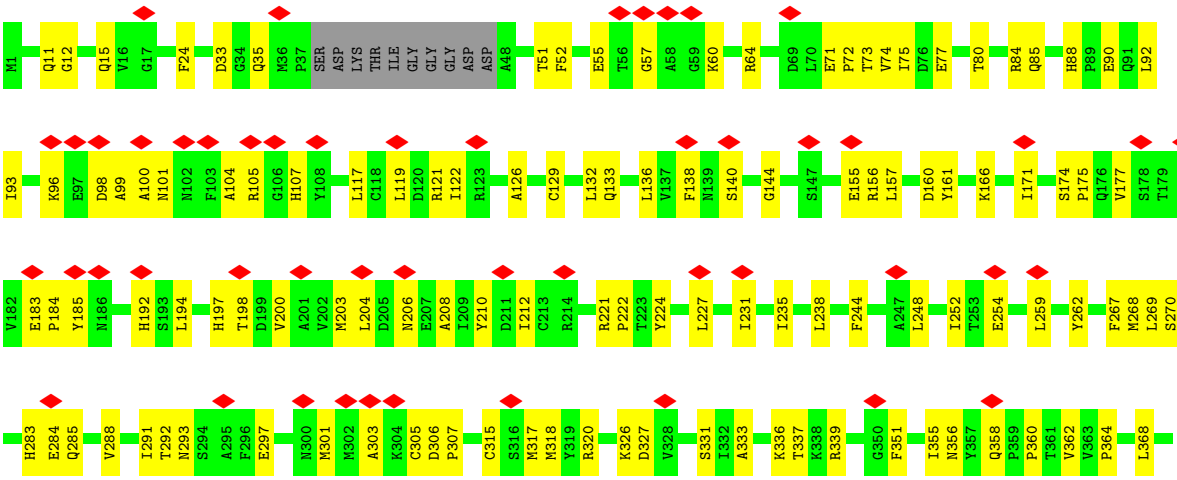


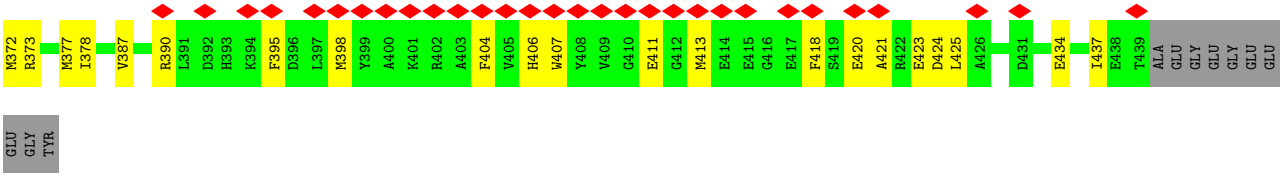


• Molecule 45: Tubulin alpha chain

Chain FA:



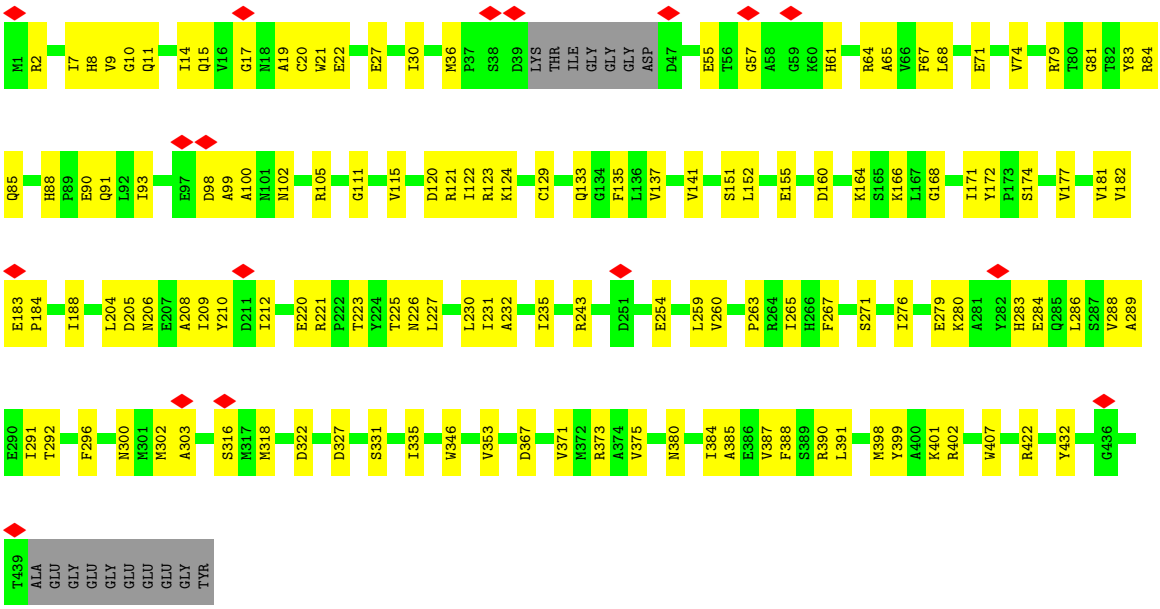




• Molecule 45: Tubulin alpha chain

Chain FC:

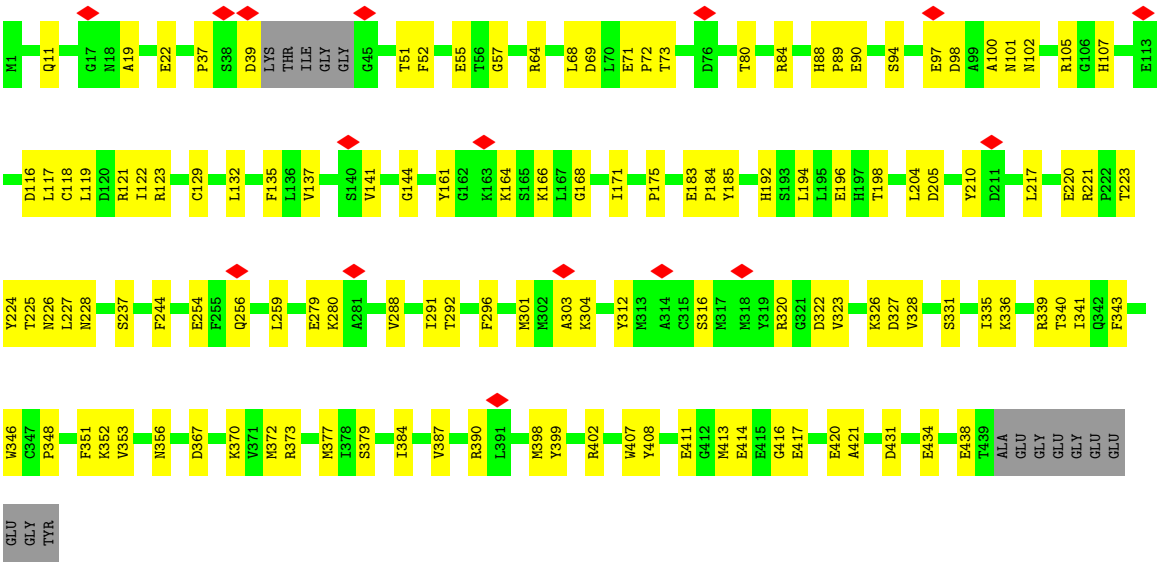




• Molecule 45: Tubulin alpha chain

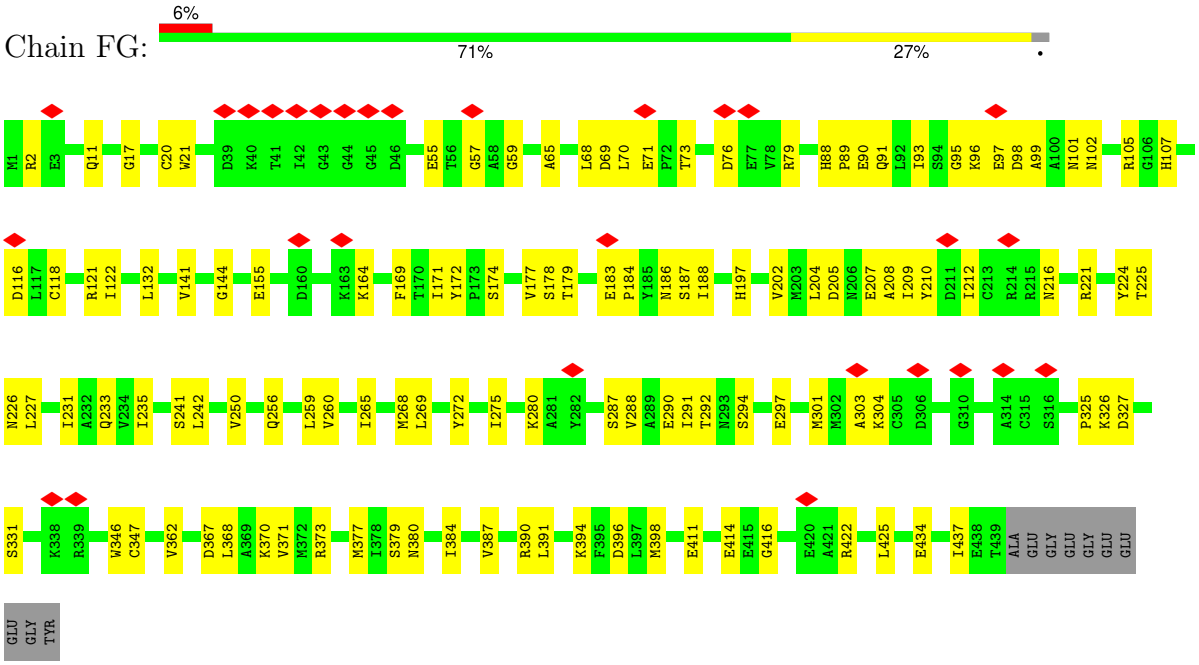
Chain FE:





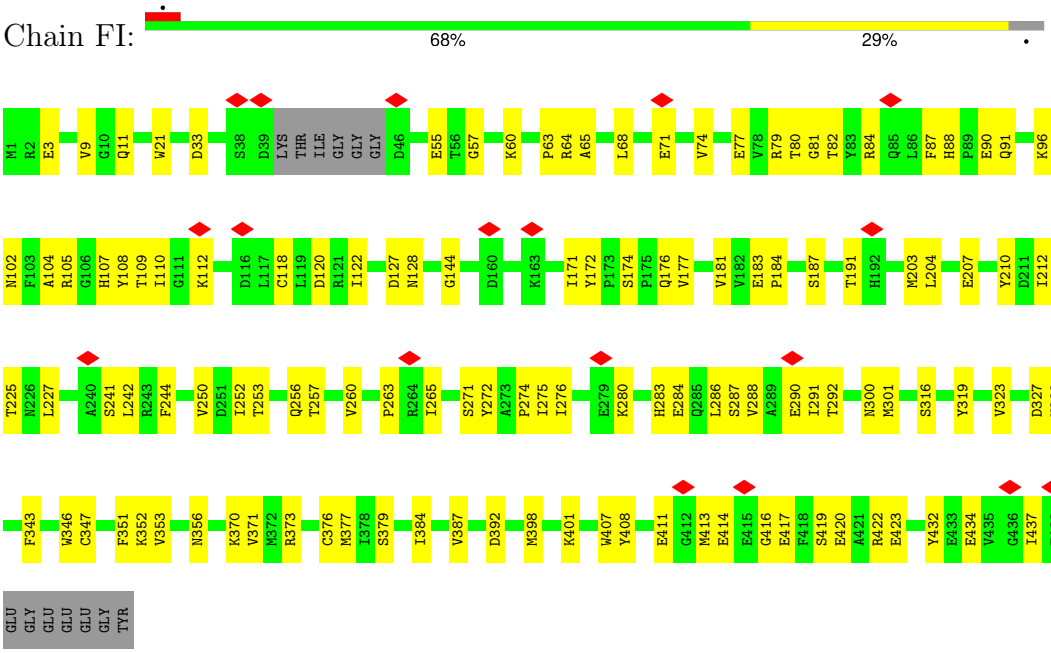
• Molecule 45: Tubulin alpha chain

Chain FG:



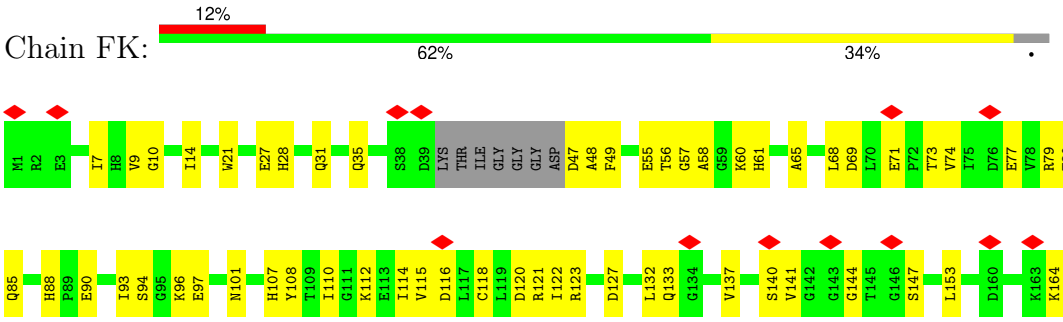
• Molecule 45: Tubulin alpha chain

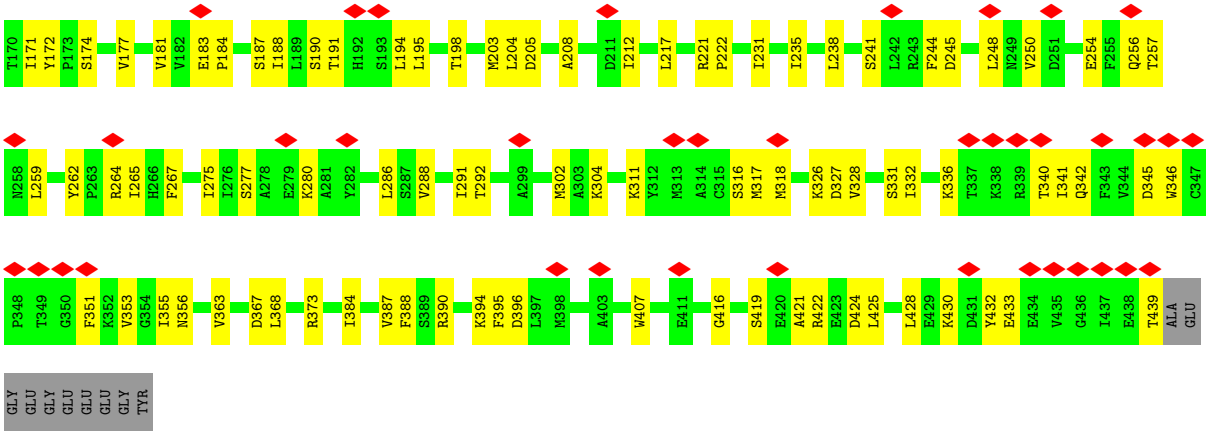
Chain FI:



• Molecule 45: Tubulin alpha chain

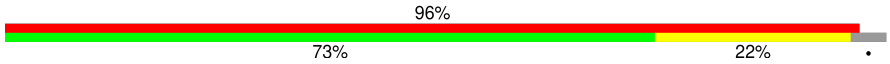
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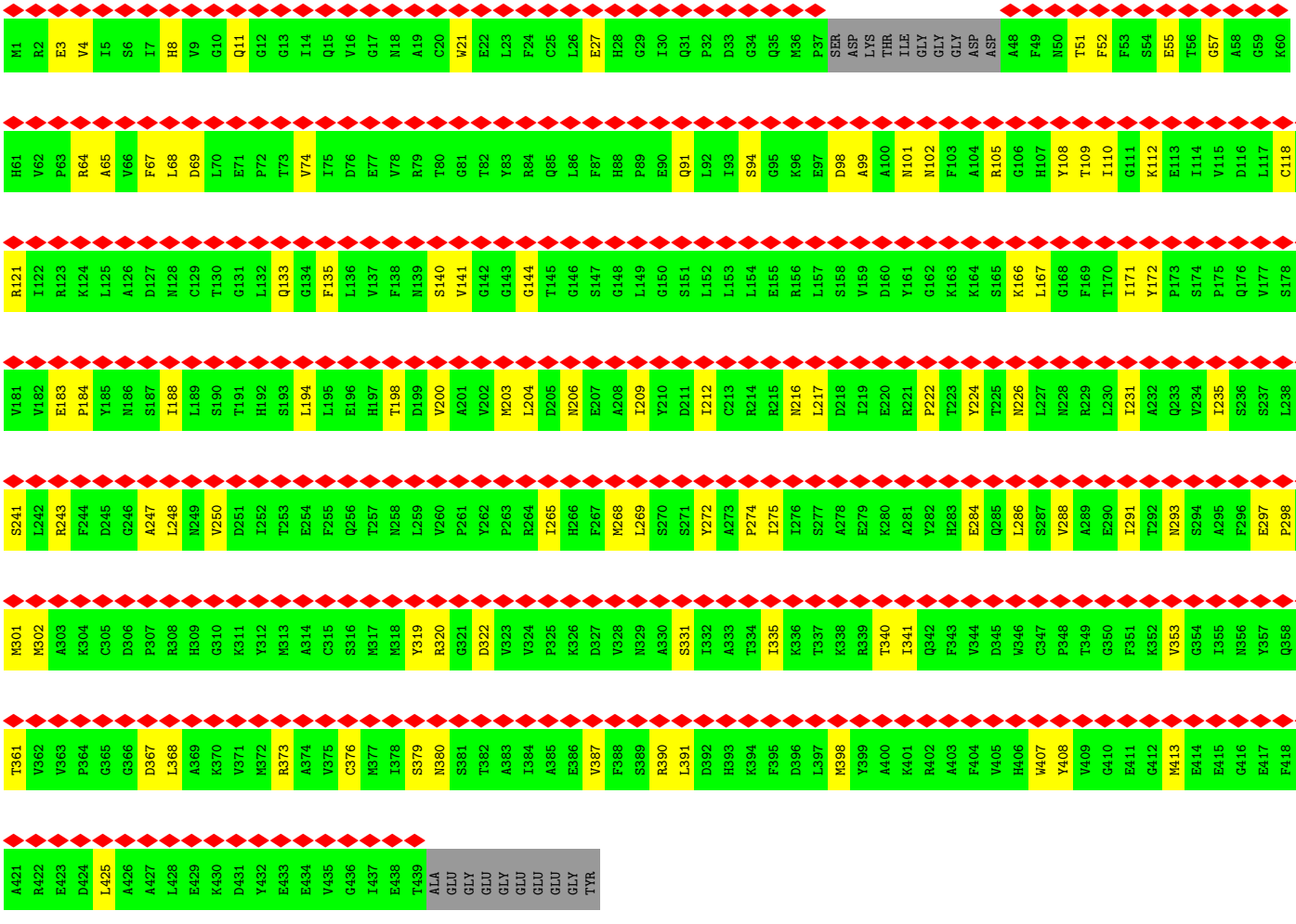




• Molecule 45: Tubulin alpha chain

Chain FM:

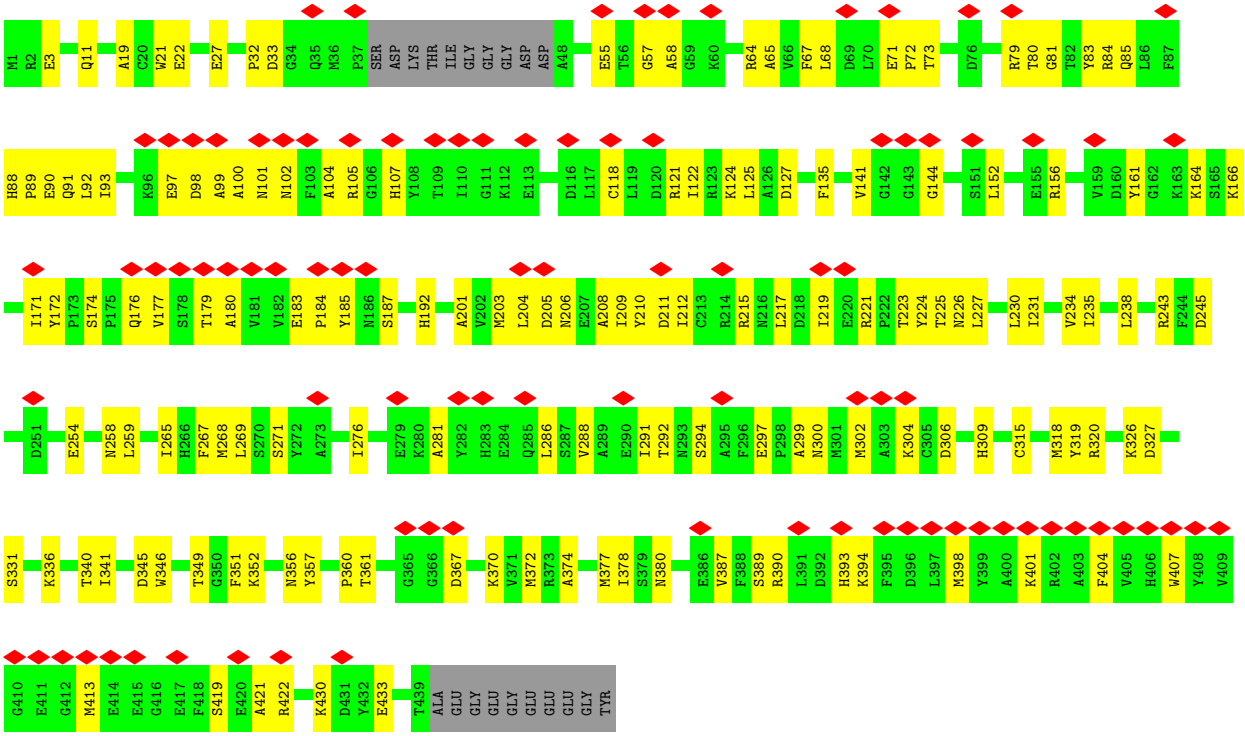




• Molecule 45: Tubulin alpha chain

Chain GA:

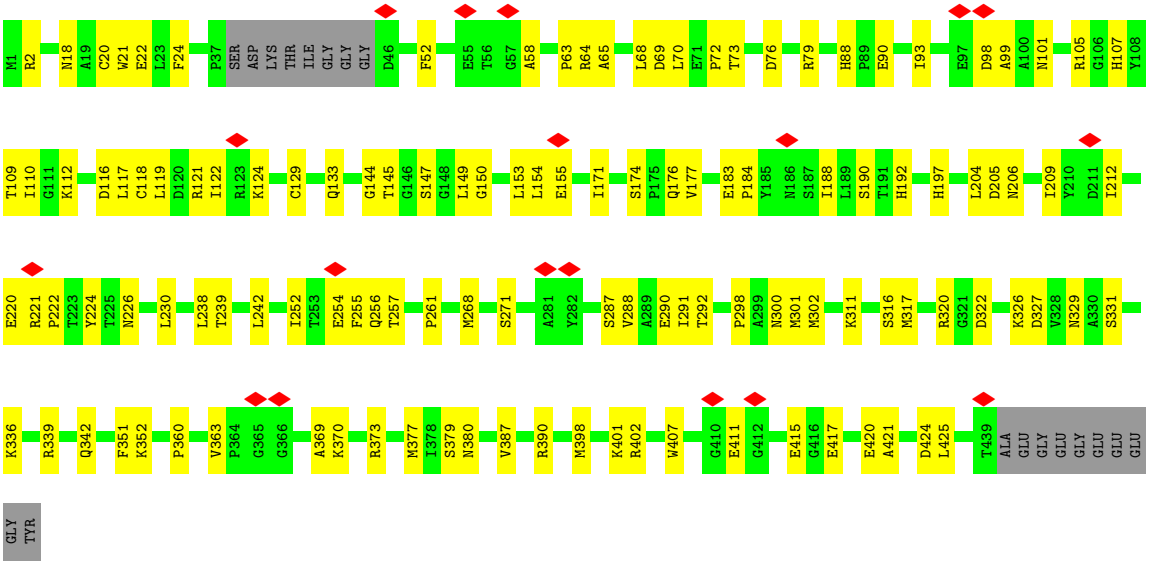




• Molecule 45: Tubulin alpha chain

Chain GC:



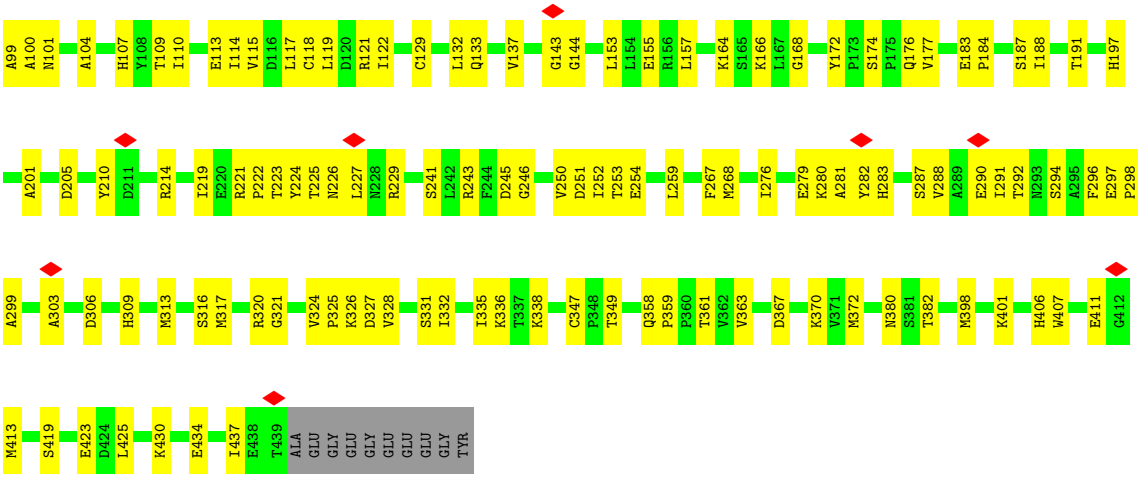


• Molecule 45: Tubulin alpha chain

Chain GE:



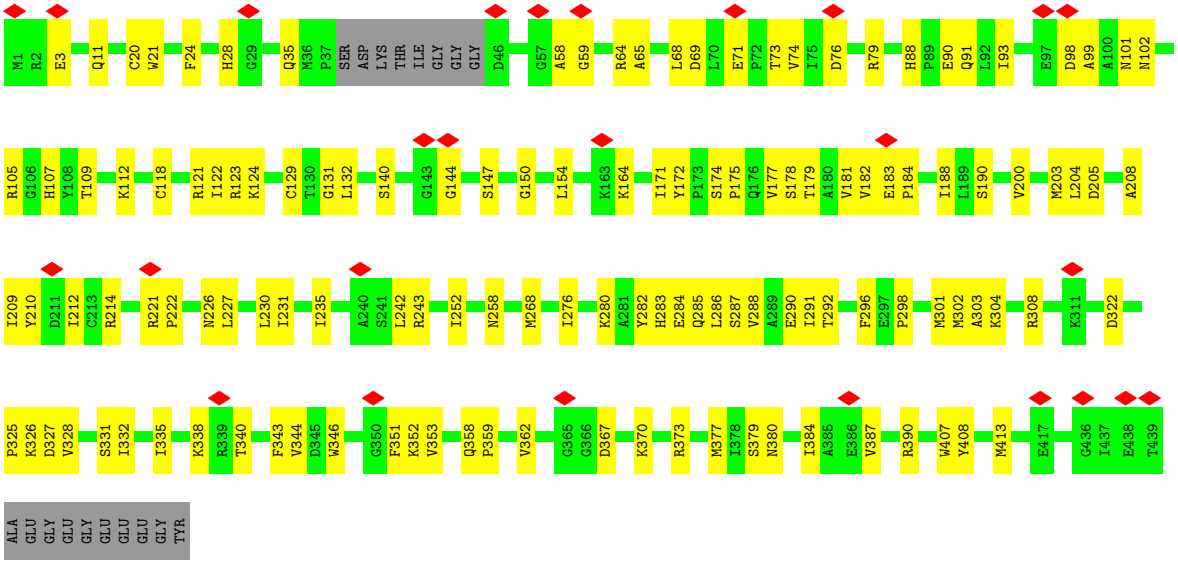




• Molecule 45: Tubulin alpha chain

Chain GG:

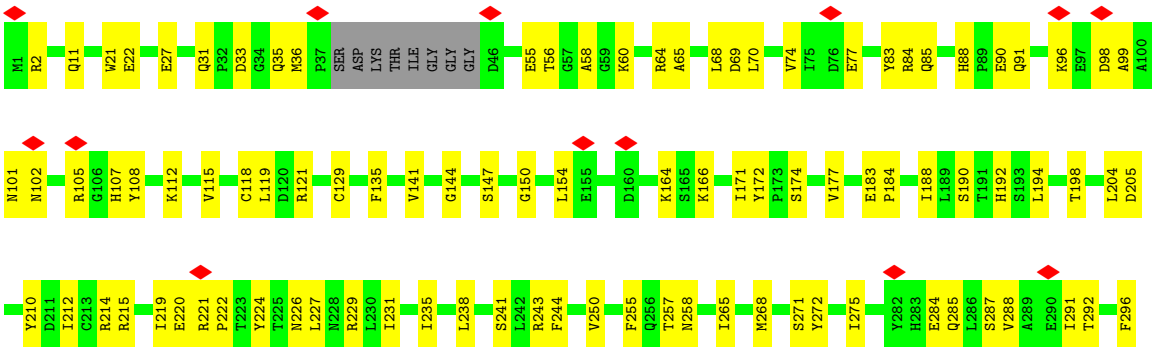


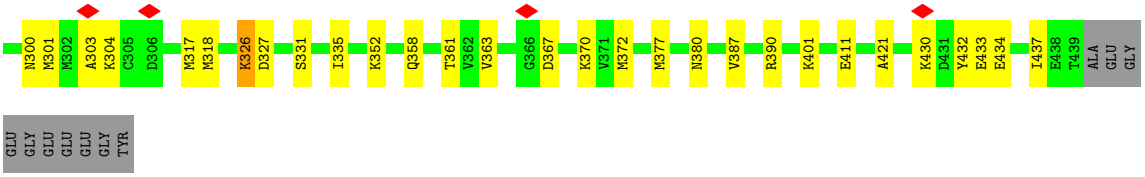


• Molecule 45: Tubulin alpha chain

Chain GI:



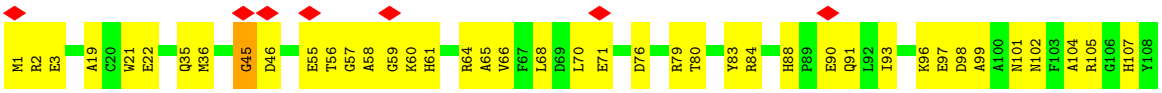


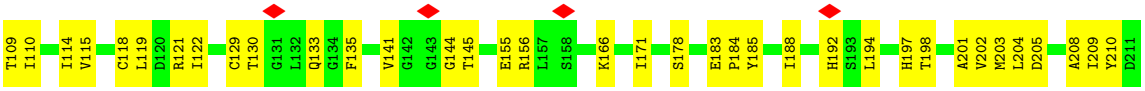


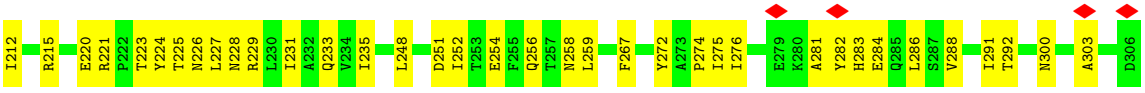
• Molecule 45: Tubulin alpha chain

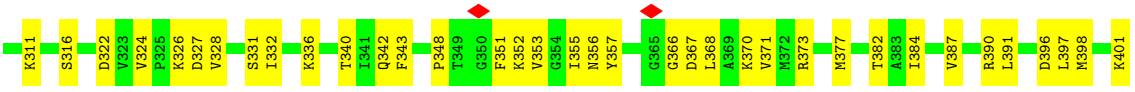
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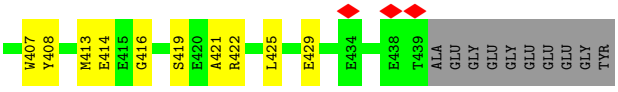






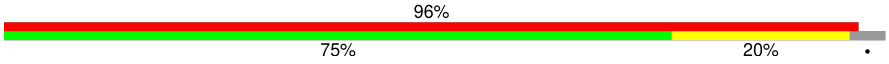


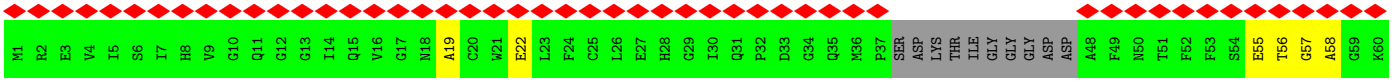


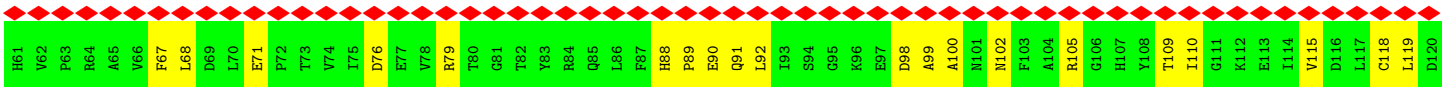


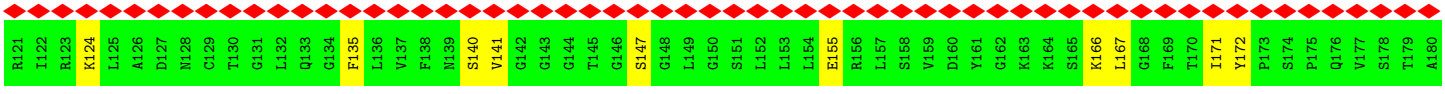
• Molecule 45: Tubulin alpha chain

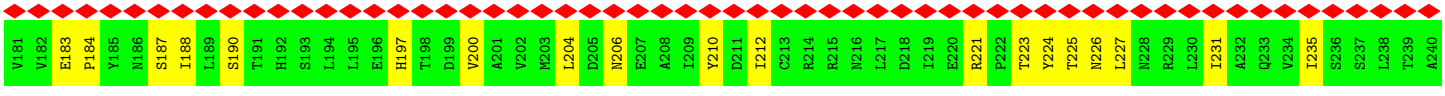
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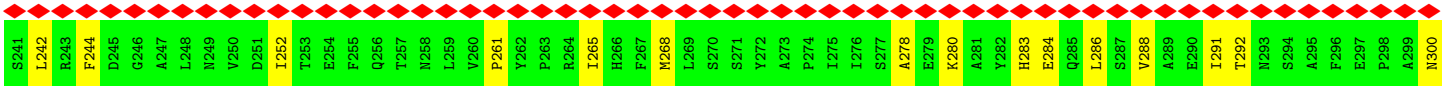


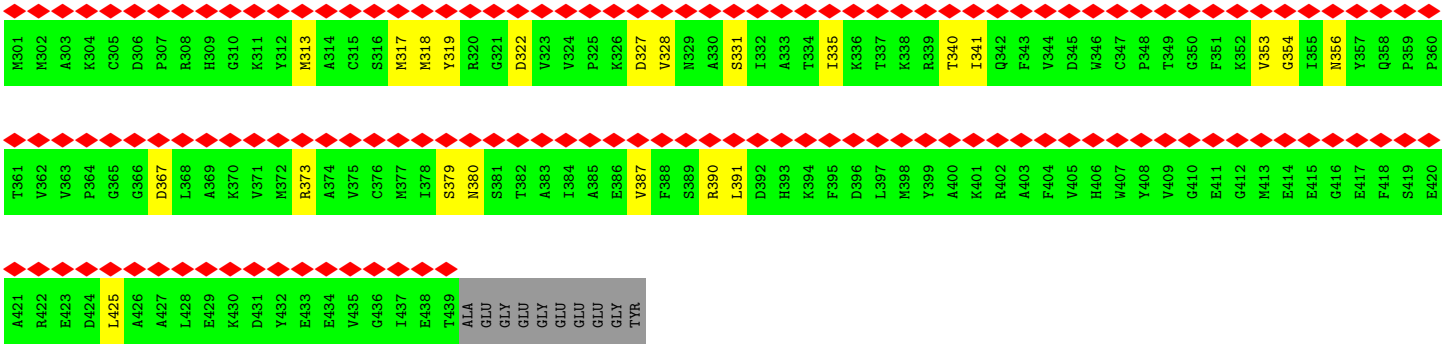








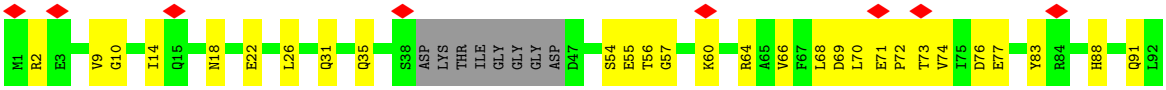


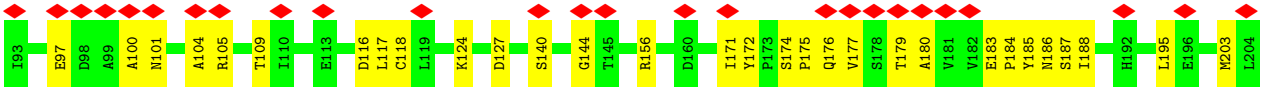


• Molecule 45: Tubulin alpha chain

Chain HA:

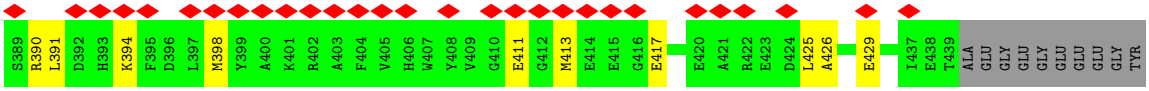








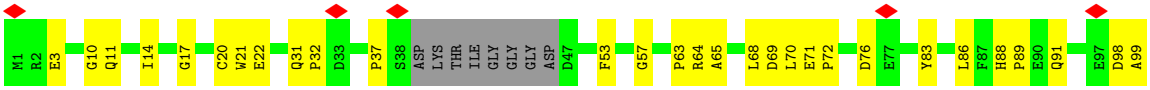


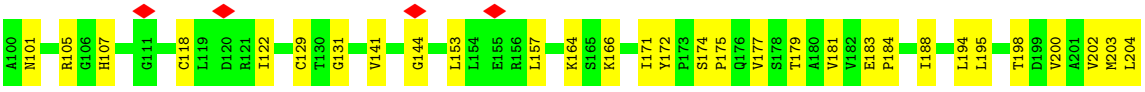


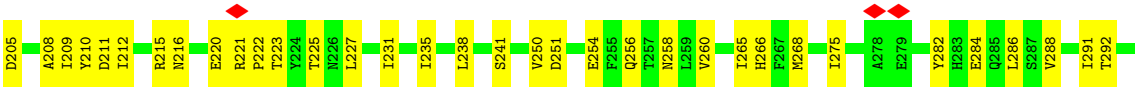
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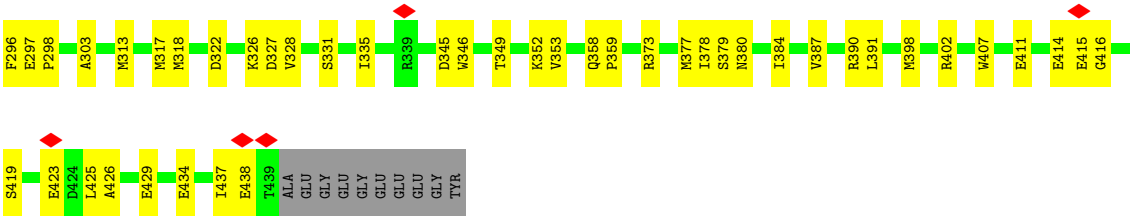
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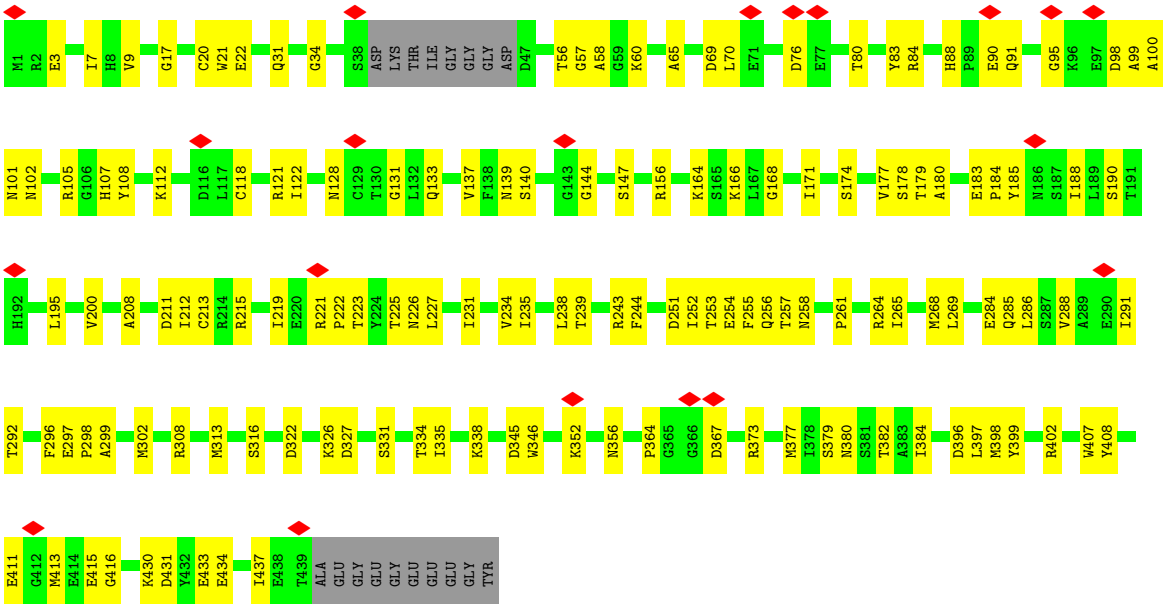




• Molecule 45: Tubulin alpha chain

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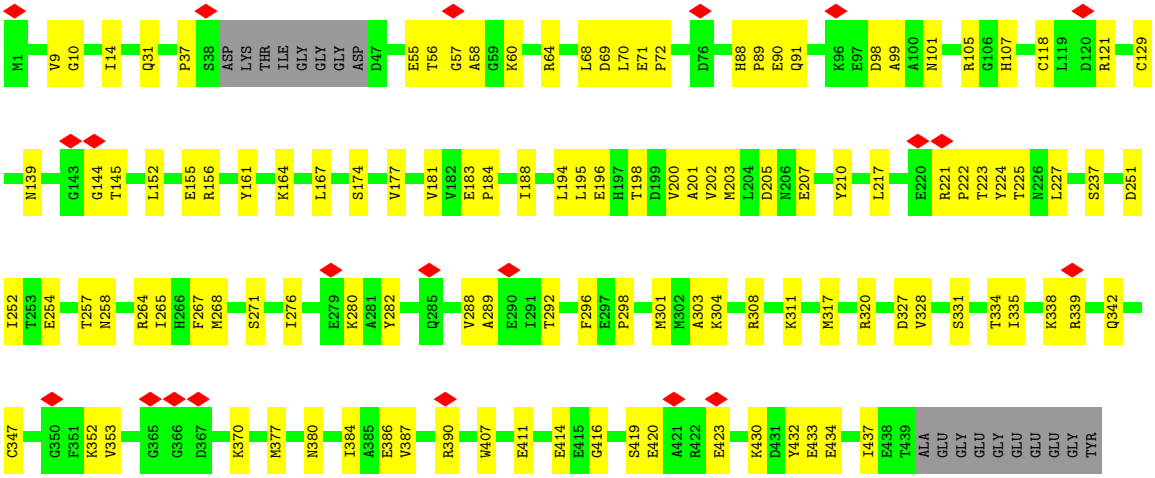




• Molecule 45: Tubulin alpha chain

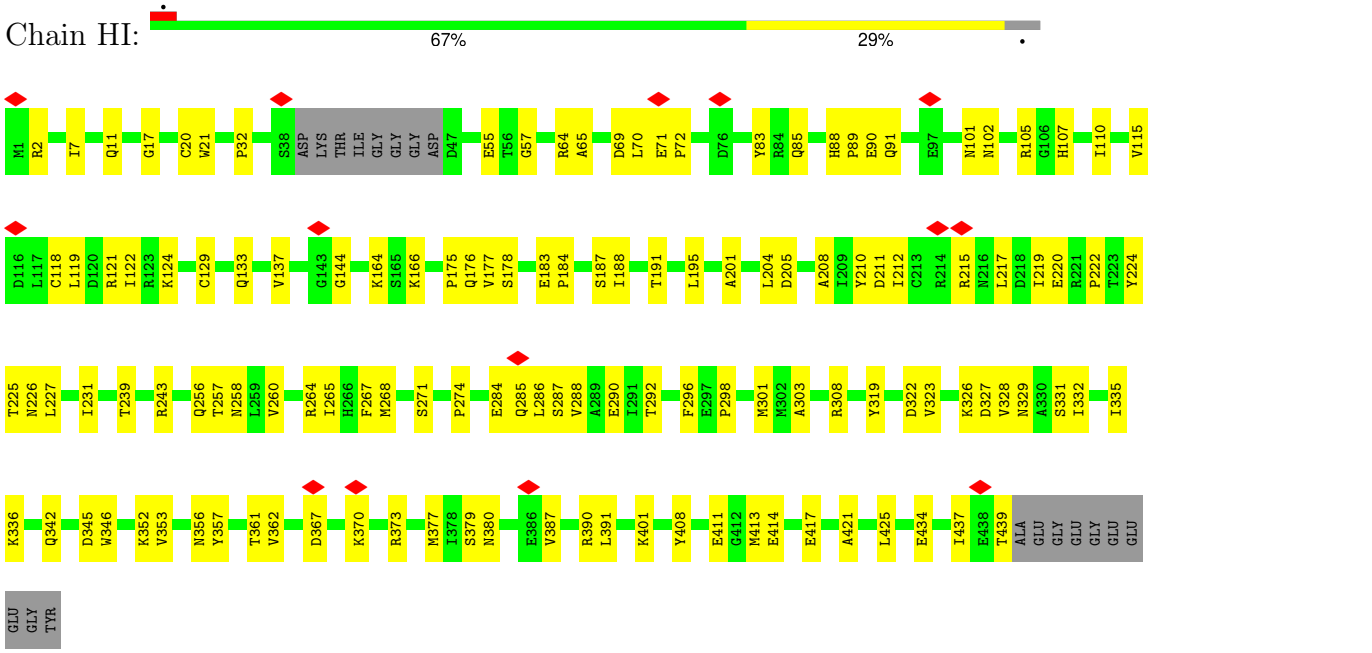
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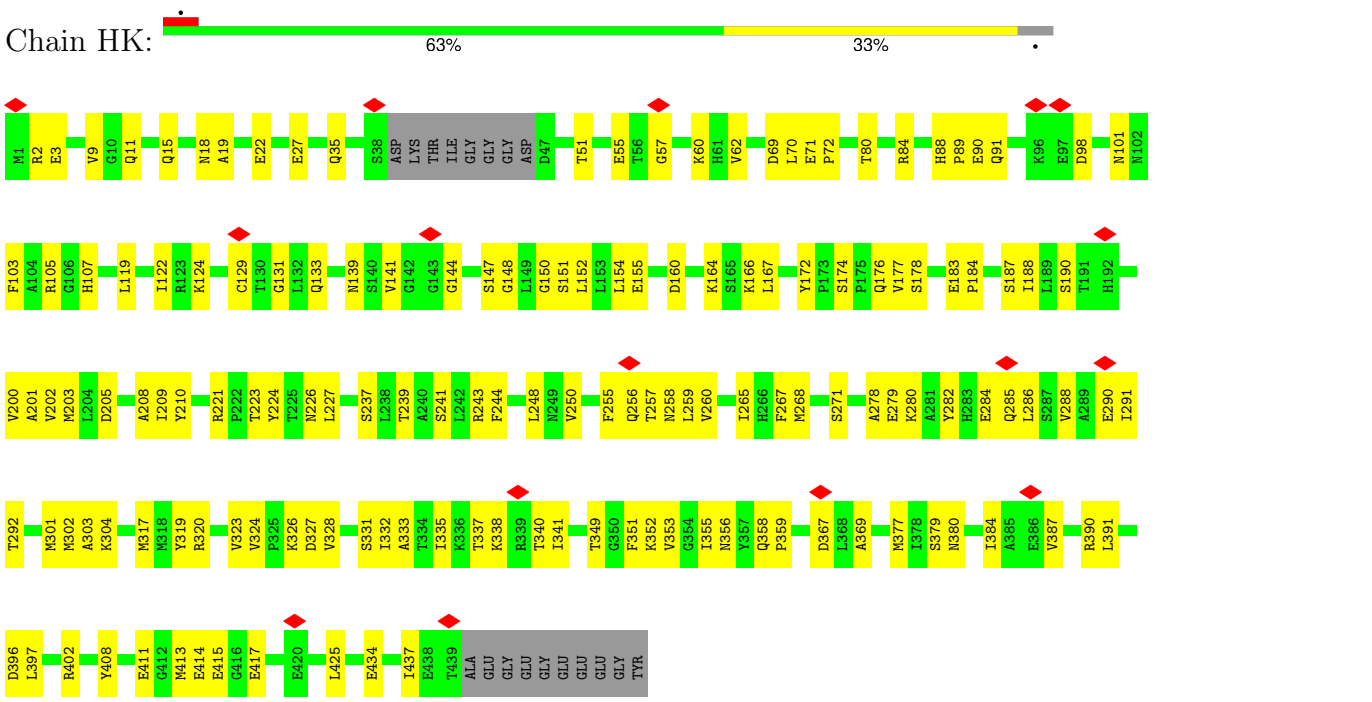
• Molecule 45: Tubulin alpha chain

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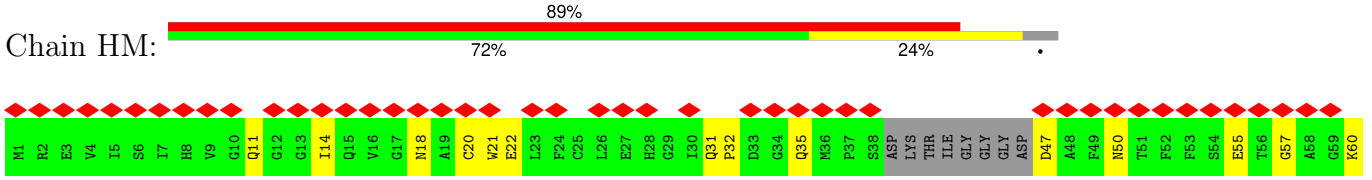
• Molecule 45: Tubulin alpha chain

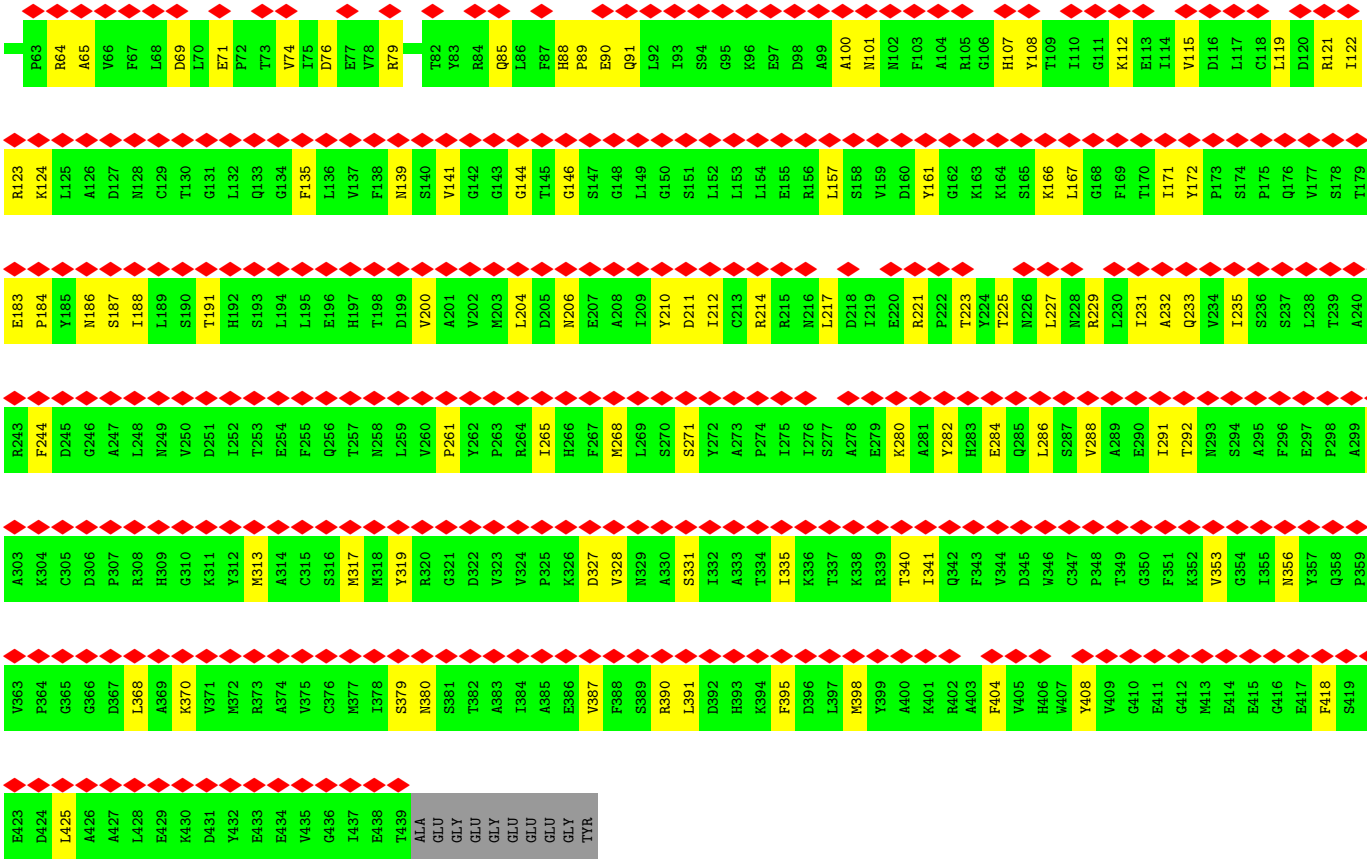
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• Molecule 45: Tubulin alpha chain

Chain HM:

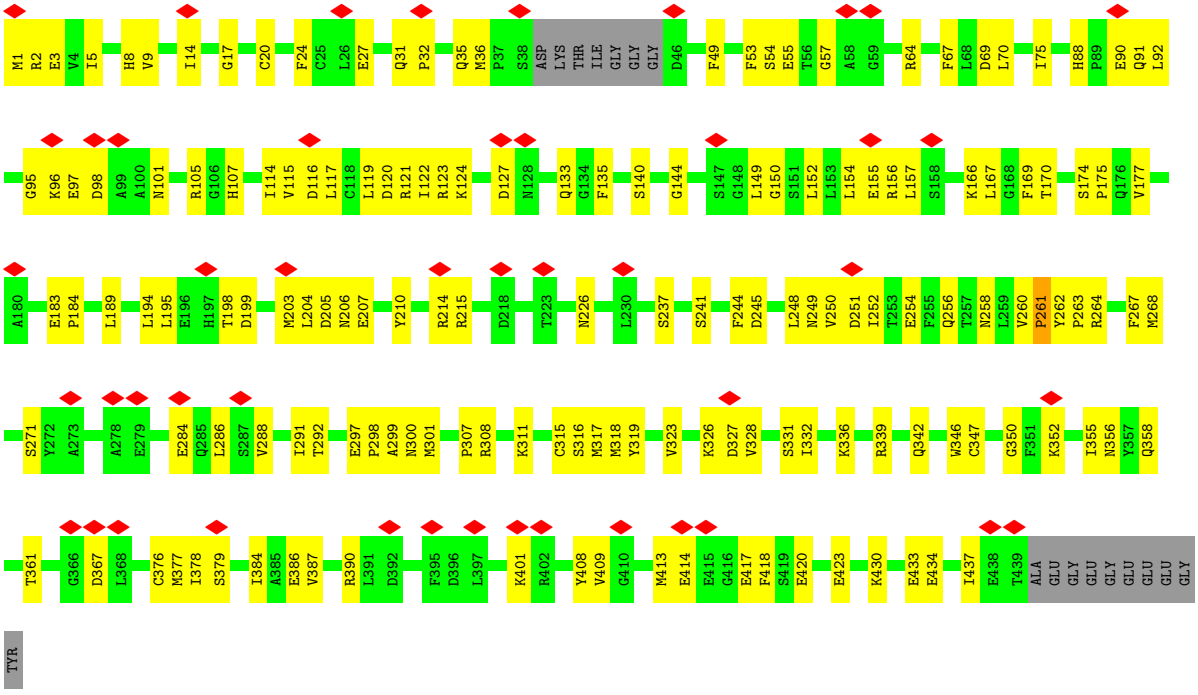




- Molecule 45: Tubulin alpha chain

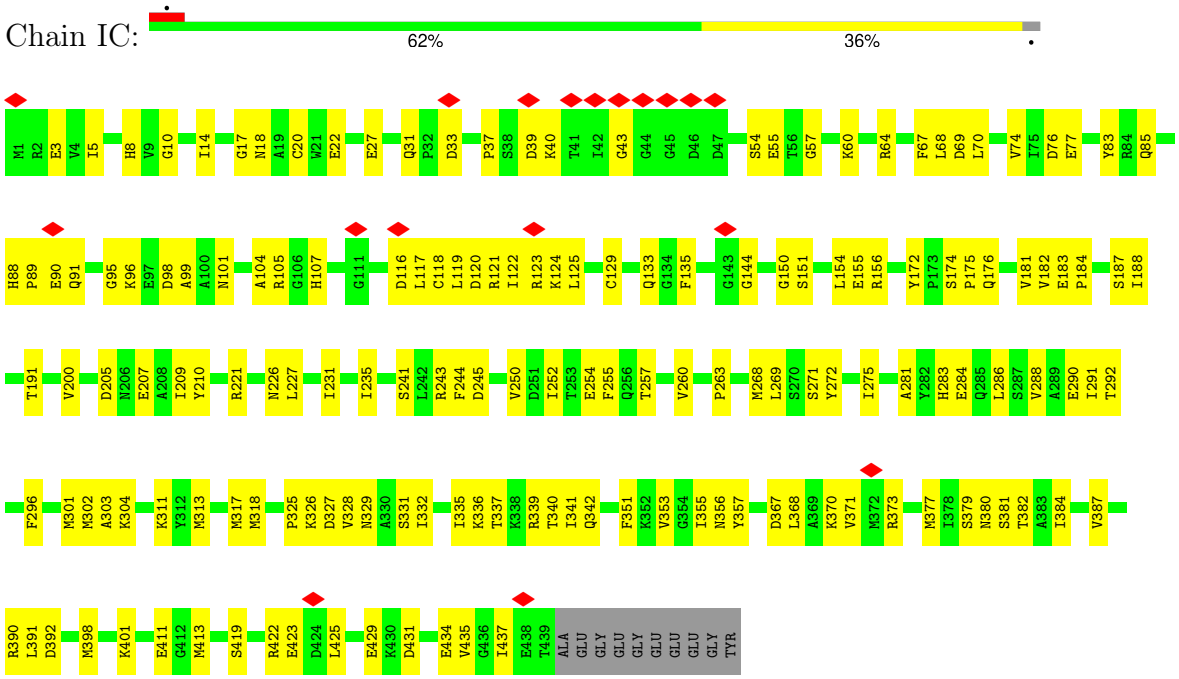
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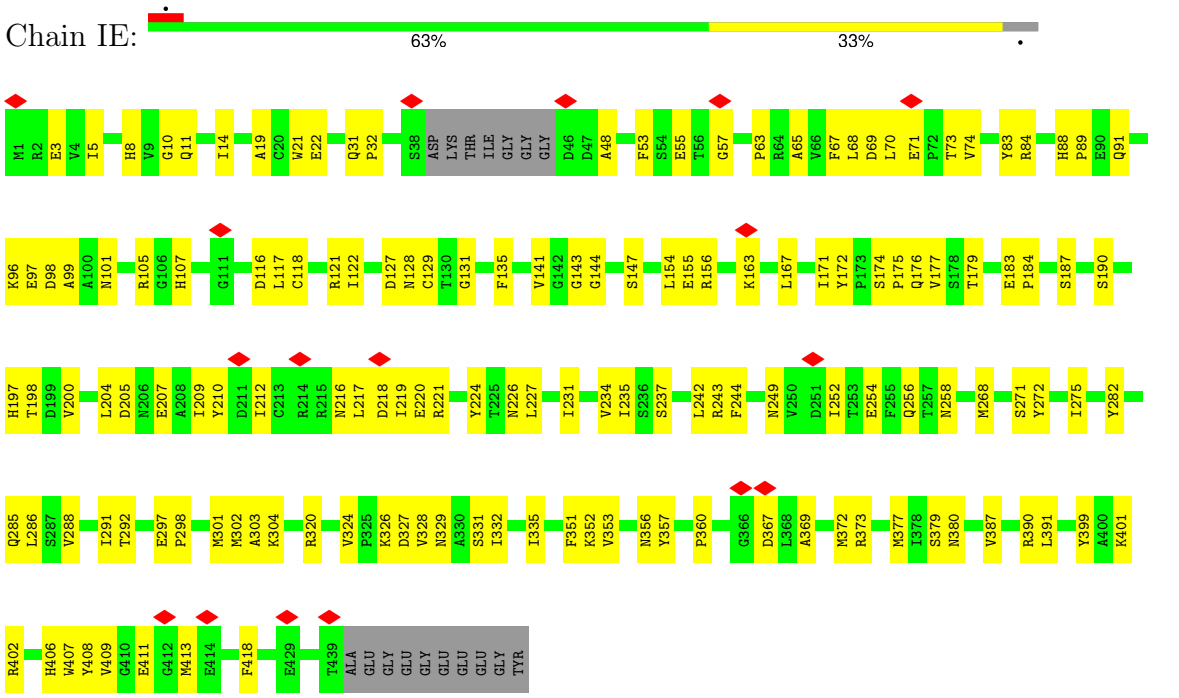
• Molecule 45: Tubulin alpha chain

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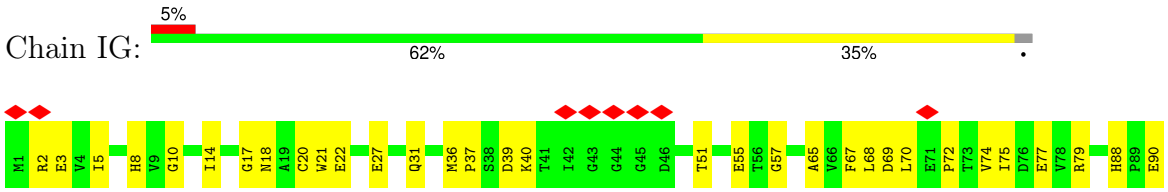
• Molecule 45: Tubulin alpha chain

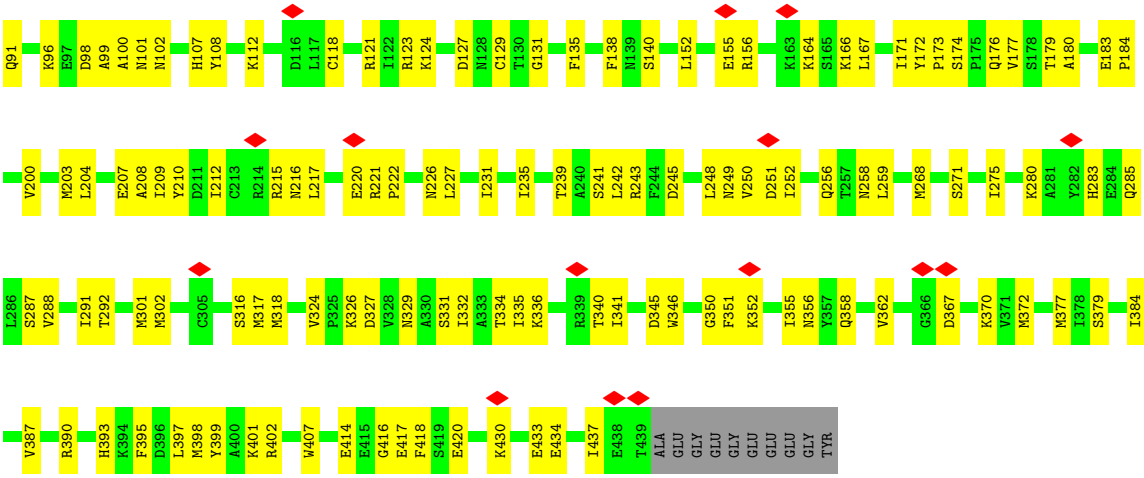
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• Molecule 45: Tubulin alpha chain

Chain IG:

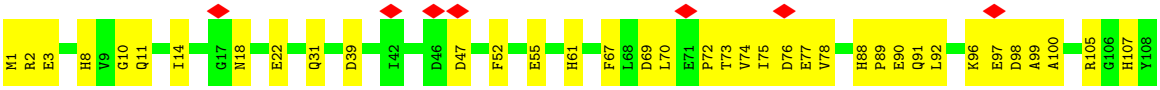


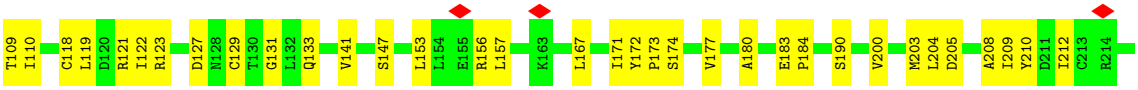


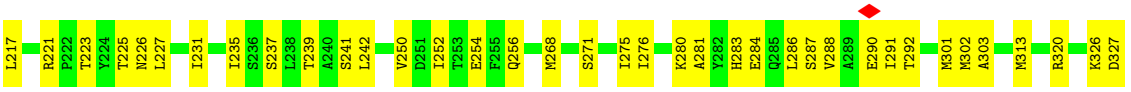
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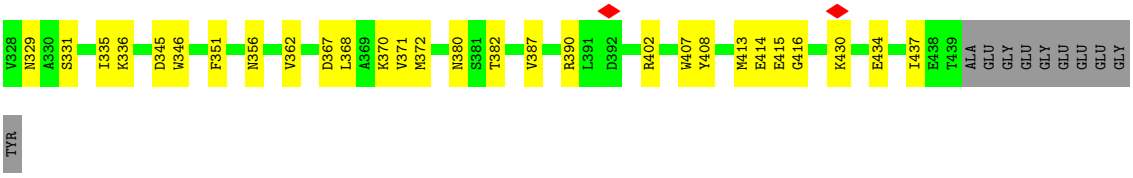
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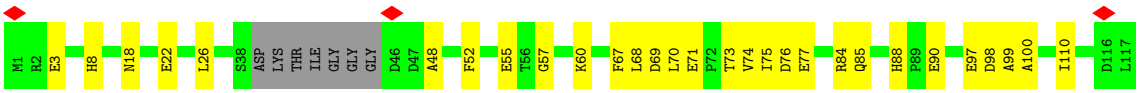


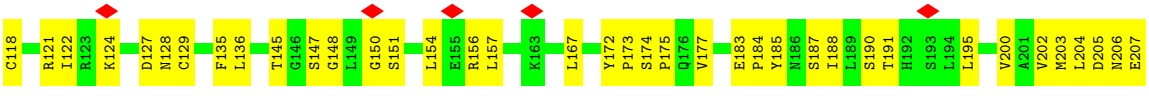


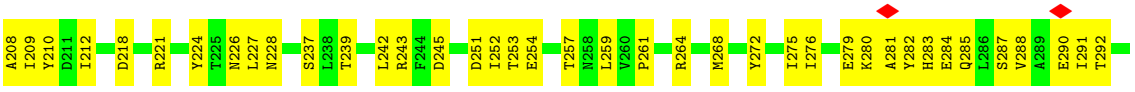
• Molecule 45: Tubulin alpha chain

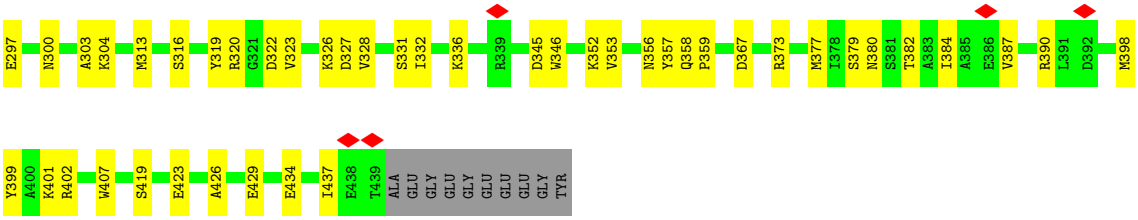
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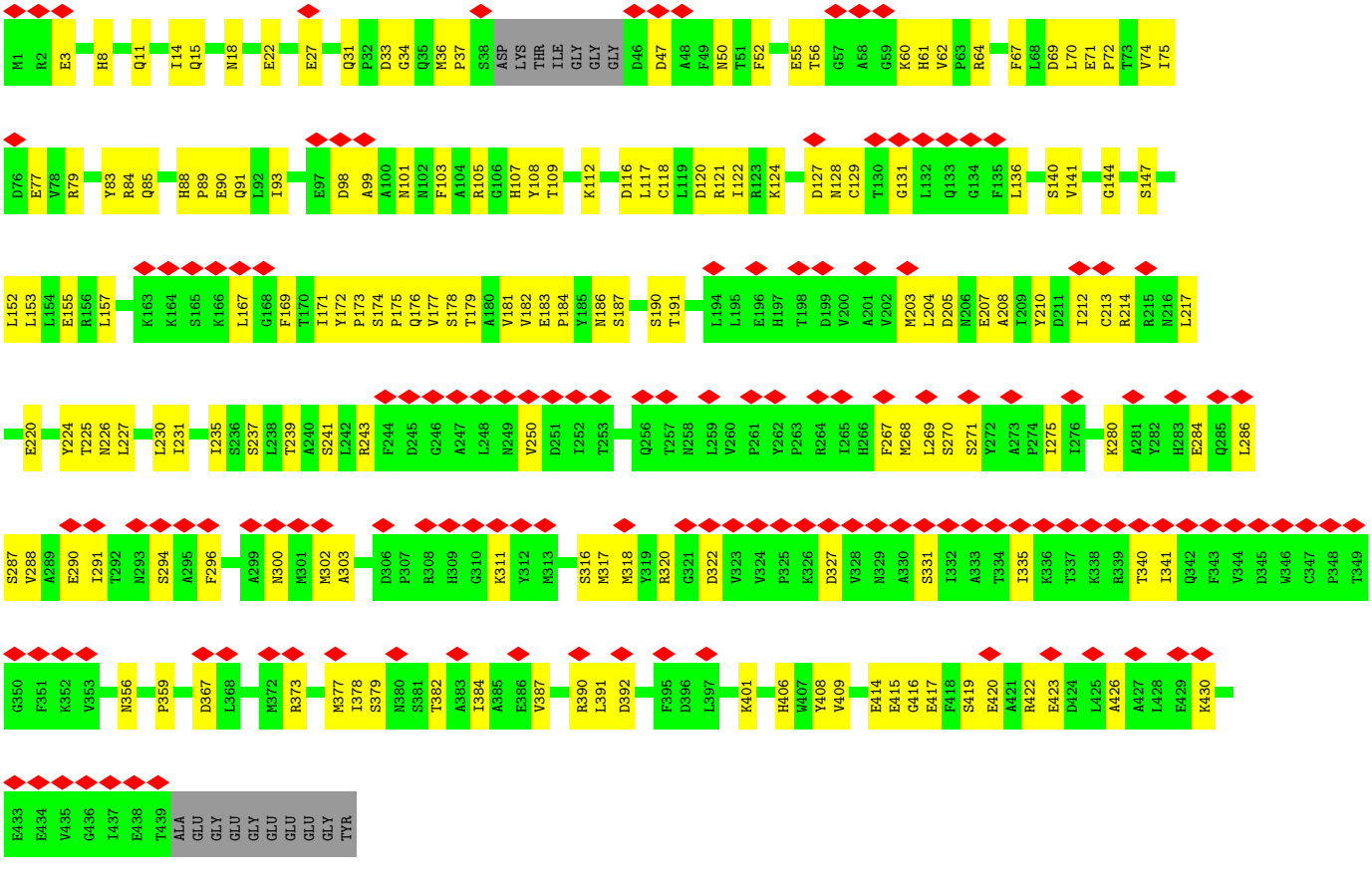




• Molecule 45: Tubulin alpha chain

Chain IM:

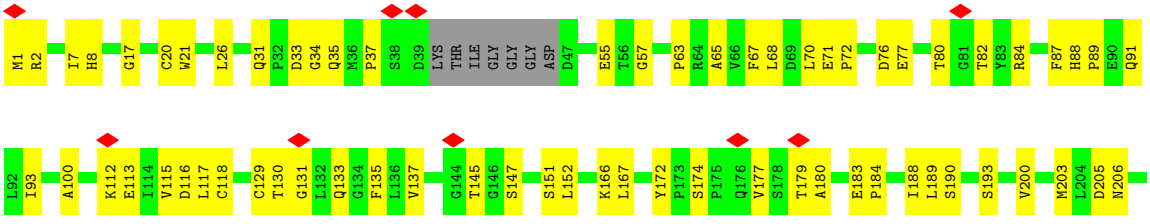


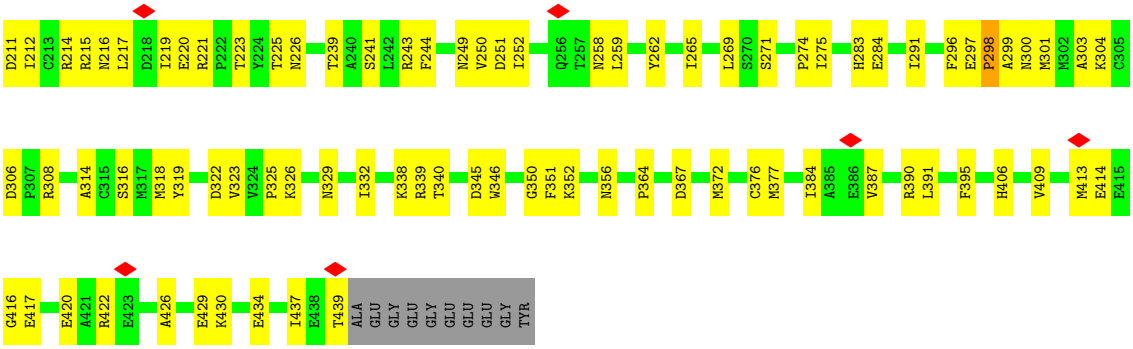


• Molecule 45: Tubulin alpha chain

Chain JA:



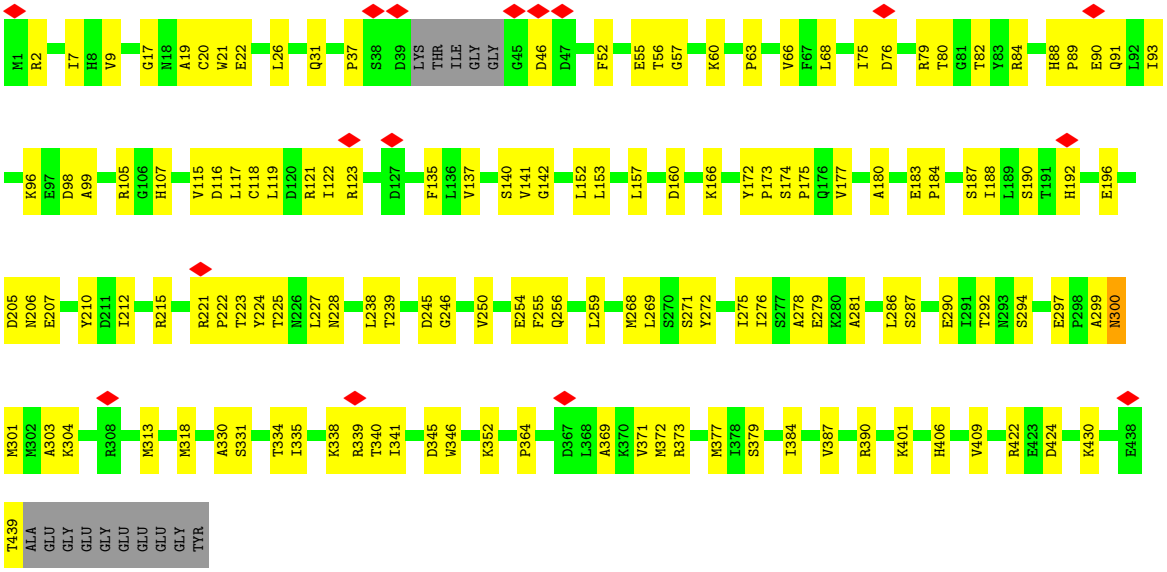




• Molecule 45: Tubulin alpha chain

Chain JC:

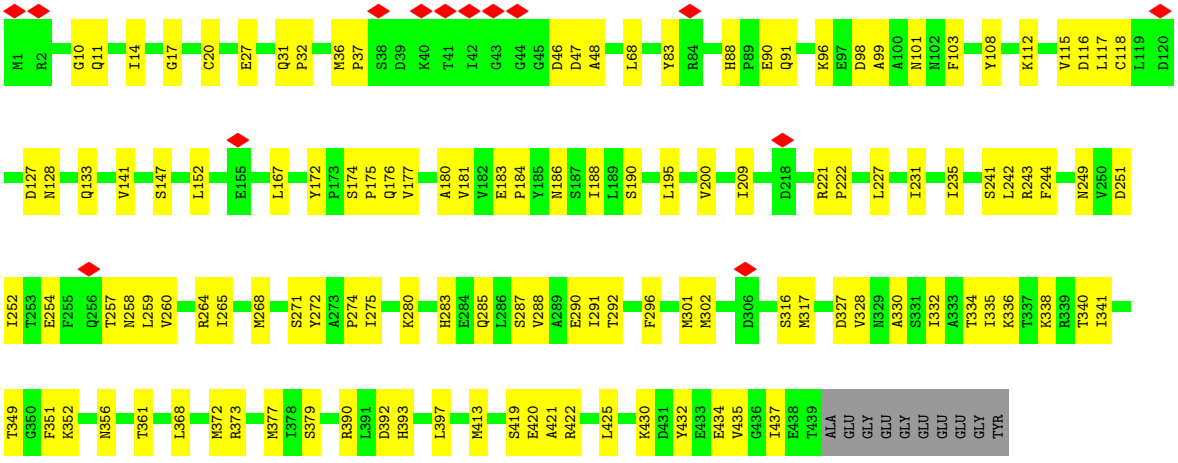




• Molecule 45: Tubulin alpha chain

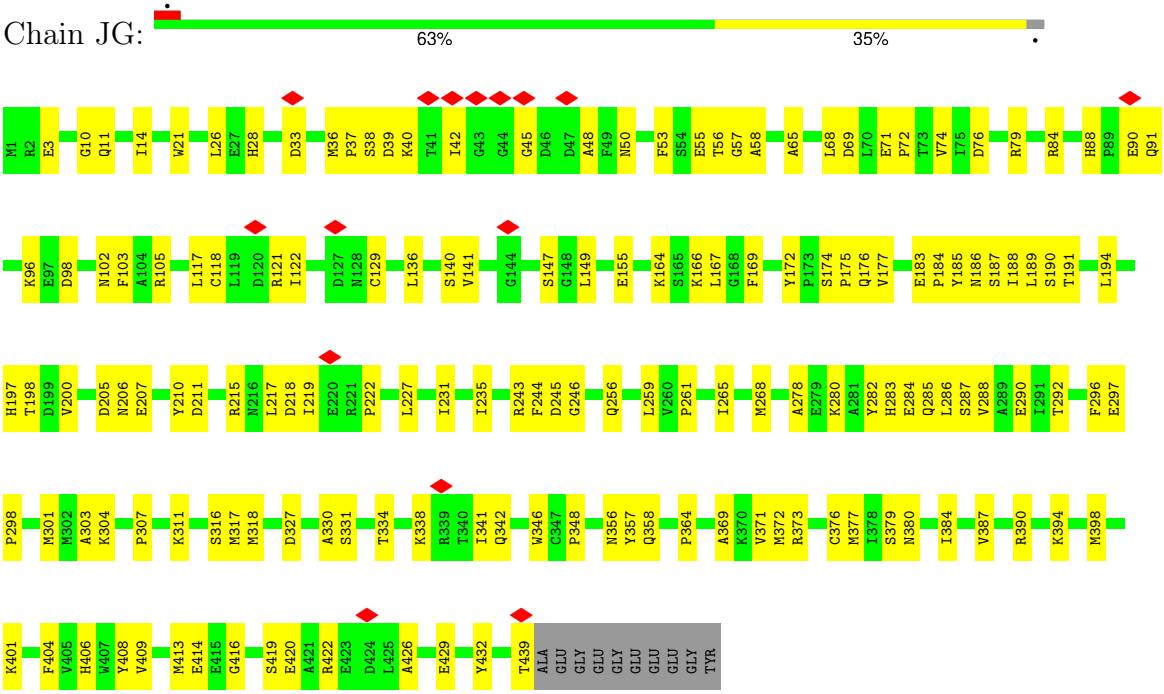
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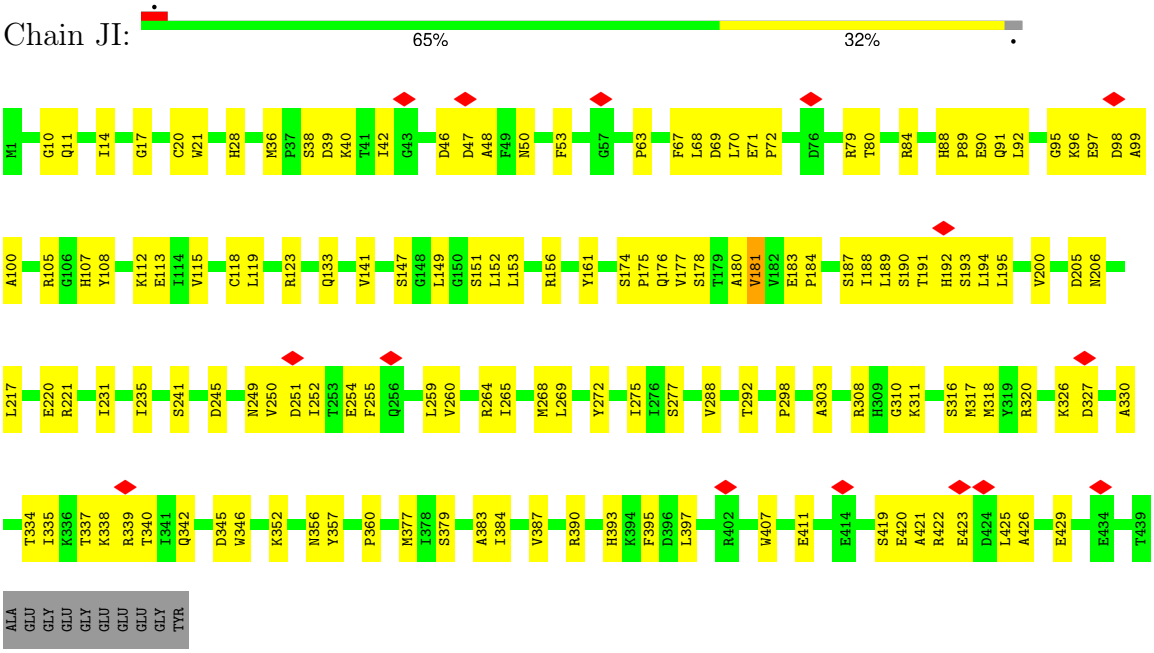
• Molecule 45: Tubulin alpha chain

Chain JG:



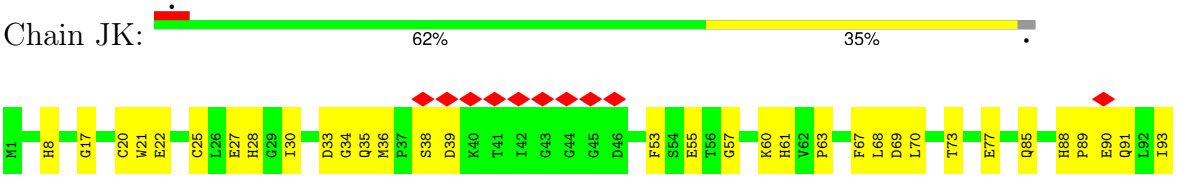
• Molecule 45: Tubulin alpha chain

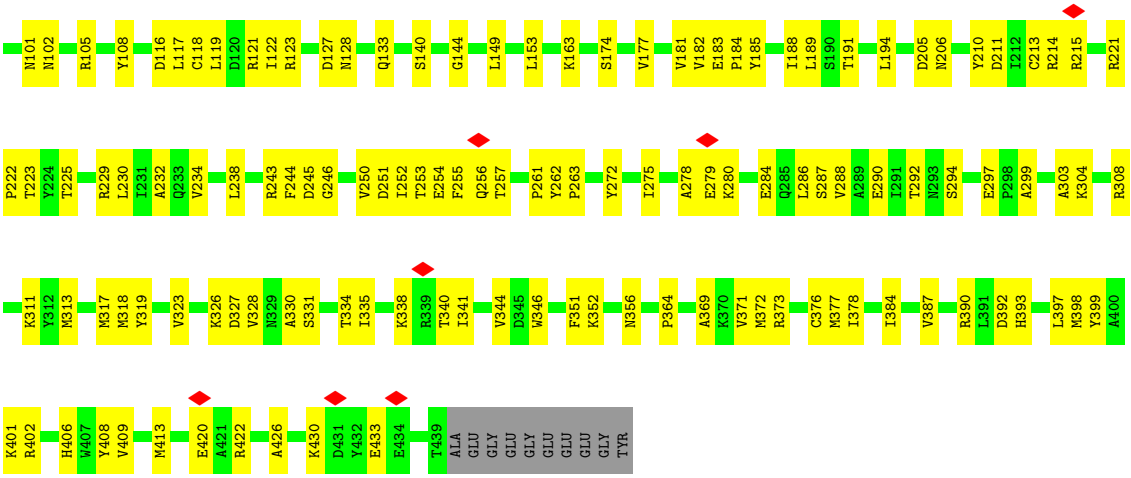
Chain JI:



• Molecule 45: Tubulin alpha chain

Chain JK:

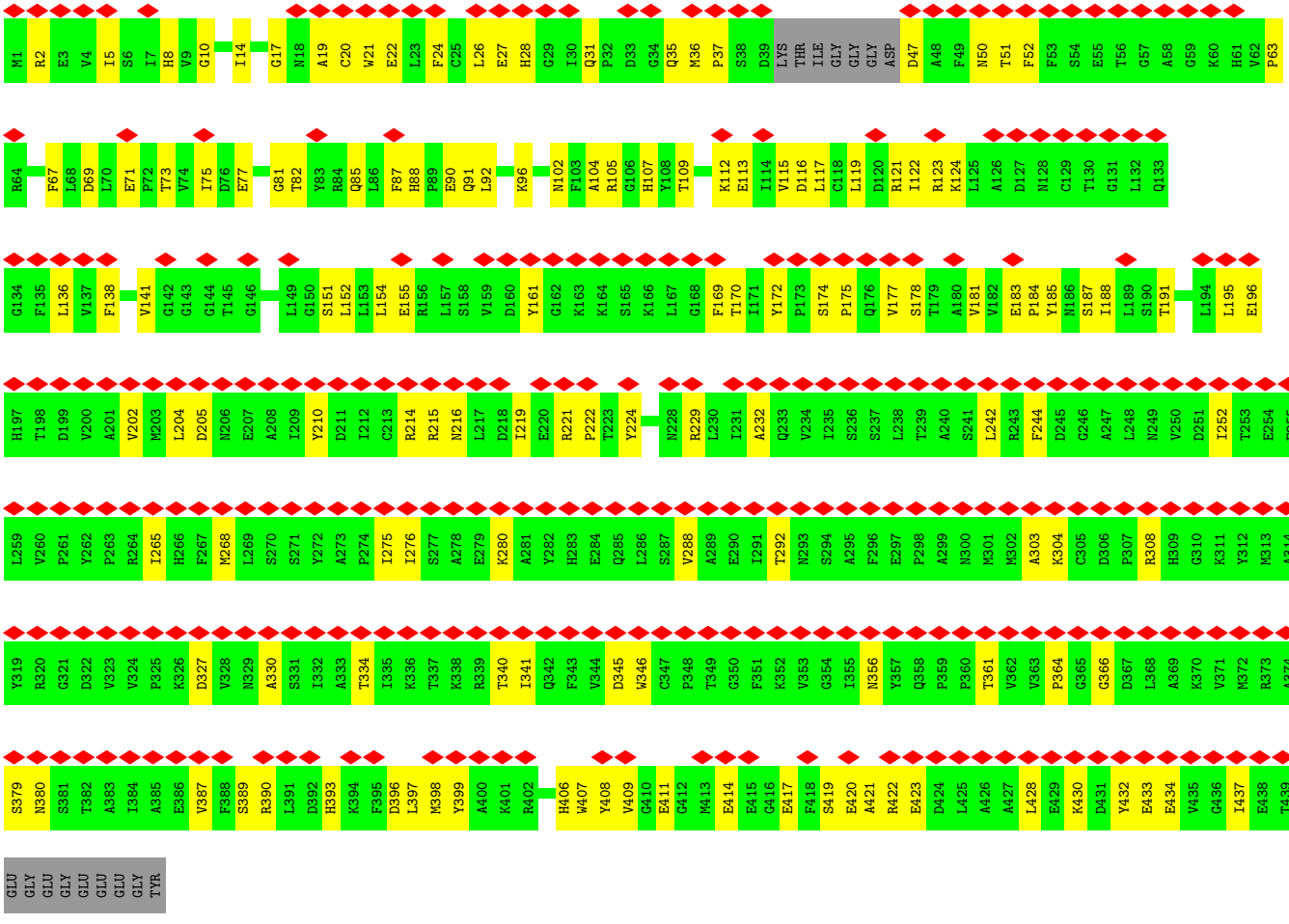




• Molecule 45: Tubulin alpha chain

Chain JM:

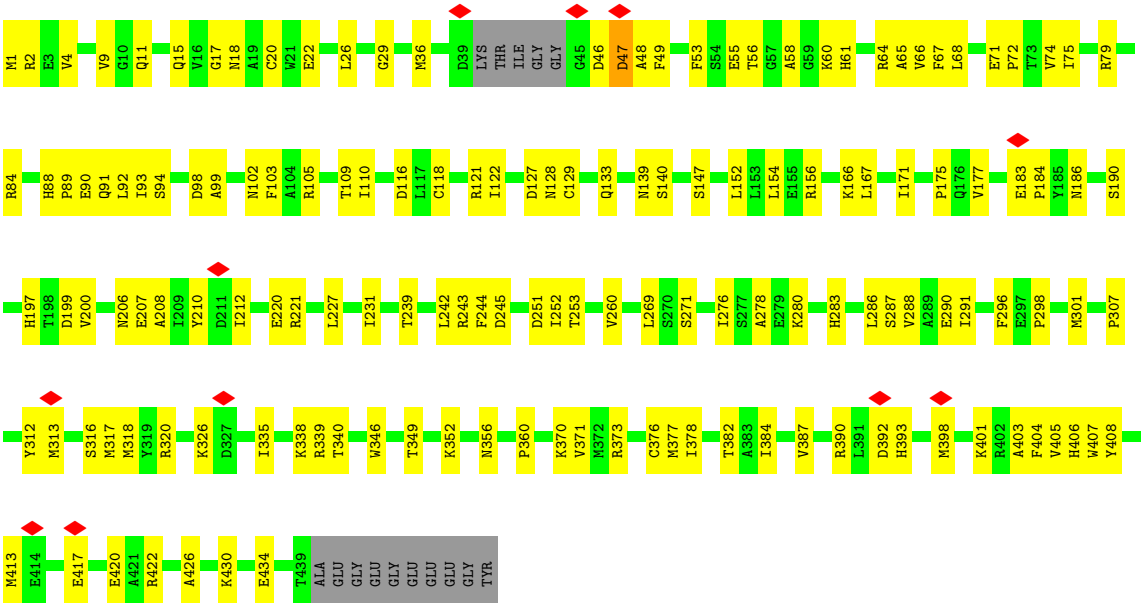




• Molecule 45: Tubulin alpha chain

Chain KA:

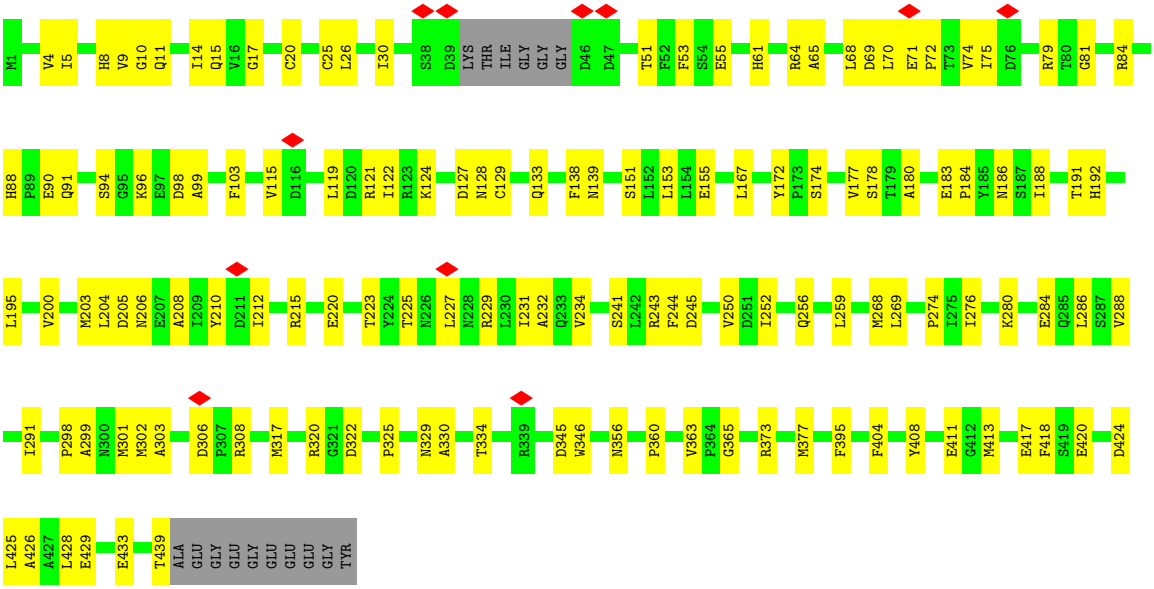




• Molecule 45: Tubulin alpha chain

Chain KC:

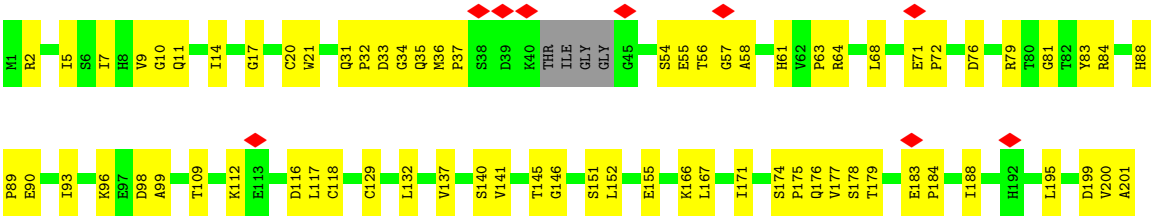


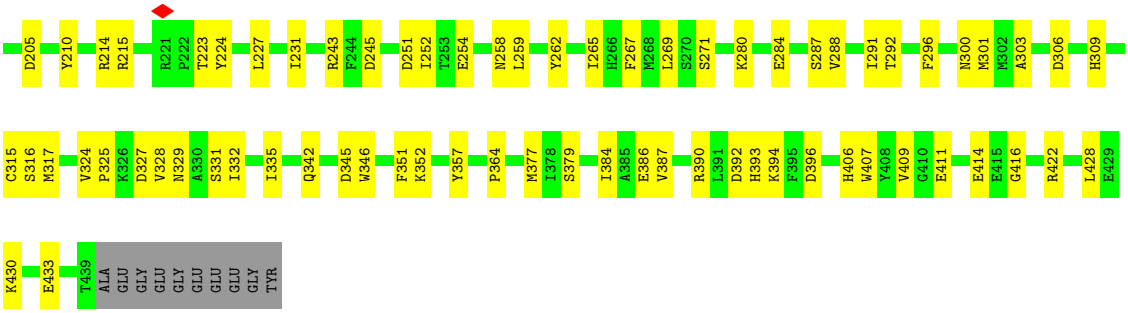


• Molecule 45: Tubulin alpha chain

Chain KE:



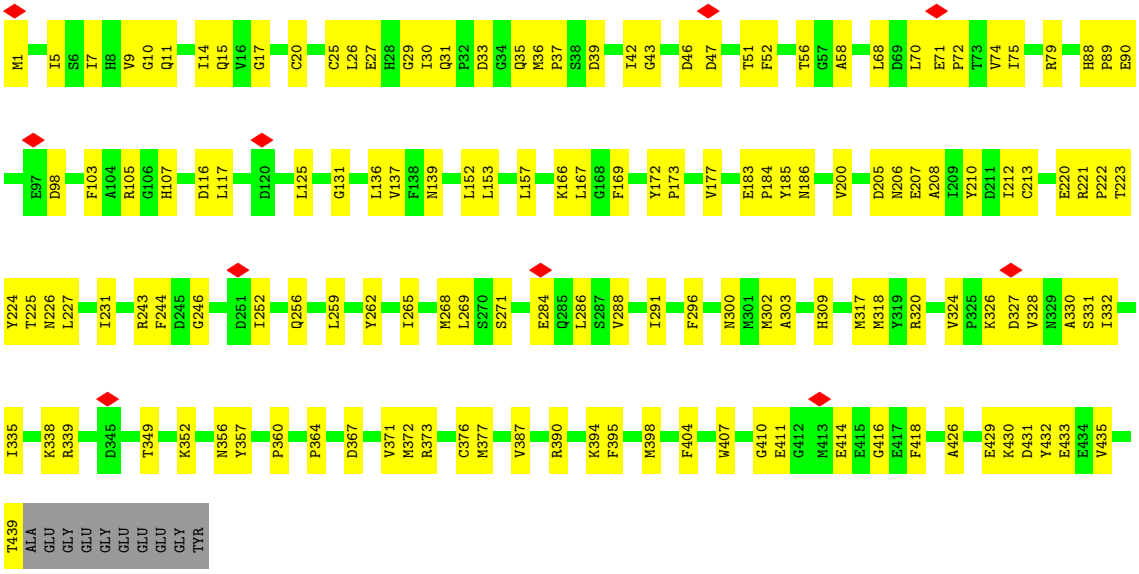




• Molecule 45: Tubulin alpha chain

Chain KG:

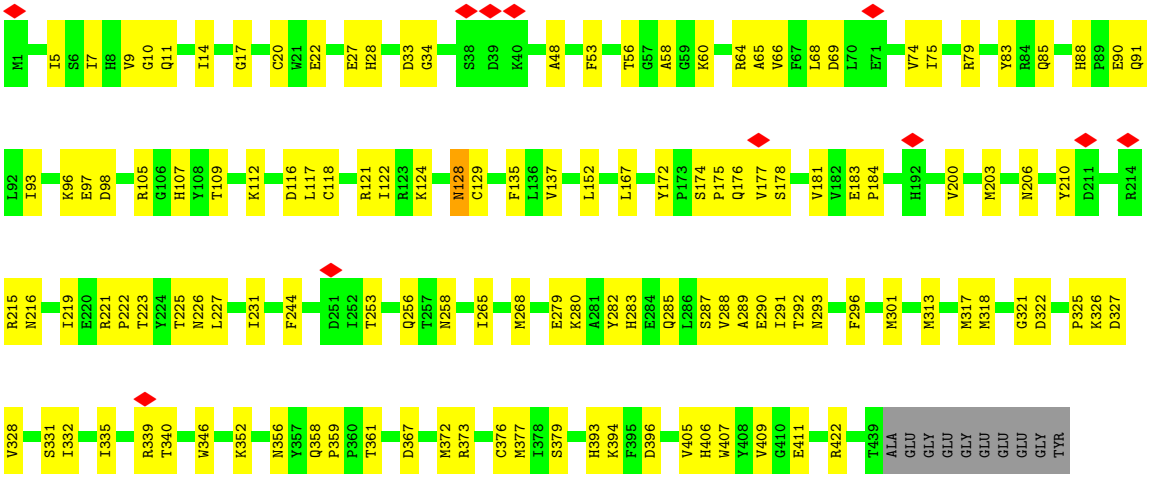




• Molecule 45: Tubulin alpha chain

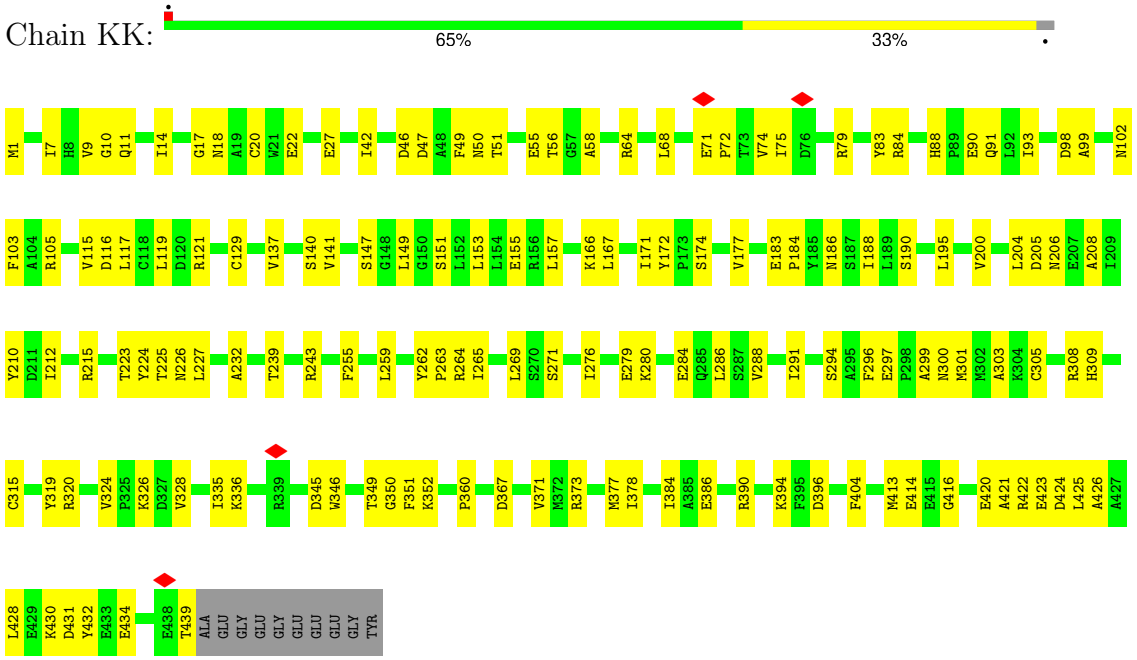
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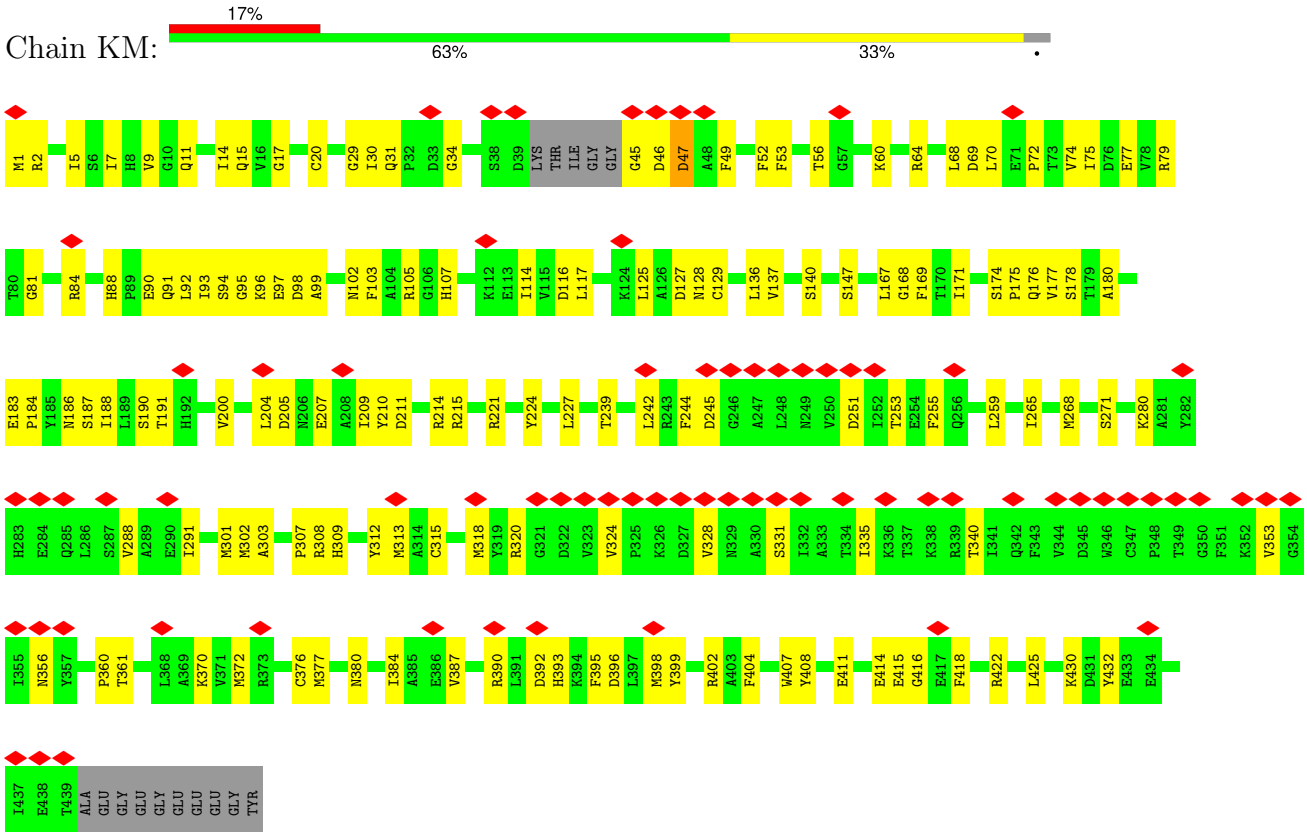
• Molecule 45: Tubulin alpha chain

Chain KK:



• Molecule 45: Tubulin alpha chain

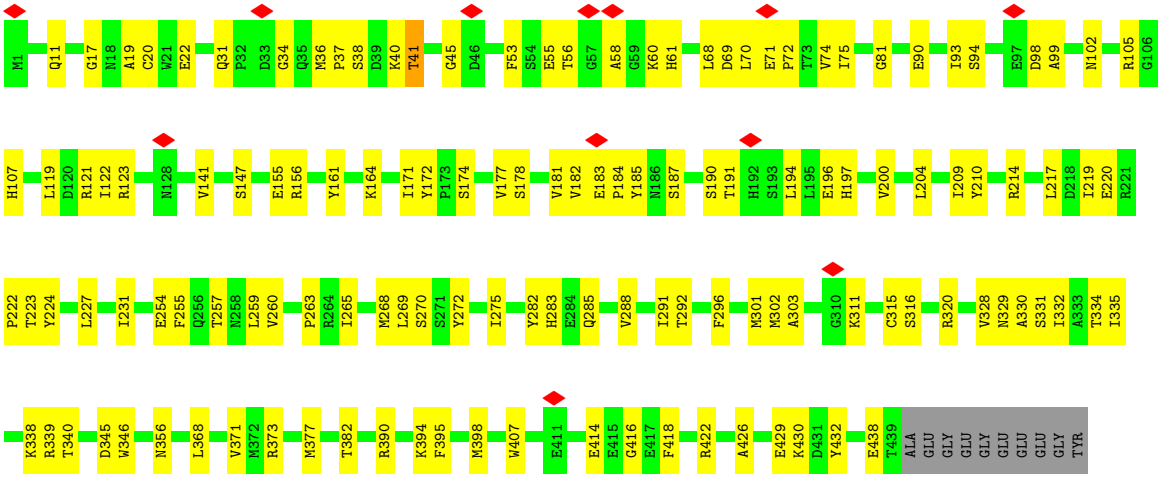
Chain KM:



• Molecule 45: Tubulin alpha chain

Chain LA:

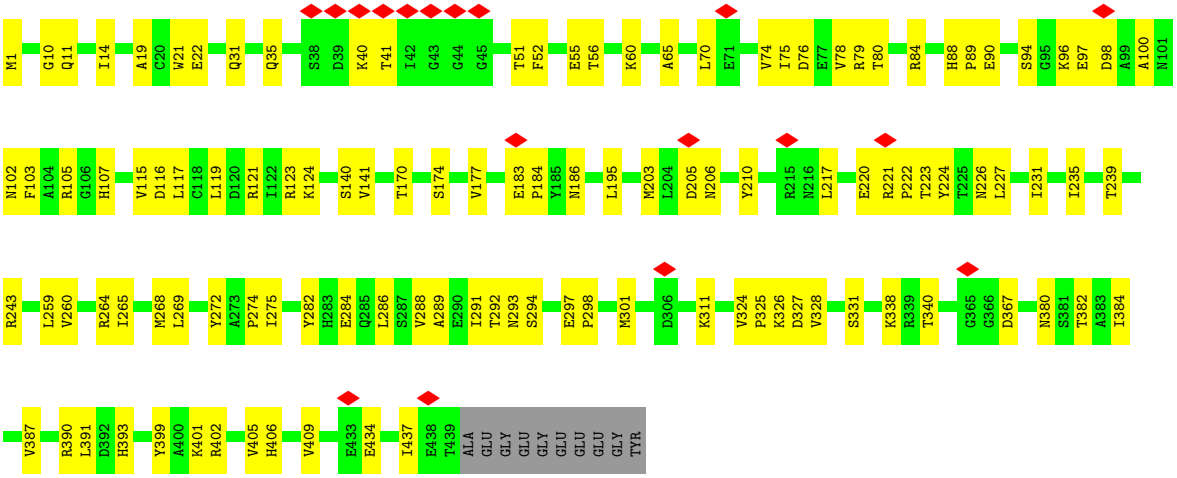




• Molecule 45: Tubulin alpha chain

Chain LC:

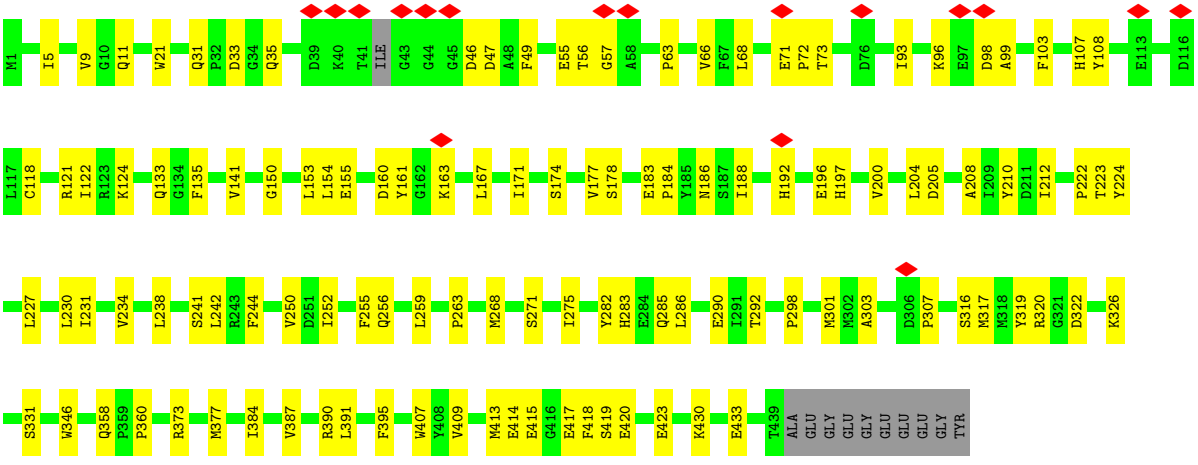




• Molecule 45: Tubulin alpha chain

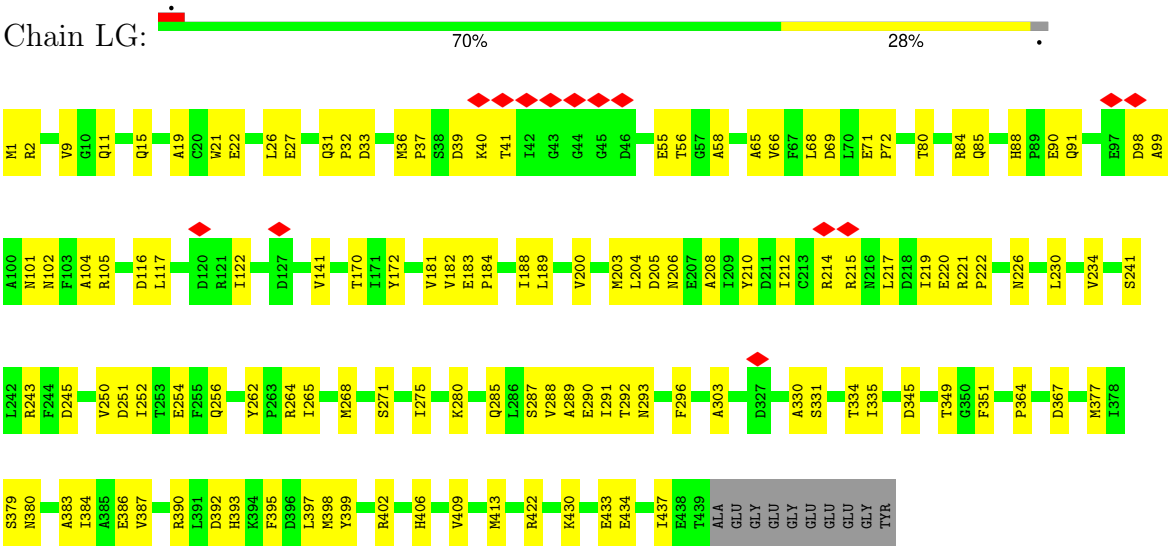
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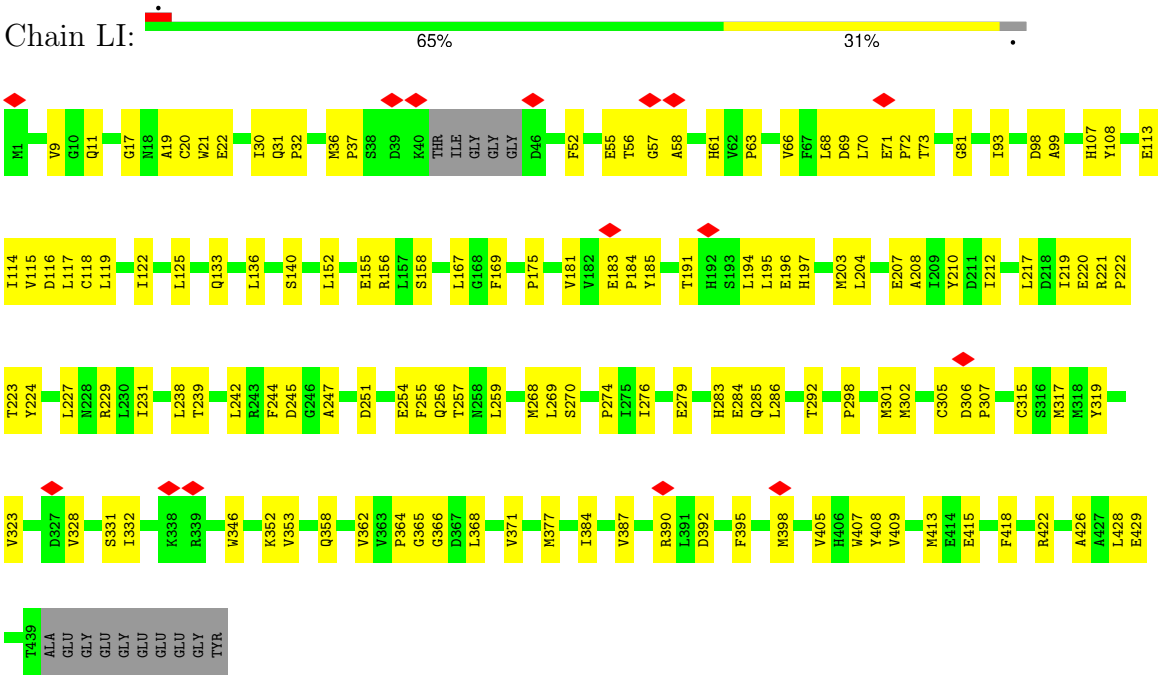
• Molecule 45: Tubulin alpha chain

Chain LG:



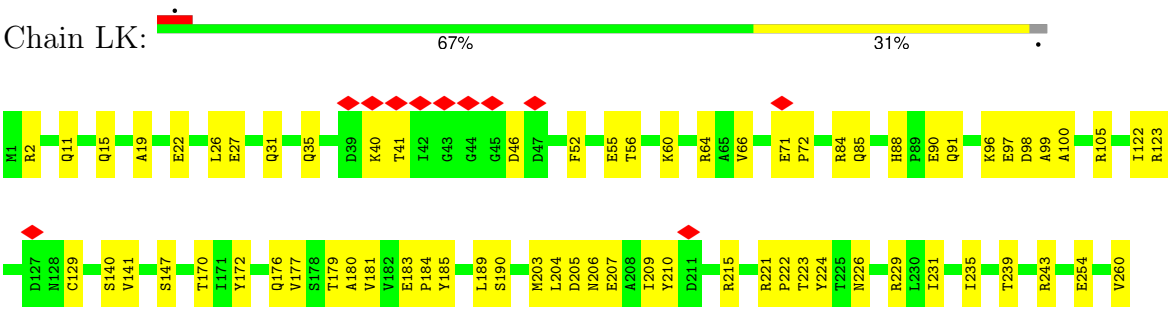
• Molecule 45: Tubulin alpha chain

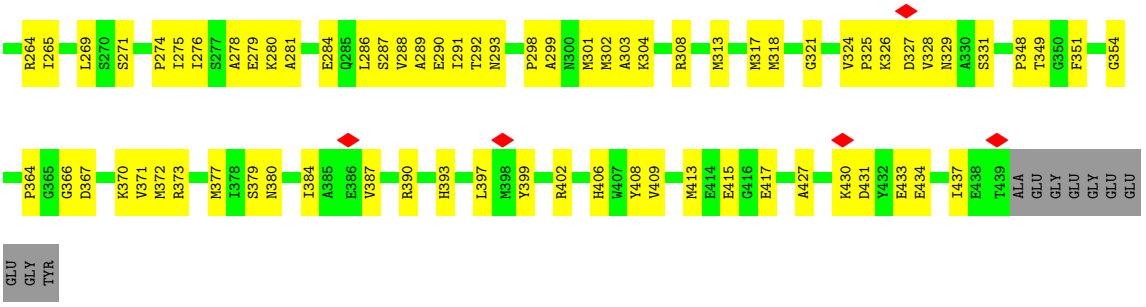
Chain LI:



• Molecule 45: Tubulin alpha chain

Chain LK:

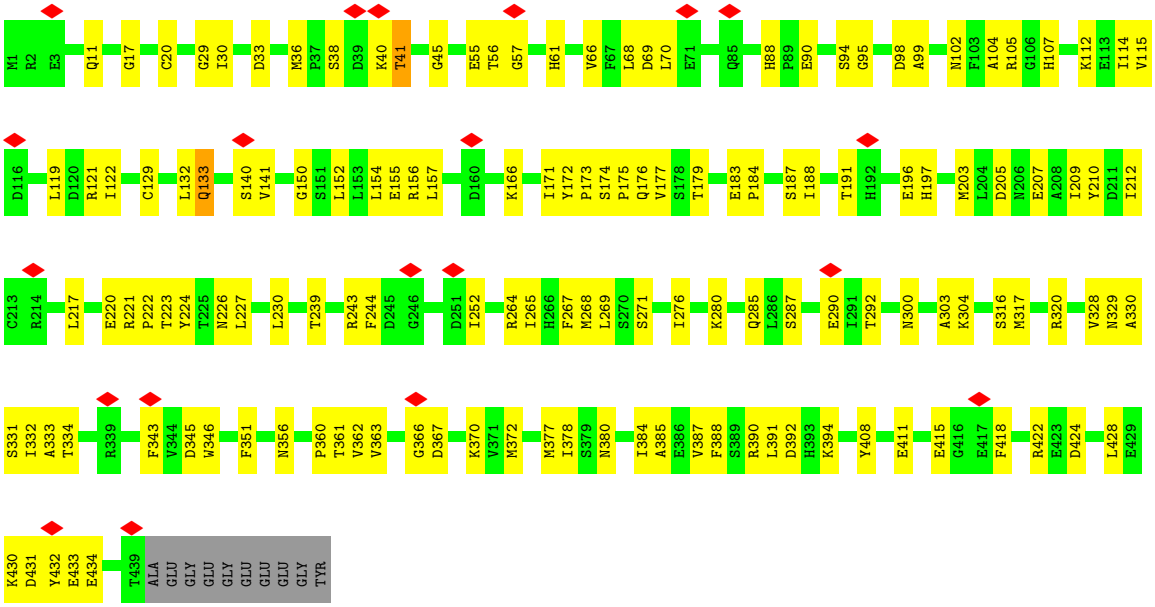




• Molecule 45: Tubulin alpha chain

Chain LM:

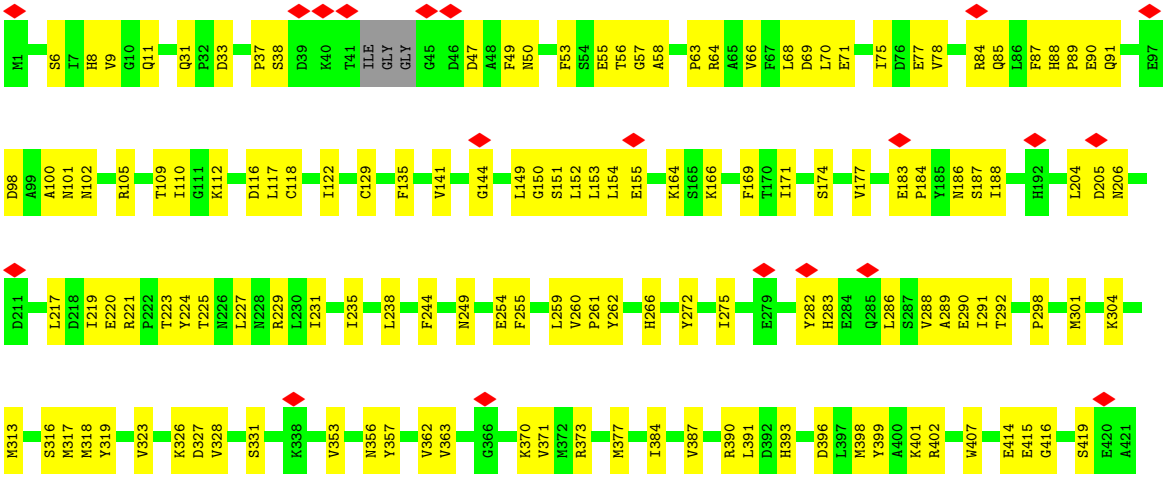


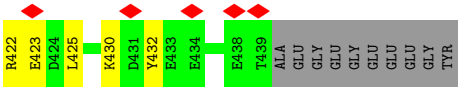


• Molecule 45: Tubulin alpha chain

Chain MA:



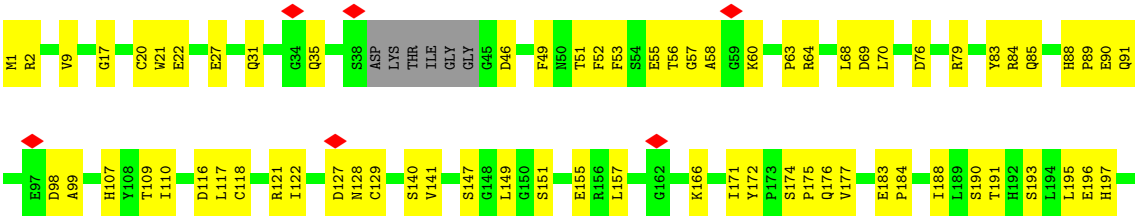




• Molecule 45: Tubulin alpha chain

Chain MC:

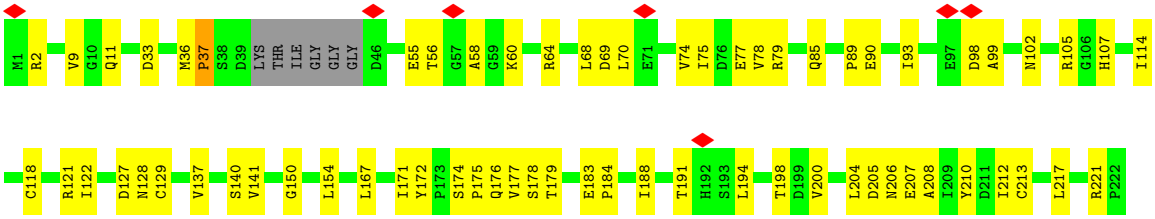




• Molecule 45: Tubulin alpha chain

Chain ME:

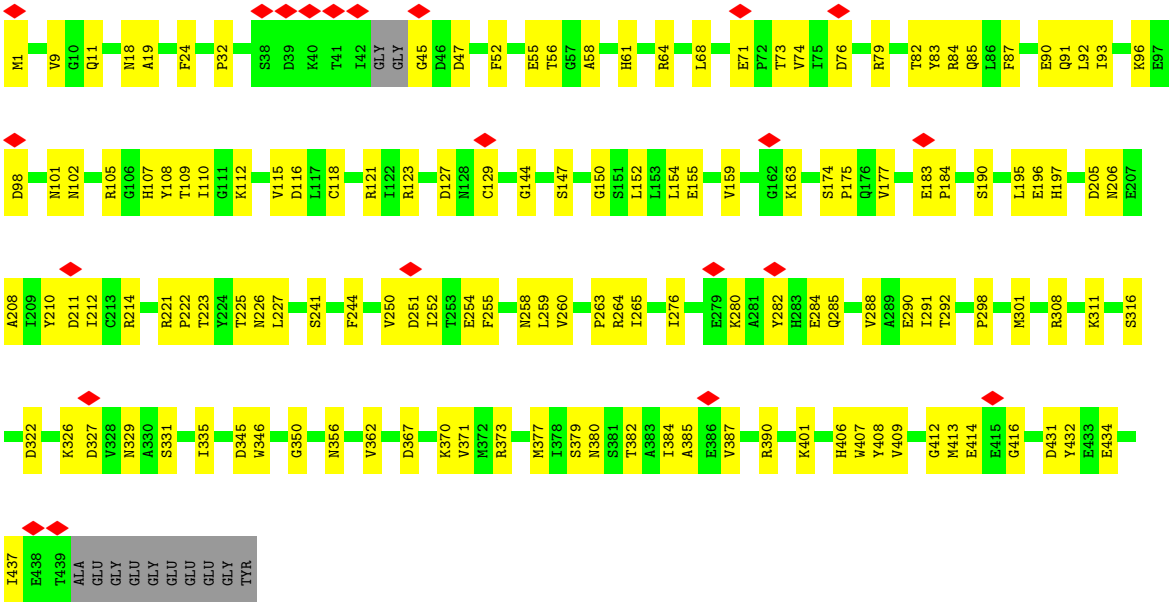




• Molecule 45: Tubulin alpha chain

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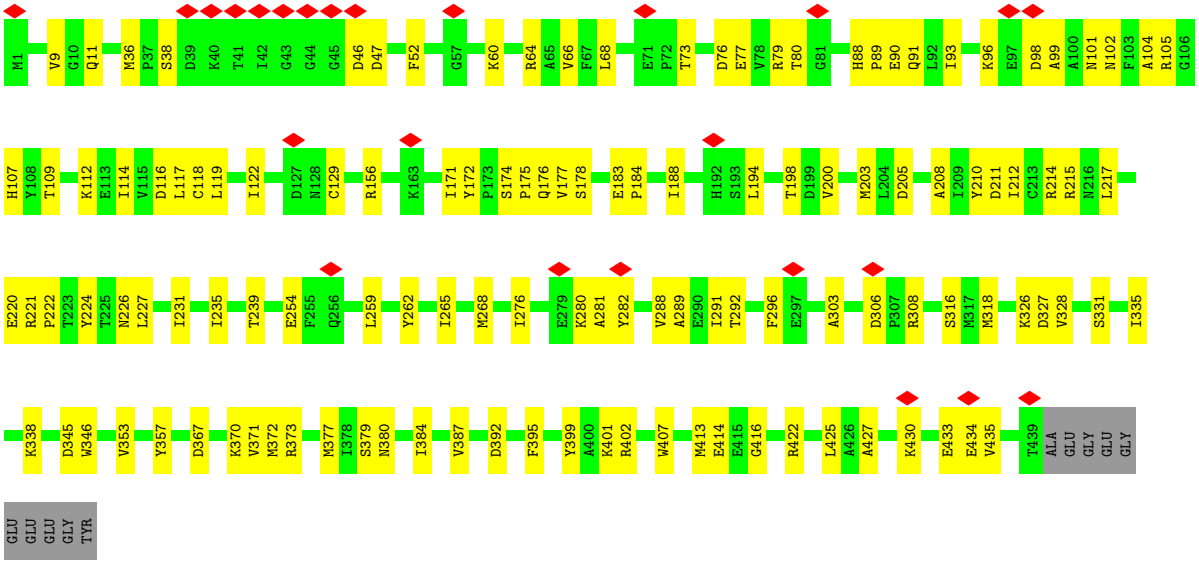




• Molecule 45: Tubulin alpha chain

Chain MI:

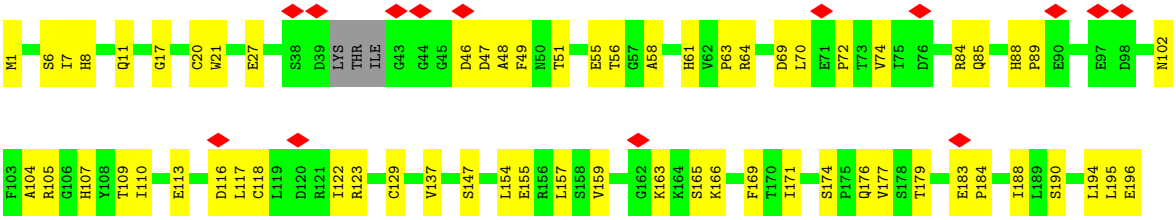


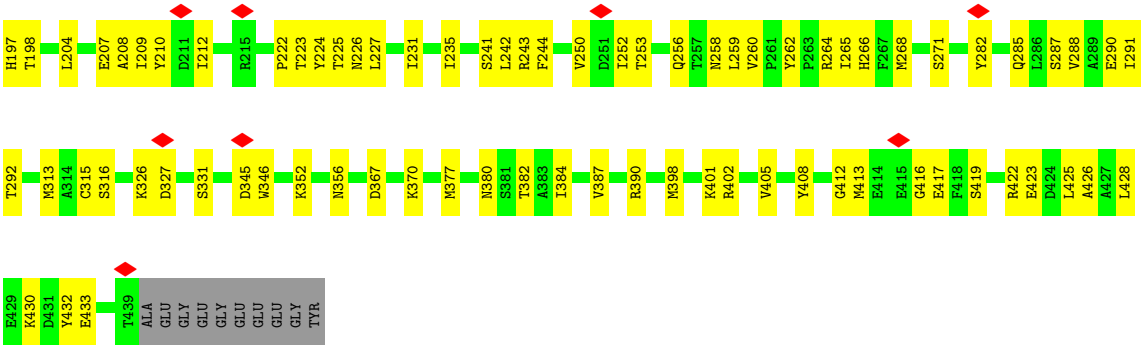


• Molecule 45: Tubulin alpha chain

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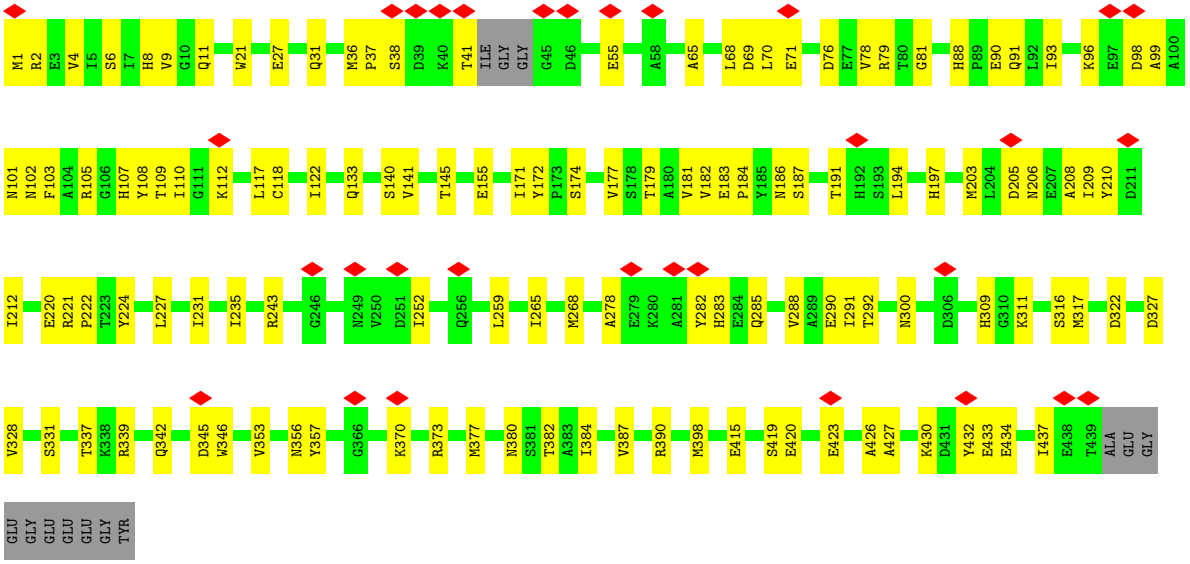




• Molecule 45: Tubulin alpha chain

Chain MM:

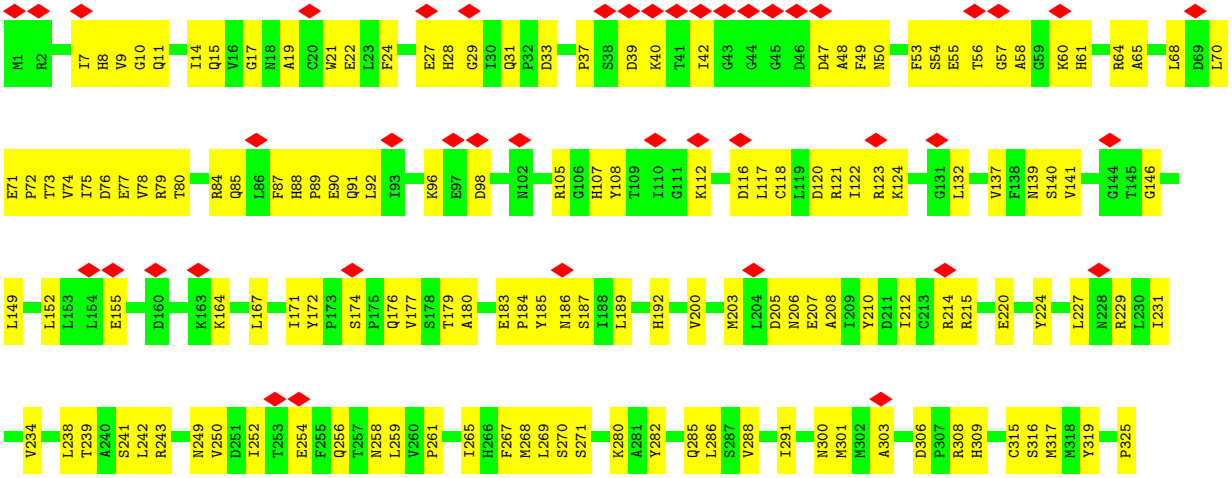


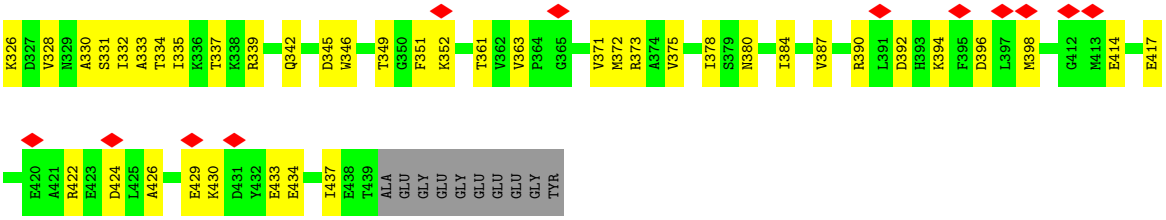


• Molecule 45: Tubulin alpha chain

Chain NA:



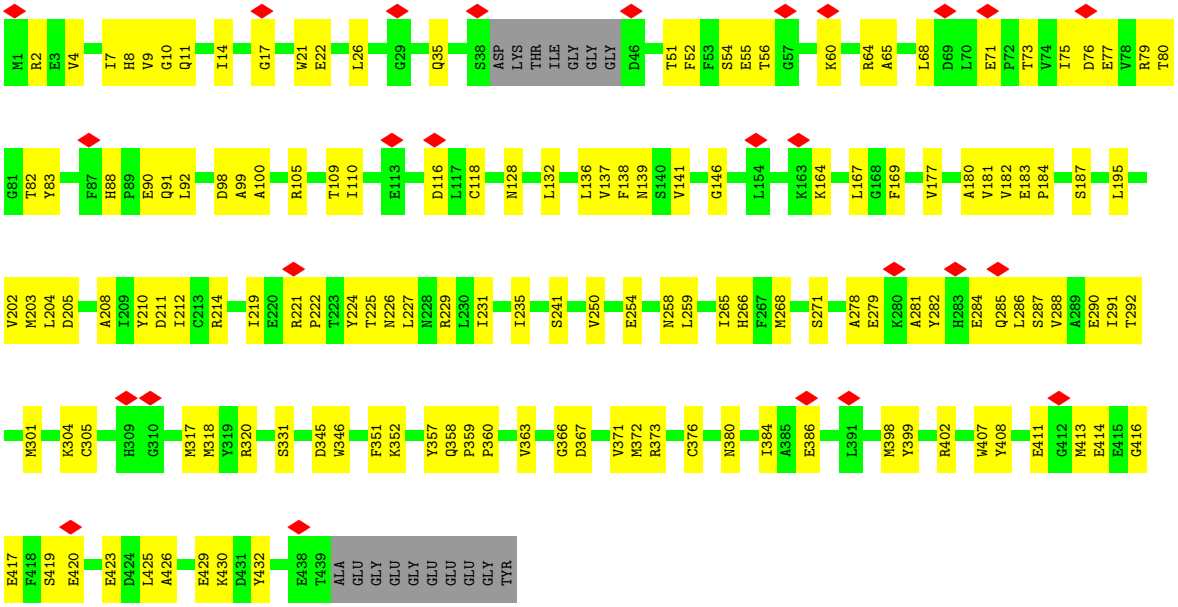




• Molecule 45: Tubulin alpha chain

Chain NC:

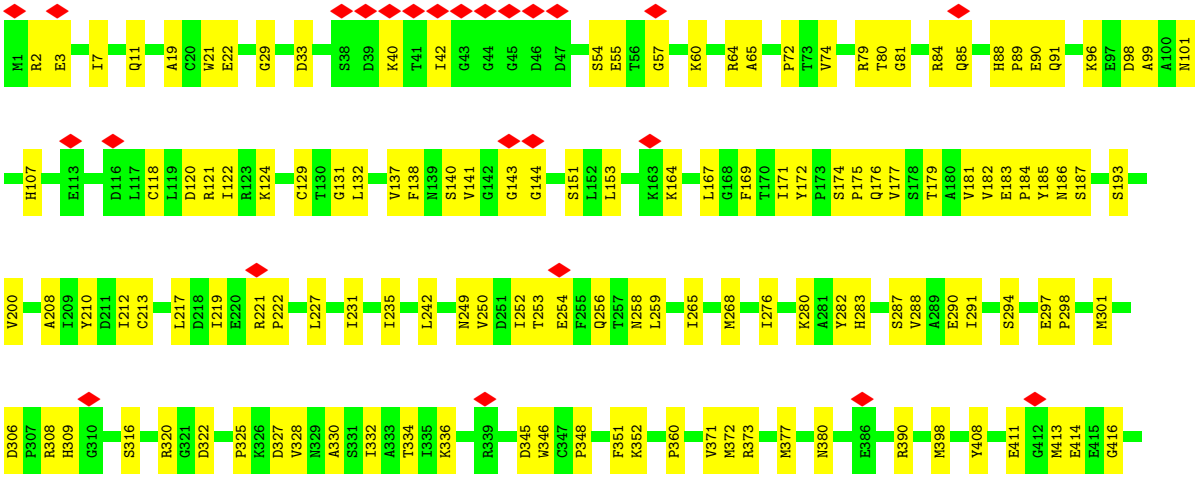


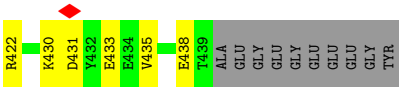


• Molecule 45: Tubulin alpha chain

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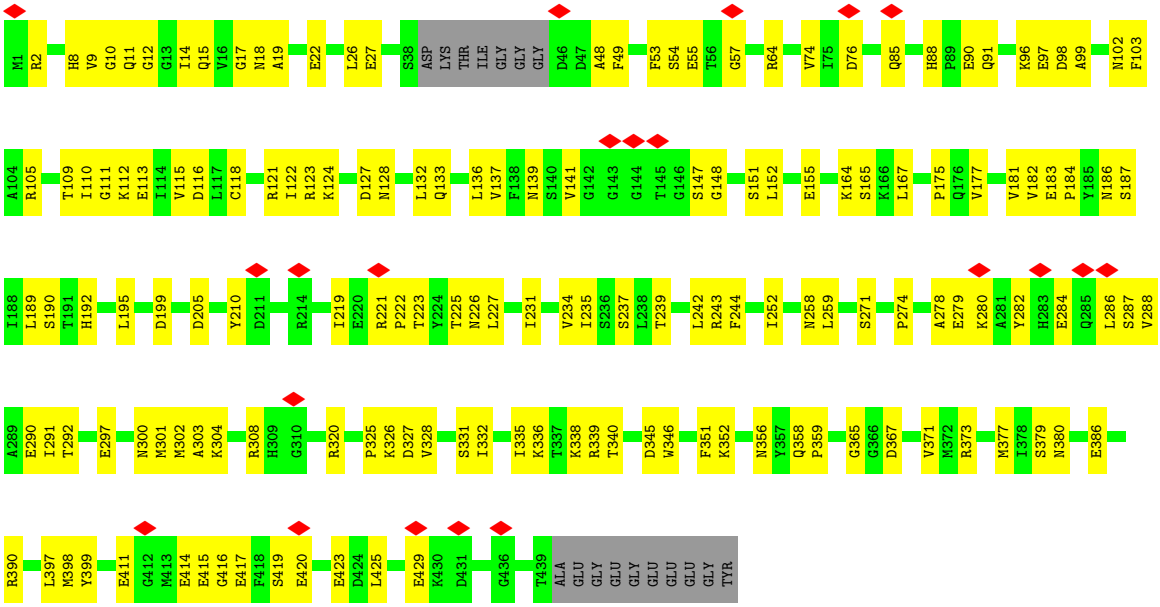




• Molecule 45: Tubulin alpha chain

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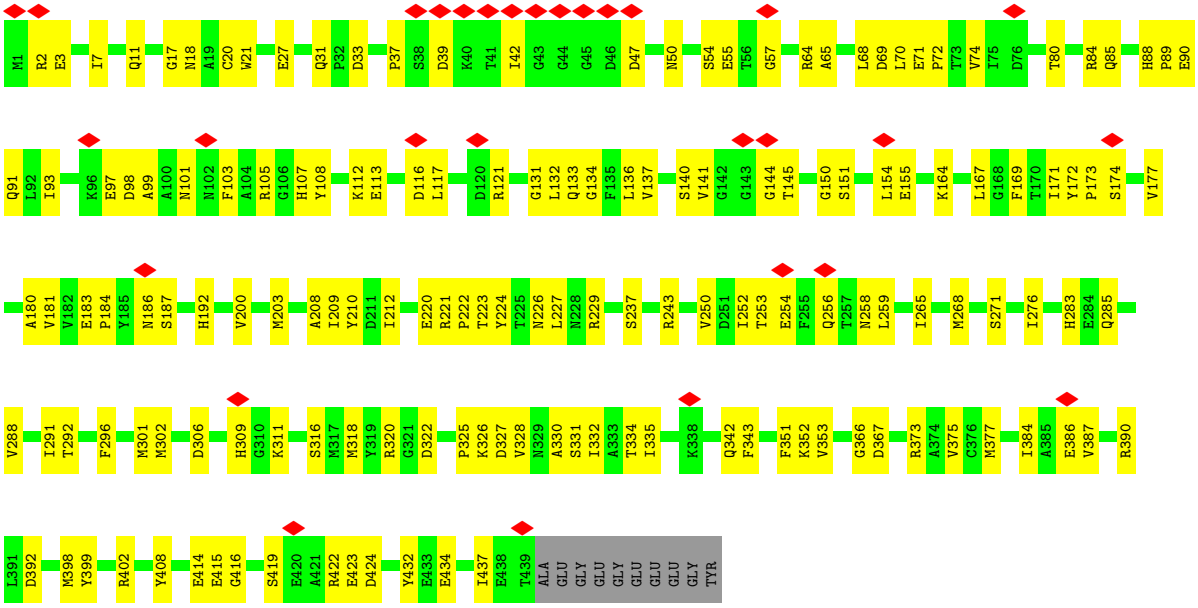




• Molecule 45: Tubulin alpha chain

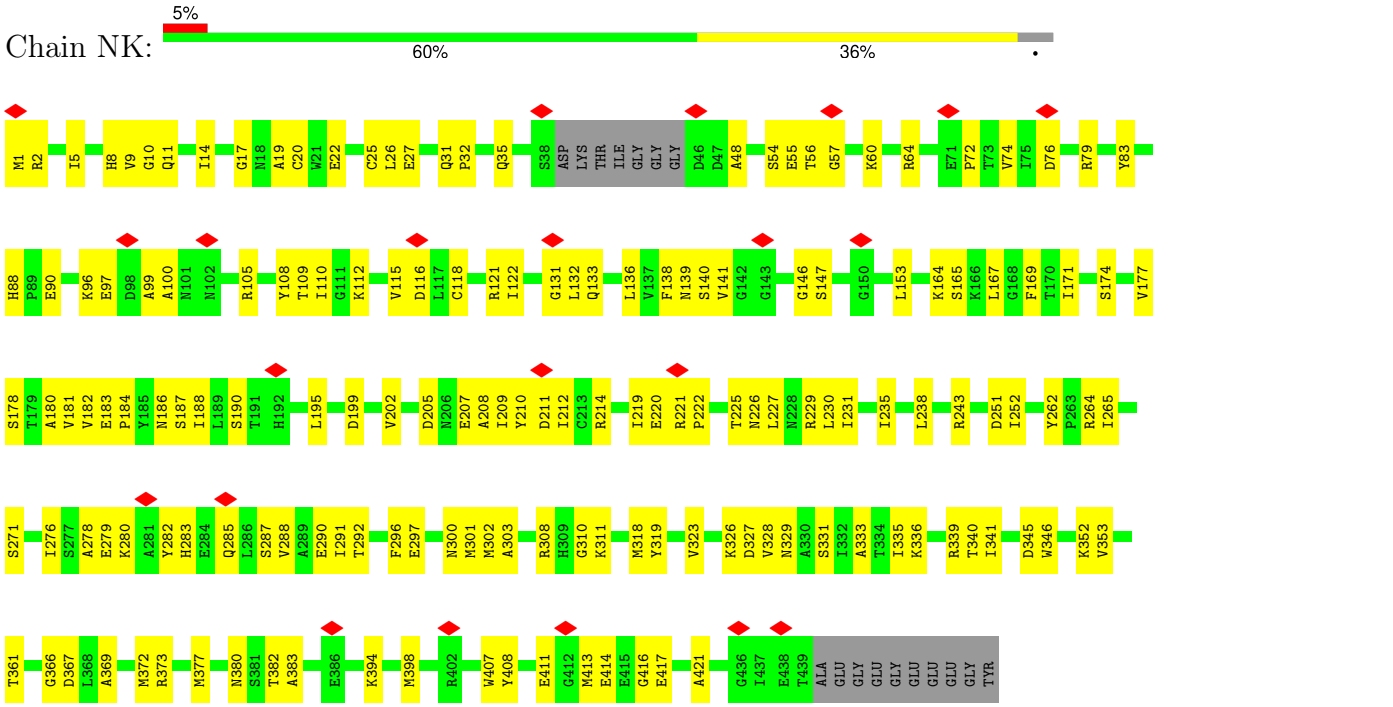
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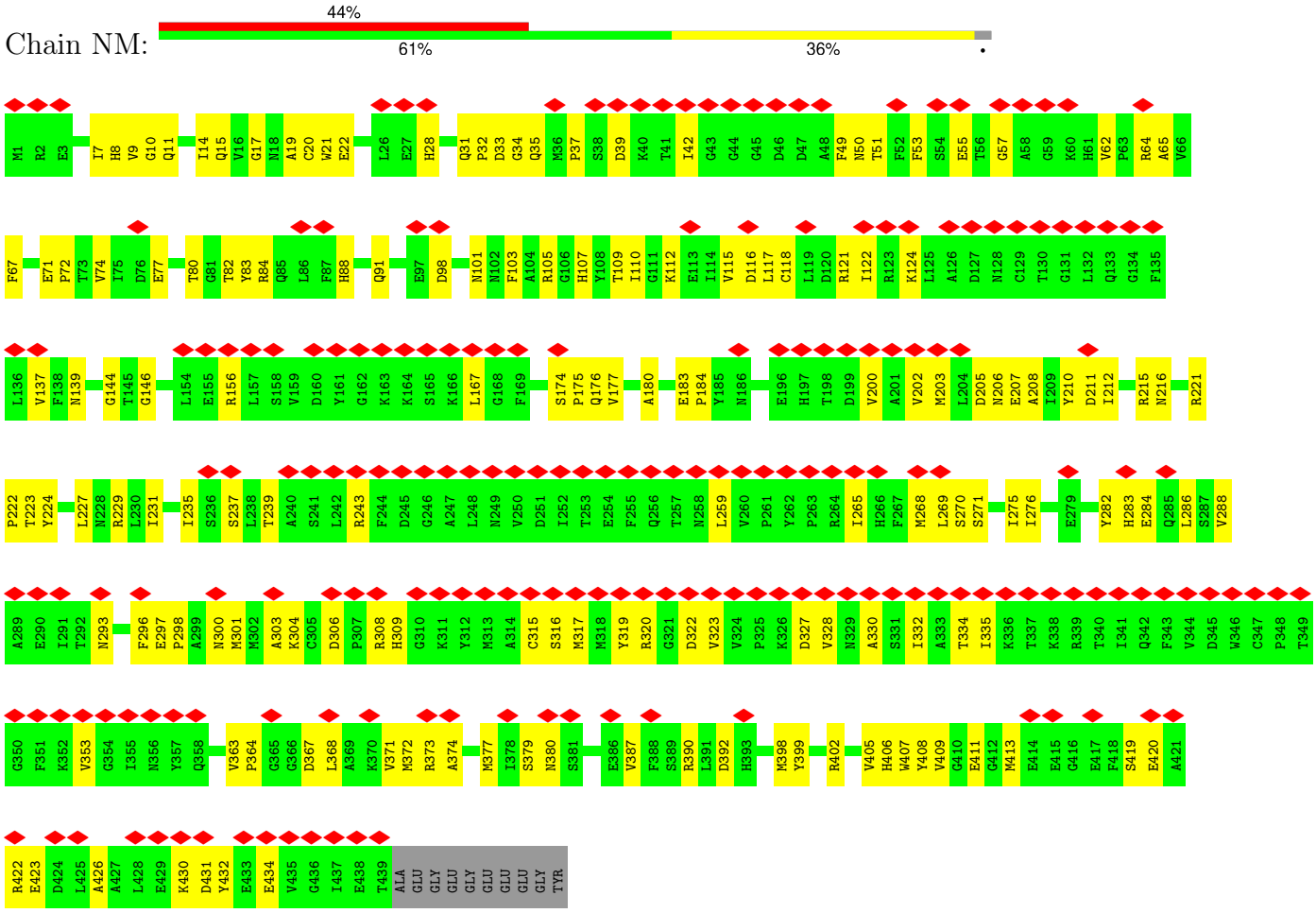
• Molecule 45: Tubulin alpha chain

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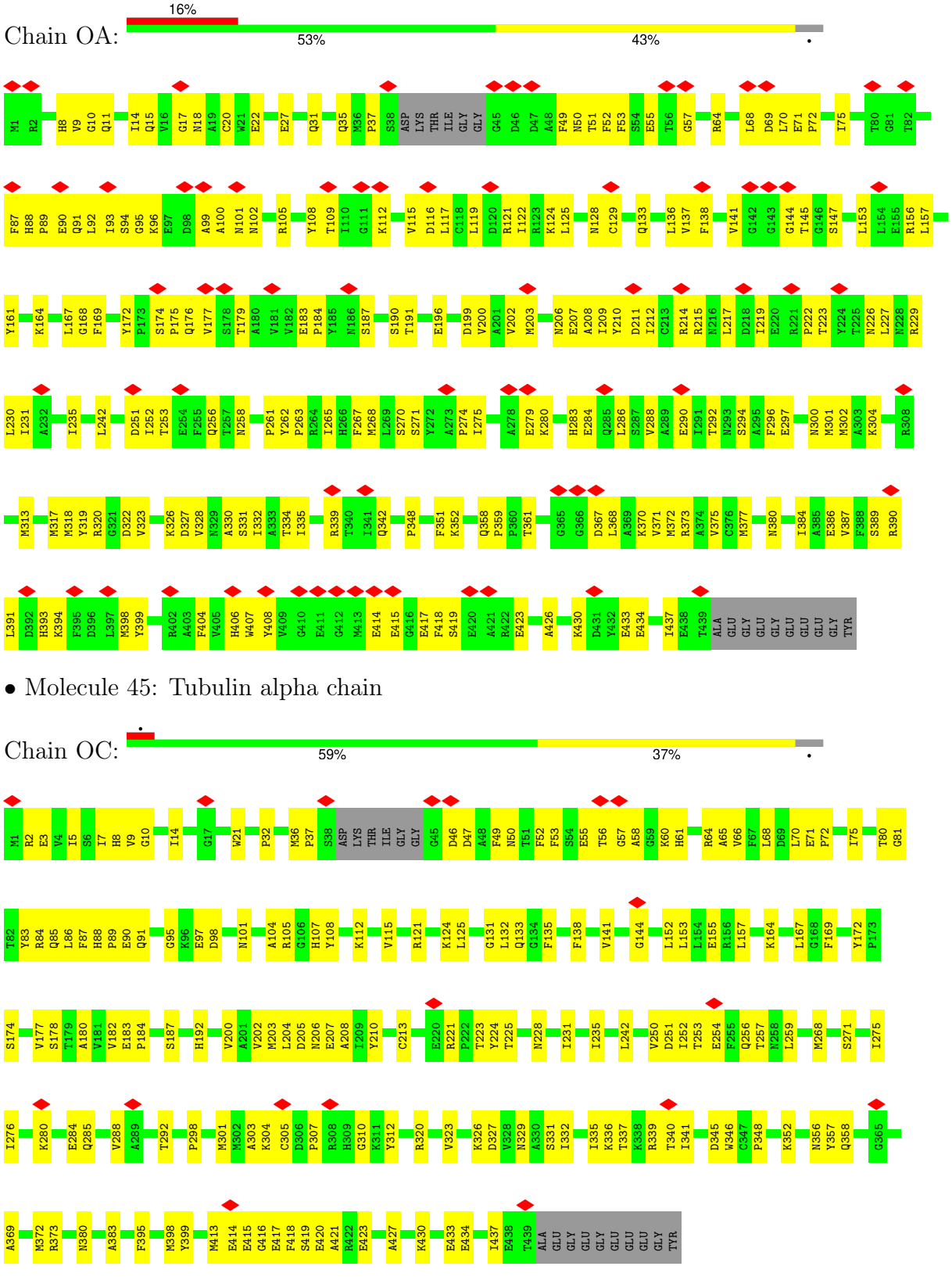
• Molecule 45: Tubulin alpha chain

Chain NM:



• Molecule 45: Tubulin alpha chain

Chain OA:

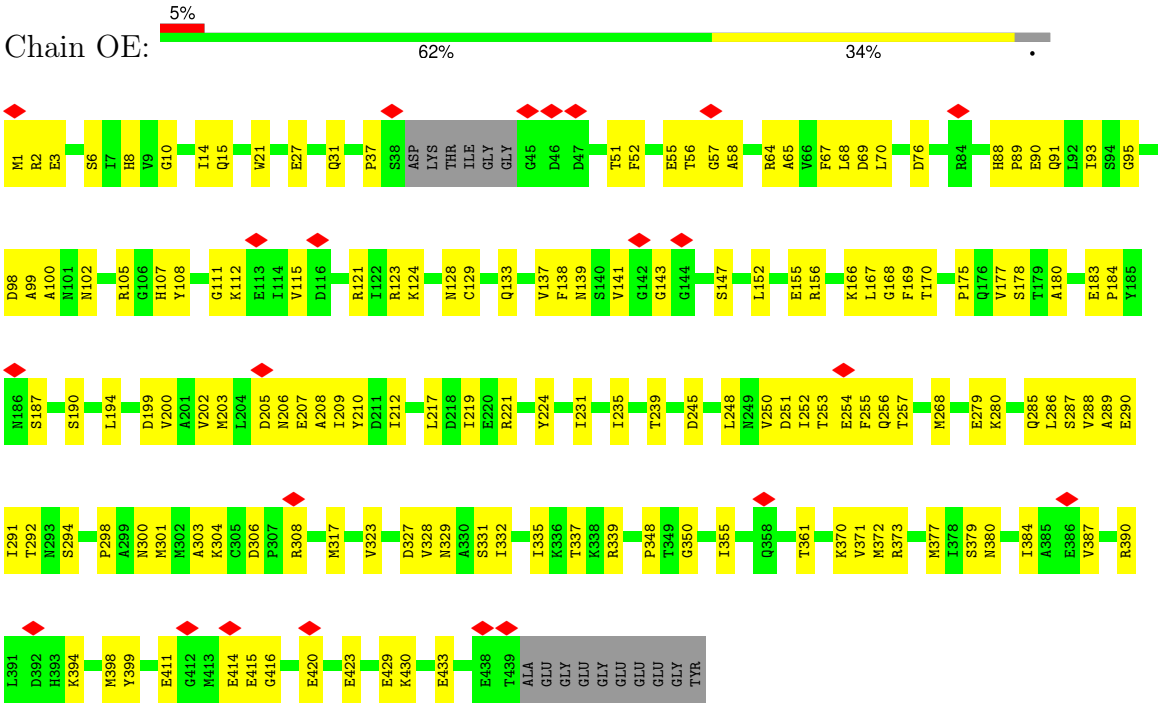


• Molecule 45: Tubulin alpha chain

Chain OC:

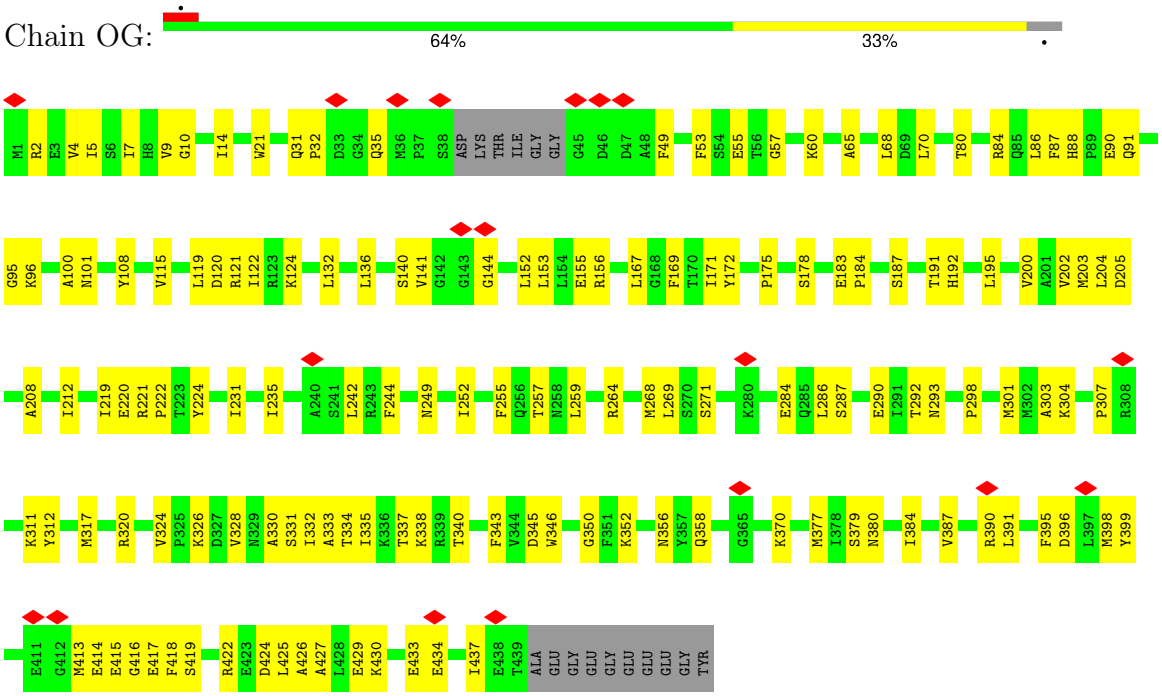
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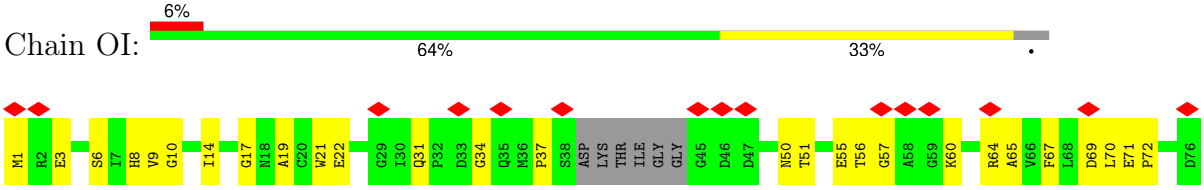
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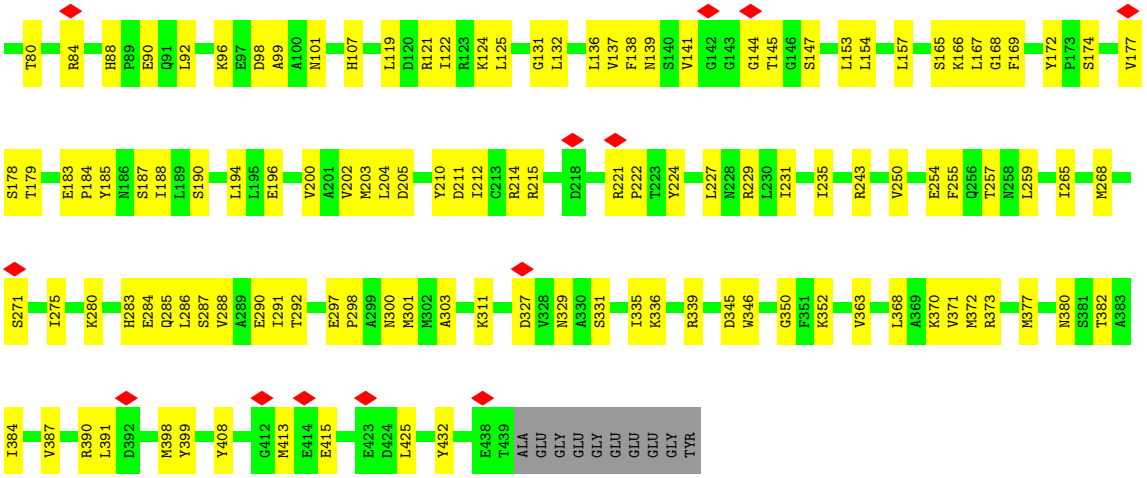
Chain OG:



• Molecule 45: Tubulin alpha chain

Chain OI:

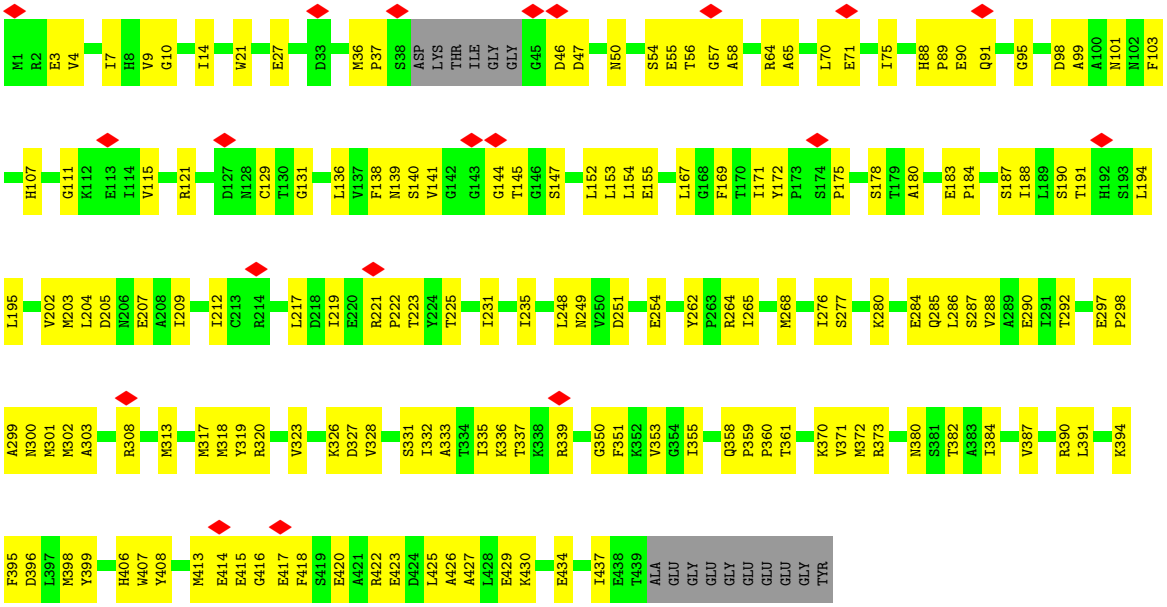




• Molecule 45: Tubulin alpha chain

Chain OK:

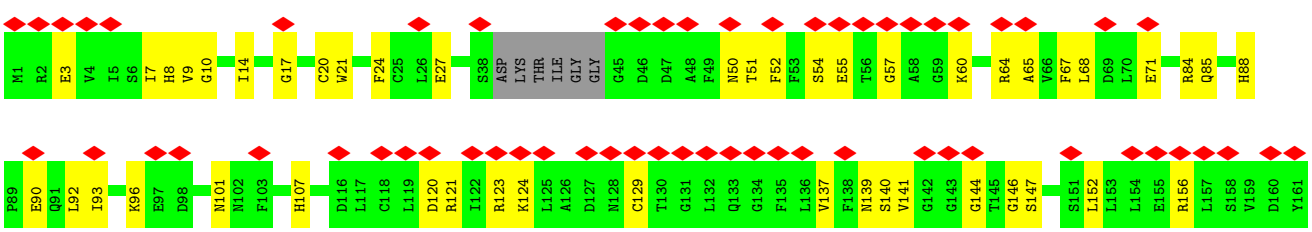


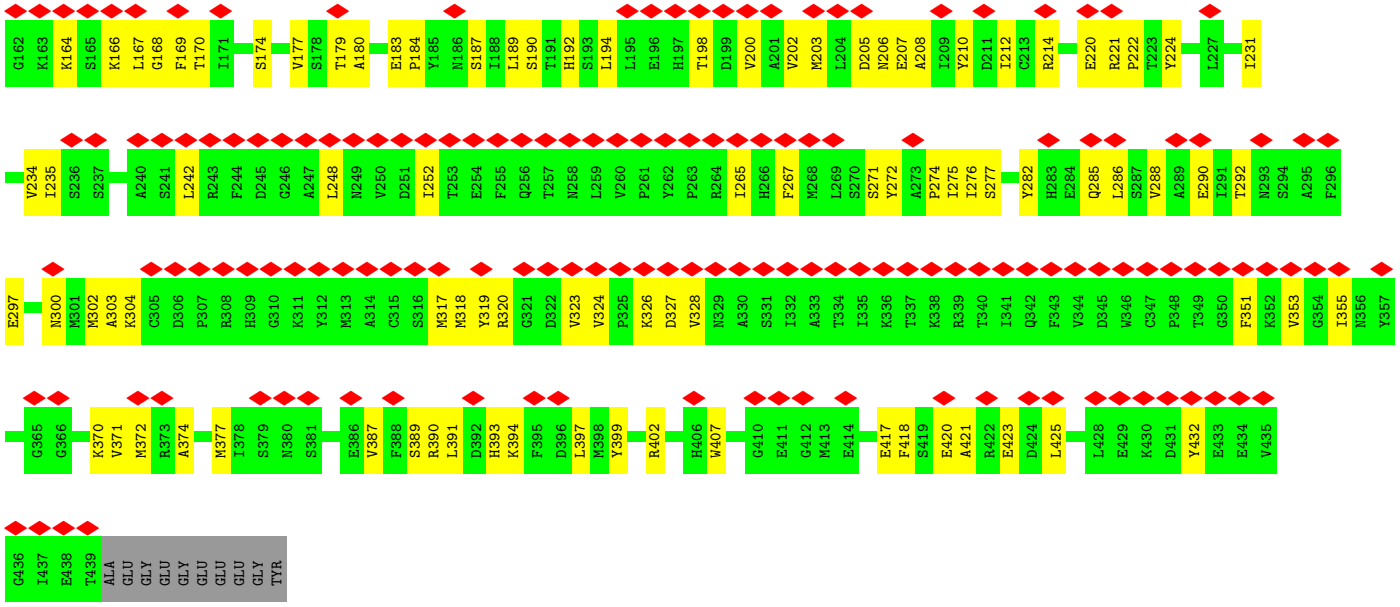


• Molecule 45: Tubulin alpha chain

Chain OM:



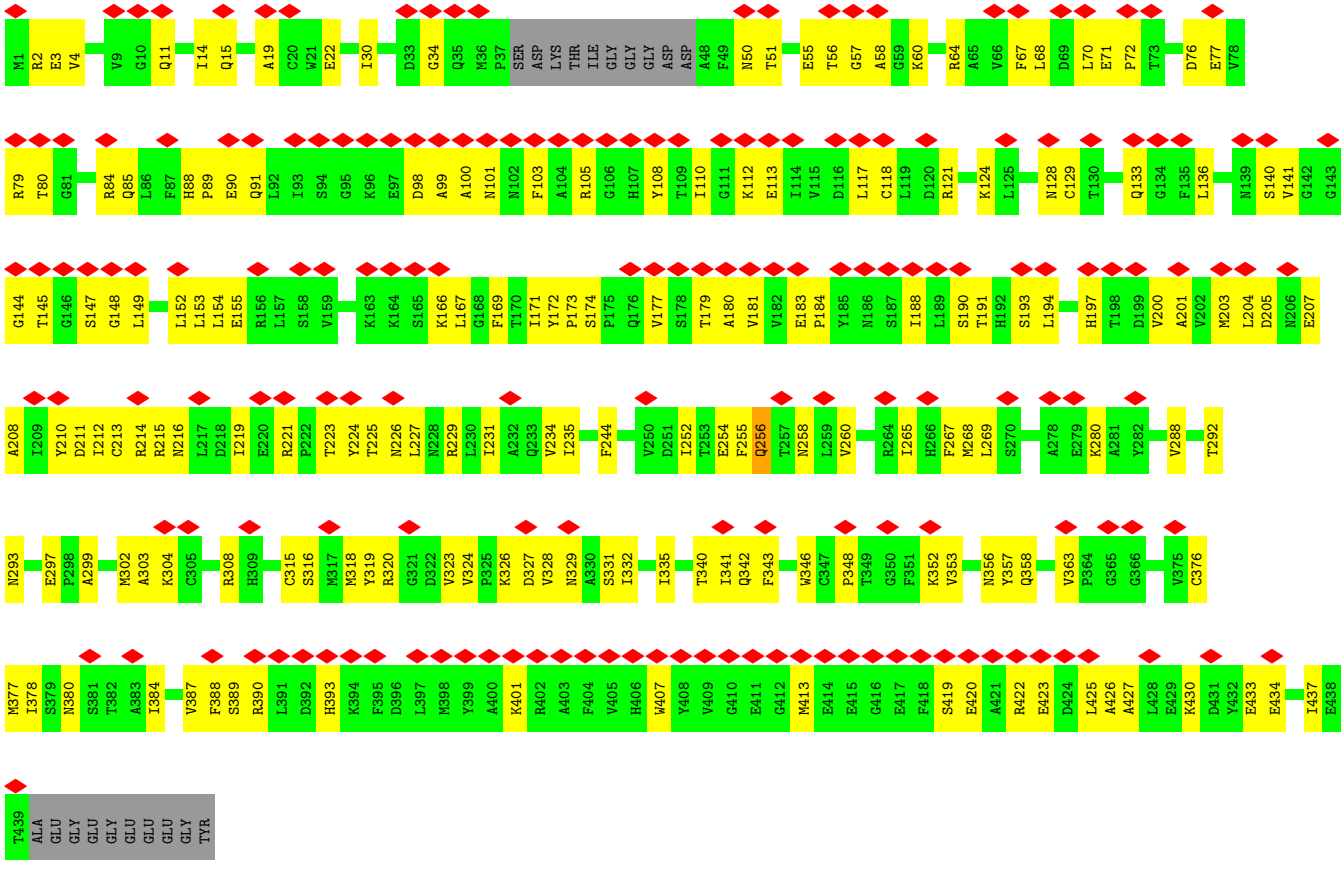




• Molecule 45: Tubulin alpha chain

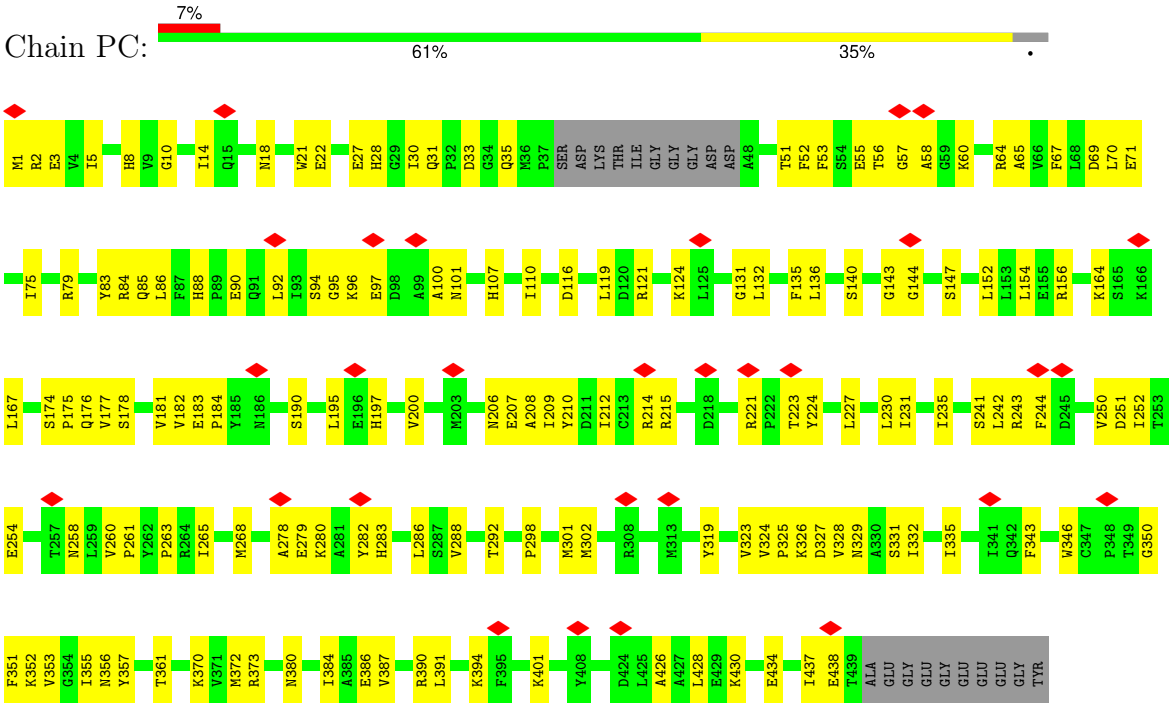
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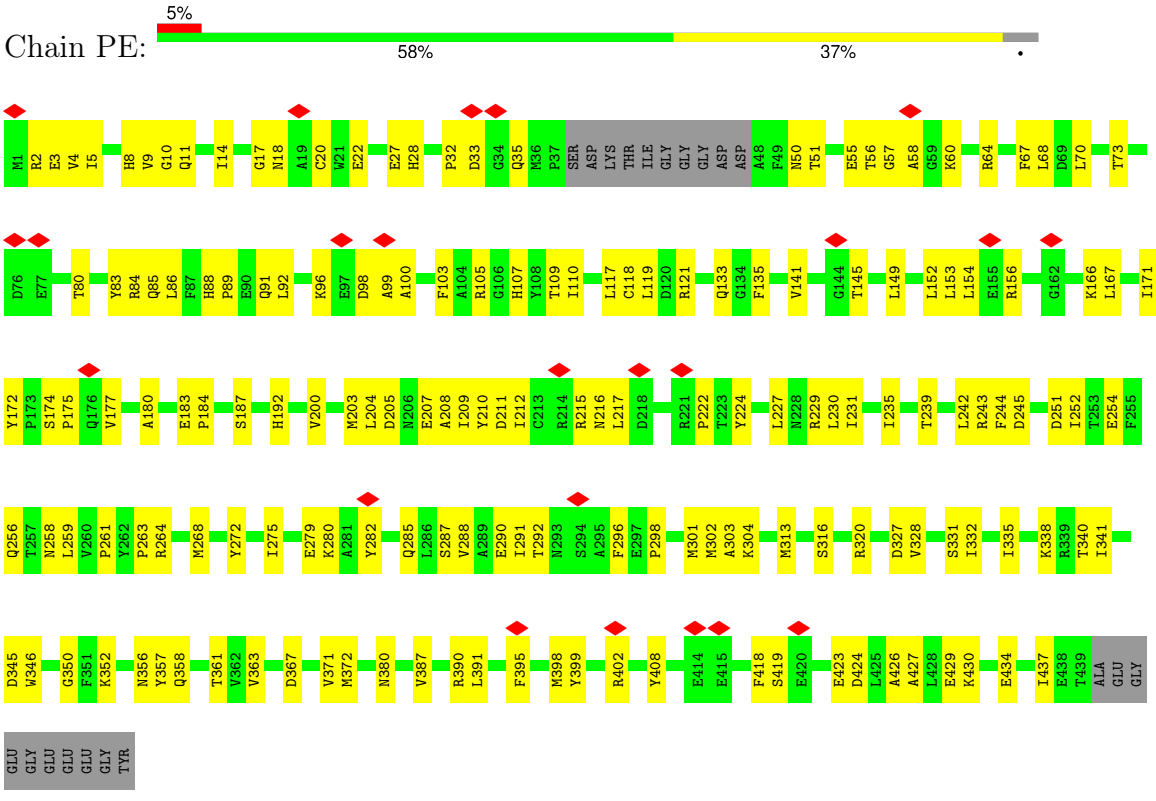
• Molecule 45: Tubulin alpha chain

Chain PC:



• Molecule 45: Tubulin alpha chain

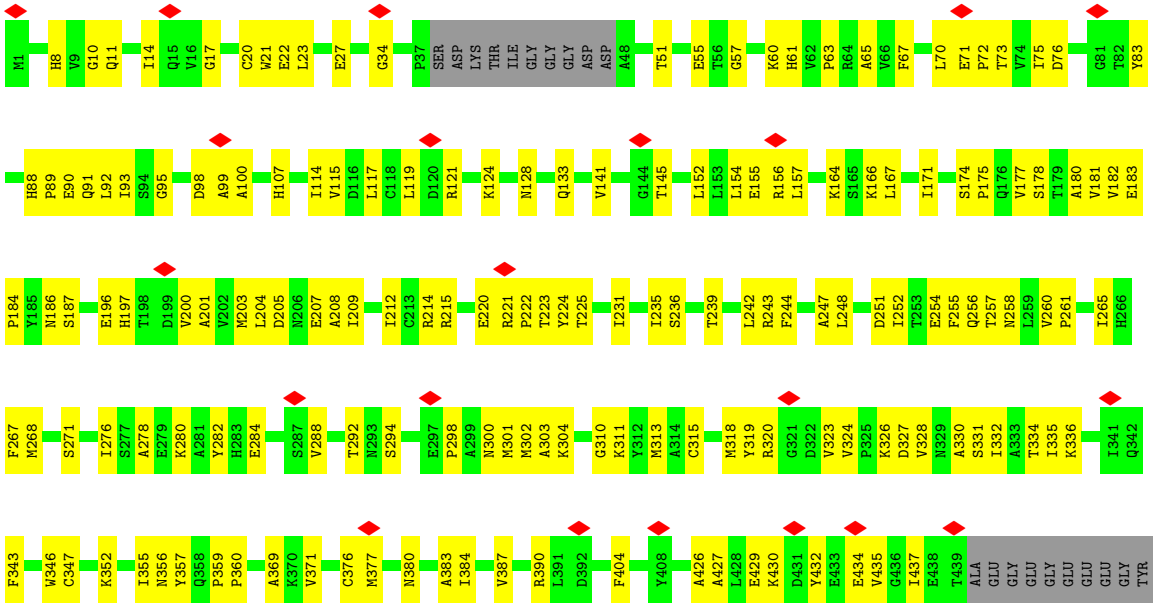
Chain PE:



• Molecule 45: Tubulin alpha chain

Chain PG:

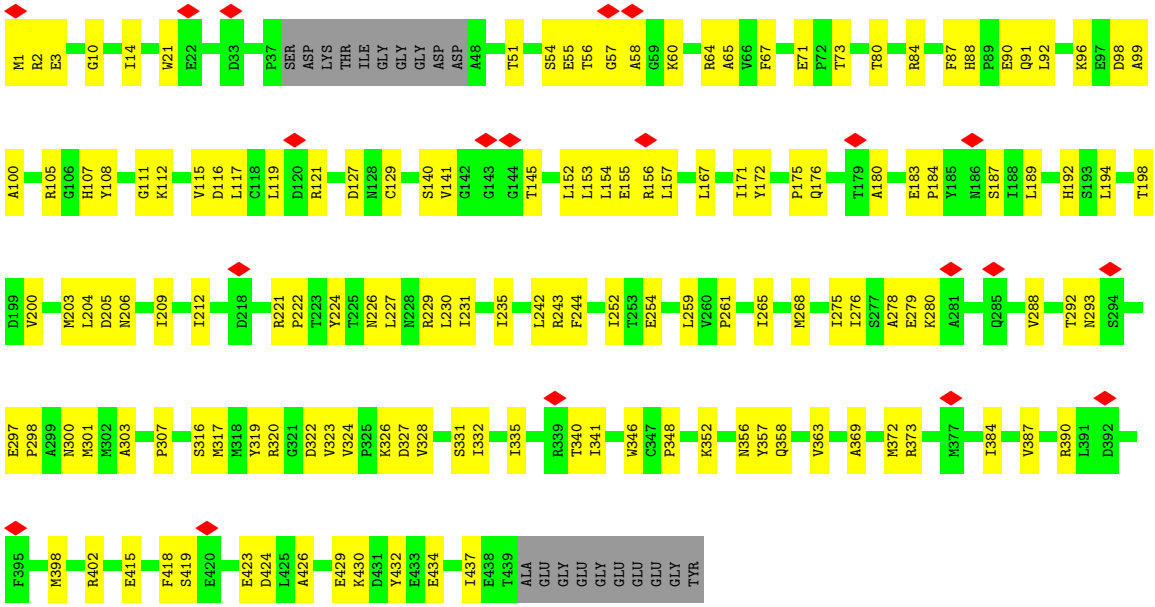




• Molecule 45: Tubulin alpha chain

Chain PI:

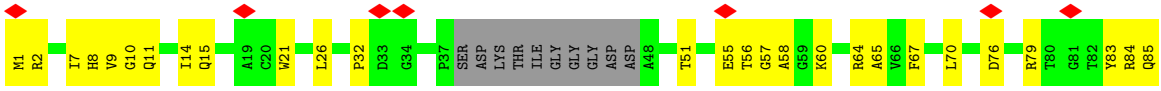


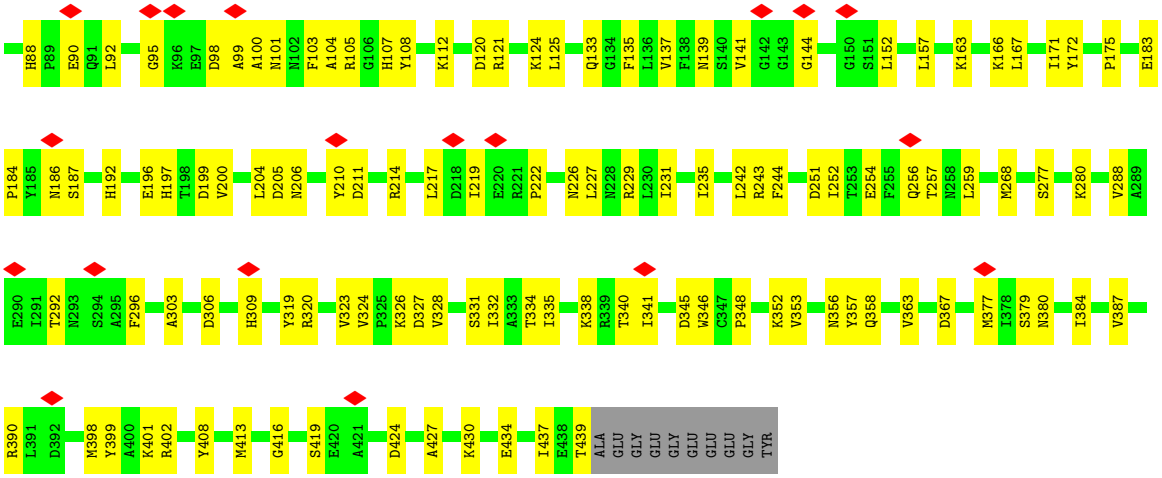


• Molecule 45: Tubulin alpha chain

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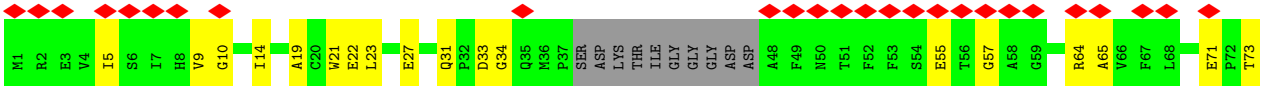


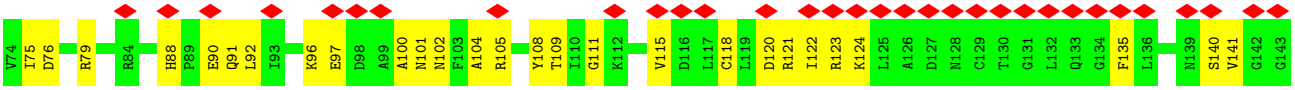


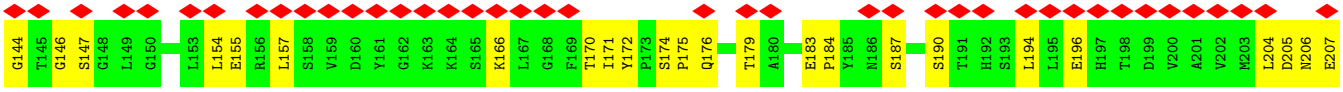
• Molecule 45: Tubulin alpha chain

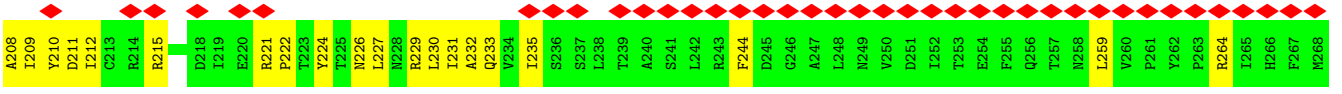
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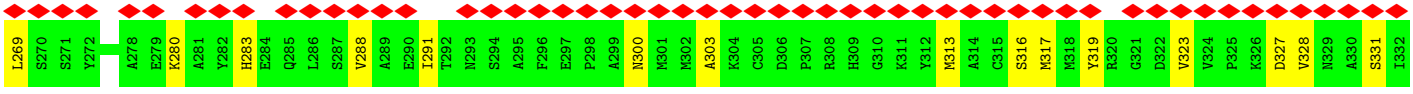


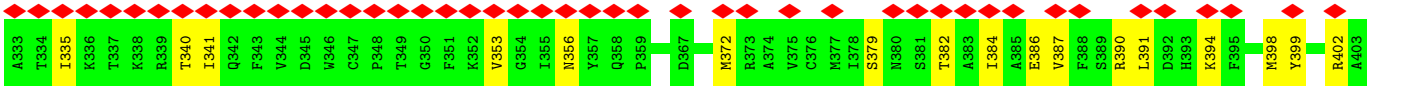


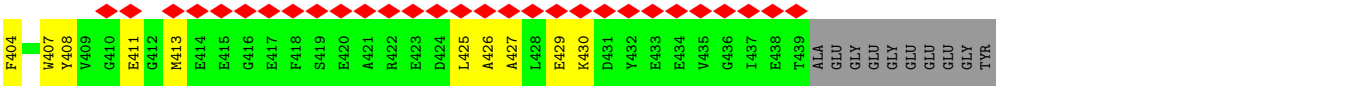








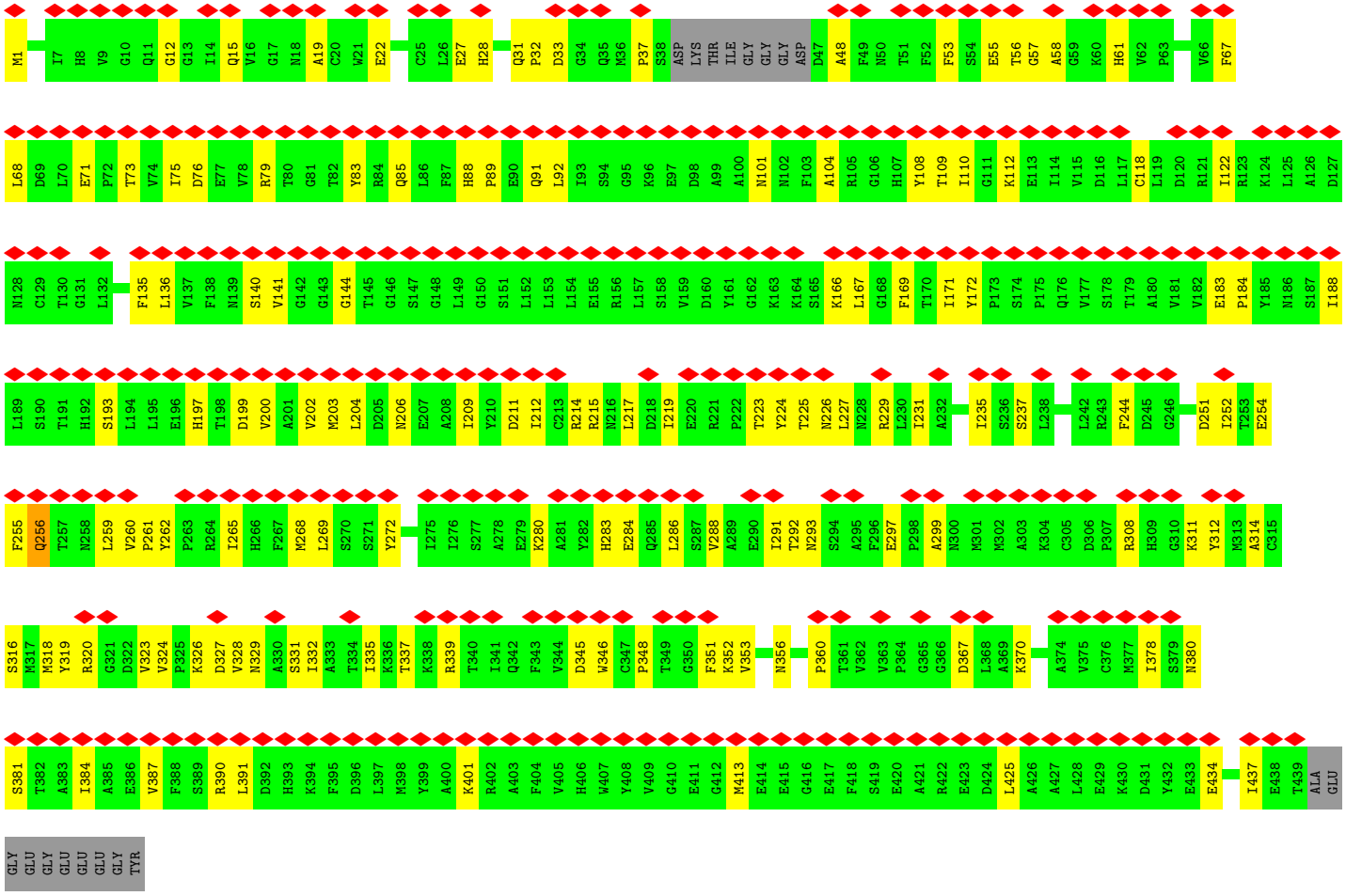




• Molecule 45: Tubulin alpha chain

Chain QA:

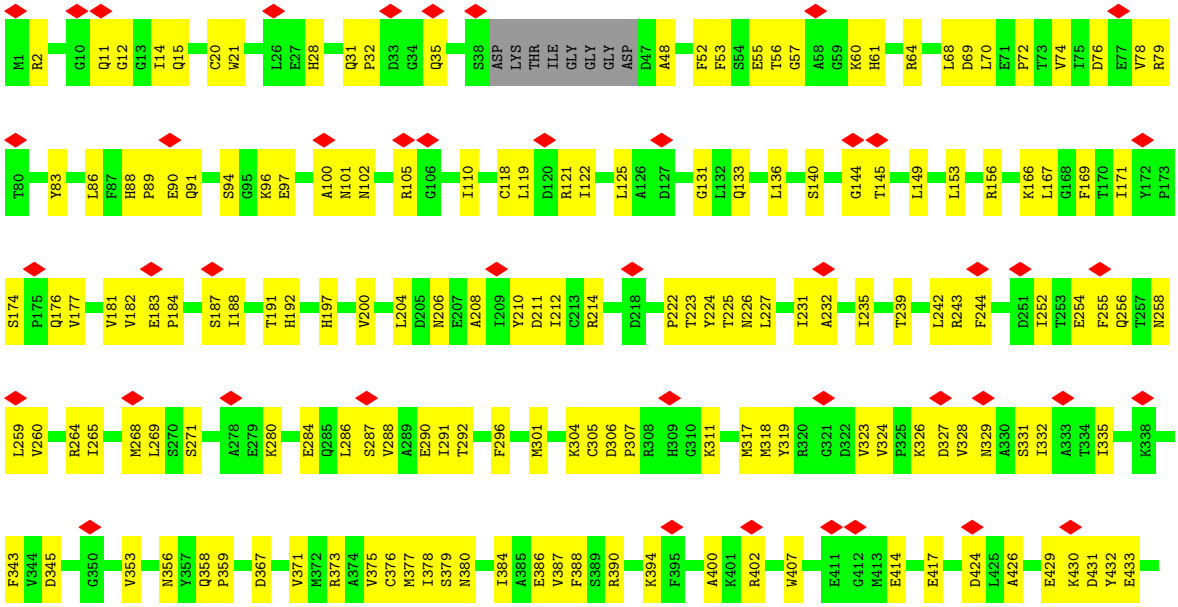


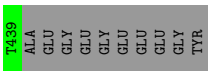


• Molecule 45: Tubulin alpha chain

Chain QC:



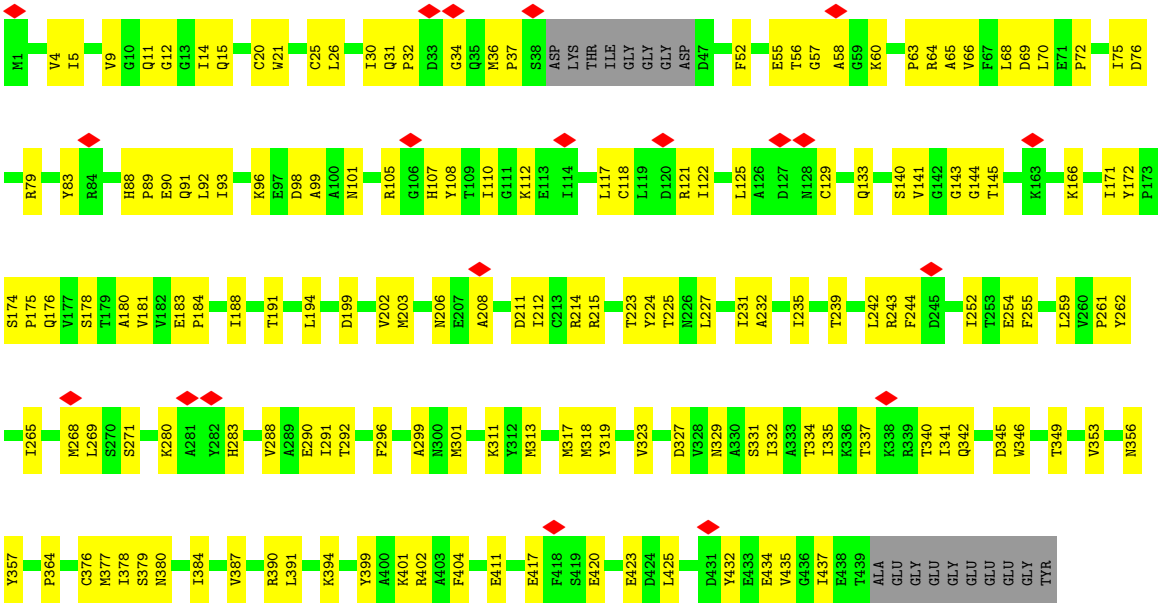




• Molecule 45: Tubulin alpha chain

Chain QE:

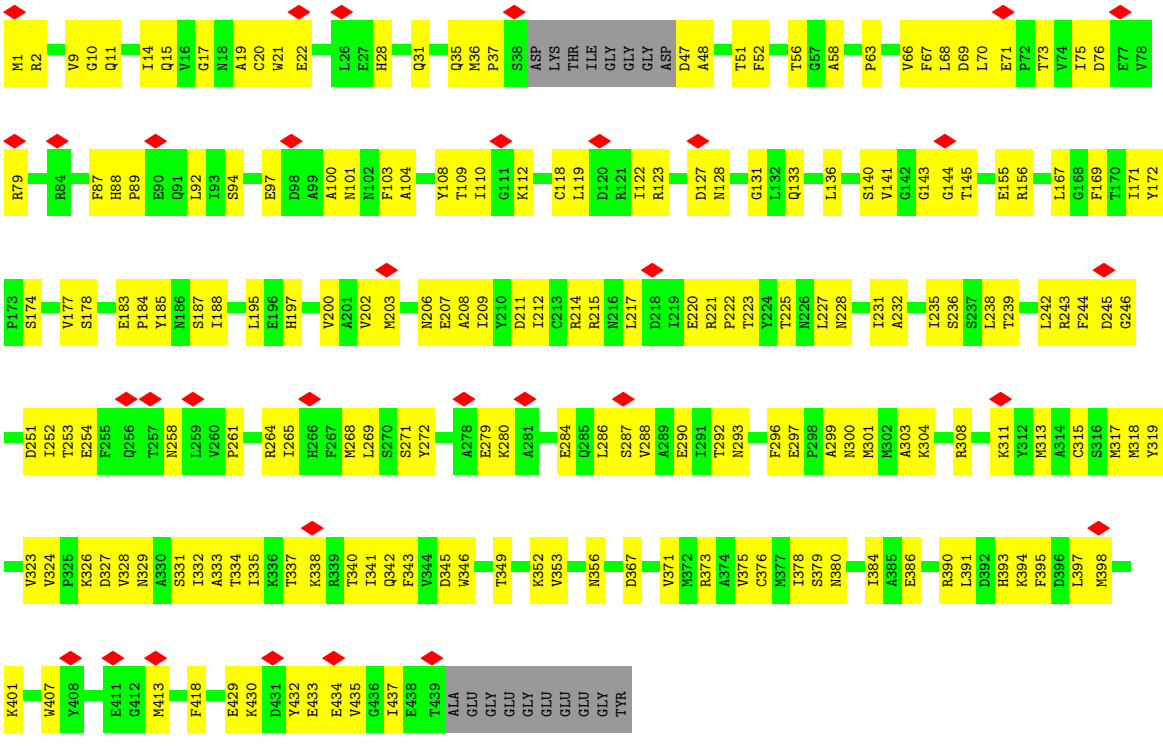




• Molecule 45: Tubulin alpha chain

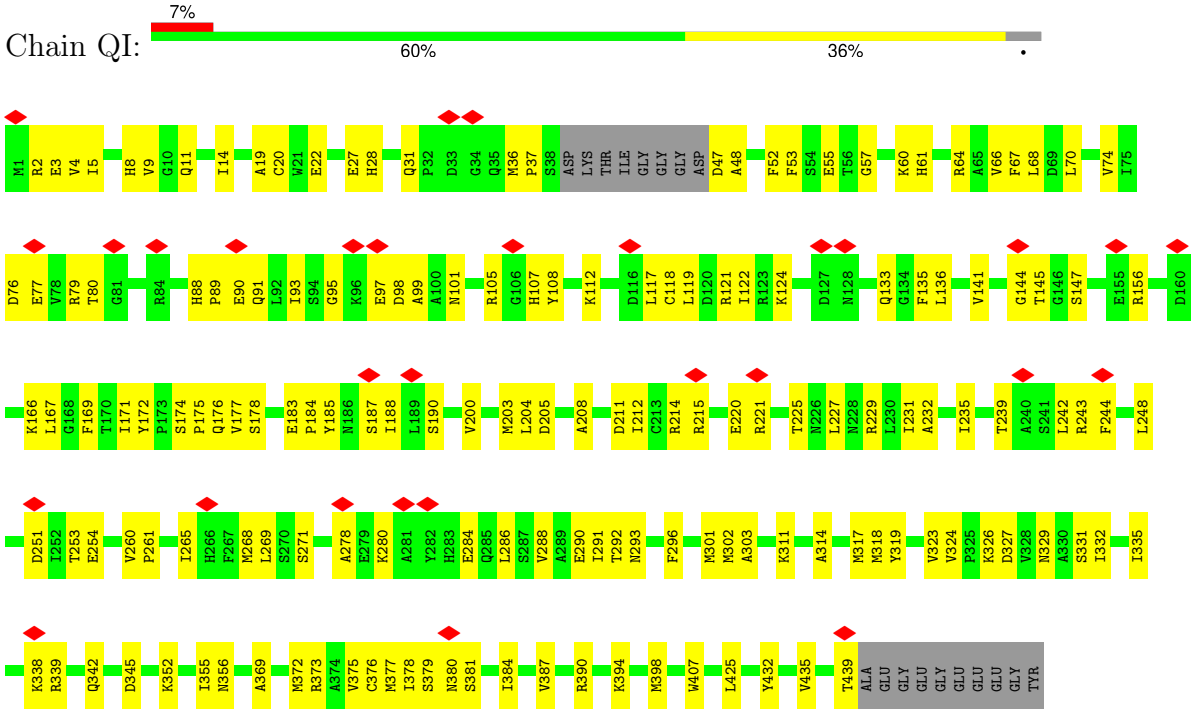
Chain QG:





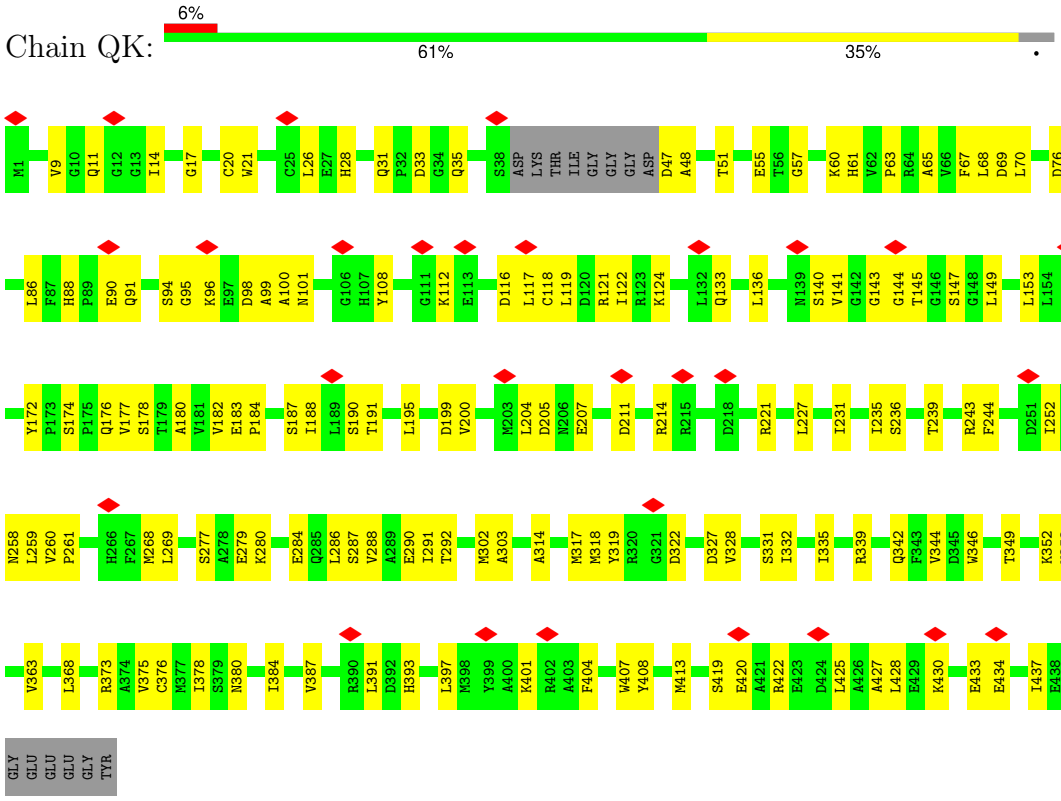
• Molecule 45: Tubulin alpha chain

Chain QI:



• Molecule 45: Tubulin alpha chain

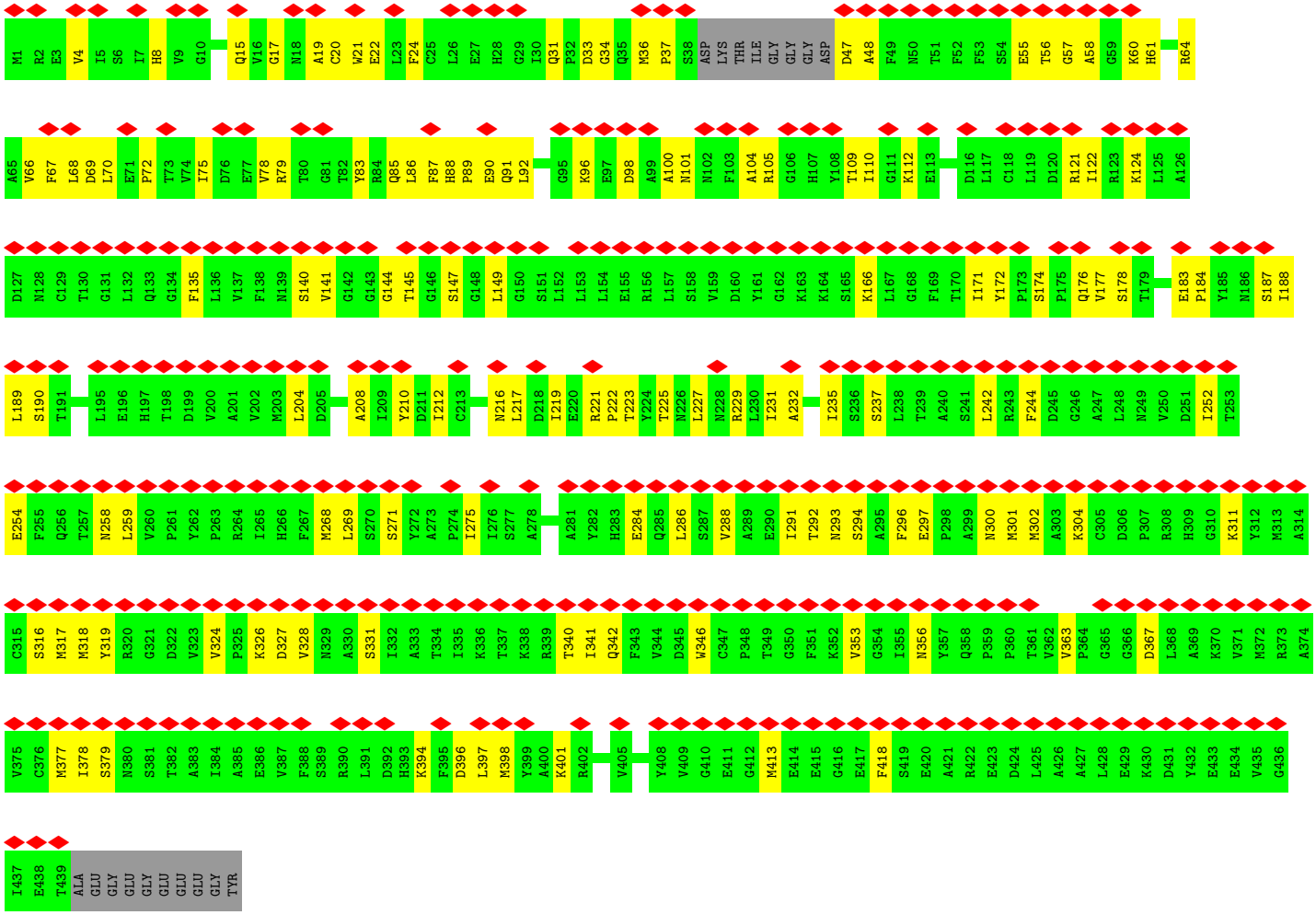
Chain QK:



• Molecule 45: Tubulin alpha chain

Chain QM:

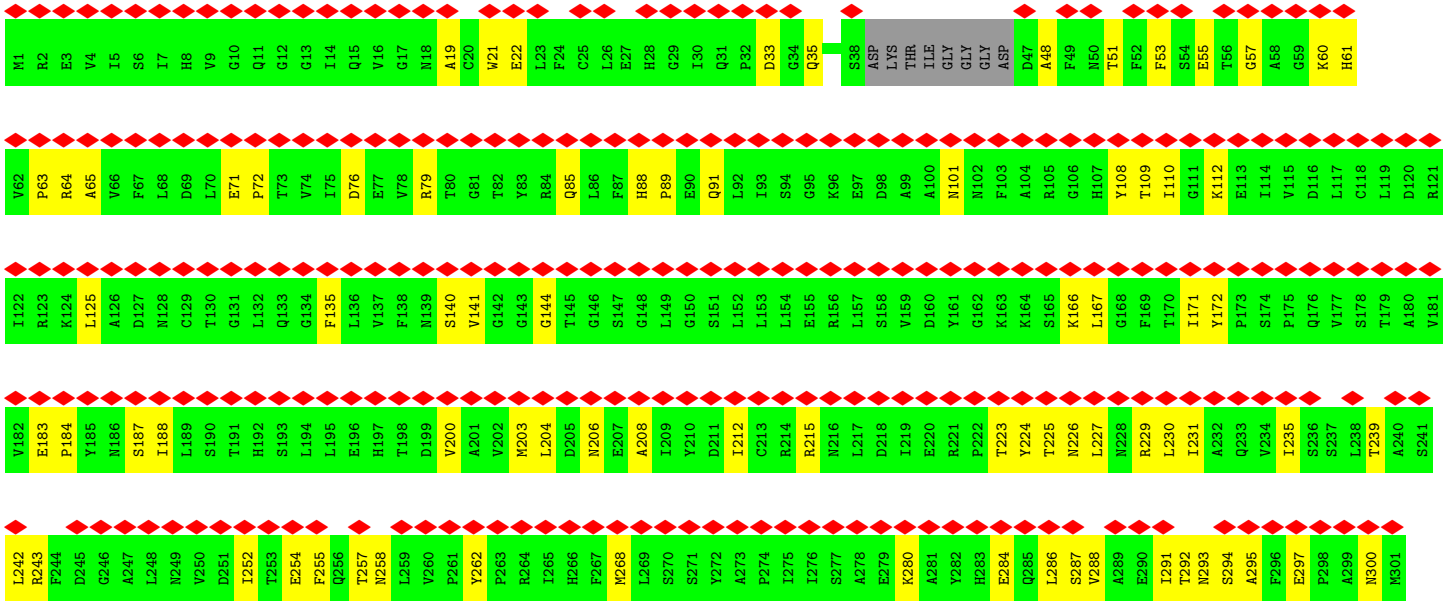


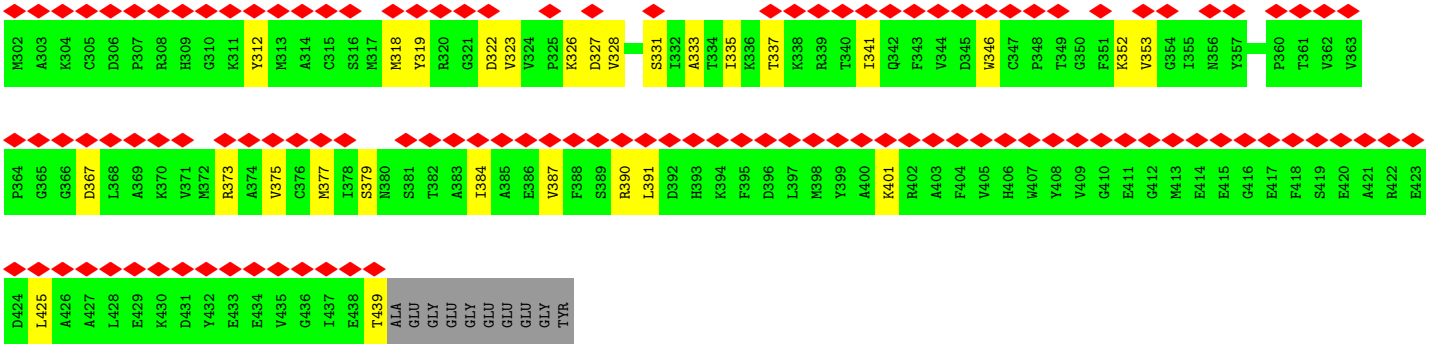


• Molecule 45: Tubulin alpha chain

Chain RA:



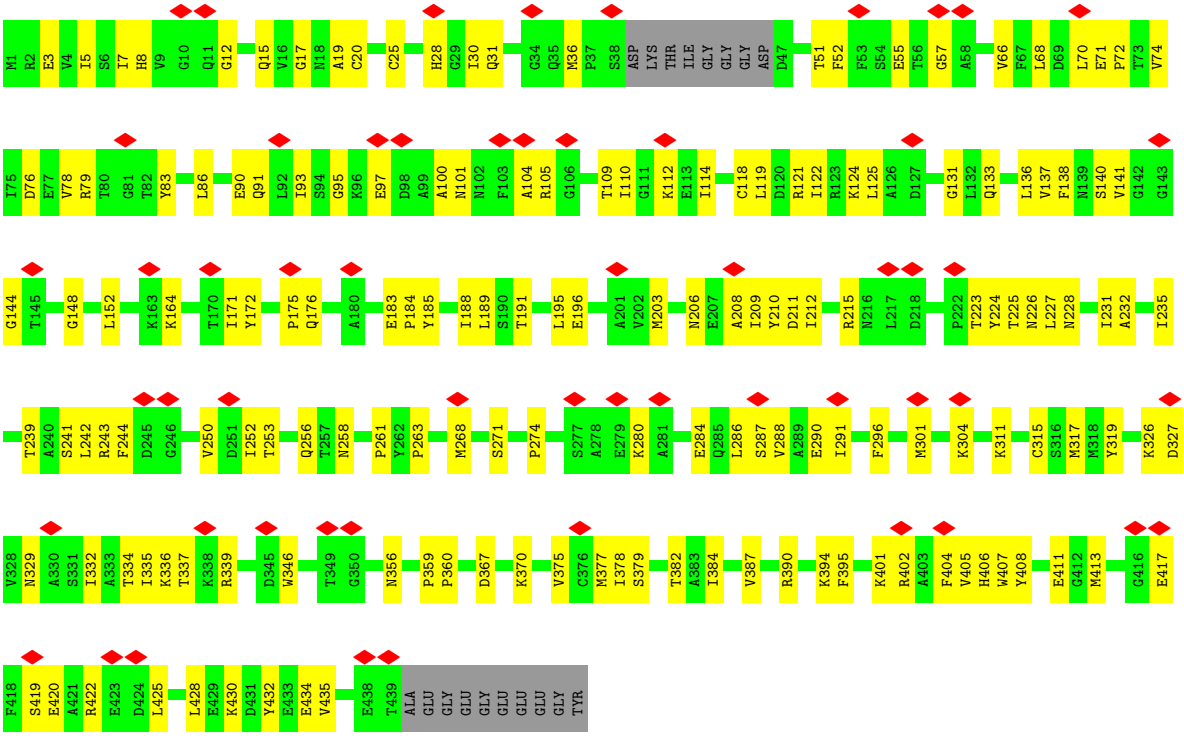




• Molecule 45: Tubulin alpha chain

Chain RC:

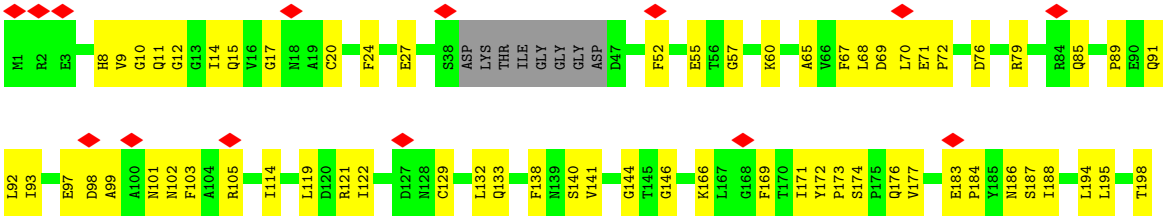


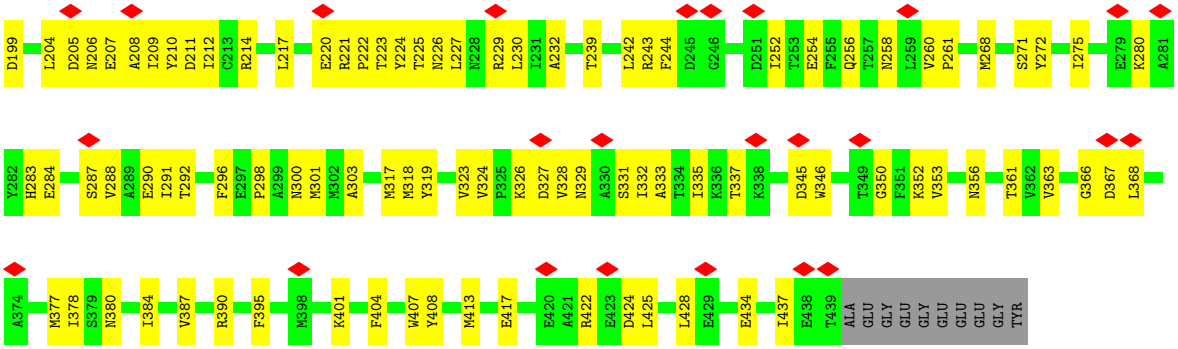


• Molecule 45: Tubulin alpha chain

Chain RE:



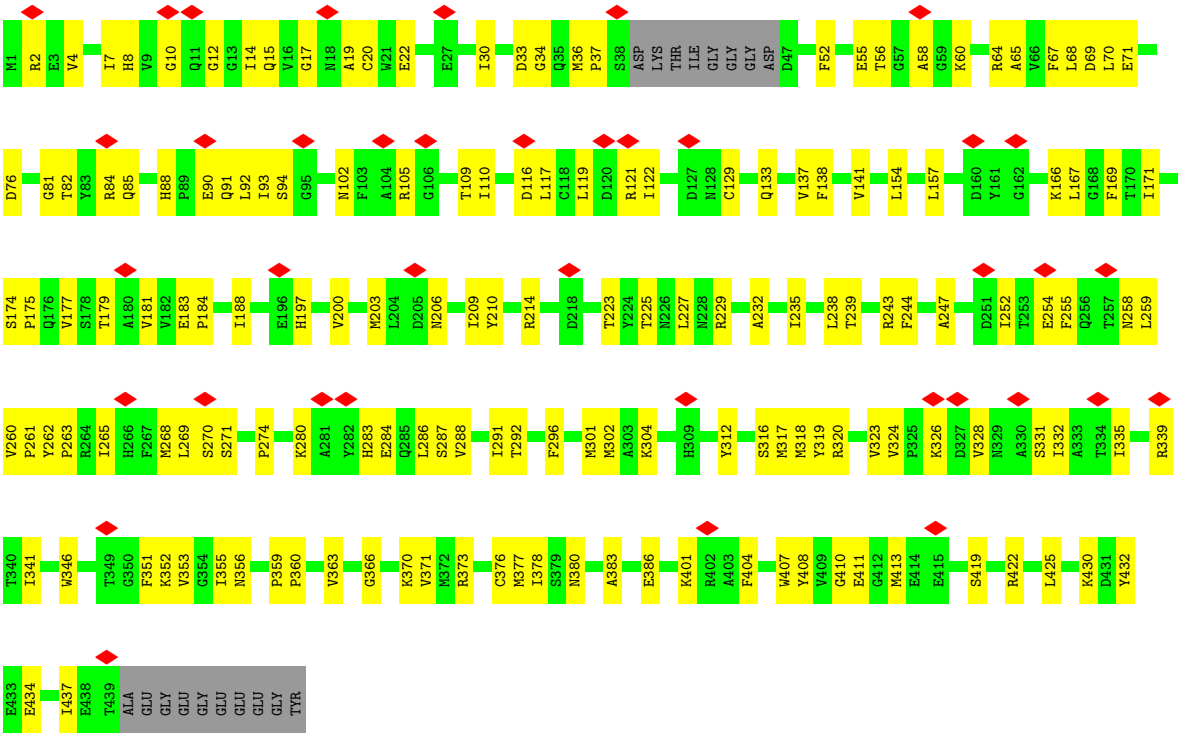




• Molecule 45: Tubulin alpha chain

Chain RG:

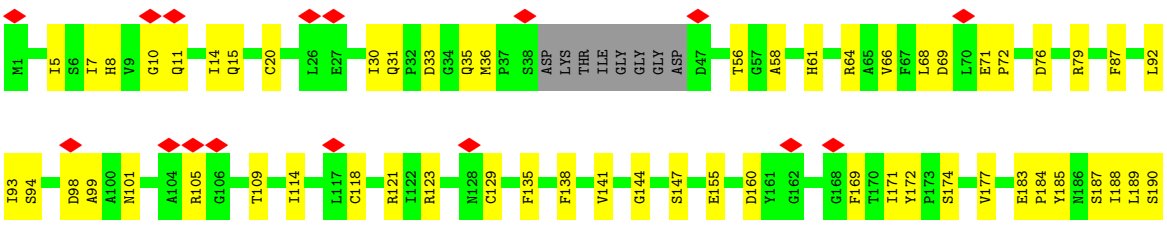


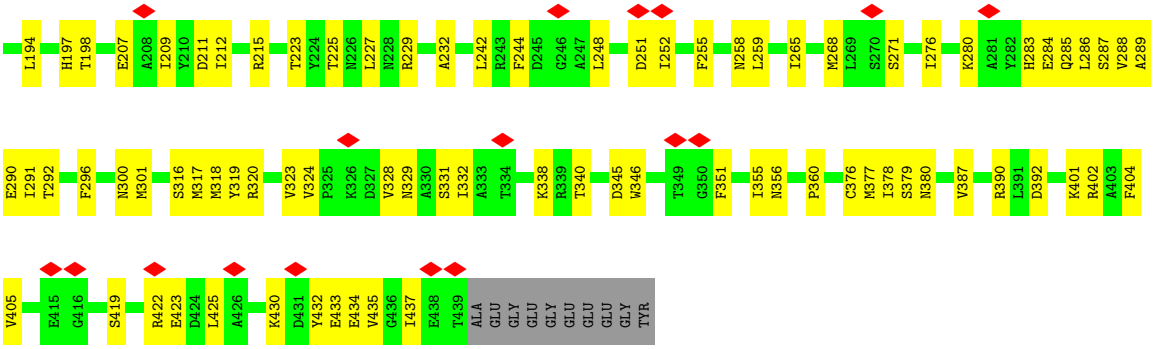


• Molecule 45: Tubulin alpha chain

Chain RI:



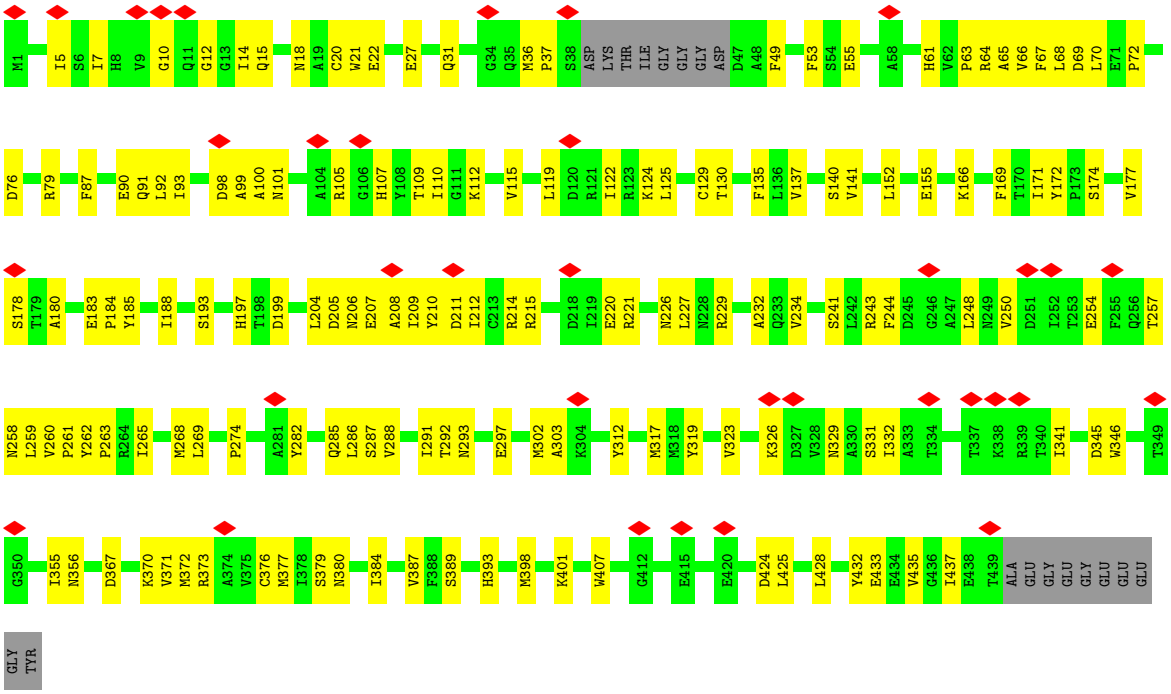




• Molecule 45: Tubulin alpha chain

Chain RK:

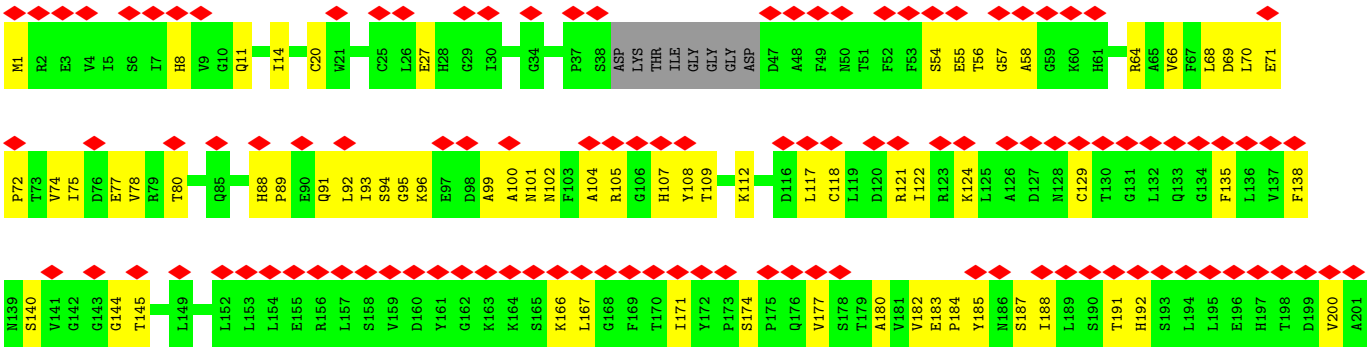


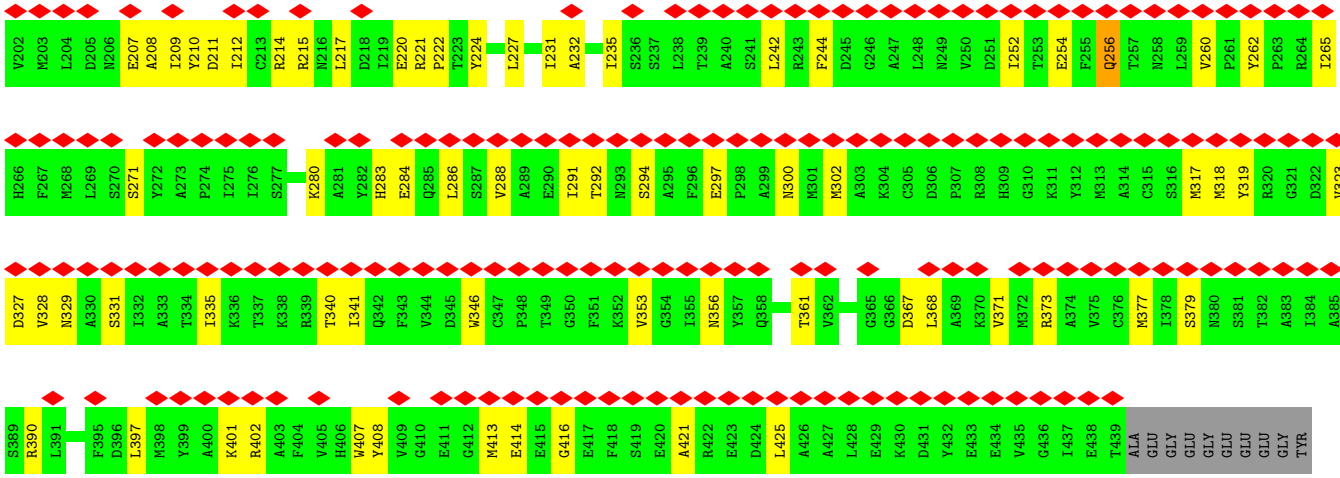


• Molecule 45: Tubulin alpha chain

Chain RM:

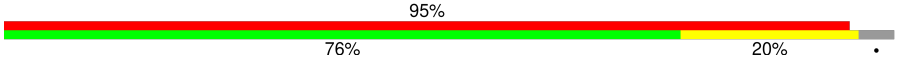


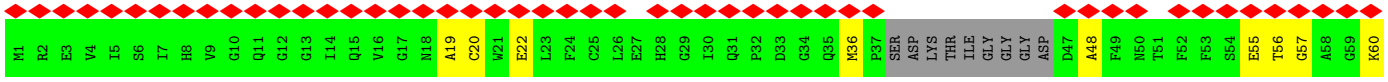


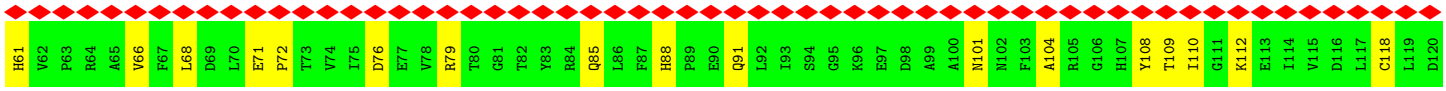


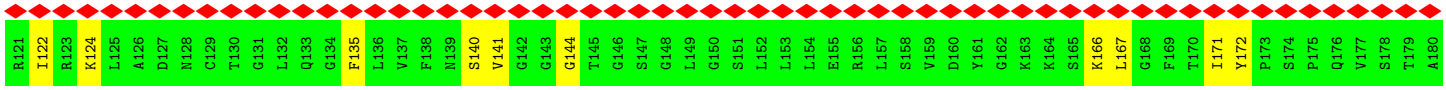
- Molecule 45: Tubulin alpha chain

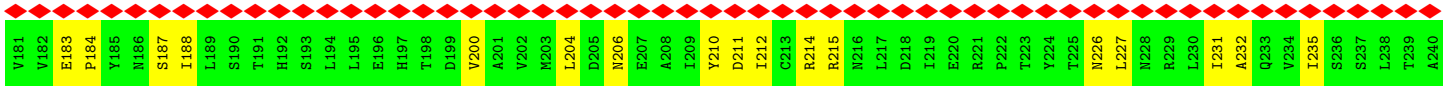
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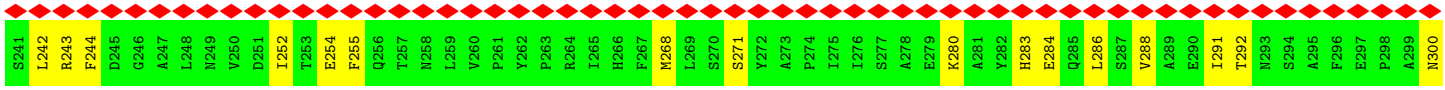


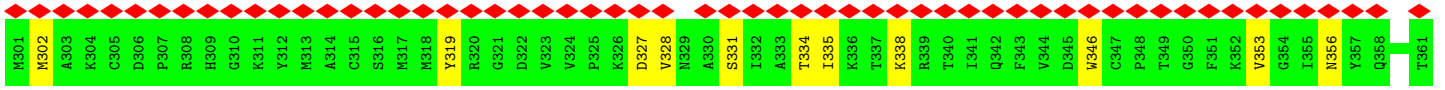


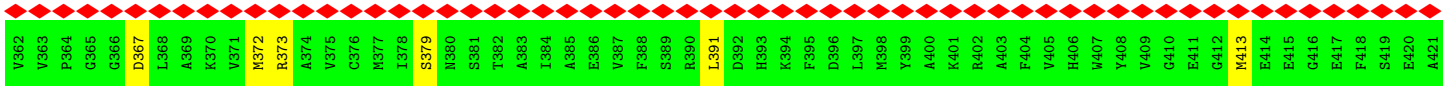


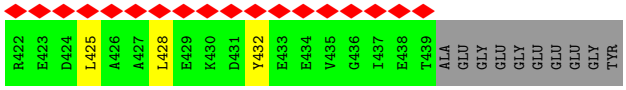








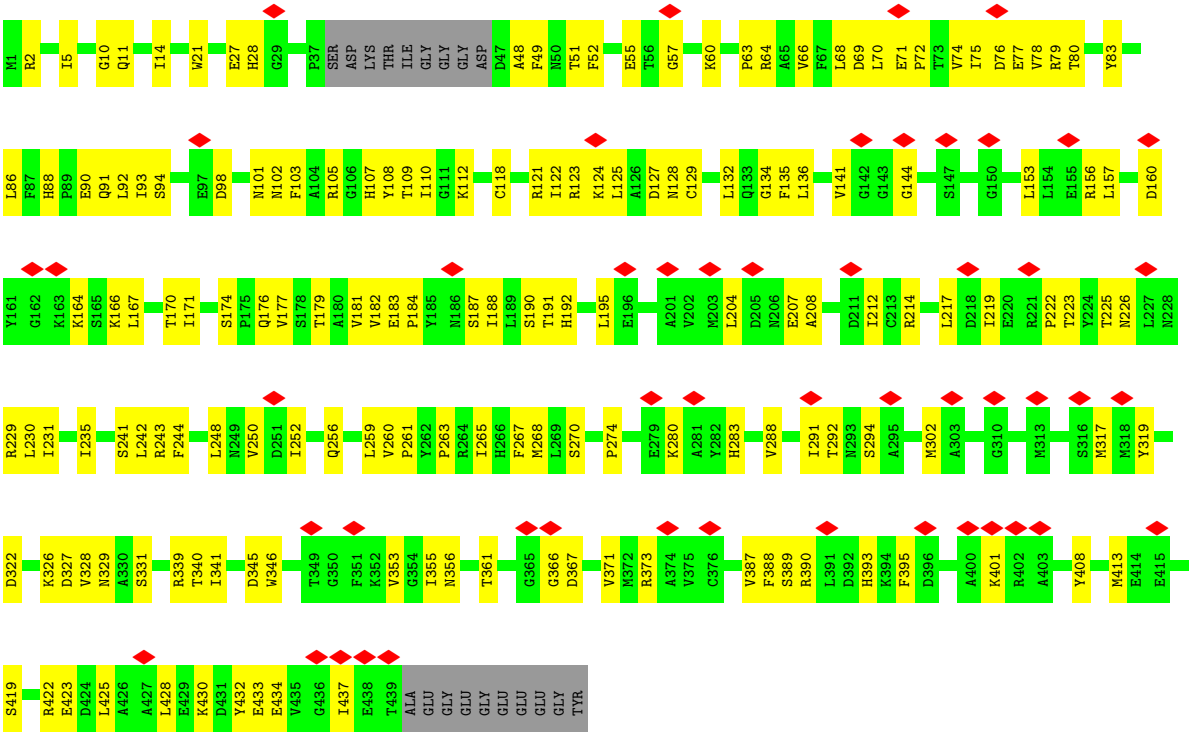




- Molecule 45: Tubulin alpha chain

Chain SC:

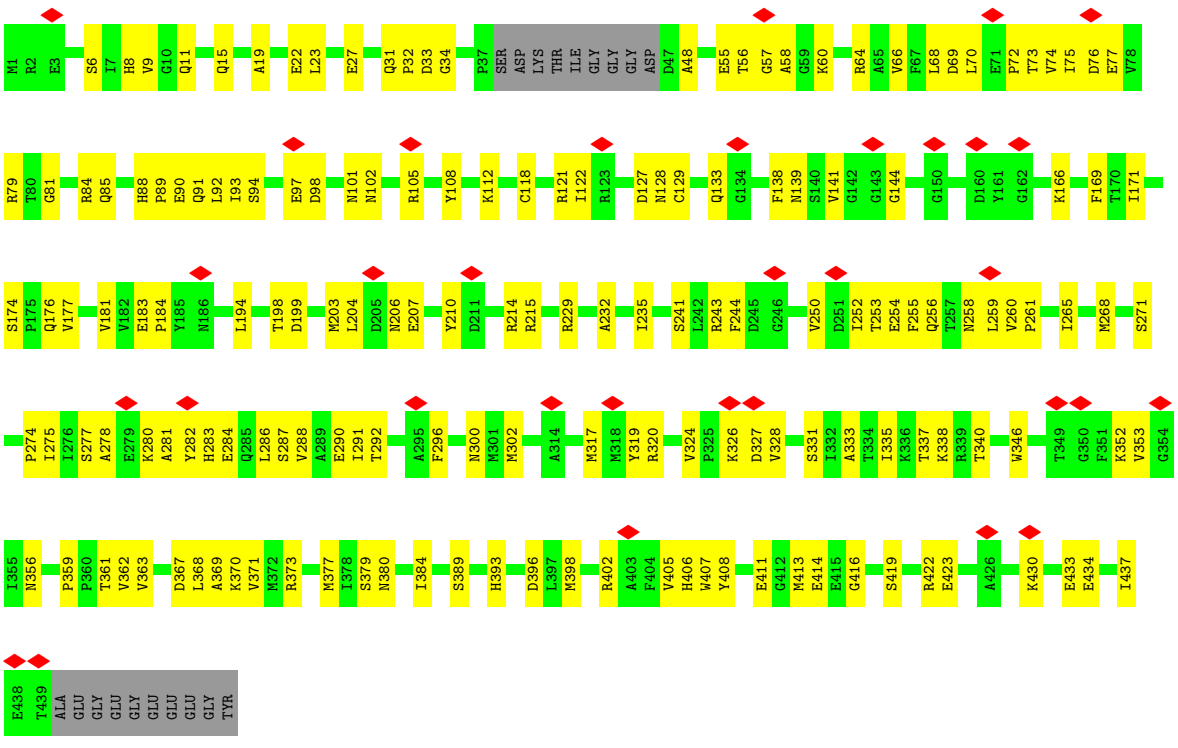




• Molecule 45: Tubulin alpha chain

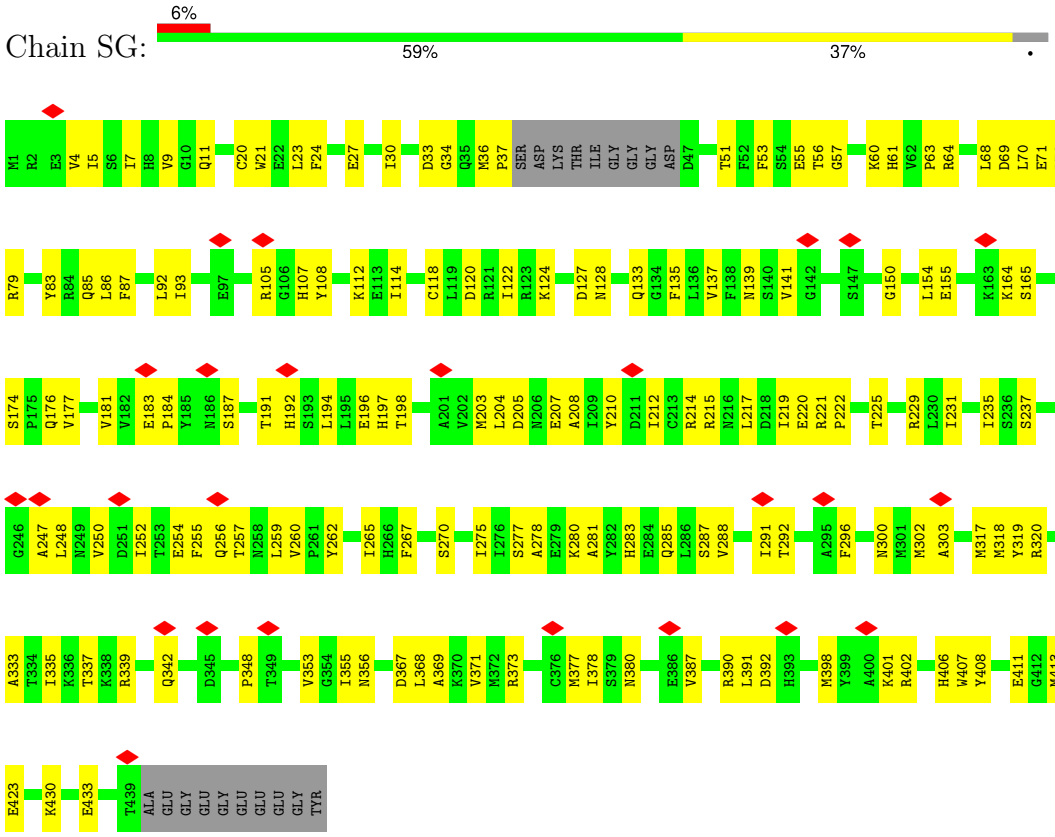
Chain SE:





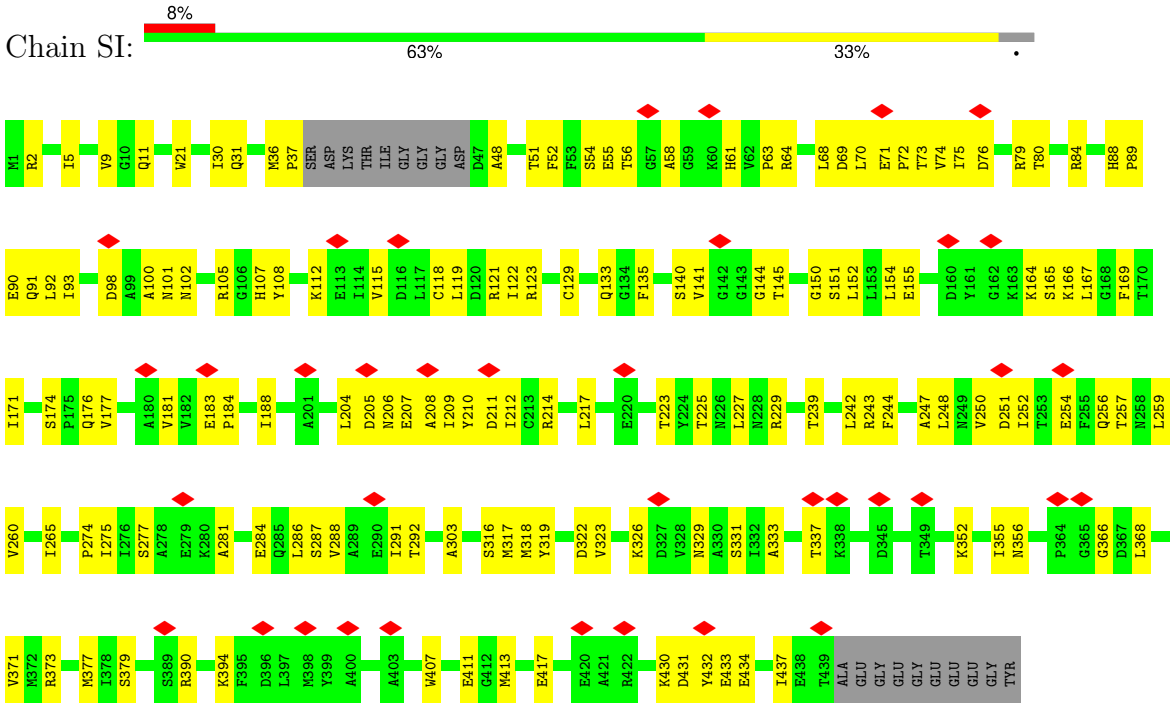
• Molecule 45: Tubulin alpha chain

Chain SG:



• Molecule 45: Tubulin alpha chain

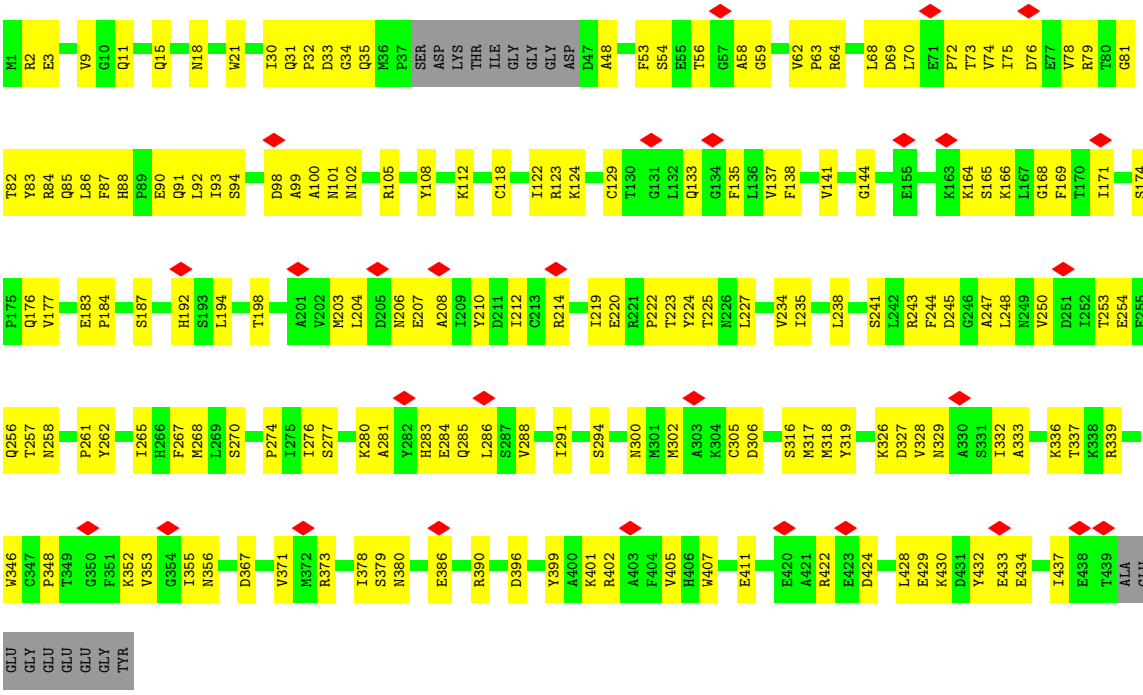
Chain SI:



• Molecule 45: Tubulin alpha chain

Chain SK:

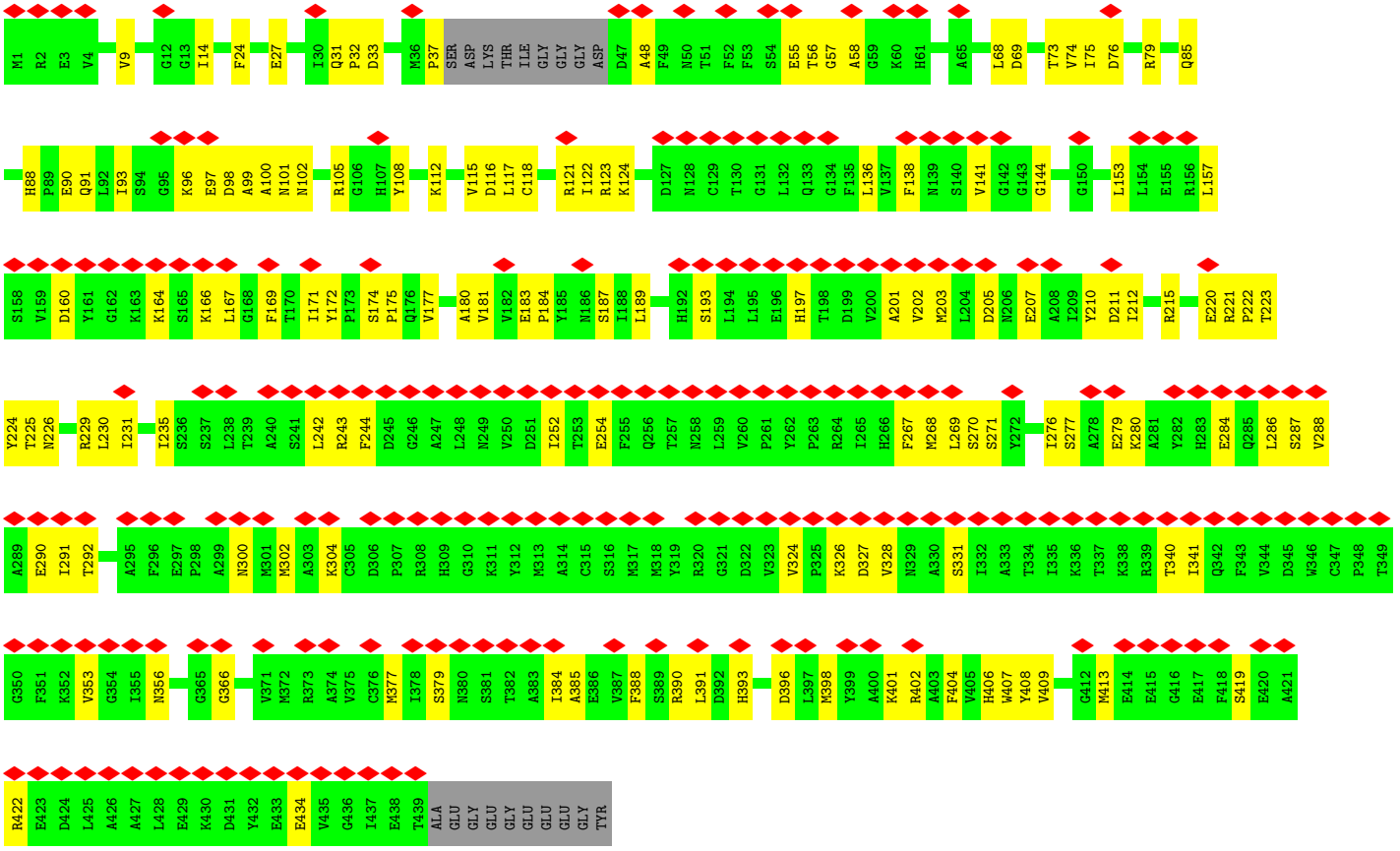




• Molecule 45: Tubulin alpha chain

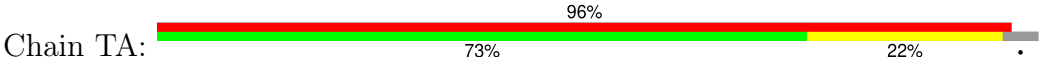
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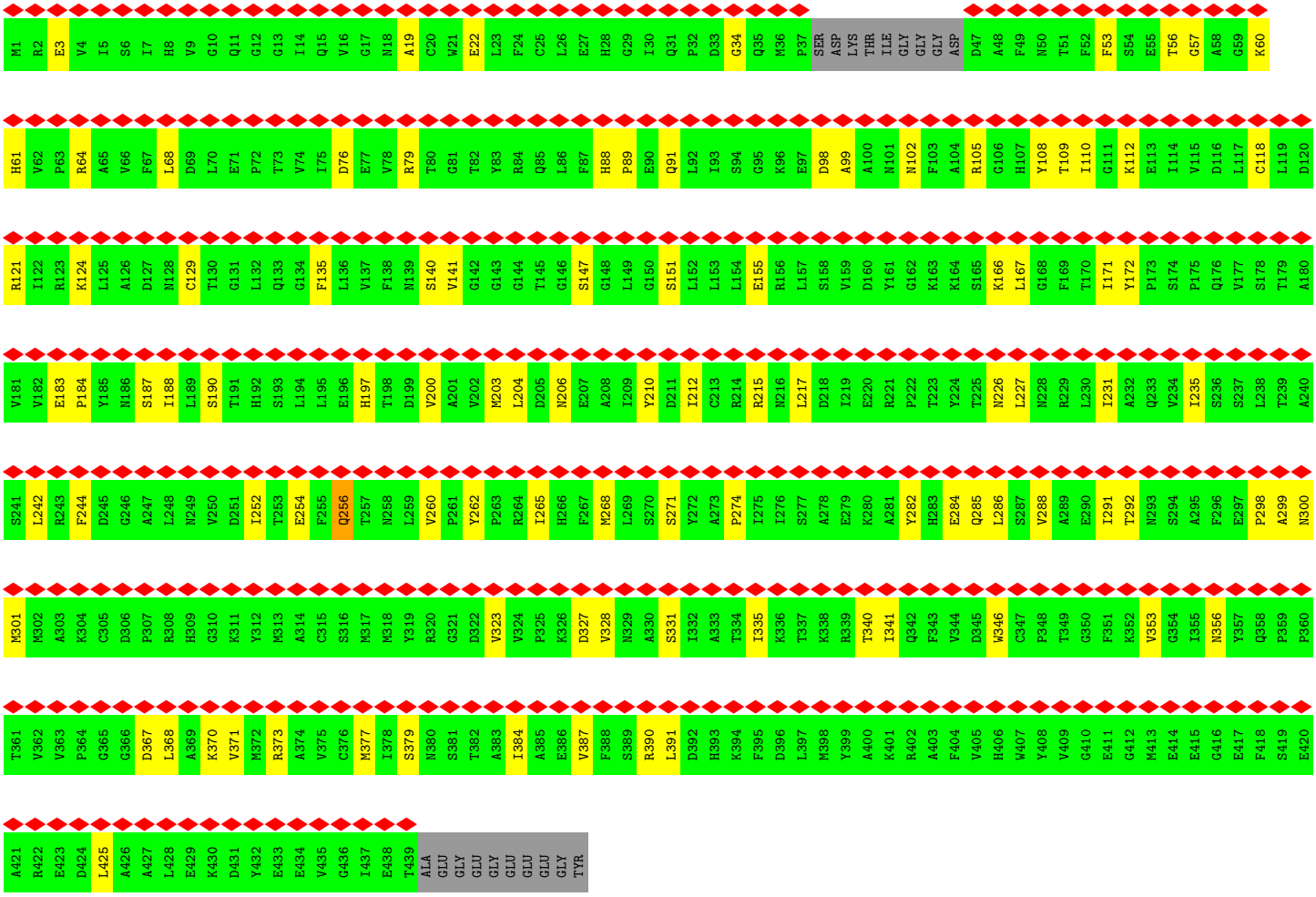




• Molecule 45: Tubulin alpha chain

Chain TA:

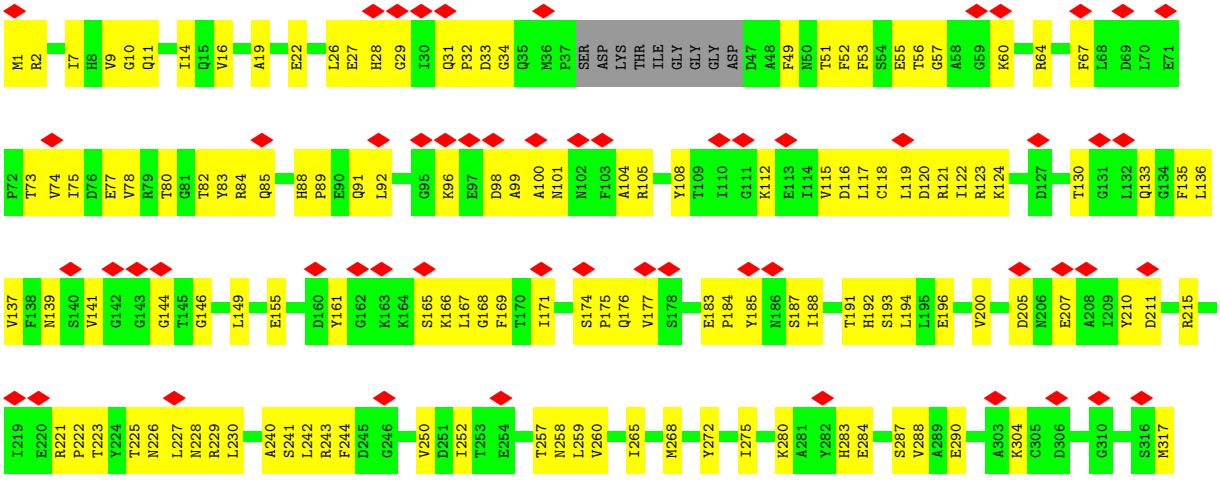


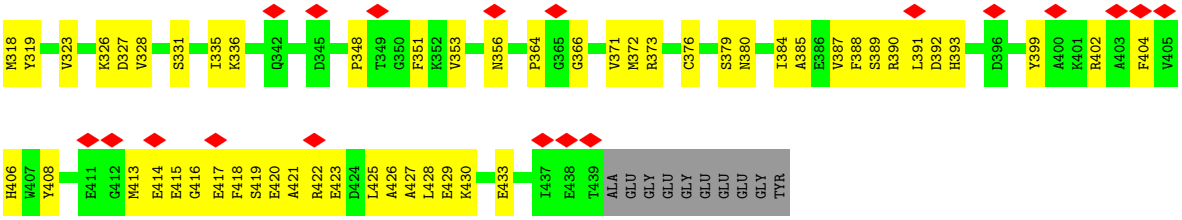


• Molecule 45: Tubulin alpha chain

Chain TC:



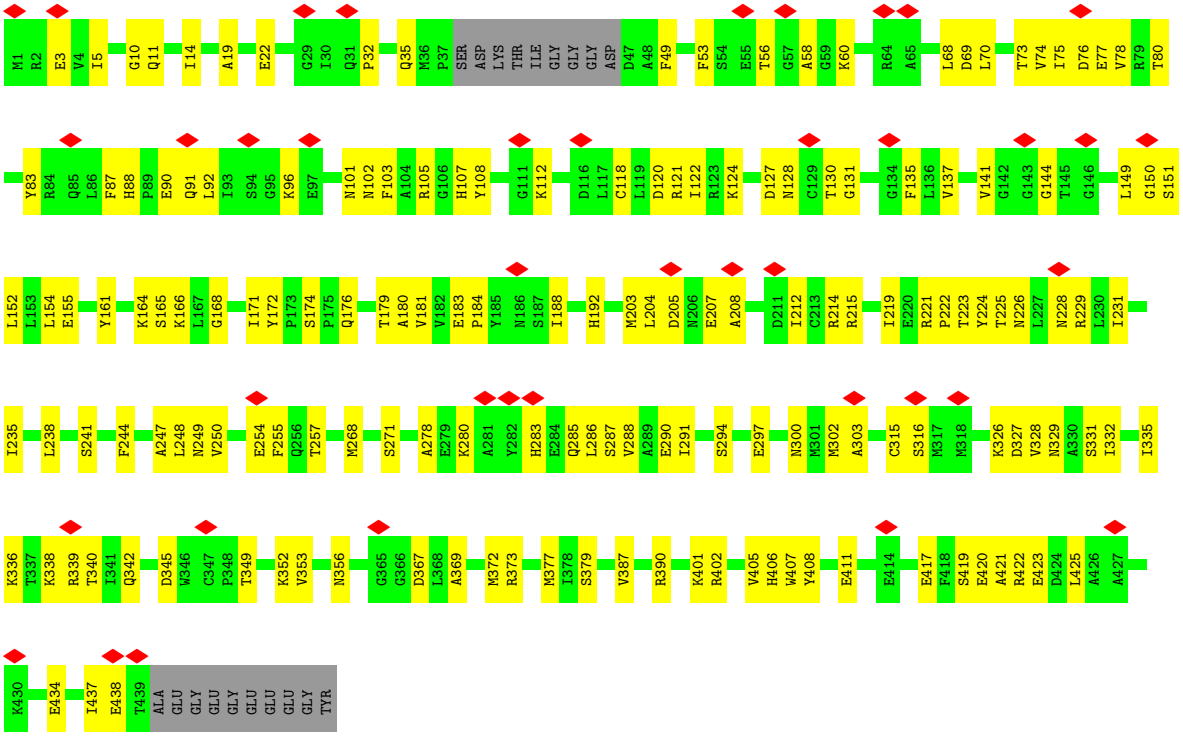




• Molecule 45: Tubulin alpha chain

Chain TE:

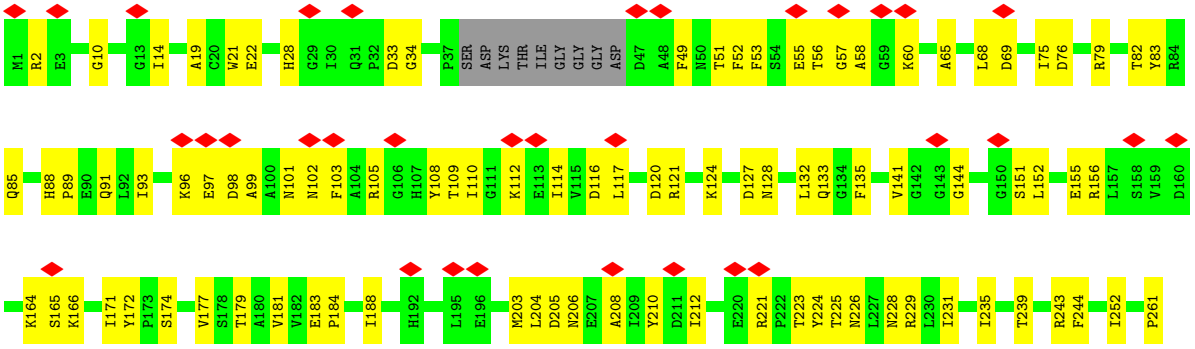


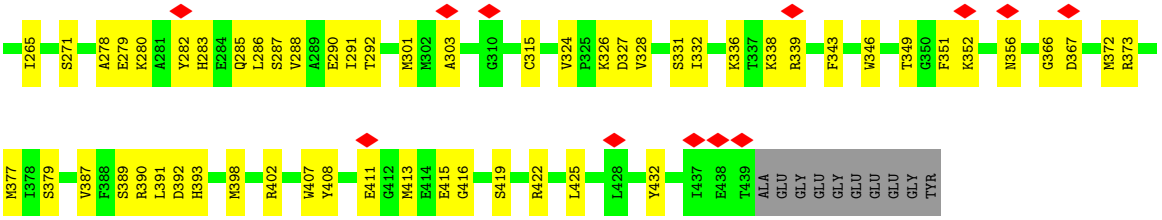


• Molecule 45: Tubulin alpha chain

Chain TG:



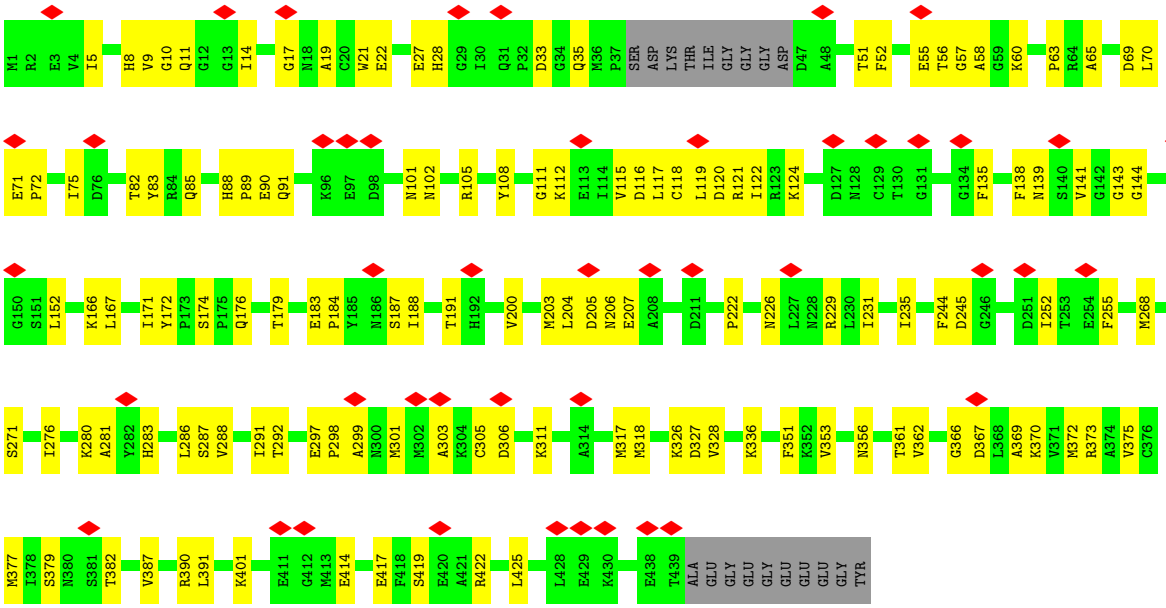




• Molecule 45: Tubulin alpha chain

Chain TI:

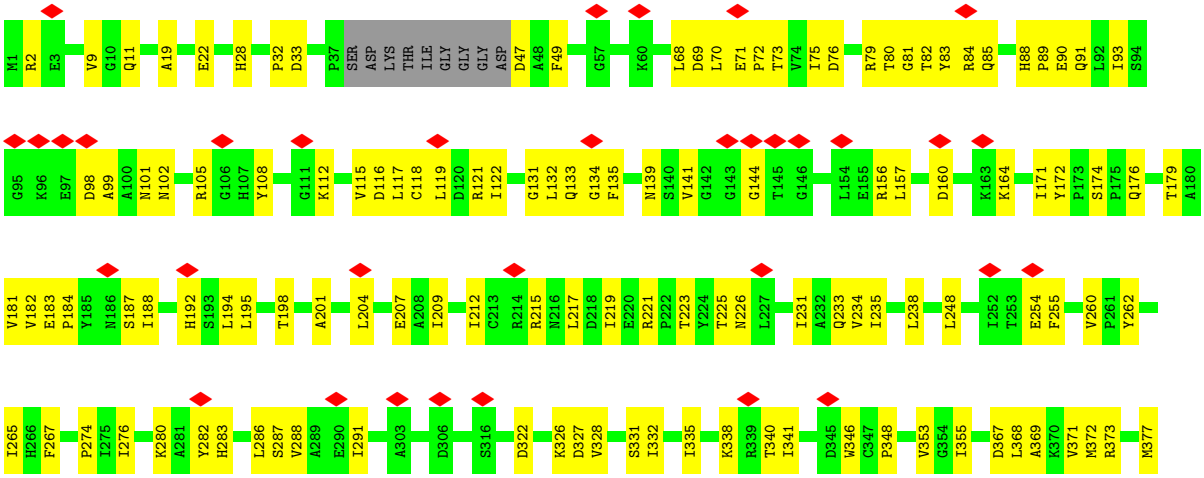


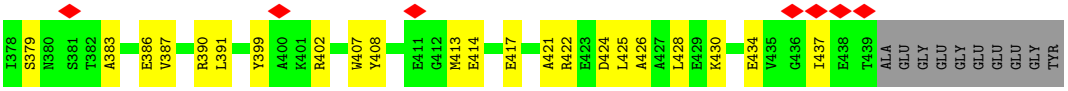


• Molecule 45: Tubulin alpha chain

Chain TK:



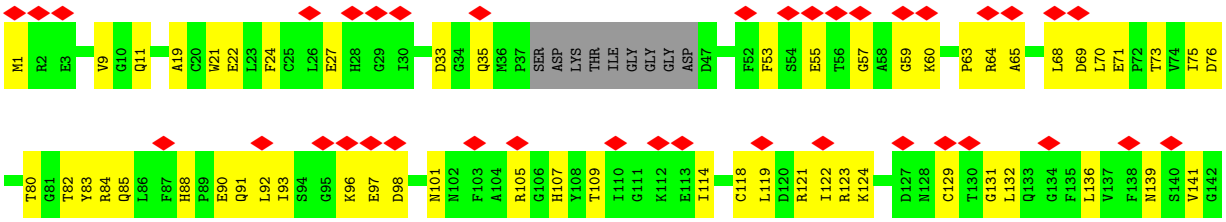




• Molecule 45: Tubulin alpha chain

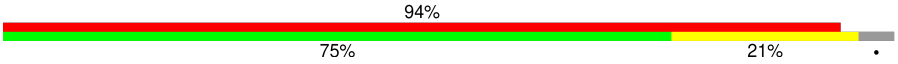
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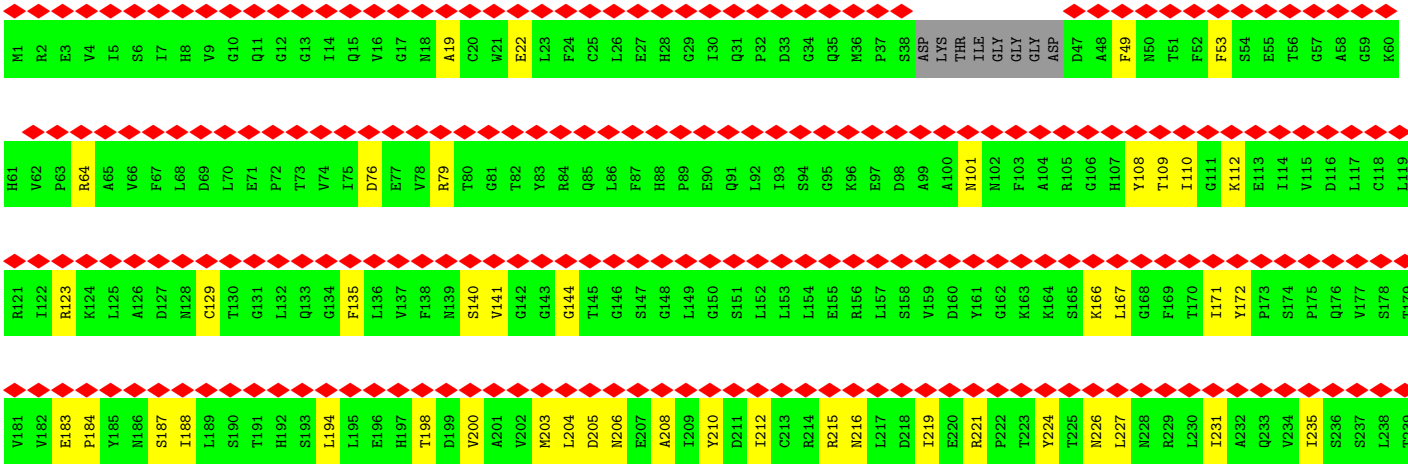


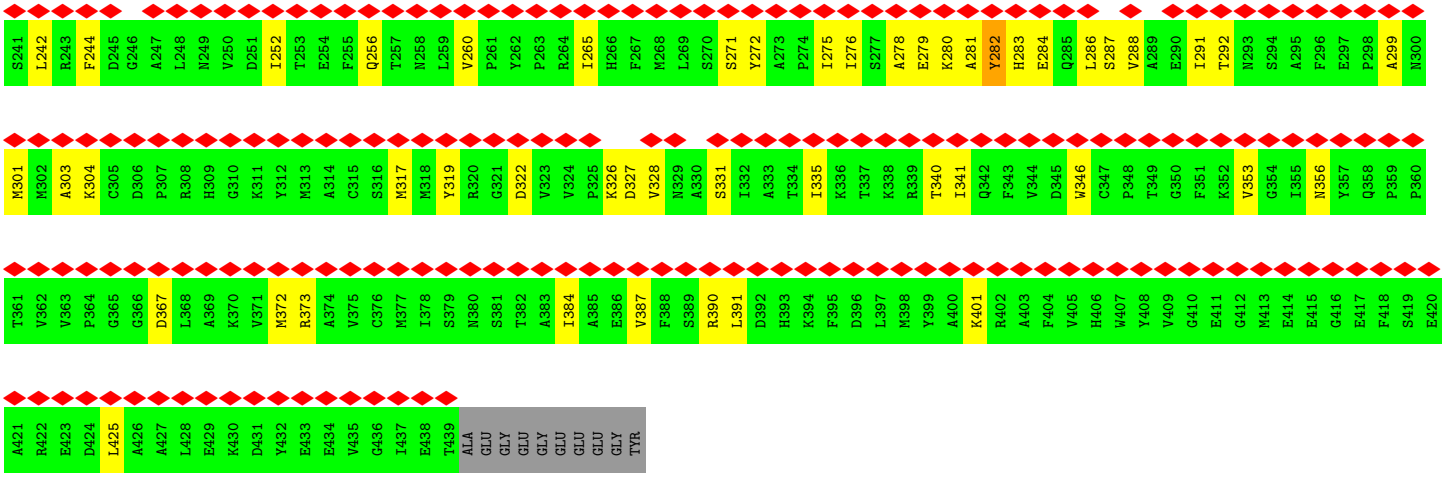


• Molecule 45: Tubulin alpha chain

Chain UA:



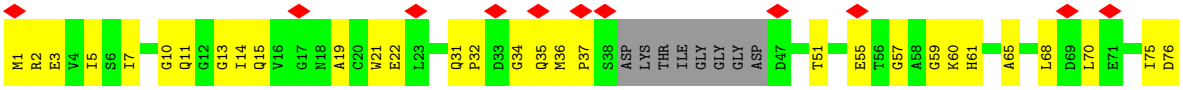


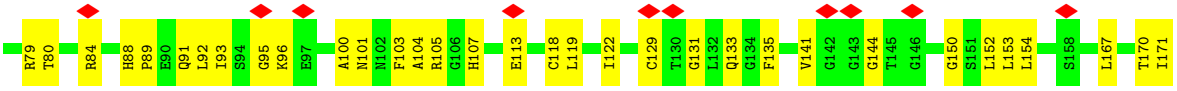


• Molecule 45: Tubulin alpha chain

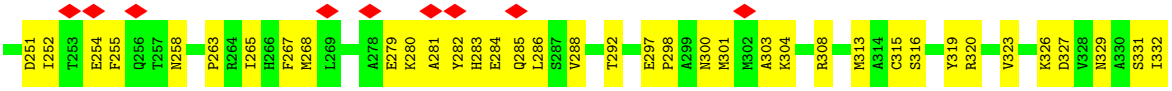
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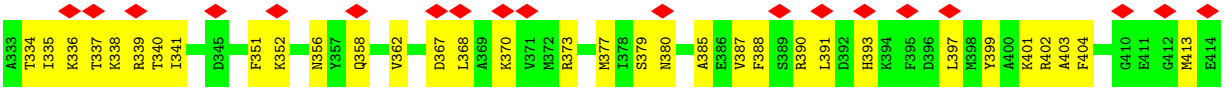


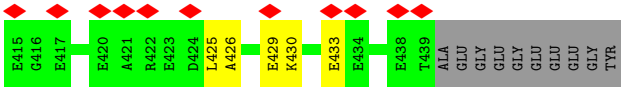








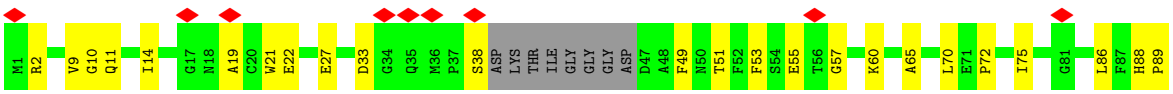


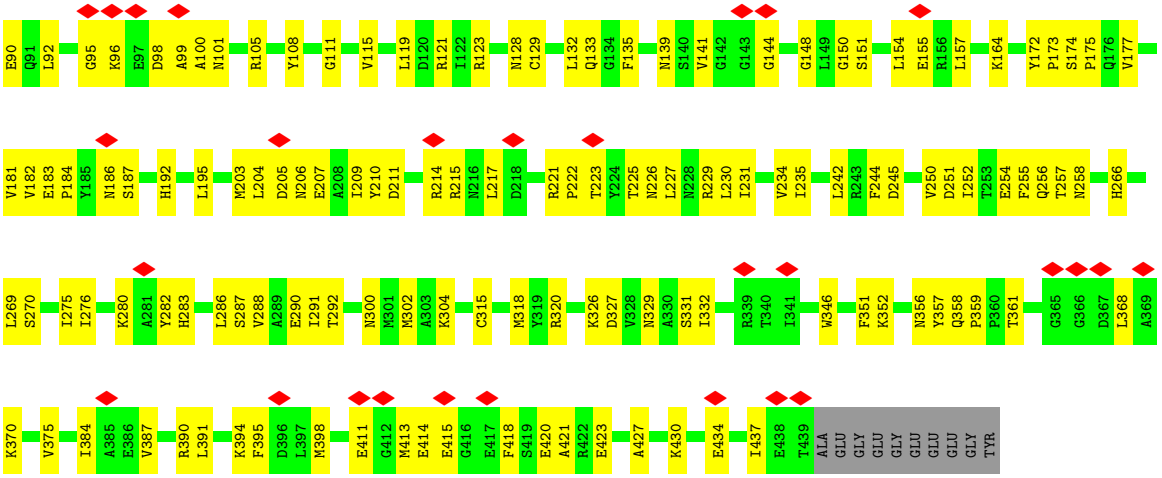


• Molecule 45: Tubulin alpha chain

Chain UE:



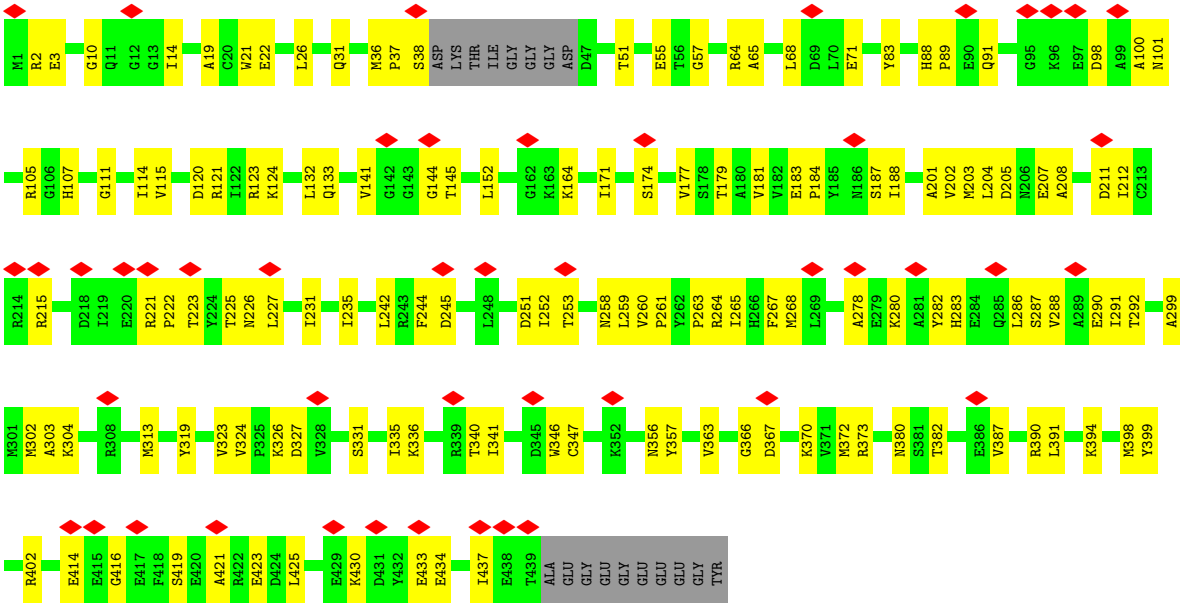




• Molecule 45: Tubulin alpha chain

Chain UG:

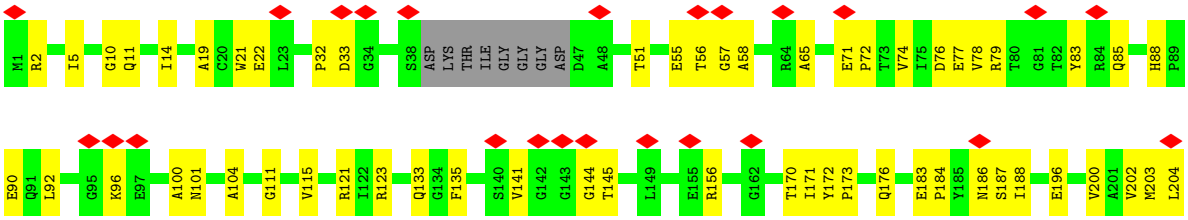


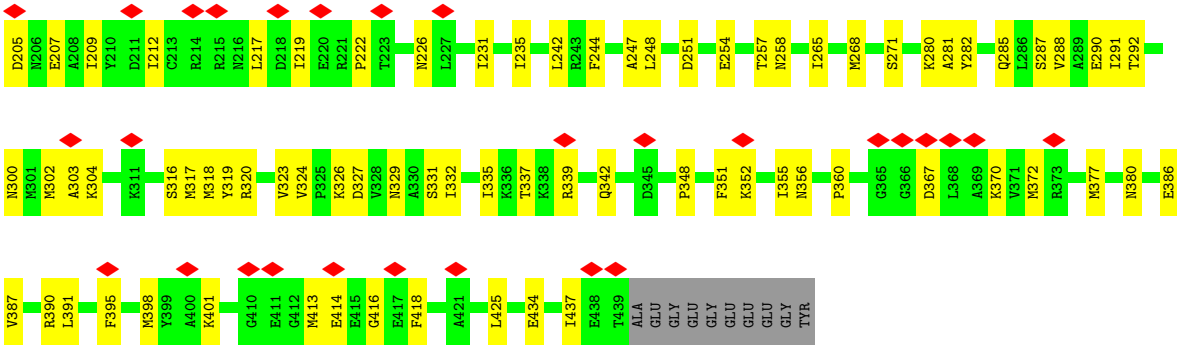


• Molecule 45: Tubulin alpha chain

Chain UI:



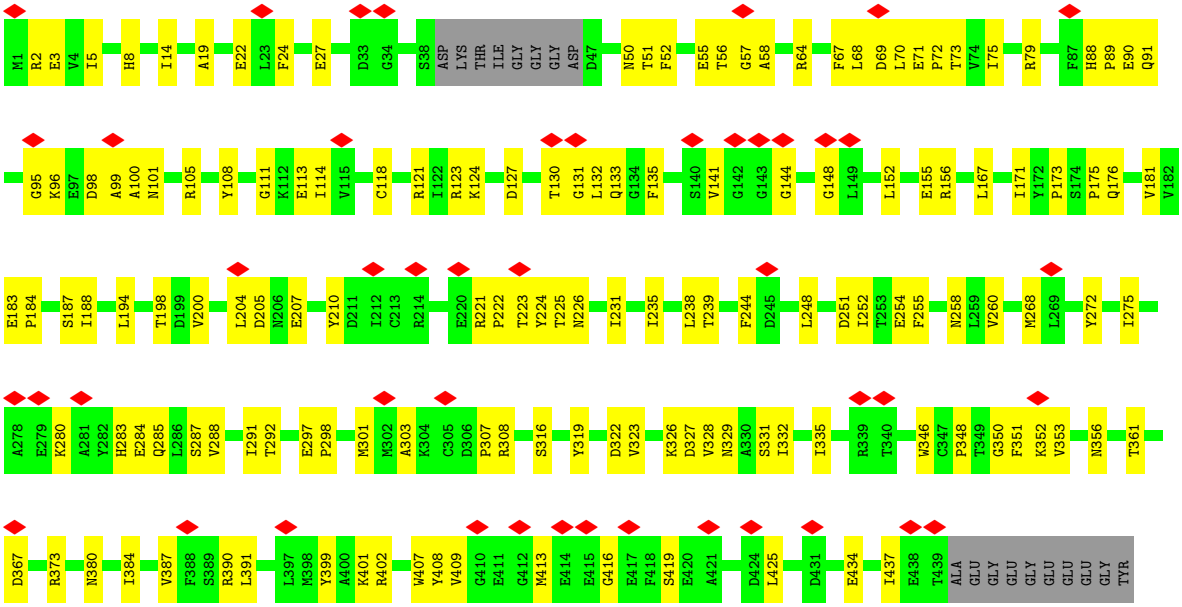




• Molecule 45: Tubulin alpha chain

Chain UK:

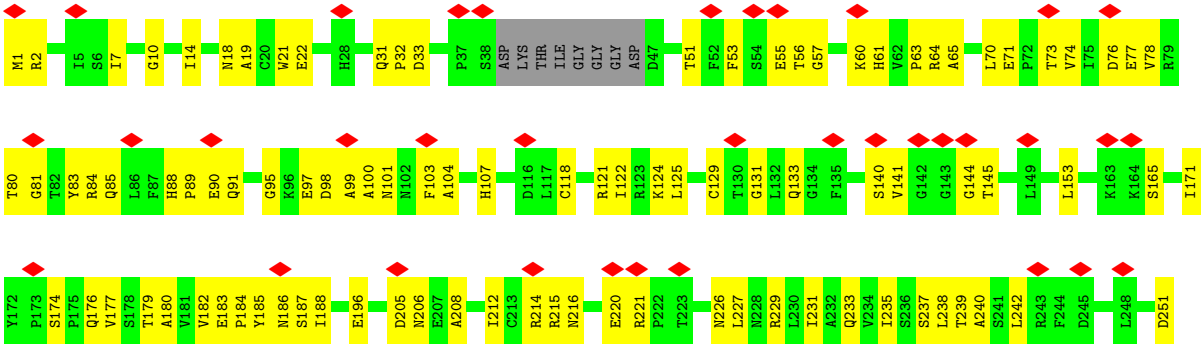


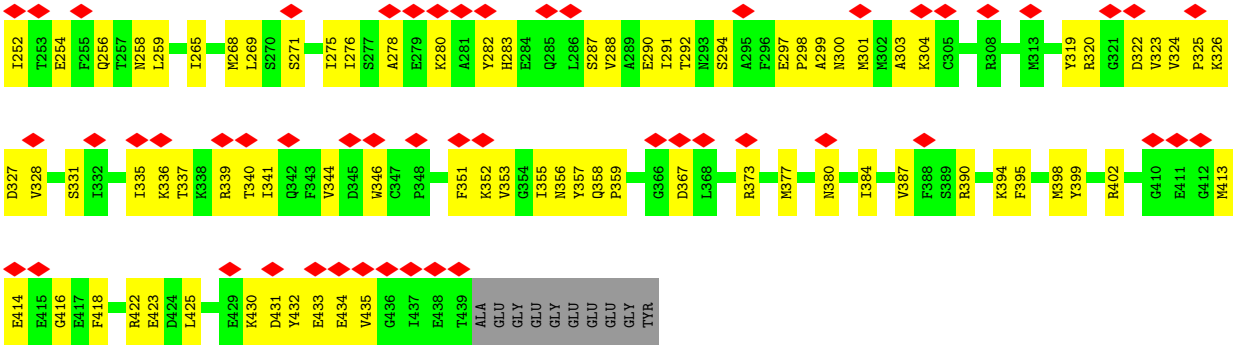


• Molecule 45: Tubulin alpha chain

Chain UM:



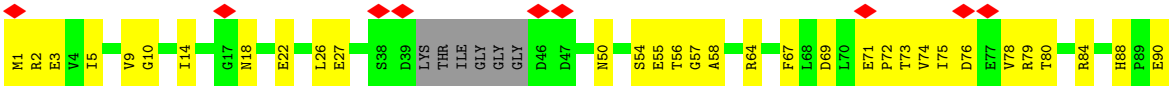


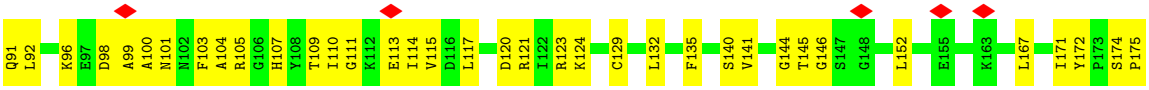


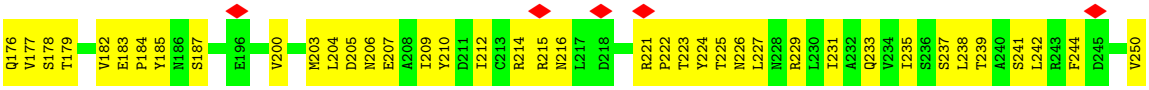
• Molecule 45: Tubulin alpha chain

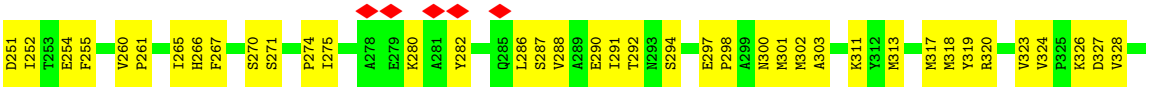
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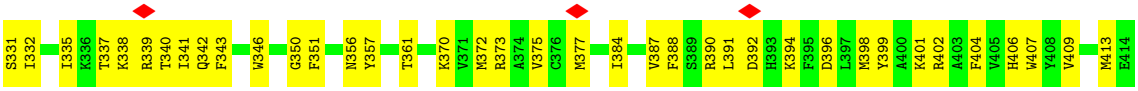


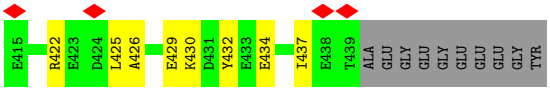








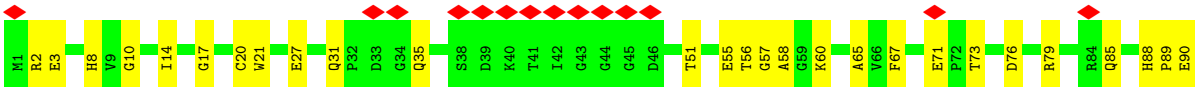


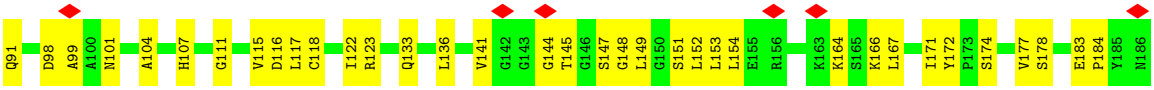


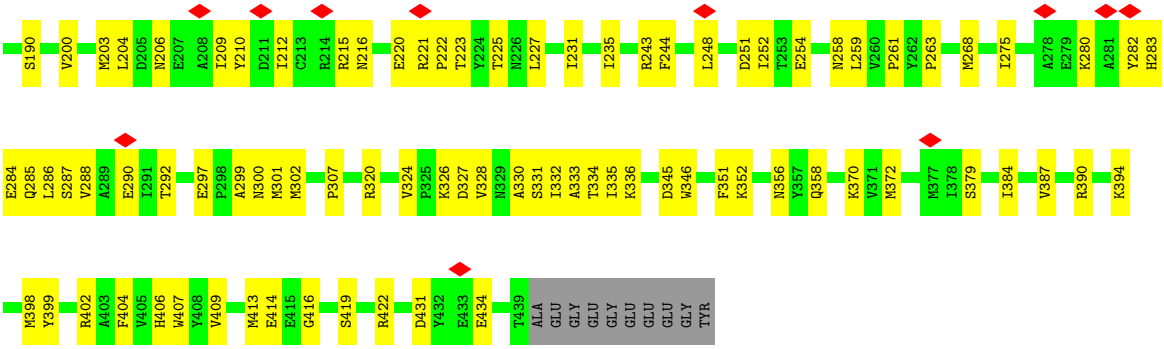
• Molecule 45: Tubulin alpha chain

Chain VC:





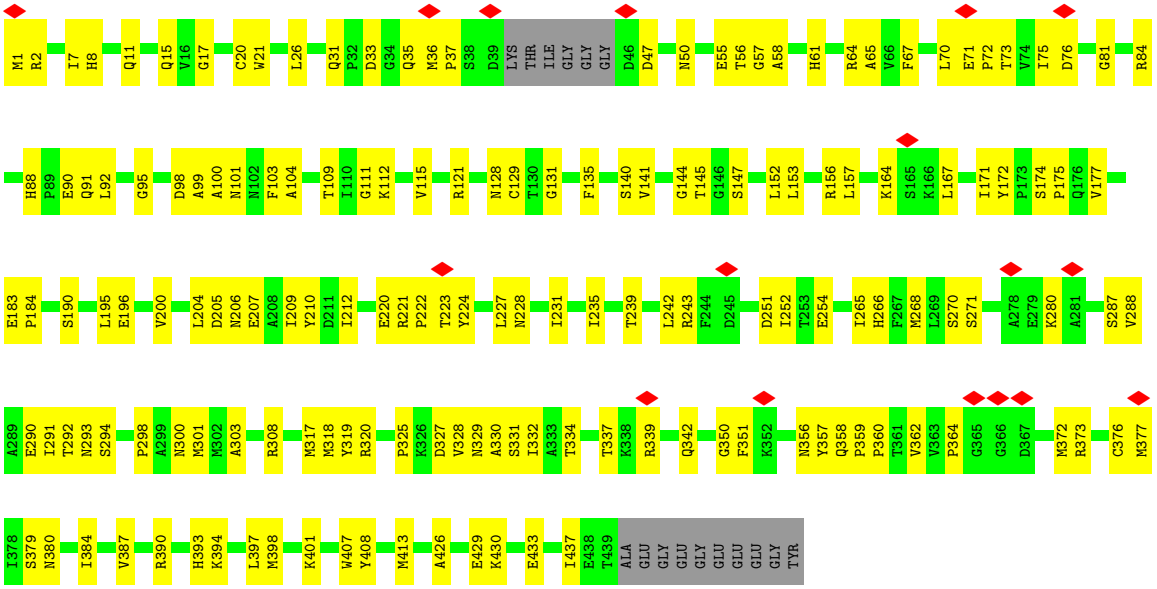




• Molecule 45: Tubulin alpha chain

Chain VE:

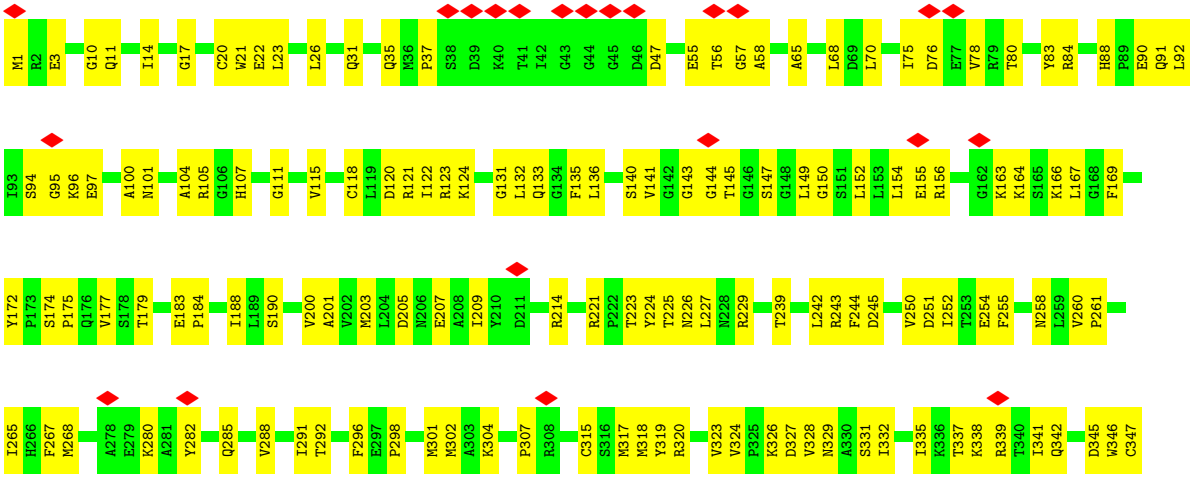


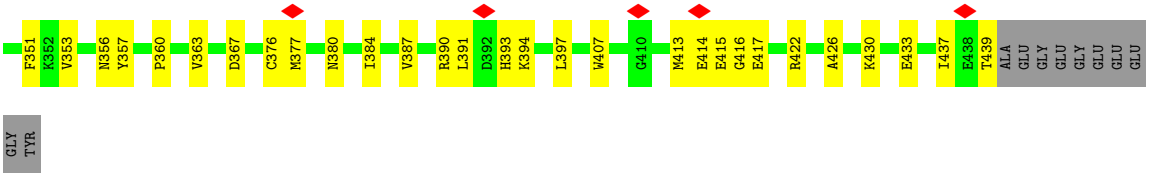


• Molecule 45: Tubulin alpha chain

Chain VG:



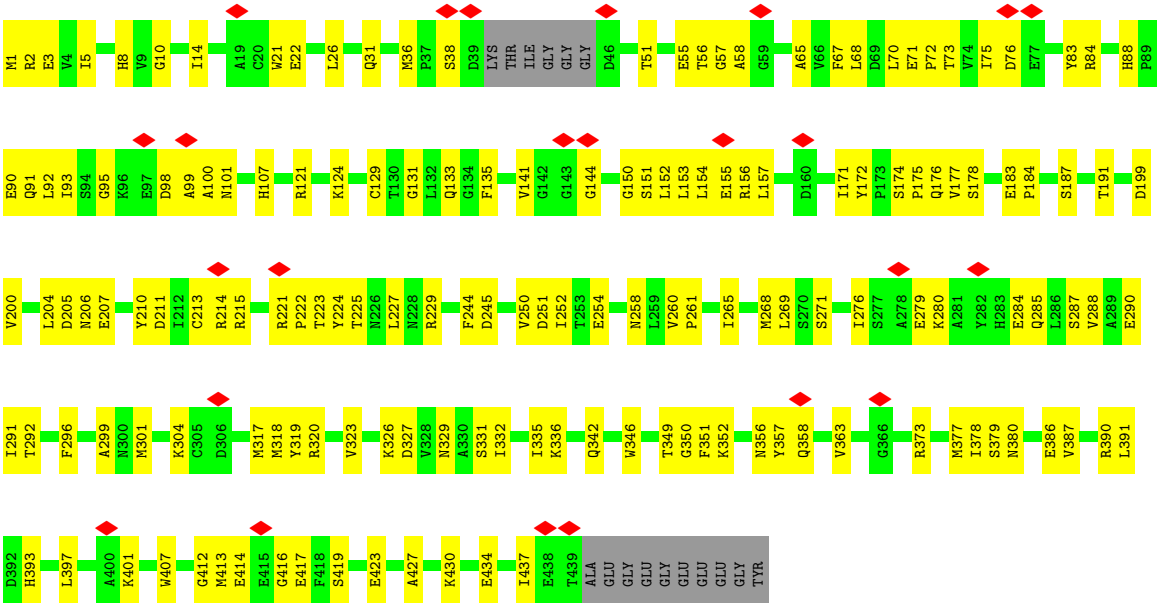




• Molecule 45: Tubulin alpha chain

Chain VI:

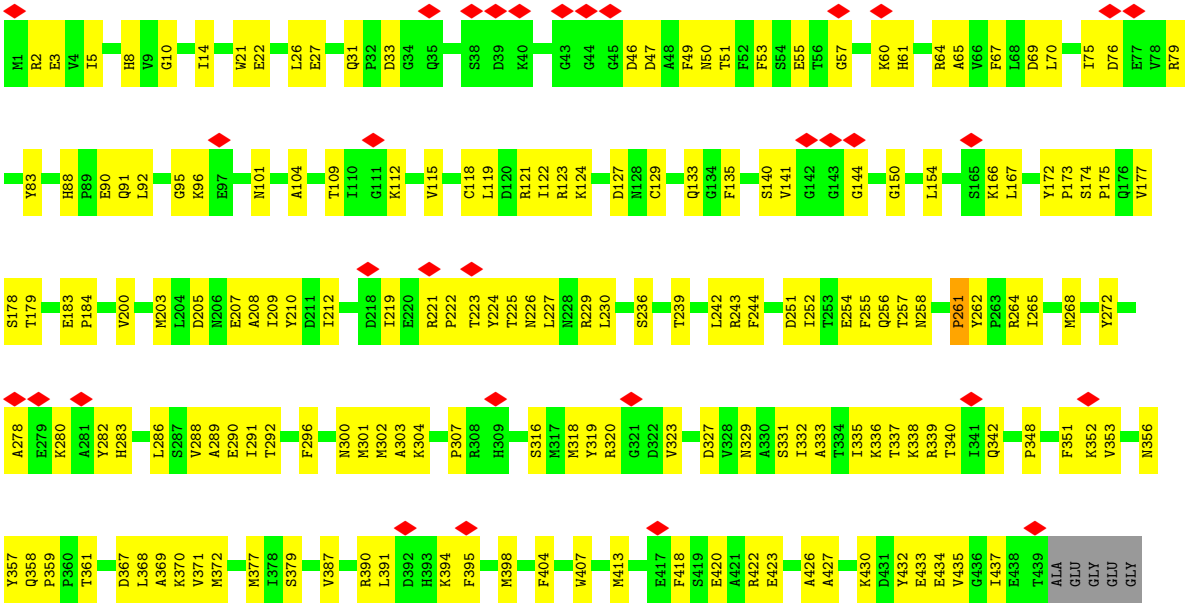




• Molecule 45: Tubulin alpha chain

Chain VK:

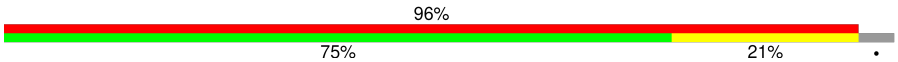


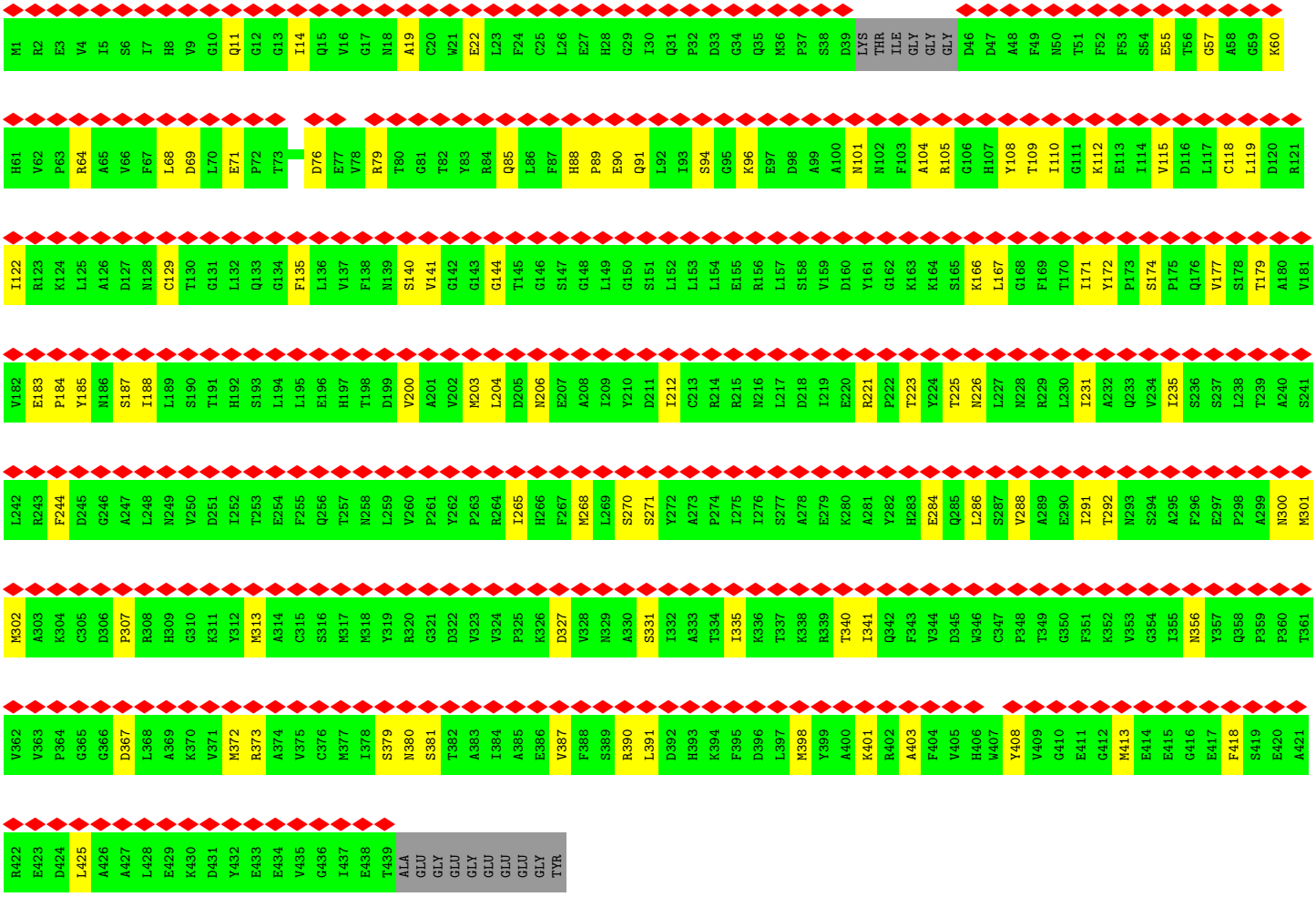




• Molecule 45: Tubulin alpha chain

Chain VM:

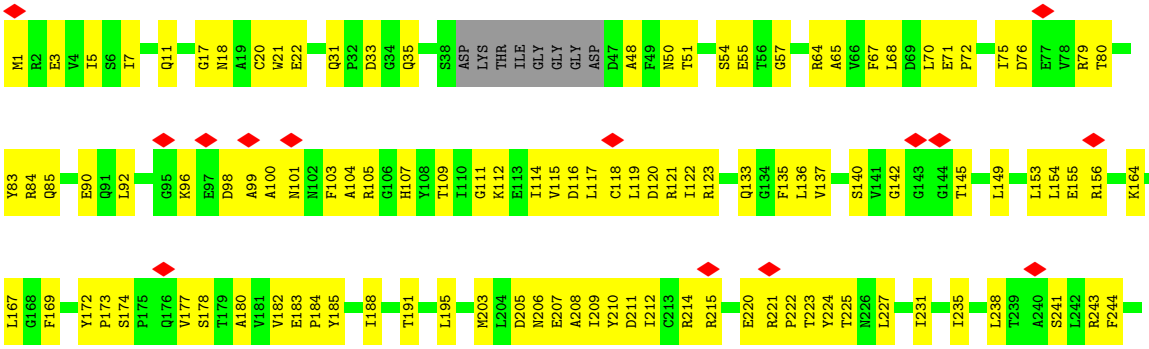


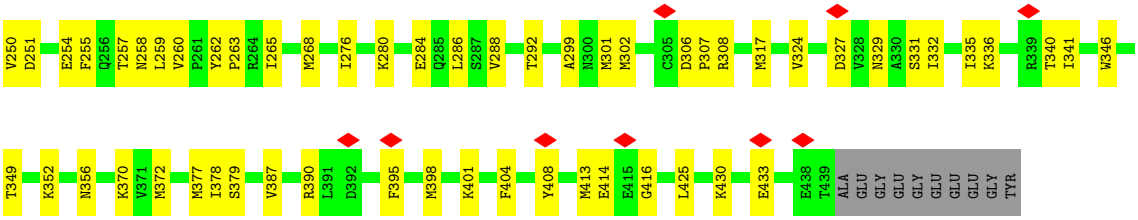


• Molecule 45: Tubulin alpha chain

Chain WA:

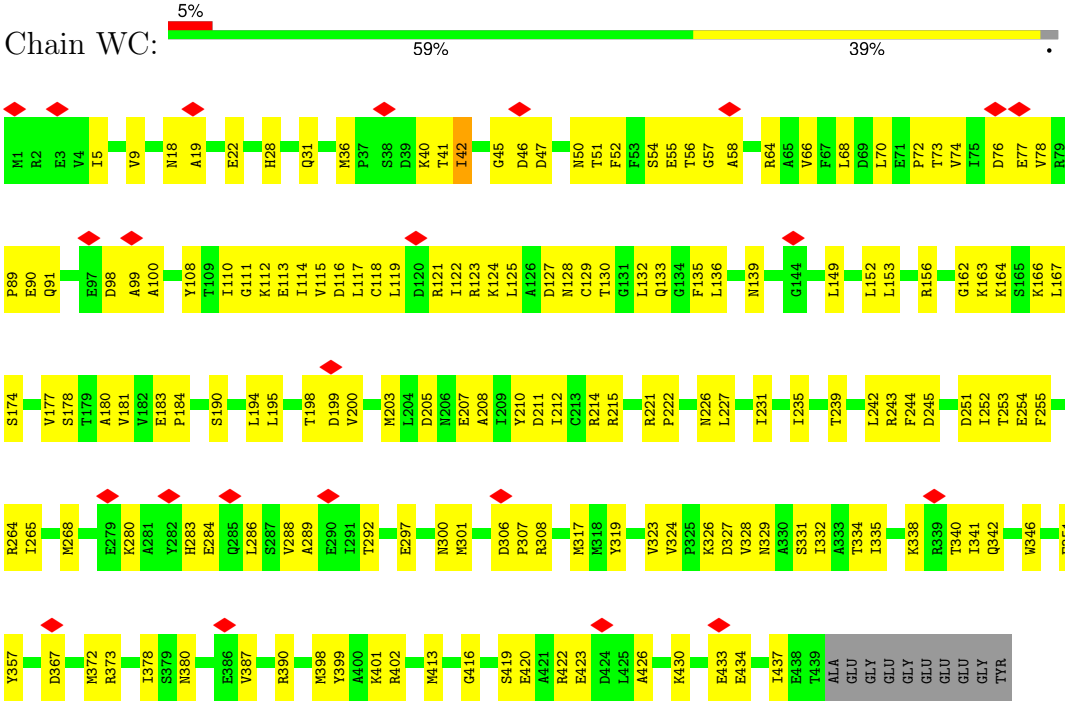






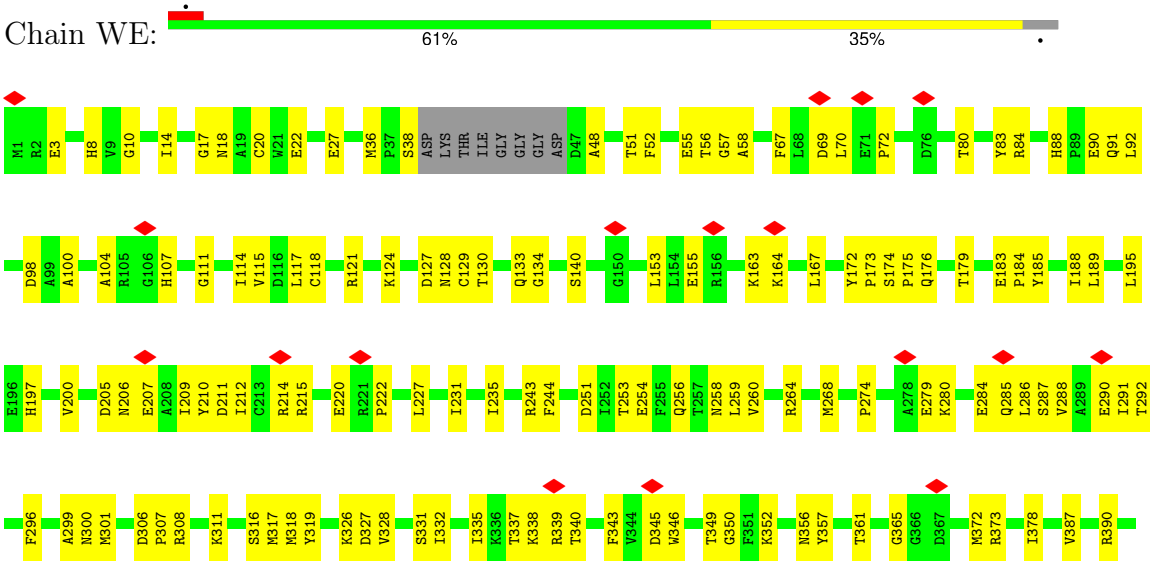
• Molecule 45: Tubulin alpha chain

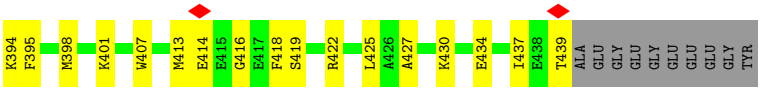
Chain WC:



• Molecule 45: Tubulin alpha chain

Chain WE:

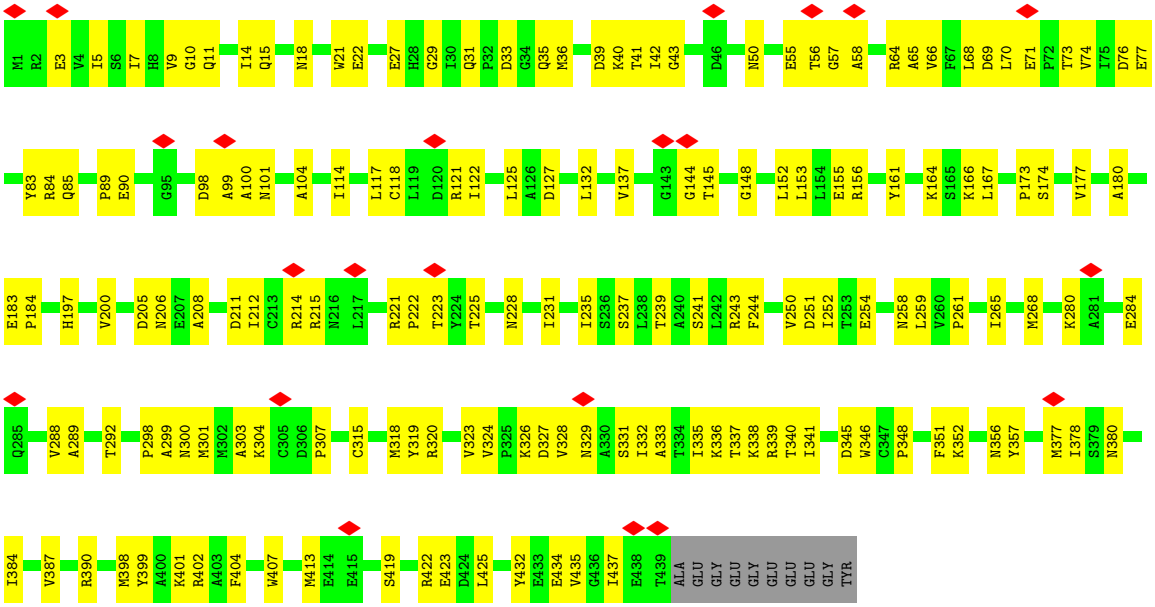




• Molecule 45: Tubulin alpha chain

Chain WG:

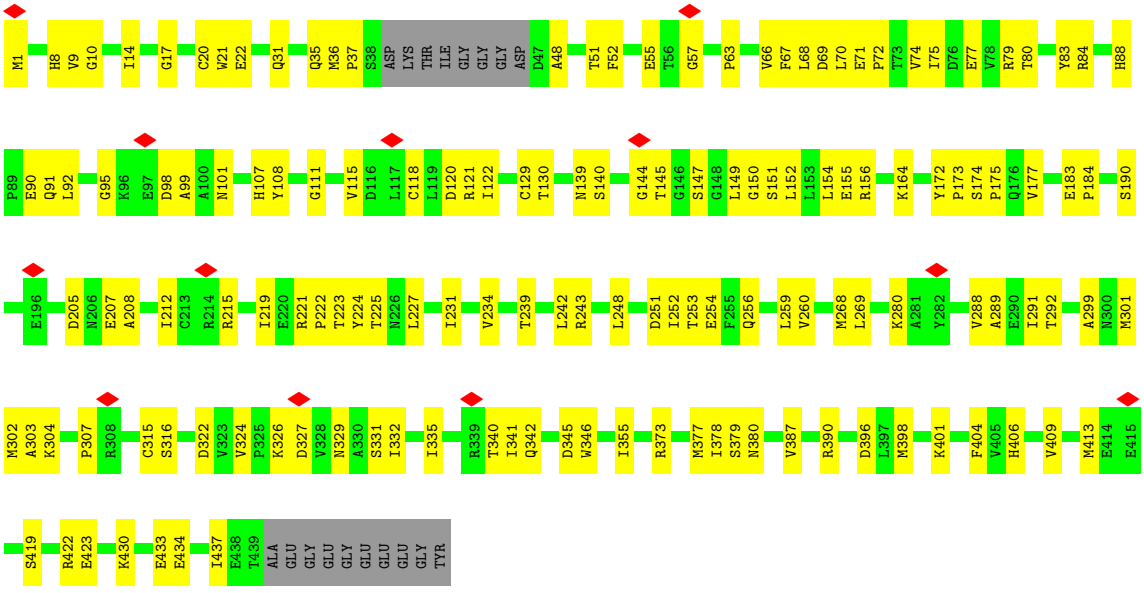




• Molecule 45: Tubulin alpha chain

Chain WI:

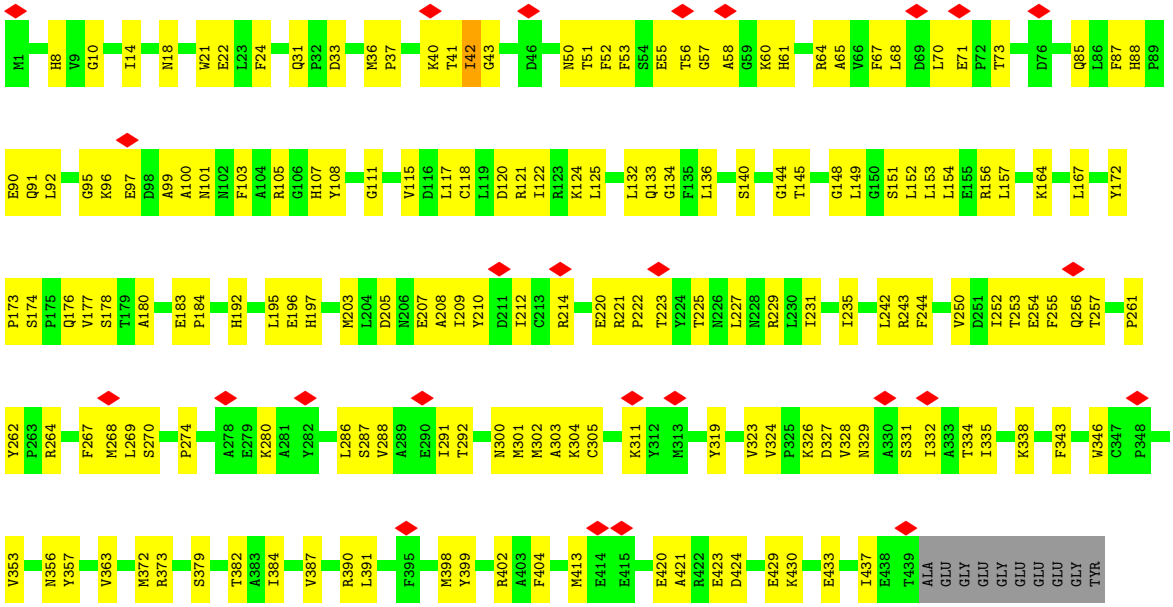




• Molecule 45: Tubulin alpha chain

Chain WK:

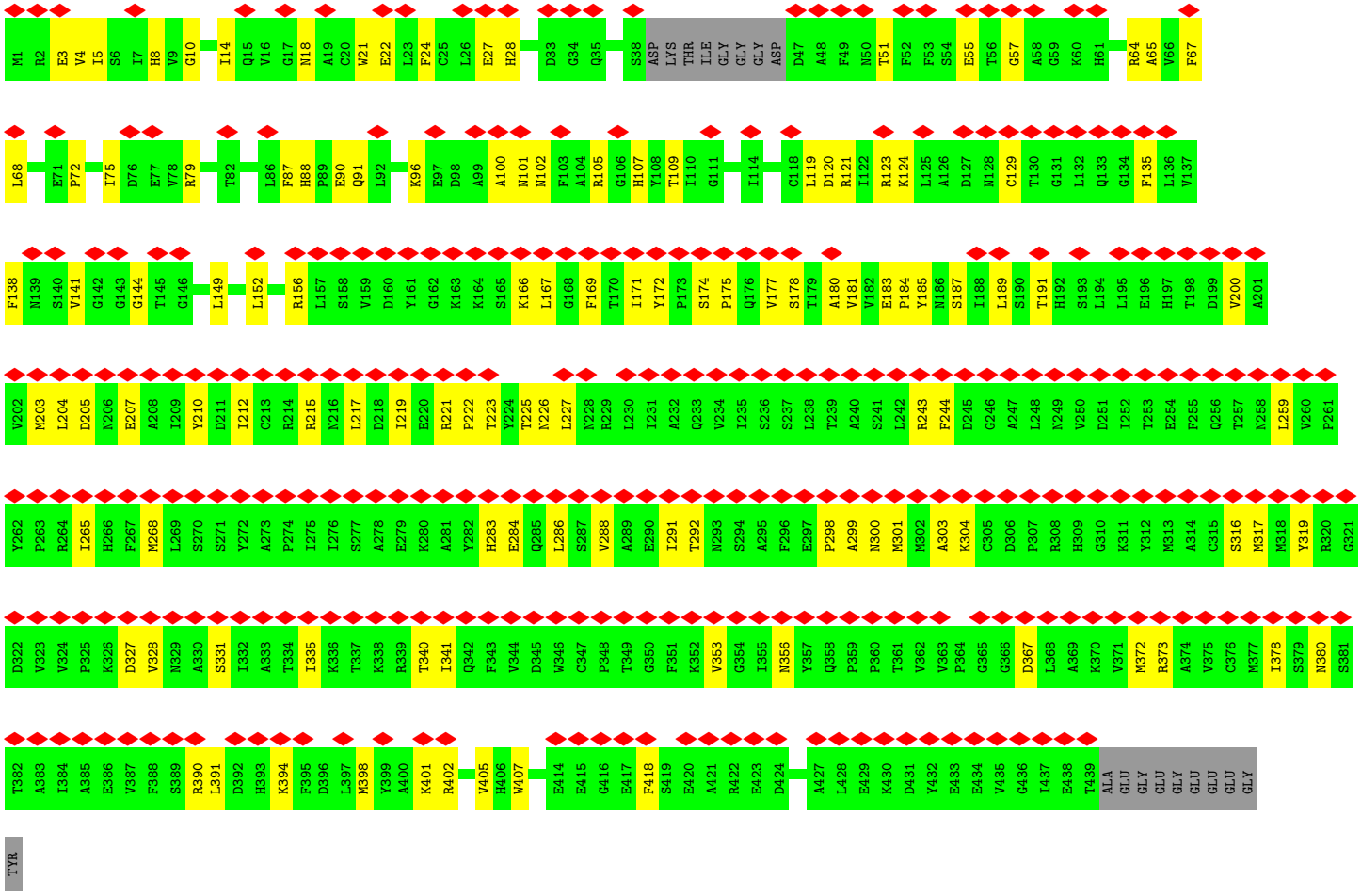




• Molecule 45: Tubulin alpha chain

Chain WM:





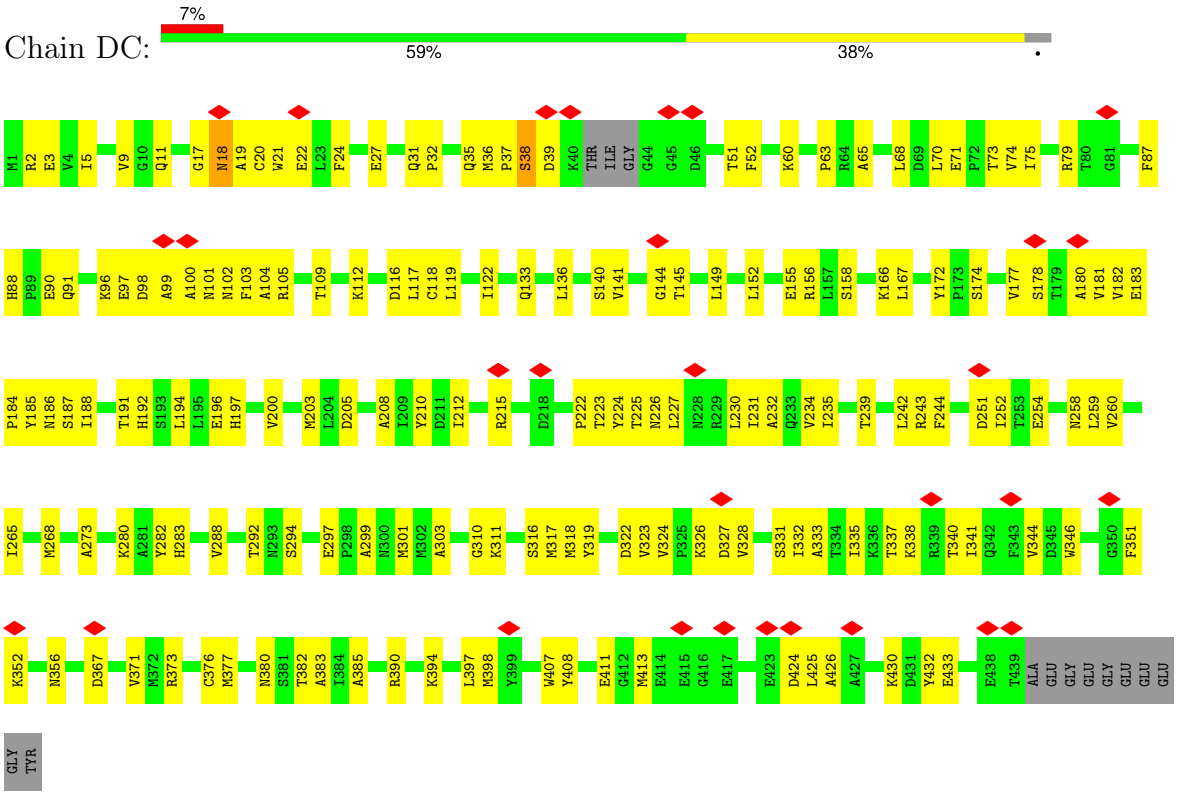
• Molecule 45: Tubulin alpha chain

Chain CE:



• Molecule 45: Tubulin alpha chain

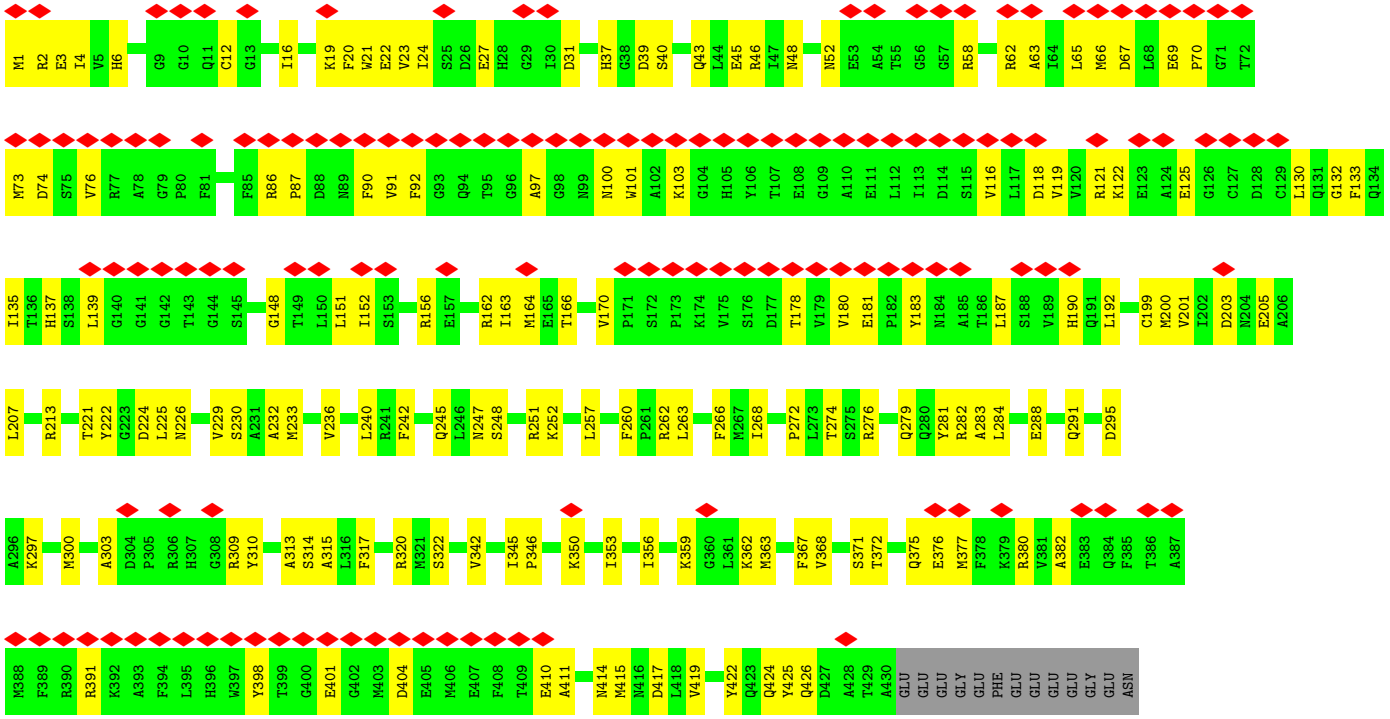
Chain DC:



• Molecule 46: Tubulin beta chain

Chain AB:

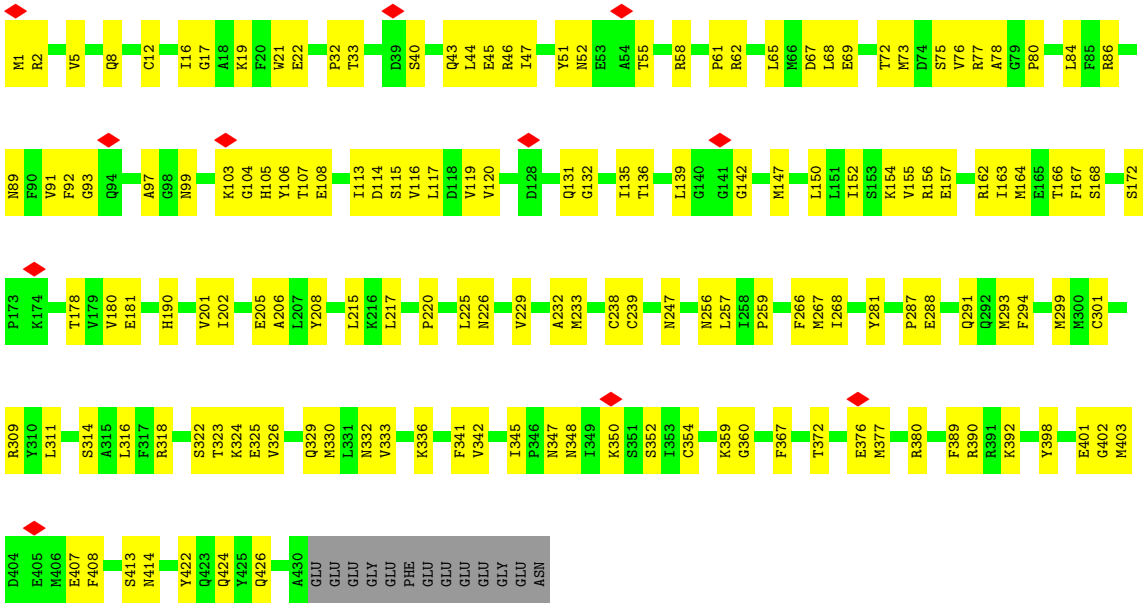




• Molecule 46: Tubulin beta chain

Chain AD:

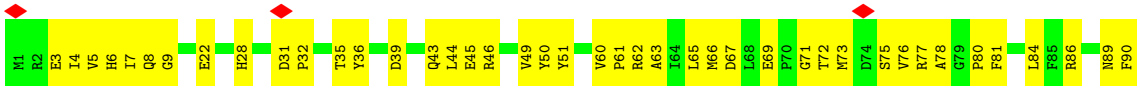


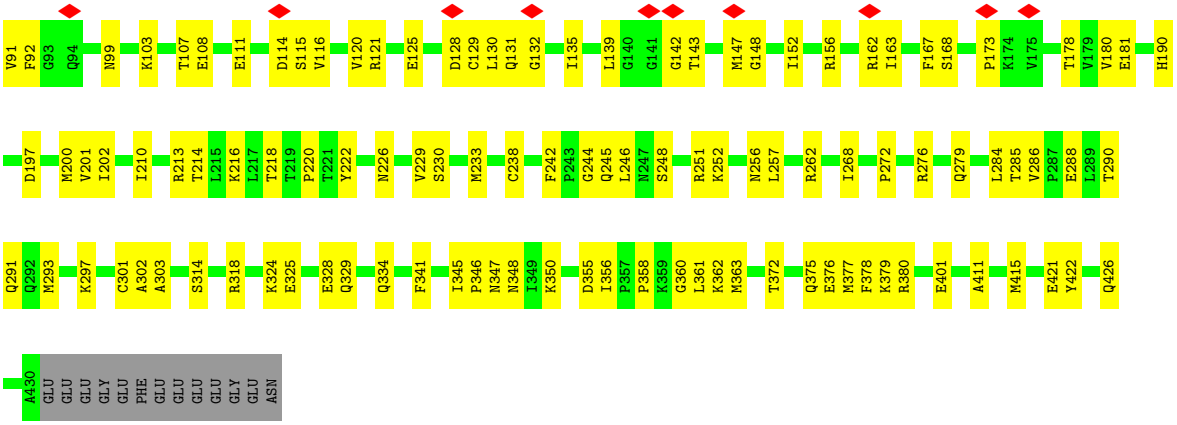


• Molecule 46: Tubulin beta chain

Chain AF:





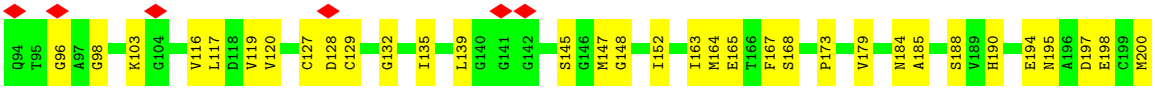


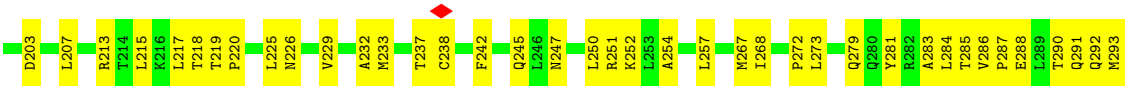
• Molecule 46: Tubulin beta chain

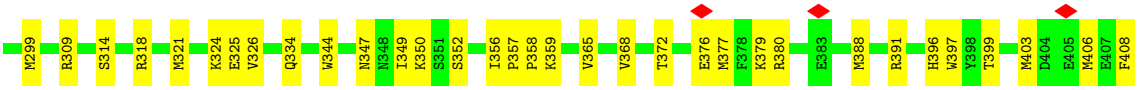
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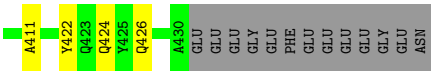








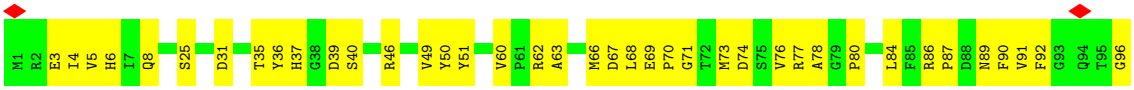


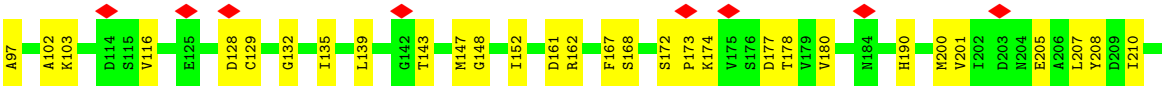


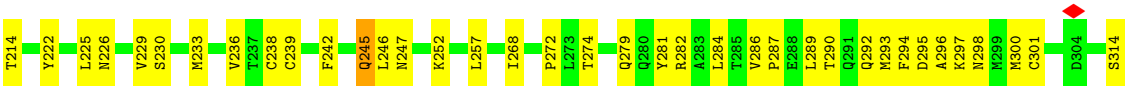
• Molecule 46: Tubulin beta chain

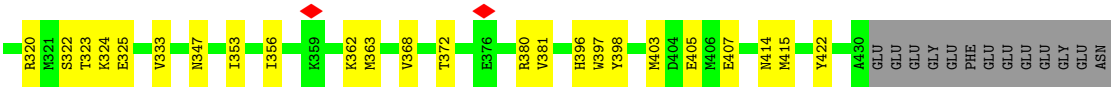
Chain AJ:







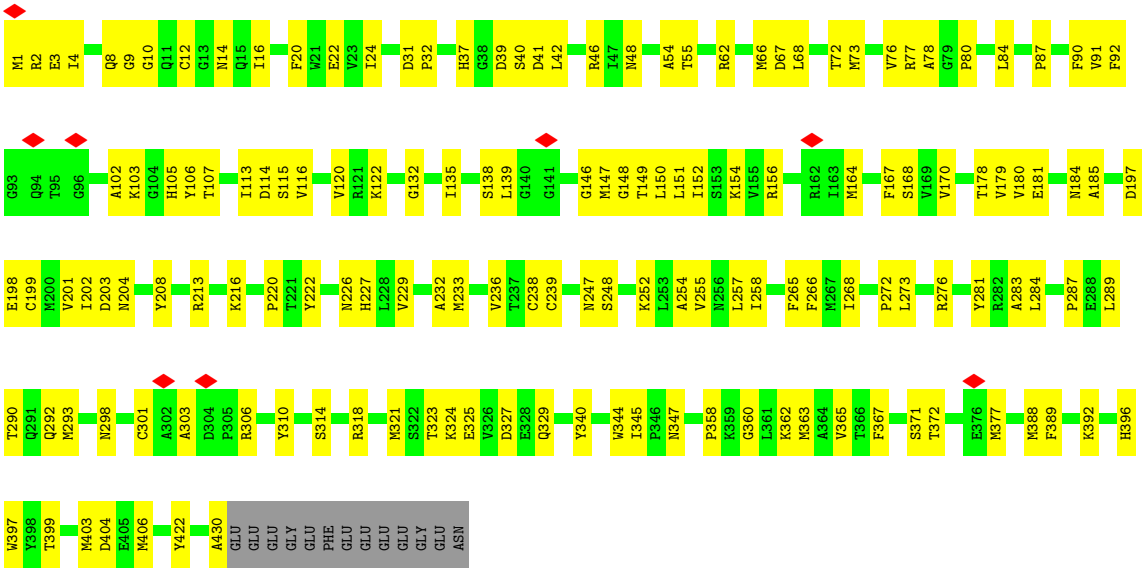




• Molecule 46: Tubulin beta chain

Chain AL:

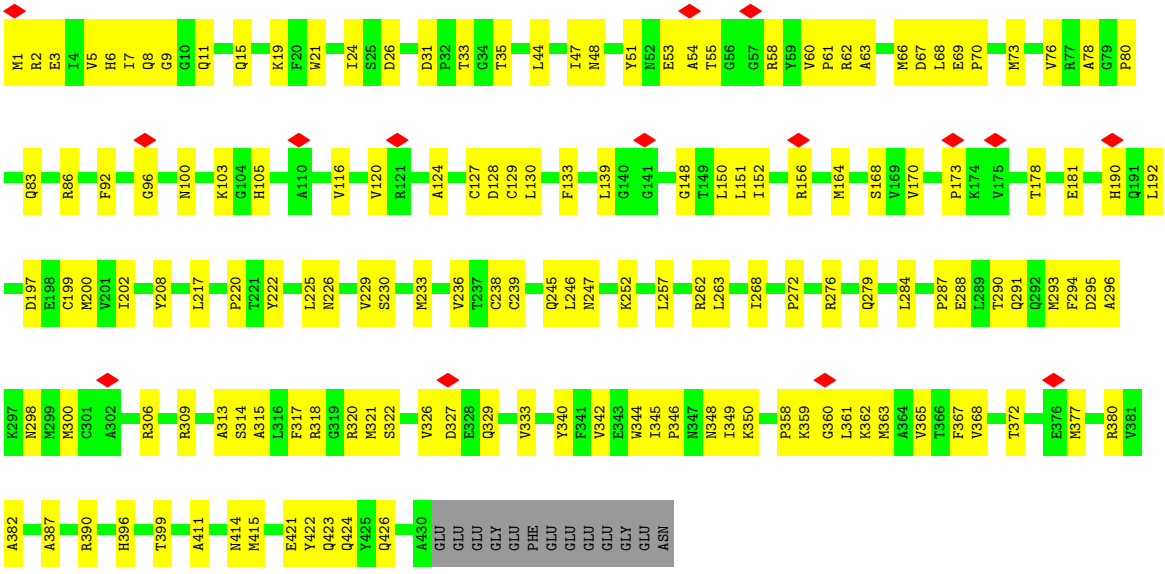




• Molecule 46: Tubulin beta chain

Chain AN:

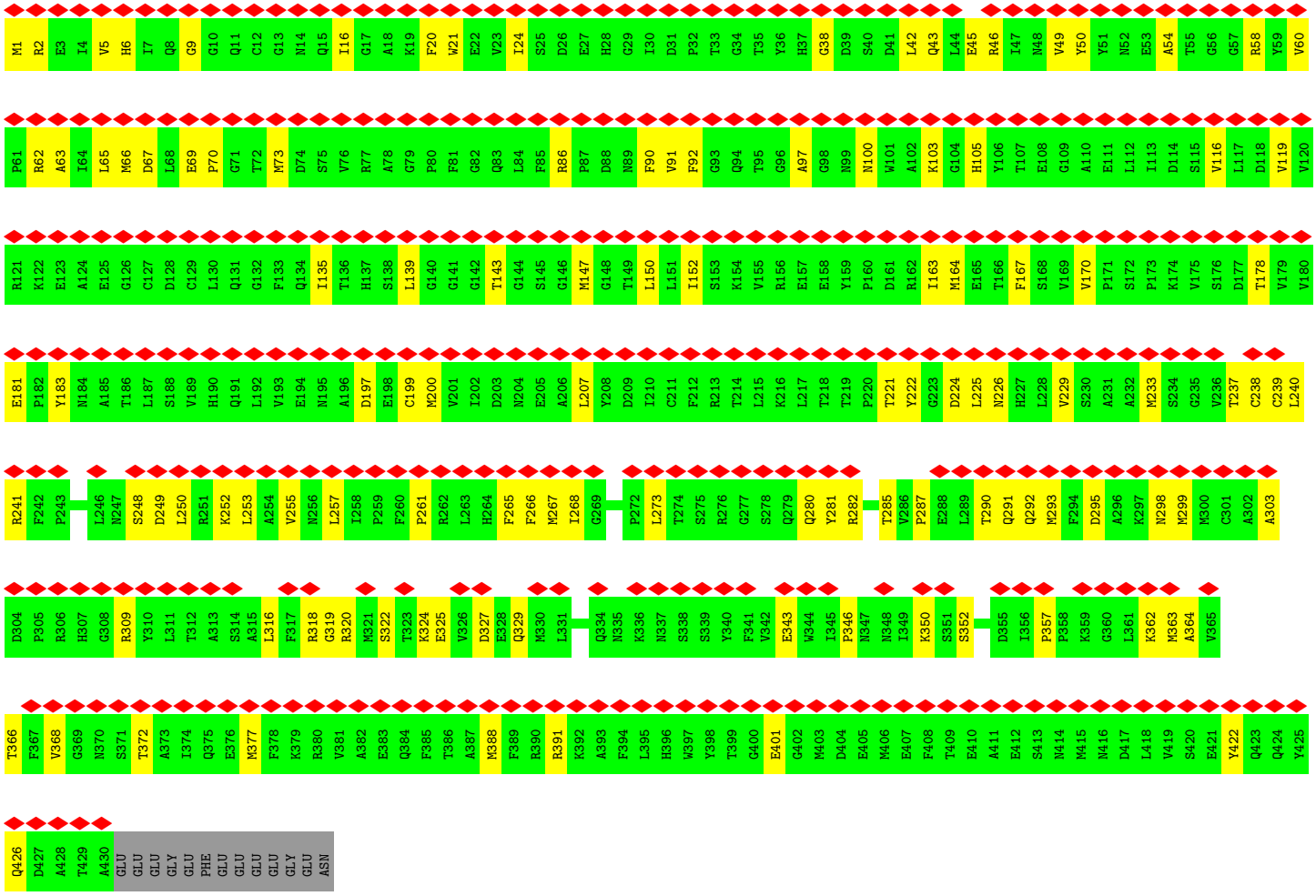




• Molecule 46: Tubulin beta chain

Chain BB:

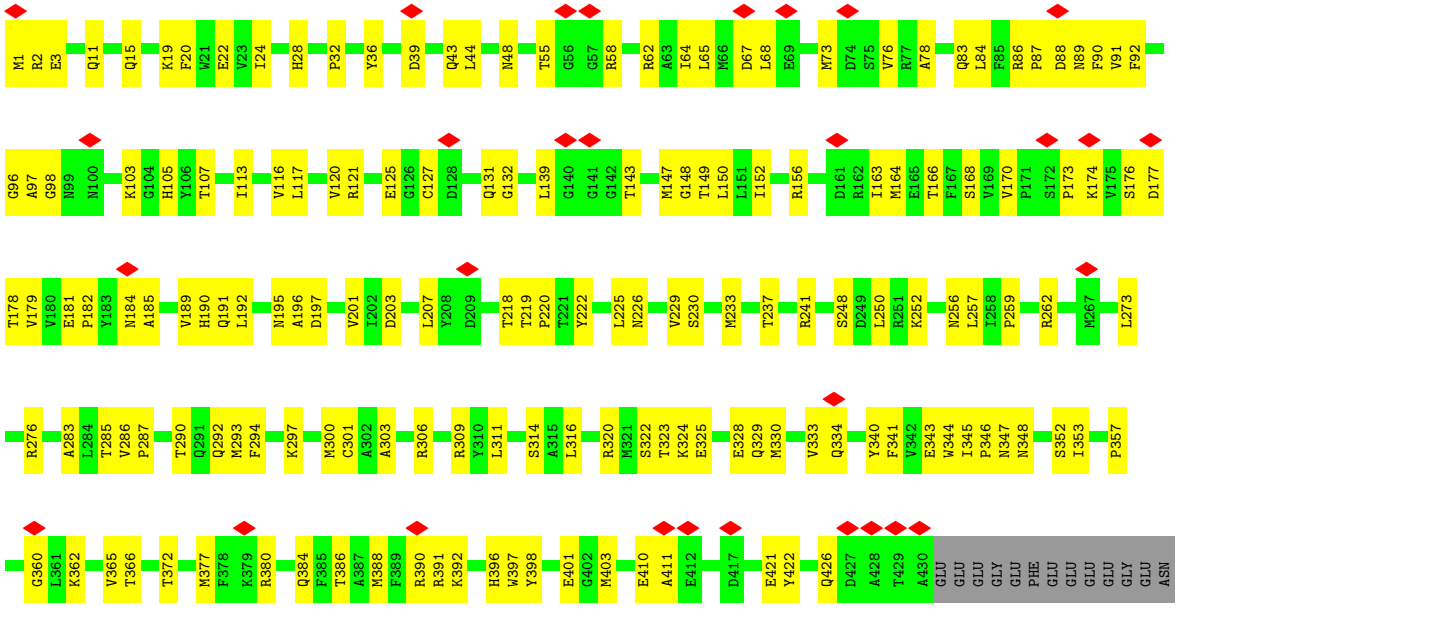




• Molecule 46: Tubulin beta chain

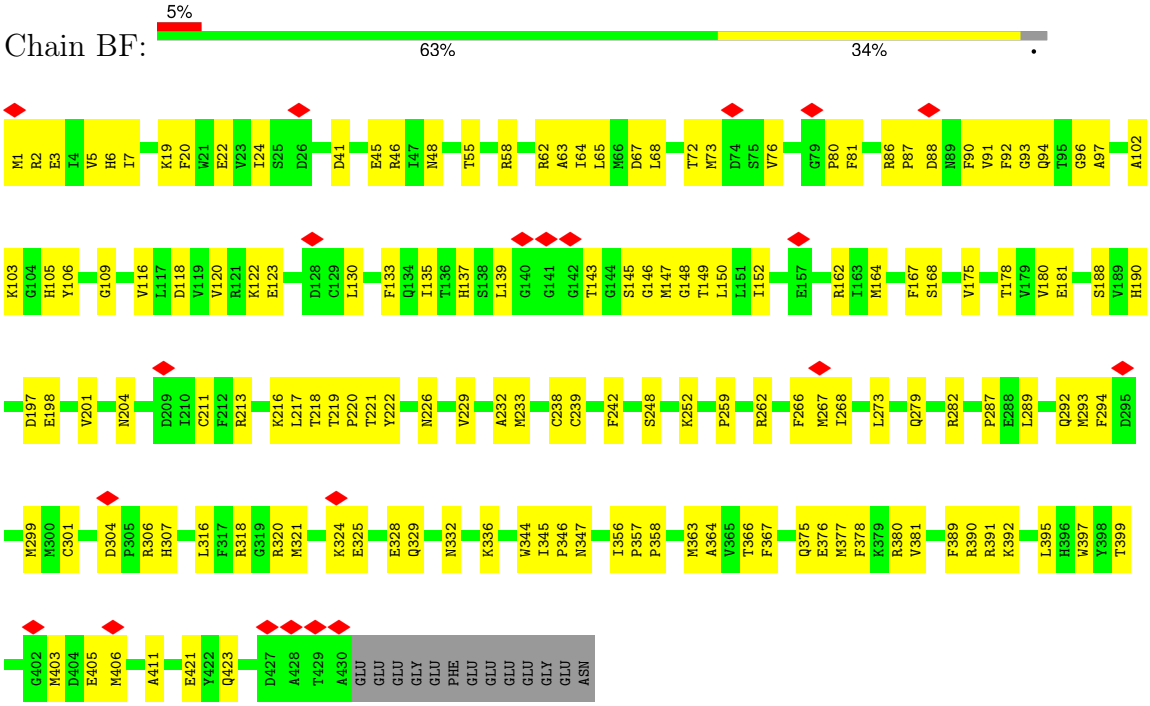
Chain BD:





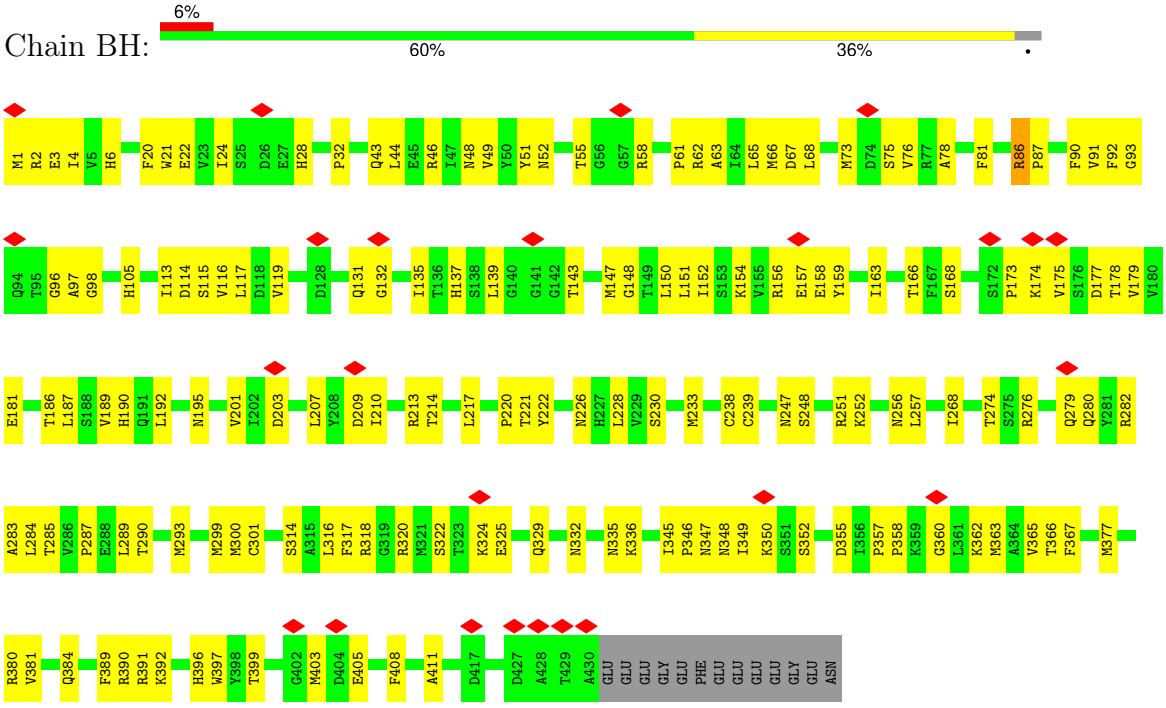
• Molecule 46: Tubulin beta chain

Chain BF:



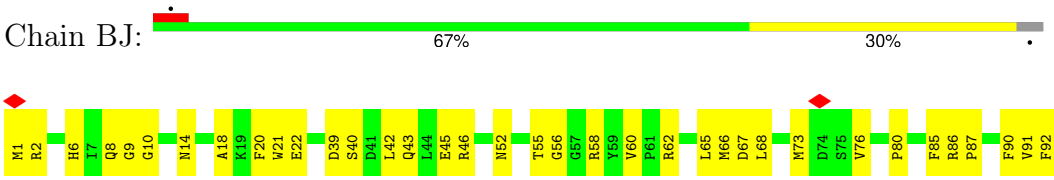
• Molecule 46: Tubulin beta chain

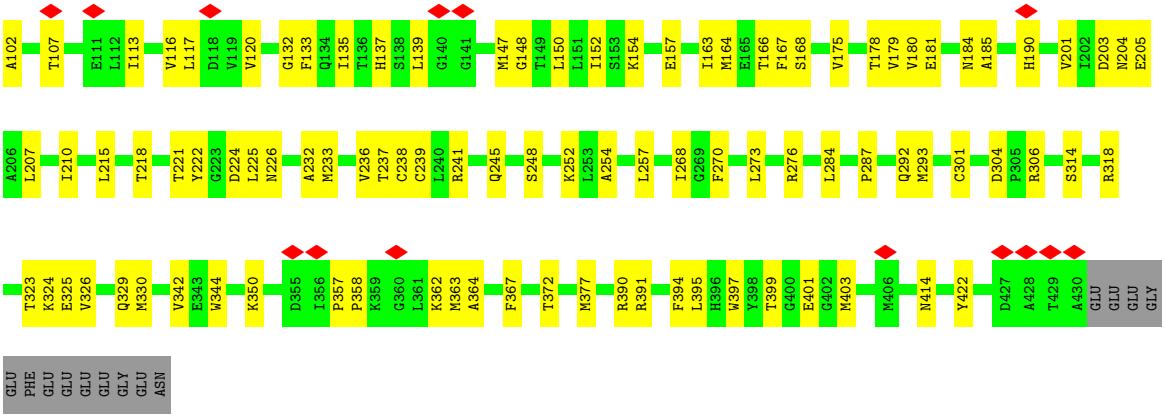
Chain BH:



• Molecule 46: Tubulin beta chain

Chain BJ:

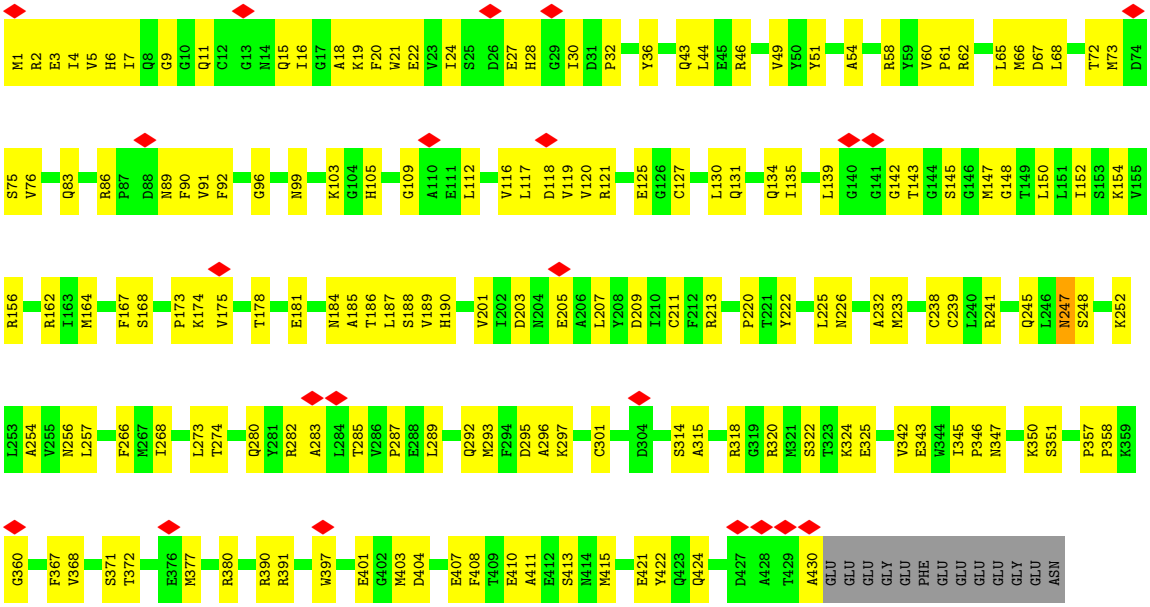




• Molecule 46: Tubulin beta chain

Chain BL:

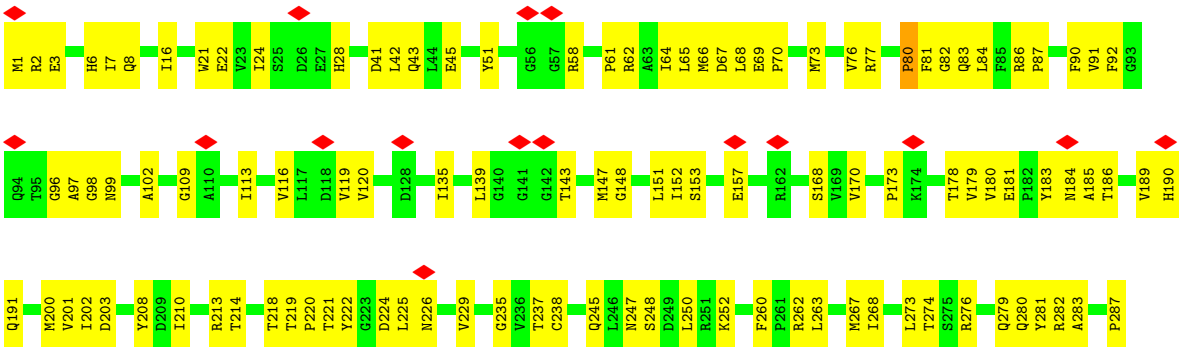


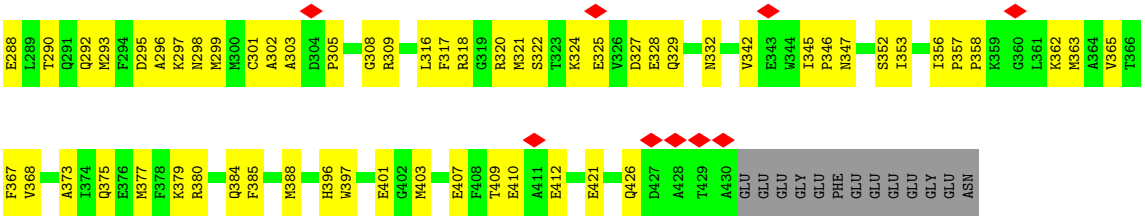


• Molecule 46: Tubulin beta chain

Chain BN:



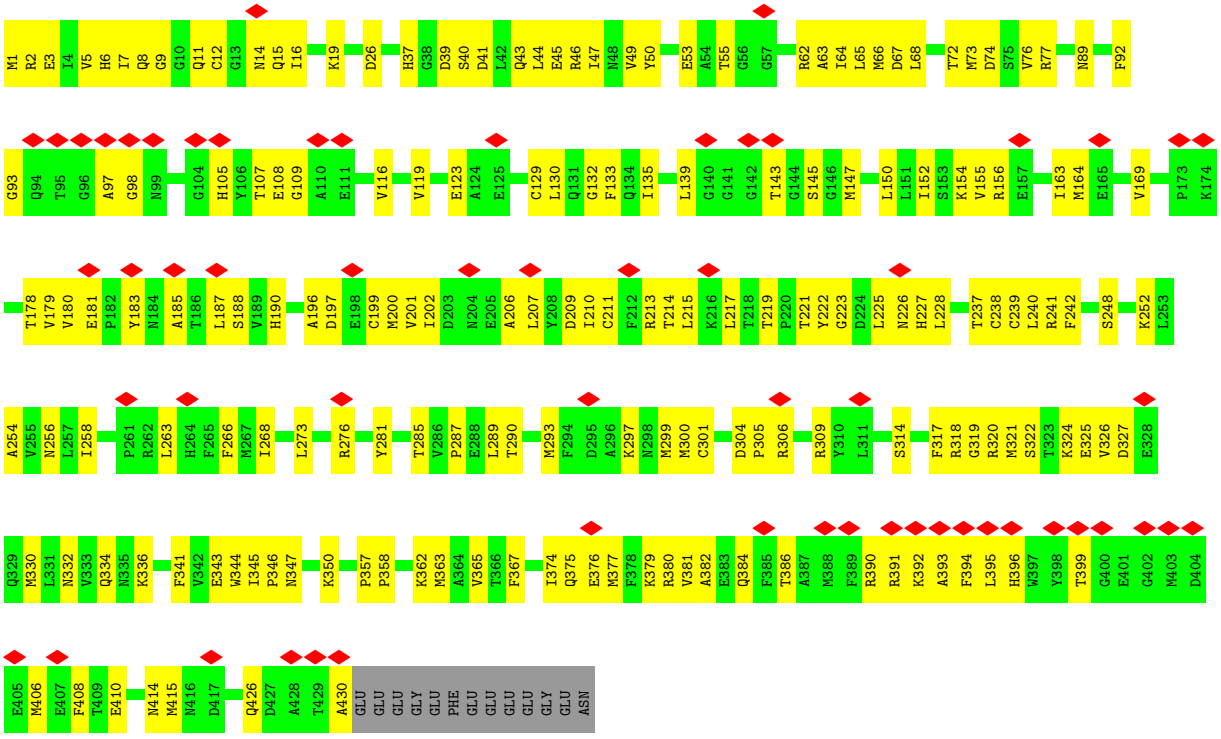




• Molecule 46: Tubulin beta chain

Chain CB:

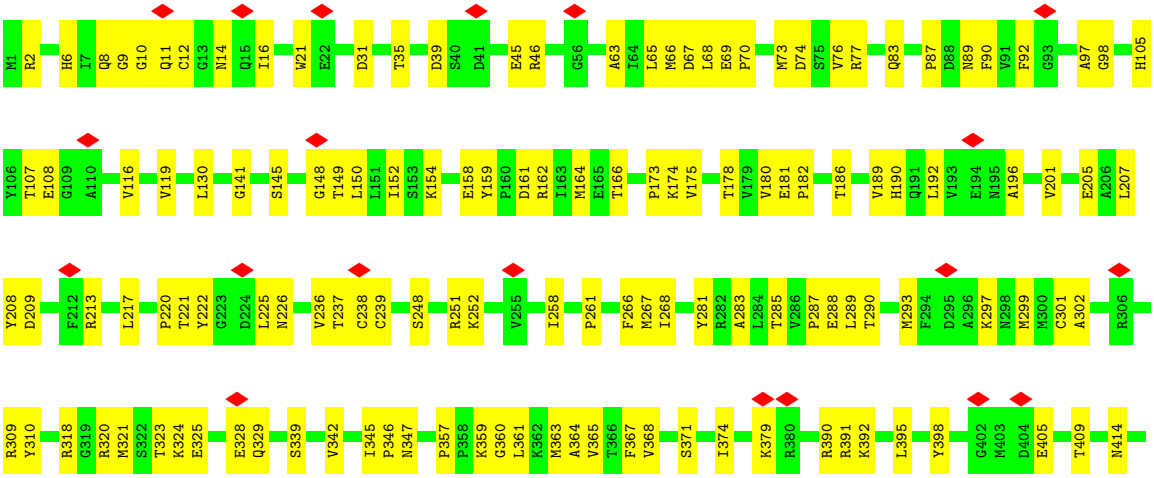


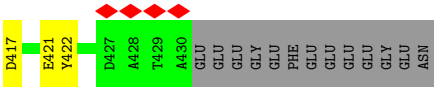


• Molecule 46: Tubulin beta chain

Chain CD:



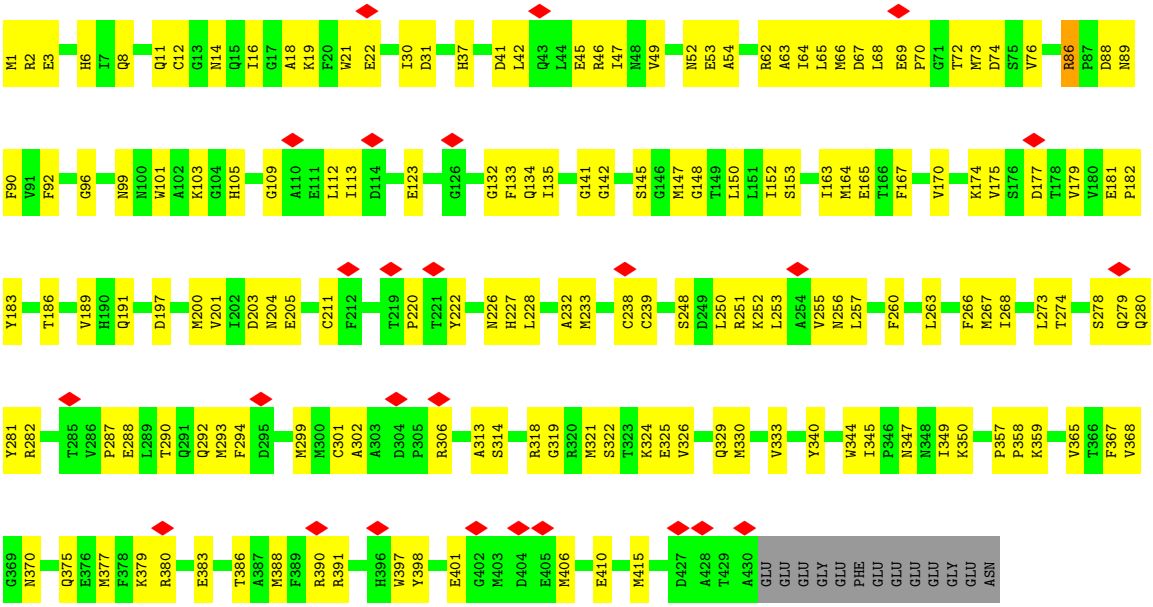




• Molecule 46: Tubulin beta chain

Chain CF:

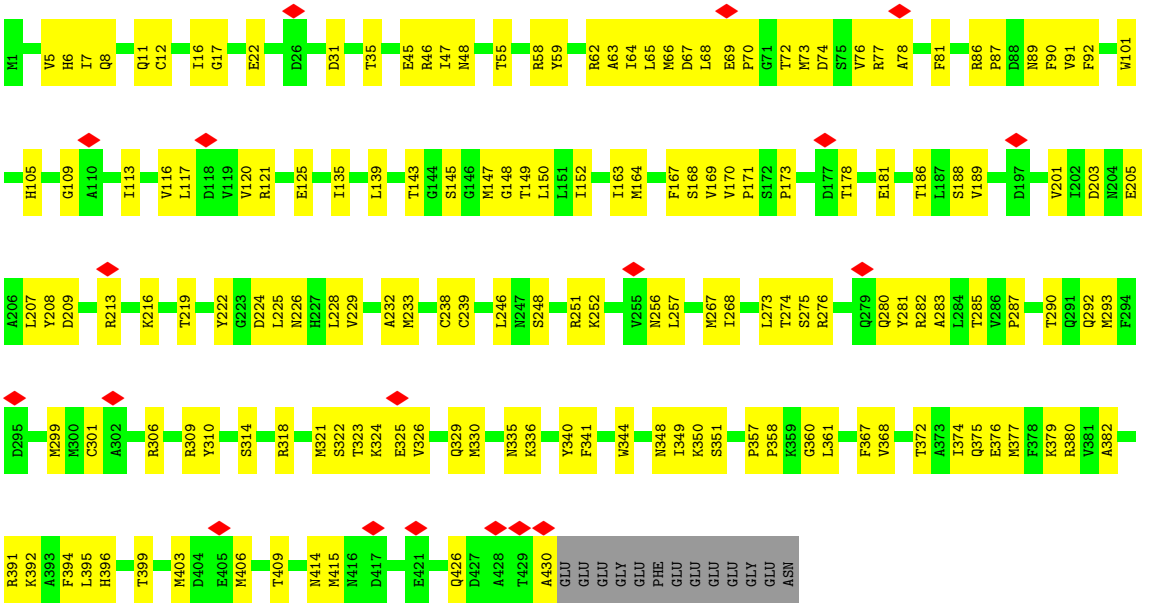




• Molecule 46: Tubulin beta chain

Chain CH:

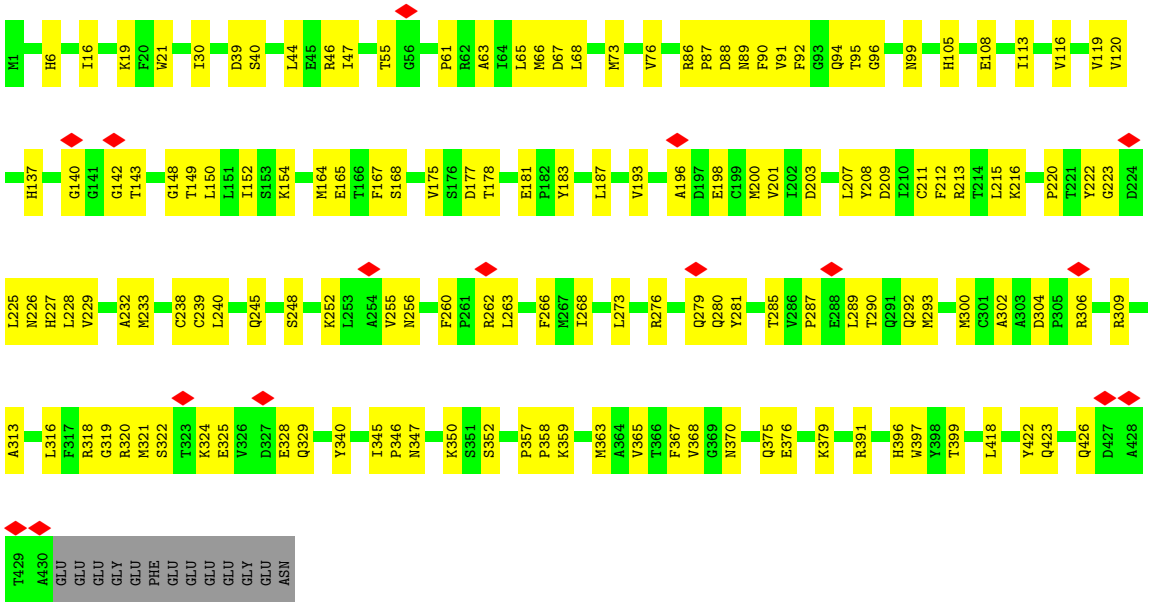




• Molecule 46: Tubulin beta chain

Chain CJ:

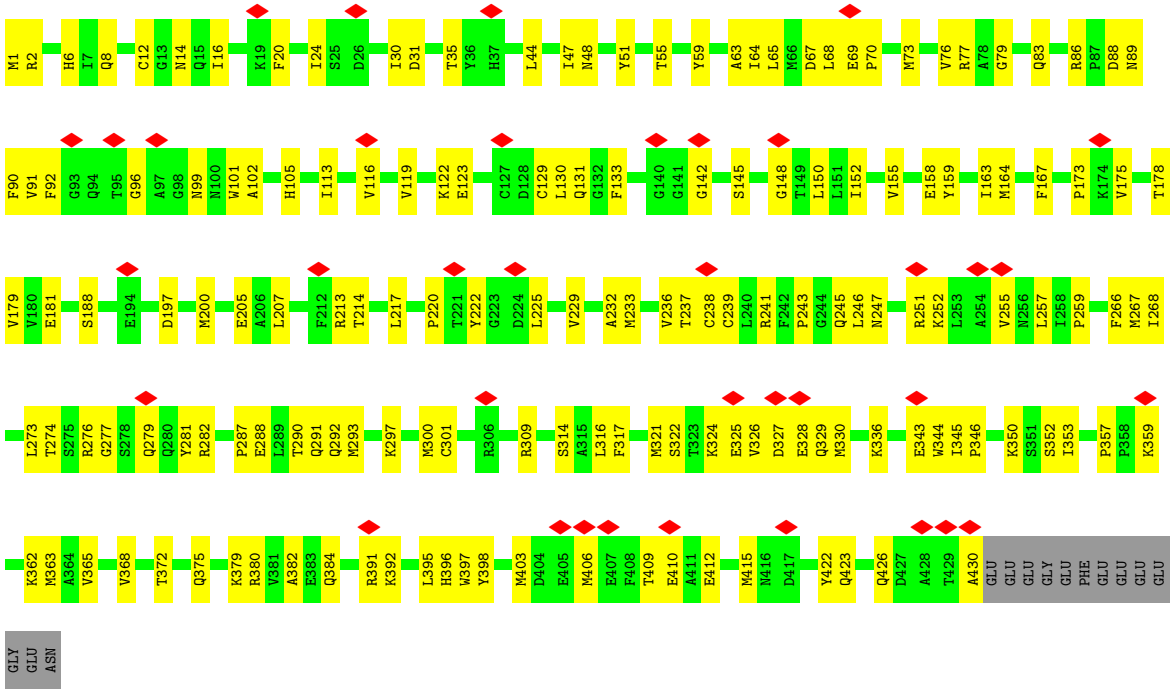




• Molecule 46: Tubulin beta chain

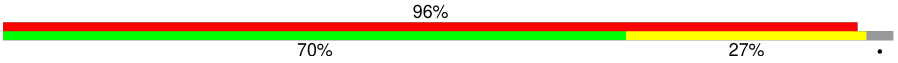
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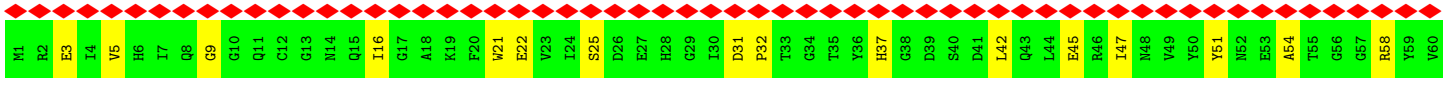


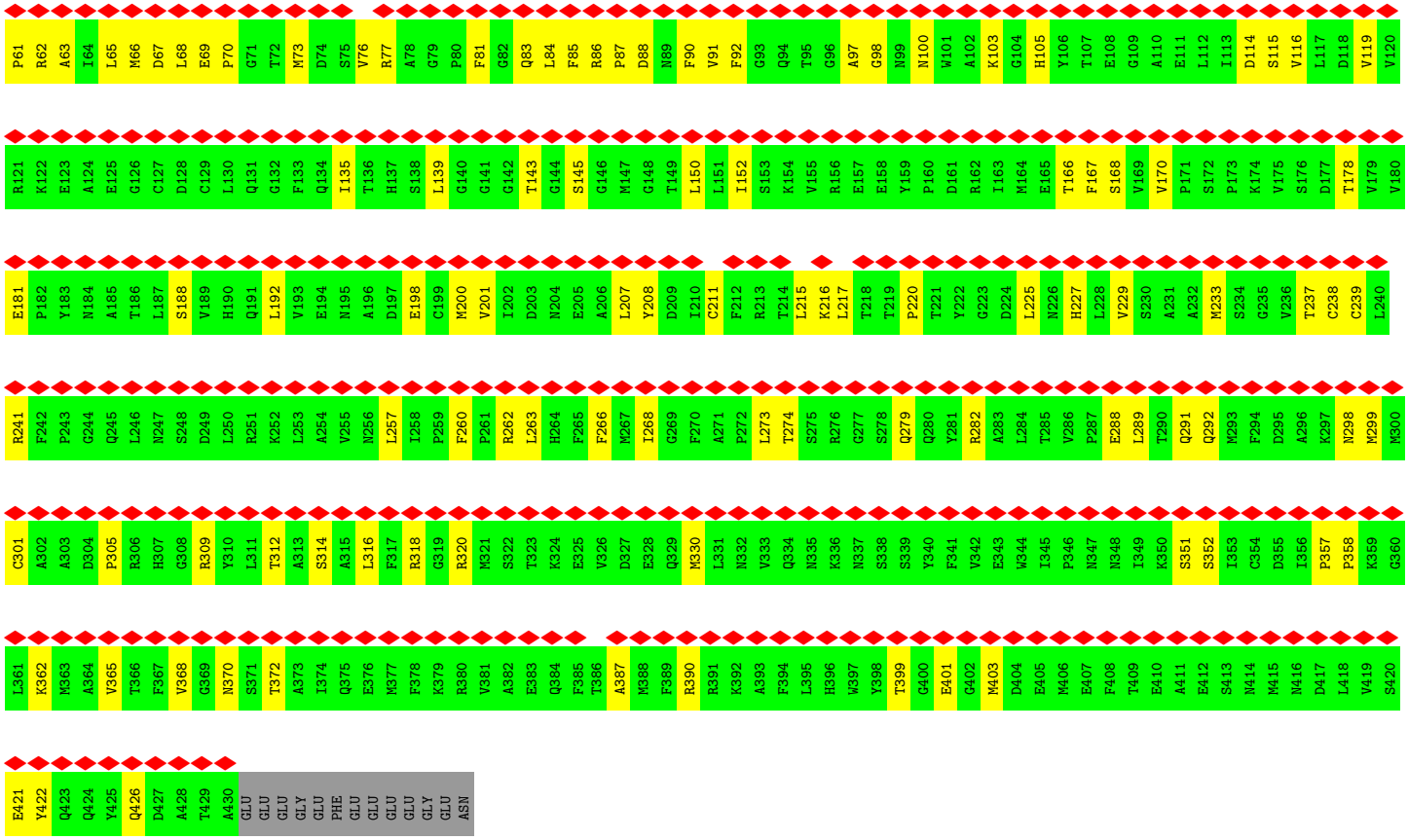


• Molecule 46: Tubulin beta chain

Chain CN:



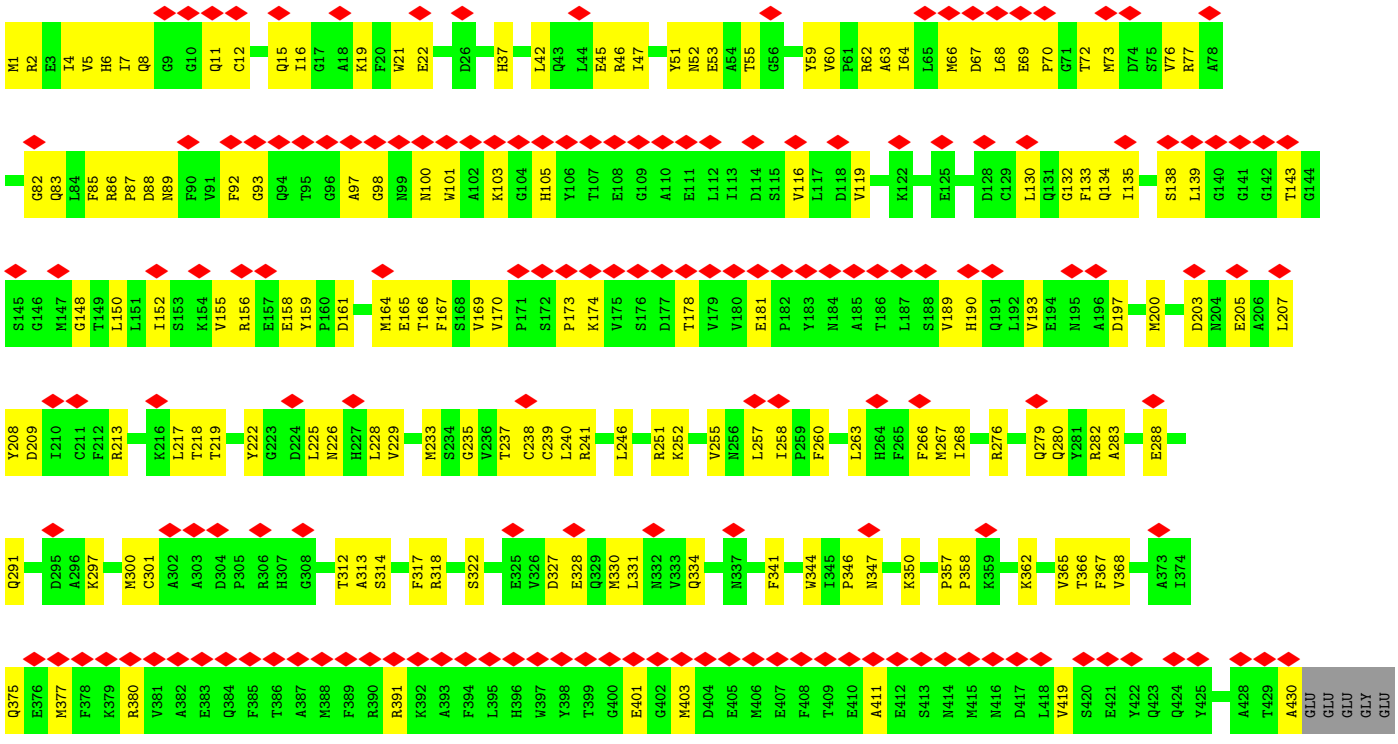




• Molecule 46: Tubulin beta chain

Chain DB:



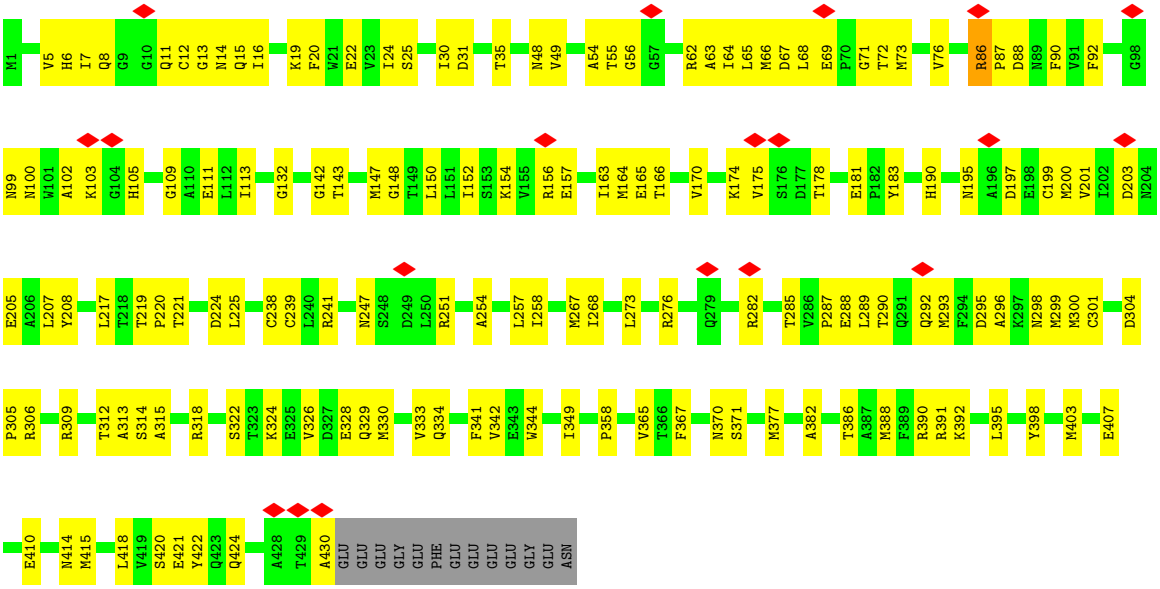




• Molecule 46: Tubulin beta chain

Chain DD:

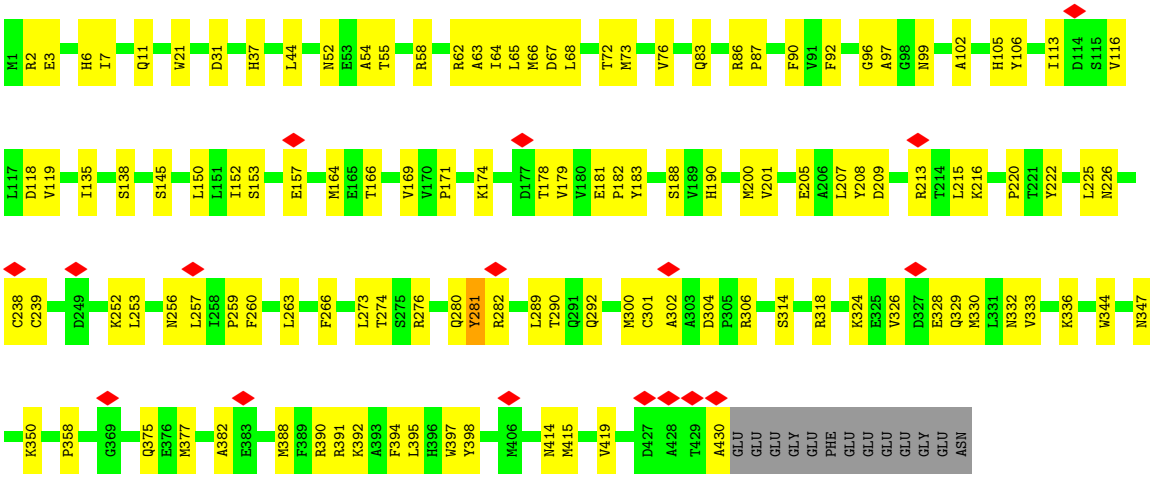




• Molecule 46: Tubulin beta chain

Chain DF:

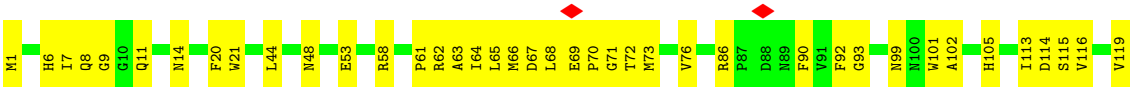


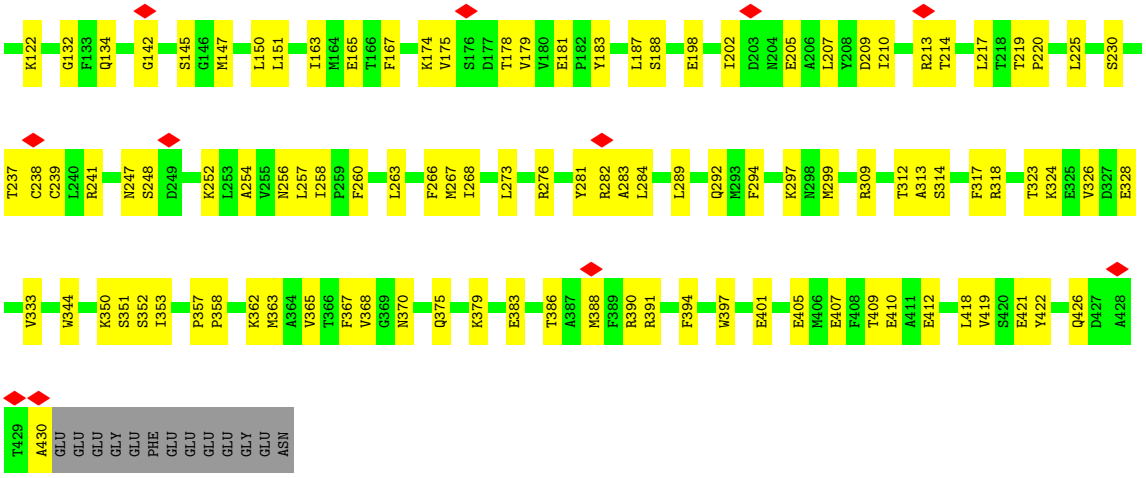


• Molecule 46: Tubulin beta chain

Chain DH:



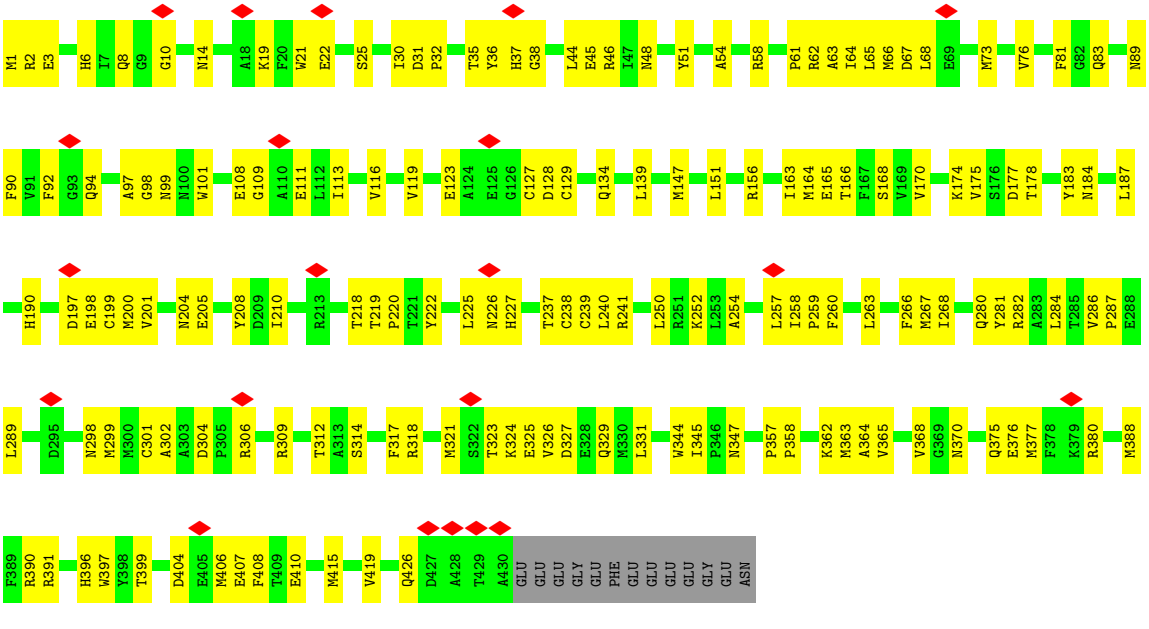




• Molecule 46: Tubulin beta chain

Chain DJ:

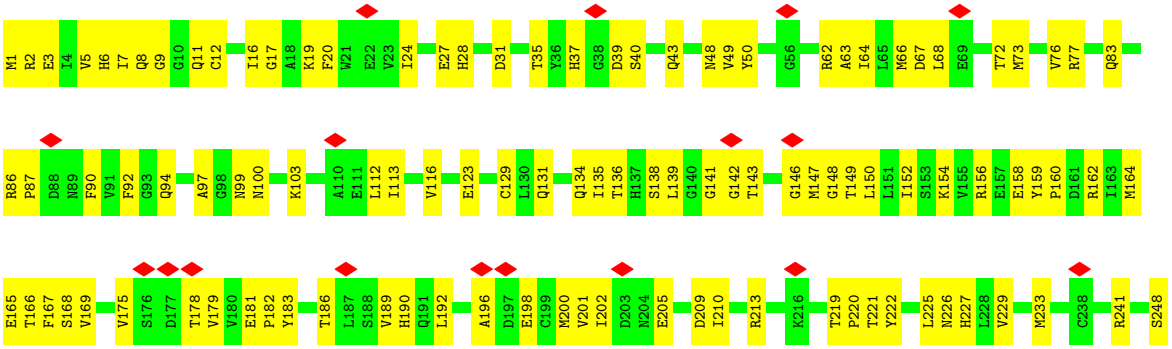


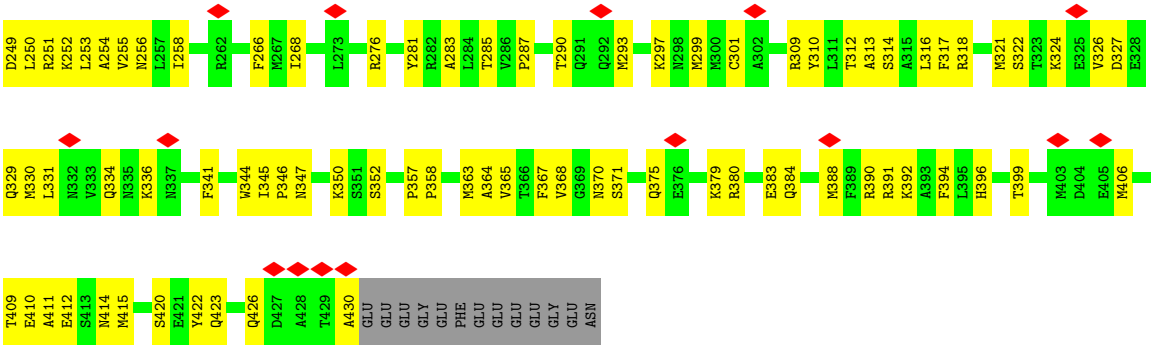


• Molecule 46: Tubulin beta chain

Chain DL:

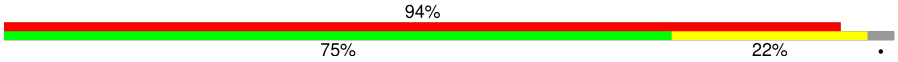


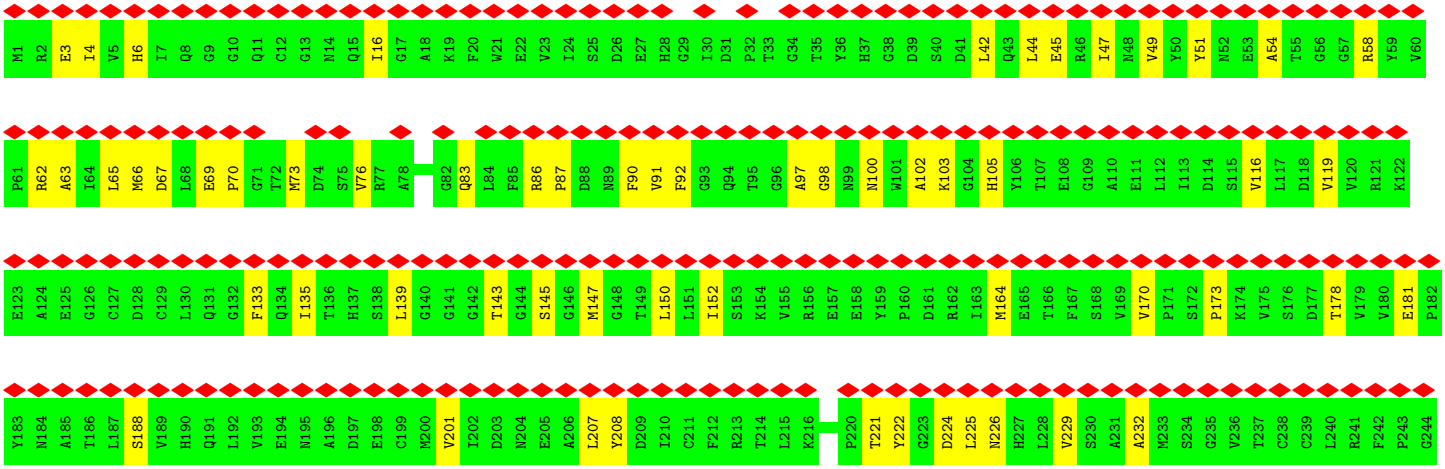




• Molecule 46: Tubulin beta chain

Chain DN:

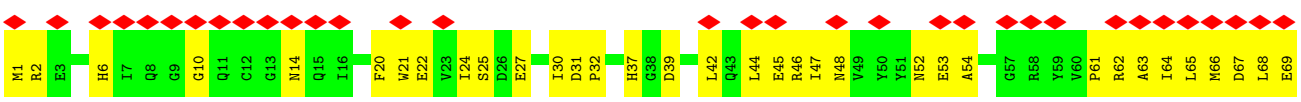


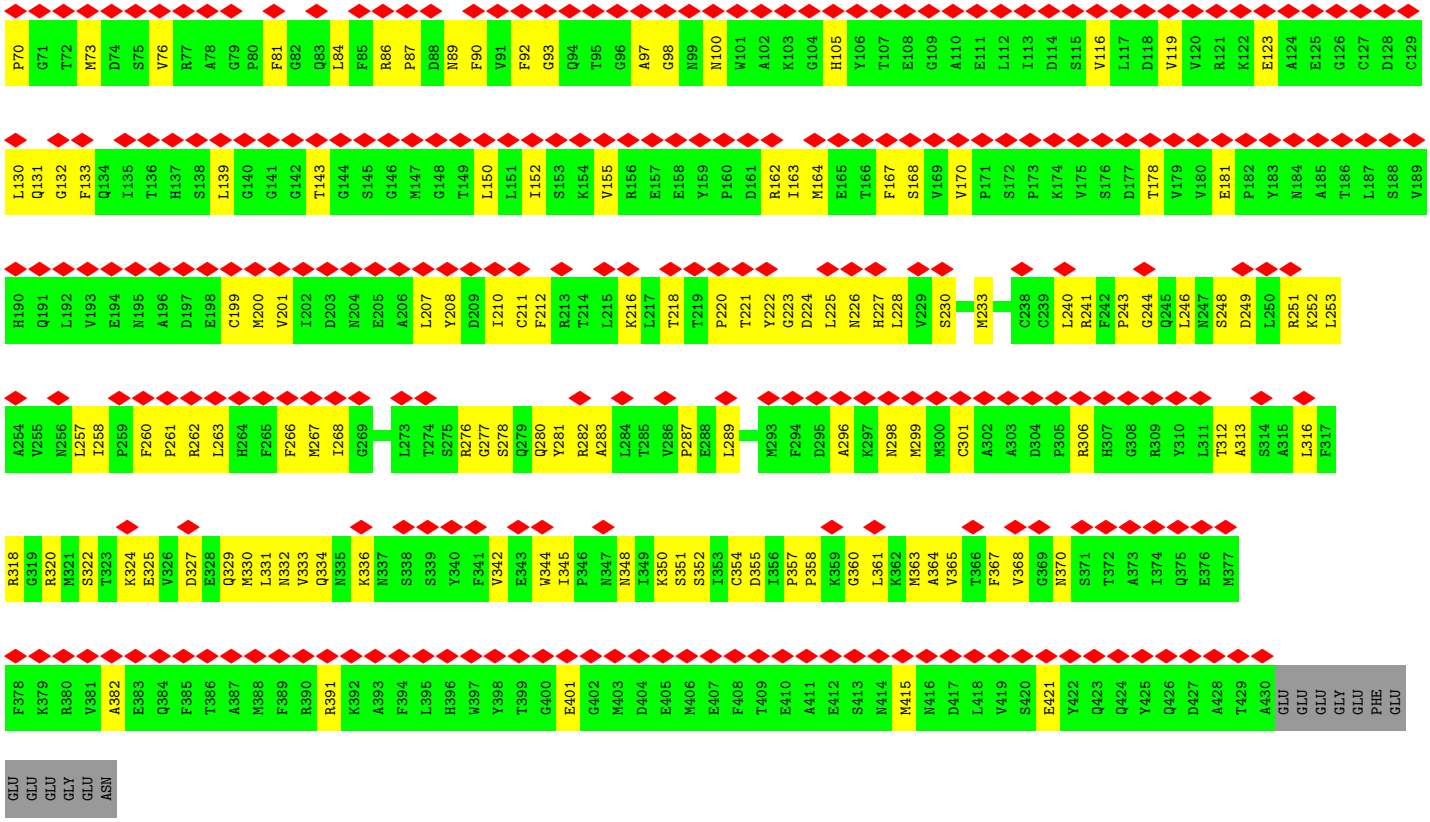


• Molecule 46: Tubulin beta chain

Chain EB:



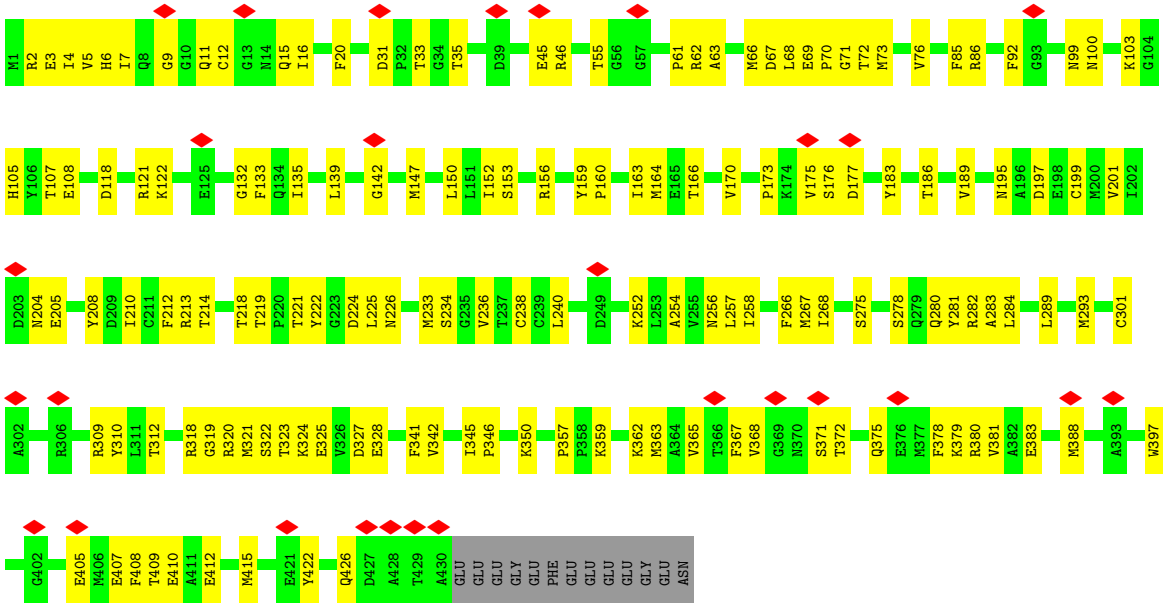




• Molecule 46: Tubulin beta chain

Chain ED:

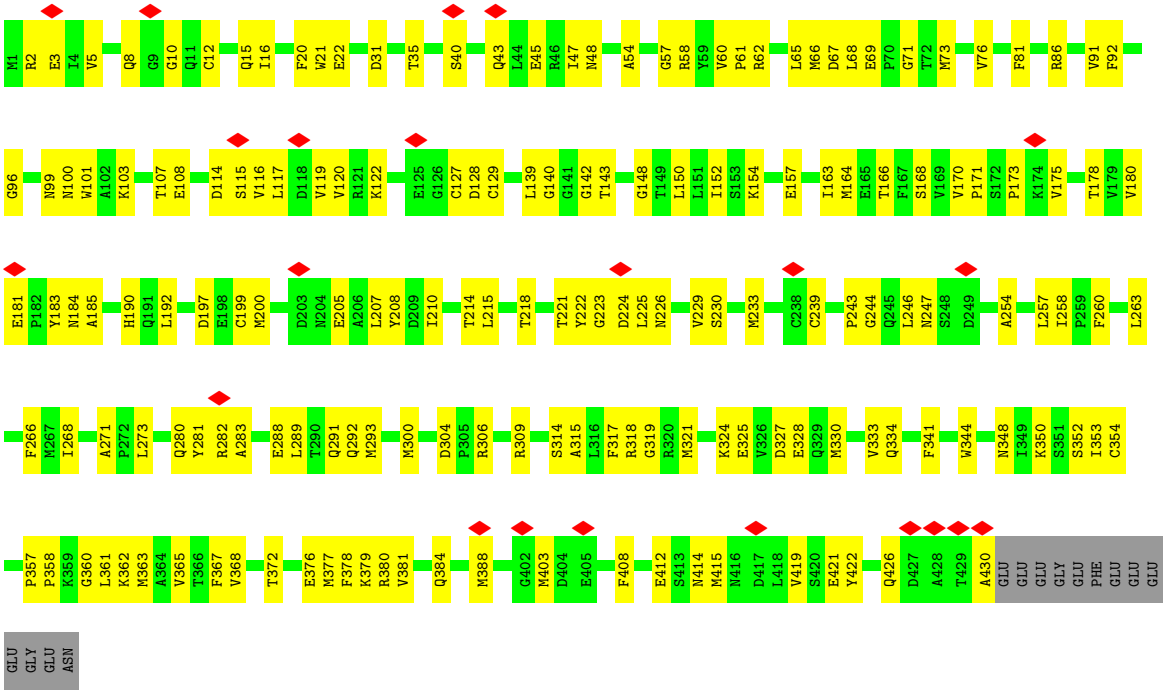




• Molecule 46: Tubulin beta chain

Chain EF:

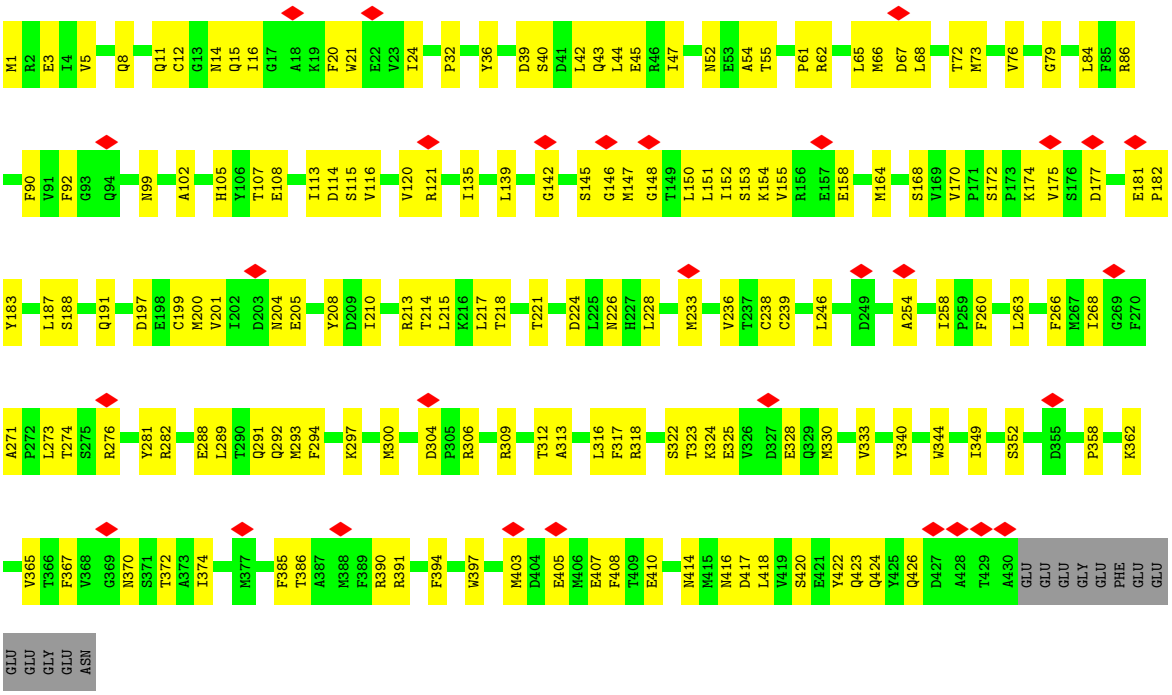




• Molecule 46: Tubulin beta chain

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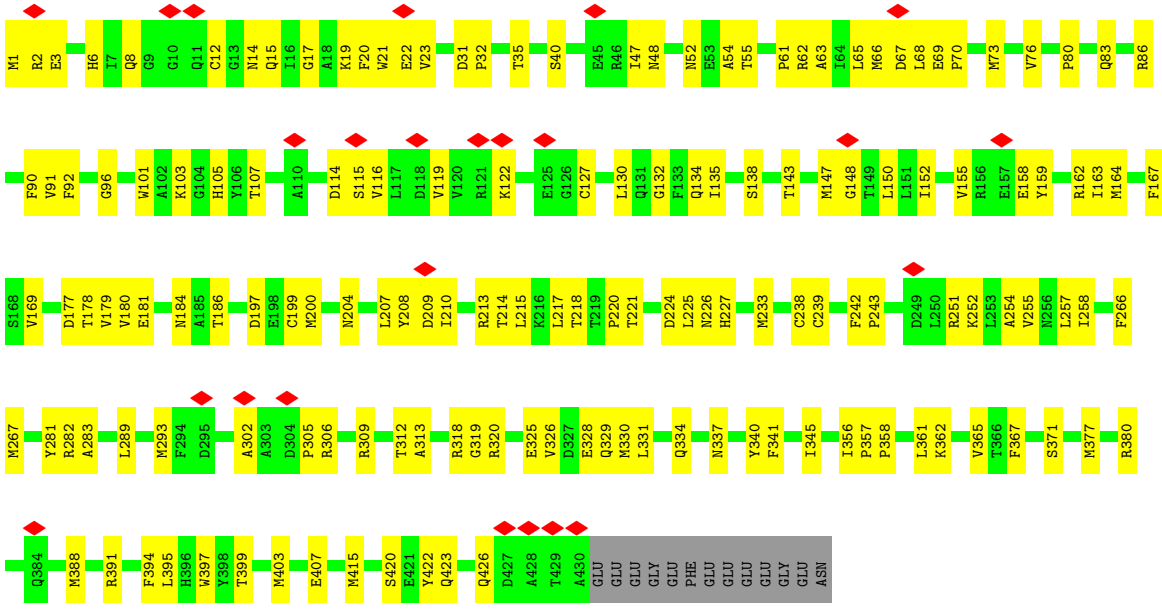




• Molecule 46: Tubulin beta chain

Chain EJ:

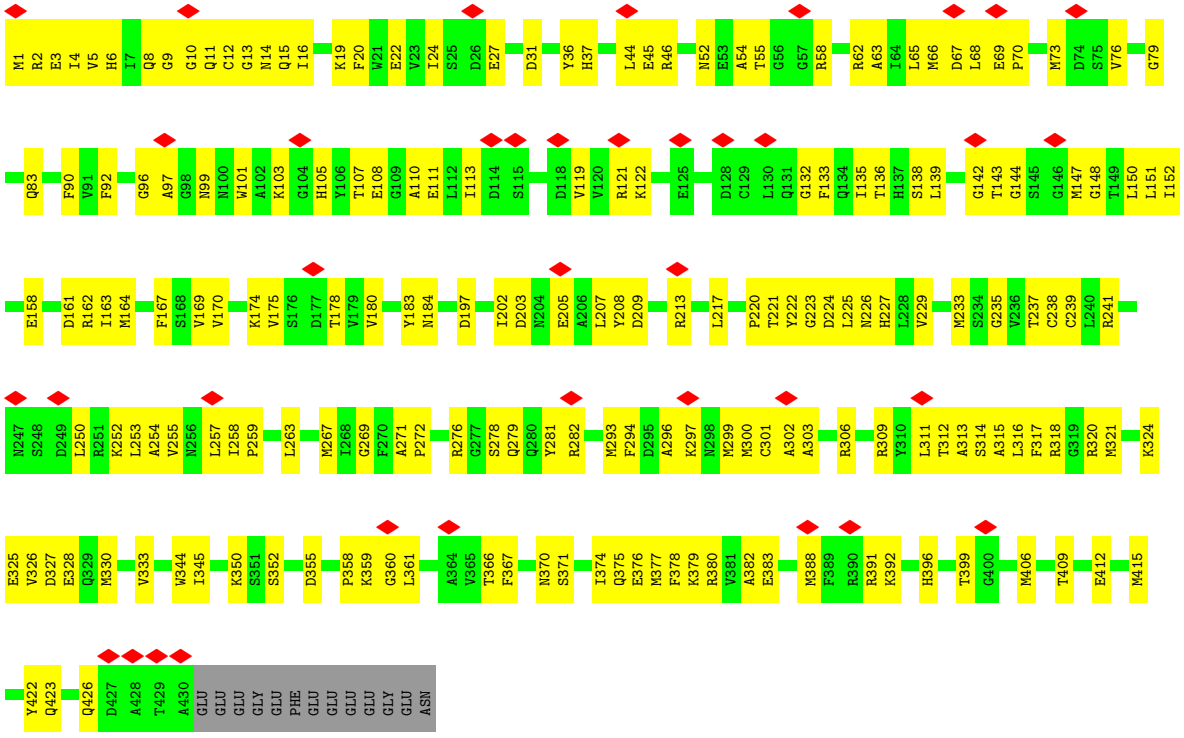




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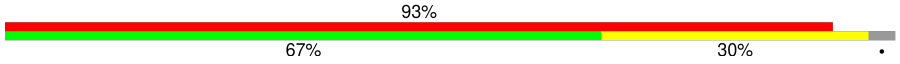
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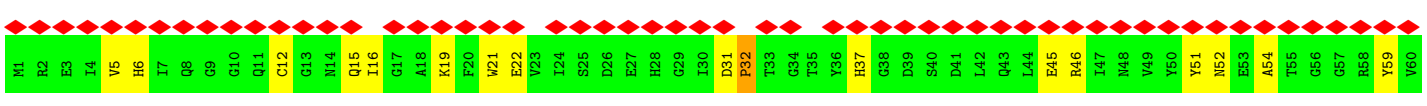


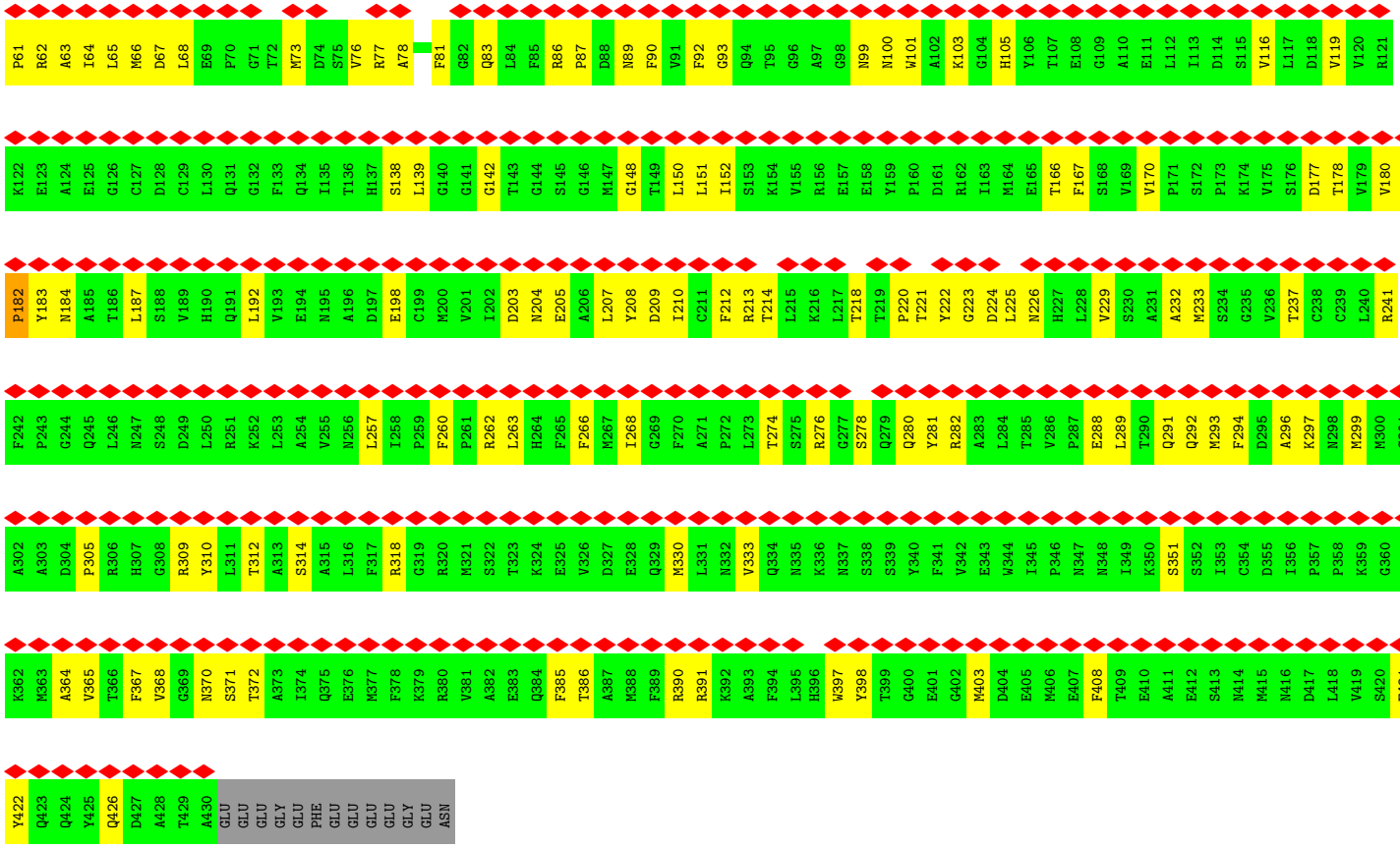


• Molecule 46: Tubulin beta chain

Chain EN:



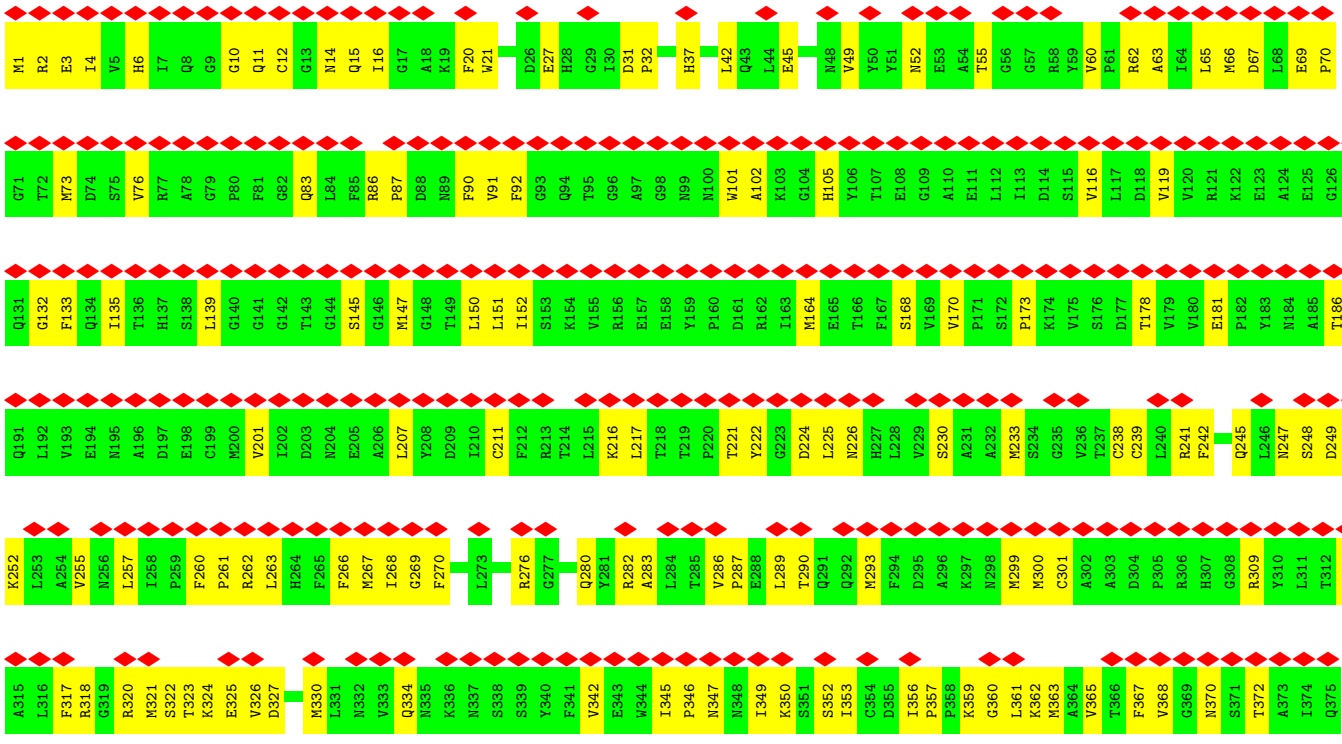


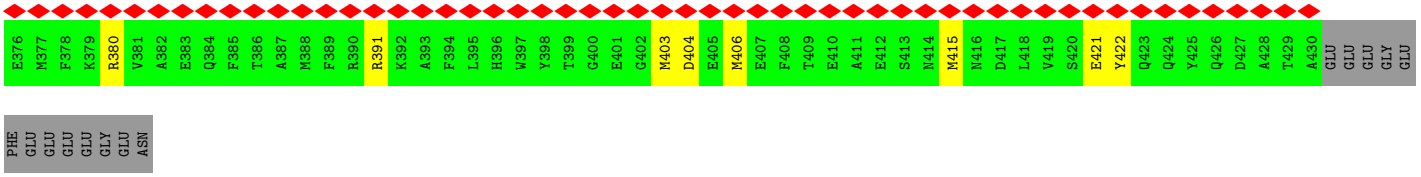


- Molecule 46: Tubulin beta chain

Chain FB:



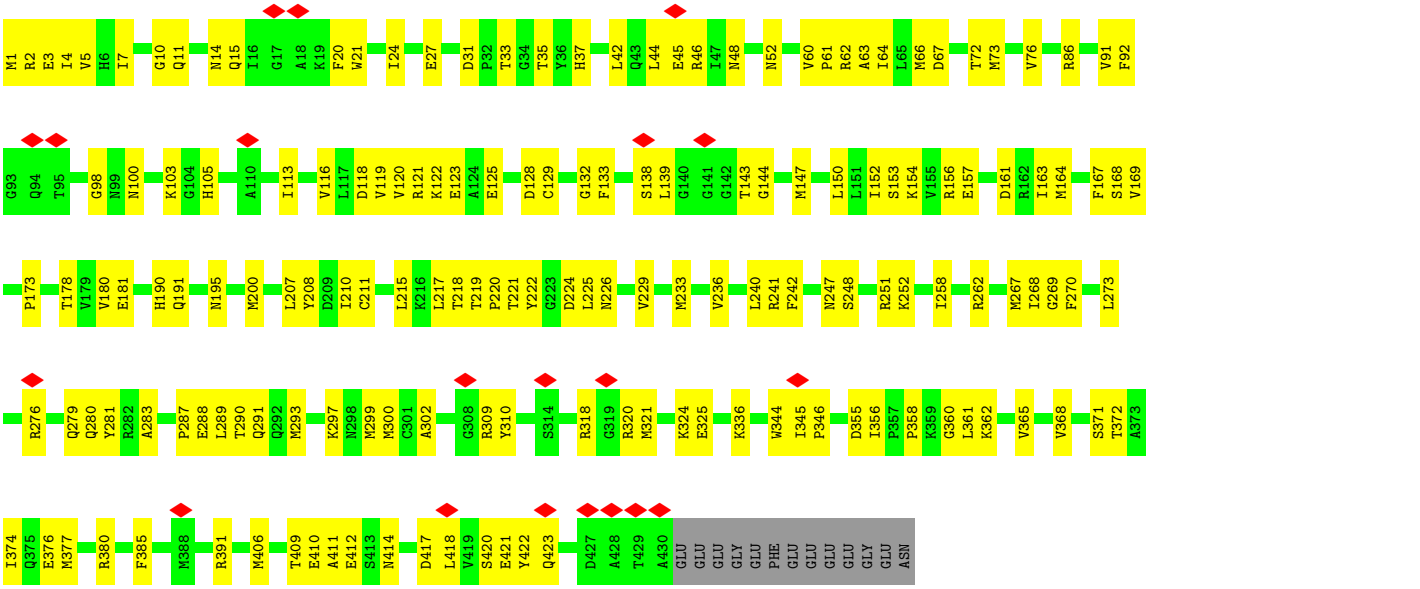




• Molecule 46: Tubulin beta chain

Chain FD:

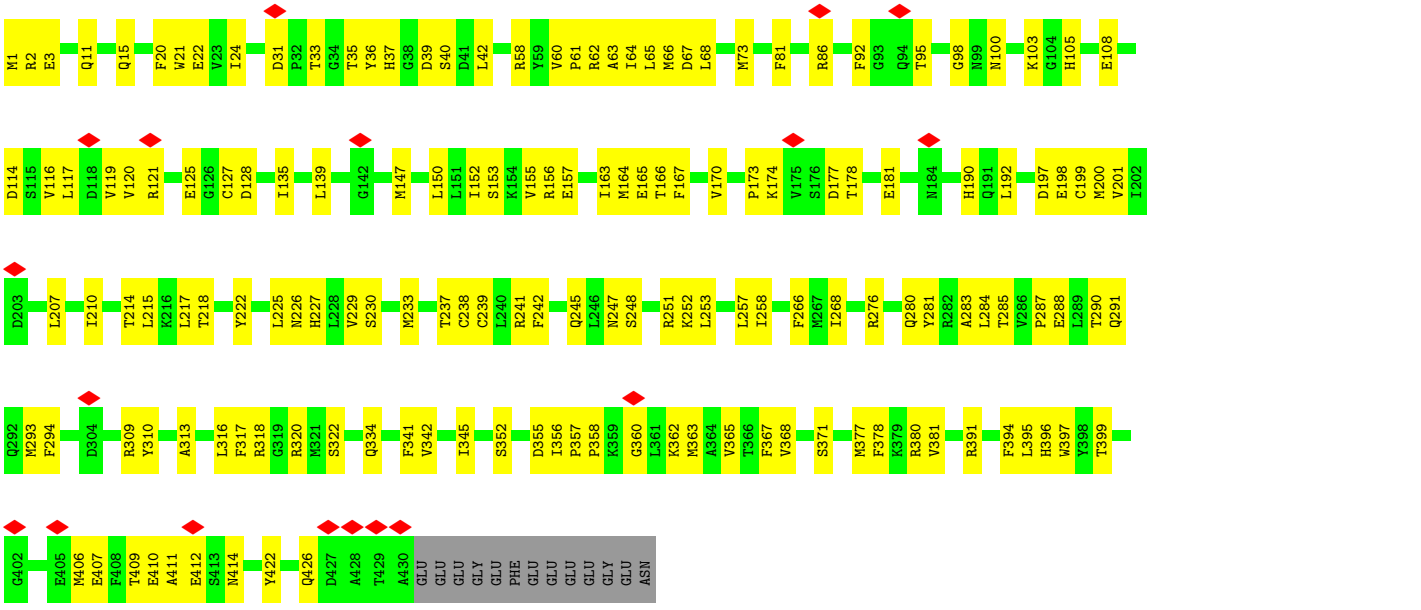




• Molecule 46: Tubulin beta chain

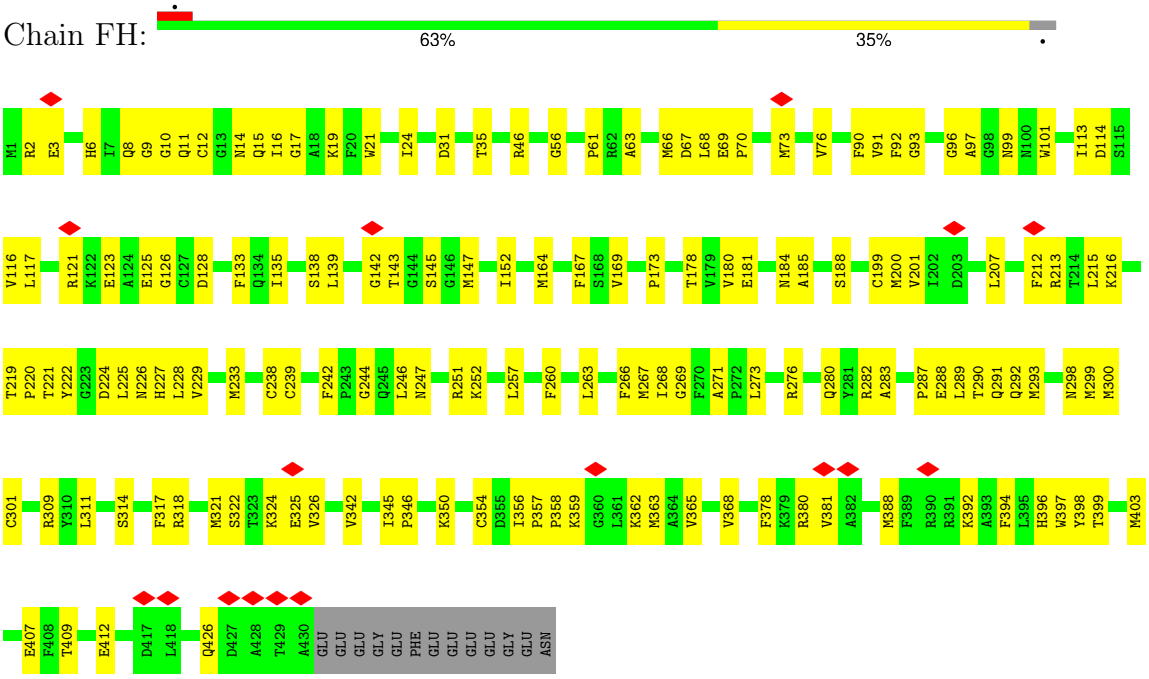
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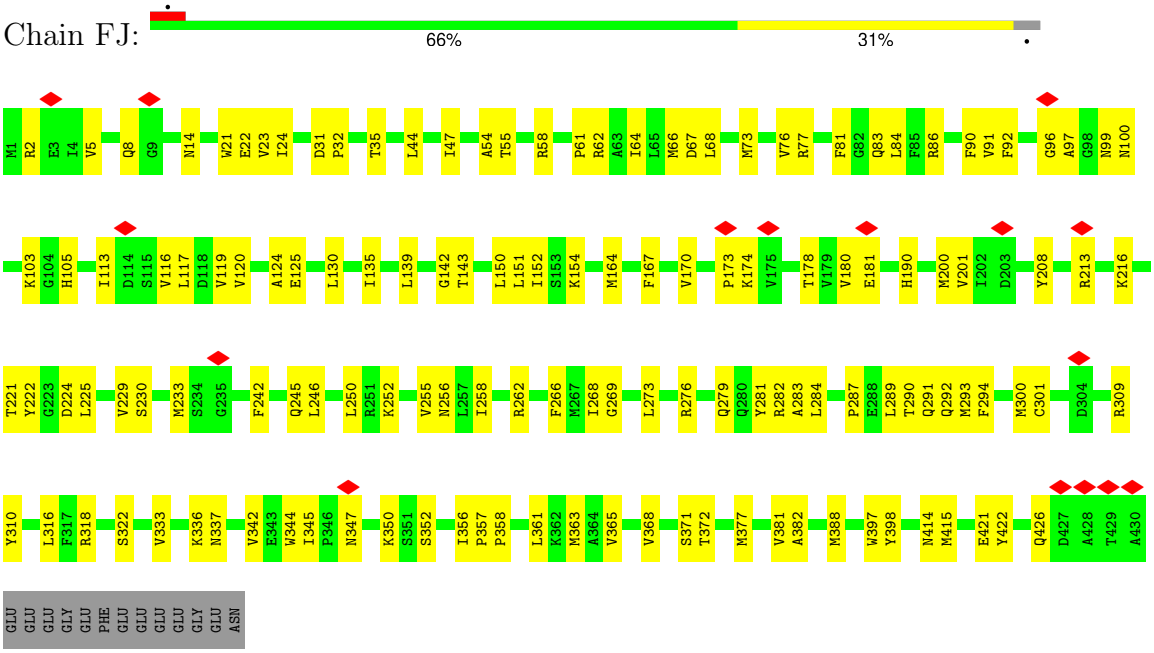
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Chain FH:



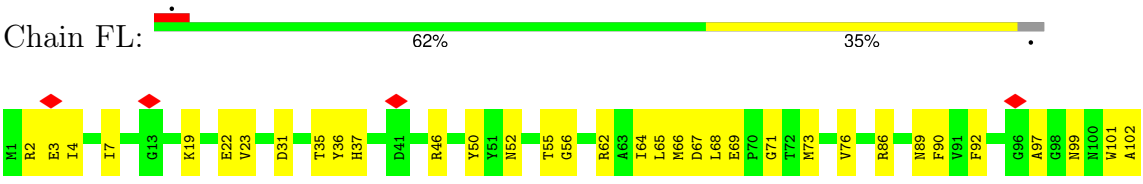
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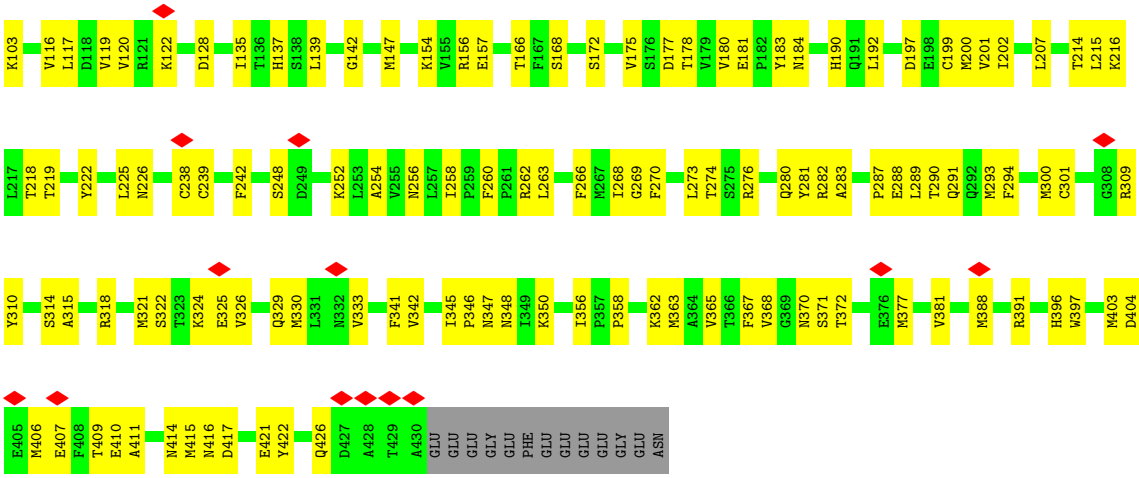
Chain FJ:



• Molecule 46: Tubulin beta chain

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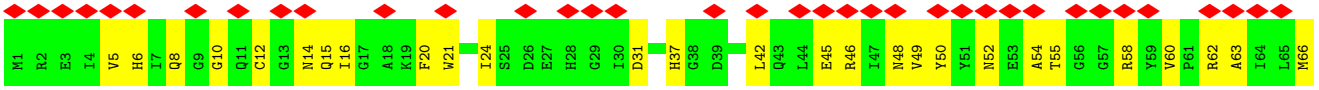


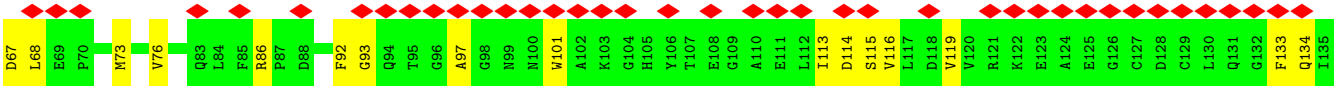


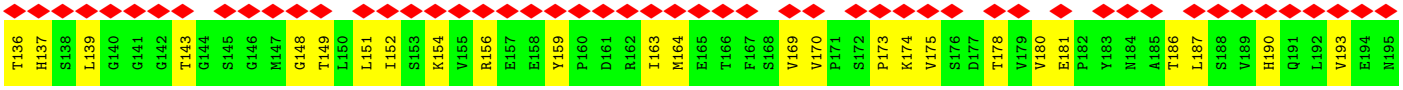
• Molecule 46: Tubulin beta chain

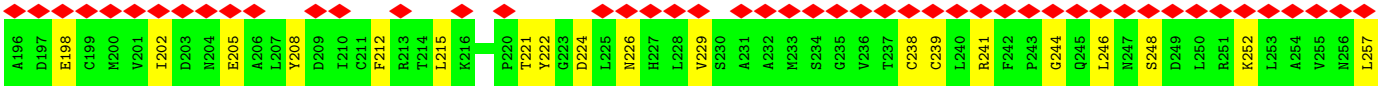
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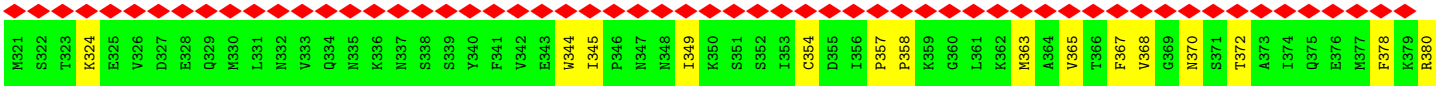


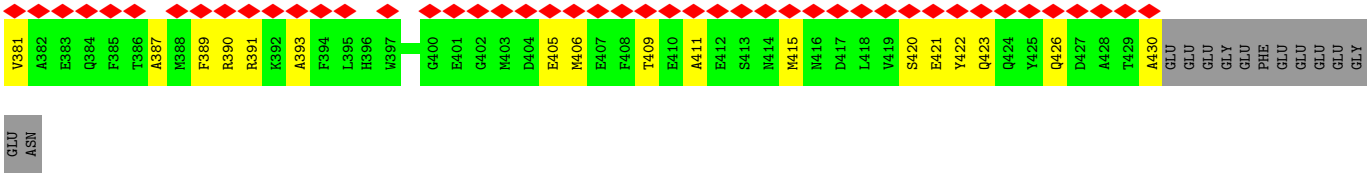








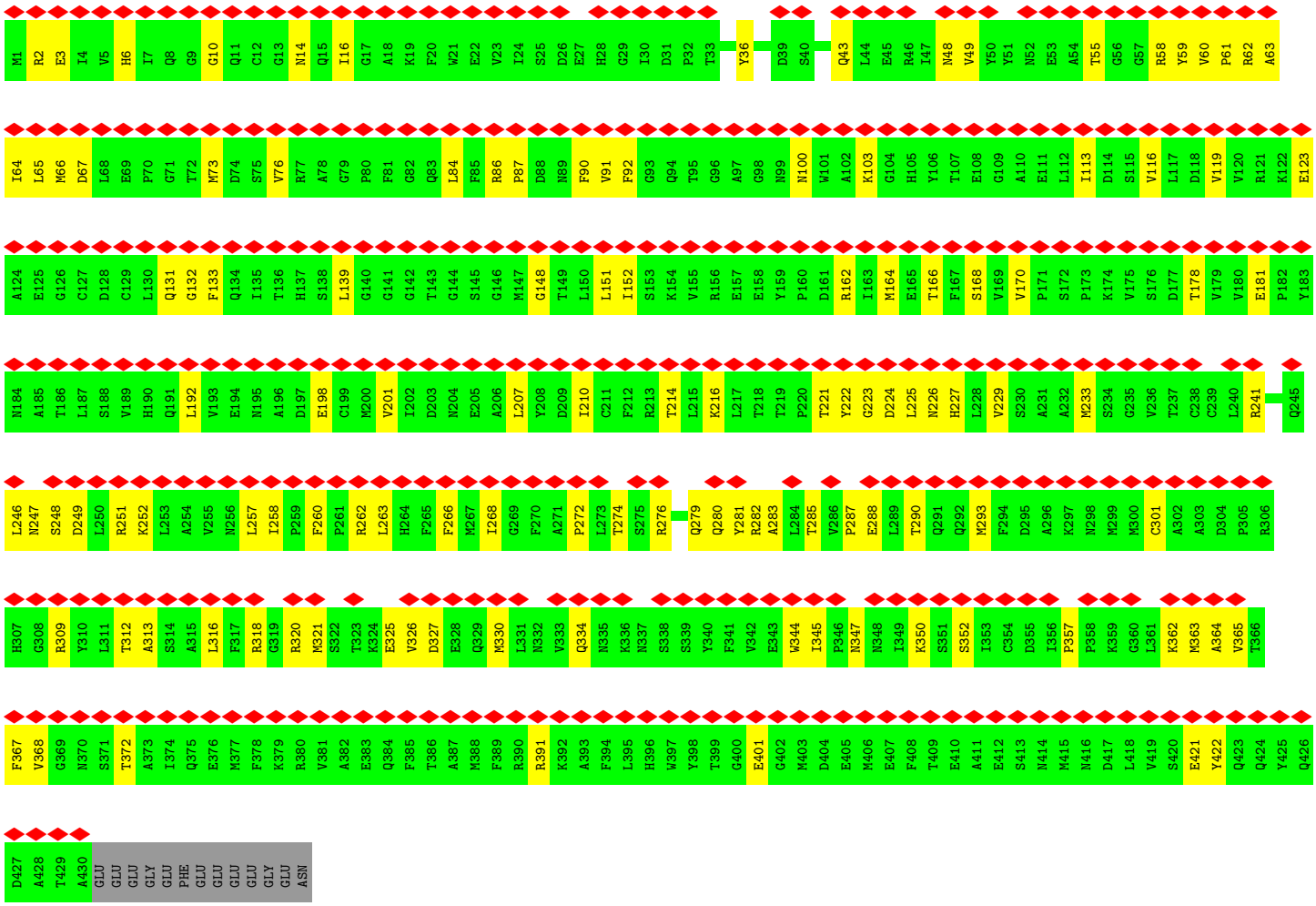




• Molecule 46: Tubulin beta chain

Chain GB:

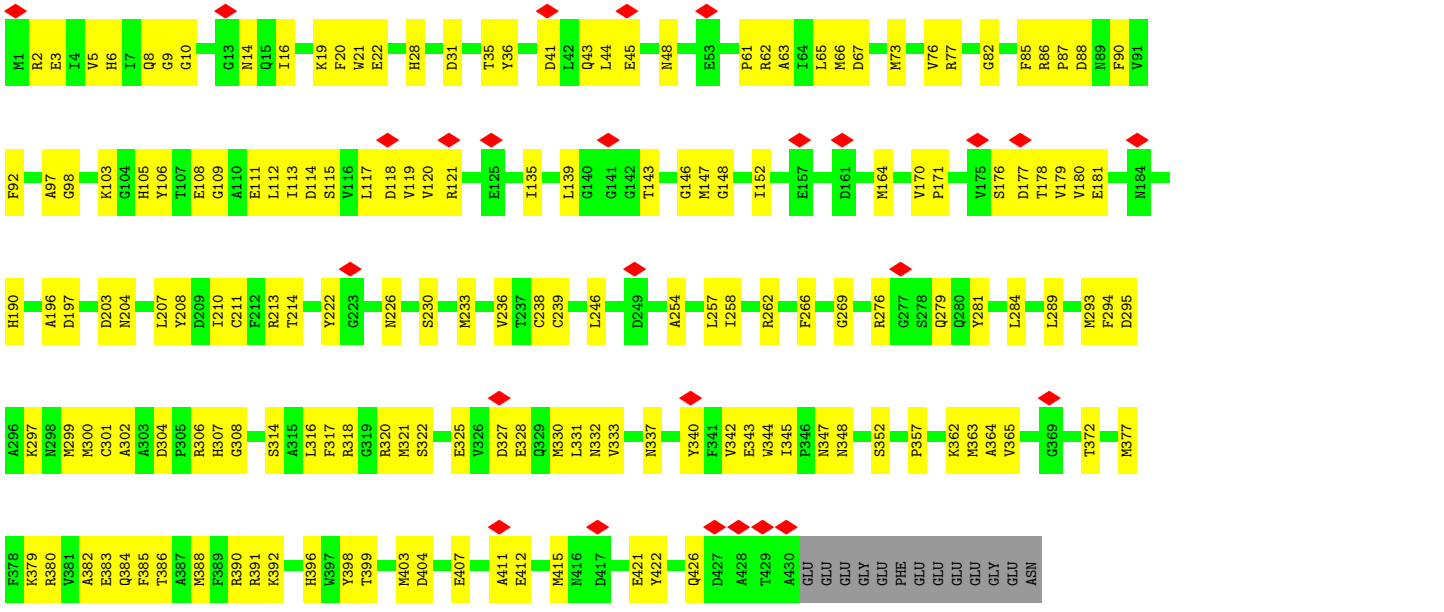




• Molecule 46: Tubulin beta chain

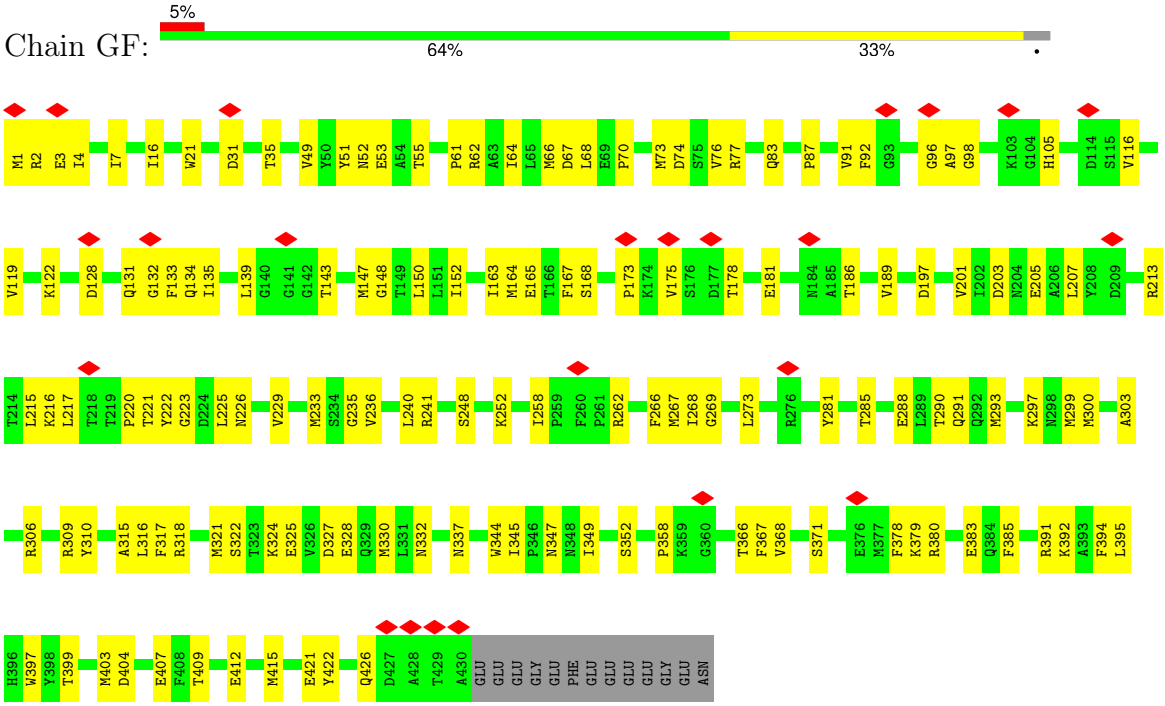
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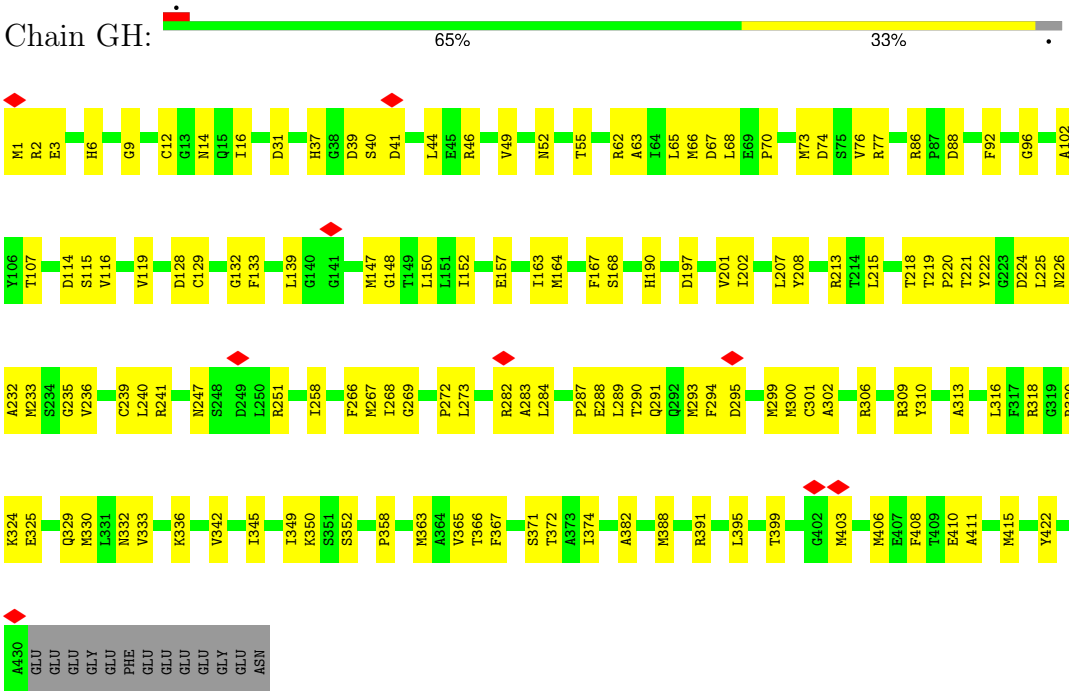
• Molecule 46: Tubulin beta chain

Chain GF:



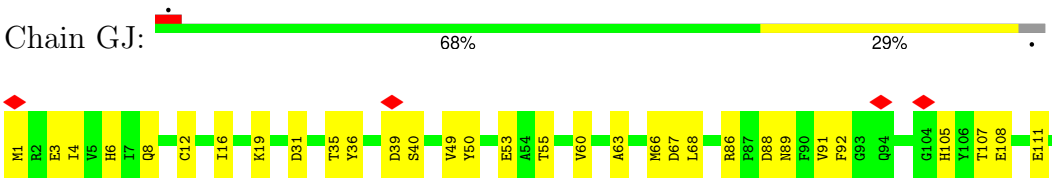
• Molecule 46: Tubulin beta chain

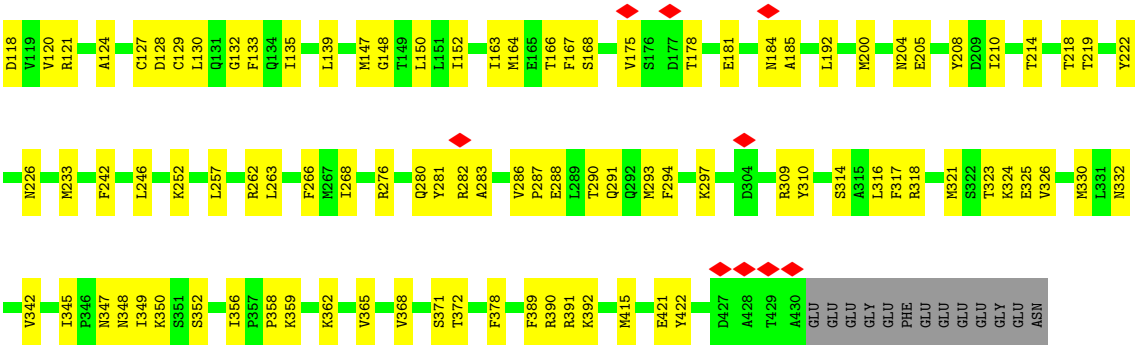
Chain GH:



• Molecule 46: Tubulin beta chain

Chain GJ:

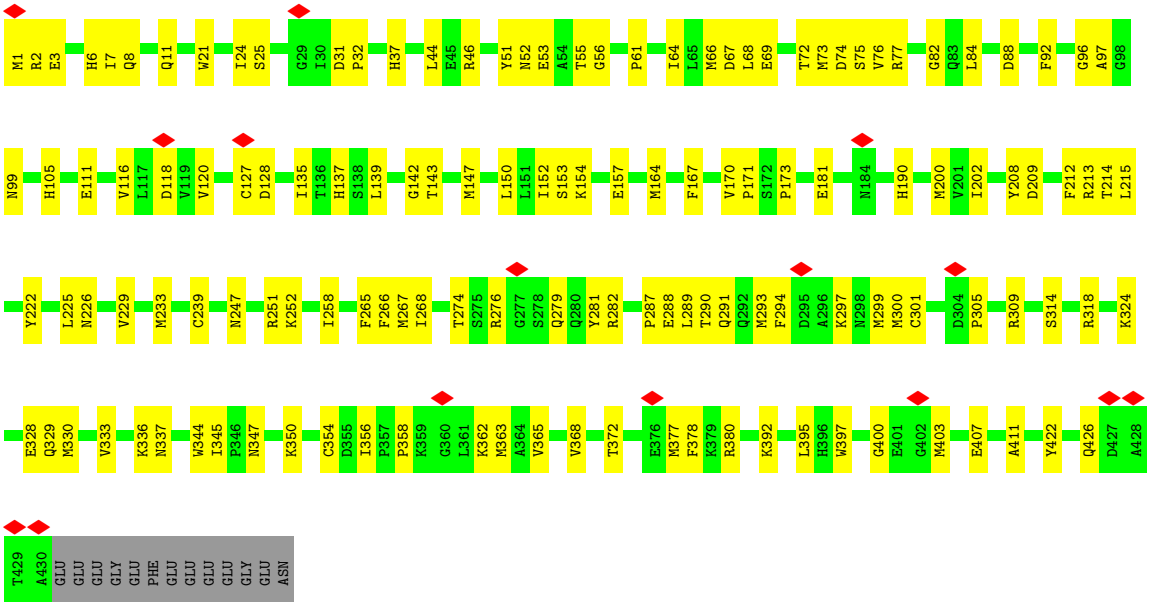




• Molecule 46: Tubulin beta chain

Chain GL:

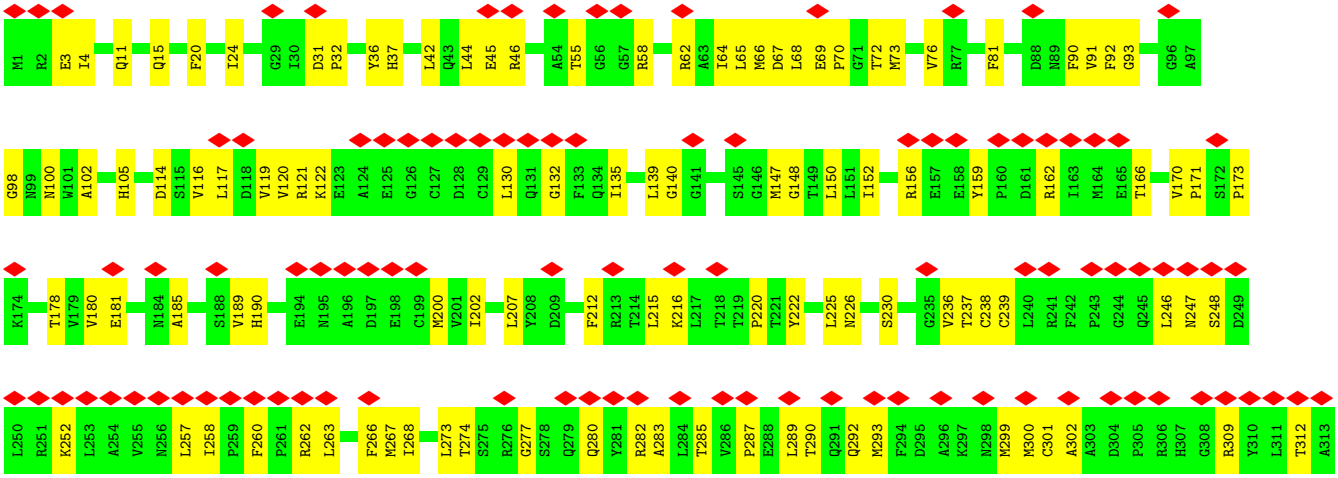


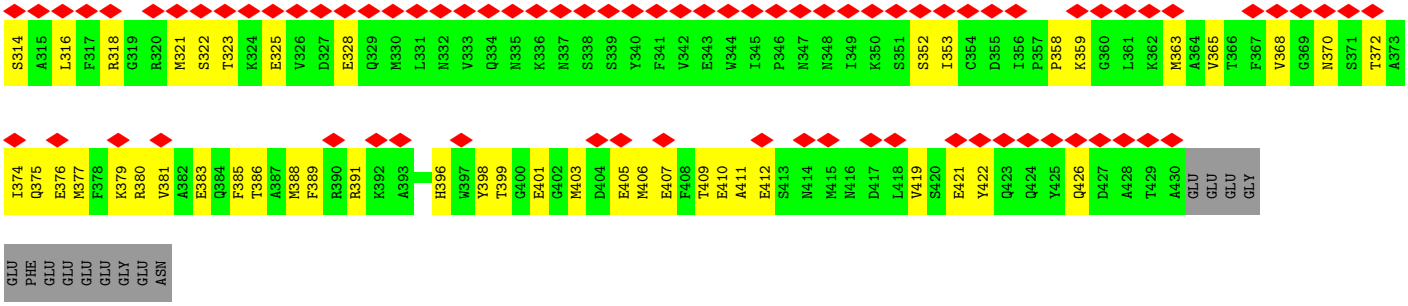


• Molecule 46: Tubulin beta chain

Chain GN:



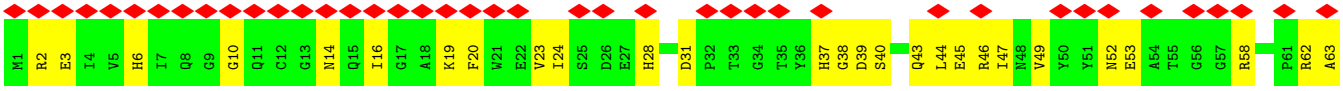


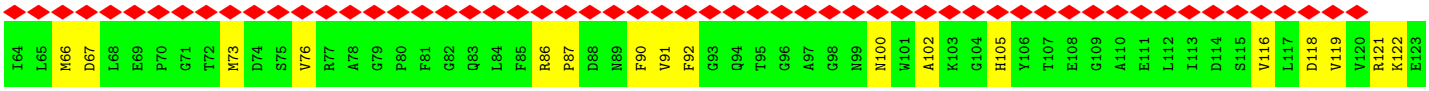


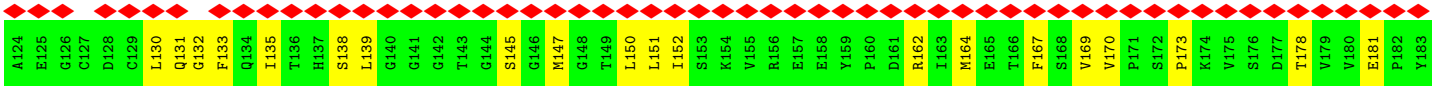
• Molecule 46: Tubulin beta chain

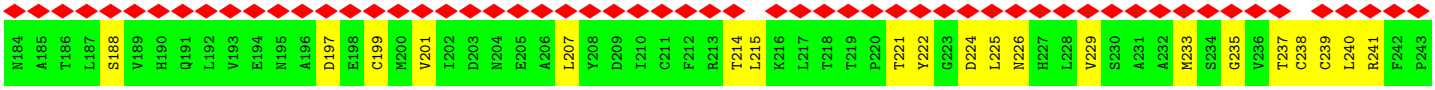
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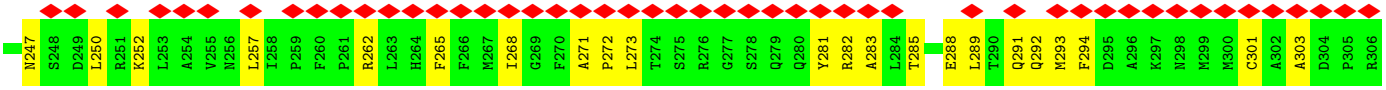


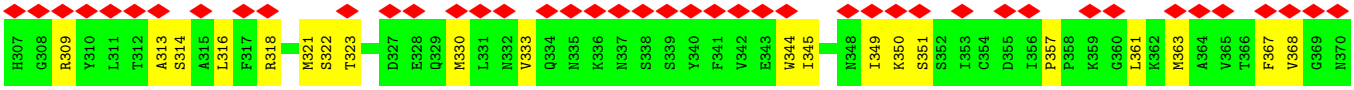


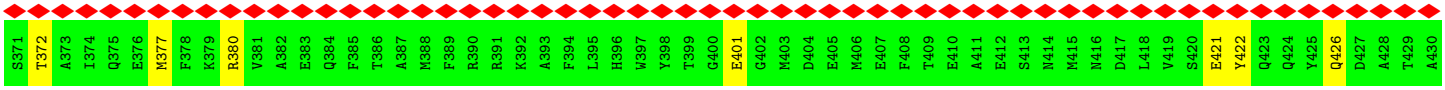










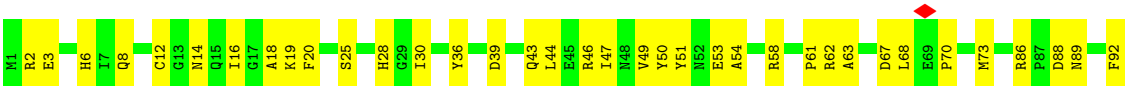


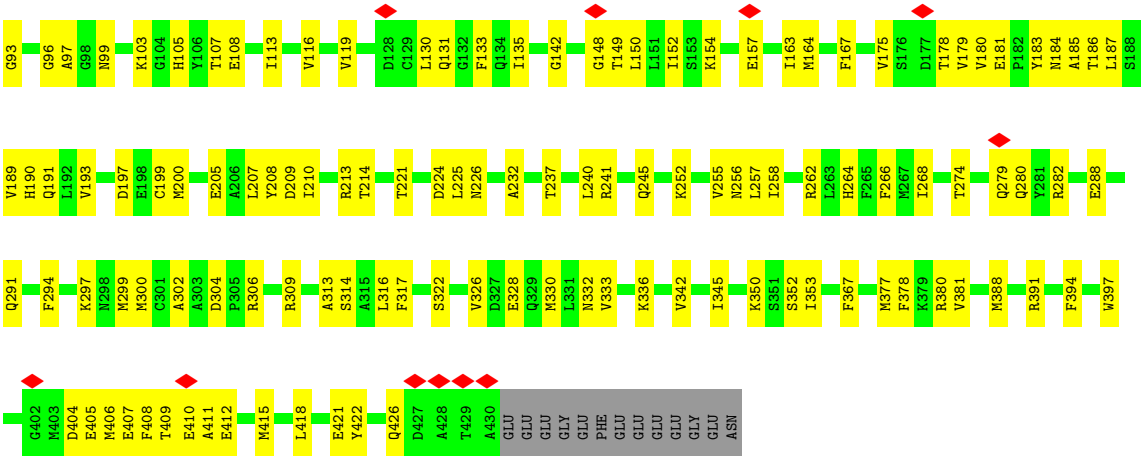


• Molecule 46: Tubulin beta chain

Chain HD:



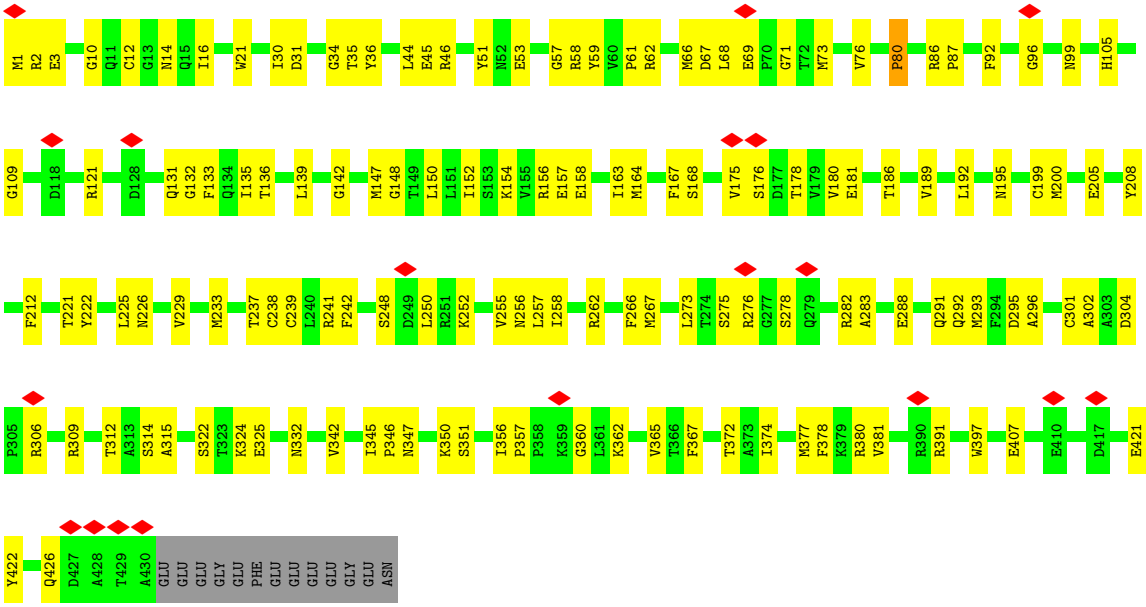




• Molecule 46: Tubulin beta chain

Chain HF:

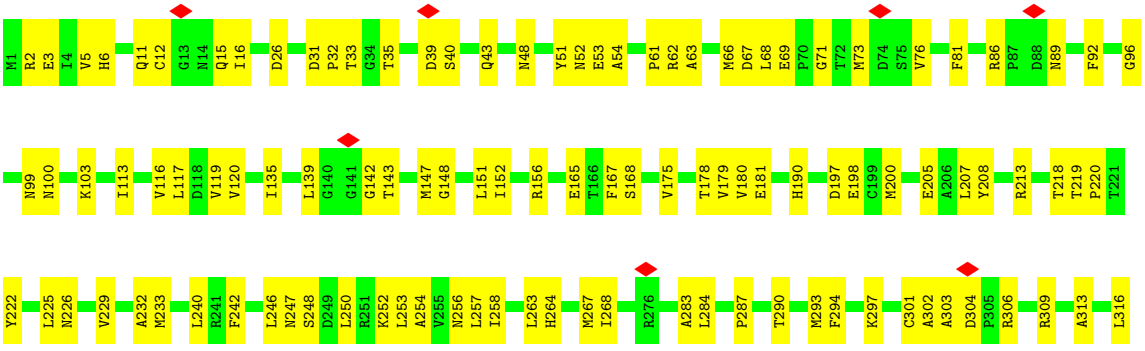


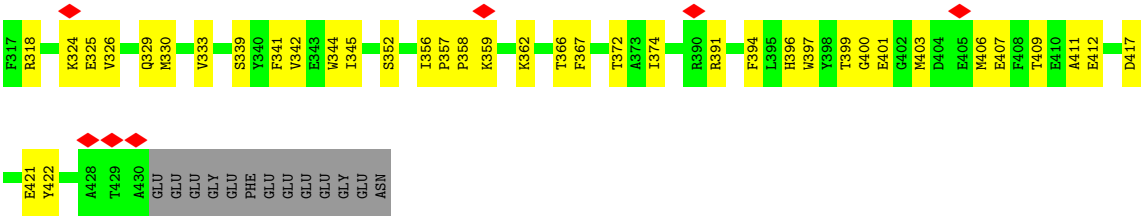


• Molecule 46: Tubulin beta chain

Chain HH:



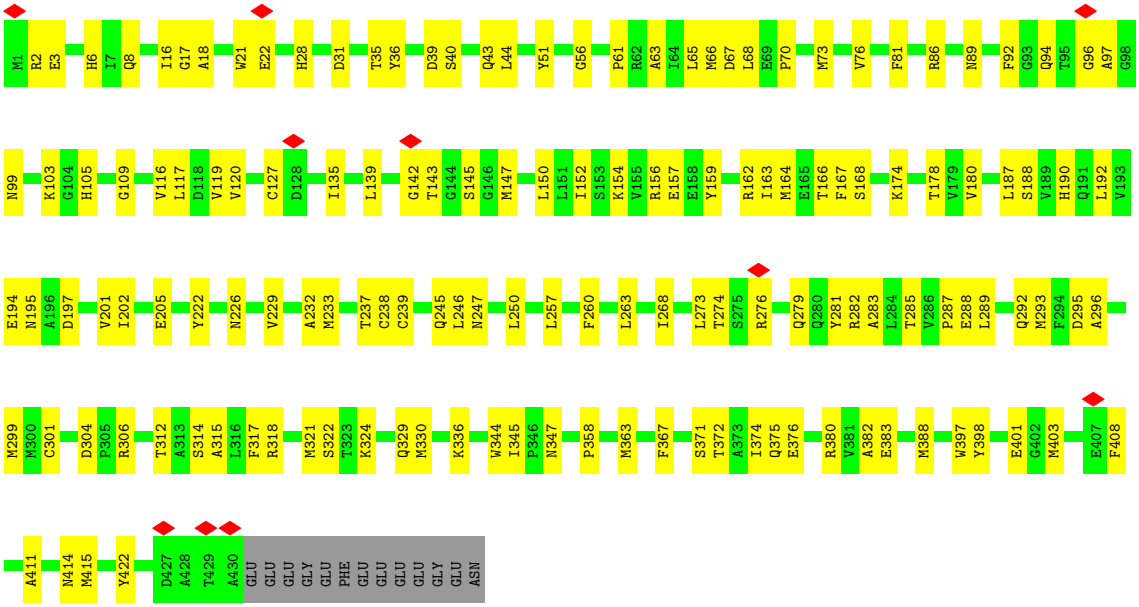




• Molecule 46: Tubulin beta chain

Chain HJ:

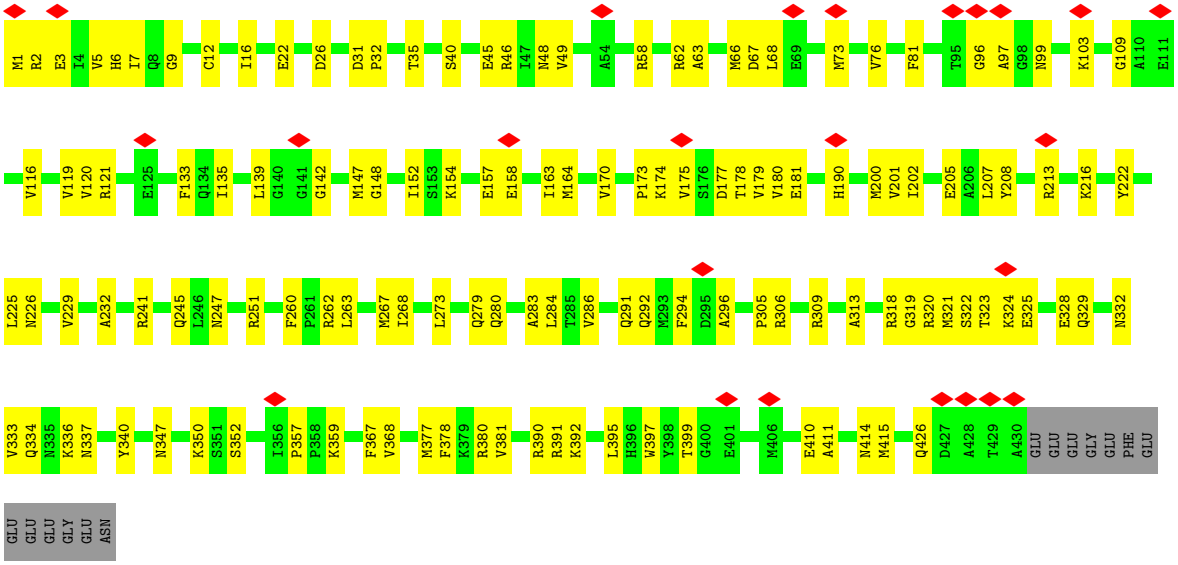




• Molecule 46: Tubulin beta chain

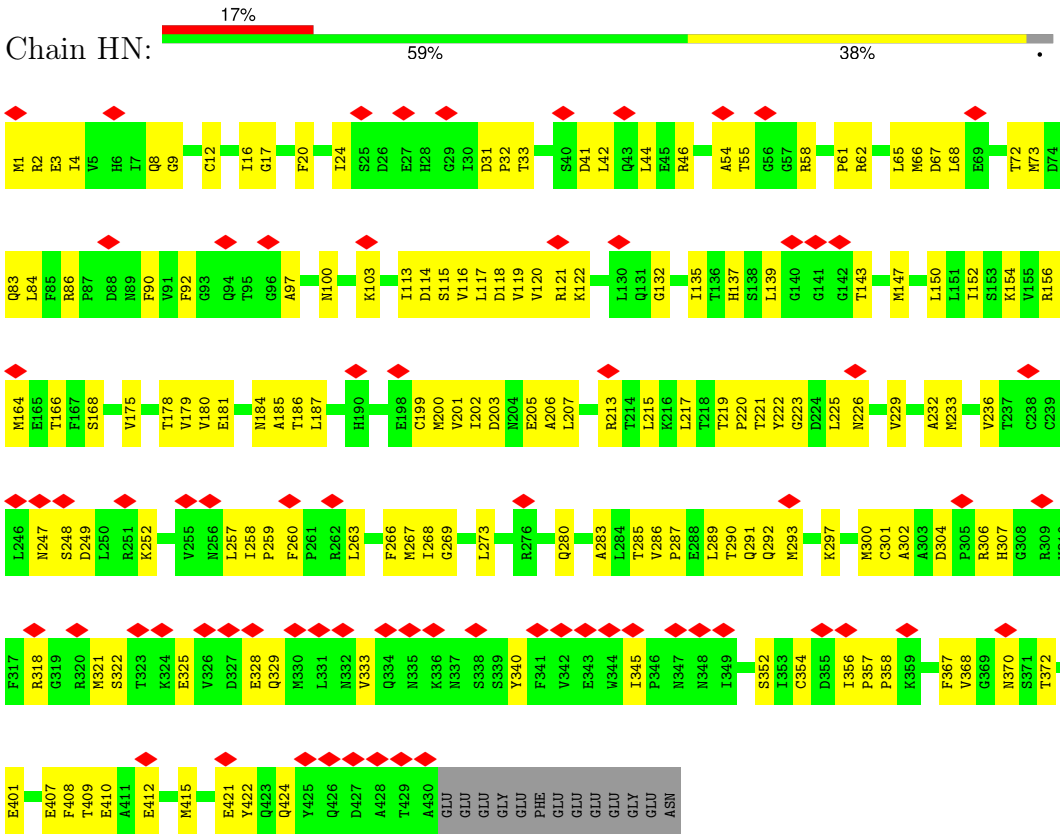
Chain HL:





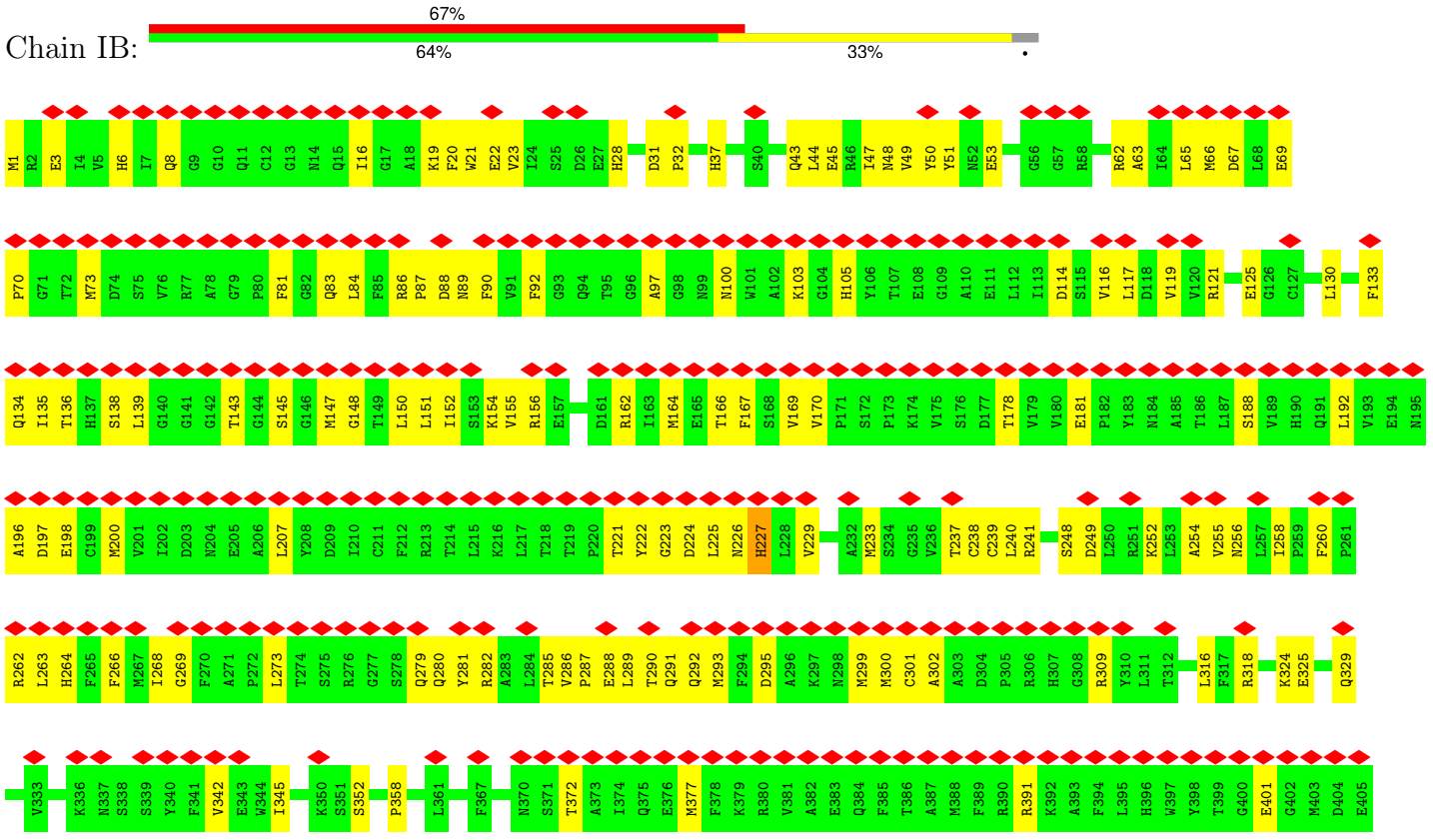
• Molecule 46: Tubulin beta chain

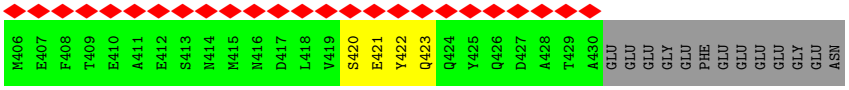
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• Molecule 46: Tubulin beta chain

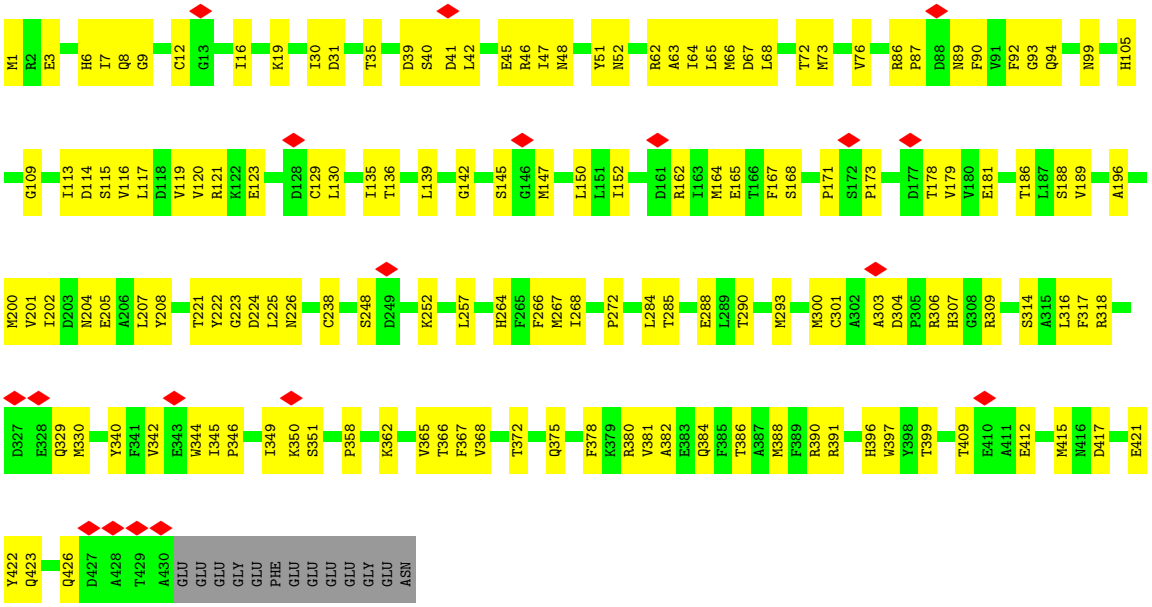
Chain IB:





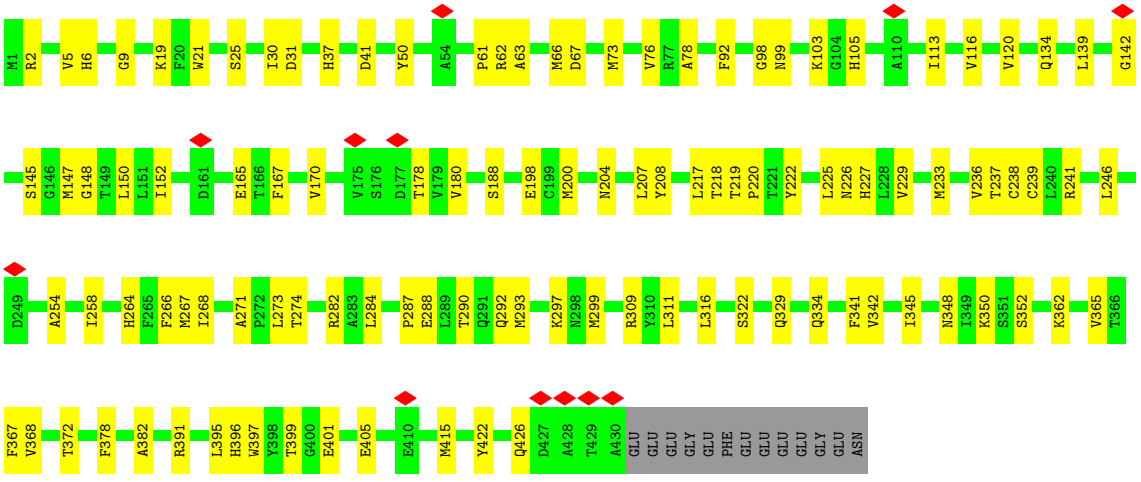
• Molecule 46: Tubulin beta chain





• Molecule 46: Tubulin beta chain

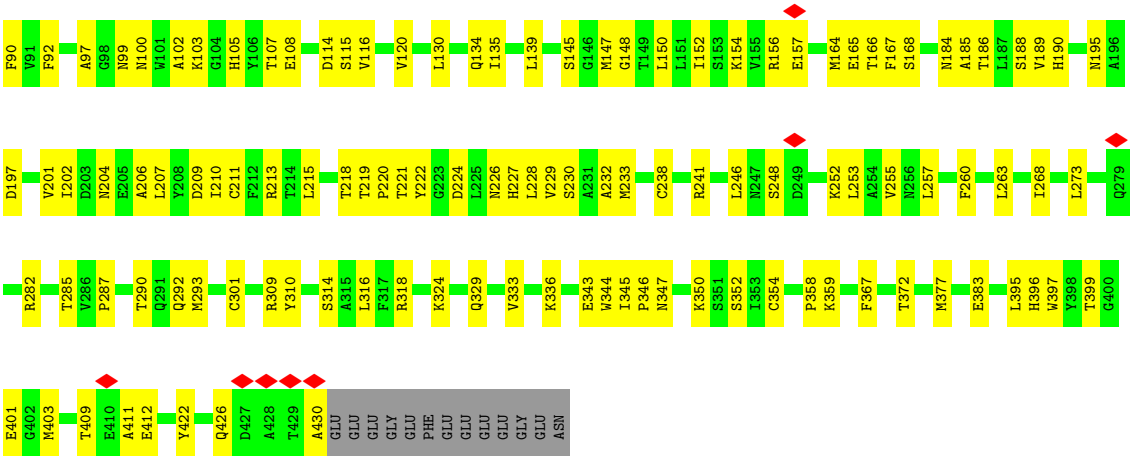




• Molecule 46: Tubulin beta chain



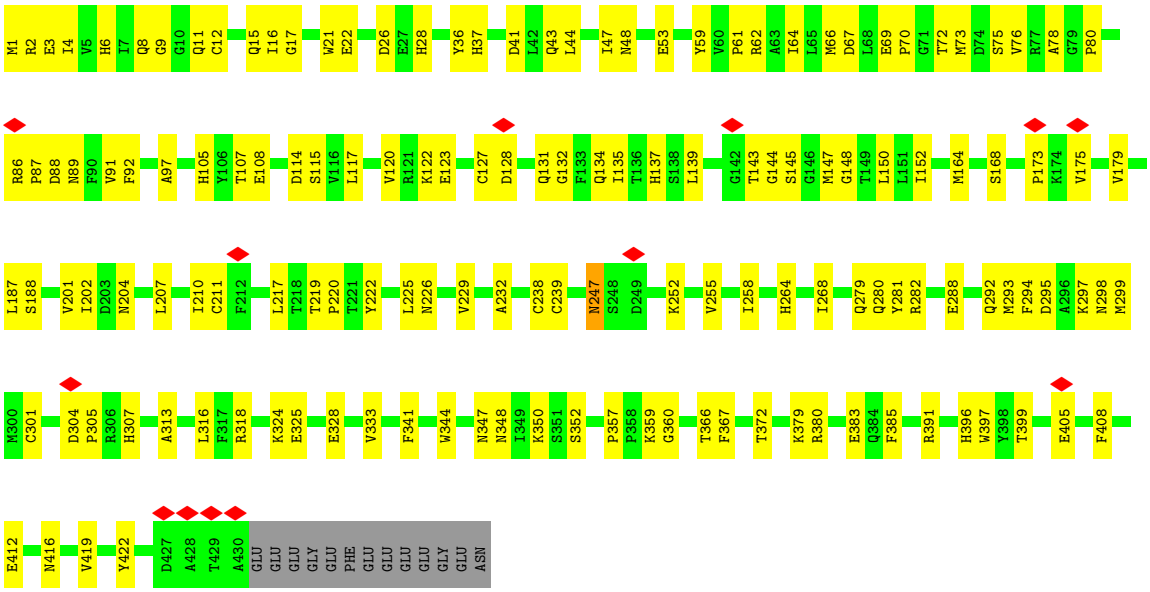




• Molecule 46: Tubulin beta chain

Chain IJ:

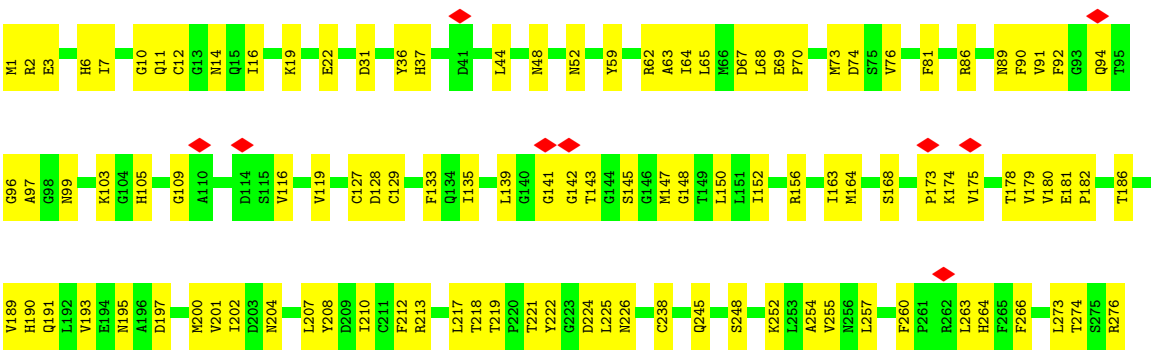


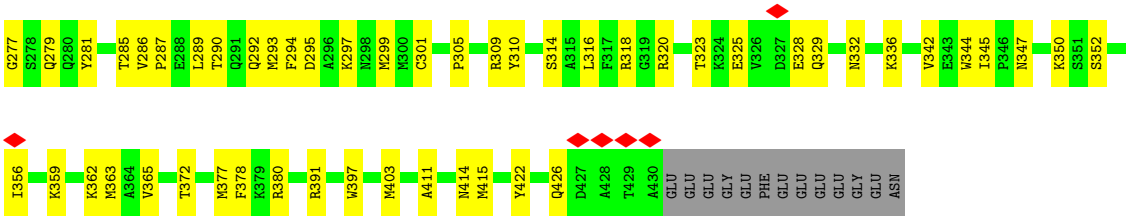


• Molecule 46: Tubulin beta chain

Chain IL:

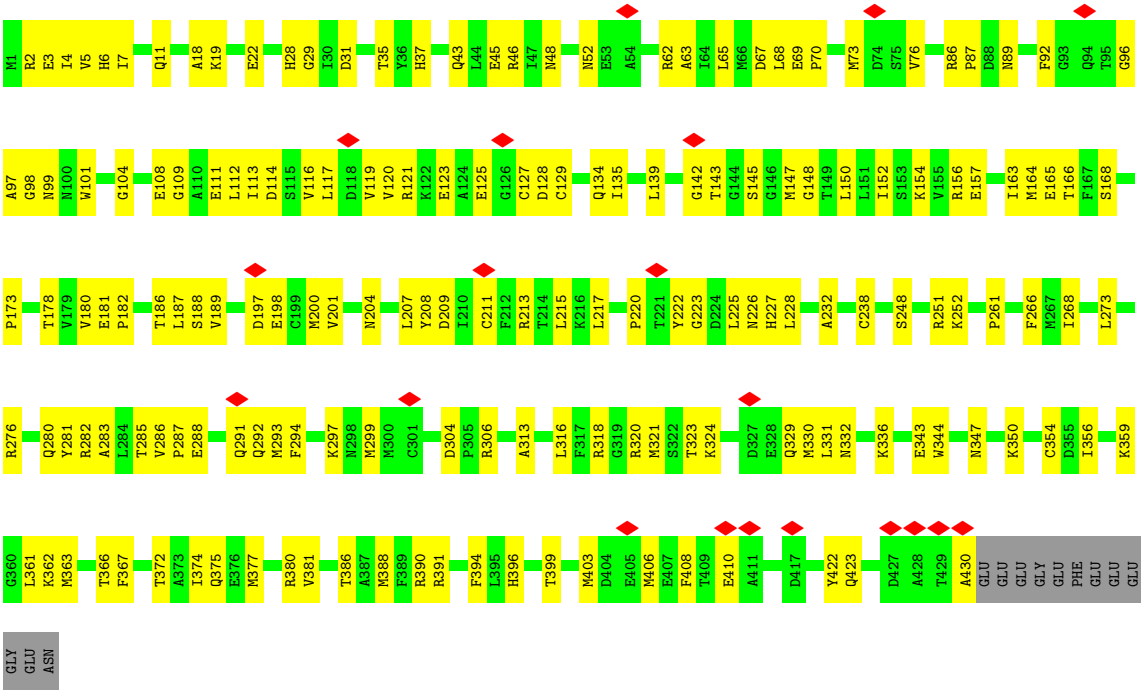






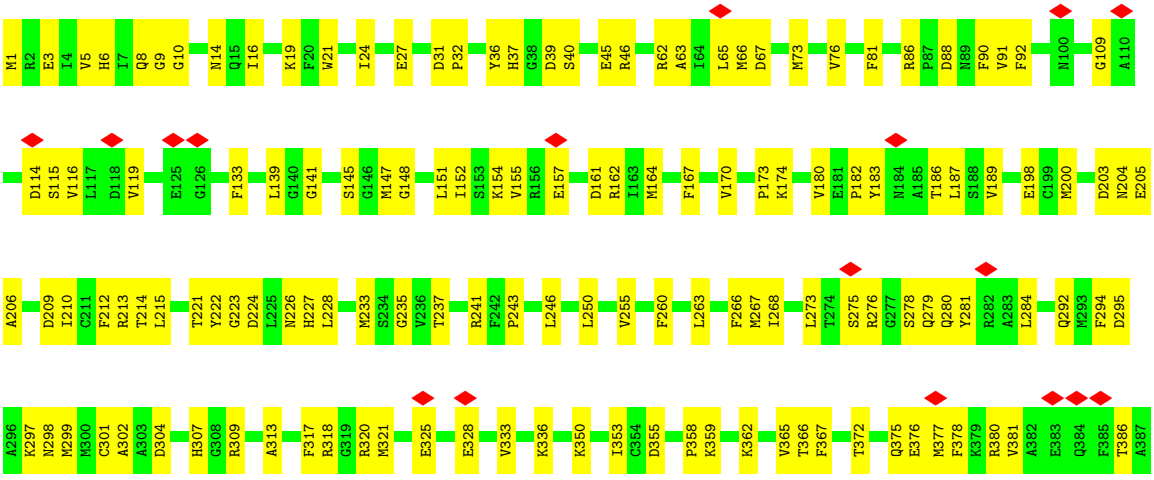
• Molecule 46: Tubulin beta chain

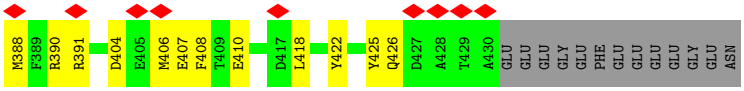




• Molecule 46: Tubulin beta chain



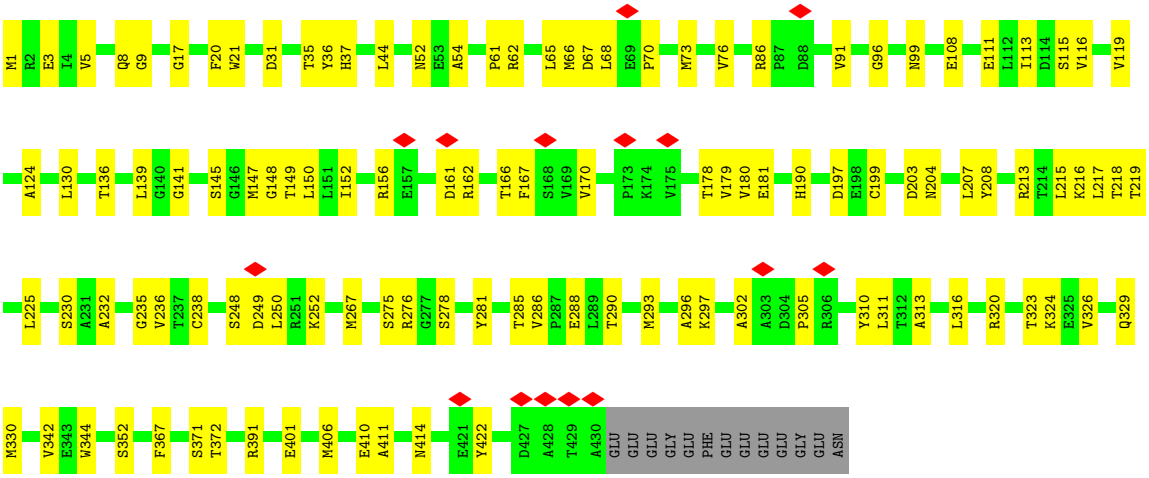




• Molecule 46: Tubulin beta chain

Chain JD:

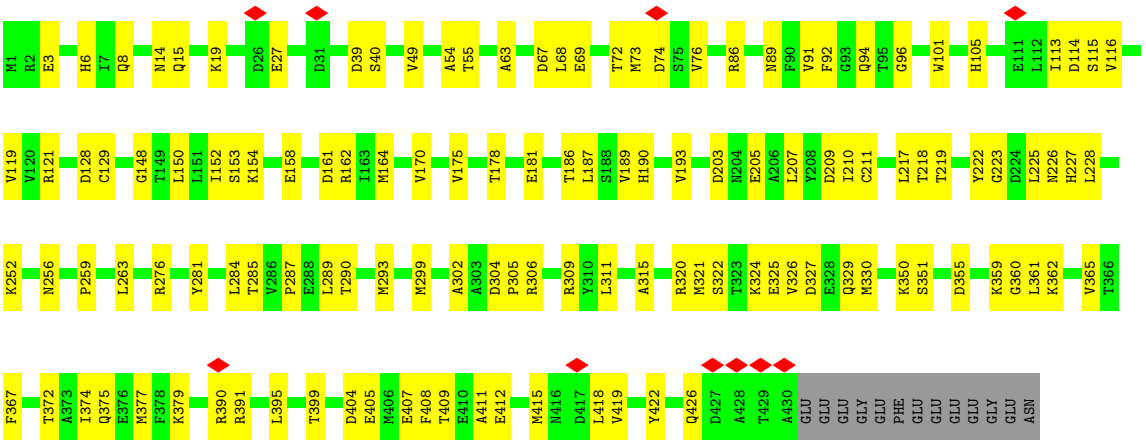




• Molecule 46: Tubulin beta chain

Chain JF:

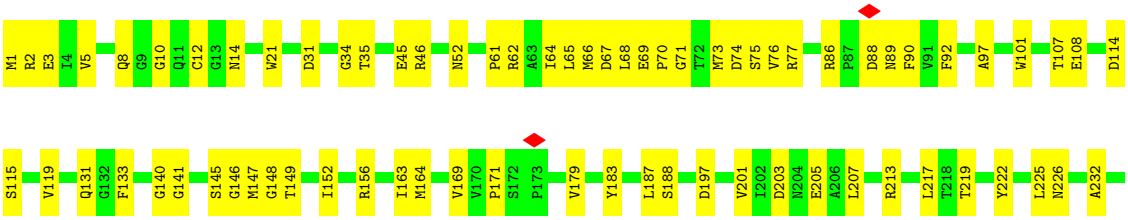


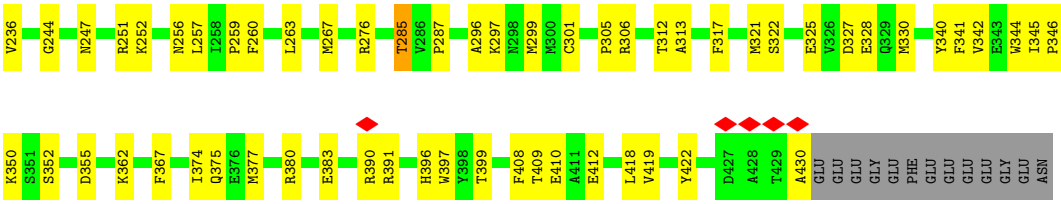


• Molecule 46: Tubulin beta chain

Chain JH:



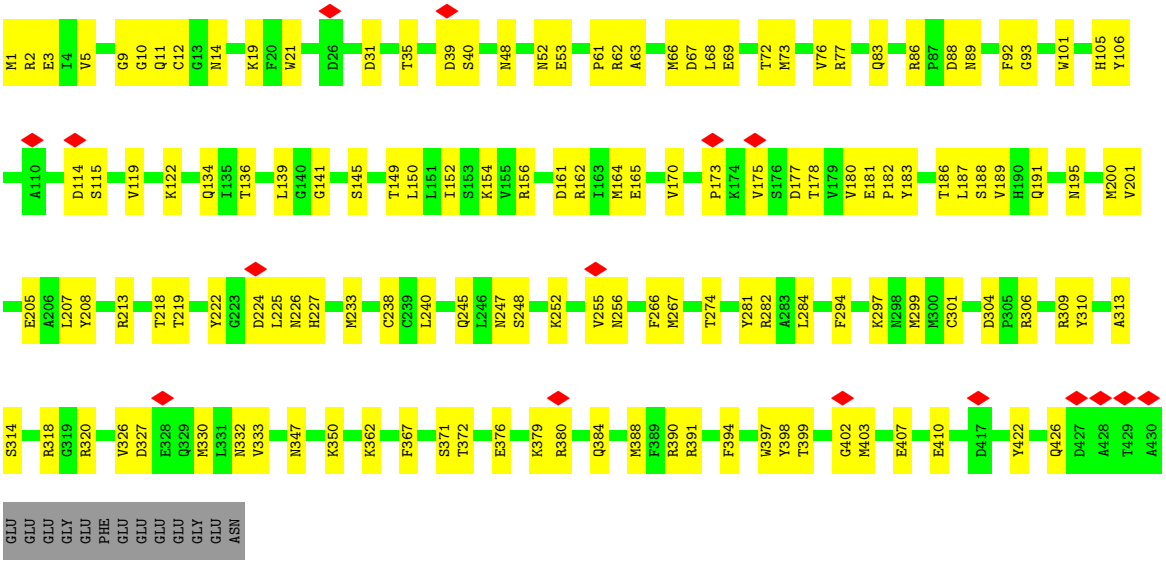




• Molecule 46: Tubulin beta chain

Chain JJ:

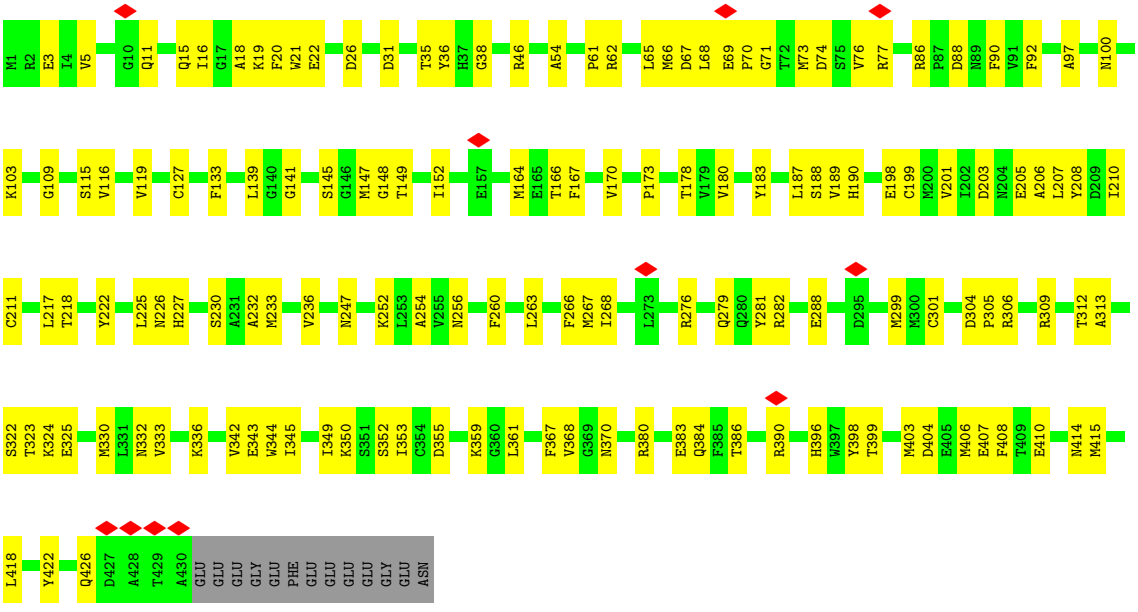




• Molecule 46: Tubulin beta chain

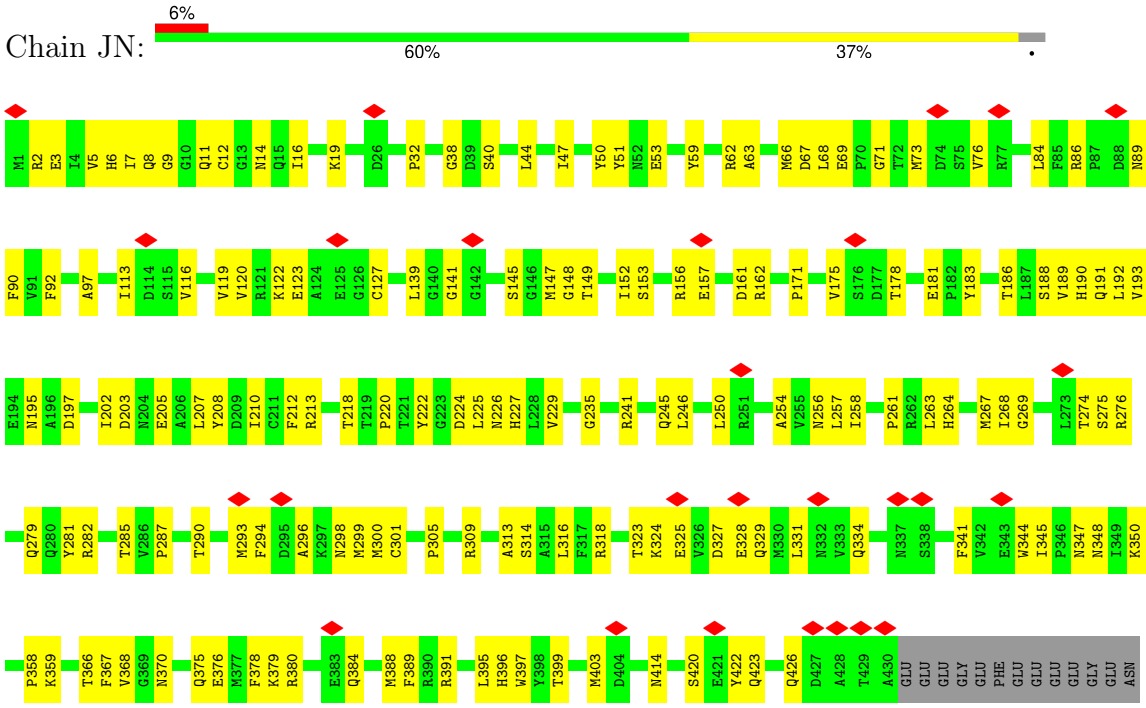
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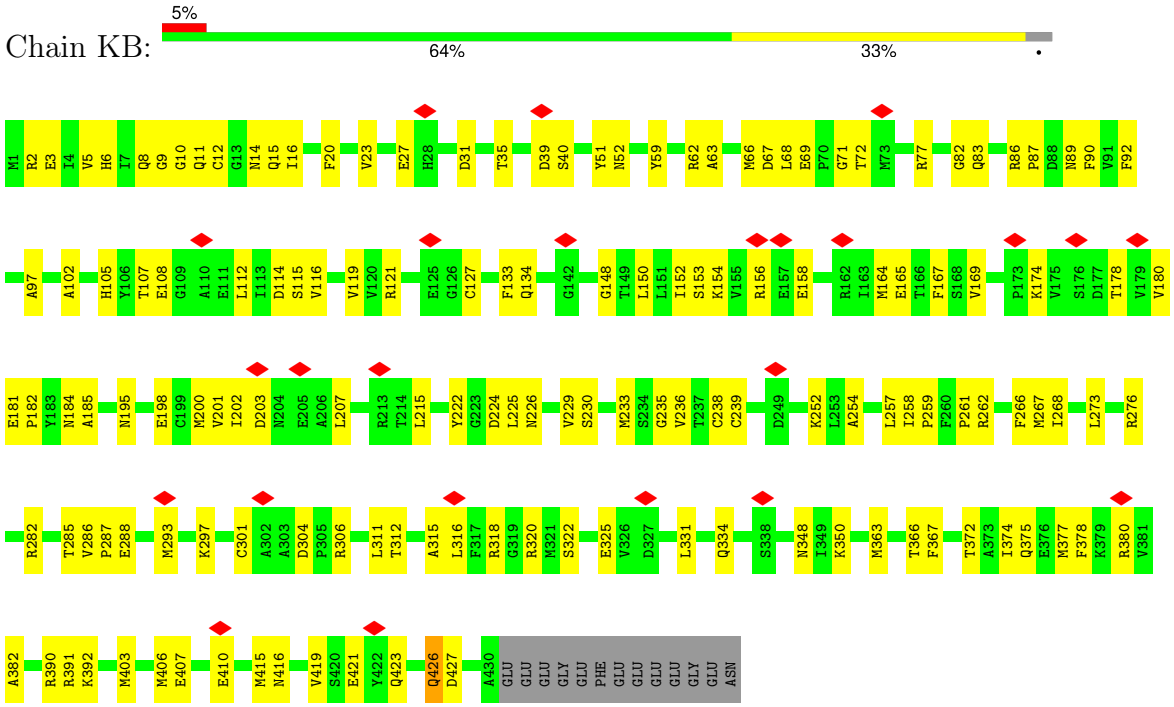
• Molecule 46: Tubulin beta chain

Chain JN:



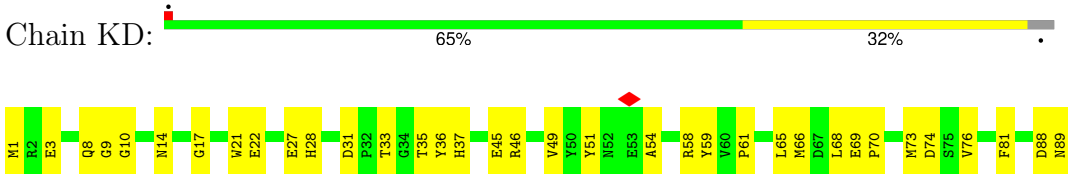
• Molecule 46: Tubulin beta chain

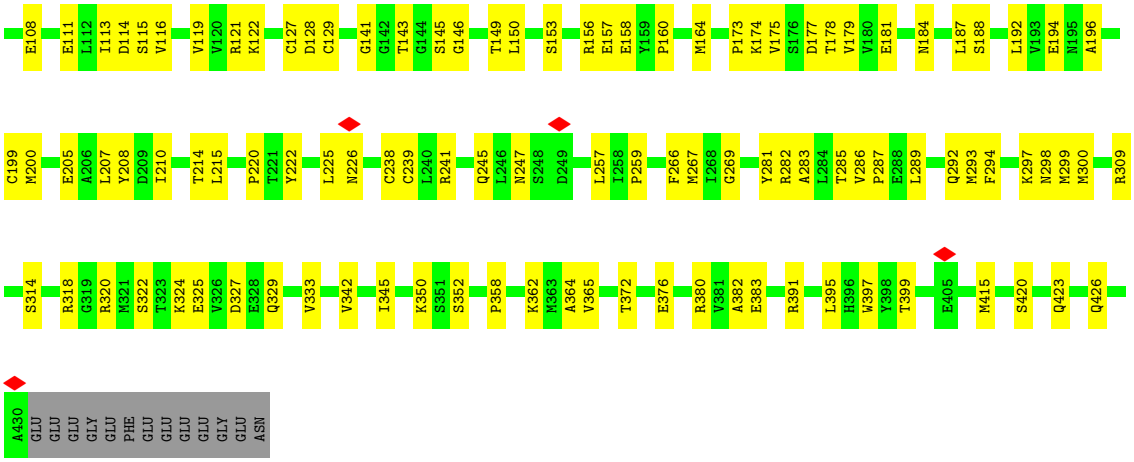
Chain KB:



• Molecule 46: Tubulin beta chain

Chain KD:

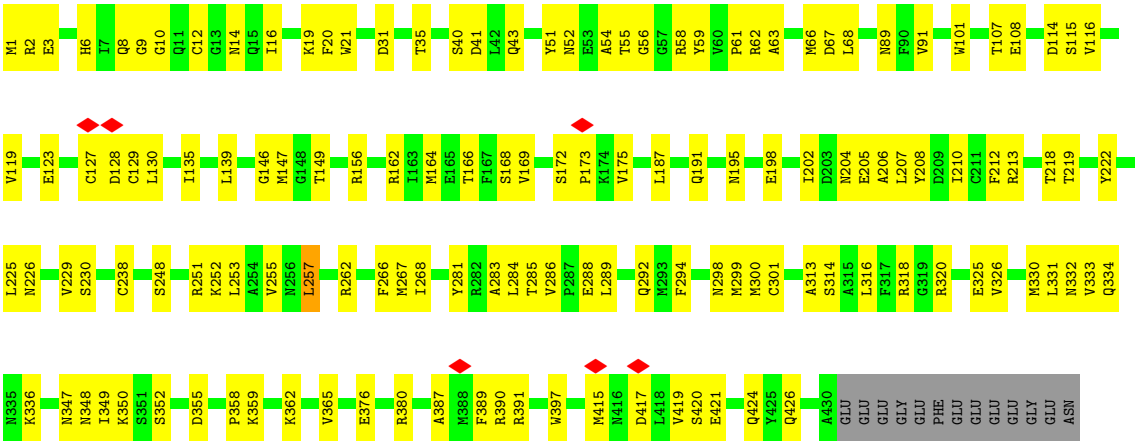




• Molecule 46: Tubulin beta chain

Chain KF:

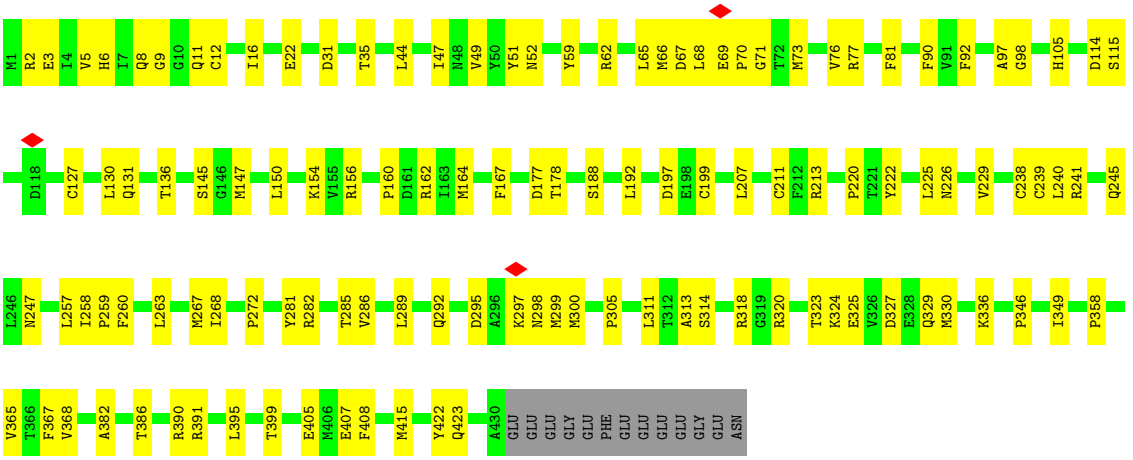




• Molecule 46: Tubulin beta chain

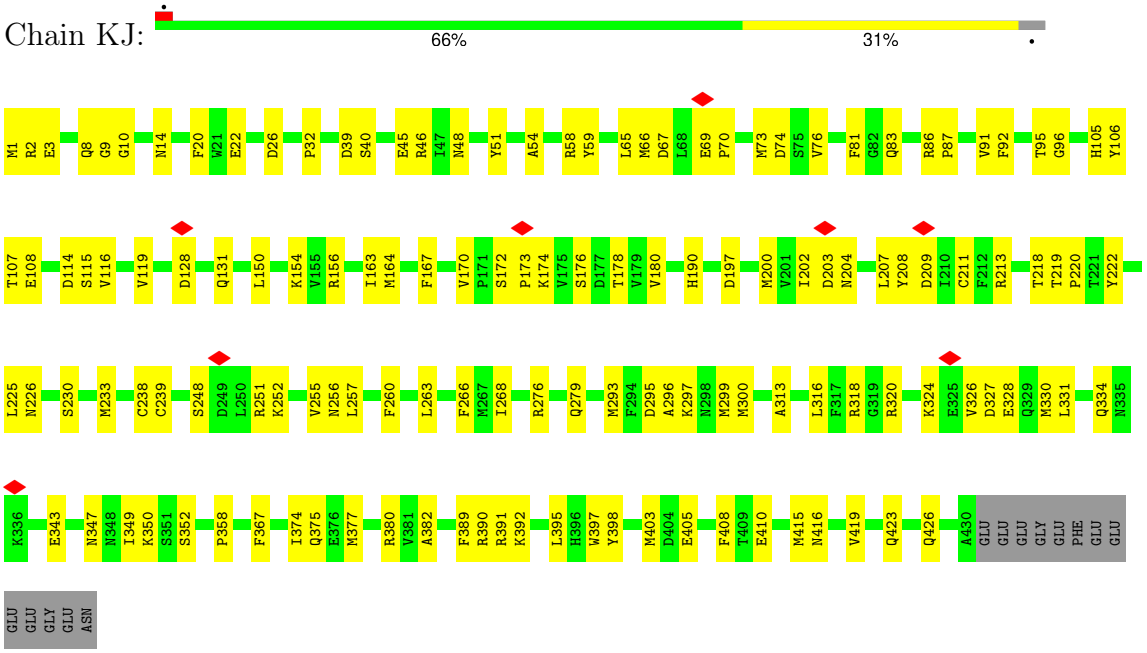
Chain KH:





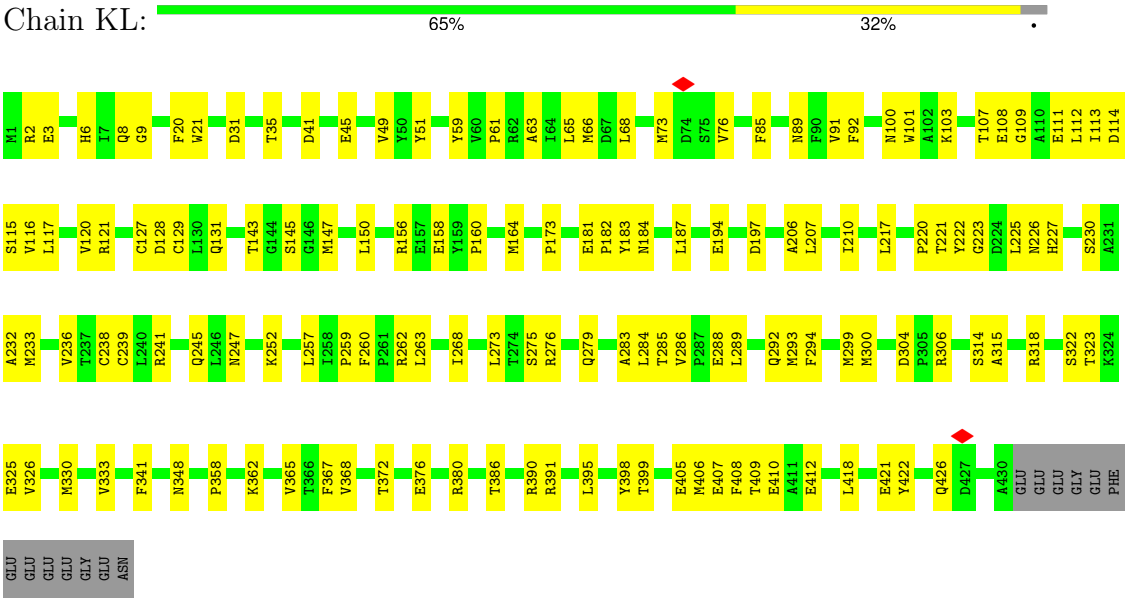
• Molecule 46: Tubulin beta chain

Chain KJ:



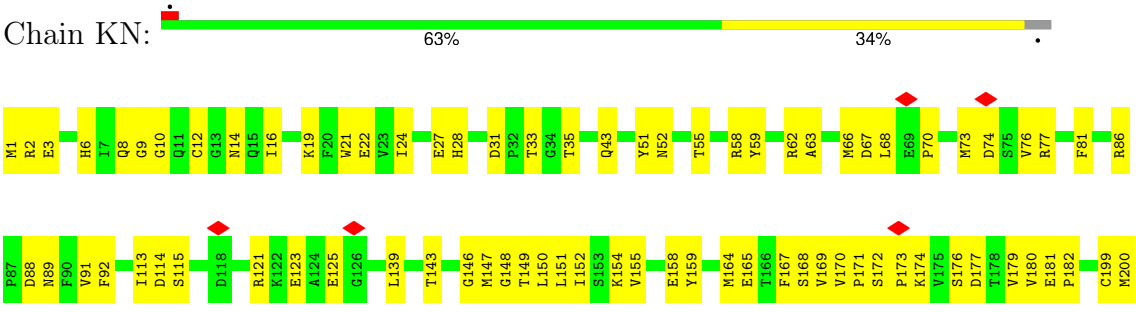
• Molecule 46: Tubulin beta chain

Chain KL:



• Molecule 46: Tubulin beta chain

Chain KN:

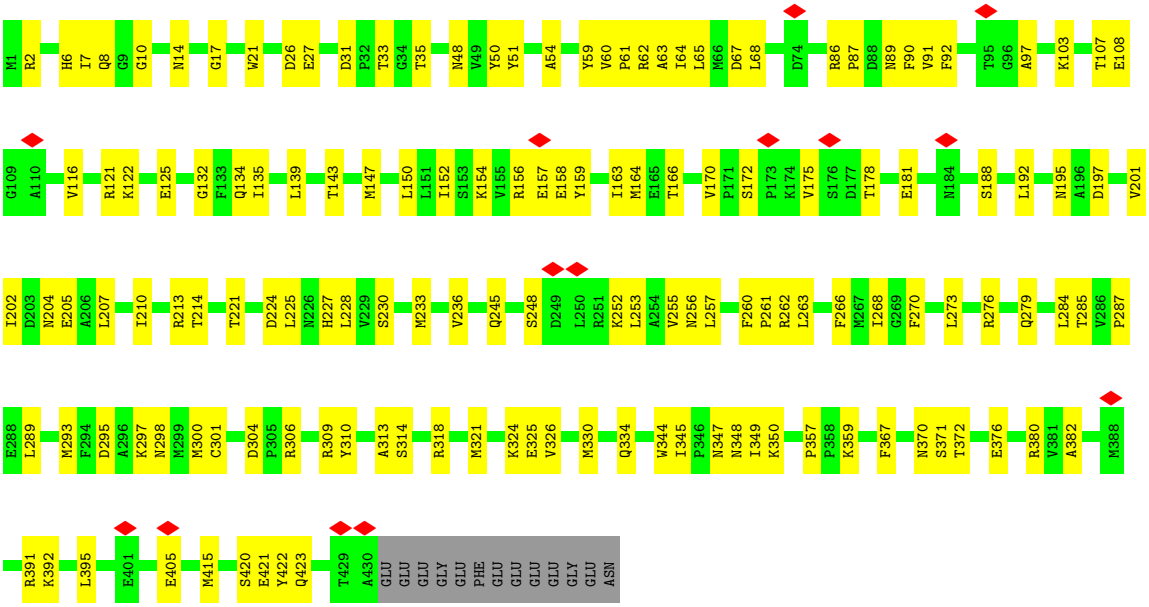




• Molecule 46: Tubulin beta chain

Chain LB:

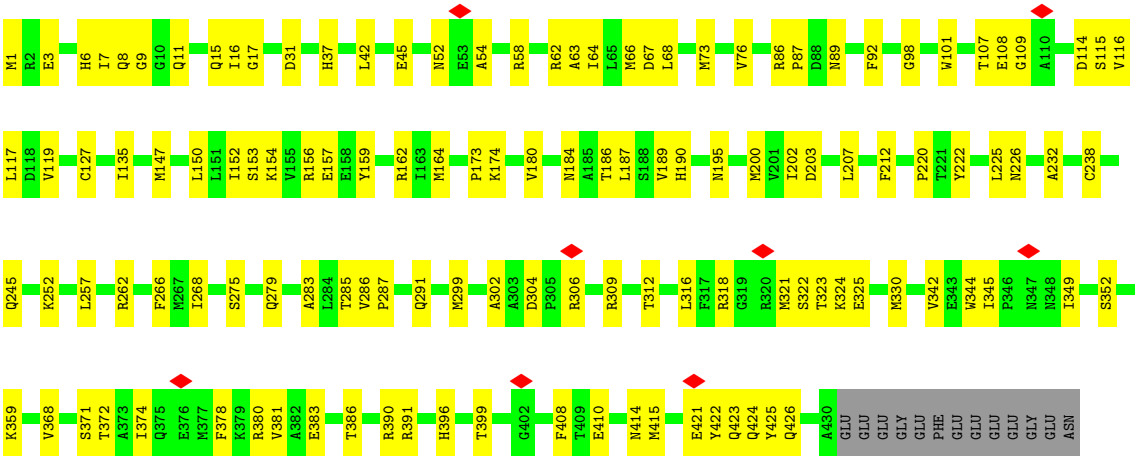




• Molecule 46: Tubulin beta chain

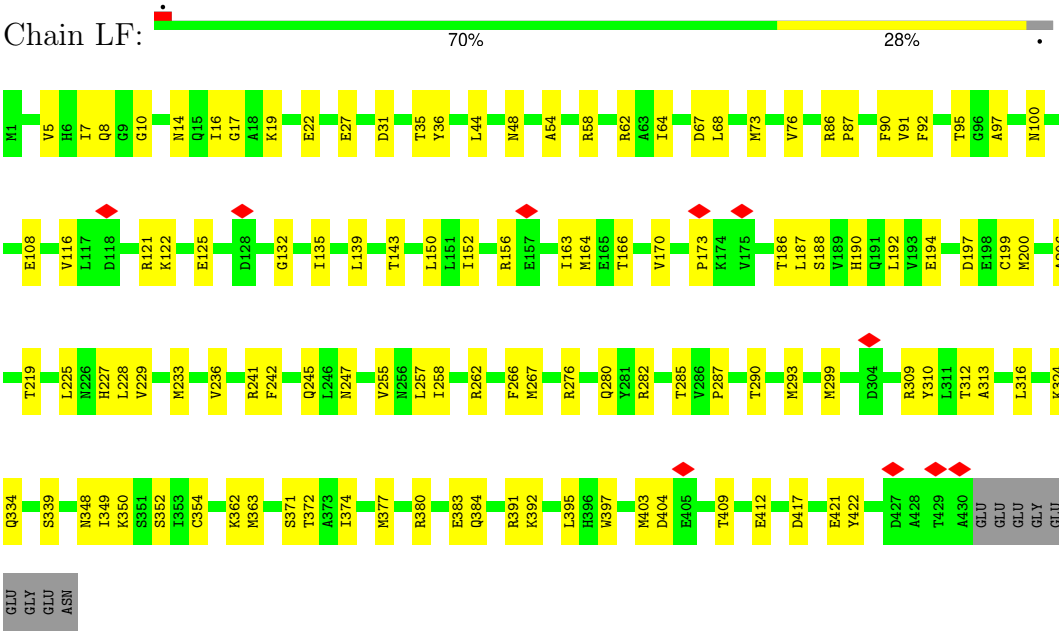
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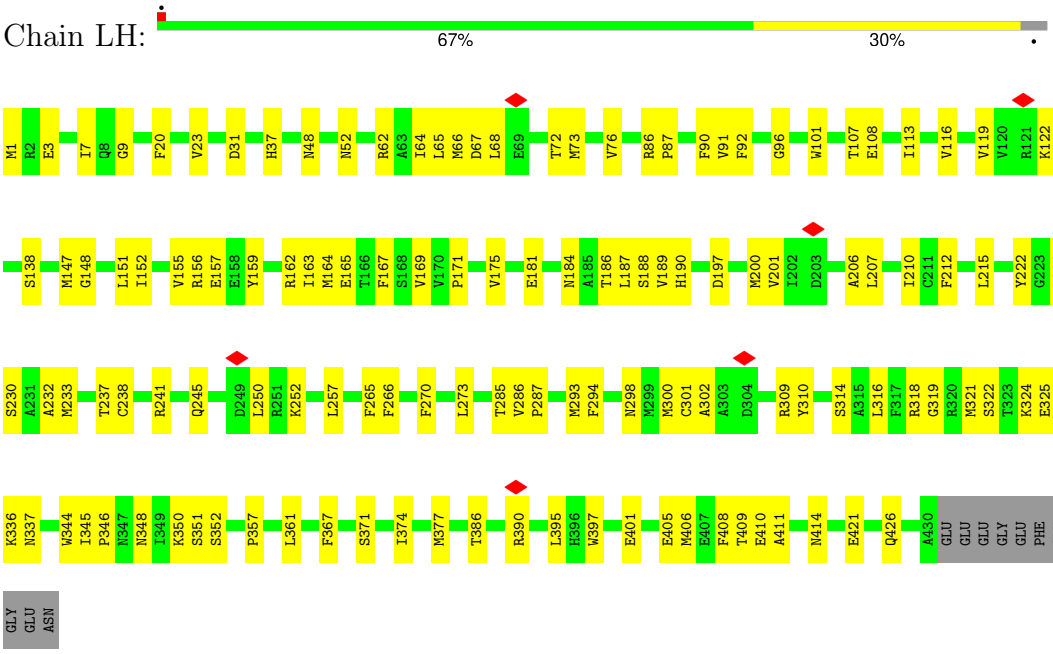
• Molecule 46: Tubulin beta chain

Chain LF:



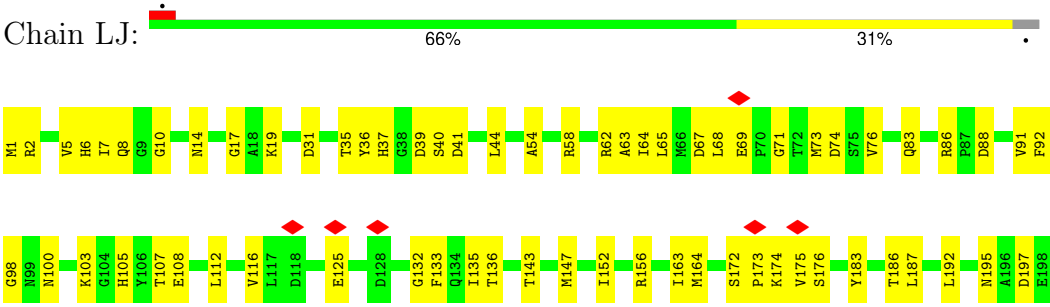
• Molecule 46: Tubulin beta chain

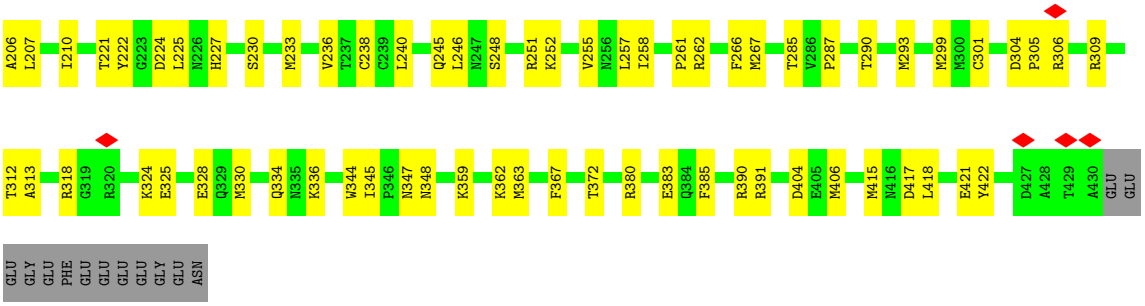
Chain LH:



• Molecule 46: Tubulin beta chain

Chain LJ:

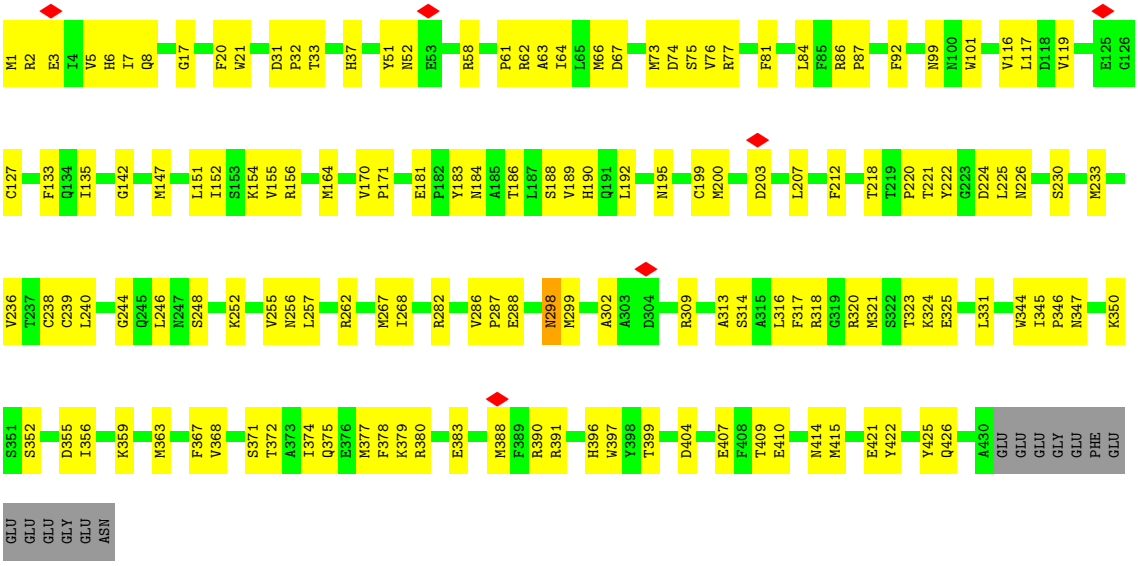




• Molecule 46: Tubulin beta chain

Chain LL:

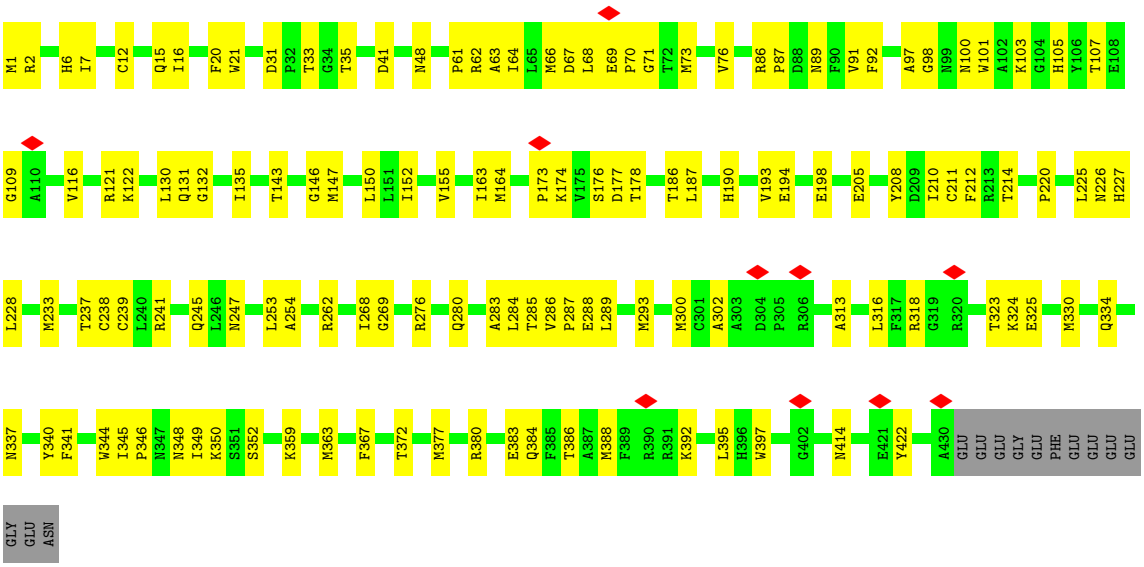




• Molecule 46: Tubulin beta chain

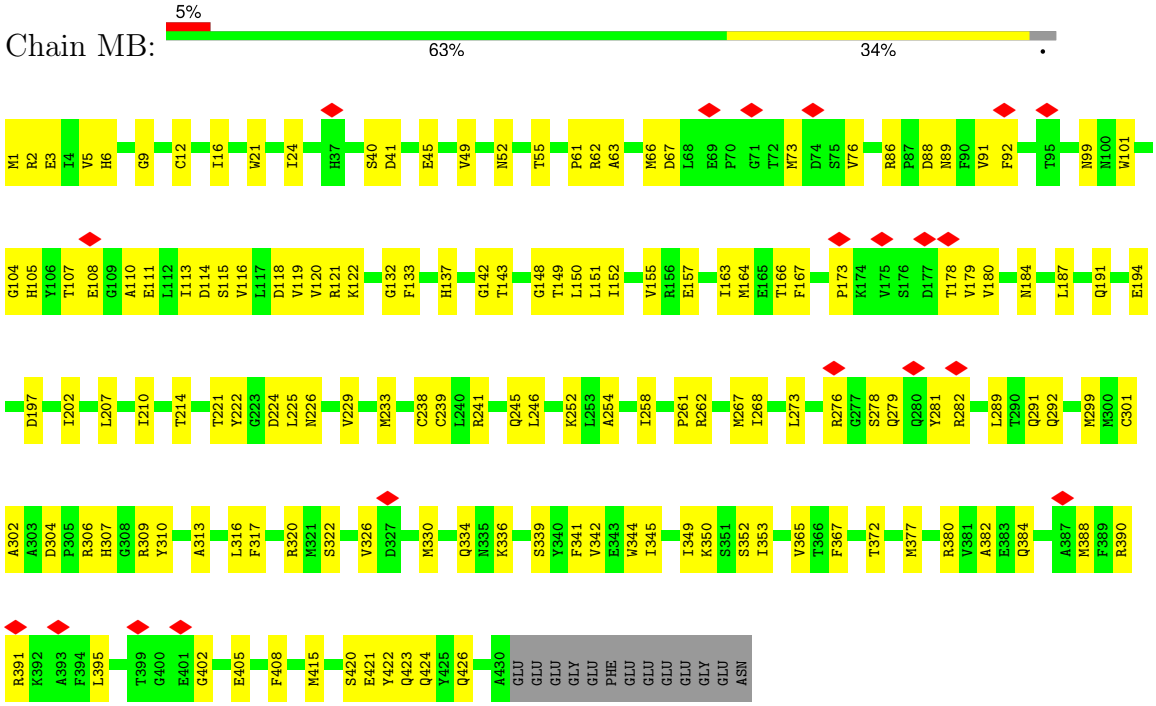
Chain LN:





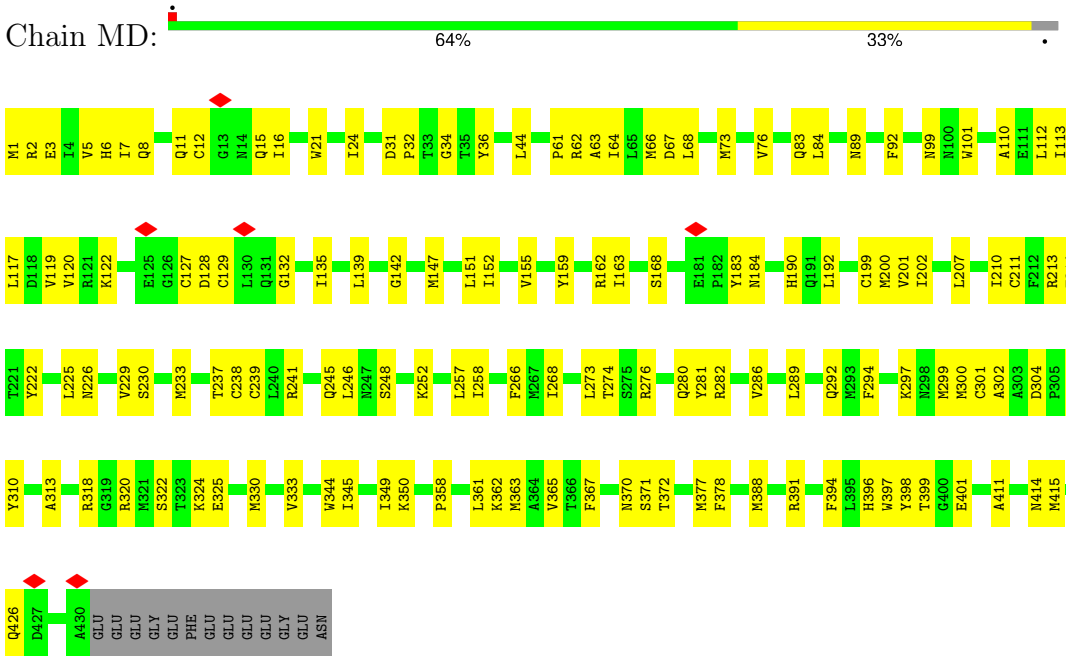
• Molecule 46: Tubulin beta chain

Chain MB:



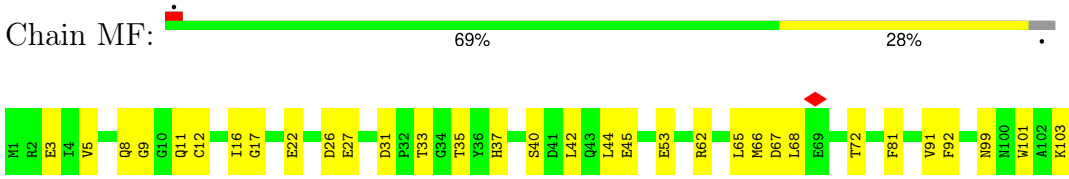
• Molecule 46: Tubulin beta chain

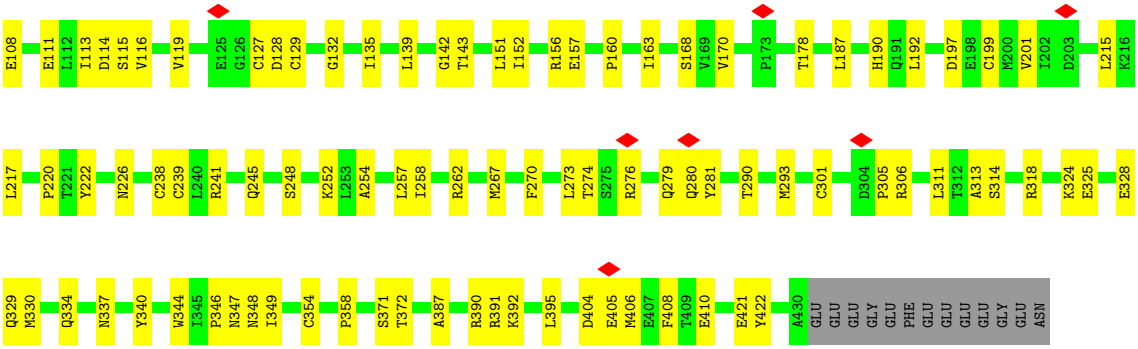
Chain MD:



• Molecule 46: Tubulin beta chain

Chain MF:

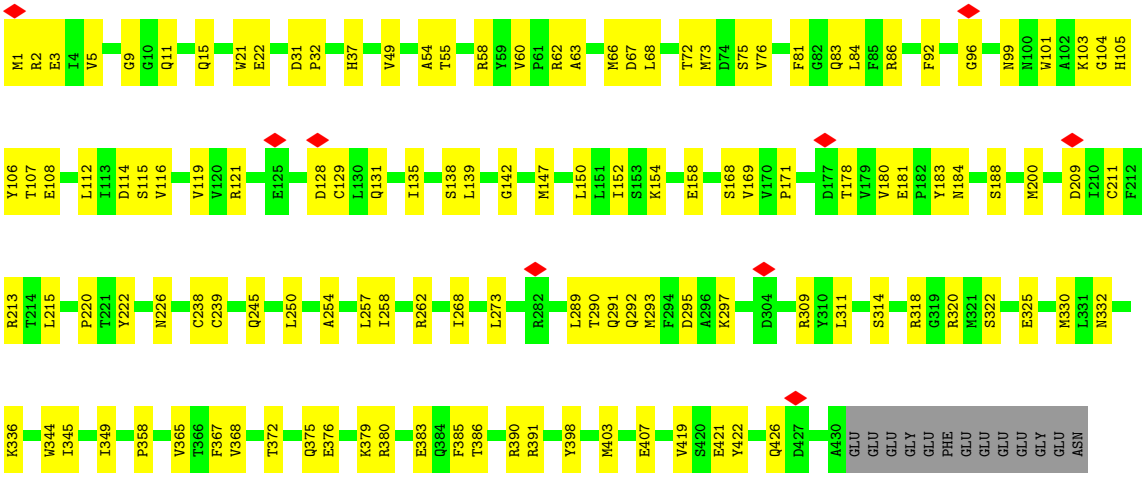




• Molecule 46: Tubulin beta chain

Chain MH:

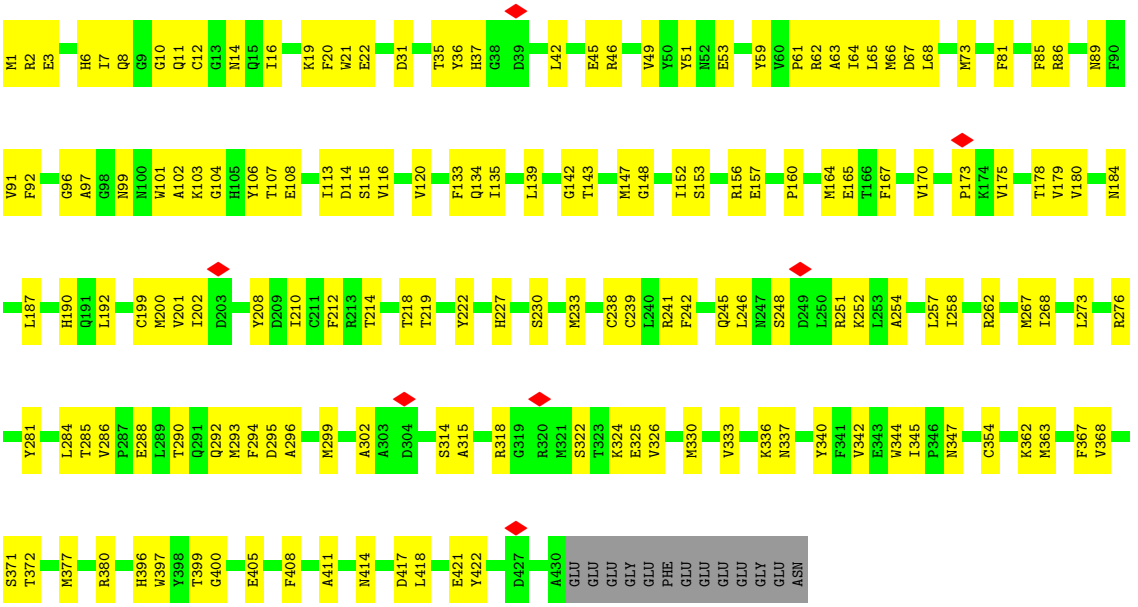




• Molecule 46: Tubulin beta chain

Chain MJ:

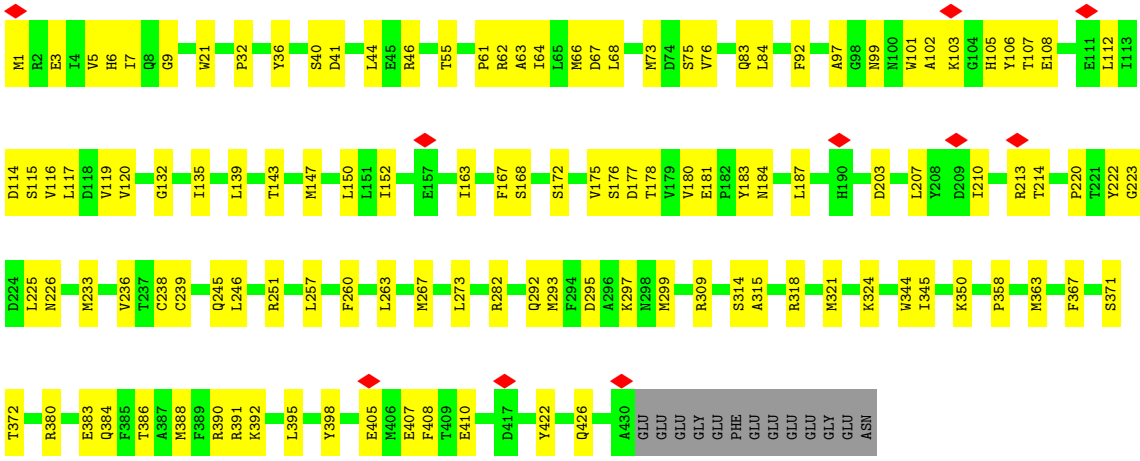




• Molecule 46: Tubulin beta chain

Chain ML:

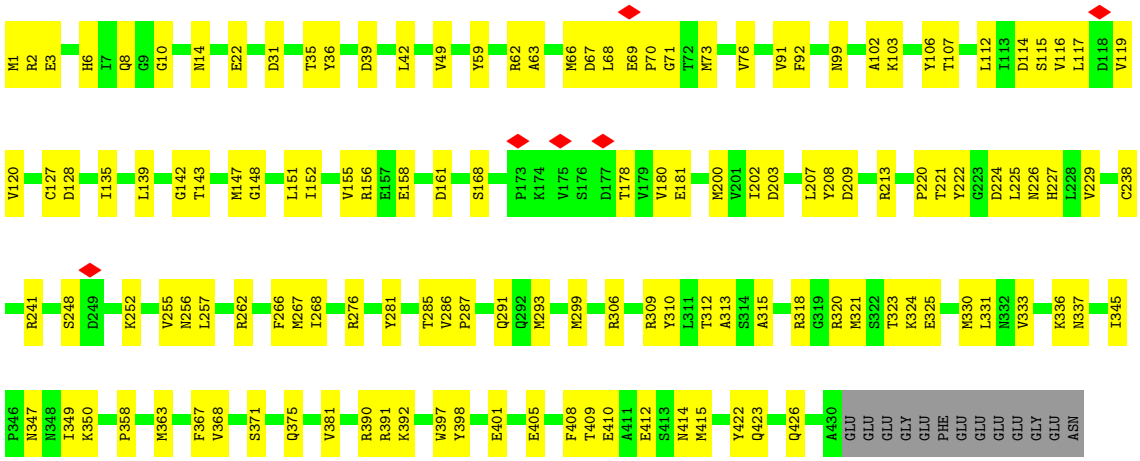




• Molecule 46: Tubulin beta chain

Chain MN:

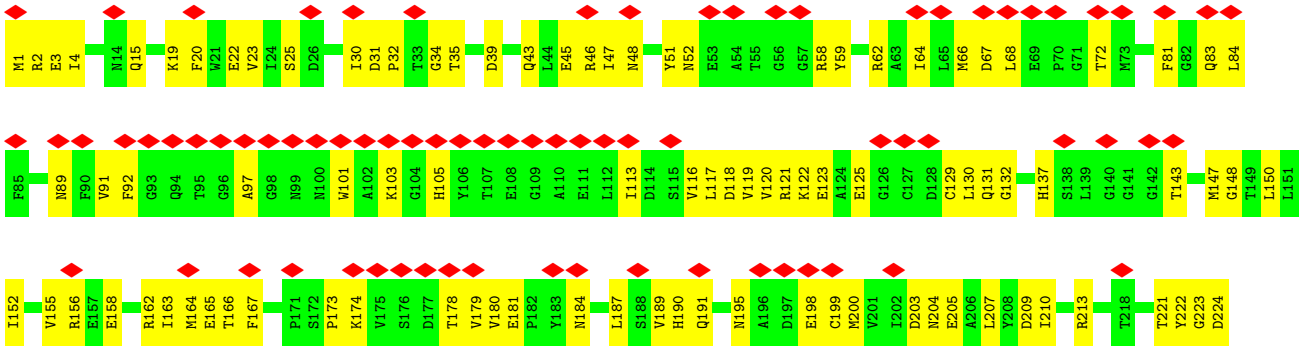


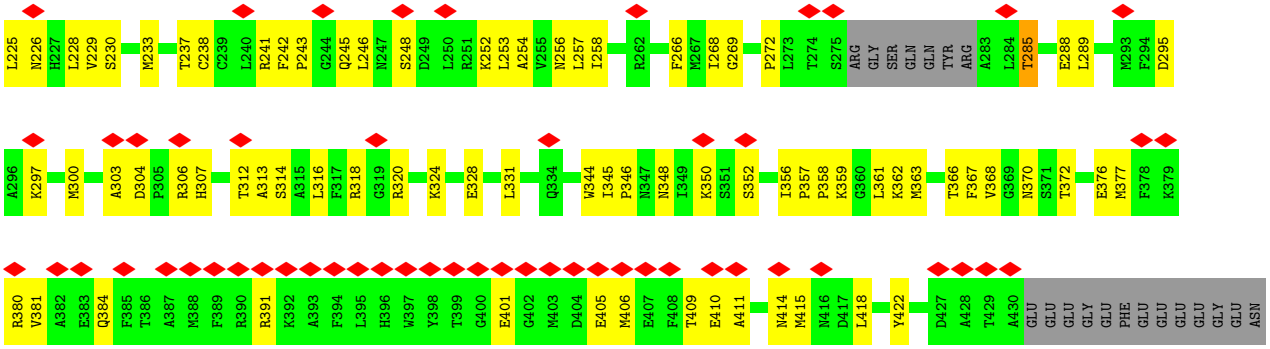


• Molecule 46: Tubulin beta chain

Chain NB:



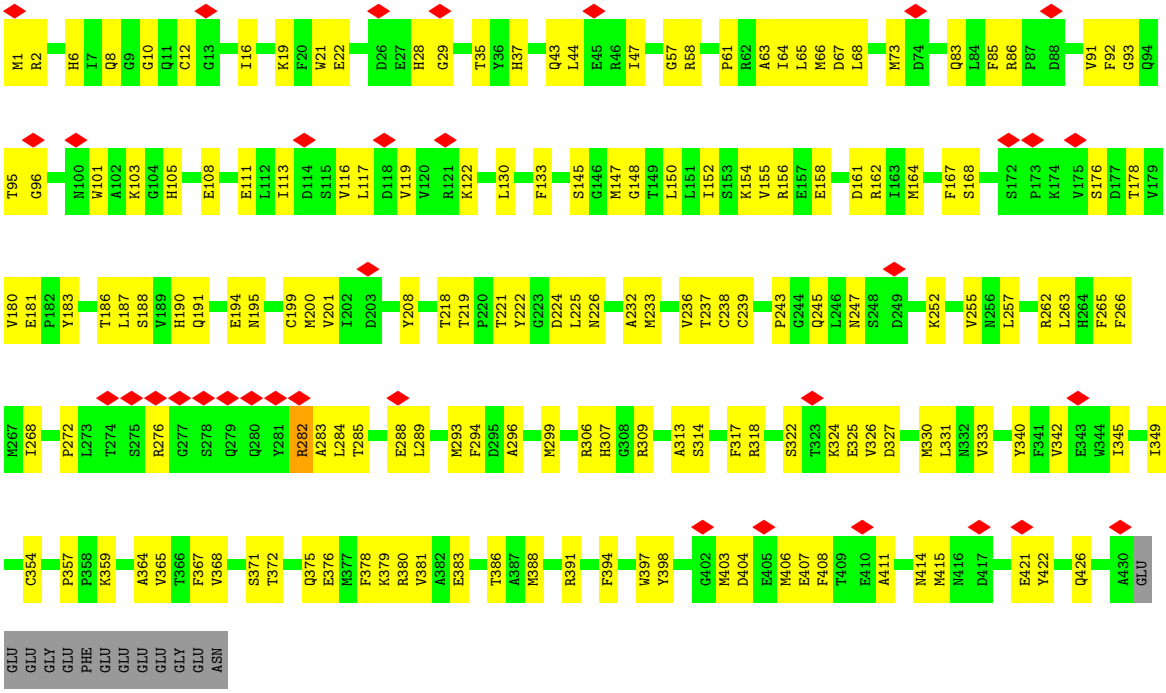




• Molecule 46: Tubulin beta chain

Chain ND:

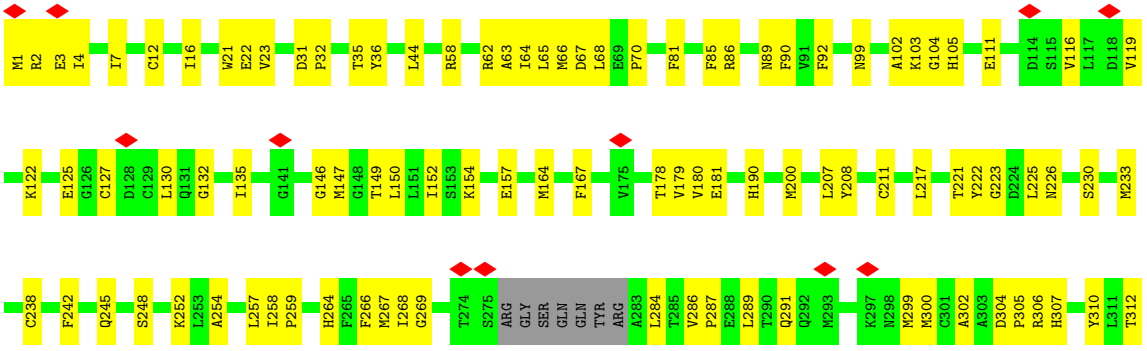


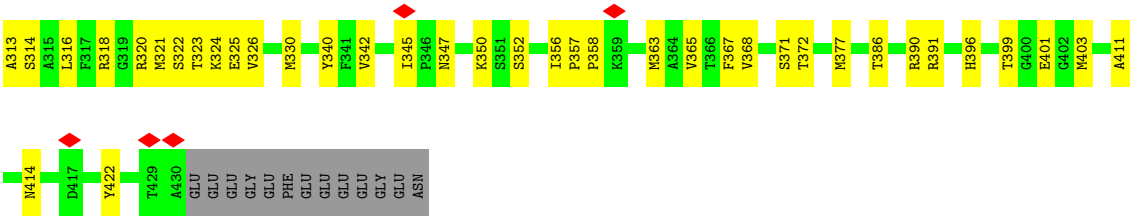


• Molecule 46: Tubulin beta chain

Chain NF:



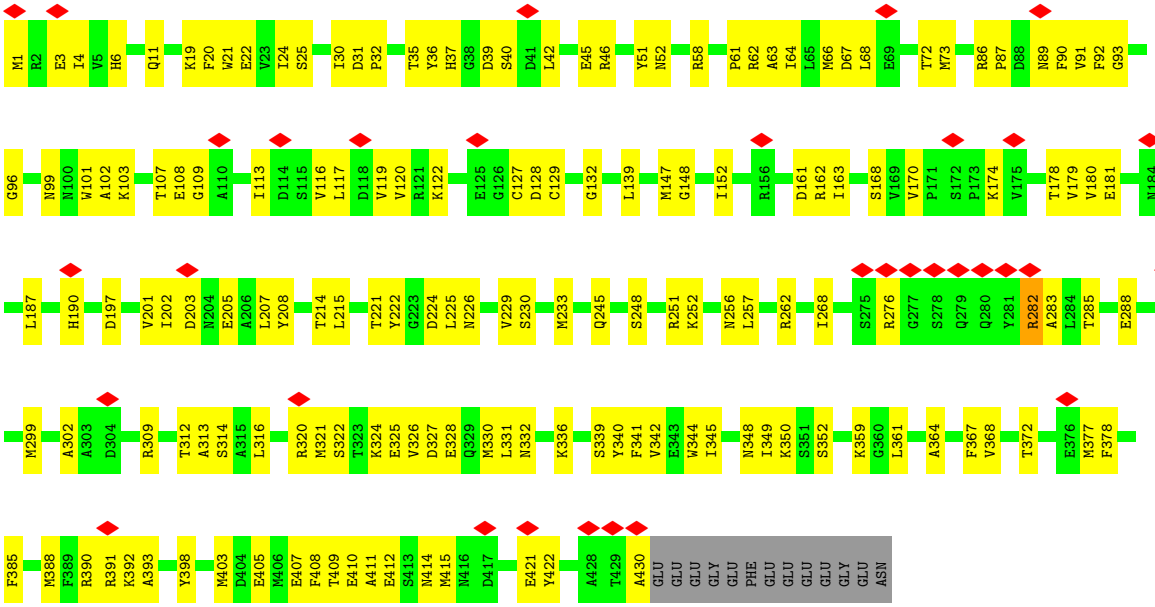




• Molecule 46: Tubulin beta chain

Chain NH:

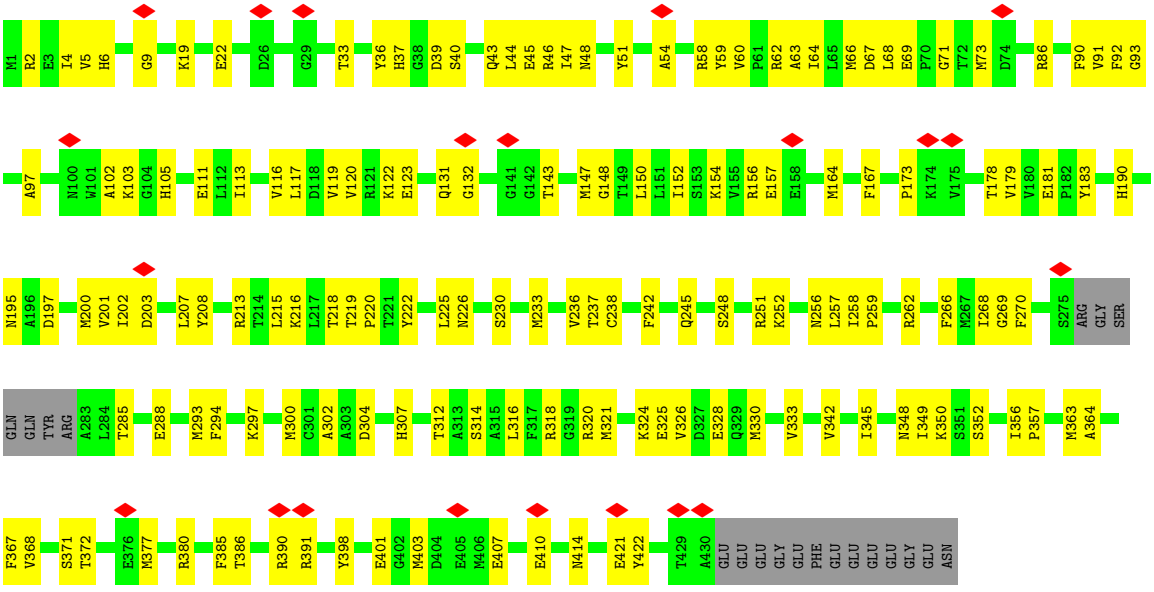




• Molecule 46: Tubulin beta chain

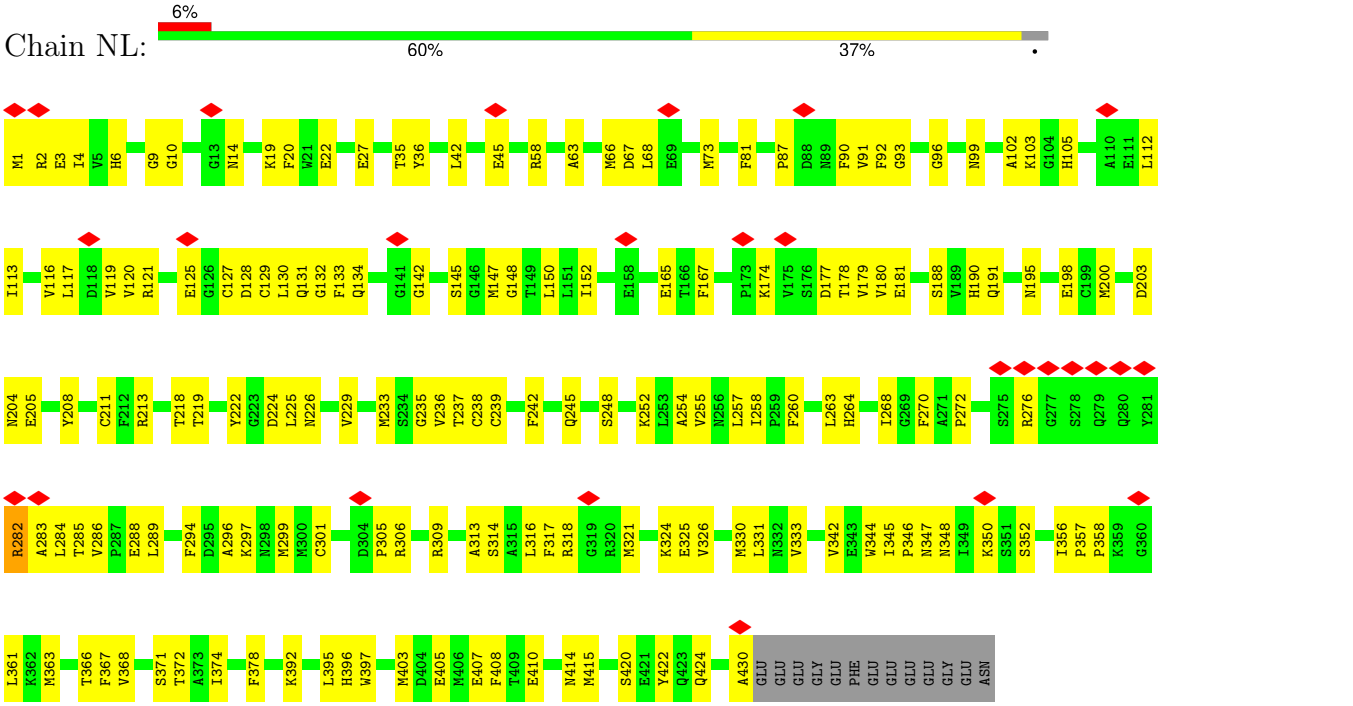
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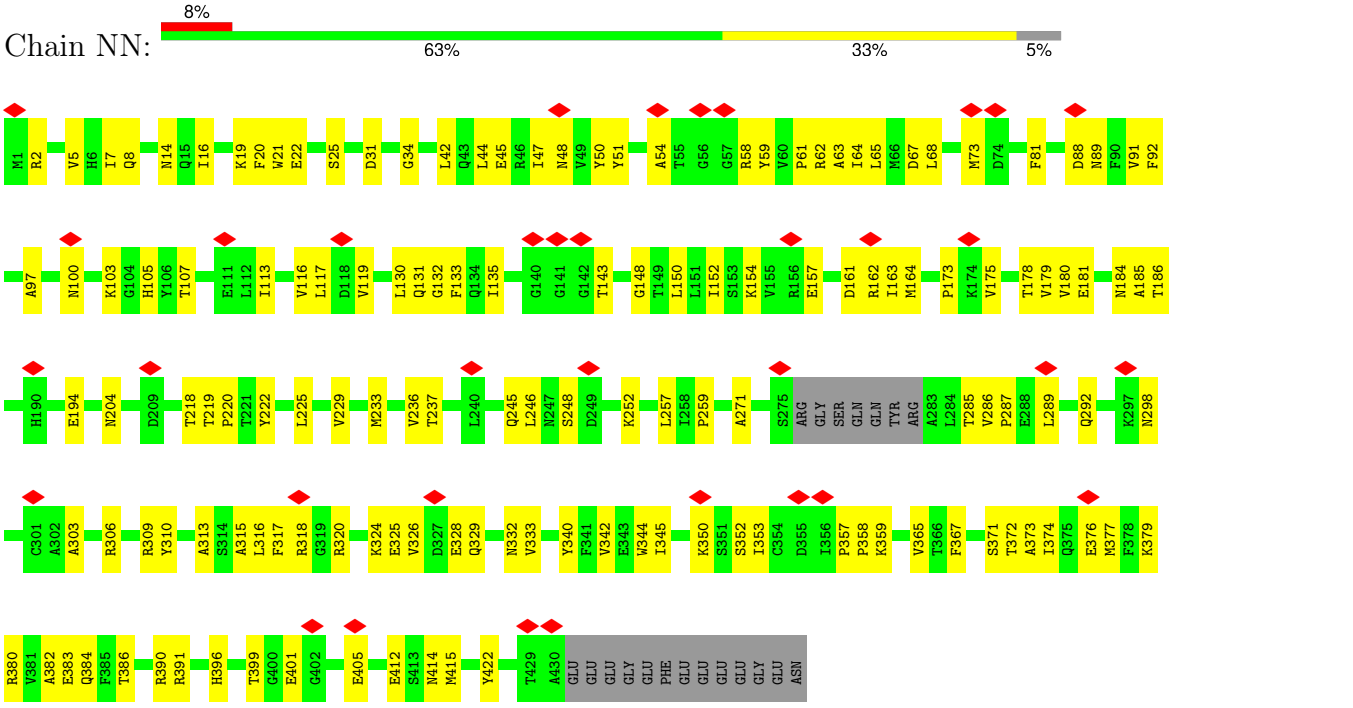
• Molecule 46: Tubulin beta chain

Chain NL:



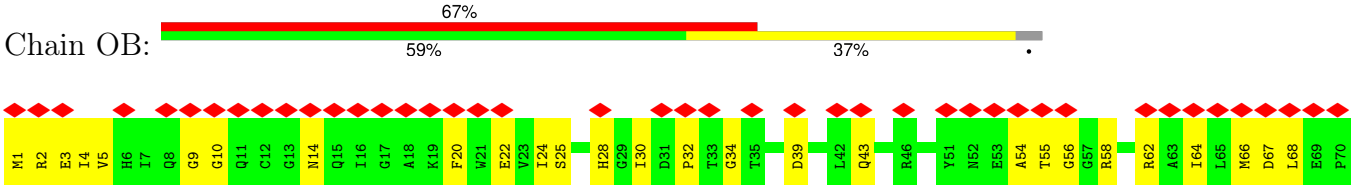
• Molecule 46: Tubulin beta chain

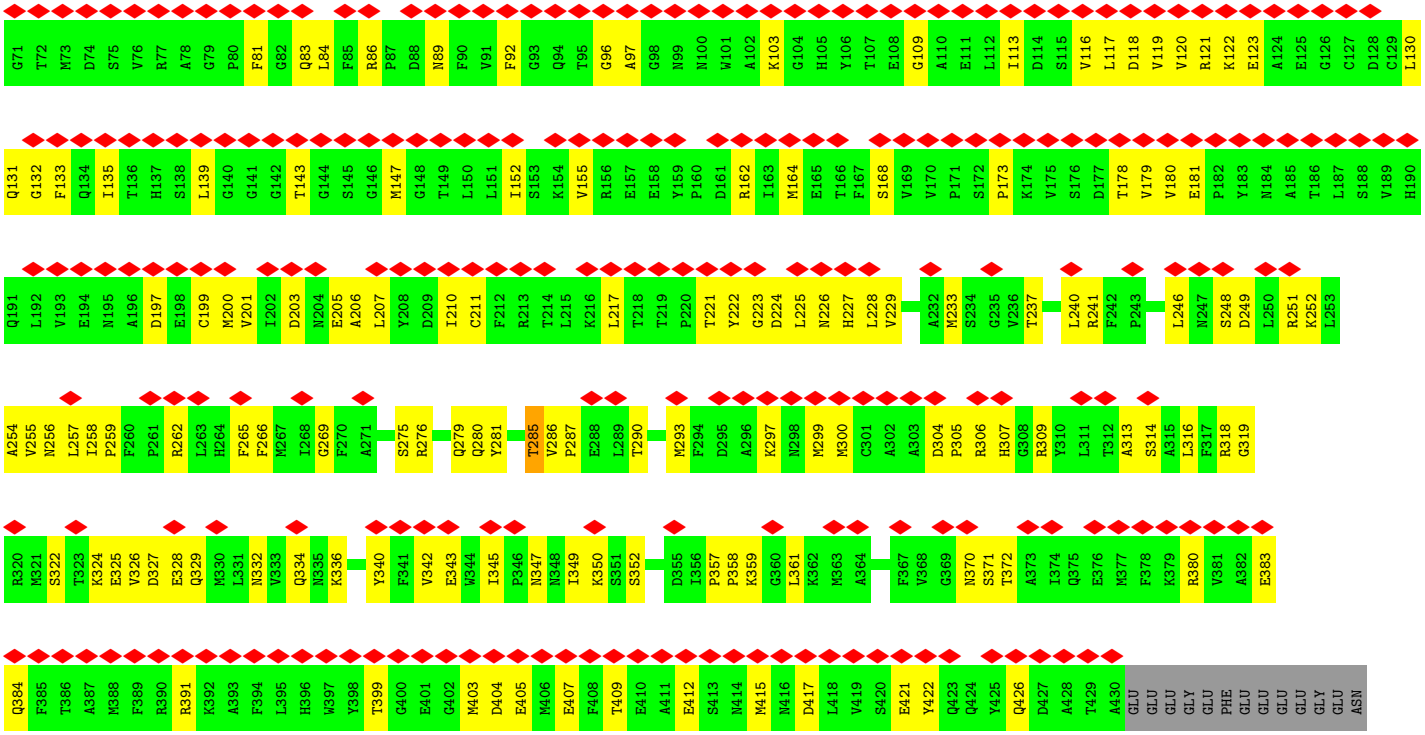
Chain NN:



• Molecule 46: Tubulin beta chain

Chain OB:

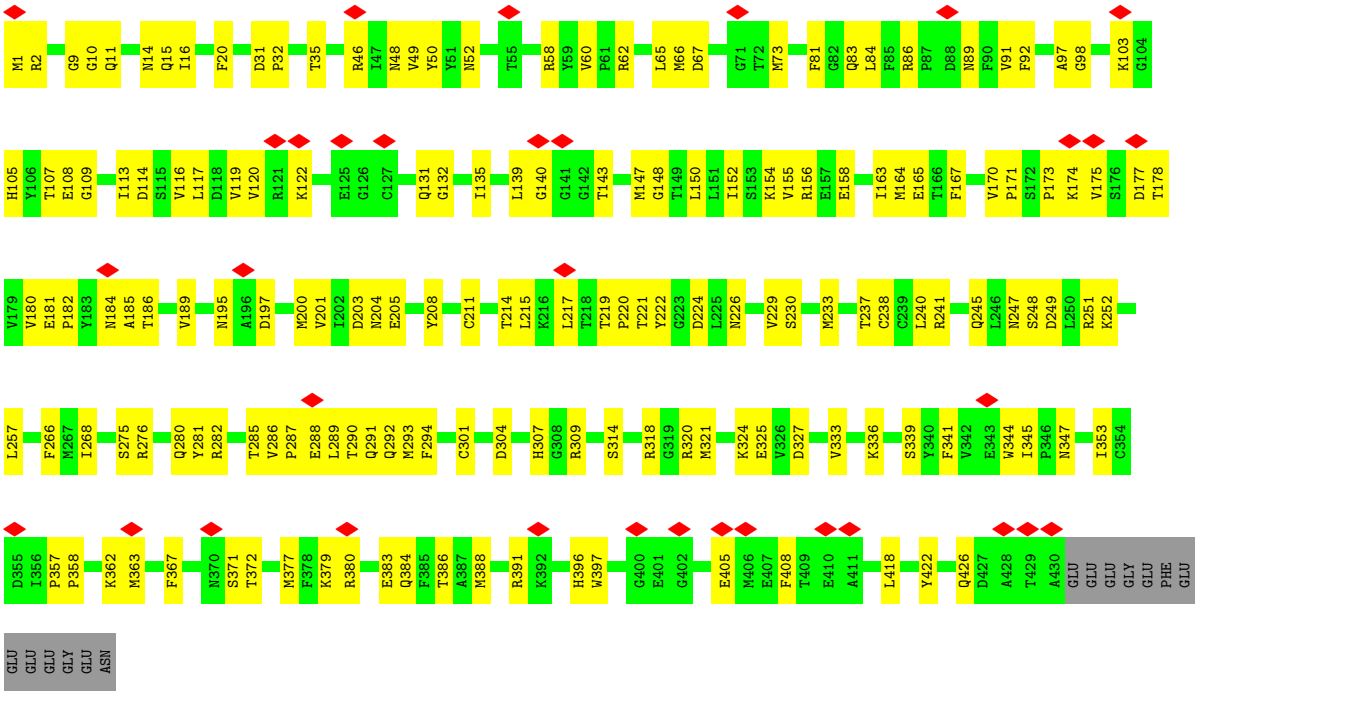




• Molecule 46: Tubulin beta chain

Chain OD:

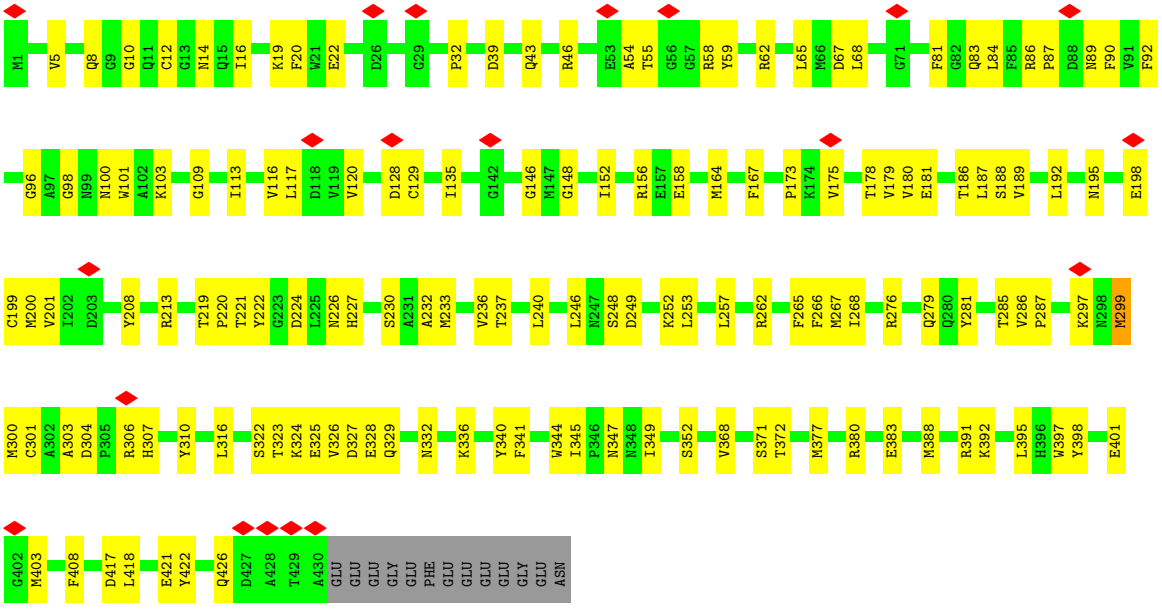




• Molecule 46: Tubulin beta chain

Chain OF:

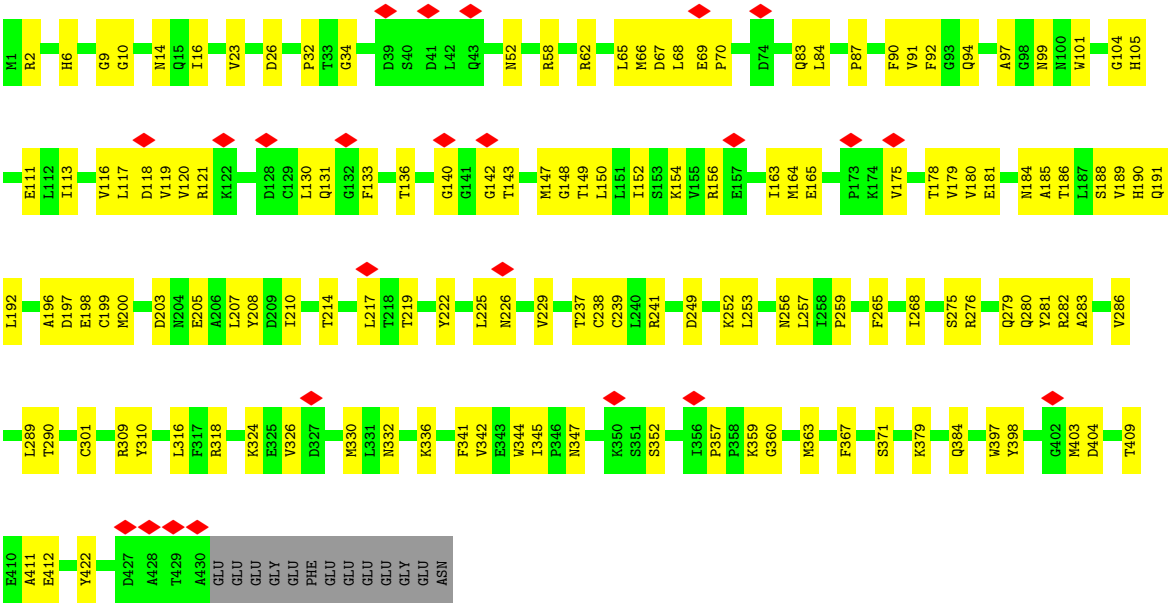




• Molecule 46: Tubulin beta chain

Chain OH:

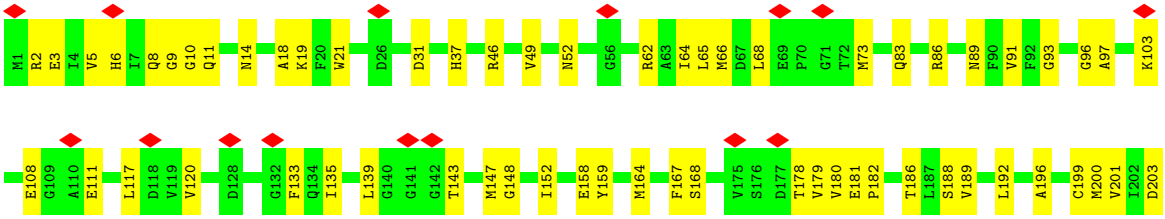


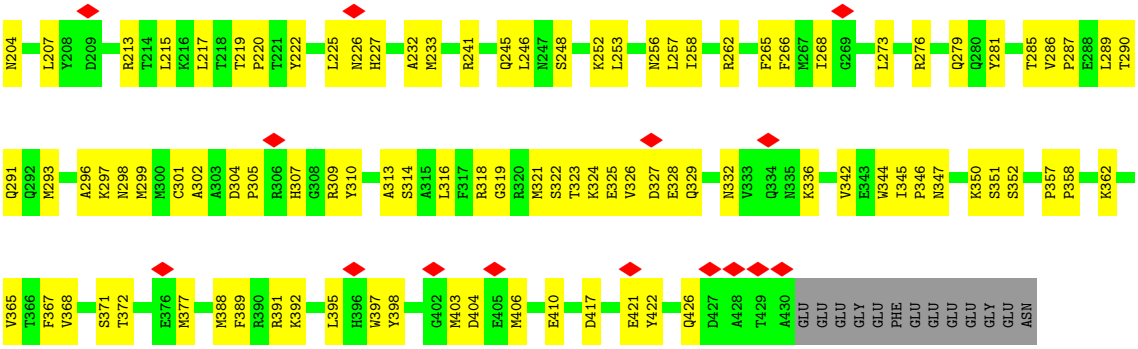


• Molecule 46: Tubulin beta chain

Chain OJ:



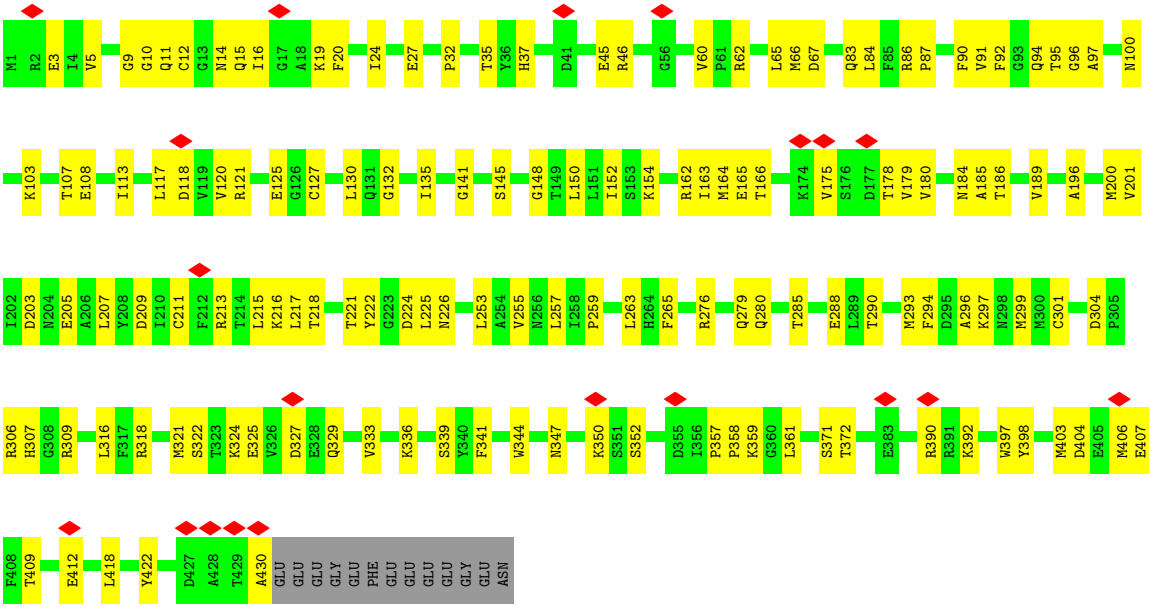




• Molecule 46: Tubulin beta chain

Chain OL:

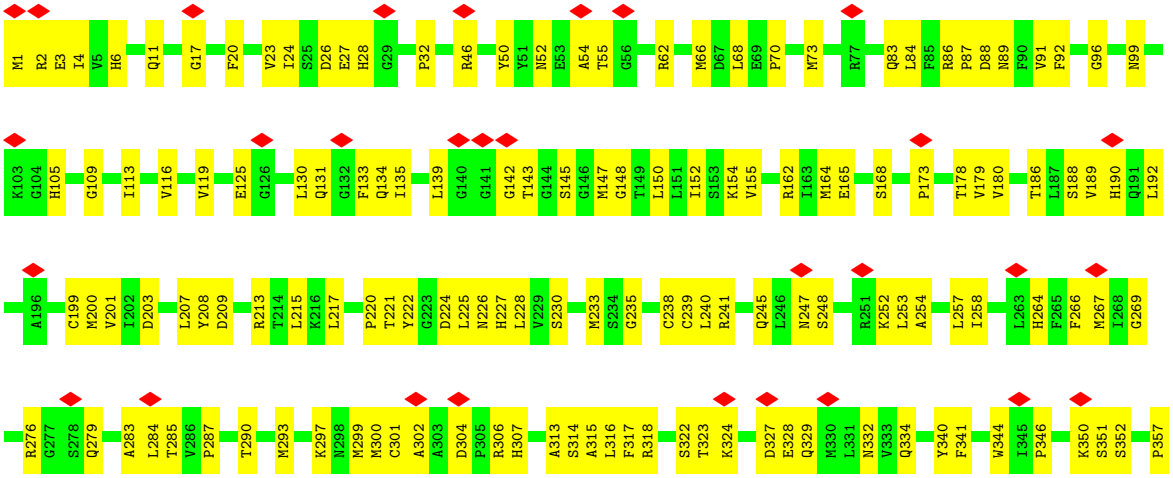


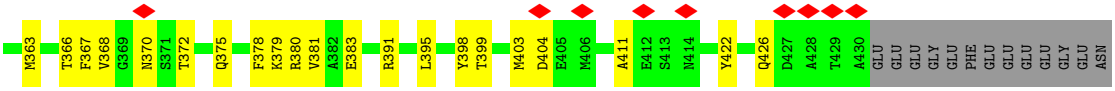


• Molecule 46: Tubulin beta chain

Chain ON:



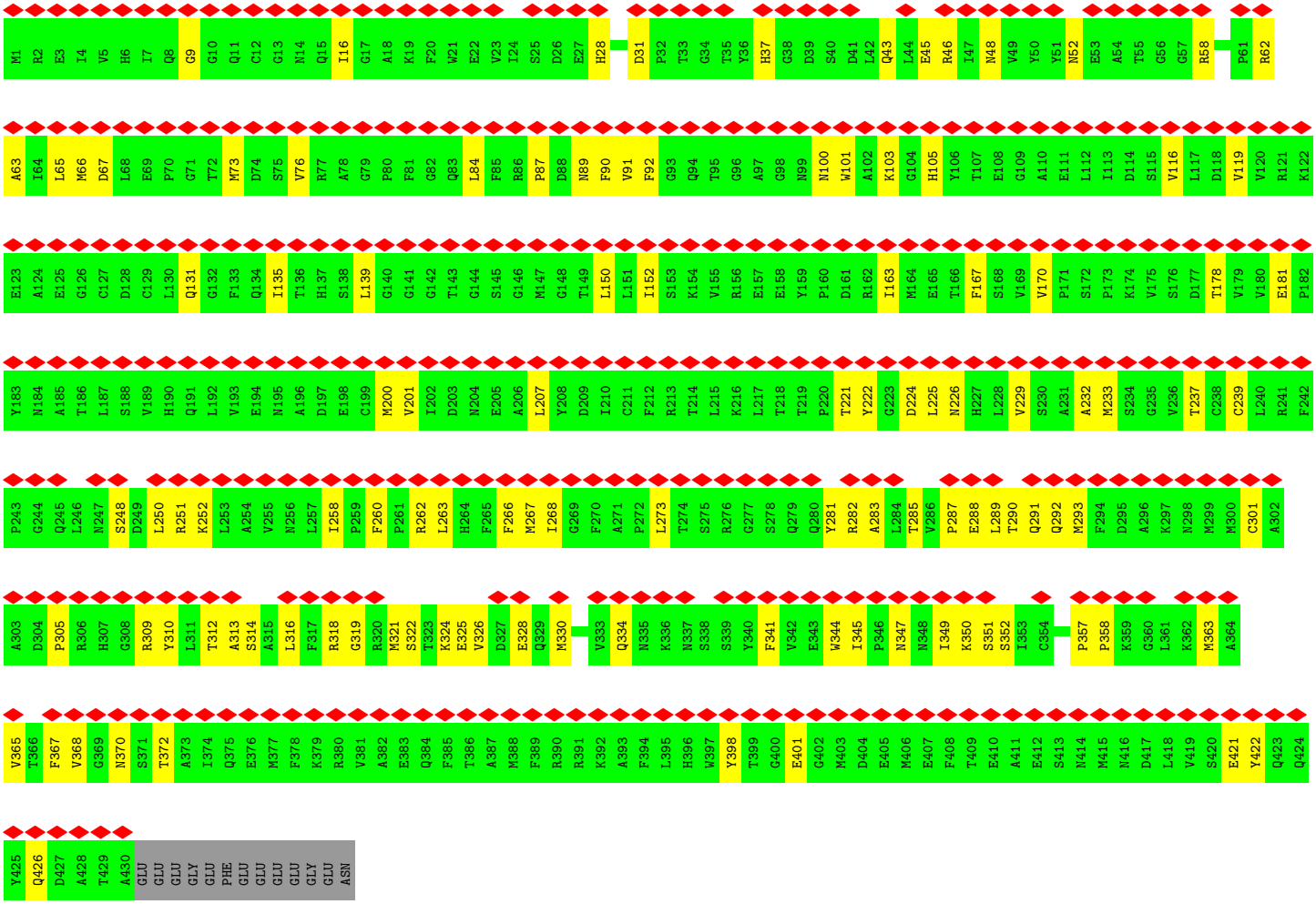




• Molecule 46: Tubulin beta chain

Chain PB:

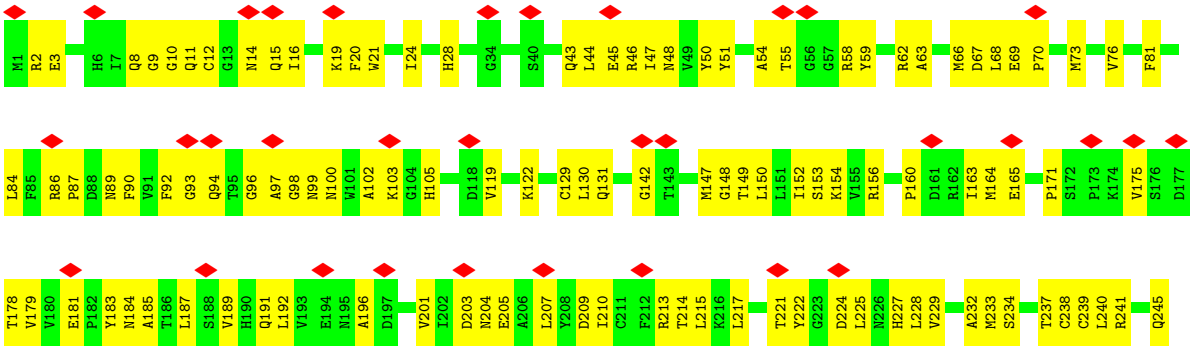


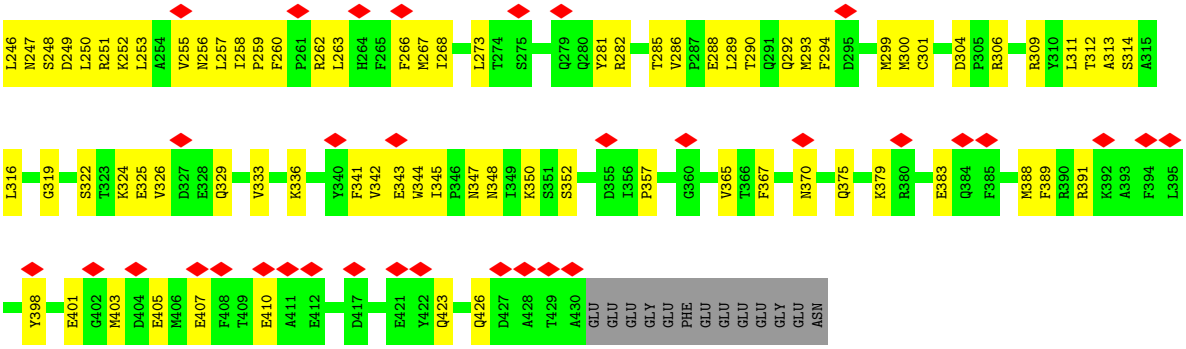


• Molecule 46: Tubulin beta chain

Chain PD:



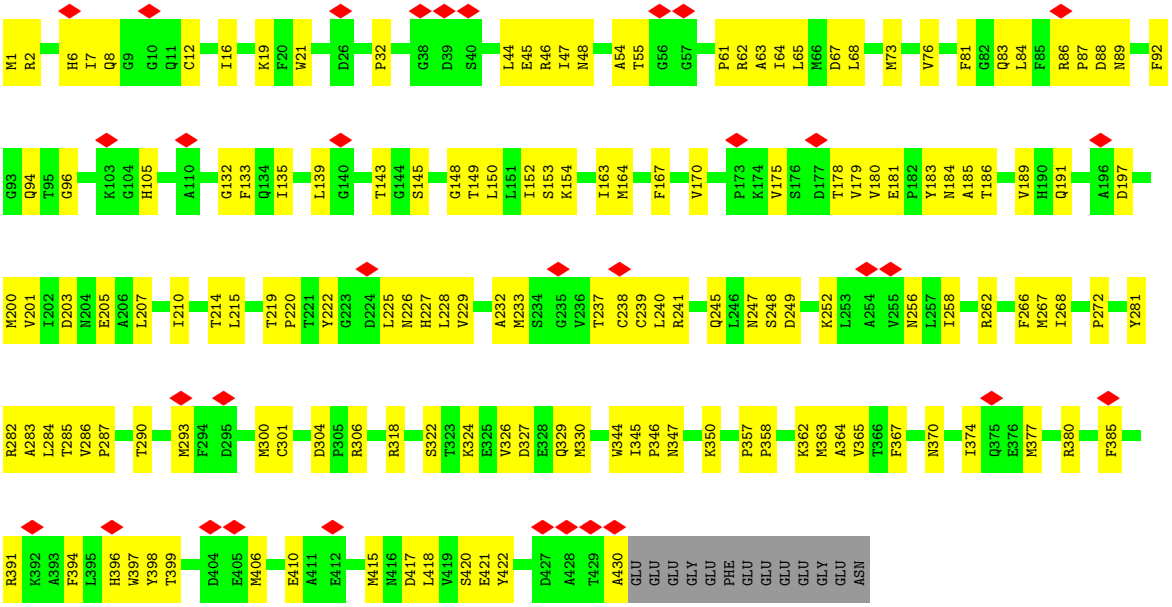




• Molecule 46: Tubulin beta chain

Chain PF:

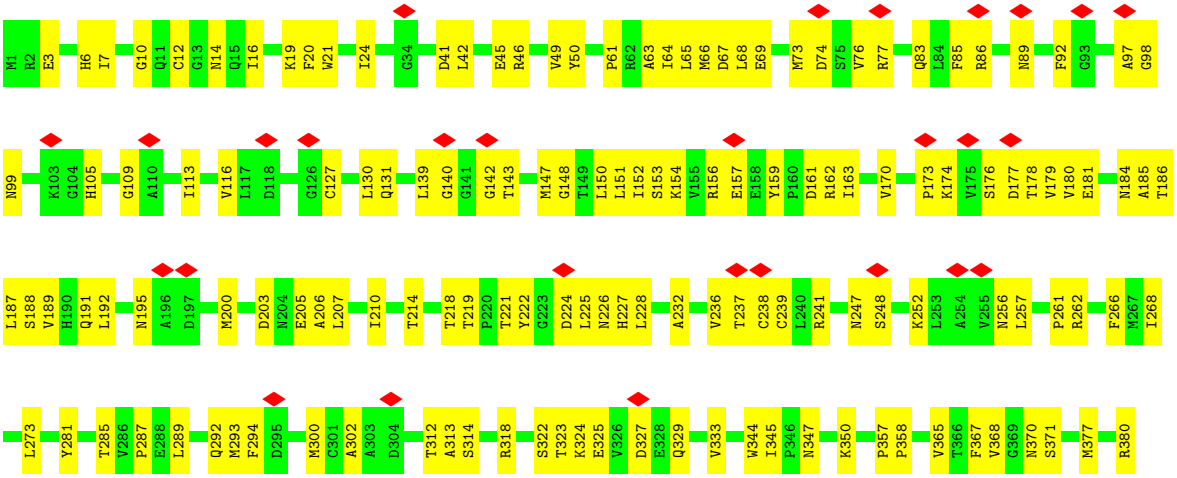


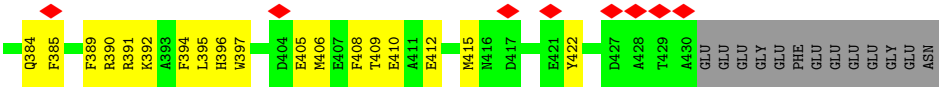


• Molecule 46: Tubulin beta chain

Chain PH:



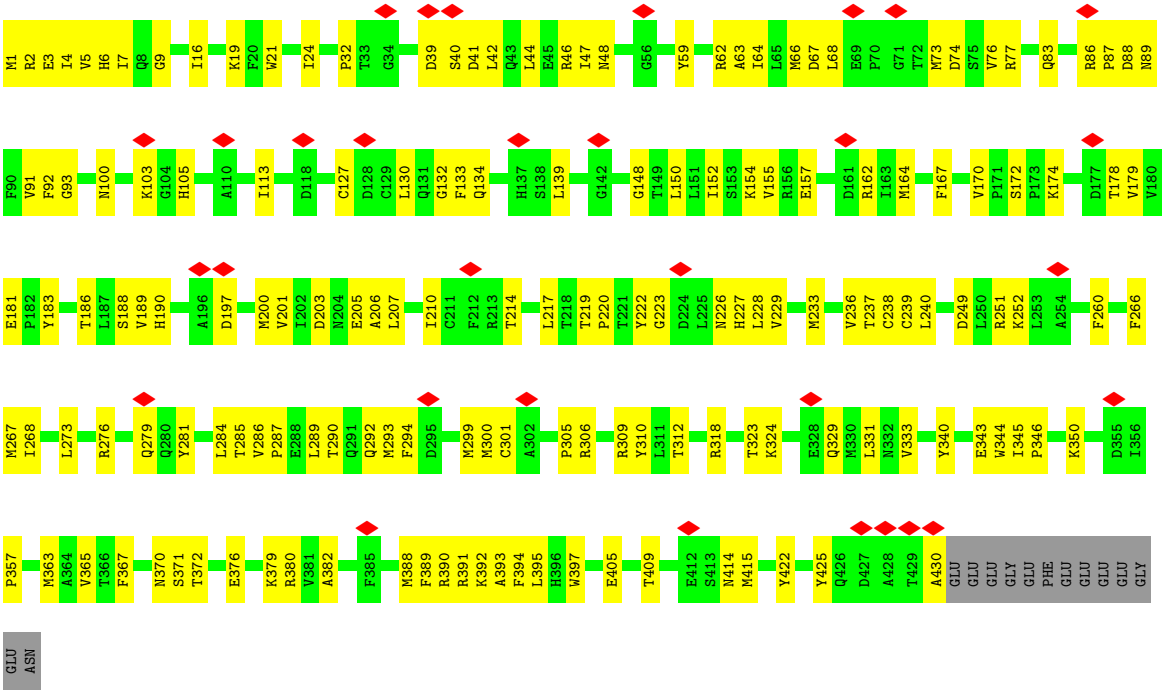




• Molecule 46: Tubulin beta chain

Chain PJ:

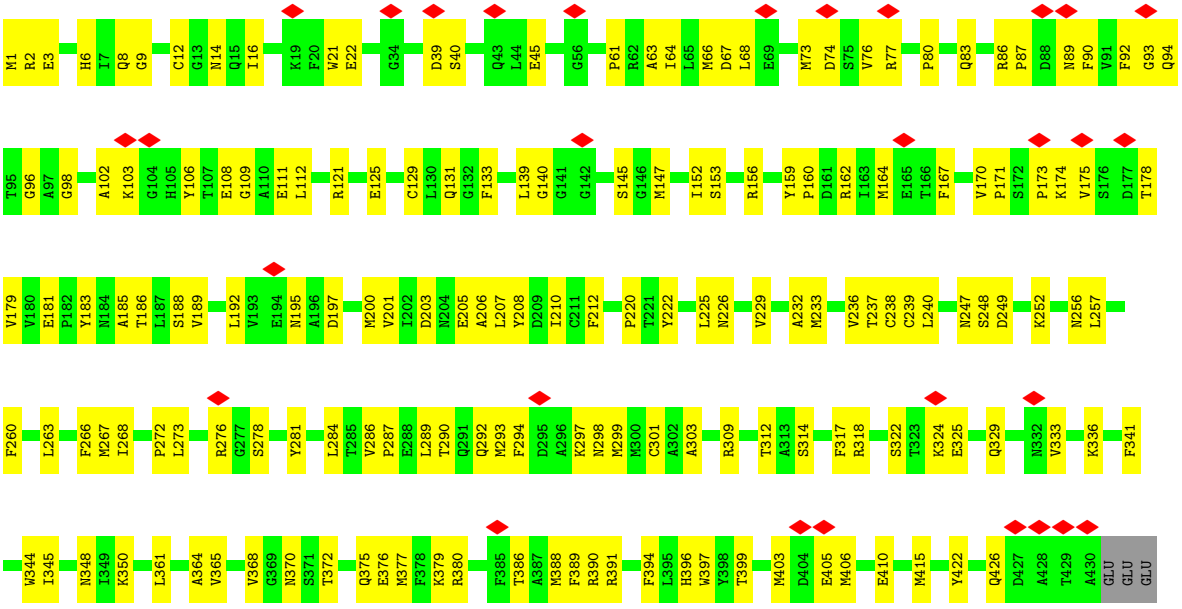




• Molecule 46: Tubulin beta chain

Chain PL:



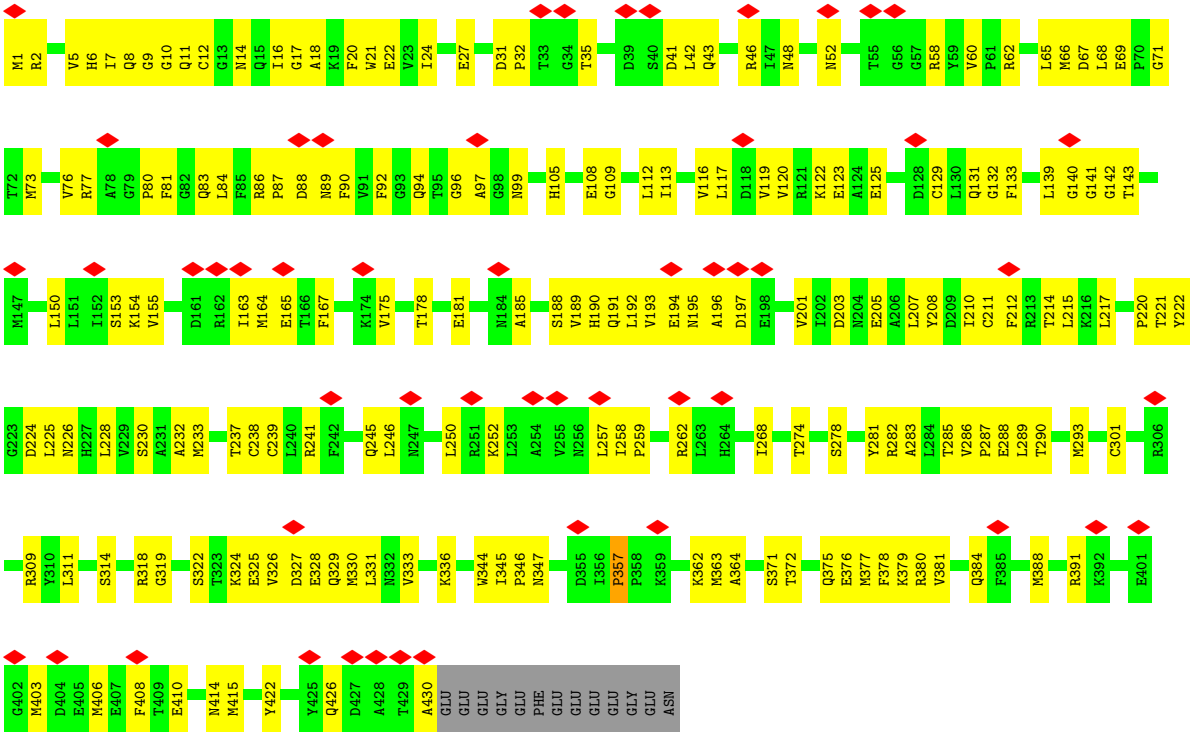




• Molecule 46: Tubulin beta chain

Chain PN:

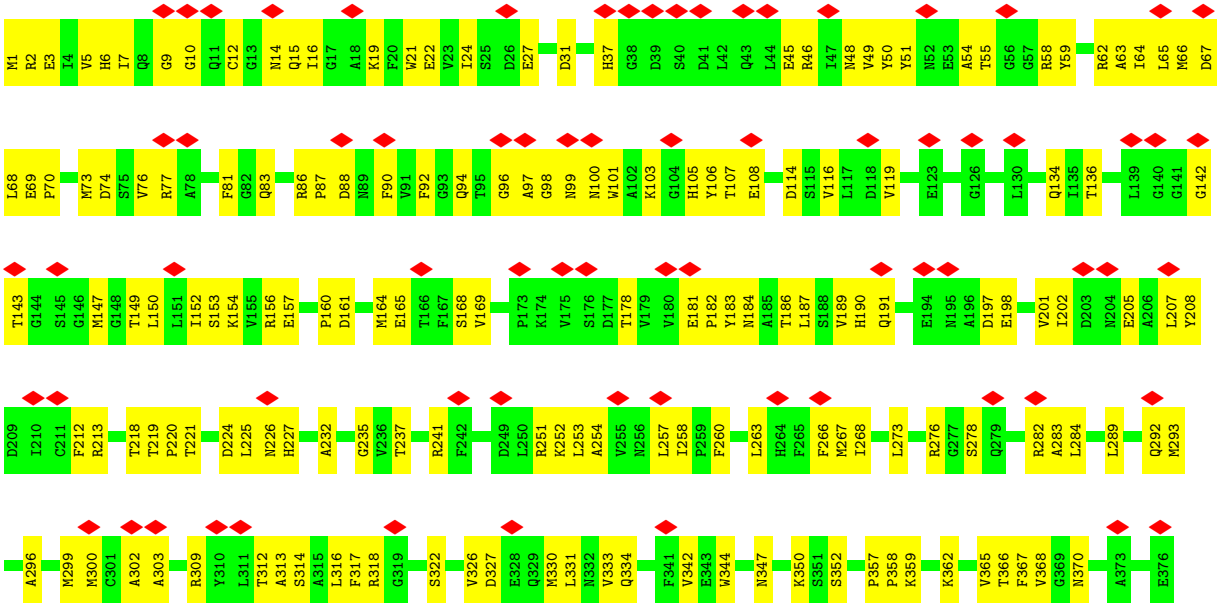


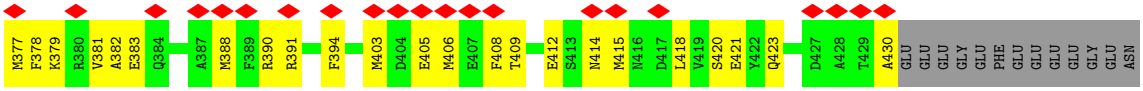


• Molecule 46: Tubulin beta chain

Chain QB:



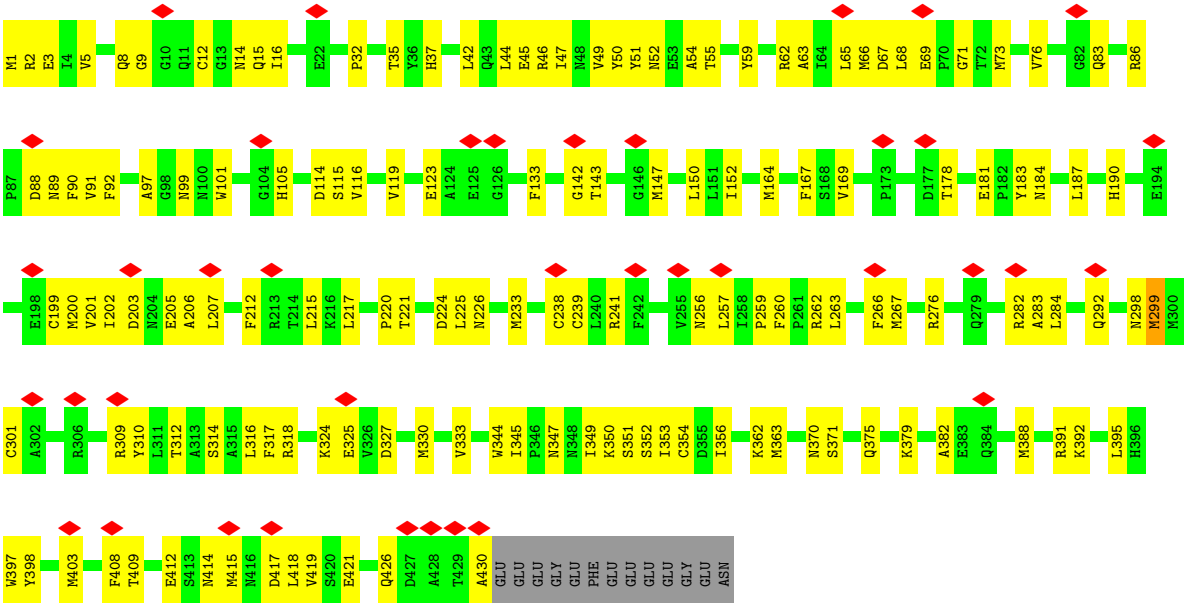




• Molecule 46: Tubulin beta chain

Chain QD:

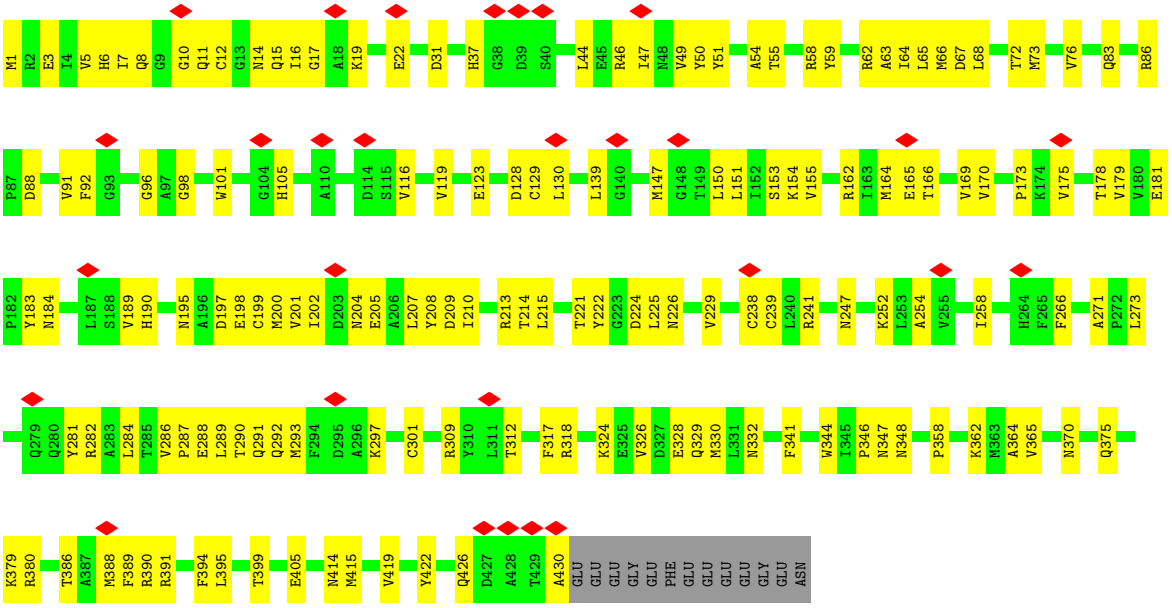




• Molecule 46: Tubulin beta chain

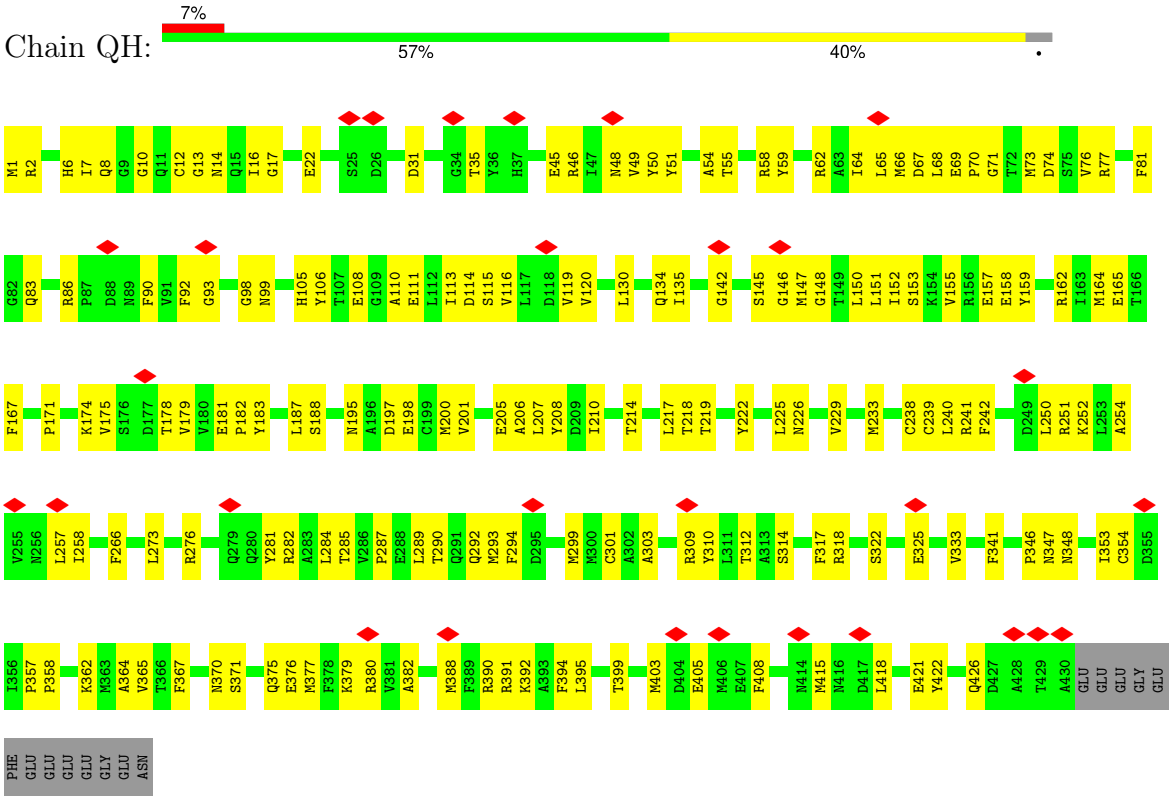
Chain QF:





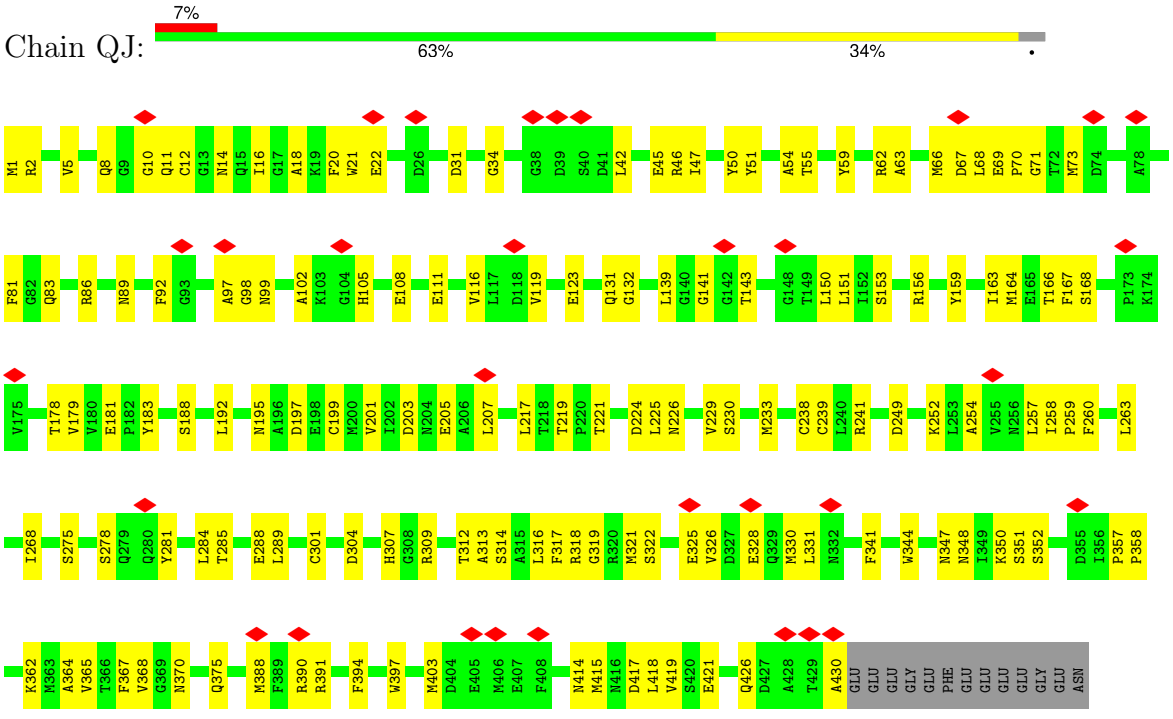
• Molecule 46: Tubulin beta chain

Chain QH:



• Molecule 46: Tubulin beta chain

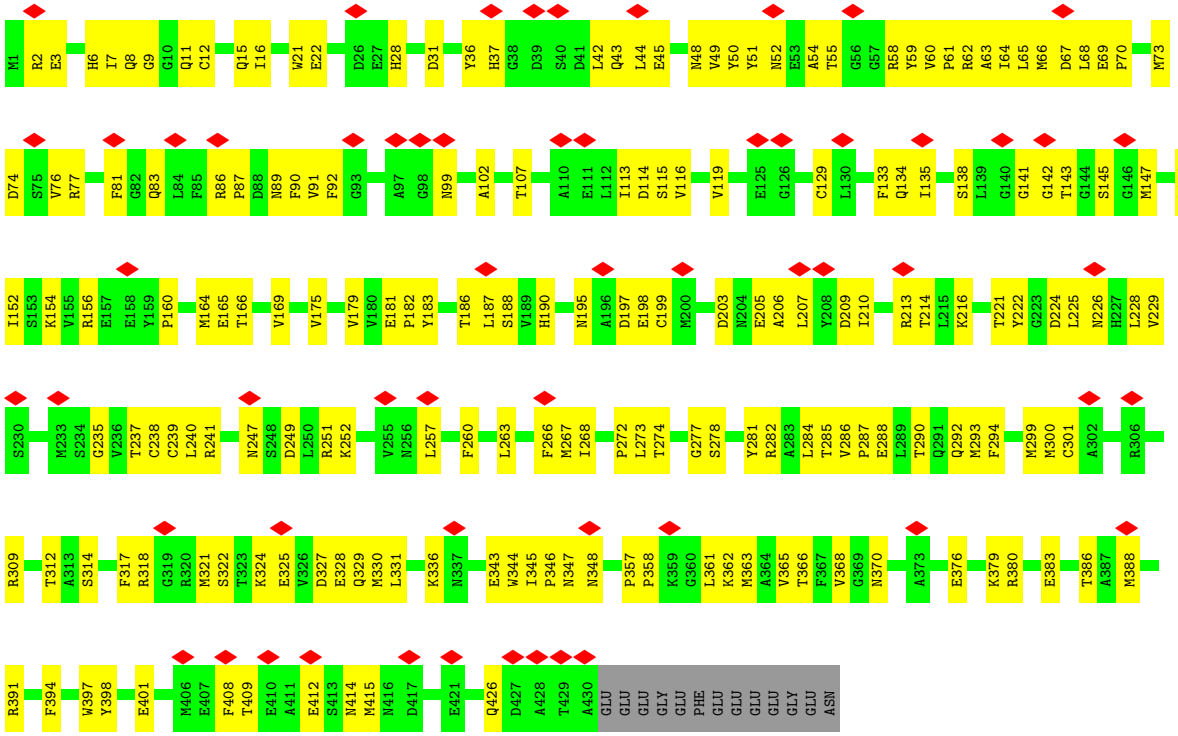
Chain QJ:



• Molecule 46: Tubulin beta chain

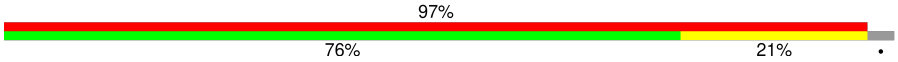
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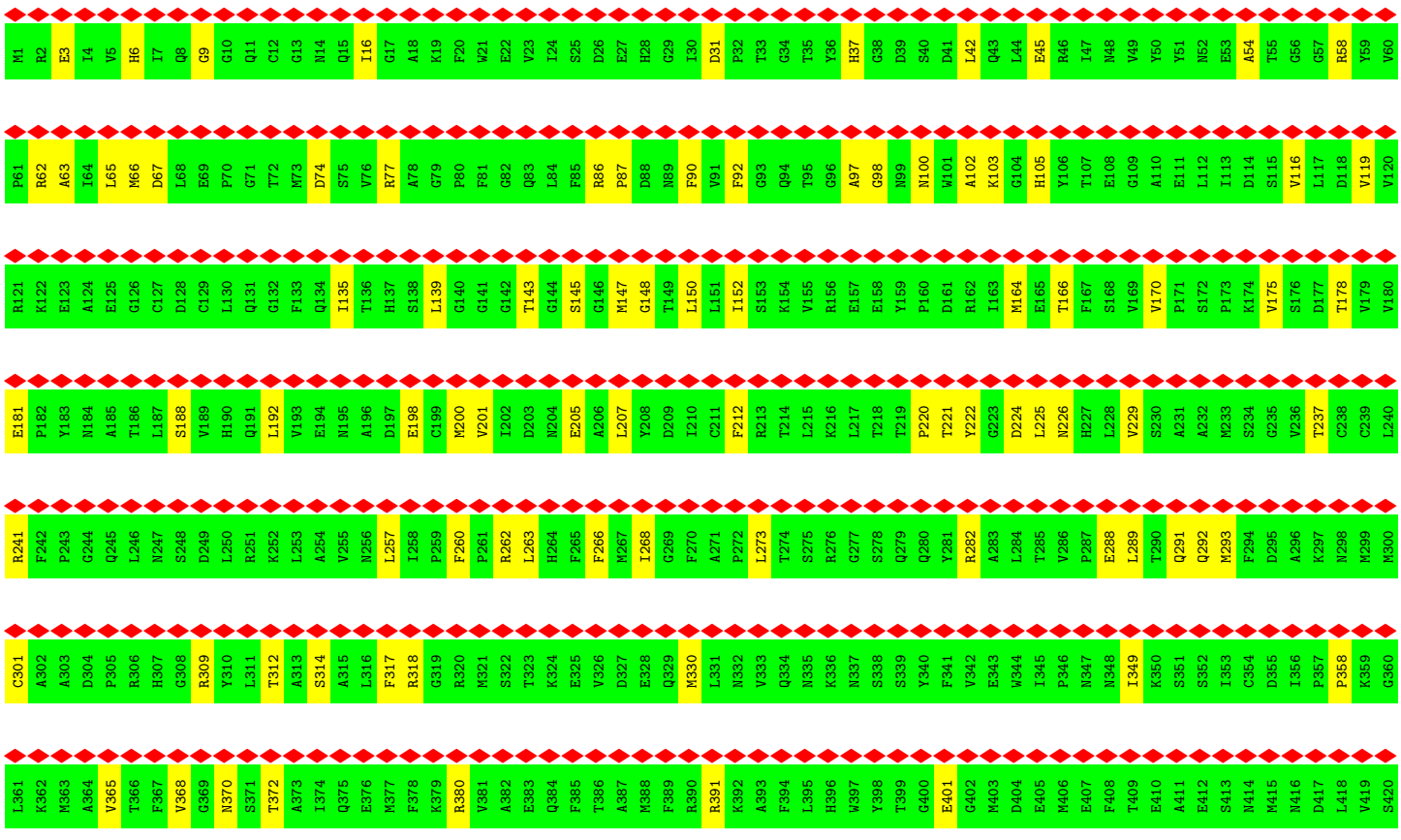


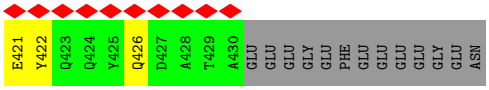


• Molecule 46: Tubulin beta chain

Chain QN:



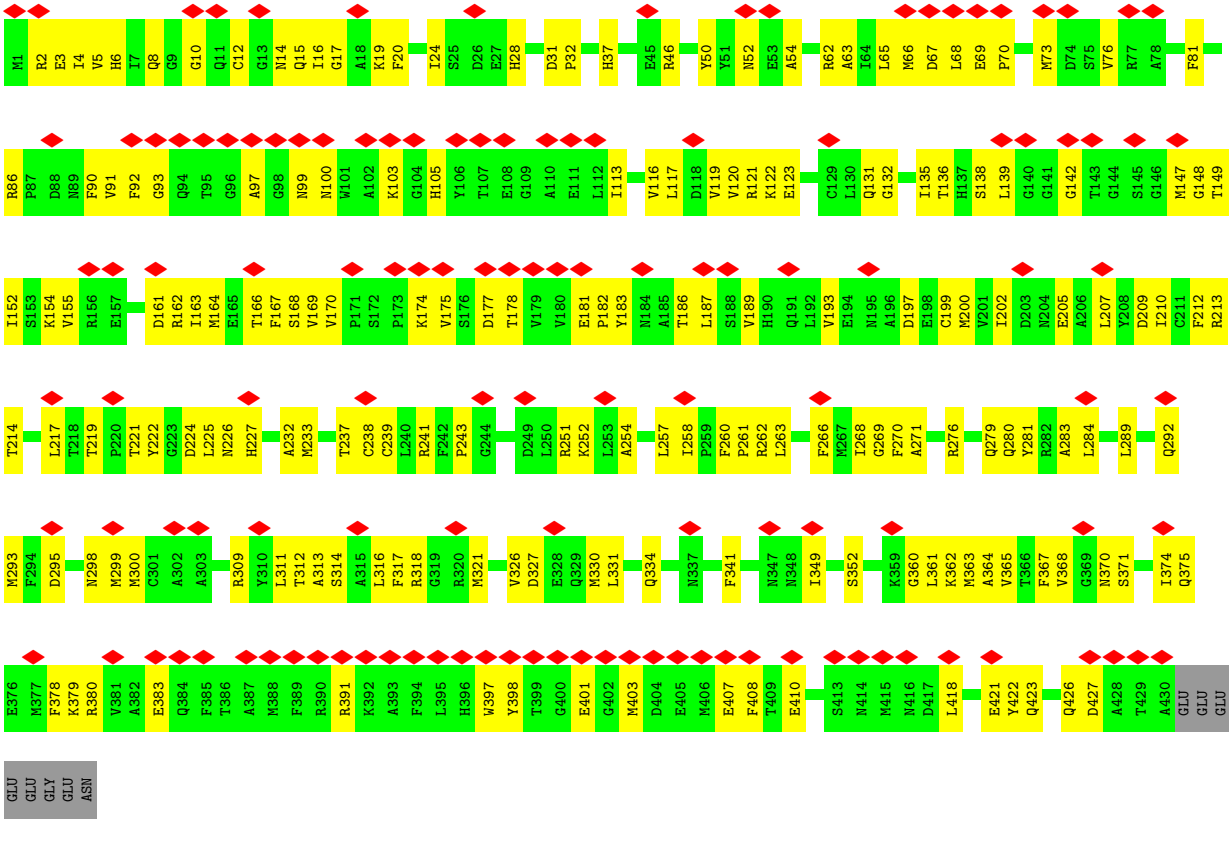




• Molecule 46: Tubulin beta chain

Chain RB:

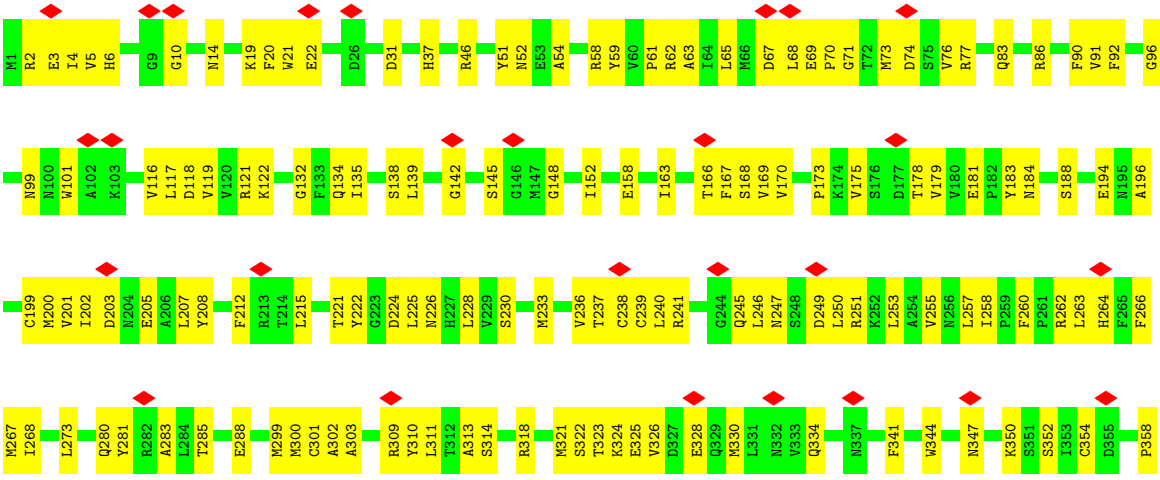


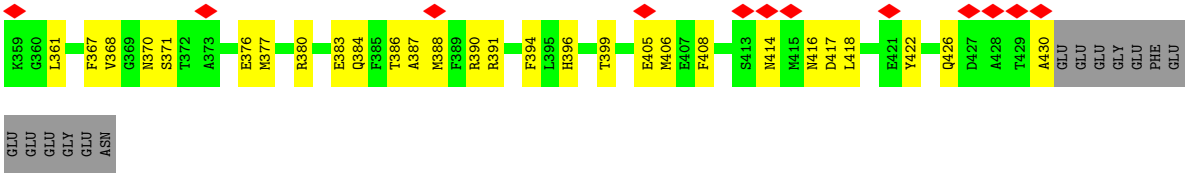


• Molecule 46: Tubulin beta chain

Chain RD:



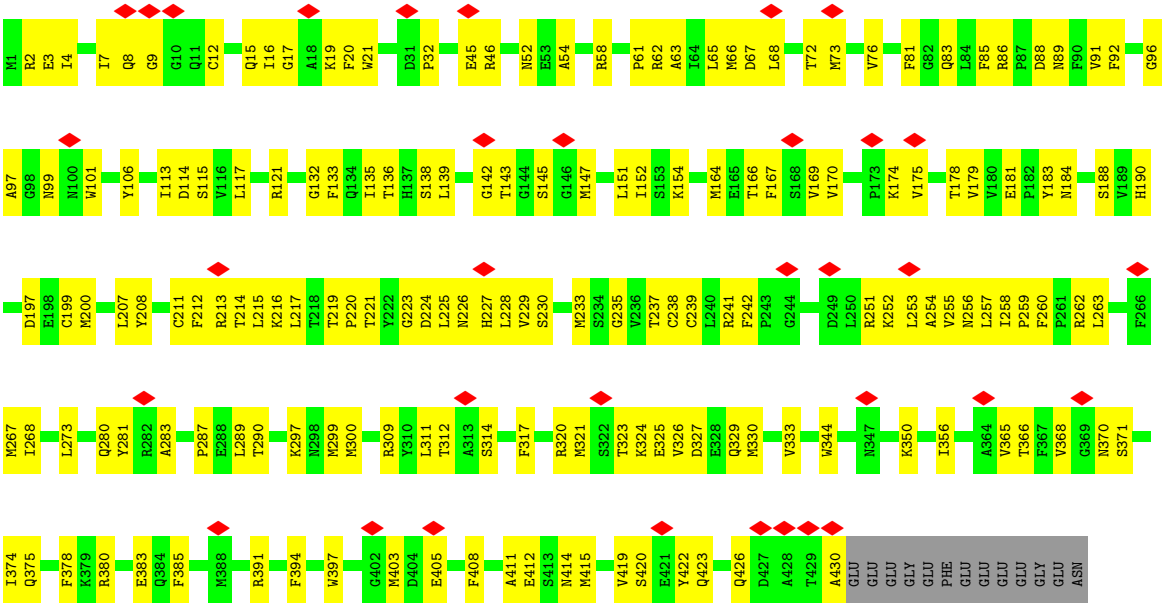




• Molecule 46: Tubulin beta chain

Chain RF:

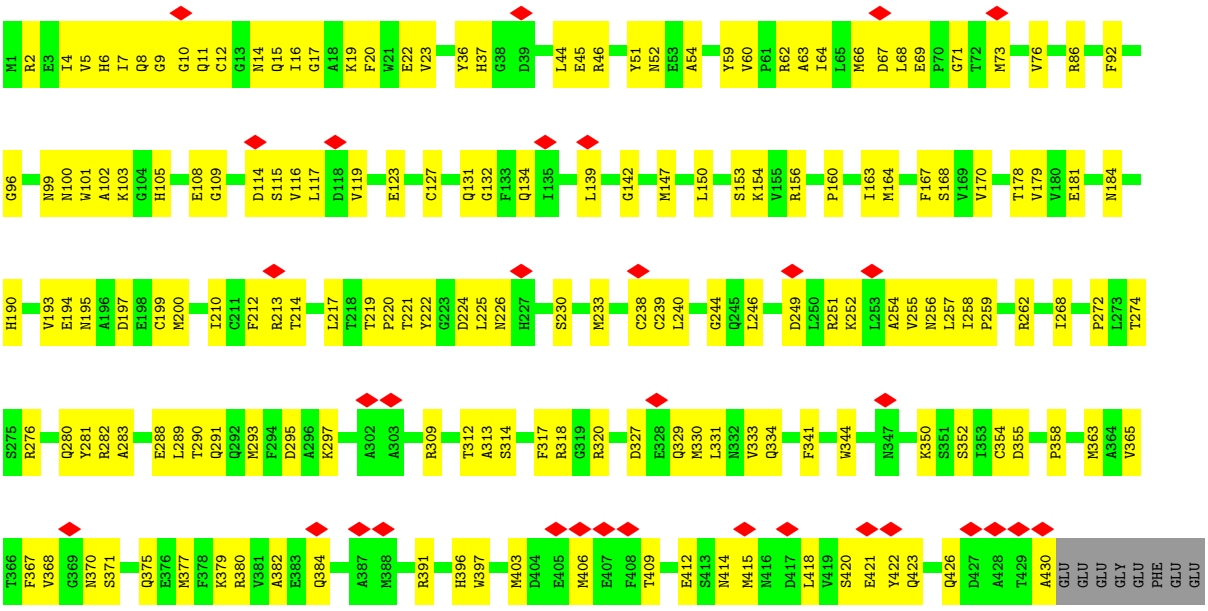




• Molecule 46: Tubulin beta chain

Chain RH:



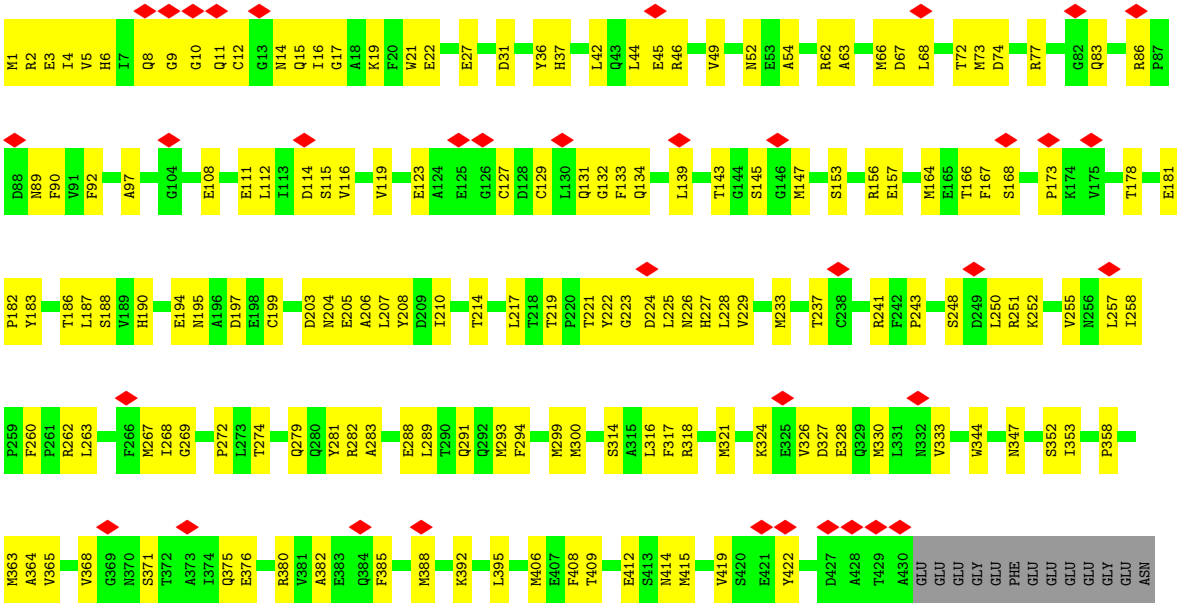




• Molecule 46: Tubulin beta chain

Chain RJ:

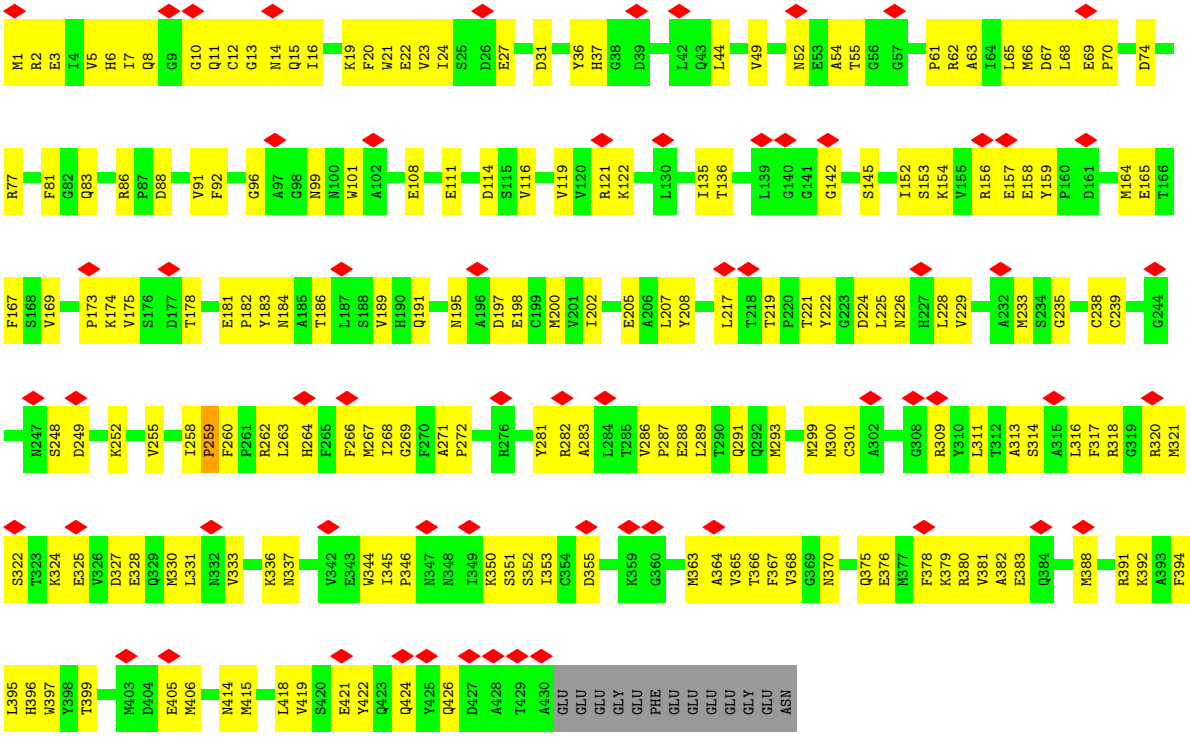




• Molecule 46: Tubulin beta chain

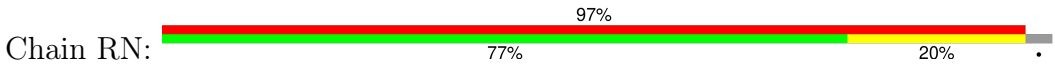
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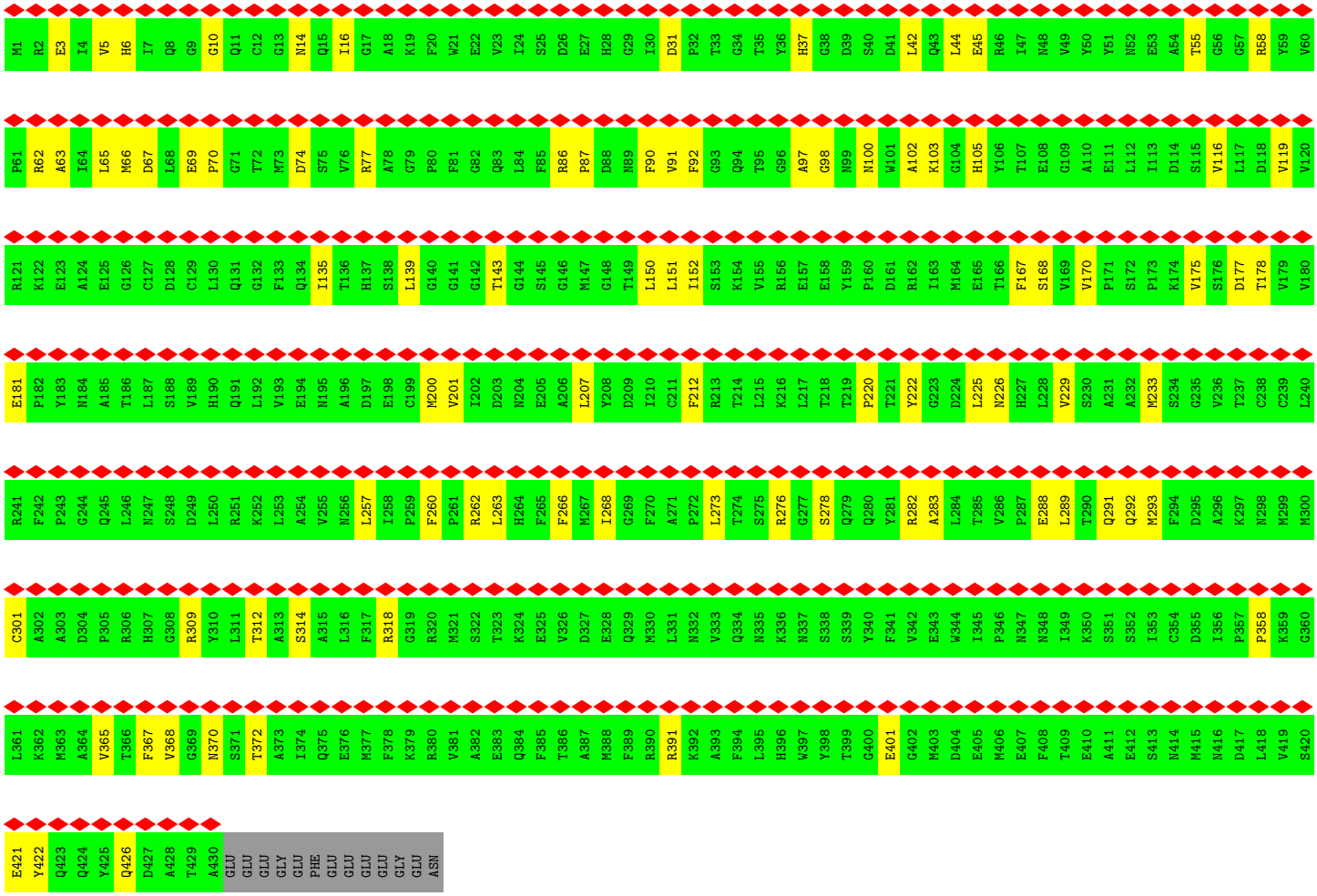




• Molecule 46: Tubulin beta chain

Chain RN:

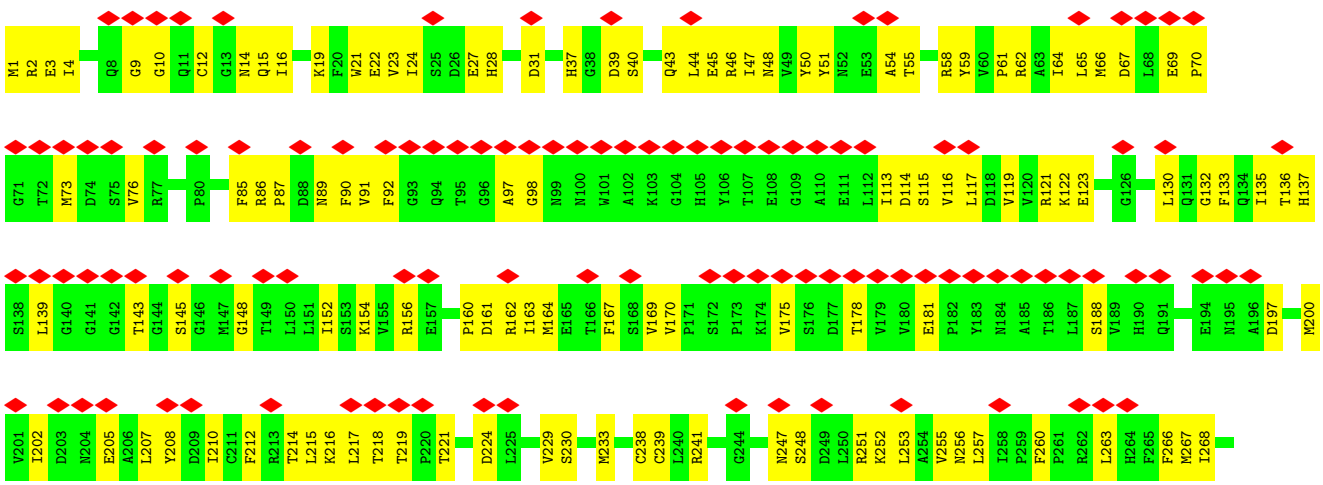


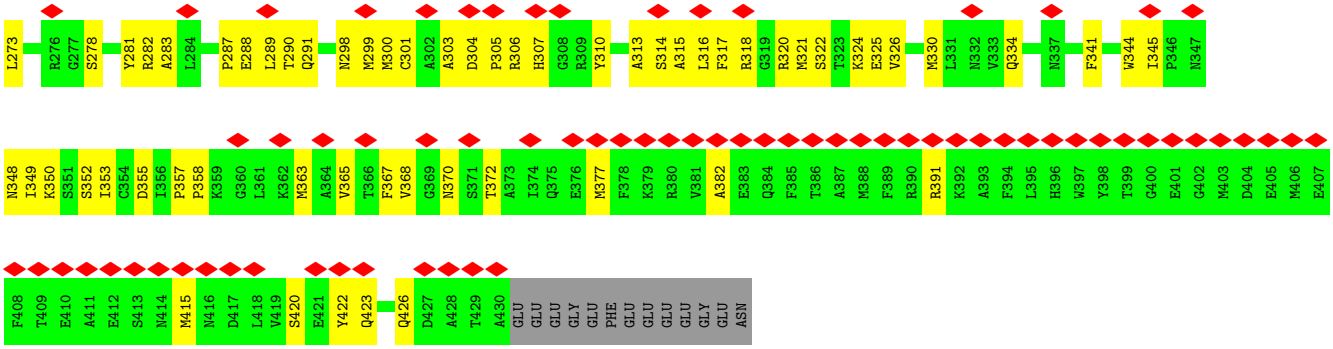


• Molecule 46: Tubulin beta chain

Chain SB:



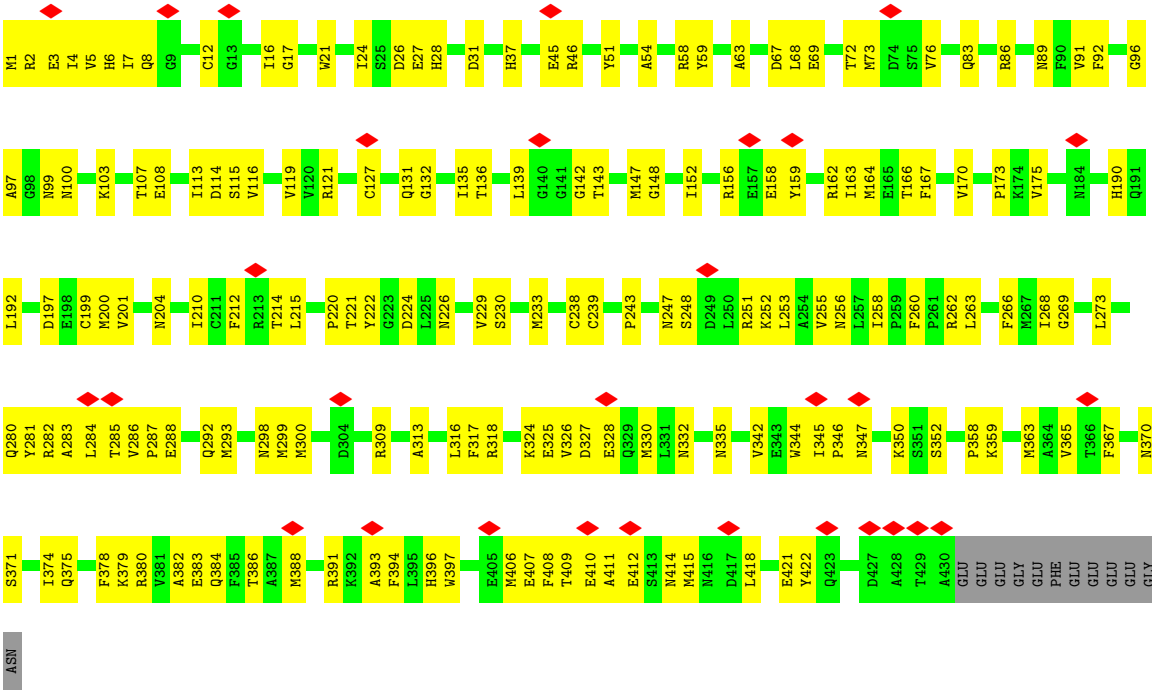




• Molecule 46: Tubulin beta chain

Chain SD:

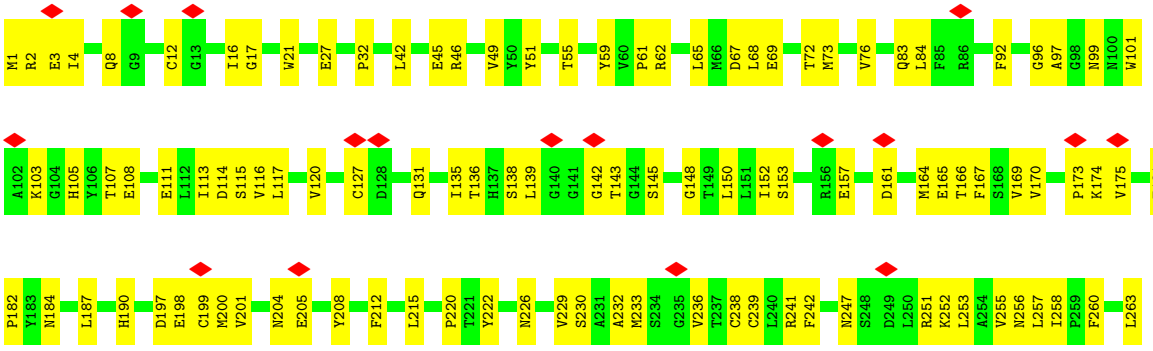


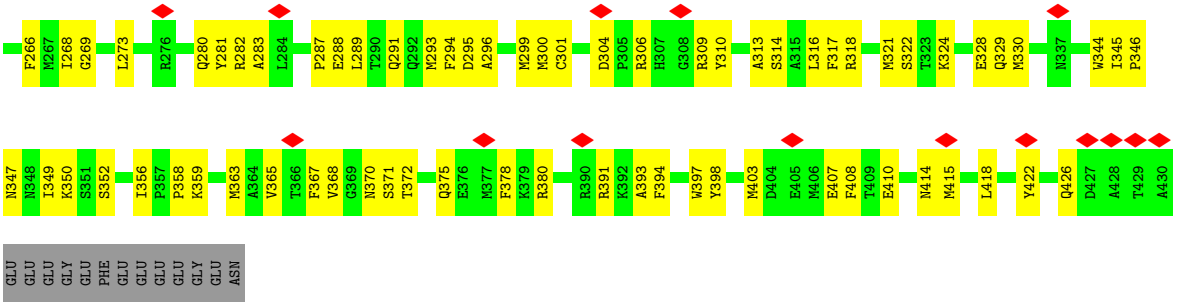


• Molecule 46: Tubulin beta chain

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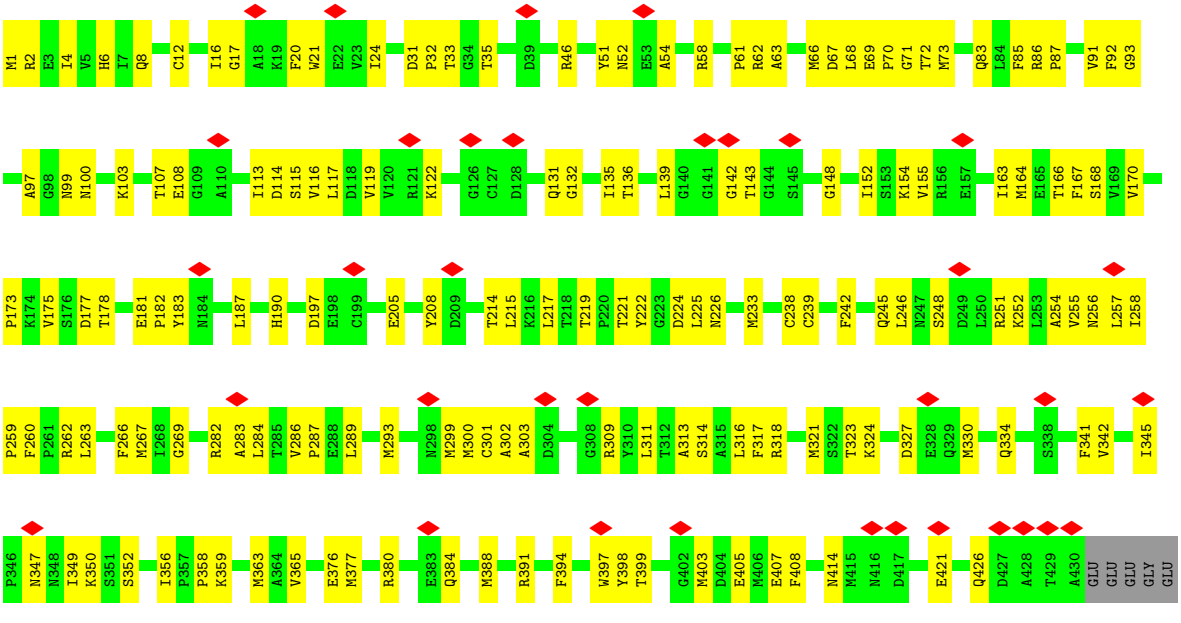




• Molecule 46: Tubulin beta chain

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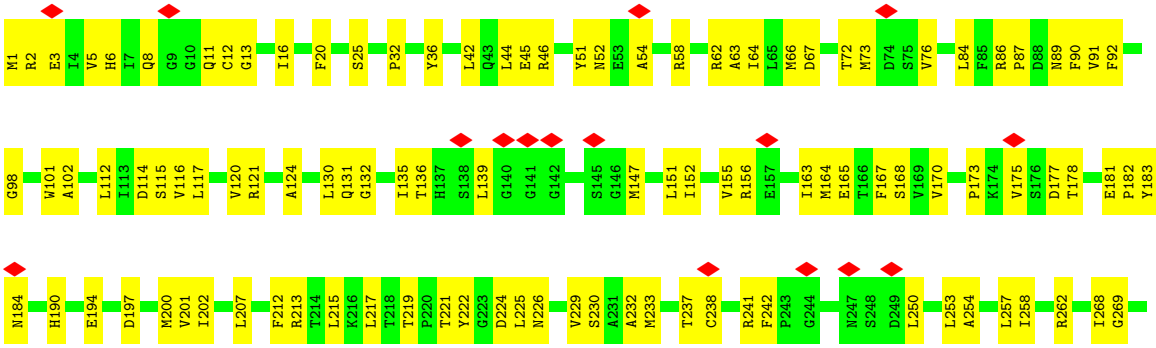


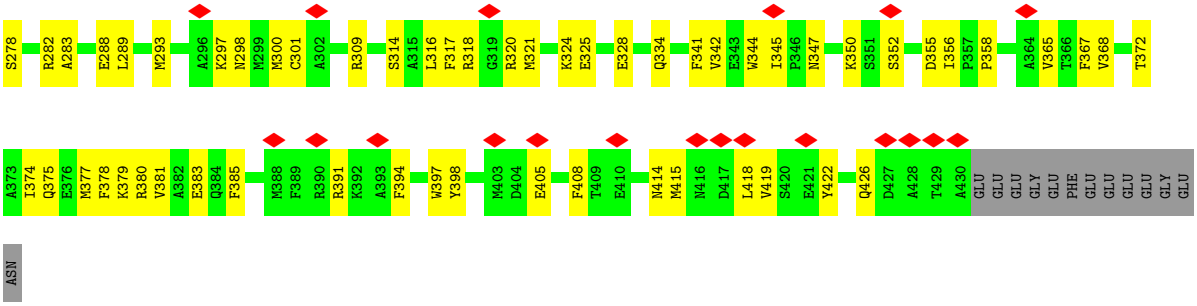


• Molecule 46: Tubulin beta chain

Chain SJ:



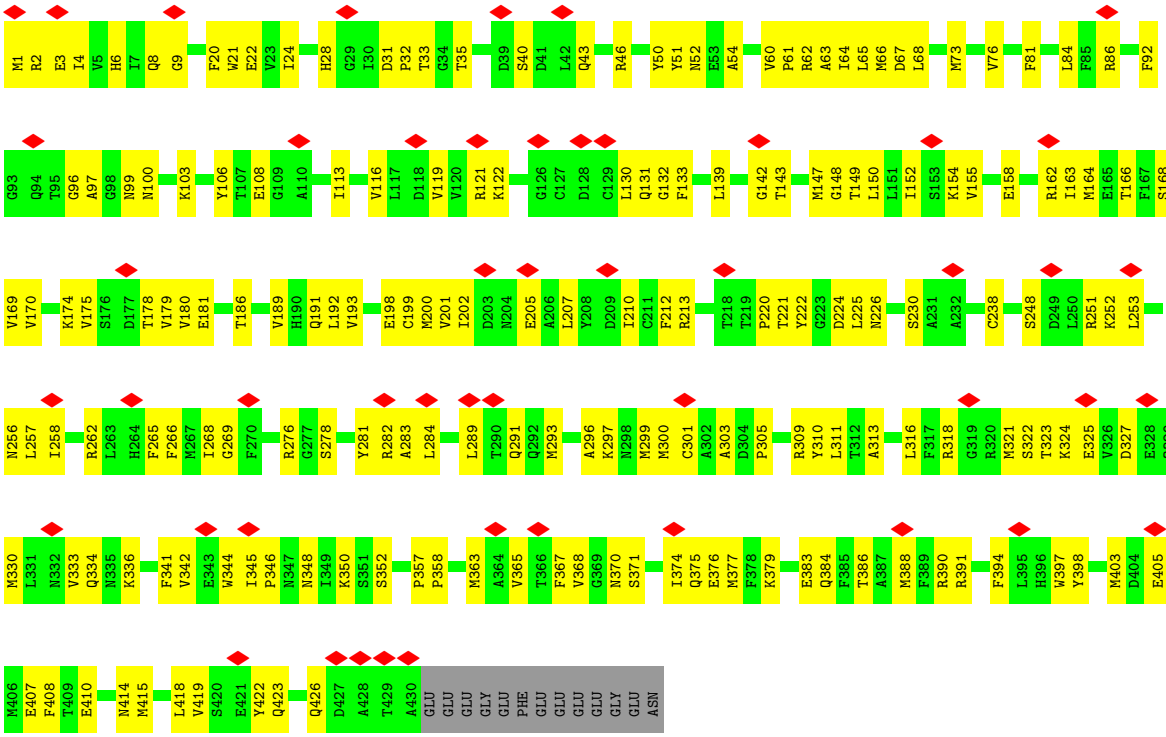




• Molecule 46: Tubulin beta chain

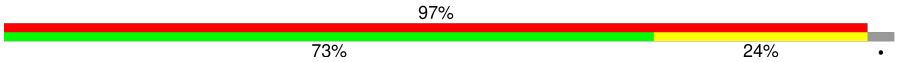
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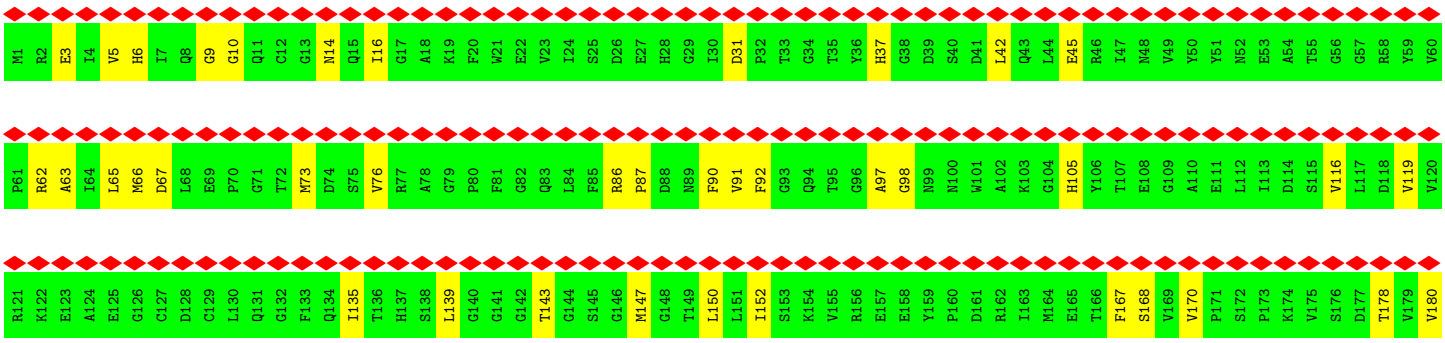


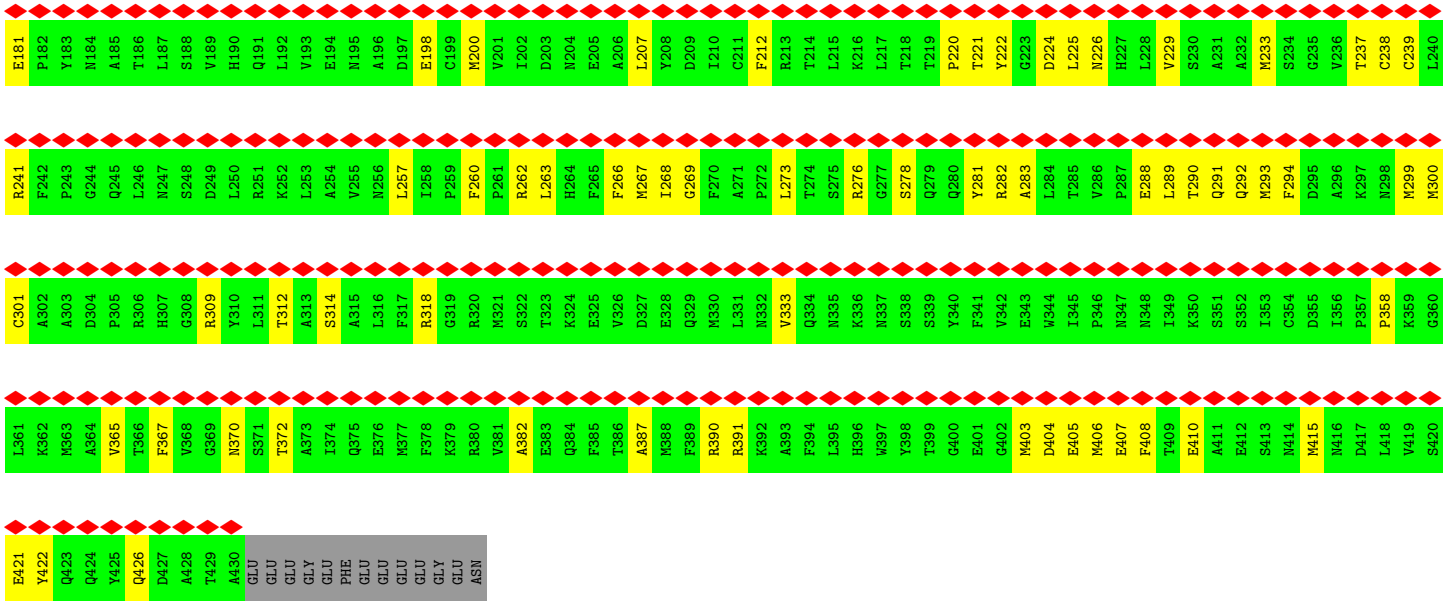


• Molecule 46: Tubulin beta chain

Chain SN:



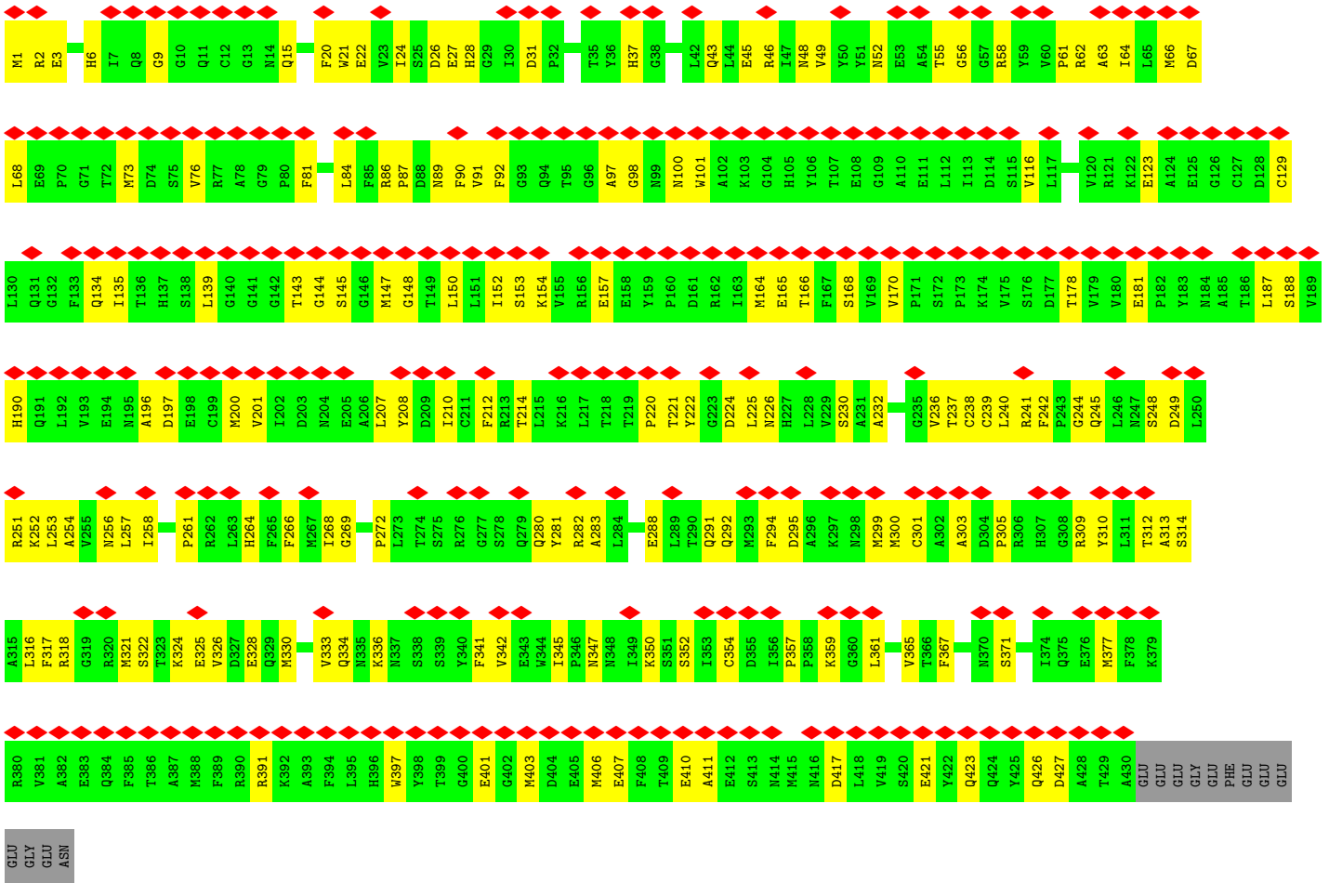




- Molecule 46: Tubulin beta chain

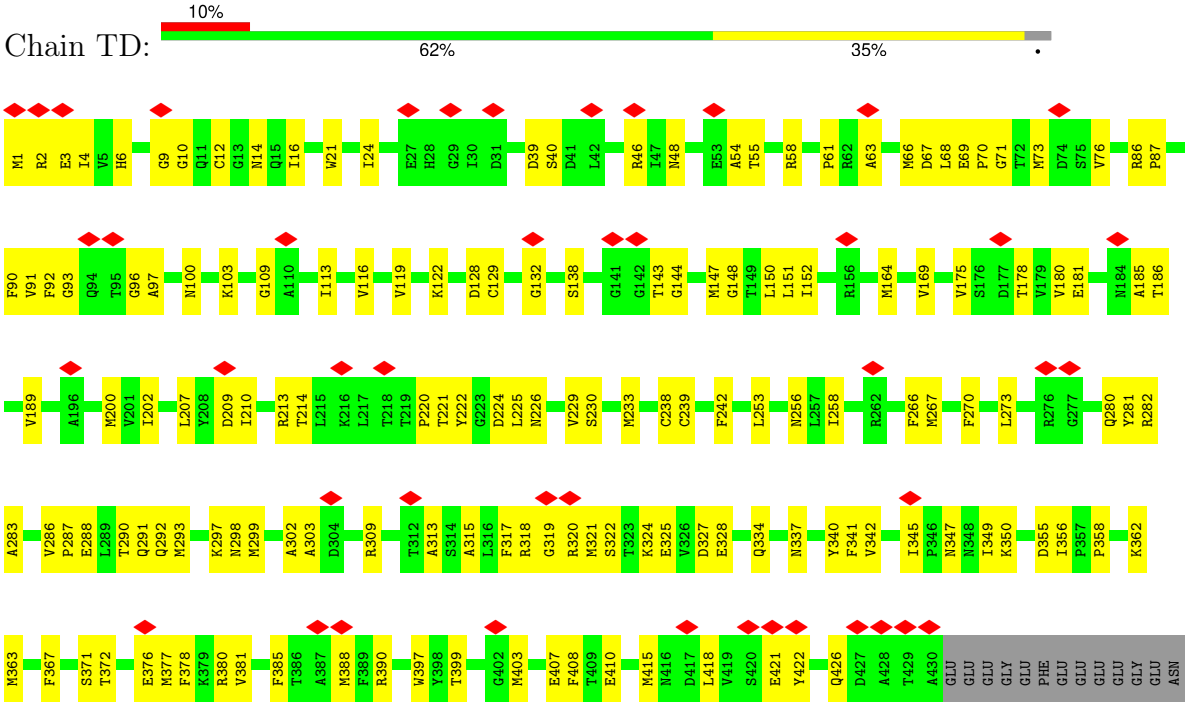
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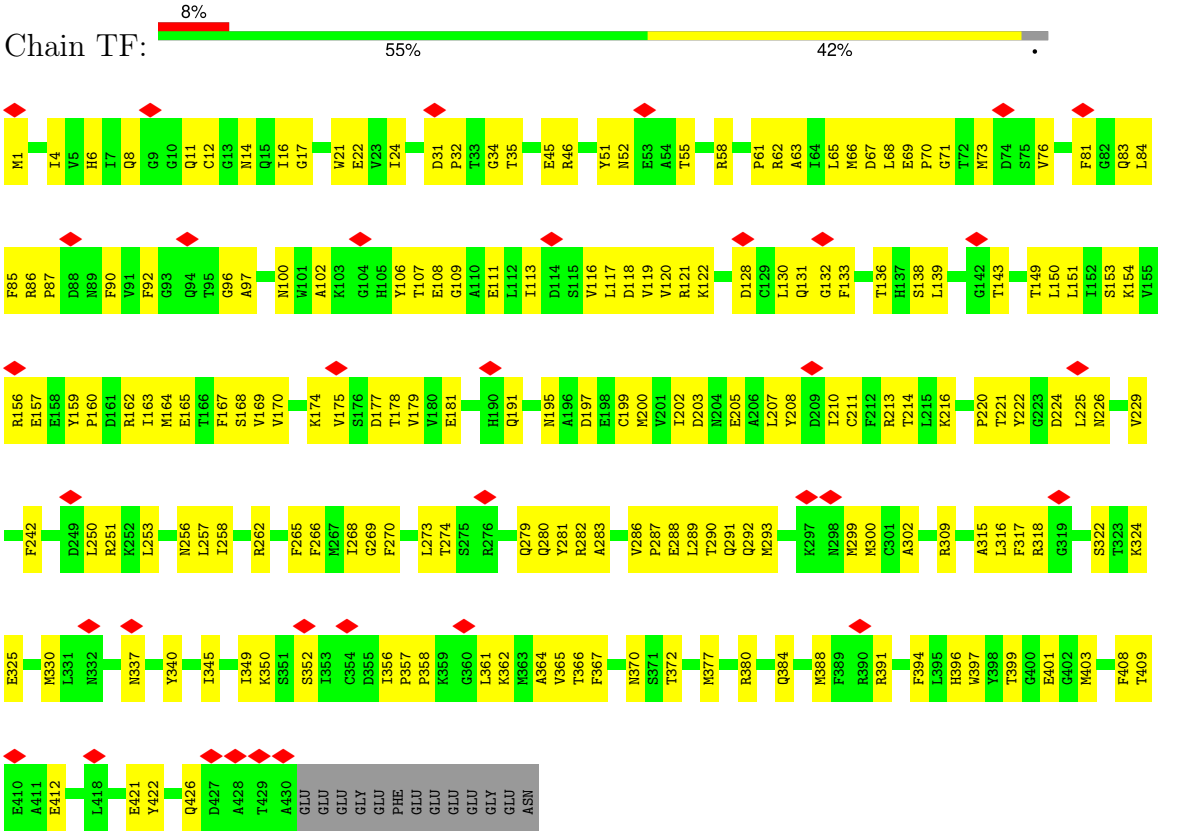
• Molecule 46: Tubulin beta chain

Chain TD:



• Molecule 46: Tubulin beta chain

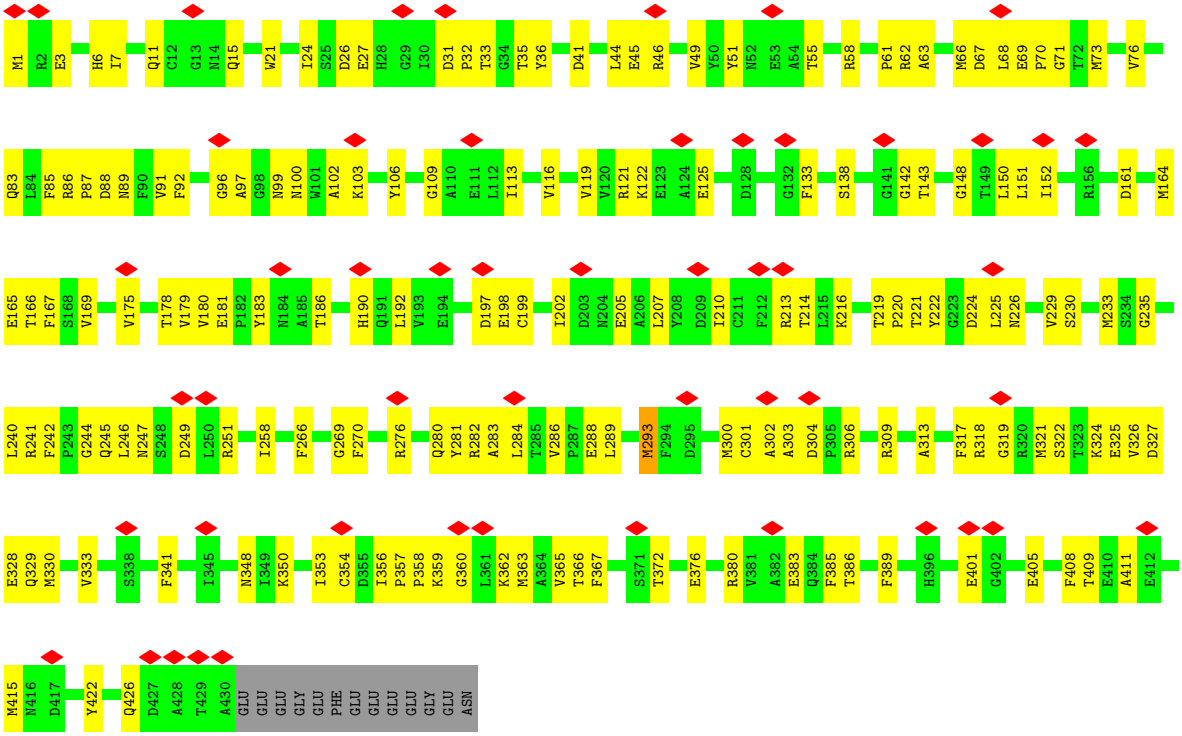
Chain TF:



• Molecule 46: Tubulin beta chain

Chain TH:

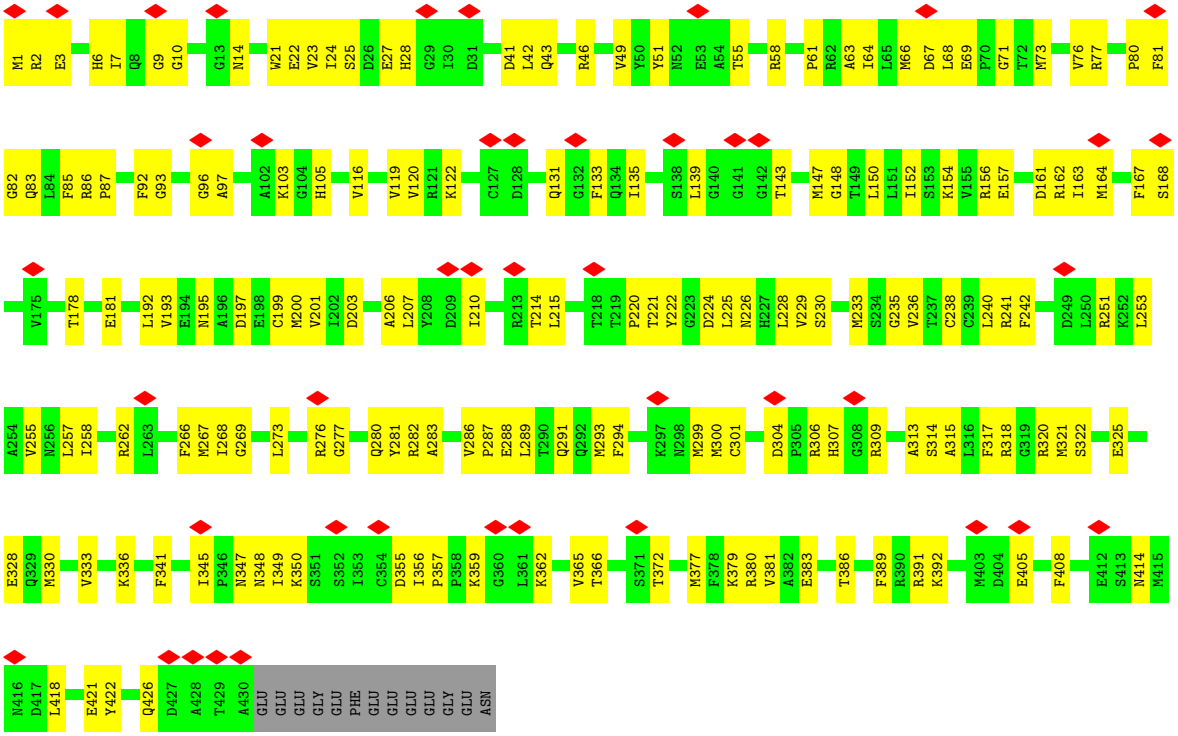




• Molecule 46: Tubulin beta chain

Chain TJ:

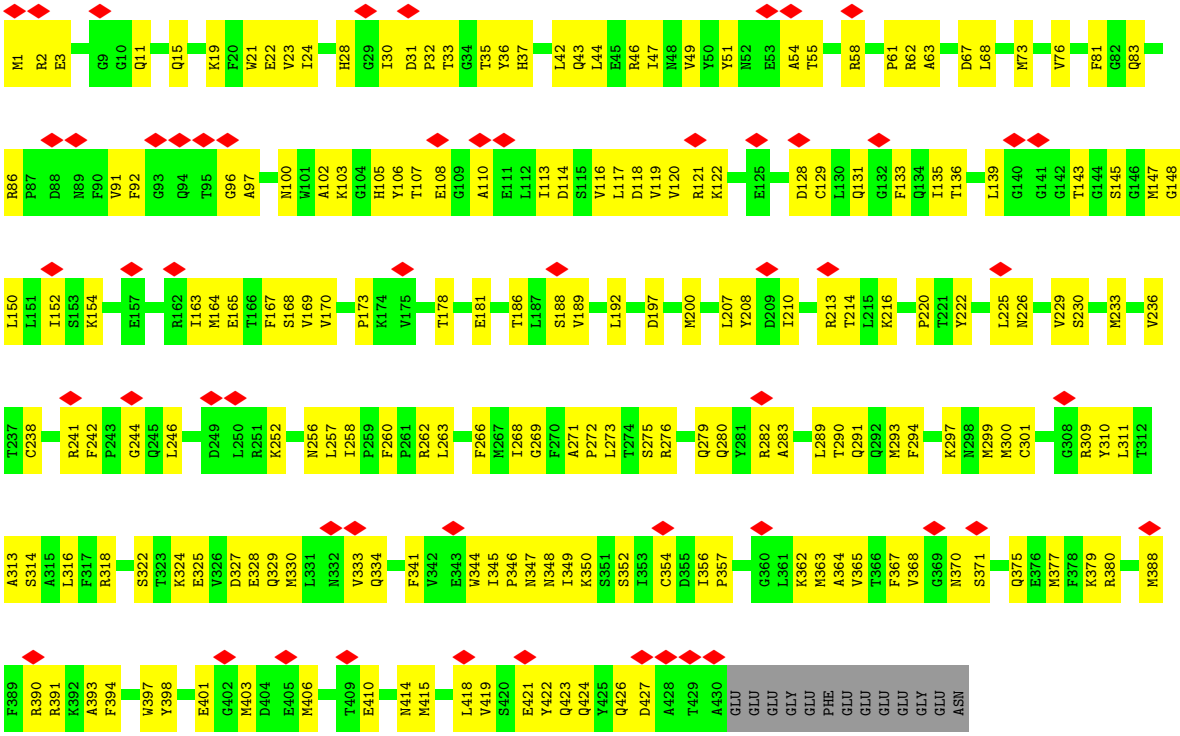




• Molecule 46: Tubulin beta chain

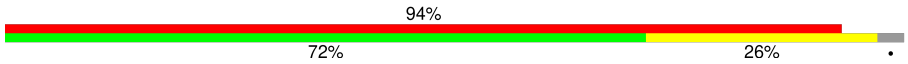
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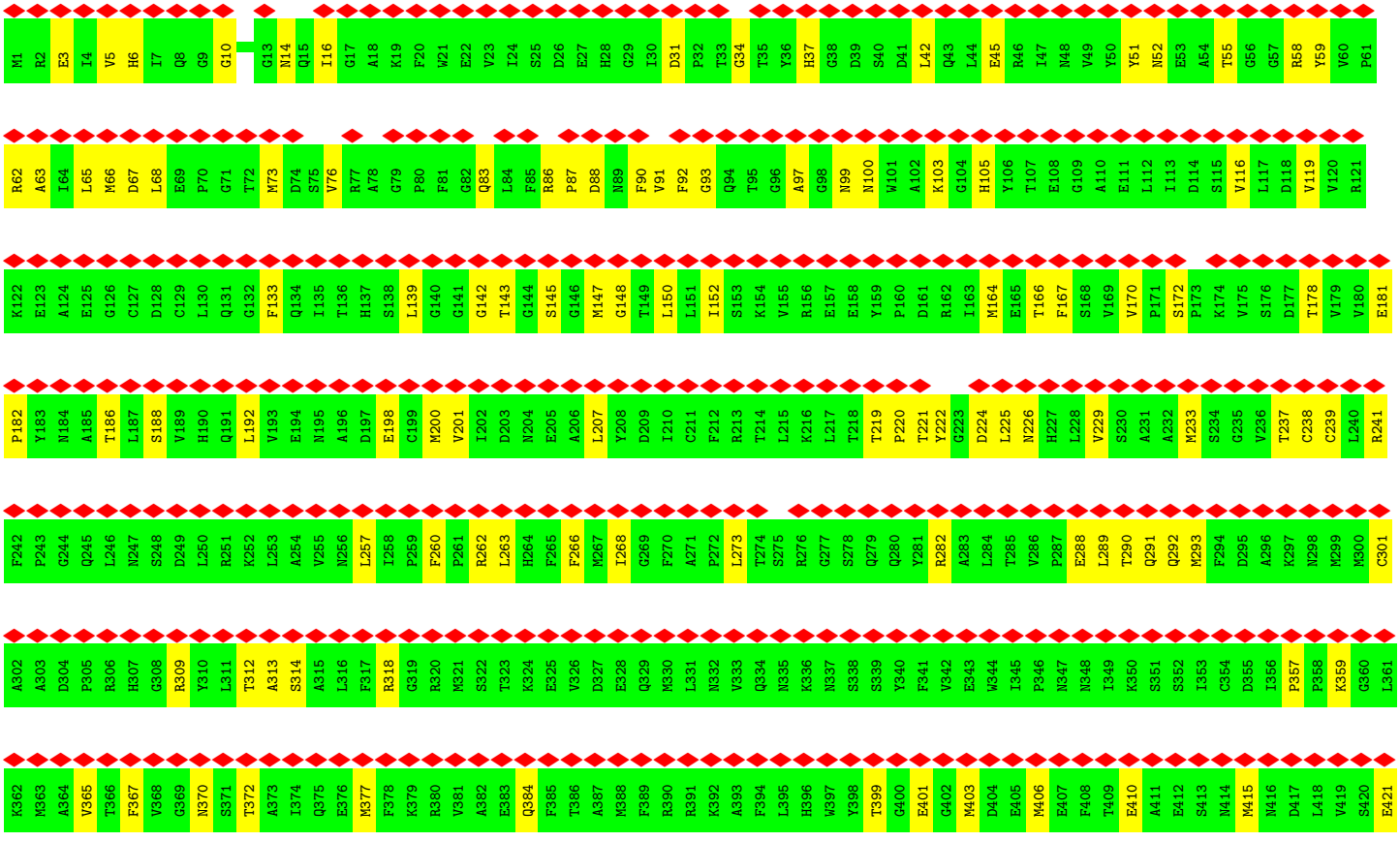


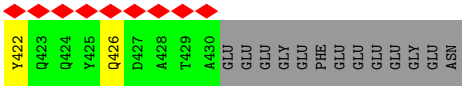


• Molecule 46: Tubulin beta chain

Chain TN:



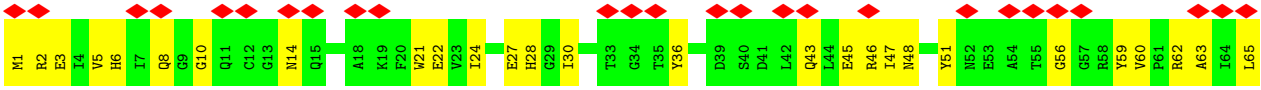


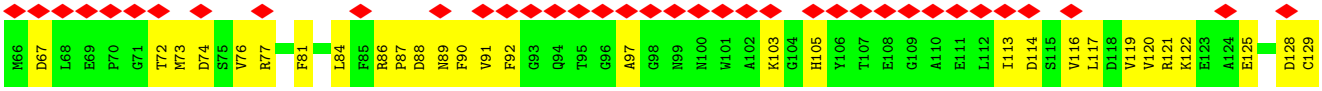


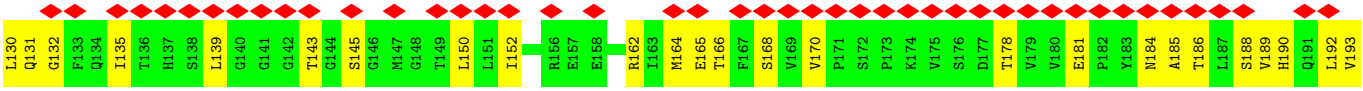
• Molecule 46: Tubulin beta chain

Chain UB:

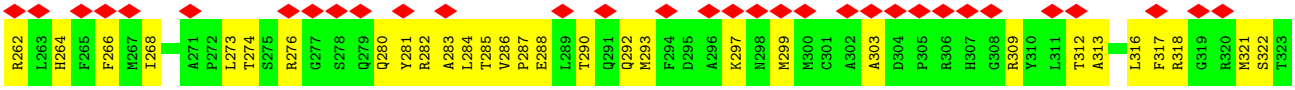


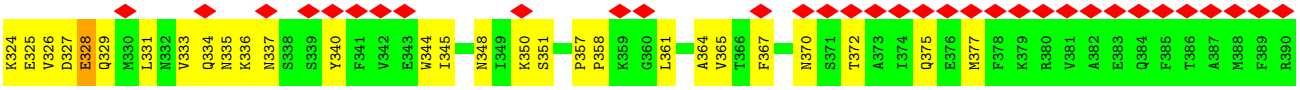


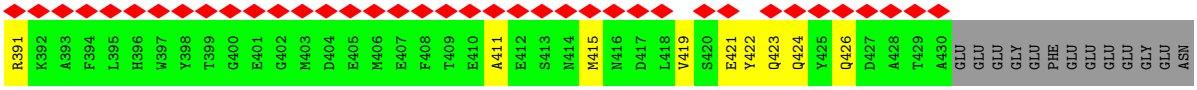










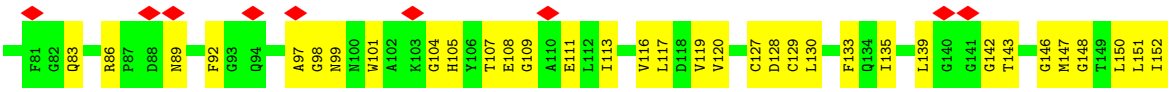


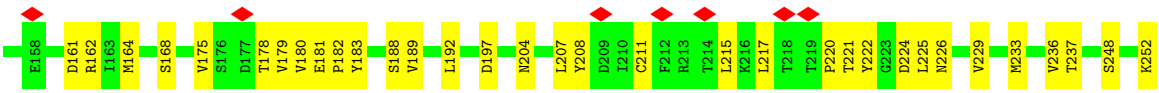
• Molecule 46: Tubulin beta chain

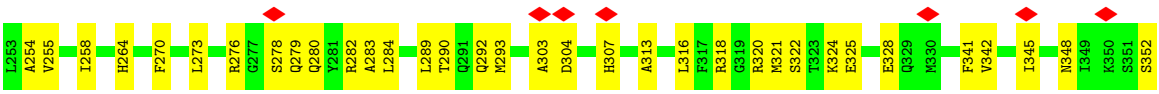
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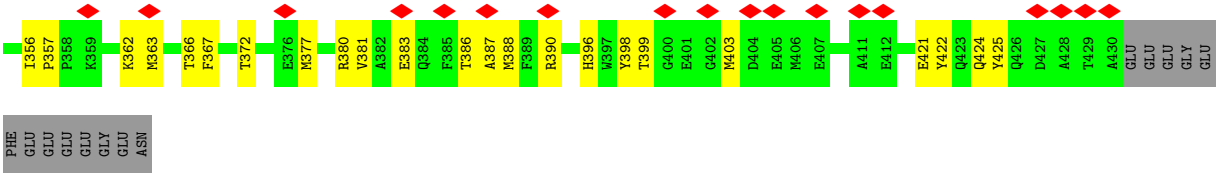








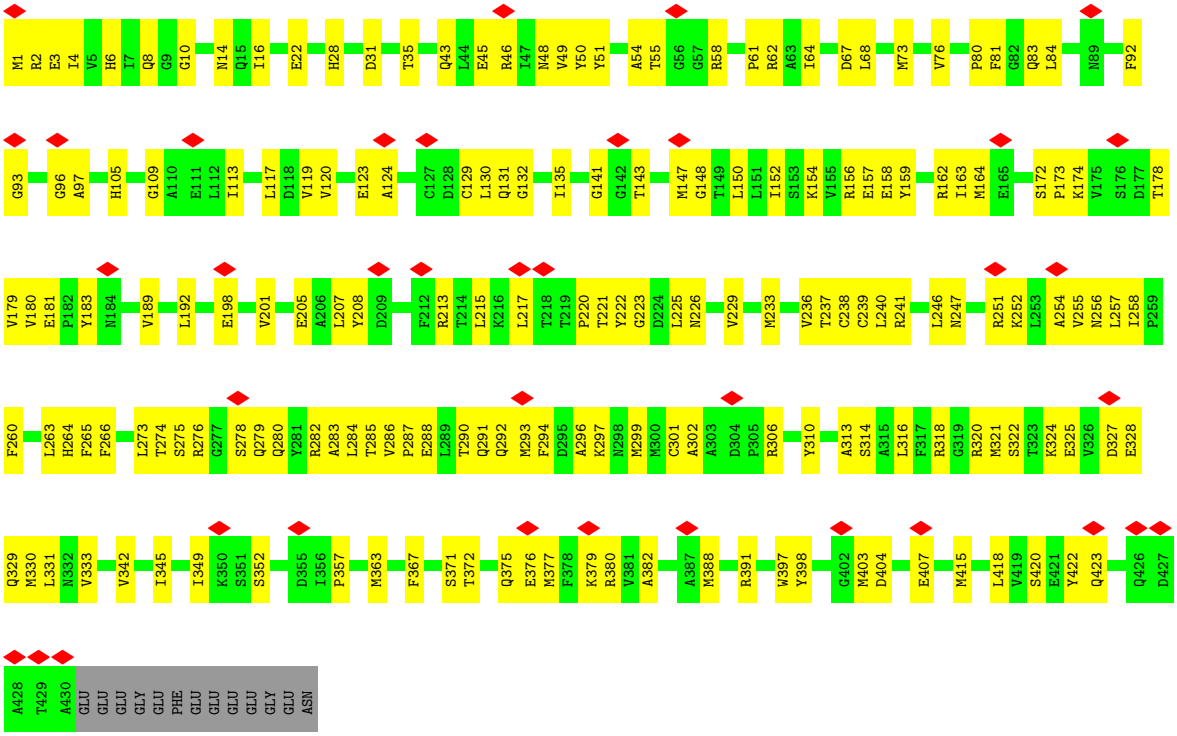




• Molecule 46: Tubulin beta chain

Chain UF:

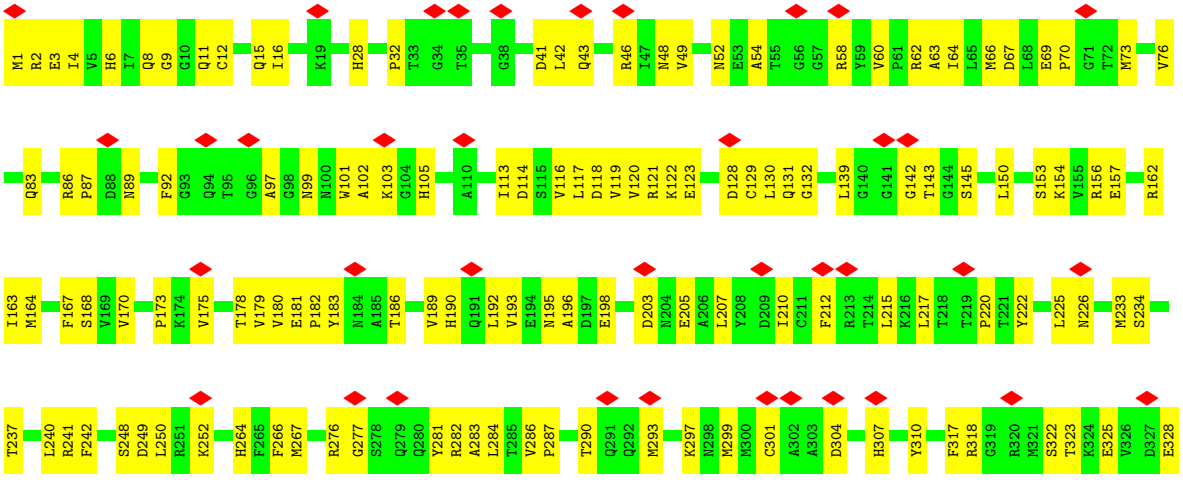


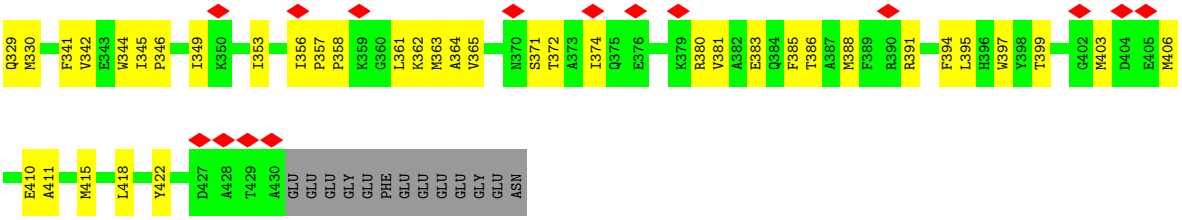


• Molecule 46: Tubulin beta chain

Chain UH:



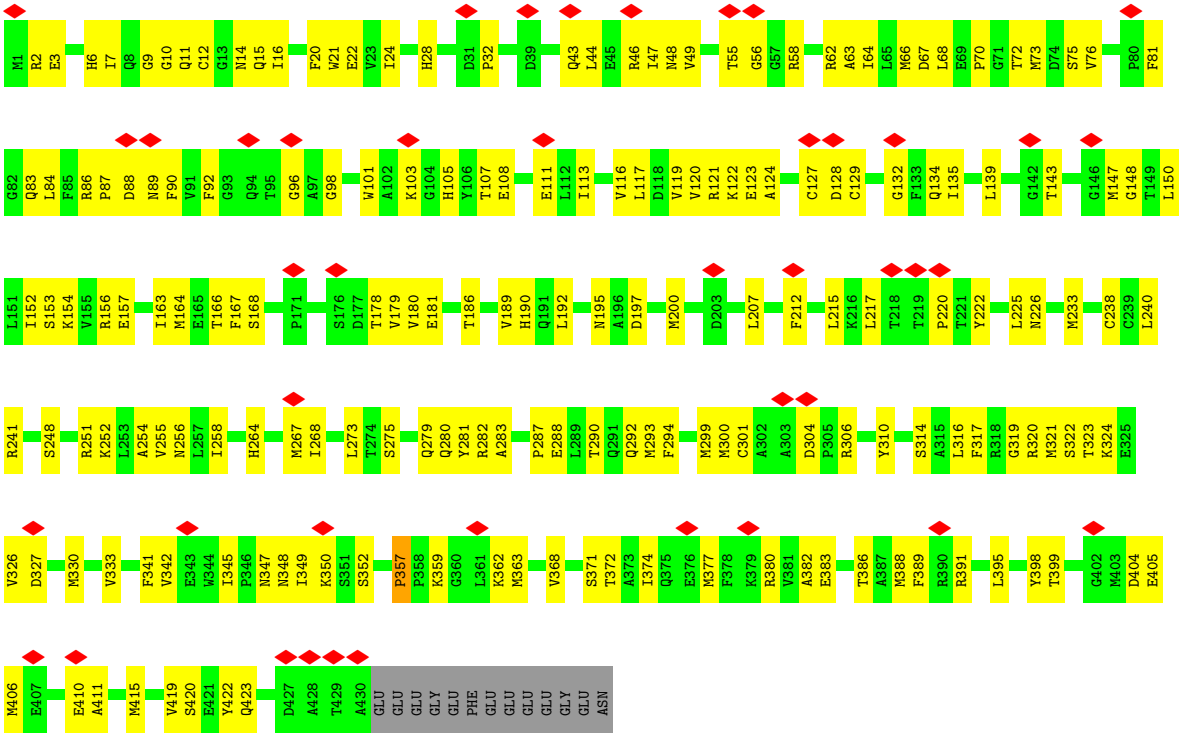




• Molecule 46: Tubulin beta chain

Chain UJ:

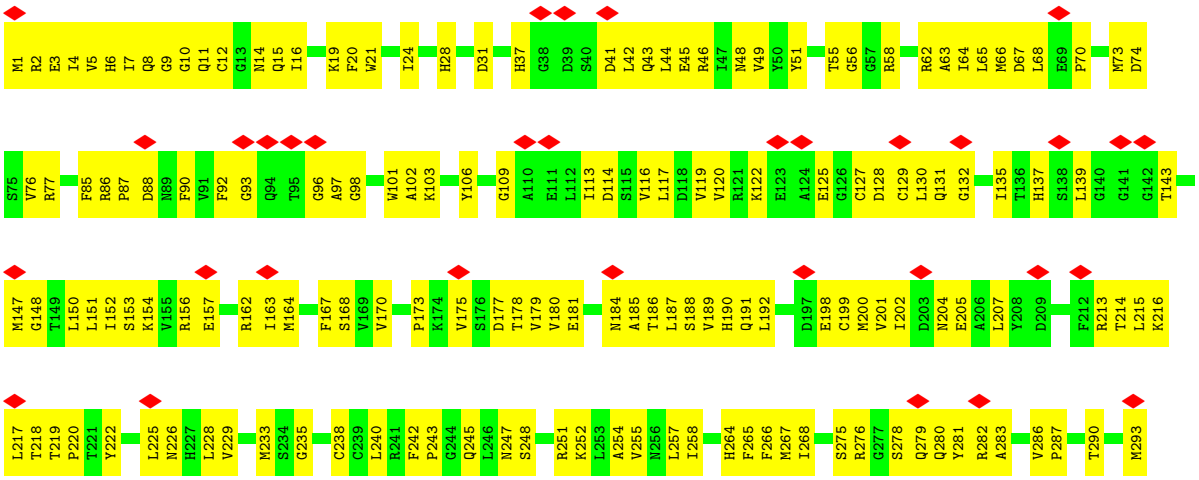


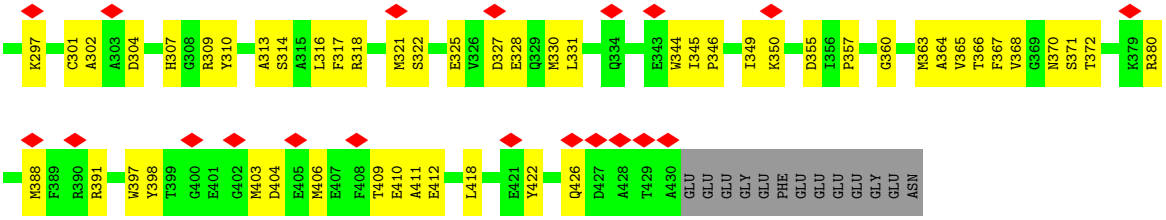


• Molecule 46: Tubulin beta chain

Chain UL:



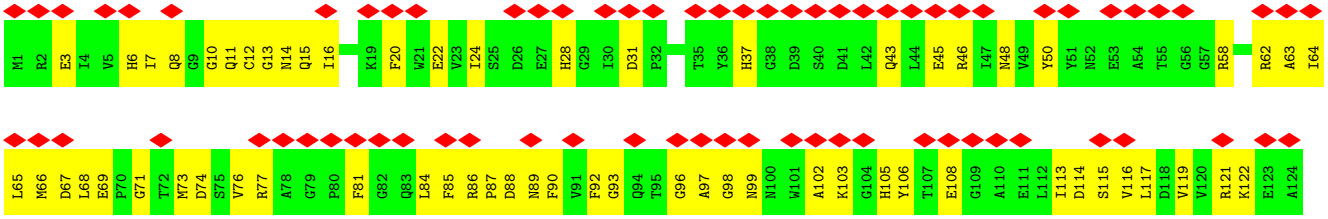




• Molecule 46: Tubulin beta chain

Chain UN:

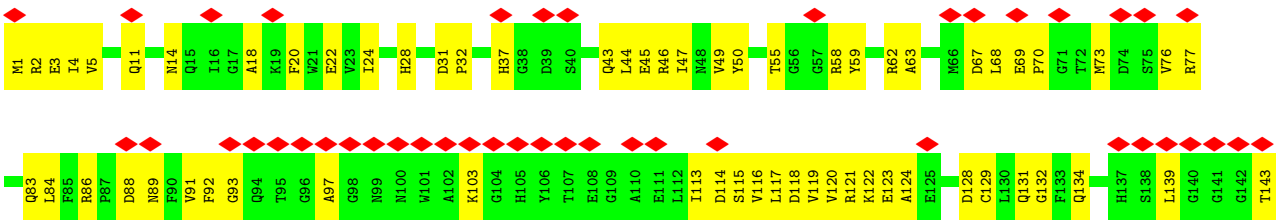


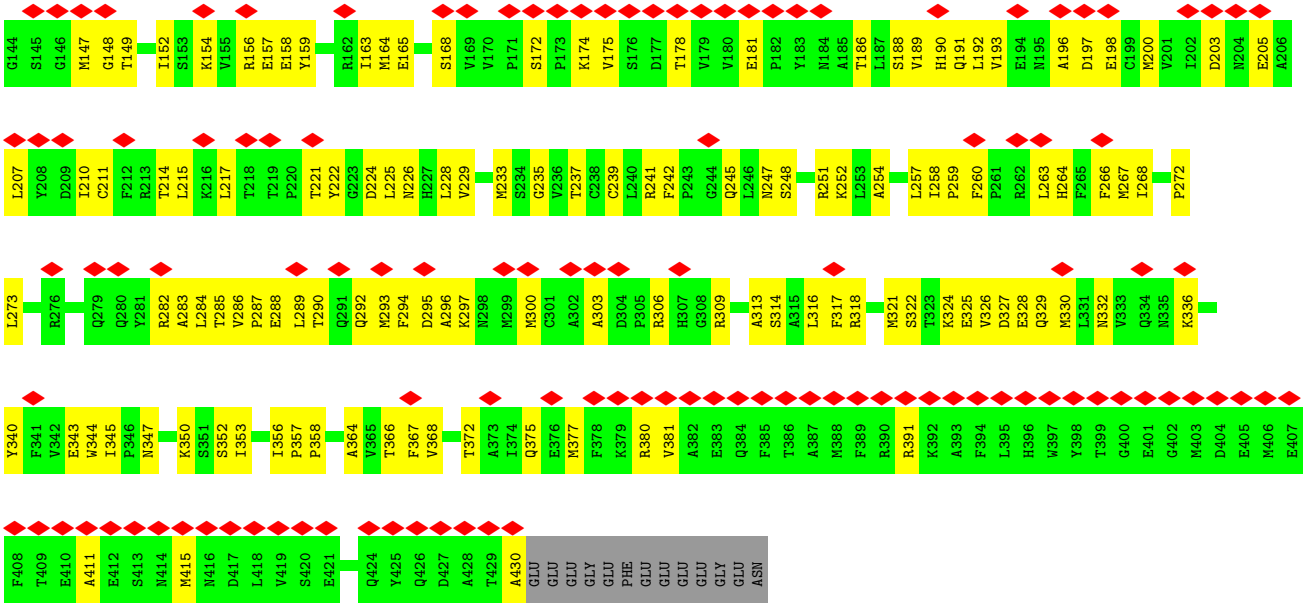


• Molecule 46: Tubulin beta chain

Chain VB:



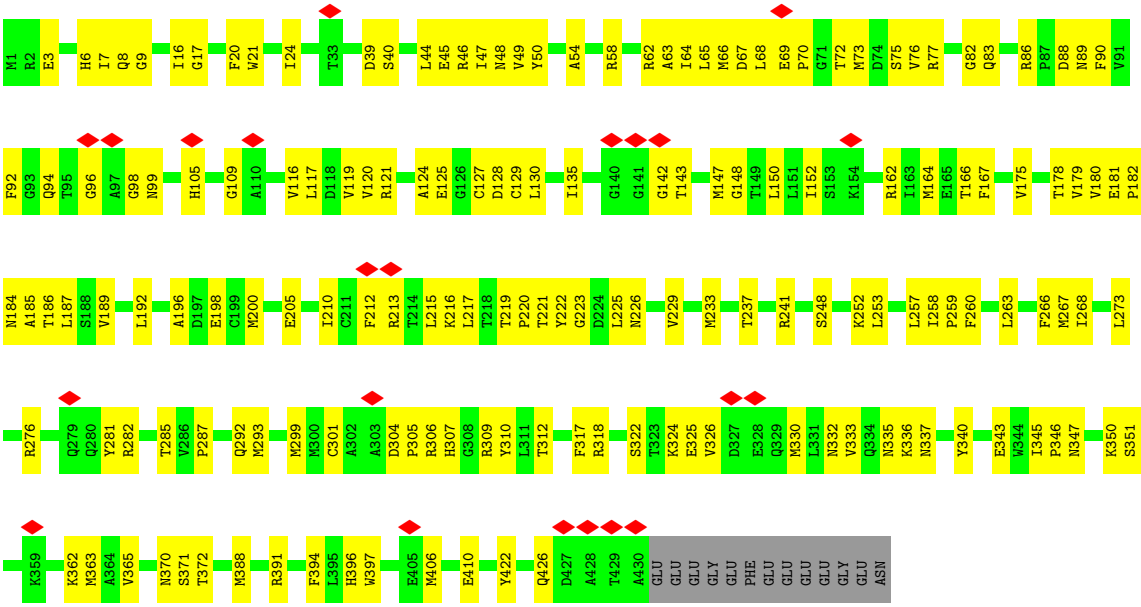




• Molecule 46: Tubulin beta chain

Chain VD:

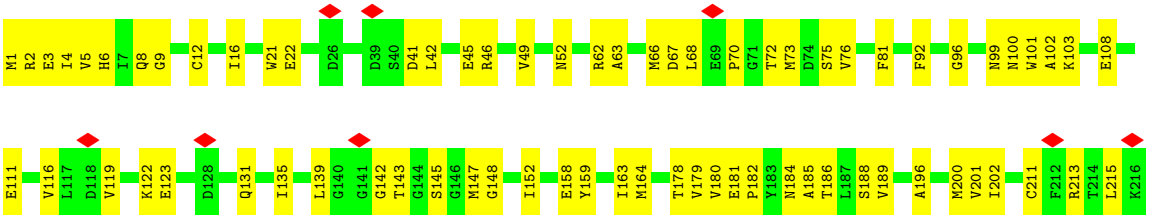


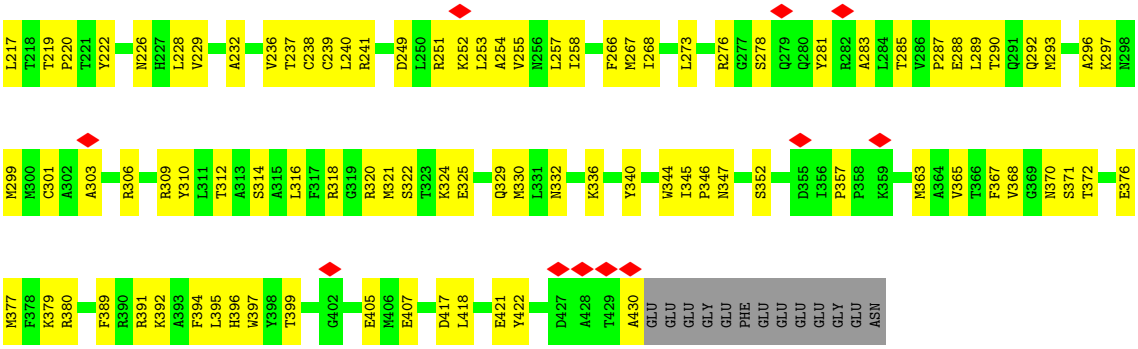


• Molecule 46: Tubulin beta chain

Chain VF:



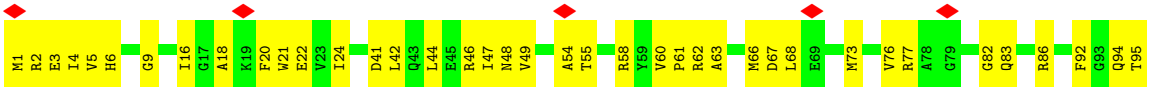




• Molecule 46: Tubulin beta chain

Chain VH:

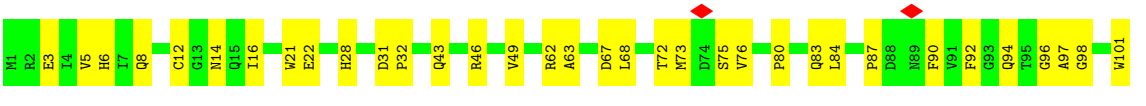


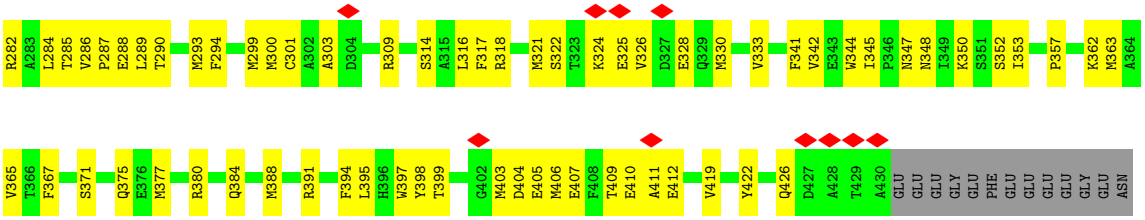


• Molecule 46: Tubulin beta chain

Chain VJ:



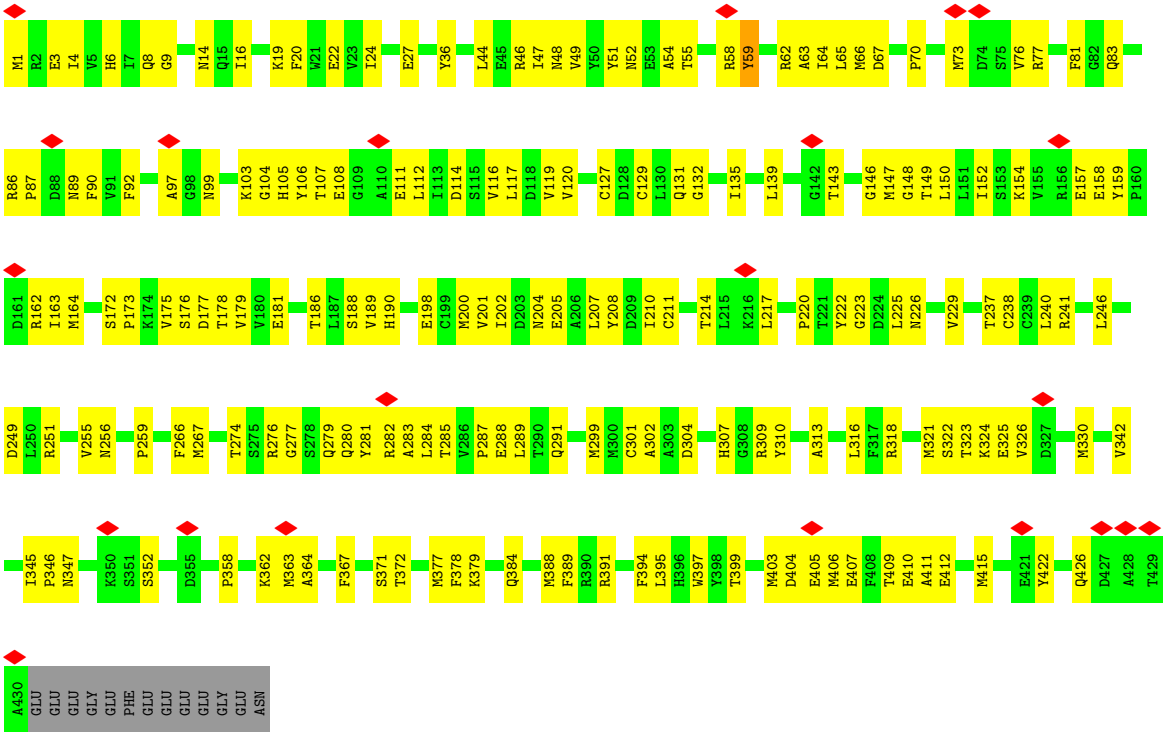




• Molecule 46: Tubulin beta chain

Chain VL:

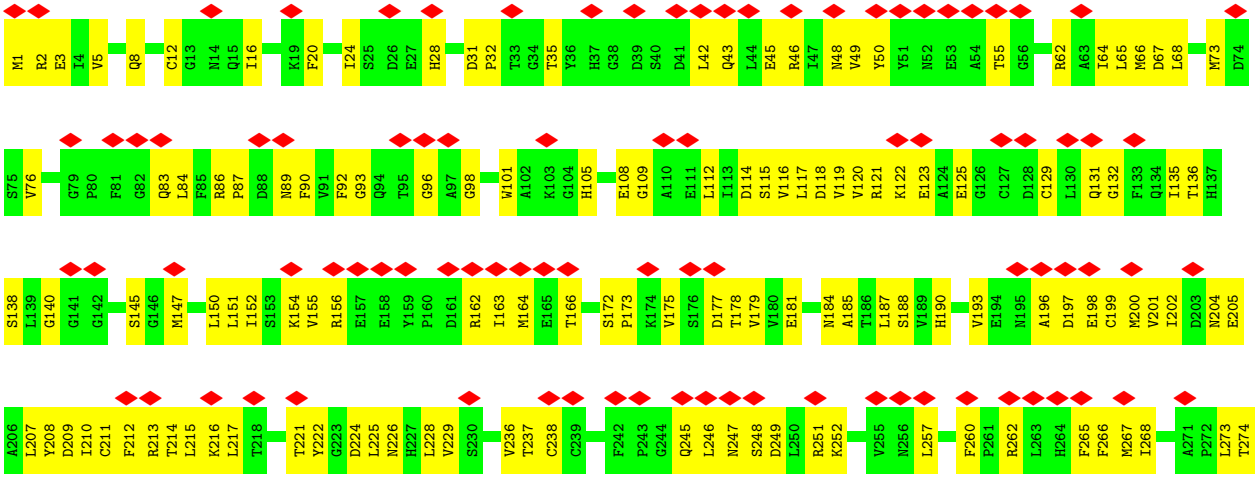


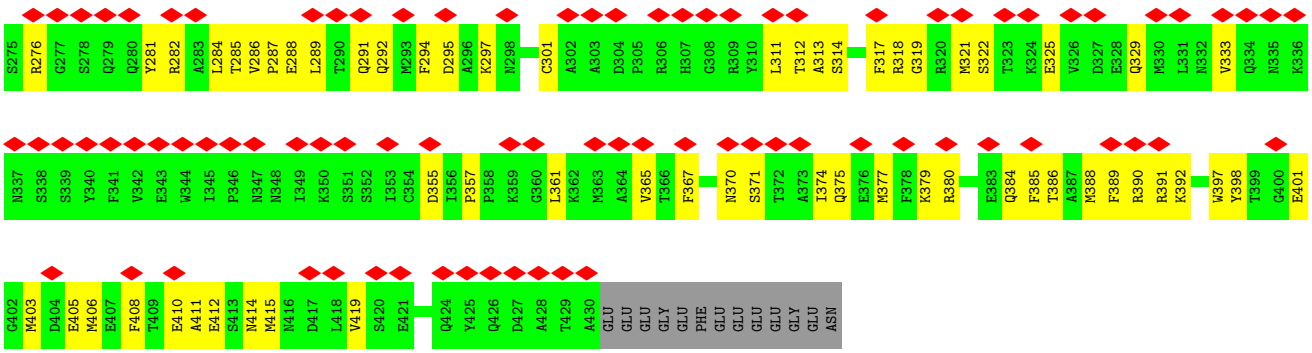


• Molecule 46: Tubulin beta chain

Chain VN:



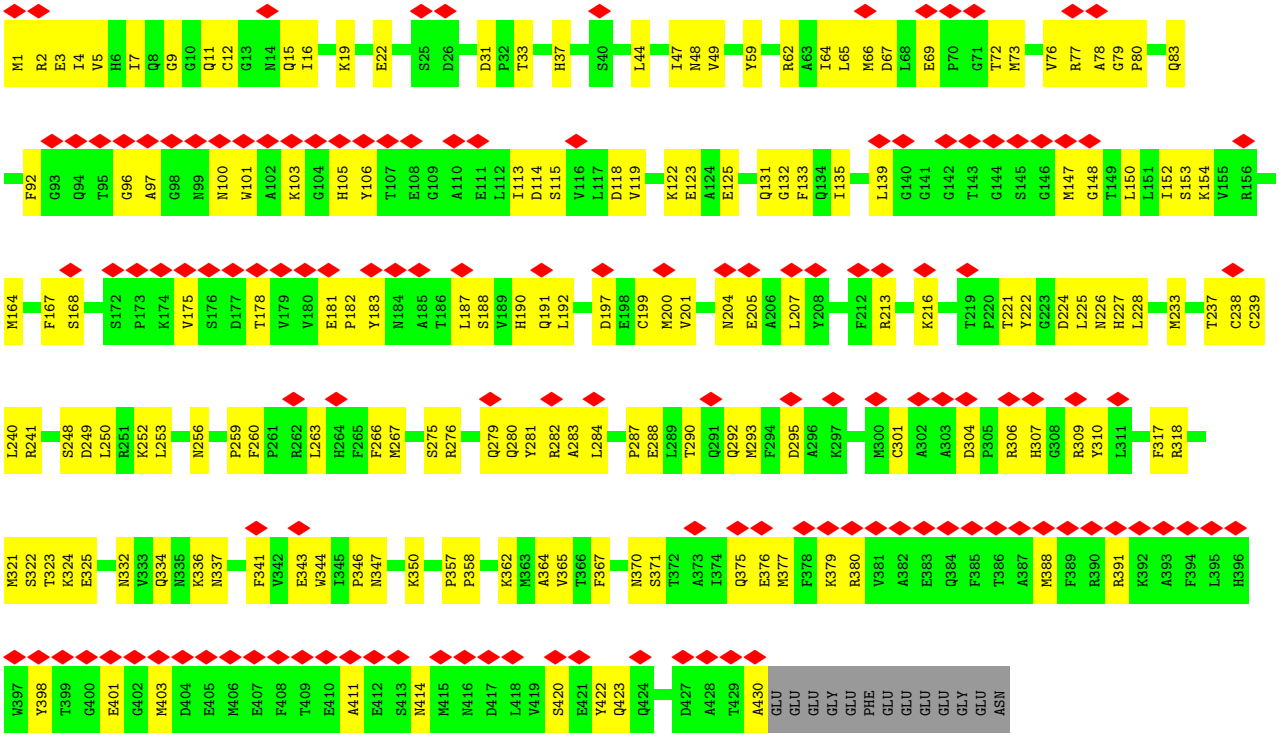




• Molecule 46: Tubulin beta chain

Chain WB:

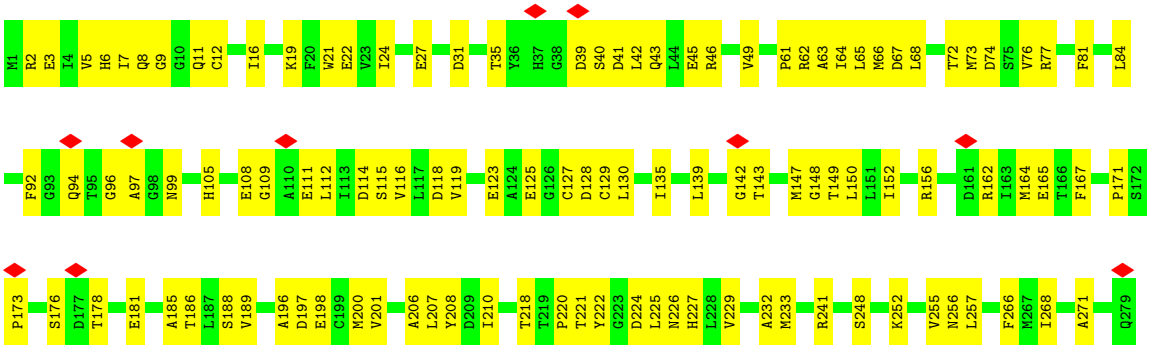


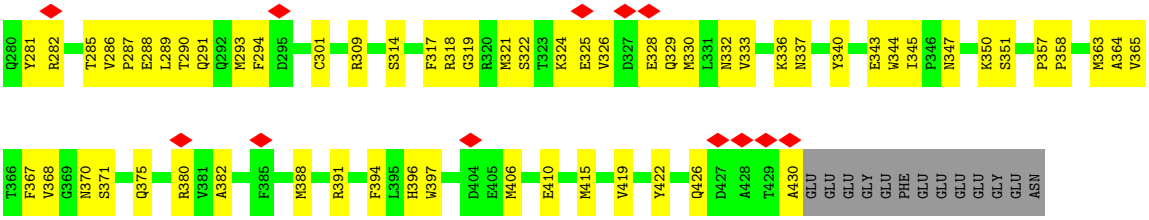


• Molecule 46: Tubulin beta chain

Chain WD:



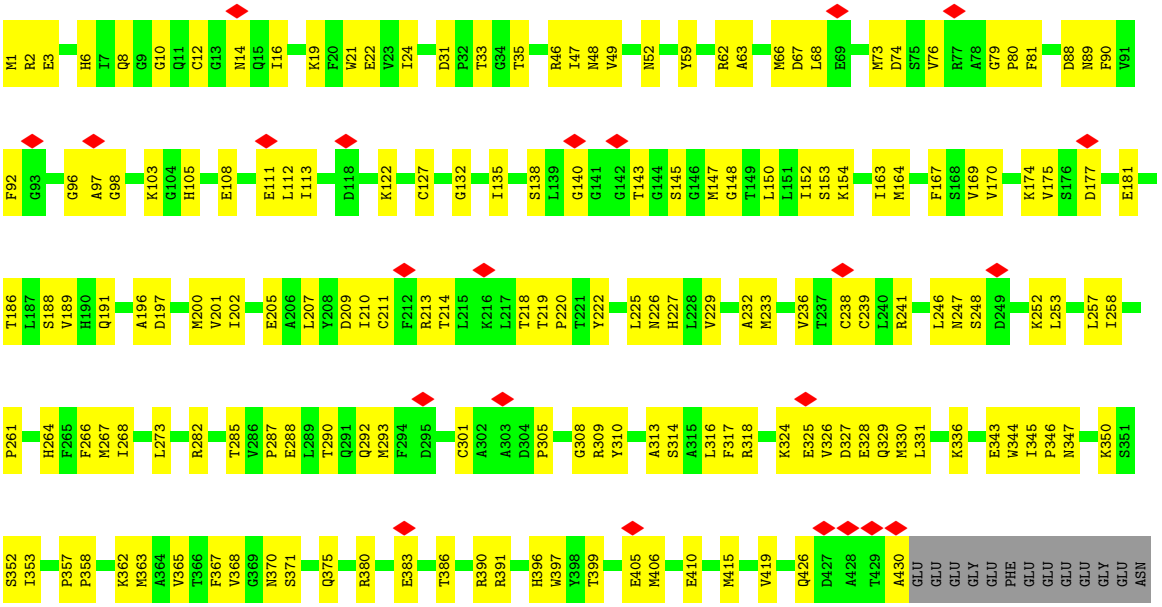




• Molecule 46: Tubulin beta chain

Chain WF:

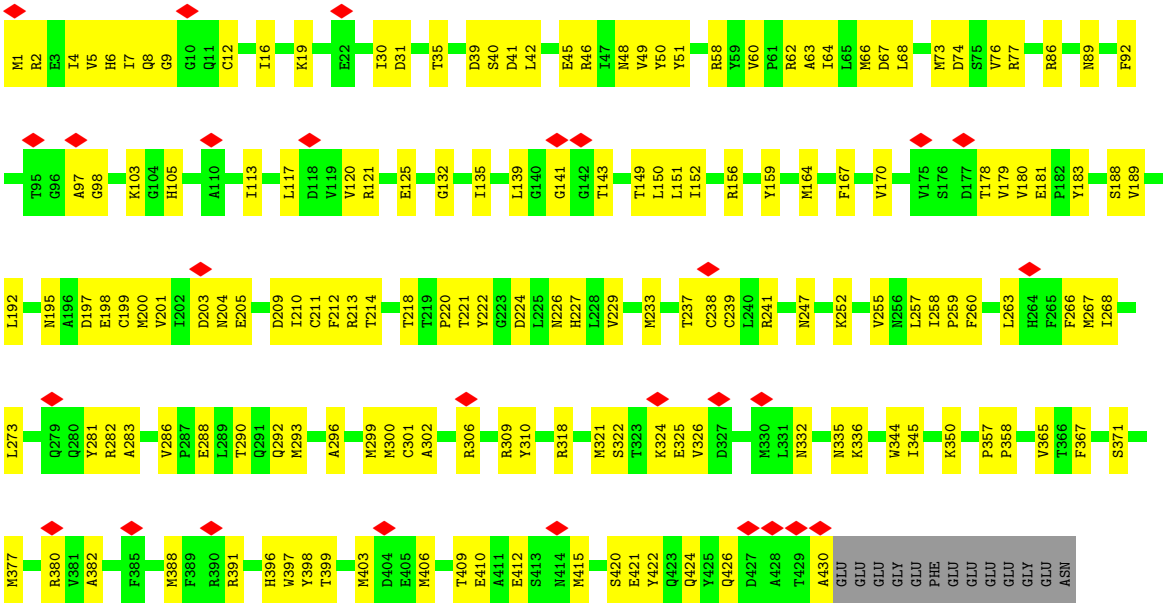




• Molecule 46: Tubulin beta chain

Chain WH:

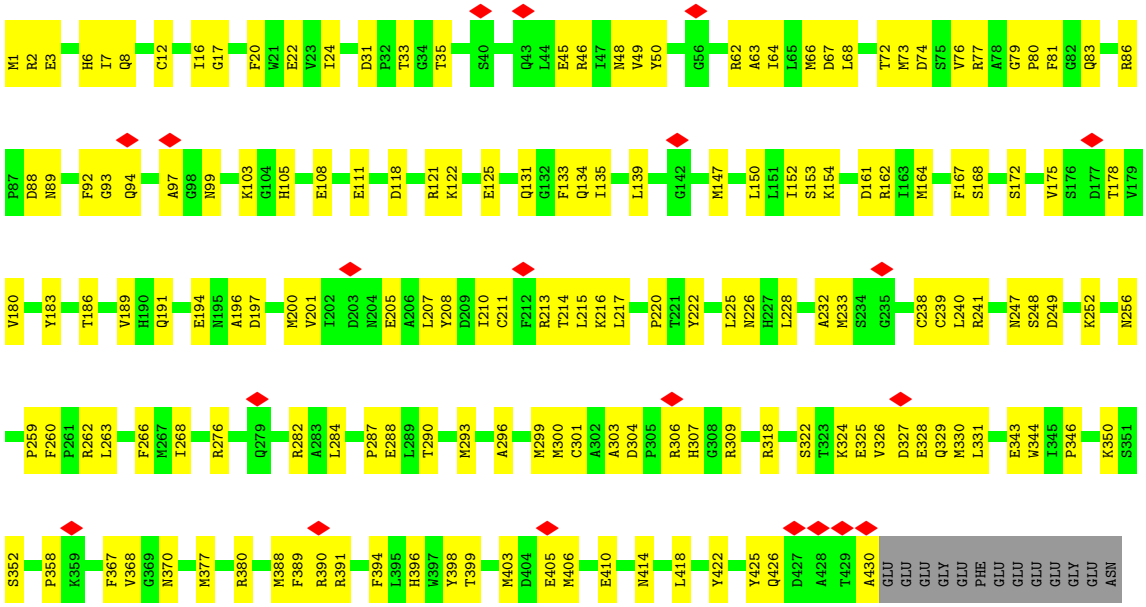




• Molecule 46: Tubulin beta chain

Chain WJ:

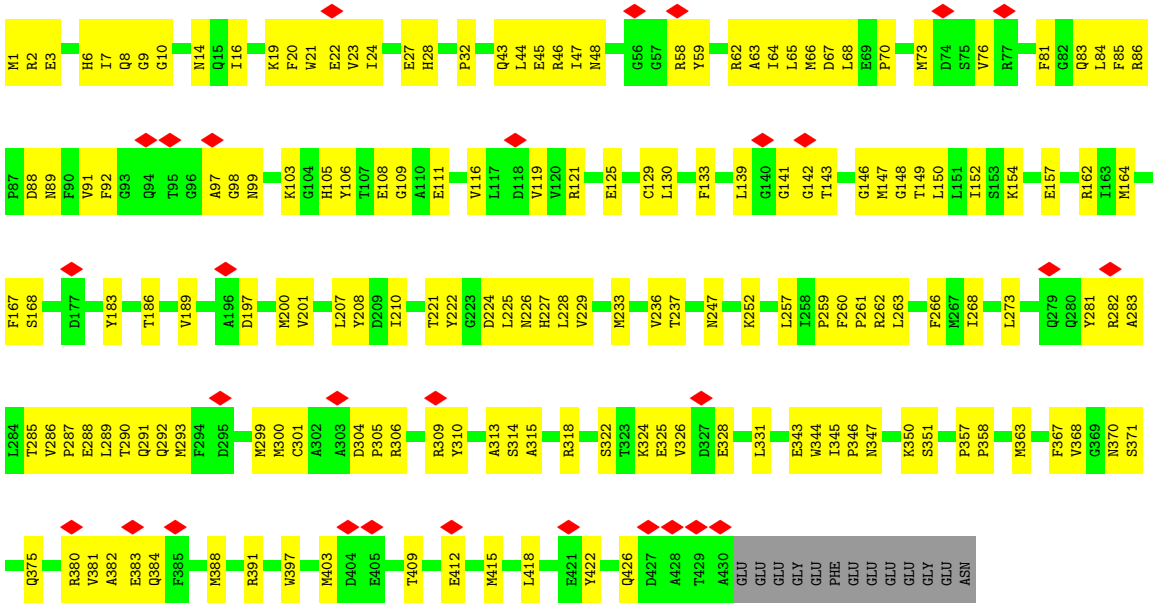




• Molecule 46: Tubulin beta chain

Chain WL:

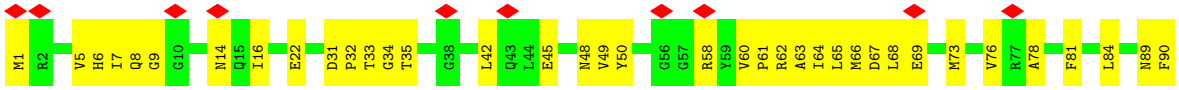


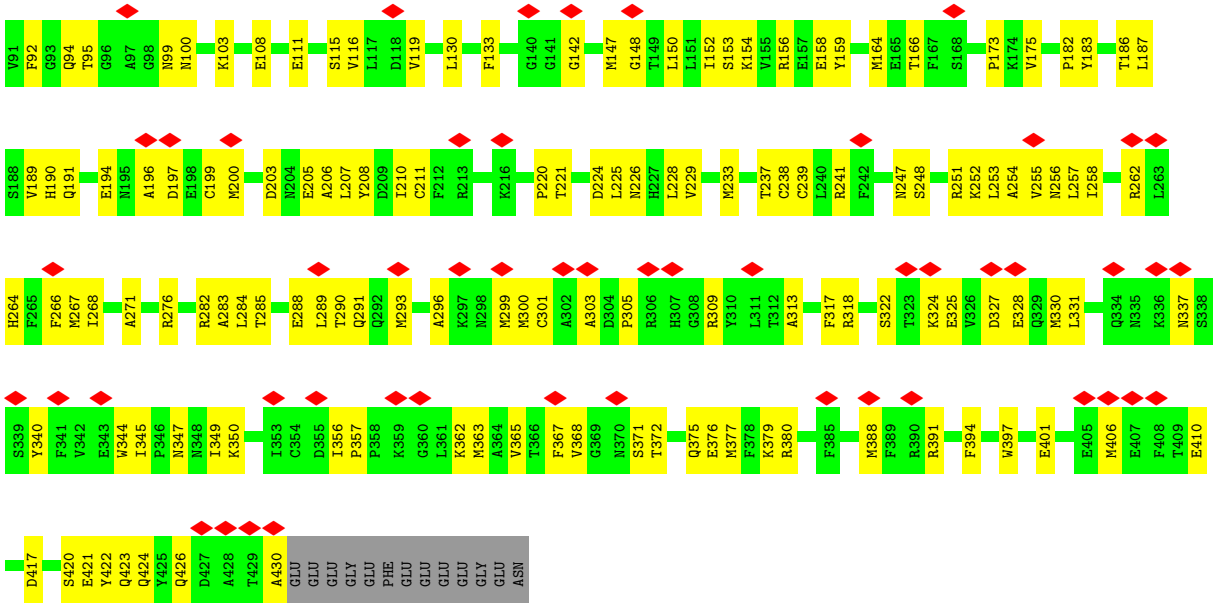


• Molecule 46: Tubulin beta chain

Chain WN:






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S188 V189 H190 Q191 E194 N195 A196 D197 E198 C199 M200 D203 W204 E205 A206 L207 Y208 D209 I210 C211 F212 R213 K216 P220 T221 D224 L225 N226 H227 L228 V229 M233 T237 C238 C239 L240 R241 F242 N247 S248 R251 K252 L253 A254 V255 N256 L257 I258 R262 L263
H264 F265 F266 M267 I268 A271 R276 R282 A283 L284 T285 E288 L289 T290 Q291 Q292 M293 A296 K297 N298 M299 M300 C301 A302 A303 D304 P305 R306 H307 G308 R309 Y310 L311 T312 A313 F317 R318 S322 T323 K324 E325 V326 D327 E328 Q329 M330 L331 Q334 N335 K336 N337 S338
S339 Y340 F341 V342 E343 W344 I345 P346 N347 N348 I349 K350 I353 C354 D355 I356 P357 P358 K359 G360 L361 K362 M363 A364 V365 T366 F367 V368 G369 N370 S371 T372 Q375 E376 M377 F378 K379 R380 F385 M388 F389 R390 R391 F394 W397 E401 E405 M406 E407 F408 T409 E410
D417 S420 E421 Y422 Q423 Q424 Y425 Q426 D427 A428 T429 A430 GLU GLU GLU GLY GLU PHE GLU GLU GLU GLU GLY GLU ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	148365	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.356	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	701.44, 701.44, 701.44	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0A	0.22	0/1272	0.66	1/1730 (0.1%)
1	1A	0.23	0/1272	0.63	2/1730 (0.1%)
1	2A	0.24	0/1272	0.68	1/1730 (0.1%)
1	3A	0.21	0/1272	0.60	2/1730 (0.1%)
2	0B	0.21	0/2674	0.63	1/3619 (0.0%)
3	0C	0.23	0/764	0.69	0/1029
3	1C	0.23	0/764	0.74	2/1029 (0.2%)
4	0D	0.23	0/1653	0.72	1/2238 (0.0%)
4	1D	0.24	0/1653	0.73	3/2238 (0.1%)
4	2D	0.25	0/1653	0.81	4/2238 (0.2%)
5	0E	0.20	0/1584	0.56	0/2133
5	1E	0.22	0/1584	0.61	2/2133 (0.1%)
5	2E	0.21	0/1584	0.60	0/2133
5	3E	0.19	0/1584	0.51	0/2133
6	0F	0.26	0/1699	0.76	2/2294 (0.1%)
7	0G	0.21	0/1409	0.71	2/1895 (0.1%)
7	1G	0.22	0/1136	0.71	2/1530 (0.1%)
8	0H	0.25	0/1060	0.72	0/1404
8	1H	0.25	0/3741	0.66	1/4955 (0.0%)
9	0N	0.19	0/2355	0.45	0/3181
9	1N	0.18	0/3884	0.44	0/5240
9	2N	0.16	0/2355	0.43	1/3181 (0.0%)
10	0Q	0.20	0/1583	0.53	0/2138
10	1Q	0.21	0/1583	0.56	0/2138
10	2Q	0.20	0/1583	0.50	0/2138
10	3Q	0.21	0/1583	0.54	2/2138 (0.1%)
10	4Q	0.21	0/1583	0.53	0/2138
10	5Q	0.20	0/1583	0.50	0/2138
10	6Q	0.20	0/1583	0.54	0/2138
11	0S	0.18	0/2361	0.48	1/3199 (0.0%)
11	1S	0.20	0/2361	0.50	0/3199
11	2S	0.21	0/2361	0.56	2/3199 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	3S	0.19	0/2361	0.50	0/3199
12	0T	0.17	0/2176	0.50	0/2931
12	1T	0.19	0/2379	0.49	0/3209
12	2T	0.21	0/2379	0.50	0/3209
12	3T	0.24	0/2379	0.48	0/3209
13	0U	0.18	0/4866	0.51	0/6583
13	1U	0.19	0/4866	0.51	0/6583
13	2U	0.19	0/4866	0.51	0/6583
13	3U	0.19	0/4866	0.54	0/6583
14	0V	0.16	0/1784	0.49	0/2393
14	1V	0.19	0/2213	0.58	0/2978
14	2V	0.20	0/2213	0.58	0/2978
14	3V	0.18	0/2213	0.54	0/2978
15	0X	0.27	0/946	0.73	1/1255 (0.1%)
15	1X	0.25	0/1216	0.65	2/1614 (0.1%)
15	2X	0.22	0/1216	0.57	1/1614 (0.1%)
15	3X	0.21	0/1216	0.55	1/1614 (0.1%)
15	4X	0.21	0/1216	0.53	0/1614
16	1B	0.18	0/4148	0.48	2/5587 (0.0%)
16	2B	0.18	0/2483	0.53	2/3339 (0.1%)
16	3B	0.19	0/2480	0.56	1/3333 (0.0%)
17	1F	0.21	0/1119	0.69	2/1513 (0.1%)
18	1I	0.22	0/1574	0.62	0/2125
19	1J	0.21	0/3090	0.61	0/4148
20	1K	0.20	0/2454	0.48	0/3260
20	2K	0.20	0/2528	0.54	0/3351
21	1L	0.18	0/6961	0.55	0/9360
21	2L	0.18	0/5243	0.53	3/7046 (0.0%)
21	3L	0.20	0/1685	0.62	0/2266
22	1M	0.19	0/3041	0.48	0/4100
22	2M	0.19	0/3041	0.50	0/4100
23	1O	0.83	1/2039 (0.0%)	0.69	4/2687 (0.1%)
23	2O	0.21	0/3185	0.58	0/4204
23	3O	0.20	0/2407	0.55	2/3180 (0.1%)
24	1P	0.22	0/3080	0.60	1/4069 (0.0%)
24	2P	0.23	0/1649	0.67	1/2186 (0.0%)
25	1R	0.17	0/4366	0.46	1/5904 (0.0%)
25	2R	0.17	0/4366	0.45	1/5904 (0.0%)
25	3R	0.18	0/4366	0.48	1/5904 (0.0%)
26	1W	0.19	0/1952	0.44	0/2606
26	2W	0.31	0/1008	0.78	2/1349 (0.1%)
27	2C	0.19	0/2511	0.55	2/3378 (0.1%)
27	3C	0.15	0/2511	0.48	2/3378 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	4C	0.16	0/2511	0.47	0/3378
28	2F	0.21	0/766	0.61	0/1025
29	2G	0.20	0/861	0.57	1/1146 (0.1%)
30	2H	0.18	0/507	0.57	0/672
30	3H	2.74	6/507 (1.2%)	0.57	0/672
30	4H	0.17	0/507	0.53	0/672
31	2I	0.23	0/1178	0.62	0/1583
31	3I	0.23	0/729	0.67	1/975 (0.1%)
32	3D	0.17	0/1878	0.44	0/2538
33	4F	0.20	0/1664	0.60	5/2251 (0.2%)
34	4R	0.33	2/5205 (0.0%)	0.52	2/7042 (0.0%)
34	5R	0.17	0/5205	0.44	0/7042
34	6R	0.14	0/5205	0.38	0/7042
34	7R	0.15	0/5205	0.40	0/7042
35	4S	0.19	0/1572	0.51	0/2122
35	5S	0.19	0/1572	0.52	0/2122
36	5A	0.20	0/1299	0.61	1/1757 (0.1%)
36	5B	0.20	0/1299	0.61	2/1757 (0.1%)
36	5C	0.19	0/1299	0.56	0/1757
36	5D	0.20	0/934	0.70	2/1265 (0.2%)
37	5E	0.20	0/1603	0.63	1/2157 (0.0%)
37	5F	0.23	0/1792	0.66	0/2415
37	5G	0.20	0/1792	0.59	0/2415
37	5H	0.21	0/1241	0.71	0/1677
39	6F	0.19	0/1170	0.54	0/1571
40	6G	0.23	0/1809	0.70	3/2426 (0.1%)
41	6H	0.23	0/1391	0.64	0/1858
44	8R	0.25	0/1135	0.50	0/1581
45	AA	0.18	0/3480	0.46	0/4716
45	AC	0.19	0/3480	0.45	0/4716
45	AE	0.19	0/3480	0.44	0/4716
45	AG	0.18	0/3480	0.46	3/4716 (0.1%)
45	AI	0.19	0/3480	0.43	0/4716
45	AK	0.19	0/3480	0.44	2/4716 (0.0%)
45	AM	0.17	0/3480	0.42	0/4716
45	BA	0.16	0/3435	0.44	0/4655
45	BC	0.19	0/3435	0.46	0/4655
45	BE	0.19	0/3435	0.47	0/4655
45	BG	0.18	0/3435	0.44	0/4655
45	BI	0.18	0/3435	0.44	0/4655
45	BK	0.18	0/3435	0.45	0/4655
45	BM	0.17	0/3435	0.45	0/4655
45	CA	0.15	0/3480	0.41	0/4716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
45	CC	0.17	0/3480	0.45	0/4716
45	CE	0.19	0/3480	0.44	0/4716
45	CG	0.18	0/3480	0.44	0/4716
45	CI	0.17	0/3480	0.43	0/4716
45	CK	0.17	0/3480	0.45	0/4716
45	CM	0.16	0/3480	0.43	0/4716
45	DA	0.12	0/3443	0.36	0/4666
45	DC	0.17	0/3460	0.47	1/4687 (0.0%)
45	DE	0.17	0/3443	0.44	0/4666
45	DG	0.17	0/3460	0.44	0/4687
45	DI	0.16	0/3443	0.42	0/4666
45	DK	0.17	0/3460	0.45	0/4687
45	DM	0.16	0/3443	0.44	0/4666
45	EA	0.12	0/3480	0.37	0/4716
45	EC	0.17	0/3480	0.47	0/4716
45	EE	0.16	0/3480	0.43	0/4716
45	EG	0.15	0/3480	0.41	0/4716
45	EI	0.15	0/3480	0.42	0/4716
45	EK	0.17	0/3480	0.44	0/4716
45	EM	0.18	0/3480	0.47	1/4716 (0.0%)
45	FA	0.17	0/3413	0.43	1/4625 (0.0%)
45	FC	0.18	0/3435	0.43	0/4655
45	FE	0.18	0/3447	0.41	0/4671
45	FG	0.18	0/3480	0.42	0/4716
45	FI	0.18	0/3443	0.41	0/4666
45	FK	0.16	0/3435	0.43	0/4655
45	FM	0.12	0/3413	0.36	0/4625
45	GA	0.15	0/3413	0.43	0/4625
45	GC	0.19	0/3429	0.46	0/4647
45	GE	0.20	0/3429	0.44	0/4647
45	GG	0.19	0/3429	0.41	0/4647
45	GI	0.19	0/3429	0.42	1/4647 (0.0%)
45	GK	0.18	0/3480	0.45	2/4716 (0.0%)
45	GM	0.12	0/3413	0.34	0/4625
45	HA	0.17	0/3427	0.47	0/4644
45	HC	0.18	0/3427	0.40	0/4644
45	HE	0.20	0/3427	0.43	0/4644
45	HG	0.19	0/3427	0.43	0/4644
45	HI	0.19	0/3427	0.42	0/4644
45	HK	0.19	0/3427	0.44	2/4644 (0.0%)
45	HM	0.12	0/3427	0.34	0/4644
45	IA	0.19	0/3435	0.46	1/4655 (0.0%)
45	IC	0.19	0/3480	0.47	0/4716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
45	IE	0.20	0/3435	0.43	0/4655
45	IG	0.19	0/3480	0.47	0/4716
45	II	0.21	0/3480	0.47	0/4716
45	IK	0.19	0/3435	0.46	0/4655
45	IM	0.16	0/3435	0.43	0/4655
45	JA	0.19	0/3435	0.43	1/4655 (0.0%)
45	JC	0.19	0/3447	0.42	0/4671
45	JE	0.19	0/3480	0.40	0/4716
45	JG	0.18	0/3480	0.43	1/4716 (0.0%)
45	JI	0.19	0/3476	0.43	1/4710 (0.0%)
45	JK	0.20	0/3480	0.48	0/4716
45	JM	0.15	0/3435	0.43	0/4655
45	KA	0.16	0/3447	0.40	0/4671
45	KC	0.17	0/3443	0.42	0/4666
45	KE	0.18	0/3456	0.42	0/4682
45	KG	0.18	0/3480	0.43	0/4716
45	KI	0.19	0/3480	0.43	0/4716
45	KK	0.18	0/3480	0.42	0/4716
45	KM	0.16	0/3447	0.42	0/4671
45	LA	0.17	0/3480	0.45	0/4716
45	LC	0.17	0/3480	0.39	0/4716
45	LE	0.18	0/3471	0.42	0/4702
45	LG	0.16	0/3480	0.38	0/4716
45	LI	0.18	0/3452	0.41	0/4677
45	LK	0.18	0/3480	0.41	0/4716
45	LM	0.17	0/3480	0.43	0/4716
45	MA	0.18	0/3463	0.43	0/4692
45	MC	0.19	0/3439	0.42	0/4660
45	ME	0.19	0/3443	0.44	0/4666
45	MG	0.18	0/3471	0.42	0/4703
45	MI	0.18	0/3480	0.44	0/4716
45	MK	0.19	0/3455	0.42	0/4681
45	MM	0.16	0/3463	0.40	0/4692
45	NA	0.17	0/3480	0.46	0/4716
45	NC	0.16	0/3435	0.39	0/4655
45	NE	0.17	0/3480	0.42	0/4716
45	NG	0.15	0/3435	0.39	0/4655
45	NI	0.17	0/3480	0.42	0/4716
45	NK	0.17	0/3435	0.45	0/4655
45	NM	0.16	0/3480	0.44	0/4716
45	OA	0.17	0/3439	0.46	0/4660
45	OC	0.18	0/3439	0.44	0/4660
45	OE	0.17	0/3439	0.43	0/4660

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
45	OG	0.16	0/3439	0.39	0/4660
45	OI	0.16	0/3439	0.42	0/4660
45	OK	0.17	0/3439	0.42	0/4660
45	OM	0.15	0/3439	0.44	0/4660
45	PA	0.17	0/3413	0.45	0/4625
45	PC	0.16	0/3413	0.43	0/4625
45	PE	0.16	0/3413	0.43	0/4625
45	PG	0.17	0/3413	0.43	0/4625
45	PI	0.17	0/3413	0.44	0/4625
45	PK	0.16	0/3413	0.42	0/4625
45	PM	0.16	0/3413	0.46	0/4625
45	QA	0.15	0/3427	0.44	0/4644
45	QC	0.17	0/3427	0.45	0/4644
45	QE	0.17	0/3427	0.42	0/4644
45	QG	0.18	0/3427	0.45	0/4644
45	QI	0.17	0/3427	0.42	0/4644
45	QK	0.17	0/3427	0.44	0/4644
45	QM	0.16	0/3427	0.44	0/4644
45	RA	0.13	0/3427	0.40	0/4644
45	RC	0.16	0/3427	0.45	0/4644
45	RE	0.26	1/3427 (0.0%)	0.51	4/4644 (0.1%)
45	RG	0.17	0/3427	0.44	0/4644
45	RI	0.16	0/3427	0.41	0/4644
45	RK	0.17	0/3427	0.46	0/4644
45	RM	0.15	0/3427	0.44	0/4644
45	SA	0.12	0/3421	0.36	0/4636
45	SC	0.15	0/3421	0.41	0/4636
45	SE	0.16	0/3421	0.41	0/4636
45	SG	0.18	0/3421	0.44	0/4636
45	SI	0.17	0/3421	0.42	0/4636
45	SK	0.18	0/3421	0.45	0/4636
45	SM	0.14	0/3421	0.41	0/4636
45	TA	0.12	0/3421	0.36	0/4636
45	TC	0.17	0/3421	0.47	0/4636
45	TE	0.19	0/3421	0.48	0/4636
45	TG	0.16	0/3421	0.42	1/4636 (0.0%)
45	TI	0.16	0/3421	0.43	0/4636
45	TK	0.17	0/3421	0.42	0/4636
45	TM	0.18	0/3421	0.47	0/4636
45	UA	1.19	6/3427 (0.2%)	0.38	0/4644
45	UC	0.16	0/3427	0.45	0/4644
45	UE	0.17	0/3427	0.47	0/4644
45	UG	0.17	0/3427	0.45	0/4644

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
45	UI	0.18	0/3427	0.46	0/4644
45	UK	0.17	0/3427	0.45	0/4644
45	UM	0.17	0/3427	0.47	0/4644
45	VA	0.18	0/3443	0.48	0/4666
45	VC	0.16	0/3480	0.41	0/4716
45	VE	0.17	0/3443	0.41	0/4666
45	VG	0.19	0/3480	0.44	0/4716
45	VI	0.18	0/3443	0.46	0/4666
45	VK	0.24	1/3480 (0.0%)	0.52	4/4716 (0.1%)
45	VM	0.12	0/3443	0.34	0/4666
45	WA	0.18	0/3427	0.49	0/4644
45	WC	0.18	0/3480	0.47	0/4716
45	WE	0.17	0/3427	0.42	0/4644
45	WG	0.18	0/3480	0.46	1/4716 (0.0%)
45	WI	0.17	0/3427	0.42	0/4644
45	WK	0.18	0/3480	0.48	0/4716
45	WM	0.15	0/3427	0.44	0/4644
46	AB	0.17	0/3439	0.43	0/4655
46	AD	0.20	0/3439	0.43	0/4655
46	AF	0.19	0/3439	0.42	0/4655
46	AH	0.19	0/3439	0.42	0/4655
46	AJ	0.19	0/3439	0.42	0/4655
46	AL	0.19	0/3439	0.39	0/4655
46	AN	0.18	0/3439	0.43	0/4655
46	BB	0.13	0/3439	0.36	0/4655
46	BD	0.19	0/3439	0.44	0/4655
46	BF	0.18	0/3439	0.41	0/4655
46	BH	0.21	0/3439	0.48	0/4655
46	BJ	0.19	0/3439	0.42	0/4655
46	BL	0.19	0/3439	0.45	0/4655
46	BN	0.19	0/3439	0.47	1/4655 (0.0%)
46	CB	0.18	0/3439	0.46	0/4655
46	CD	0.18	0/3439	0.44	0/4655
46	CF	0.41	2/3439 (0.1%)	0.57	2/4655 (0.0%)
46	CH	0.17	0/3439	0.44	0/4655
46	CJ	0.17	0/3439	0.41	0/4655
46	CL	0.18	0/3439	0.46	0/4655
46	CN	0.12	0/3439	0.32	0/4655
46	DB	0.15	0/3439	0.42	0/4655
46	DD	0.18	0/3439	0.45	1/4655 (0.0%)
46	DF	1.06	6/3439 (0.2%)	0.43	0/4655
46	DH	0.17	0/3439	0.41	0/4655
46	DJ	0.17	0/3439	0.42	0/4655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
46	DL	0.17	0/3439	0.45	0/4655
46	DN	0.12	0/3439	0.32	0/4655
46	EB	0.14	0/3439	0.37	0/4655
46	ED	0.17	0/3439	0.44	0/4655
46	EF	0.17	0/3439	0.46	0/4655
46	EH	0.16	0/3439	0.41	0/4655
46	EJ	0.16	0/3439	0.40	0/4655
46	EL	0.18	0/3439	0.48	0/4655
46	EN	0.17	0/3439	0.41	3/4655 (0.1%)
46	FB	0.13	0/3439	0.36	0/4655
46	FD	0.20	0/3439	0.48	0/4655
46	FF	0.20	0/3439	0.43	0/4655
46	FH	0.19	0/3439	0.45	0/4655
46	FJ	0.19	0/3439	0.41	0/4655
46	FL	0.19	0/3439	0.45	0/4655
46	FN	0.14	0/3439	0.40	0/4655
46	GB	0.13	0/3439	0.37	0/4655
46	GD	0.19	0/3439	0.46	0/4655
46	GF	0.20	0/3439	0.42	0/4655
46	GH	0.21	0/3439	0.44	0/4655
46	GJ	0.19	0/3439	0.42	0/4655
46	GL	0.18	0/3439	0.42	0/4655
46	GN	0.16	0/3439	0.43	0/4655
46	HB	0.13	0/3439	0.36	0/4655
46	HD	0.18	0/3439	0.42	0/4655
46	HF	0.22	0/3439	0.48	2/4655 (0.0%)
46	HH	0.19	0/3439	0.41	0/4655
46	HJ	0.20	0/3439	0.42	0/4655
46	HL	0.19	0/3439	0.41	0/4655
46	HN	0.16	0/3439	0.41	0/4655
46	IB	0.16	0/3439	0.43	0/4655
46	ID	0.18	0/3439	0.41	0/4655
46	IF	0.19	0/3439	0.41	0/4655
46	IH	0.20	0/3439	0.43	0/4655
46	IJ	0.20	0/3439	0.43	0/4655
46	IL	0.19	0/3439	0.41	0/4655
46	IN	0.19	0/3439	0.46	0/4655
46	JB	0.17	0/3439	0.41	0/4655
46	JD	0.19	0/3439	0.43	0/4655
46	JF	0.19	0/3439	0.39	0/4655
46	JH	0.18	0/3439	0.43	2/4655 (0.0%)
46	JJ	0.19	0/3439	0.43	0/4655
46	JL	0.19	0/3439	0.42	0/4655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
46	JN	0.19	0/3439	0.46	0/4655
46	KB	0.16	0/3439	0.41	1/4655 (0.0%)
46	KD	0.17	0/3439	0.41	0/4655
46	KF	0.18	0/3439	0.43	3/4655 (0.1%)
46	KH	0.19	0/3439	0.42	2/4655 (0.0%)
46	KJ	0.19	0/3439	0.48	4/4655 (0.1%)
46	KL	0.18	0/3439	0.41	0/4655
46	KN	0.18	0/3439	0.44	2/4655 (0.0%)
46	LB	0.15	0/3439	0.38	0/4655
46	LD	0.17	0/3439	0.40	0/4655
46	LF	0.18	0/3439	0.44	0/4655
46	LH	0.17	0/3439	0.40	0/4655
46	LJ	0.19	0/3439	0.43	0/4655
46	LL	0.19	0/3439	0.41	0/4655
46	LN	0.18	0/3439	0.41	0/4655
46	MB	0.18	0/3439	0.43	0/4655
46	MD	0.19	0/3439	0.39	0/4655
46	MF	0.20	0/3439	0.43	0/4655
46	MH	0.19	0/3439	0.42	0/4655
46	MJ	0.21	0/3439	0.44	0/4655
46	ML	0.18	0/3439	0.38	0/4655
46	MN	0.18	0/3439	0.39	0/4655
46	NB	0.16	0/3375	0.47	2/4569 (0.0%)
46	ND	0.19	0/3439	0.49	1/4655 (0.0%)
46	NF	0.16	0/3375	0.42	0/4569
46	NH	0.17	0/3439	0.43	1/4655 (0.0%)
46	NJ	0.17	0/3375	0.43	0/4569
46	NL	0.18	0/3439	0.44	1/4655 (0.0%)
46	NN	0.17	0/3375	0.42	0/4569
46	OB	0.16	0/3439	0.43	2/4655 (0.0%)
46	OD	0.17	0/3439	0.45	0/4655
46	OF	0.16	0/3439	0.41	1/4655 (0.0%)
46	OH	0.16	0/3439	0.42	0/4655
46	OJ	0.16	0/3439	0.40	0/4655
46	OL	0.18	0/3439	0.43	0/4655
46	ON	0.16	0/3439	0.43	0/4655
46	PB	0.12	0/3439	0.33	0/4655
46	PD	0.17	0/3439	0.47	0/4655
46	PF	0.17	0/3439	0.41	0/4655
46	PH	0.19	0/3439	0.44	0/4655
46	PJ	0.16	0/3439	0.41	0/4655
46	PL	0.17	0/3439	0.43	0/4655
46	PN	0.18	0/3439	0.50	2/4655 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
46	QB	0.17	0/3439	0.44	0/4655
46	QD	0.16	0/3439	0.41	0/4655
46	QF	0.17	0/3439	0.44	0/4655
46	QH	0.17	0/3439	0.43	0/4655
46	QJ	0.16	0/3439	0.43	0/4655
46	QL	0.18	0/3439	0.45	0/4655
46	QN	0.11	0/3439	0.31	0/4655
46	RB	0.17	0/3439	0.44	0/4655
46	RD	0.17	0/3439	0.40	0/4655
46	RF	0.18	0/3439	0.44	0/4655
46	RH	0.17	0/3439	0.43	0/4655
46	RJ	0.17	0/3439	0.41	0/4655
46	RL	0.27	1/3439 (0.0%)	0.58	4/4655 (0.1%)
46	RN	0.11	0/3439	0.30	0/4655
46	SB	0.16	0/3439	0.45	0/4655
46	SD	0.19	0/3439	0.44	0/4655
46	SF	0.18	0/3439	0.43	0/4655
46	SH	0.18	0/3439	0.43	0/4655
46	SJ	0.18	0/3439	0.41	0/4655
46	SL	0.19	0/3439	0.47	0/4655
46	SN	0.12	0/3439	0.32	0/4655
46	TB	0.17	0/3439	0.46	0/4655
46	TD	0.17	0/3439	0.44	0/4655
46	TF	0.17	0/3439	0.43	0/4655
46	TH	0.16	0/3439	0.42	1/4655 (0.0%)
46	TJ	0.17	0/3439	0.43	0/4655
46	TL	0.17	0/3439	0.46	0/4655
46	TN	0.12	0/3439	0.33	0/4655
46	UB	0.18	0/3439	0.45	1/4655 (0.0%)
46	UD	0.17	0/3439	0.43	0/4655
46	UF	0.17	0/3439	0.41	0/4655
46	UH	0.18	0/3439	0.44	0/4655
46	UJ	0.19	0/3439	0.49	1/4655 (0.0%)
46	UL	0.18	0/3439	0.45	0/4655
46	UN	0.16	0/3439	0.44	0/4655
46	VB	0.17	0/3439	0.49	0/4655
46	VD	0.19	0/3439	0.45	0/4655
46	VF	0.18	0/3439	0.43	0/4655
46	VH	0.17	0/3439	0.44	0/4655
46	VJ	0.18	0/3439	0.43	0/4655
46	VL	0.18	0/3439	0.47	2/4655 (0.0%)
46	VN	0.17	0/3439	0.44	0/4655
46	WB	0.17	0/3439	0.47	0/4655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
46	WD	0.19	0/3439	0.45	0/4655
46	WF	0.18	0/3439	0.43	0/4655
46	WH	0.17	0/3439	0.44	0/4655
46	WJ	0.19	0/3439	0.47	0/4655
46	WL	0.19	0/3439	0.44	0/4655
46	WN	0.18	0/3439	0.44	0/4655
All	All	0.21	26/1335252 (0.0%)	0.45	151/1806584 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0A	0	1
1	1A	0	1
1	2A	0	1
1	3A	0	1
2	0B	0	3
4	1D	0	1
4	2D	0	1
5	0E	0	1
5	1E	0	1
6	0F	0	4
7	0G	0	2
7	1G	0	1
10	2Q	0	1
11	0S	0	1
13	0U	0	1
13	1U	0	1
13	3U	0	1
21	1L	0	2
21	2L	0	2
23	1O	0	1
25	1R	0	1
25	2R	0	1
25	3R	0	1
31	3I	0	1
33	4F	0	1
40	6G	0	2
44	8R	0	1
45	BI	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	EA	0	1
45	EE	0	1
45	EI	0	1
45	EM	0	1
45	PA	0	1
45	QA	0	1
45	RM	0	1
45	TA	0	1
46	BH	0	1
46	QD	0	1
46	UF	0	1
All	All	0	48

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	UA	282	TYR	CD2-CE2	41.47	2.63	1.38
23	1O	266	GLU	CA-C	35.74	1.94	1.52
46	DF	281	TYR	CD2-CE2	33.38	2.38	1.38
45	UA	282	TYR	CD1-CE1	31.01	2.31	1.38
46	DF	281	TYR	CD1-CE1	30.10	2.29	1.38

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	4R	147	ARG	CD-NE-CZ	21.14	153.99	124.40
46	CF	86	ARG	CD-NE-CZ	20.44	153.02	124.40
45	VK	261	PRO	CA-N-CD	-12.04	95.14	112.00
46	RL	173	PRO	N-CD-CG	-11.58	85.83	103.20
45	RE	89	PRO	CA-N-CD	-11.56	95.81	112.00

There are no chirality outliers.

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0A	70	HIS	Peptide
2	0B	222	GLU	Peptide
2	0B	223	LYS	Peptide
2	0B	322	ARG	Peptide
5	0E	43	VAL	Peptide

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	0A	1229	0	1156	68	0
1	1A	1229	0	1156	56	0
1	2A	1229	0	1156	58	0
1	3A	1229	0	1156	60	0
2	0B	2615	0	2539	126	0
3	0C	747	0	746	45	0
3	1C	747	0	746	40	0
4	0D	1619	0	1606	109	0
4	1D	1619	0	1606	99	0
4	2D	1619	0	1606	103	0
5	0E	1557	0	1513	65	0
5	1E	1557	0	1513	70	0
5	2E	1557	0	1513	90	0
5	3E	1557	0	1513	80	0
6	0F	1665	0	1658	112	0
7	0G	1378	0	1332	86	0
7	1G	1109	0	1072	69	0
8	0H	1046	0	1051	60	0
8	1H	3706	0	3719	230	0
9	0N	2305	0	2251	103	0
9	1N	3805	0	3734	141	0
9	2N	2305	0	2251	90	0
10	0Q	1548	0	1575	63	0
10	1Q	1548	0	1575	78	0
10	2Q	1548	0	1575	68	0
10	3Q	1548	0	1575	68	0
10	4Q	1548	0	1575	76	0
10	5Q	1548	0	1575	62	0
10	6Q	1548	0	1575	67	0
11	0S	2310	0	2349	94	0
11	1S	2310	0	2349	121	0
11	2S	2310	0	2349	108	0
11	3S	2310	0	2349	93	0
12	0T	2124	0	2067	80	0
12	1T	2321	0	2267	110	0
12	2T	2321	0	2267	122	0
12	3T	2321	0	2267	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	0U	4774	0	4750	217	0
13	1U	4774	0	4750	208	0
13	2U	4774	0	4750	224	0
13	3U	4774	0	4750	232	0
14	0V	1750	0	1740	49	0
14	1V	2168	0	2164	93	0
14	2V	2168	0	2164	122	0
14	3V	2168	0	2164	76	0
15	0X	935	0	911	50	0
15	1X	1202	0	1179	73	0
15	2X	1202	0	1179	49	0
15	3X	1202	0	1179	48	0
15	4X	1202	0	1179	61	0
16	1B	4066	0	4014	130	0
16	2B	2439	0	2418	92	0
16	3B	2437	0	2415	107	0
17	1F	1093	0	1080	66	0
18	1I	1546	0	1485	76	0
19	1J	3025	0	2936	184	0
20	1K	2425	0	2432	123	0
20	2K	2506	0	2541	119	0
21	1L	6842	0	6888	308	0
21	2L	5151	0	5185	216	0
21	3L	1660	0	1672	76	0
22	1M	2978	0	2957	99	0
22	2M	2978	0	2957	98	0
23	1O	2032	0	2152	160	0
23	2O	3173	0	3302	237	0
23	3O	2397	0	2483	112	0
24	1P	3060	0	3181	196	0
24	2P	1633	0	1646	102	0
25	1R	4244	0	4119	145	0
25	2R	4244	0	4119	159	0
25	3R	4244	0	4119	156	0
26	1W	1924	0	1867	74	0
26	2W	990	0	967	102	0
27	2C	2467	0	2457	101	0
27	3C	2467	0	2457	96	0
27	4C	2467	0	2457	102	0
28	2F	746	0	702	34	0
29	2G	848	0	871	45	0
30	2H	501	0	513	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	3H	501	0	513	72	0
30	4H	501	0	513	17	0
31	2I	1150	0	1150	81	0
31	3I	712	0	722	54	0
32	3D	1835	0	1817	52	0
33	4F	1618	0	1562	71	0
34	4R	5070	0	4976	167	0
34	5R	5070	0	4976	174	0
34	6R	5070	0	4976	152	0
34	7R	5070	0	4976	166	0
35	4S	1537	0	1565	94	0
35	5S	1537	0	1565	73	0
36	5A	1261	0	1230	49	0
36	5B	1261	0	1230	56	0
36	5C	1261	0	1230	53	0
36	5D	908	0	886	36	0
37	5E	1566	0	1570	78	0
37	5F	1750	0	1753	110	0
37	5G	1750	0	1753	85	0
37	5H	1210	0	1191	76	0
38	5I	515	0	109	0	0
38	5J	545	0	115	1	0
38	5K	400	0	84	0	0
39	6F	1140	0	1077	50	0
40	6G	1769	0	1772	127	0
41	6H	1362	0	1278	59	0
42	8L	1925	0	391	4	0
42	8N	1790	0	362	0	0
43	8P	1815	0	369	4	0
44	8R	2020	0	1200	24	0
45	AA	3408	0	3347	101	0
45	AC	3408	0	3347	132	0
45	AE	3408	0	3347	120	0
45	AG	3408	0	3347	101	0
45	AI	3408	0	3347	82	0
45	AK	3408	0	3347	96	0
45	AM	3408	0	3347	111	0
45	BA	3364	0	3302	136	0
45	BC	3364	0	3302	114	0
45	BE	3364	0	3302	119	0
45	BG	3364	0	3302	112	0
45	BI	3364	0	3302	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	BK	3364	0	3302	125	0
45	BM	3364	0	3302	131	0
45	CA	3408	0	3347	115	0
45	CC	3408	0	3347	138	0
45	CE	3408	0	3347	110	0
45	CG	3408	0	3347	135	0
45	CI	3408	0	3347	106	0
45	CK	3408	0	3347	116	0
45	CM	3408	0	3347	106	0
45	DA	3372	0	3305	67	0
45	DC	3389	0	3325	140	0
45	DE	3372	0	3306	117	0
45	DG	3389	0	3325	119	0
45	DI	3372	0	3306	115	0
45	DK	3389	0	3325	129	0
45	DM	3372	0	3306	142	0
45	EA	3408	0	3347	56	0
45	EC	3408	0	3347	172	0
45	EE	3408	0	3347	115	0
45	EG	3408	0	3347	122	0
45	EI	3408	0	3346	103	0
45	EK	3408	0	3347	109	0
45	EM	3408	0	3347	132	0
45	FA	3342	0	3289	115	0
45	FC	3364	0	3302	106	0
45	FE	3376	0	3309	89	0
45	FG	3408	0	3347	96	0
45	FI	3372	0	3306	98	0
45	FK	3364	0	3302	122	0
45	FM	3342	0	3289	60	0
45	GA	3342	0	3289	126	0
45	GC	3358	0	3297	96	0
45	GE	3358	0	3297	137	0
45	GG	3358	0	3297	115	0
45	GI	3358	0	3297	97	0
45	GK	3408	0	3347	117	0
45	GM	3342	0	3289	61	0
45	HA	3356	0	3298	109	0
45	HC	3356	0	3298	102	0
45	HE	3356	0	3298	118	0
45	HG	3356	0	3298	97	0
45	HI	3356	0	3298	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	HK	3356	0	3298	120	0
45	HM	3356	0	3298	76	0
45	IA	3364	0	3302	128	0
45	IC	3408	0	3347	121	0
45	IE	3364	0	3302	126	0
45	IG	3408	0	3347	140	0
45	II	3408	0	3347	109	0
45	IK	3364	0	3302	117	0
45	IM	3364	0	3302	136	0
45	JA	3364	0	3302	114	0
45	JC	3376	0	3309	107	0
45	JE	3408	0	3347	92	0
45	JG	3408	0	3347	116	0
45	JI	3404	0	3337	107	0
45	JK	3408	0	3347	125	0
45	JM	3364	0	3302	110	0
45	KA	3376	0	3309	120	0
45	KC	3372	0	3306	93	0
45	KE	3385	0	3322	113	0
45	KG	3408	0	3347	129	0
45	KI	3408	0	3347	101	0
45	KK	3408	0	3347	112	0
45	KM	3376	0	3309	133	0
45	LA	3408	0	3347	103	0
45	LC	3408	0	3347	103	0
45	LE	3400	0	3335	94	0
45	LG	3408	0	3347	101	0
45	LI	3381	0	3319	116	0
45	LK	3408	0	3347	117	0
45	LM	3408	0	3347	97	0
45	MA	3392	0	3329	107	0
45	MC	3368	0	3305	109	0
45	ME	3372	0	3306	111	0
45	MG	3400	0	3340	114	0
45	MI	3408	0	3347	105	0
45	MK	3384	0	3315	108	0
45	MM	3392	0	3329	103	0
45	NA	3408	0	3347	159	0
45	NC	3364	0	3302	112	0
45	NE	3408	0	3347	111	0
45	NG	3364	0	3302	120	0
45	NI	3408	0	3347	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	NK	3364	0	3302	132	0
45	NM	3408	0	3347	142	0
45	OA	3368	0	3305	169	0
45	OC	3368	0	3305	139	0
45	OE	3368	0	3305	133	0
45	OG	3368	0	3305	113	0
45	OI	3368	0	3305	116	0
45	OK	3368	0	3305	136	0
45	OM	3368	0	3305	124	0
45	PA	3342	0	3288	148	0
45	PC	3342	0	3289	134	0
45	PE	3342	0	3289	141	0
45	PG	3342	0	3289	148	0
45	PI	3342	0	3289	123	0
45	PK	3342	0	3289	114	0
45	PM	3342	0	3289	107	0
45	QA	3356	0	3298	110	0
45	QC	3356	0	3298	129	0
45	QE	3356	0	3298	126	0
45	QG	3356	0	3298	159	0
45	QI	3356	0	3298	143	0
45	QK	3356	0	3298	131	0
45	QM	3356	0	3298	122	0
45	RA	3356	0	3298	76	0
45	RC	3356	0	3298	128	0
45	RE	3356	0	3298	135	0
45	RG	3356	0	3298	150	0
45	RI	3356	0	3298	98	0
45	RK	3356	0	3298	120	0
45	RM	3356	0	3298	111	0
45	SA	3350	0	3293	58	0
45	SC	3350	0	3293	127	0
45	SE	3350	0	3293	125	0
45	SG	3350	0	3293	137	0
45	SI	3350	0	3293	116	0
45	SK	3350	0	3293	152	0
45	SM	3350	0	3293	116	0
45	TA	3350	0	3293	69	0
45	TC	3350	0	3293	154	0
45	TE	3350	0	3293	143	0
45	TG	3350	0	3293	119	0
45	TI	3350	0	3293	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	TK	3350	0	3293	121	0
45	TM	3350	0	3293	143	0
45	UA	3356	0	3298	111	0
45	UC	3356	0	3298	152	0
45	UE	3356	0	3298	137	0
45	UG	3356	0	3298	128	0
45	UI	3356	0	3298	114	0
45	UK	3356	0	3298	141	0
45	UM	3356	0	3298	143	0
45	VA	3372	0	3306	192	0
45	VC	3408	0	3347	120	0
45	VE	3372	0	3306	125	0
45	VG	3408	0	3347	161	0
45	VI	3372	0	3306	136	0
45	VK	3408	0	3347	160	0
45	VM	3372	0	3306	70	0
45	WA	3356	0	3297	144	0
45	WC	3408	0	3347	164	0
45	WE	3356	0	3298	125	0
45	WG	3408	0	3347	139	0
45	WI	3356	0	3298	110	0
45	WK	3408	0	3347	146	0
45	WM	3356	0	3298	96	0
46	AB	3366	0	3257	128	0
46	AD	3366	0	3257	127	0
46	AF	3366	0	3257	112	0
46	AH	3366	0	3257	114	0
46	AJ	3366	0	3257	101	0
46	AL	3366	0	3257	111	0
46	AN	3366	0	3257	129	0
46	BB	3366	0	3257	93	0
46	BD	3366	0	3257	151	0
46	BF	3366	0	3257	134	0
46	BH	3366	0	3257	153	0
46	BJ	3366	0	3257	114	0
46	BL	3366	0	3257	132	0
46	BN	3366	0	3257	177	0
46	CB	3366	0	3257	175	0
46	CD	3366	0	3257	118	0
46	CF	3366	0	3257	185	0
46	CH	3366	0	3257	126	0
46	CJ	3366	0	3257	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	CL	3366	0	3257	138	0
46	CN	3366	0	3257	90	0
46	DB	3366	0	3257	134	0
46	DD	3366	0	3257	124	0
46	DF	3366	0	3257	136	0
46	DH	3366	0	3257	117	0
46	DJ	3366	0	3257	131	0
46	DL	3366	0	3257	170	0
46	DN	3366	0	3257	69	0
46	EB	3366	0	3257	137	0
46	ED	3366	0	3257	128	0
46	EF	3366	0	3257	155	0
46	EH	3366	0	3257	138	0
46	EJ	3366	0	3257	132	0
46	EL	3366	0	3257	157	0
46	EN	3366	0	3257	103	0
46	FB	3366	0	3257	128	0
46	FD	3366	0	3257	143	0
46	FF	3366	0	3257	131	0
46	FH	3366	0	3257	134	0
46	FJ	3366	0	3257	118	0
46	FL	3366	0	3257	140	0
46	FN	3366	0	3257	104	0
46	GB	3366	0	3257	97	0
46	GD	3366	0	3257	136	0
46	GF	3366	0	3257	127	0
46	GH	3366	0	3257	122	0
46	GJ	3366	0	3257	108	0
46	GL	3366	0	3257	112	0
46	GN	3366	0	3257	116	0
46	HB	3366	0	3257	108	0
46	HD	3366	0	3257	133	0
46	HF	3366	0	3257	131	0
46	HH	3366	0	3257	130	0
46	HJ	3366	0	3257	120	0
46	HL	3366	0	3257	126	0
46	HN	3366	0	3257	134	0
46	IB	3366	0	3257	115	0
46	ID	3366	0	3257	132	0
46	IF	3366	0	3257	86	0
46	IH	3366	0	3257	132	0
46	IJ	3366	0	3257	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	IL	3366	0	3257	125	0
46	IN	3366	0	3257	147	0
46	JB	3366	0	3257	104	0
46	JD	3366	0	3257	89	0
46	JF	3366	0	3257	101	0
46	JH	3366	0	3257	108	0
46	JJ	3366	0	3257	109	0
46	JL	3366	0	3257	118	0
46	JN	3366	0	3257	146	0
46	KB	3366	0	3257	114	0
46	KD	3366	0	3257	99	0
46	KF	3366	0	3257	111	0
46	KH	3366	0	3257	105	0
46	KJ	3366	0	3257	107	0
46	KL	3366	0	3257	103	0
46	KN	3366	0	3257	129	0
46	LB	3366	0	3257	109	0
46	LD	3366	0	3257	111	0
46	LF	3366	0	3257	104	0
46	LH	3366	0	3257	102	0
46	LJ	3366	0	3257	115	0
46	LL	3366	0	3257	118	0
46	LN	3366	0	3257	109	0
46	MB	3366	0	3257	130	0
46	MD	3366	0	3257	113	0
46	MF	3366	0	3257	117	0
46	MH	3366	0	3257	97	0
46	MJ	3366	0	3257	149	0
46	ML	3366	0	3257	84	0
46	MN	3366	0	3257	119	0
46	NB	3304	0	3197	159	0
46	ND	3366	0	3257	153	0
46	NF	3304	0	3197	100	0
46	NH	3366	0	3257	140	0
46	NJ	3304	0	3197	128	0
46	NL	3366	0	3257	152	0
46	NN	3304	0	3197	122	0
46	OB	3366	0	3257	134	0
46	OD	3366	0	3257	146	0
46	OF	3366	0	3255	125	0
46	OH	3366	0	3257	109	0
46	OJ	3366	0	3257	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	OL	3366	0	3257	115	0
46	ON	3366	0	3257	164	0
46	PB	3366	0	3257	90	0
46	PD	3366	0	3255	157	0
46	PF	3366	0	3257	130	0
46	PH	3366	0	3257	128	0
46	PJ	3366	0	3257	140	0
46	PL	3366	0	3257	143	0
46	PN	3366	0	3257	164	0
46	QB	3366	0	3257	163	0
46	QD	3366	0	3257	124	0
46	QF	3366	0	3257	135	0
46	QH	3366	0	3257	148	0
46	QJ	3366	0	3257	126	0
46	QL	3366	0	3257	172	0
46	QN	3366	0	3257	69	0
46	RB	3366	0	3257	150	0
46	RD	3366	0	3257	136	0
46	RF	3366	0	3257	155	0
46	RH	3366	0	3257	139	0
46	RJ	3366	0	3257	135	0
46	RL	3366	0	3257	182	0
46	RN	3366	0	3257	69	0
46	SB	3366	0	3257	145	0
46	SD	3366	0	3257	148	0
46	SF	3366	0	3257	148	0
46	SH	3366	0	3257	138	0
46	SJ	3366	0	3257	141	0
46	SL	3366	0	3257	172	0
46	SN	3366	0	3257	72	0
46	TB	3366	0	3257	156	0
46	TD	3366	0	3257	145	0
46	TF	3366	0	3257	159	0
46	TH	3366	0	3257	136	0
46	TJ	3366	0	3257	145	0
46	TL	3366	0	3257	189	0
46	TN	3366	0	3257	78	0
46	UB	3366	0	3257	168	0
46	UD	3366	0	3257	143	0
46	UF	3366	0	3257	158	0
46	UH	3366	0	3257	146	0
46	UJ	3366	0	3257	174	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	UL	3366	0	3257	183	0
46	UN	3366	0	3257	132	0
46	VB	3366	0	3257	157	0
46	VD	3366	0	3257	149	0
46	VF	3366	0	3257	145	0
46	VH	3366	0	3257	154	0
46	VJ	3366	0	3257	139	0
46	VL	3366	0	3257	173	0
46	VN	3366	0	3257	169	0
46	WB	3366	0	3257	155	0
46	WD	3366	0	3257	151	0
46	WF	3366	0	3257	150	0
46	WH	3366	0	3257	131	0
46	WJ	3366	0	3257	136	0
46	WL	3366	0	3257	137	0
46	WN	3366	0	3257	158	0
47	AA	32	0	12	3	0
47	AC	32	0	12	1	0
47	AE	32	0	12	0	0
47	AG	32	0	12	1	0
47	AI	32	0	12	1	0
47	AK	32	0	12	1	0
47	AM	32	0	12	2	0
47	BA	32	0	12	1	0
47	BC	32	0	12	0	0
47	BE	32	0	12	4	0
47	BG	32	0	12	1	0
47	BI	32	0	12	3	0
47	BK	32	0	12	1	0
47	BM	32	0	12	2	0
47	CA	32	0	12	2	0
47	CC	32	0	12	1	0
47	CE	32	0	12	1	0
47	CG	32	0	12	2	0
47	CI	32	0	12	2	0
47	CK	32	0	12	1	0
47	CM	32	0	12	1	0
47	DA	32	0	12	2	0
47	DC	32	0	12	3	0
47	DE	32	0	12	2	0
47	DG	32	0	12	3	0
47	DI	32	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	DK	32	0	12	3	0
47	DM	32	0	12	2	0
47	EA	32	0	12	2	0
47	EC	32	0	12	3	0
47	EE	32	0	12	1	0
47	EG	32	0	12	2	0
47	EI	32	0	12	1	0
47	EK	32	0	12	3	0
47	EM	32	0	12	2	0
47	FA	32	0	12	3	0
47	FC	32	0	12	2	0
47	FE	32	0	12	1	0
47	FG	32	0	12	1	0
47	FI	32	0	12	0	0
47	FK	32	0	12	1	0
47	FM	32	0	12	2	0
47	GA	32	0	12	0	0
47	GC	32	0	12	1	0
47	GE	32	0	12	1	0
47	GG	32	0	12	1	0
47	GI	32	0	12	1	0
47	GK	32	0	12	1	0
47	GM	32	0	12	2	0
47	HA	32	0	12	1	0
47	HC	32	0	12	0	0
47	HE	32	0	12	2	0
47	HG	32	0	12	2	0
47	HI	32	0	12	0	0
47	HK	32	0	12	0	0
47	HM	32	0	12	1	0
47	IA	32	0	12	1	0
47	IC	32	0	12	0	0
47	IE	32	0	12	3	0
47	IG	32	0	12	2	0
47	II	32	0	12	0	0
47	IK	32	0	12	3	0
47	IM	32	0	12	3	0
47	JA	32	0	12	1	0
47	JC	32	0	12	2	0
47	JE	32	0	12	0	0
47	JG	32	0	12	2	0
47	JI	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	JK	32	0	12	2	0
47	JM	32	0	12	0	0
47	KA	32	0	12	2	0
47	KC	32	0	12	2	0
47	KE	32	0	12	2	0
47	KG	32	0	12	2	0
47	KI	32	0	12	1	0
47	KK	32	0	12	0	0
47	KM	32	0	12	3	0
47	LA	32	0	12	1	0
47	LC	32	0	12	3	0
47	LE	32	0	12	0	0
47	LG	32	0	12	2	0
47	LI	32	0	12	1	0
47	LK	32	0	12	3	0
47	LM	32	0	12	1	0
47	MA	32	0	12	0	0
47	MC	32	0	12	1	0
47	ME	32	0	12	1	0
47	MG	32	0	12	0	0
47	MI	32	0	12	0	0
47	MK	32	0	12	0	0
47	MM	32	0	12	4	0
47	NA	32	0	12	3	0
47	NC	32	0	12	0	0
47	NE	32	0	12	1	0
47	NG	32	0	12	1	0
47	NI	32	0	12	0	0
47	NK	32	0	12	1	0
47	NM	32	0	12	2	0
47	OA	32	0	12	0	0
47	OC	32	0	12	1	0
47	OF	32	0	12	4	0
47	OG	32	0	12	4	0
47	OI	32	0	12	3	0
47	OK	32	0	12	1	0
47	OM	32	0	12	1	0
47	PA	32	0	12	2	0
47	PD	32	0	12	3	0
47	PE	32	0	12	1	0
47	PG	32	0	12	4	0
47	PI	32	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	PK	32	0	12	4	0
47	PM	32	0	12	2	0
47	QA	32	0	12	2	0
47	QC	32	0	12	3	0
47	QE	32	0	12	5	0
47	QG	32	0	12	5	0
47	QI	32	0	12	3	0
47	QK	32	0	12	2	0
47	QM	32	0	12	2	0
47	RA	32	0	12	2	0
47	RC	32	0	12	3	0
47	RE	32	0	12	3	0
47	RG	32	0	12	2	0
47	RI	32	0	12	1	0
47	RK	32	0	12	3	0
47	RM	32	0	12	2	0
47	SA	32	0	12	2	0
47	SC	32	0	12	2	0
47	SE	32	0	12	2	0
47	SG	32	0	12	0	0
47	SI	32	0	12	2	0
47	SK	32	0	12	4	0
47	SM	32	0	12	1	0
47	TA	32	0	12	2	0
47	TC	32	0	12	3	0
47	TE	32	0	12	1	0
47	TG	32	0	12	1	0
47	TI	32	0	12	1	0
47	TK	32	0	12	2	0
47	TM	32	0	12	2	0
47	UA	32	0	12	2	0
47	UC	32	0	12	1	0
47	UE	32	0	12	3	0
47	UG	32	0	12	1	0
47	UI	32	0	12	2	0
47	UK	32	0	12	0	0
47	UM	32	0	12	1	0
47	VA	32	0	12	3	0
47	VC	32	0	12	2	0
47	VE	32	0	12	4	0
47	VG	32	0	12	4	0
47	VI	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	VK	32	0	12	1	0
47	VM	32	0	12	2	0
47	WA	32	0	12	3	0
47	WC	32	0	12	0	0
47	WE	32	0	12	1	0
47	WG	32	0	12	1	0
47	WI	32	0	12	3	0
47	WK	32	0	12	2	0
47	WM	32	0	12	1	0
48	AA	1	0	0	0	0
48	AC	1	0	0	0	0
48	AE	1	0	0	0	0
48	AG	1	0	0	0	0
48	AI	1	0	0	0	0
48	AK	1	0	0	0	0
48	AM	1	0	0	0	0
48	BA	1	0	0	0	0
48	BC	1	0	0	0	0
48	BE	1	0	0	0	0
48	BG	1	0	0	0	0
48	BI	1	0	0	0	0
48	BK	1	0	0	0	0
48	BM	1	0	0	0	0
48	CA	1	0	0	0	0
48	CC	1	0	0	0	0
48	CE	1	0	0	0	0
48	CG	1	0	0	0	0
48	CI	1	0	0	0	0
48	CK	1	0	0	0	0
48	CM	1	0	0	0	0
48	DA	1	0	0	0	0
48	DC	1	0	0	0	0
48	DE	1	0	0	0	0
48	DG	1	0	0	0	0
48	DI	1	0	0	0	0
48	DK	1	0	0	0	0
48	DM	1	0	0	0	0
48	EA	1	0	0	0	0
48	EC	1	0	0	0	0
48	EE	1	0	0	0	0
48	EG	1	0	0	0	0
48	EI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	EK	1	0	0	0	0
48	EM	1	0	0	0	0
48	FA	1	0	0	0	0
48	FC	1	0	0	0	0
48	FE	1	0	0	0	0
48	FG	1	0	0	0	0
48	FI	1	0	0	0	0
48	FL	1	0	0	0	0
48	FM	1	0	0	0	0
48	GB	1	0	0	0	0
48	GC	1	0	0	0	0
48	GE	1	0	0	0	0
48	GG	1	0	0	0	0
48	GI	1	0	0	0	0
48	GL	1	0	0	0	0
48	GN	1	0	0	0	0
48	HA	1	0	0	0	0
48	HC	1	0	0	0	0
48	HE	1	0	0	0	0
48	HG	1	0	0	0	0
48	HI	1	0	0	0	0
48	HK	1	0	0	0	0
48	HM	1	0	0	0	0
48	IA	1	0	0	0	0
48	IC	1	0	0	0	0
48	IE	1	0	0	0	0
48	IG	1	0	0	0	0
48	II	1	0	0	0	0
48	IK	1	0	0	0	0
48	IM	1	0	0	0	0
48	JA	1	0	0	0	0
48	JC	1	0	0	0	0
48	JE	1	0	0	0	0
48	JG	1	0	0	0	0
48	JI	1	0	0	0	0
48	JK	1	0	0	0	0
48	JM	1	0	0	0	0
48	KA	1	0	0	0	0
48	KC	1	0	0	0	0
48	KE	1	0	0	0	0
48	KG	1	0	0	0	0
48	KI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	KK	1	0	0	0	0
48	KM	1	0	0	0	0
48	LA	1	0	0	0	0
48	LC	1	0	0	0	0
48	LE	1	0	0	0	0
48	LG	1	0	0	0	0
48	LI	1	0	0	0	0
48	LK	1	0	0	0	0
48	LM	1	0	0	0	0
48	MA	1	0	0	0	0
48	MC	1	0	0	0	0
48	ME	1	0	0	0	0
48	MG	1	0	0	0	0
48	MI	1	0	0	0	0
48	MK	1	0	0	0	0
48	MM	1	0	0	0	0
48	NA	1	0	0	0	0
48	ND	1	0	0	0	0
48	NE	1	0	0	0	0
48	NG	1	0	0	0	0
48	NI	1	0	0	0	0
48	NK	1	0	0	0	0
48	NM	1	0	0	0	0
48	OA	1	0	0	0	0
48	OC	1	0	0	0	0
48	OE	1	0	0	0	0
48	OG	1	0	0	0	0
48	OI	1	0	0	0	0
48	OK	1	0	0	0	0
48	OM	1	0	0	0	0
48	PA	1	0	0	0	0
48	PC	1	0	0	0	0
48	PE	1	0	0	0	0
48	PG	1	0	0	0	0
48	PI	1	0	0	0	0
48	PK	1	0	0	0	0
48	PN	1	0	0	0	0
48	QA	1	0	0	0	0
48	QC	1	0	0	0	0
48	QE	1	0	0	0	0
48	QG	1	0	0	0	0
48	QI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	QK	1	0	0	0	0
48	QM	1	0	0	0	0
48	RA	1	0	0	0	0
48	RC	1	0	0	0	0
48	RD	1	0	0	0	0
48	RG	1	0	0	0	0
48	RI	1	0	0	0	0
48	RK	1	0	0	0	0
48	RM	1	0	0	0	0
48	SA	1	0	0	0	0
48	SC	1	0	0	0	0
48	SE	1	0	0	0	0
48	SG	1	0	0	0	0
48	SI	1	0	0	0	0
48	SK	1	0	0	0	0
48	SM	1	0	0	0	0
48	TA	1	0	0	0	0
48	TB	1	0	0	0	0
48	TE	1	0	0	0	0
48	TF	1	0	0	0	0
48	TI	1	0	0	0	0
48	TK	1	0	0	0	0
48	TL	1	0	0	0	0
48	UA	1	0	0	0	0
48	UC	1	0	0	0	0
48	UE	1	0	0	0	0
48	UG	1	0	0	0	0
48	UI	1	0	0	0	0
48	UK	1	0	0	0	0
48	UM	1	0	0	0	0
48	VA	1	0	0	0	0
48	VC	1	0	0	0	0
48	VE	1	0	0	0	0
48	VG	1	0	0	0	0
48	VI	1	0	0	0	0
48	VK	1	0	0	0	0
48	VM	1	0	0	0	0
48	WA	1	0	0	0	0
48	WC	1	0	0	0	0
48	WE	1	0	0	0	0
48	WG	1	0	0	0	0
48	WI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	WK	1	0	0	0	0
48	WM	1	0	0	0	0
49	AB	28	0	12	0	0
49	AD	28	0	12	0	0
49	AF	28	0	12	1	0
49	AH	28	0	12	2	0
49	AJ	28	0	12	2	0
49	AL	28	0	12	1	0
49	AN	28	0	12	1	0
49	BB	28	0	12	0	0
49	BD	28	0	12	2	0
49	BF	28	0	12	4	0
49	BH	28	0	12	2	0
49	BJ	28	0	12	2	0
49	BL	28	0	12	2	0
49	BN	28	0	12	0	0
49	CB	28	0	12	2	0
49	CD	28	0	12	2	0
49	CF	28	0	12	6	0
49	CH	28	0	12	1	0
49	CJ	28	0	12	4	0
49	CL	28	0	12	0	0
49	CN	28	0	12	0	0
49	DB	28	0	12	0	0
49	DD	28	0	12	2	0
49	DF	28	0	12	1	0
49	DH	28	0	12	2	0
49	DJ	28	0	12	2	0
49	DL	28	0	12	1	0
49	DN	28	0	12	1	0
49	EB	28	0	12	0	0
49	ED	28	0	12	1	0
49	EF	28	0	12	1	0
49	EH	28	0	12	4	0
49	EJ	28	0	12	0	0
49	EL	28	0	12	3	0
49	EN	28	0	12	5	0
49	FB	28	0	12	0	0
49	FD	28	0	12	0	0
49	FF	28	0	12	2	0
49	FH	28	0	12	4	0
49	FJ	28	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	FL	28	0	12	2	0
49	FN	28	0	12	1	0
49	GB	28	0	12	0	0
49	GD	28	0	12	2	0
49	GF	28	0	12	1	0
49	GH	28	0	12	0	0
49	GJ	28	0	12	1	0
49	GL	28	0	12	3	0
49	GN	28	0	12	1	0
49	HB	28	0	12	1	0
49	HD	28	0	12	1	0
49	HF	28	0	12	2	0
49	HH	28	0	12	2	0
49	HJ	28	0	12	2	0
49	HL	28	0	12	1	0
49	HN	28	0	12	1	0
49	IB	28	0	12	1	0
49	ID	28	0	12	0	0
49	IF	28	0	12	1	0
49	IH	28	0	12	3	0
49	IJ	28	0	12	3	0
49	IL	28	0	12	4	0
49	IN	28	0	12	3	0
49	JB	28	0	12	0	0
49	JD	28	0	12	1	0
49	JF	28	0	12	1	0
49	JH	28	0	12	1	0
49	JJ	28	0	12	3	0
49	JL	28	0	12	1	0
49	JN	28	0	12	1	0
49	KB	28	0	12	0	0
49	KD	28	0	12	0	0
49	KF	28	0	12	1	0
49	KH	28	0	12	1	0
49	KJ	28	0	12	0	0
49	KL	28	0	12	0	0
49	KN	28	0	12	0	0
49	LB	28	0	12	0	0
49	LD	28	0	12	0	0
49	LF	28	0	12	0	0
49	LH	28	0	12	0	0
49	LJ	28	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	LL	28	0	12	1	0
49	LN	28	0	12	2	0
49	MB	28	0	12	0	0
49	MD	28	0	12	0	0
49	MF	28	0	12	2	0
49	MH	28	0	12	1	0
49	MJ	28	0	12	3	0
49	ML	28	0	12	0	0
49	MN	28	0	12	0	0
49	NB	28	0	12	1	0
49	ND	28	0	12	0	0
49	NF	28	0	12	0	0
49	NH	28	0	12	0	0
49	NJ	28	0	12	1	0
49	NL	28	0	12	0	0
49	NN	28	0	12	0	0
49	OB	28	0	12	2	0
49	OD	28	0	12	2	0
49	OF	28	0	12	3	0
49	OH	28	0	12	0	0
49	OJ	28	0	12	2	0
49	OL	28	0	12	1	0
49	ON	28	0	12	2	0
49	PB	28	0	12	1	0
49	PD	28	0	12	0	0
49	PF	28	0	12	0	0
49	PH	28	0	12	2	0
49	PJ	28	0	12	1	0
49	PL	28	0	12	0	0
49	PN	28	0	12	3	0
49	QB	28	0	12	1	0
49	QD	28	0	12	1	0
49	QF	28	0	12	6	0
49	QH	28	0	12	1	0
49	QJ	28	0	12	3	0
49	QL	28	0	12	1	0
49	QN	28	0	12	1	0
49	RB	28	0	12	1	0
49	RD	28	0	12	0	0
49	RF	28	0	12	0	0
49	RH	28	0	12	1	0
49	RJ	28	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	RL	28	0	12	1	0
49	RN	28	0	12	1	0
49	SB	28	0	12	1	0
49	SD	28	0	12	0	0
49	SF	28	0	12	1	0
49	SH	28	0	12	0	0
49	SJ	28	0	12	1	0
49	SL	28	0	12	0	0
49	SN	28	0	12	1	0
49	TB	28	0	12	0	0
49	TD	28	0	12	1	0
49	TF	28	0	12	1	0
49	TH	28	0	12	1	0
49	TJ	28	0	12	1	0
49	TL	28	0	12	1	0
49	TN	28	0	12	1	0
49	UB	28	0	12	0	0
49	UD	28	0	12	2	0
49	UF	28	0	12	5	0
49	UH	28	0	12	1	0
49	UJ	28	0	12	3	0
49	UL	28	0	12	2	0
49	UN	28	0	12	1	0
49	VB	28	0	12	1	0
49	VD	28	0	12	1	0
49	VF	28	0	12	2	0
49	VH	28	0	12	2	0
49	VJ	28	0	12	4	0
49	VL	28	0	12	3	0
49	VN	28	0	12	2	0
49	WB	28	0	12	0	0
49	WD	28	0	12	3	0
49	WF	28	0	12	1	0
49	WH	28	0	12	2	0
49	WJ	28	0	12	0	0
49	WL	28	0	12	2	0
49	WN	28	0	12	0	0
All	All	1325153	0	1283777	44224	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 17.

The worst 5 of 44224 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)
46:DF:281:TYR:CD1	46:DF:281:TYR:CG	1.80	1.67
46:DF:281:TYR:CG	46:DF:281:TYR:CD2	1.80	1.65
45:UA:282:TYR:CD1	45:UA:282:TYR:CG	1.83	1.64
30:3H:174:PHE:CD1	30:3H:174:PHE:CG	1.79	1.62
30:3H:174:PHE:CG	30:3H:174:PHE:CD2	1.79	1.62

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	0A	148/236 (63%)	118 (80%)	25 (17%)	5 (3%)	3	23
1	1A	148/236 (63%)	118 (80%)	26 (18%)	4 (3%)	4	28
1	2A	148/236 (63%)	117 (79%)	26 (18%)	5 (3%)	3	23
1	3A	148/236 (63%)	121 (82%)	24 (16%)	3 (2%)	6	33
2	0B	317/329 (96%)	245 (77%)	64 (20%)	8 (2%)	4	29
3	0C	93/156 (60%)	72 (77%)	17 (18%)	4 (4%)	2	20
3	1C	93/156 (60%)	70 (75%)	19 (20%)	4 (4%)	2	20
4	0D	198/225 (88%)	150 (76%)	40 (20%)	8 (4%)	2	21
4	1D	198/225 (88%)	149 (75%)	40 (20%)	9 (4%)	2	19
4	2D	198/225 (88%)	145 (73%)	44 (22%)	9 (4%)	2	19
5	0E	187/191 (98%)	174 (93%)	10 (5%)	3 (2%)	7	37
5	1E	187/191 (98%)	169 (90%)	14 (8%)	4 (2%)	5	32
5	2E	187/191 (98%)	168 (90%)	17 (9%)	2 (1%)	11	44
5	3E	187/191 (98%)	175 (94%)	10 (5%)	2 (1%)	11	44
6	0F	202/219 (92%)	160 (79%)	37 (18%)	5 (2%)	4	29
7	0G	162/183 (88%)	123 (76%)	33 (20%)	6 (4%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	1G	129/183 (70%)	100 (78%)	25 (19%)	4 (3%)	3 25
8	0H	118/447 (26%)	107 (91%)	9 (8%)	2 (2%)	7 36
8	1H	423/447 (95%)	402 (95%)	19 (4%)	2 (0%)	24 61
9	0N	278/492 (56%)	265 (95%)	13 (5%)	0	100 100
9	1N	457/492 (93%)	444 (97%)	12 (3%)	1 (0%)	43 76
9	2N	278/492 (56%)	270 (97%)	8 (3%)	0	100 100
10	0Q	184/195 (94%)	171 (93%)	13 (7%)	0	100 100
10	1Q	184/195 (94%)	172 (94%)	12 (6%)	0	100 100
10	2Q	184/195 (94%)	166 (90%)	18 (10%)	0	100 100
10	3Q	184/195 (94%)	172 (94%)	12 (6%)	0	100 100
10	4Q	184/195 (94%)	167 (91%)	17 (9%)	0	100 100
10	5Q	184/195 (94%)	169 (92%)	15 (8%)	0	100 100
10	6Q	184/195 (94%)	166 (90%)	18 (10%)	0	100 100
11	0S	284/319 (89%)	258 (91%)	26 (9%)	0	100 100
11	1S	284/319 (89%)	258 (91%)	25 (9%)	1 (0%)	30 65
11	2S	284/319 (89%)	262 (92%)	20 (7%)	2 (1%)	18 55
11	3S	284/319 (89%)	263 (93%)	21 (7%)	0	100 100
12	0T	255/298 (86%)	241 (94%)	14 (6%)	0	100 100
12	1T	283/298 (95%)	257 (91%)	26 (9%)	0	100 100
12	2T	283/298 (95%)	263 (93%)	20 (7%)	0	100 100
12	3T	283/298 (95%)	261 (92%)	22 (8%)	0	100 100
13	0U	605/656 (92%)	550 (91%)	55 (9%)	0	100 100
13	1U	605/656 (92%)	550 (91%)	55 (9%)	0	100 100
13	2U	605/656 (92%)	553 (91%)	52 (9%)	0	100 100
13	3U	605/656 (92%)	551 (91%)	54 (9%)	0	100 100
14	0V	203/269 (76%)	176 (87%)	24 (12%)	3 (2%)	8 39
14	1V	259/269 (96%)	221 (85%)	30 (12%)	8 (3%)	3 25
14	2V	259/269 (96%)	215 (83%)	38 (15%)	6 (2%)	5 31
14	3V	259/269 (96%)	223 (86%)	30 (12%)	6 (2%)	5 31
15	0X	108/142 (76%)	104 (96%)	3 (3%)	1 (1%)	14 49
15	1X	139/142 (98%)	132 (95%)	6 (4%)	1 (1%)	18 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	2X	139/142 (98%)	133 (96%)	5 (4%)	1 (1%)	18 55
15	3X	139/142 (98%)	132 (95%)	6 (4%)	1 (1%)	18 55
15	4X	139/142 (98%)	131 (94%)	8 (6%)	0	100 100
16	1B	496/498 (100%)	469 (95%)	24 (5%)	3 (1%)	21 58
16	2B	293/498 (59%)	271 (92%)	21 (7%)	1 (0%)	36 70
16	3B	291/498 (58%)	267 (92%)	24 (8%)	0	100 100
17	1F	132/173 (76%)	114 (86%)	14 (11%)	4 (3%)	3 25
18	1I	182/263 (69%)	150 (82%)	30 (16%)	2 (1%)	11 44
19	1J	364/422 (86%)	307 (84%)	49 (14%)	8 (2%)	5 31
20	1K	275/489 (56%)	273 (99%)	1 (0%)	1 (0%)	30 65
20	2K	284/489 (58%)	282 (99%)	2 (1%)	0	100 100
21	1L	808/940 (86%)	708 (88%)	92 (11%)	8 (1%)	12 46
21	2L	604/940 (64%)	533 (88%)	65 (11%)	6 (1%)	12 46
21	3L	198/940 (21%)	170 (86%)	24 (12%)	4 (2%)	6 33
22	1M	367/372 (99%)	343 (94%)	22 (6%)	2 (0%)	24 61
22	2M	367/372 (99%)	351 (96%)	15 (4%)	1 (0%)	36 70
23	1O	235/494 (48%)	230 (98%)	5 (2%)	0	100 100
23	2O	366/494 (74%)	363 (99%)	2 (0%)	1 (0%)	36 70
23	3O	275/494 (56%)	273 (99%)	2 (1%)	0	100 100
24	1P	353/507 (70%)	348 (99%)	4 (1%)	1 (0%)	36 70
24	2P	188/507 (37%)	187 (100%)	1 (0%)	0	100 100
25	1R	502/516 (97%)	469 (93%)	32 (6%)	1 (0%)	43 76
25	2R	502/516 (97%)	475 (95%)	26 (5%)	1 (0%)	43 76
25	3R	502/516 (97%)	472 (94%)	29 (6%)	1 (0%)	43 76
26	1W	222/280 (79%)	218 (98%)	4 (2%)	0	100 100
26	2W	114/280 (41%)	106 (93%)	8 (7%)	0	100 100
27	2C	298/300 (99%)	279 (94%)	17 (6%)	2 (1%)	18 55
27	3C	298/300 (99%)	278 (93%)	17 (6%)	3 (1%)	12 46
27	4C	298/300 (99%)	280 (94%)	16 (5%)	2 (1%)	18 55
28	2F	83/96 (86%)	74 (89%)	9 (11%)	0	100 100
29	2G	97/99 (98%)	92 (95%)	5 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
30	2H	59/229 (26%)	51 (86%)	7 (12%)	1 (2%)	7 36
30	3H	59/229 (26%)	52 (88%)	6 (10%)	1 (2%)	7 36
30	4H	59/229 (26%)	51 (86%)	7 (12%)	1 (2%)	7 36
31	2I	136/293 (46%)	113 (83%)	19 (14%)	4 (3%)	3 26
31	3I	83/293 (28%)	67 (81%)	14 (17%)	2 (2%)	4 30
32	3D	235/237 (99%)	224 (95%)	11 (5%)	0	100 100
33	4F	194/276 (70%)	163 (84%)	28 (14%)	3 (2%)	8 39
34	4R	607/613 (99%)	578 (95%)	29 (5%)	0	100 100
34	5R	607/613 (99%)	575 (95%)	32 (5%)	0	100 100
34	6R	607/613 (99%)	576 (95%)	31 (5%)	0	100 100
34	7R	607/613 (99%)	581 (96%)	26 (4%)	0	100 100
35	4S	186/249 (75%)	181 (97%)	5 (3%)	0	100 100
35	5S	186/249 (75%)	178 (96%)	8 (4%)	0	100 100
36	5A	155/175 (89%)	126 (81%)	29 (19%)	0	100 100
36	5B	155/175 (89%)	121 (78%)	33 (21%)	1 (1%)	21 58
36	5C	155/175 (89%)	126 (81%)	28 (18%)	1 (1%)	21 58
36	5D	112/175 (64%)	92 (82%)	20 (18%)	0	100 100
37	5E	186/247 (75%)	153 (82%)	29 (16%)	4 (2%)	5 31
37	5F	208/247 (84%)	169 (81%)	33 (16%)	6 (3%)	3 26
37	5G	208/247 (84%)	170 (82%)	34 (16%)	4 (2%)	6 34
37	5H	144/247 (58%)	114 (79%)	28 (19%)	2 (1%)	9 39
39	6F	130/145 (90%)	111 (85%)	16 (12%)	3 (2%)	5 31
40	6G	210/364 (58%)	179 (85%)	29 (14%)	2 (1%)	12 46
41	6H	151/518 (29%)	120 (80%)	27 (18%)	4 (3%)	4 28
44	8R	178/361 (49%)	173 (97%)	4 (2%)	1 (1%)	21 58
45	AA	437/449 (97%)	427 (98%)	10 (2%)	0	100 100
45	AC	437/449 (97%)	425 (97%)	12 (3%)	0	100 100
45	AE	437/449 (97%)	424 (97%)	13 (3%)	0	100 100
45	AG	437/449 (97%)	421 (96%)	16 (4%)	0	100 100
45	AI	437/449 (97%)	422 (97%)	15 (3%)	0	100 100
45	AK	437/449 (97%)	425 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	AM	437/449 (97%)	419 (96%)	18 (4%)	0	100	100
45	BA	428/449 (95%)	416 (97%)	12 (3%)	0	100	100
45	BC	428/449 (95%)	414 (97%)	14 (3%)	0	100	100
45	BE	428/449 (95%)	415 (97%)	13 (3%)	0	100	100
45	BG	428/449 (95%)	418 (98%)	10 (2%)	0	100	100
45	BI	428/449 (95%)	413 (96%)	15 (4%)	0	100	100
45	BK	428/449 (95%)	412 (96%)	16 (4%)	0	100	100
45	BM	428/449 (95%)	413 (96%)	15 (4%)	0	100	100
45	CA	437/449 (97%)	422 (97%)	15 (3%)	0	100	100
45	CC	437/449 (97%)	427 (98%)	10 (2%)	0	100	100
45	CE	437/449 (97%)	427 (98%)	10 (2%)	0	100	100
45	CG	437/449 (97%)	421 (96%)	16 (4%)	0	100	100
45	CI	437/449 (97%)	426 (98%)	11 (2%)	0	100	100
45	CK	437/449 (97%)	419 (96%)	18 (4%)	0	100	100
45	CM	437/449 (97%)	423 (97%)	14 (3%)	0	100	100
45	DA	429/449 (96%)	417 (97%)	12 (3%)	0	100	100
45	DC	432/449 (96%)	419 (97%)	12 (3%)	1 (0%)	43	76
45	DE	429/449 (96%)	411 (96%)	18 (4%)	0	100	100
45	DG	432/449 (96%)	419 (97%)	12 (3%)	1 (0%)	43	76
45	DI	429/449 (96%)	414 (96%)	15 (4%)	0	100	100
45	DK	432/449 (96%)	423 (98%)	8 (2%)	1 (0%)	43	76
45	DM	429/449 (96%)	417 (97%)	12 (3%)	0	100	100
45	EA	437/449 (97%)	423 (97%)	14 (3%)	0	100	100
45	EC	437/449 (97%)	418 (96%)	19 (4%)	0	100	100
45	EE	437/449 (97%)	424 (97%)	12 (3%)	1 (0%)	43	76
45	EG	437/449 (97%)	429 (98%)	8 (2%)	0	100	100
45	EI	437/449 (97%)	421 (96%)	15 (3%)	1 (0%)	43	76
45	EK	437/449 (97%)	421 (96%)	16 (4%)	0	100	100
45	EM	437/449 (97%)	421 (96%)	15 (3%)	1 (0%)	43	76
45	FA	425/449 (95%)	415 (98%)	10 (2%)	0	100	100
45	FC	428/449 (95%)	414 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	FE	430/449 (96%)	416 (97%)	14 (3%)	0	100	100
45	FG	437/449 (97%)	423 (97%)	14 (3%)	0	100	100
45	FI	429/449 (96%)	418 (97%)	11 (3%)	0	100	100
45	FK	428/449 (95%)	417 (97%)	11 (3%)	0	100	100
45	FM	425/449 (95%)	413 (97%)	12 (3%)	0	100	100
45	GA	425/449 (95%)	413 (97%)	12 (3%)	0	100	100
45	GC	427/449 (95%)	416 (97%)	11 (3%)	0	100	100
45	GE	427/449 (95%)	410 (96%)	17 (4%)	0	100	100
45	GG	427/449 (95%)	410 (96%)	17 (4%)	0	100	100
45	GI	427/449 (95%)	412 (96%)	15 (4%)	0	100	100
45	GK	437/449 (97%)	421 (96%)	16 (4%)	0	100	100
45	GM	425/449 (95%)	416 (98%)	9 (2%)	0	100	100
45	HA	427/449 (95%)	411 (96%)	16 (4%)	0	100	100
45	HC	427/449 (95%)	414 (97%)	13 (3%)	0	100	100
45	HE	427/449 (95%)	417 (98%)	10 (2%)	0	100	100
45	HG	427/449 (95%)	414 (97%)	13 (3%)	0	100	100
45	HI	427/449 (95%)	414 (97%)	13 (3%)	0	100	100
45	HK	427/449 (95%)	417 (98%)	10 (2%)	0	100	100
45	HM	427/449 (95%)	418 (98%)	9 (2%)	0	100	100
45	IA	428/449 (95%)	409 (96%)	19 (4%)	0	100	100
45	IC	437/449 (97%)	422 (97%)	15 (3%)	0	100	100
45	IE	428/449 (95%)	409 (96%)	19 (4%)	0	100	100
45	IG	437/449 (97%)	422 (97%)	15 (3%)	0	100	100
45	II	437/449 (97%)	417 (95%)	20 (5%)	0	100	100
45	IK	428/449 (95%)	414 (97%)	14 (3%)	0	100	100
45	IM	428/449 (95%)	420 (98%)	8 (2%)	0	100	100
45	JA	428/449 (95%)	414 (97%)	14 (3%)	0	100	100
45	JC	430/449 (96%)	417 (97%)	13 (3%)	0	100	100
45	JE	437/449 (97%)	420 (96%)	17 (4%)	0	100	100
45	JG	437/449 (97%)	420 (96%)	16 (4%)	1 (0%)	43	76
45	JI	437/449 (97%)	411 (94%)	24 (6%)	2 (0%)	24	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	JK	437/449 (97%)	422 (97%)	15 (3%)	0	100	100
45	JM	428/449 (95%)	418 (98%)	10 (2%)	0	100	100
45	KA	430/449 (96%)	416 (97%)	13 (3%)	1 (0%)	43	76
45	KC	429/449 (96%)	416 (97%)	13 (3%)	0	100	100
45	KE	431/449 (96%)	412 (96%)	19 (4%)	0	100	100
45	KG	437/449 (97%)	417 (95%)	19 (4%)	1 (0%)	43	76
45	KI	437/449 (97%)	422 (97%)	15 (3%)	0	100	100
45	KK	437/449 (97%)	413 (94%)	24 (6%)	0	100	100
45	KM	430/449 (96%)	418 (97%)	11 (3%)	1 (0%)	43	76
45	LA	437/449 (97%)	421 (96%)	15 (3%)	1 (0%)	43	76
45	LC	437/449 (97%)	419 (96%)	18 (4%)	0	100	100
45	LE	434/449 (97%)	416 (96%)	18 (4%)	0	100	100
45	LG	437/449 (97%)	421 (96%)	16 (4%)	0	100	100
45	LI	430/449 (96%)	411 (96%)	19 (4%)	0	100	100
45	LK	437/449 (97%)	419 (96%)	18 (4%)	0	100	100
45	LM	437/449 (97%)	422 (97%)	14 (3%)	1 (0%)	43	76
45	MA	432/449 (96%)	413 (96%)	19 (4%)	0	100	100
45	MC	429/449 (96%)	412 (96%)	17 (4%)	0	100	100
45	ME	429/449 (96%)	414 (96%)	14 (3%)	1 (0%)	43	76
45	MG	433/449 (96%)	420 (97%)	13 (3%)	0	100	100
45	MI	437/449 (97%)	422 (97%)	15 (3%)	0	100	100
45	MK	432/449 (96%)	417 (96%)	15 (4%)	0	100	100
45	MM	432/449 (96%)	418 (97%)	14 (3%)	0	100	100
45	NA	437/449 (97%)	422 (97%)	14 (3%)	1 (0%)	43	76
45	NC	428/449 (95%)	412 (96%)	16 (4%)	0	100	100
45	NE	437/449 (97%)	418 (96%)	18 (4%)	1 (0%)	43	76
45	NG	428/449 (95%)	410 (96%)	18 (4%)	0	100	100
45	NI	437/449 (97%)	422 (97%)	14 (3%)	1 (0%)	43	76
45	NK	428/449 (95%)	411 (96%)	17 (4%)	0	100	100
45	NM	437/449 (97%)	418 (96%)	18 (4%)	1 (0%)	43	76
45	OA	429/449 (96%)	413 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	OC	429/449 (96%)	418 (97%)	11 (3%)	0	100	100
45	OE	429/449 (96%)	419 (98%)	10 (2%)	0	100	100
45	OG	429/449 (96%)	420 (98%)	9 (2%)	0	100	100
45	OI	429/449 (96%)	418 (97%)	11 (3%)	0	100	100
45	OK	429/449 (96%)	412 (96%)	17 (4%)	0	100	100
45	OM	429/449 (96%)	417 (97%)	12 (3%)	0	100	100
45	PA	425/449 (95%)	411 (97%)	14 (3%)	0	100	100
45	PC	425/449 (95%)	411 (97%)	14 (3%)	0	100	100
45	PE	425/449 (95%)	407 (96%)	18 (4%)	0	100	100
45	PG	425/449 (95%)	410 (96%)	15 (4%)	0	100	100
45	PI	425/449 (95%)	413 (97%)	12 (3%)	0	100	100
45	PK	425/449 (95%)	406 (96%)	19 (4%)	0	100	100
45	PM	425/449 (95%)	411 (97%)	14 (3%)	0	100	100
45	QA	427/449 (95%)	419 (98%)	8 (2%)	0	100	100
45	QC	427/449 (95%)	418 (98%)	9 (2%)	0	100	100
45	QE	427/449 (95%)	415 (97%)	12 (3%)	0	100	100
45	QG	427/449 (95%)	417 (98%)	10 (2%)	0	100	100
45	QI	427/449 (95%)	408 (96%)	19 (4%)	0	100	100
45	QK	427/449 (95%)	415 (97%)	12 (3%)	0	100	100
45	QM	427/449 (95%)	414 (97%)	13 (3%)	0	100	100
45	RA	427/449 (95%)	420 (98%)	7 (2%)	0	100	100
45	RC	427/449 (95%)	419 (98%)	8 (2%)	0	100	100
45	RE	427/449 (95%)	414 (97%)	13 (3%)	0	100	100
45	RG	427/449 (95%)	416 (97%)	11 (3%)	0	100	100
45	RI	427/449 (95%)	414 (97%)	13 (3%)	0	100	100
45	RK	427/449 (95%)	411 (96%)	16 (4%)	0	100	100
45	RM	427/449 (95%)	418 (98%)	9 (2%)	0	100	100
45	SA	426/449 (95%)	419 (98%)	7 (2%)	0	100	100
45	SC	426/449 (95%)	410 (96%)	16 (4%)	0	100	100
45	SE	426/449 (95%)	412 (97%)	14 (3%)	0	100	100
45	SG	426/449 (95%)	411 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	SI	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
45	SK	426/449 (95%)	412 (97%)	14 (3%)	0	100	100
45	SM	426/449 (95%)	412 (97%)	14 (3%)	0	100	100
45	TA	426/449 (95%)	414 (97%)	12 (3%)	0	100	100
45	TC	426/449 (95%)	411 (96%)	15 (4%)	0	100	100
45	TE	426/449 (95%)	412 (97%)	14 (3%)	0	100	100
45	TG	426/449 (95%)	414 (97%)	12 (3%)	0	100	100
45	TI	426/449 (95%)	420 (99%)	6 (1%)	0	100	100
45	TK	426/449 (95%)	412 (97%)	14 (3%)	0	100	100
45	TM	426/449 (95%)	412 (97%)	14 (3%)	0	100	100
45	UA	427/449 (95%)	418 (98%)	9 (2%)	0	100	100
45	UC	427/449 (95%)	415 (97%)	12 (3%)	0	100	100
45	UE	427/449 (95%)	412 (96%)	15 (4%)	0	100	100
45	UG	427/449 (95%)	416 (97%)	11 (3%)	0	100	100
45	UI	427/449 (95%)	413 (97%)	14 (3%)	0	100	100
45	UK	427/449 (95%)	412 (96%)	15 (4%)	0	100	100
45	UM	427/449 (95%)	416 (97%)	11 (3%)	0	100	100
45	VA	429/449 (96%)	415 (97%)	14 (3%)	0	100	100
45	VC	437/449 (97%)	427 (98%)	10 (2%)	0	100	100
45	VE	429/449 (96%)	416 (97%)	13 (3%)	0	100	100
45	VG	437/449 (97%)	417 (95%)	20 (5%)	0	100	100
45	VI	429/449 (96%)	421 (98%)	8 (2%)	0	100	100
45	VK	437/449 (97%)	422 (97%)	15 (3%)	0	100	100
45	VM	429/449 (96%)	420 (98%)	9 (2%)	0	100	100
45	WA	427/449 (95%)	415 (97%)	12 (3%)	0	100	100
45	WC	437/449 (97%)	421 (96%)	15 (3%)	1 (0%)	43	76
45	WE	427/449 (95%)	414 (97%)	13 (3%)	0	100	100
45	WG	437/449 (97%)	418 (96%)	18 (4%)	1 (0%)	43	76
45	WI	427/449 (95%)	417 (98%)	10 (2%)	0	100	100
45	WK	437/449 (97%)	419 (96%)	17 (4%)	1 (0%)	43	76
45	WM	427/449 (95%)	415 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	AB	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	AD	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	AF	428/443 (97%)	424 (99%)	4 (1%)	0	100	100
46	AH	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	AJ	428/443 (97%)	422 (99%)	6 (1%)	0	100	100
46	AL	428/443 (97%)	422 (99%)	6 (1%)	0	100	100
46	AN	428/443 (97%)	425 (99%)	3 (1%)	0	100	100
46	BB	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	BD	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	BF	428/443 (97%)	417 (97%)	11 (3%)	0	100	100
46	BH	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	BJ	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	BL	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	BN	428/443 (97%)	415 (97%)	13 (3%)	0	100	100
46	CB	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	CD	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	CF	428/443 (97%)	410 (96%)	18 (4%)	0	100	100
46	CH	428/443 (97%)	412 (96%)	16 (4%)	0	100	100
46	CJ	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	CL	428/443 (97%)	415 (97%)	13 (3%)	0	100	100
46	CN	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
46	DB	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	DD	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	DF	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	DH	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	DJ	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	DL	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	DN	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	EB	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	ED	428/443 (97%)	413 (96%)	15 (4%)	0	100	100
46	EF	428/443 (97%)	419 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	EH	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	EJ	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	EL	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	EN	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
46	FB	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	FD	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	FF	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	FH	428/443 (97%)	411 (96%)	17 (4%)	0	100	100
46	FJ	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	FL	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	FN	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	GB	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	GD	428/443 (97%)	415 (97%)	13 (3%)	0	100	100
46	GF	428/443 (97%)	412 (96%)	16 (4%)	0	100	100
46	GH	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	GJ	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	GL	428/443 (97%)	417 (97%)	11 (3%)	0	100	100
46	GN	428/443 (97%)	422 (99%)	6 (1%)	0	100	100
46	HB	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	HD	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	HF	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	HH	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	HJ	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	HL	428/443 (97%)	417 (97%)	11 (3%)	0	100	100
46	HN	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	IB	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	ID	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	IF	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	IH	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	IJ	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	IL	428/443 (97%)	421 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	IN	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	JB	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	JD	428/443 (97%)	413 (96%)	15 (4%)	0	100	100
46	JF	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	JH	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	JJ	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	JL	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	JN	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	KB	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	KD	428/443 (97%)	417 (97%)	11 (3%)	0	100	100
46	KF	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	KH	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	KJ	428/443 (97%)	410 (96%)	18 (4%)	0	100	100
46	KL	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	KN	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	LB	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	LD	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	LF	428/443 (97%)	415 (97%)	13 (3%)	0	100	100
46	LH	428/443 (97%)	415 (97%)	13 (3%)	0	100	100
46	LJ	428/443 (97%)	413 (96%)	15 (4%)	0	100	100
46	LL	428/443 (97%)	413 (96%)	15 (4%)	0	100	100
46	LN	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	MB	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	MD	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	MF	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	MH	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	MJ	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	ML	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	MN	428/443 (97%)	417 (97%)	11 (3%)	0	100	100
46	NB	419/443 (95%)	408 (97%)	11 (3%)	0	100	100
46	ND	428/443 (97%)	414 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	NF	419/443 (95%)	407 (97%)	12 (3%)	0	100	100
46	NH	428/443 (97%)	415 (97%)	13 (3%)	0	100	100
46	NJ	419/443 (95%)	405 (97%)	14 (3%)	0	100	100
46	NL	428/443 (97%)	412 (96%)	16 (4%)	0	100	100
46	NN	419/443 (95%)	407 (97%)	12 (3%)	0	100	100
46	OB	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	OD	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	OF	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	OH	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	OJ	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	OL	428/443 (97%)	409 (96%)	19 (4%)	0	100	100
46	ON	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	PB	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	PD	428/443 (97%)	415 (97%)	13 (3%)	0	100	100
46	PF	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	PH	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	PJ	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	PL	428/443 (97%)	417 (97%)	11 (3%)	0	100	100
46	PN	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	QB	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	QD	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	QF	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	QH	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	QJ	428/443 (97%)	415 (97%)	13 (3%)	0	100	100
46	QL	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	QN	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	RB	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	RD	428/443 (97%)	415 (97%)	13 (3%)	0	100	100
46	RF	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	RH	428/443 (97%)	414 (97%)	14 (3%)	0	100	100
46	RJ	428/443 (97%)	416 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	RL	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	RN	428/443 (97%)	424 (99%)	4 (1%)	0	100	100
46	SB	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	SD	428/443 (97%)	415 (97%)	13 (3%)	0	100	100
46	SF	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	SH	428/443 (97%)	417 (97%)	11 (3%)	0	100	100
46	SJ	428/443 (97%)	417 (97%)	11 (3%)	0	100	100
46	SL	428/443 (97%)	415 (97%)	13 (3%)	0	100	100
46	SN	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	TB	428/443 (97%)	417 (97%)	11 (3%)	0	100	100
46	TD	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	TF	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	TH	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	TJ	428/443 (97%)	422 (99%)	6 (1%)	0	100	100
46	TL	428/443 (97%)	417 (97%)	11 (3%)	0	100	100
46	TN	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	UB	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	UD	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	UF	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	UH	428/443 (97%)	417 (97%)	11 (3%)	0	100	100
46	UJ	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	UL	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	UN	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	VB	428/443 (97%)	416 (97%)	12 (3%)	0	100	100
46	VD	428/443 (97%)	419 (98%)	9 (2%)	0	100	100
46	VF	428/443 (97%)	420 (98%)	8 (2%)	0	100	100
46	VH	428/443 (97%)	417 (97%)	11 (3%)	0	100	100
46	VJ	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	VL	428/443 (97%)	418 (98%)	10 (2%)	0	100	100
46	VN	428/443 (97%)	421 (98%)	7 (2%)	0	100	100
46	WB	428/443 (97%)	425 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
46	WD	428/443 (97%)	420 (98%)	8 (2%)	0	100 100
46	WF	428/443 (97%)	423 (99%)	5 (1%)	0	100 100
46	WH	428/443 (97%)	420 (98%)	8 (2%)	0	100 100
46	WJ	428/443 (97%)	421 (98%)	7 (2%)	0	100 100
46	WL	428/443 (97%)	419 (98%)	9 (2%)	0	100 100
46	WN	428/443 (97%)	417 (97%)	11 (3%)	0	100 100
All	All	164878/178239 (92%)	158526 (96%)	6118 (4%)	234 (0%)	49 81

5 of 234 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0A	20	PRO
1	0A	90	GLN
2	0B	67	THR
2	0B	208	VAL
3	0C	45	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	0A	133/213 (62%)	132 (99%)	1 (1%)	73 77
1	1A	133/213 (62%)	133 (100%)	0	100 100
1	2A	133/213 (62%)	133 (100%)	0	100 100
1	3A	133/213 (62%)	133 (100%)	0	100 100
2	0B	291/301 (97%)	290 (100%)	1 (0%)	86 85
3	0C	81/137 (59%)	81 (100%)	0	100 100
3	1C	81/137 (59%)	81 (100%)	0	100 100
4	0D	175/197 (89%)	175 (100%)	0	100 100
4	1D	175/197 (89%)	175 (100%)	0	100 100
4	2D	175/197 (89%)	175 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	0E	172/175 (98%)	172 (100%)	0	100	100
5	1E	172/175 (98%)	172 (100%)	0	100	100
5	2E	172/175 (98%)	172 (100%)	0	100	100
5	3E	172/175 (98%)	172 (100%)	0	100	100
6	0F	182/194 (94%)	182 (100%)	0	100	100
7	0G	153/167 (92%)	153 (100%)	0	100	100
7	1G	125/167 (75%)	125 (100%)	0	100	100
8	0H	111/413 (27%)	111 (100%)	0	100	100
8	1H	392/413 (95%)	391 (100%)	1 (0%)	86	85
9	0N	256/451 (57%)	256 (100%)	0	100	100
9	1N	423/451 (94%)	423 (100%)	0	100	100
9	2N	256/451 (57%)	256 (100%)	0	100	100
10	0Q	174/182 (96%)	174 (100%)	0	100	100
10	1Q	174/182 (96%)	174 (100%)	0	100	100
10	2Q	174/182 (96%)	174 (100%)	0	100	100
10	3Q	174/182 (96%)	173 (99%)	1 (1%)	78	80
10	4Q	174/182 (96%)	174 (100%)	0	100	100
10	5Q	174/182 (96%)	174 (100%)	0	100	100
10	6Q	174/182 (96%)	174 (100%)	0	100	100
11	0S	257/286 (90%)	257 (100%)	0	100	100
11	1S	257/286 (90%)	256 (100%)	1 (0%)	84	83
11	2S	257/286 (90%)	256 (100%)	1 (0%)	84	83
11	3S	257/286 (90%)	257 (100%)	0	100	100
12	0T	229/264 (87%)	229 (100%)	0	100	100
12	1T	251/264 (95%)	251 (100%)	0	100	100
12	2T	251/264 (95%)	251 (100%)	0	100	100
12	3T	251/264 (95%)	251 (100%)	0	100	100
13	0U	528/571 (92%)	527 (100%)	1 (0%)	87	87
13	1U	528/571 (92%)	528 (100%)	0	100	100
13	2U	528/571 (92%)	528 (100%)	0	100	100
13	3U	528/571 (92%)	527 (100%)	1 (0%)	87	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	0V	196/249 (79%)	196 (100%)	0	100 100
14	1V	244/249 (98%)	244 (100%)	0	100 100
14	2V	244/249 (98%)	243 (100%)	1 (0%)	84 83
14	3V	244/249 (98%)	244 (100%)	0	100 100
15	0X	98/129 (76%)	98 (100%)	0	100 100
15	1X	128/129 (99%)	128 (100%)	0	100 100
15	2X	128/129 (99%)	128 (100%)	0	100 100
15	3X	128/129 (99%)	128 (100%)	0	100 100
15	4X	128/129 (99%)	128 (100%)	0	100 100
16	1B	441/441 (100%)	441 (100%)	0	100 100
16	2B	264/441 (60%)	264 (100%)	0	100 100
16	3B	263/441 (60%)	263 (100%)	0	100 100
17	1F	121/157 (77%)	120 (99%)	1 (1%)	73 77
18	1I	172/239 (72%)	172 (100%)	0	100 100
19	1J	328/370 (89%)	328 (100%)	0	100 100
20	1K	263/463 (57%)	263 (100%)	0	100 100
20	2K	275/463 (59%)	275 (100%)	0	100 100
21	1L	771/878 (88%)	771 (100%)	0	100 100
21	2L	576/878 (66%)	575 (100%)	1 (0%)	87 87
21	3L	191/878 (22%)	191 (100%)	0	100 100
22	1M	323/325 (99%)	323 (100%)	0	100 100
22	2M	323/325 (99%)	323 (100%)	0	100 100
23	1O	228/458 (50%)	228 (100%)	0	100 100
23	2O	346/458 (76%)	346 (100%)	0	100 100
23	3O	258/458 (56%)	258 (100%)	0	100 100
24	1P	328/471 (70%)	328 (100%)	0	100 100
24	2P	173/471 (37%)	173 (100%)	0	100 100
25	1R	466/475 (98%)	466 (100%)	0	100 100
25	2R	466/475 (98%)	466 (100%)	0	100 100
25	3R	466/475 (98%)	466 (100%)	0	100 100
26	1W	211/265 (80%)	211 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	2W	109/265 (41%)	109 (100%)	0	100	100
27	2C	271/271 (100%)	271 (100%)	0	100	100
27	3C	271/271 (100%)	271 (100%)	0	100	100
27	4C	271/271 (100%)	271 (100%)	0	100	100
28	2F	81/90 (90%)	81 (100%)	0	100	100
29	2G	91/91 (100%)	91 (100%)	0	100	100
30	2H	59/212 (28%)	59 (100%)	0	100	100
30	3H	59/212 (28%)	59 (100%)	0	100	100
30	4H	59/212 (28%)	59 (100%)	0	100	100
31	2I	124/259 (48%)	124 (100%)	0	100	100
31	3I	80/259 (31%)	80 (100%)	0	100	100
32	3D	195/195 (100%)	195 (100%)	0	100	100
33	4F	179/245 (73%)	179 (100%)	0	100	100
34	4R	561/568 (99%)	561 (100%)	0	100	100
34	5R	561/568 (99%)	561 (100%)	0	100	100
34	6R	561/568 (99%)	561 (100%)	0	100	100
34	7R	561/568 (99%)	561 (100%)	0	100	100
35	4S	169/222 (76%)	169 (100%)	0	100	100
35	5S	169/222 (76%)	169 (100%)	0	100	100
36	5A	140/159 (88%)	140 (100%)	0	100	100
36	5B	140/159 (88%)	140 (100%)	0	100	100
36	5C	140/159 (88%)	140 (100%)	0	100	100
36	5D	101/159 (64%)	101 (100%)	0	100	100
37	5E	173/227 (76%)	173 (100%)	0	100	100
37	5F	194/227 (86%)	194 (100%)	0	100	100
37	5G	194/227 (86%)	194 (100%)	0	100	100
37	5H	132/227 (58%)	132 (100%)	0	100	100
39	6F	128/141 (91%)	128 (100%)	0	100	100
40	6G	194/329 (59%)	194 (100%)	0	100	100
41	6H	150/474 (32%)	148 (99%)	2 (1%)	61	72
44	8R	31/31 (100%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	AA	370/376 (98%)	370 (100%)	0	100 100
45	AC	370/376 (98%)	370 (100%)	0	100 100
45	AE	370/376 (98%)	370 (100%)	0	100 100
45	AG	370/376 (98%)	370 (100%)	0	100 100
45	AI	370/376 (98%)	370 (100%)	0	100 100
45	AK	370/376 (98%)	370 (100%)	0	100 100
45	AM	370/376 (98%)	370 (100%)	0	100 100
45	BA	366/376 (97%)	366 (100%)	0	100 100
45	BC	366/376 (97%)	366 (100%)	0	100 100
45	BE	366/376 (97%)	366 (100%)	0	100 100
45	BG	366/376 (97%)	366 (100%)	0	100 100
45	BI	366/376 (97%)	366 (100%)	0	100 100
45	BK	366/376 (97%)	366 (100%)	0	100 100
45	BM	366/376 (97%)	366 (100%)	0	100 100
45	CA	370/376 (98%)	370 (100%)	0	100 100
45	CC	370/376 (98%)	370 (100%)	0	100 100
45	CE	370/376 (98%)	370 (100%)	0	100 100
45	CG	370/376 (98%)	369 (100%)	1 (0%)	86 85
45	CI	370/376 (98%)	370 (100%)	0	100 100
45	CK	370/376 (98%)	370 (100%)	0	100 100
45	CM	370/376 (98%)	370 (100%)	0	100 100
45	DA	367/376 (98%)	367 (100%)	0	100 100
45	DC	368/376 (98%)	367 (100%)	1 (0%)	86 85
45	DE	367/376 (98%)	367 (100%)	0	100 100
45	DG	368/376 (98%)	367 (100%)	1 (0%)	86 85
45	DI	367/376 (98%)	366 (100%)	1 (0%)	86 85
45	DK	368/376 (98%)	368 (100%)	0	100 100
45	DM	367/376 (98%)	367 (100%)	0	100 100
45	EA	370/376 (98%)	370 (100%)	0	100 100
45	EC	370/376 (98%)	370 (100%)	0	100 100
45	EE	370/376 (98%)	370 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	EG	370/376 (98%)	370 (100%)	0	100	100
45	EI	370/376 (98%)	370 (100%)	0	100	100
45	EK	370/376 (98%)	370 (100%)	0	100	100
45	EM	370/376 (98%)	370 (100%)	0	100	100
45	FA	363/376 (96%)	363 (100%)	0	100	100
45	FC	366/376 (97%)	366 (100%)	0	100	100
45	FE	367/376 (98%)	367 (100%)	0	100	100
45	FG	370/376 (98%)	370 (100%)	0	100	100
45	FI	367/376 (98%)	367 (100%)	0	100	100
45	FK	366/376 (97%)	366 (100%)	0	100	100
45	FM	363/376 (96%)	363 (100%)	0	100	100
45	GA	363/376 (96%)	363 (100%)	0	100	100
45	GC	365/376 (97%)	365 (100%)	0	100	100
45	GE	365/376 (97%)	365 (100%)	0	100	100
45	GG	365/376 (97%)	365 (100%)	0	100	100
45	GI	365/376 (97%)	365 (100%)	0	100	100
45	GK	370/376 (98%)	370 (100%)	0	100	100
45	GM	363/376 (96%)	363 (100%)	0	100	100
45	HA	365/376 (97%)	365 (100%)	0	100	100
45	HC	365/376 (97%)	365 (100%)	0	100	100
45	HE	365/376 (97%)	365 (100%)	0	100	100
45	HG	365/376 (97%)	365 (100%)	0	100	100
45	HI	365/376 (97%)	365 (100%)	0	100	100
45	HK	365/376 (97%)	365 (100%)	0	100	100
45	HM	365/376 (97%)	365 (100%)	0	100	100
45	IA	366/376 (97%)	366 (100%)	0	100	100
45	IC	370/376 (98%)	370 (100%)	0	100	100
45	IE	366/376 (97%)	365 (100%)	1 (0%)	86	85
45	IG	370/376 (98%)	370 (100%)	0	100	100
45	II	370/376 (98%)	370 (100%)	0	100	100
45	IK	366/376 (97%)	366 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	IM	366/376 (97%)	366 (100%)	0	100 100
45	JA	366/376 (97%)	366 (100%)	0	100 100
45	JC	367/376 (98%)	366 (100%)	1 (0%)	86 85
45	JE	370/376 (98%)	369 (100%)	1 (0%)	86 85
45	JG	370/376 (98%)	370 (100%)	0	100 100
45	JI	369/376 (98%)	369 (100%)	0	100 100
45	JK	370/376 (98%)	370 (100%)	0	100 100
45	JM	366/376 (97%)	366 (100%)	0	100 100
45	KA	367/376 (98%)	367 (100%)	0	100 100
45	KC	367/376 (98%)	367 (100%)	0	100 100
45	KE	368/376 (98%)	368 (100%)	0	100 100
45	KG	370/376 (98%)	370 (100%)	0	100 100
45	KI	370/376 (98%)	369 (100%)	1 (0%)	86 85
45	KK	370/376 (98%)	370 (100%)	0	100 100
45	KM	367/376 (98%)	367 (100%)	0	100 100
45	LA	370/376 (98%)	370 (100%)	0	100 100
45	LC	370/376 (98%)	370 (100%)	0	100 100
45	LE	369/376 (98%)	369 (100%)	0	100 100
45	LG	370/376 (98%)	370 (100%)	0	100 100
45	LI	368/376 (98%)	368 (100%)	0	100 100
45	LK	370/376 (98%)	370 (100%)	0	100 100
45	LM	370/376 (98%)	369 (100%)	1 (0%)	86 85
45	MA	369/376 (98%)	369 (100%)	0	100 100
45	MC	366/376 (97%)	366 (100%)	0	100 100
45	ME	367/376 (98%)	367 (100%)	0	100 100
45	MG	370/376 (98%)	370 (100%)	0	100 100
45	MI	370/376 (98%)	370 (100%)	0	100 100
45	MK	367/376 (98%)	367 (100%)	0	100 100
45	MM	369/376 (98%)	369 (100%)	0	100 100
45	NA	370/376 (98%)	368 (100%)	2 (0%)	81 82
45	NC	366/376 (97%)	366 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	NE	370/376 (98%)	370 (100%)	0	100	100
45	NG	366/376 (97%)	366 (100%)	0	100	100
45	NI	370/376 (98%)	370 (100%)	0	100	100
45	NK	366/376 (97%)	366 (100%)	0	100	100
45	NM	370/376 (98%)	370 (100%)	0	100	100
45	OA	366/376 (97%)	366 (100%)	0	100	100
45	OC	366/376 (97%)	366 (100%)	0	100	100
45	OE	366/376 (97%)	365 (100%)	1 (0%)	86	85
45	OG	366/376 (97%)	366 (100%)	0	100	100
45	OI	366/376 (97%)	366 (100%)	0	100	100
45	OK	366/376 (97%)	366 (100%)	0	100	100
45	OM	366/376 (97%)	366 (100%)	0	100	100
45	PA	363/376 (96%)	363 (100%)	0	100	100
45	PC	363/376 (96%)	363 (100%)	0	100	100
45	PE	363/376 (96%)	363 (100%)	0	100	100
45	PG	363/376 (96%)	362 (100%)	1 (0%)	86	85
45	PI	363/376 (96%)	363 (100%)	0	100	100
45	PK	363/376 (96%)	363 (100%)	0	100	100
45	PM	363/376 (96%)	363 (100%)	0	100	100
45	QA	365/376 (97%)	365 (100%)	0	100	100
45	QC	365/376 (97%)	365 (100%)	0	100	100
45	QE	365/376 (97%)	365 (100%)	0	100	100
45	QG	365/376 (97%)	365 (100%)	0	100	100
45	QI	365/376 (97%)	365 (100%)	0	100	100
45	QK	365/376 (97%)	365 (100%)	0	100	100
45	QM	365/376 (97%)	365 (100%)	0	100	100
45	RA	365/376 (97%)	365 (100%)	0	100	100
45	RC	365/376 (97%)	365 (100%)	0	100	100
45	RE	365/376 (97%)	365 (100%)	0	100	100
45	RG	365/376 (97%)	365 (100%)	0	100	100
45	RI	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	RK	365/376 (97%)	365 (100%)	0	100	100
45	RM	365/376 (97%)	365 (100%)	0	100	100
45	SA	364/376 (97%)	364 (100%)	0	100	100
45	SC	364/376 (97%)	364 (100%)	0	100	100
45	SE	364/376 (97%)	364 (100%)	0	100	100
45	SG	364/376 (97%)	364 (100%)	0	100	100
45	SI	364/376 (97%)	364 (100%)	0	100	100
45	SK	364/376 (97%)	364 (100%)	0	100	100
45	SM	364/376 (97%)	364 (100%)	0	100	100
45	TA	364/376 (97%)	364 (100%)	0	100	100
45	TC	364/376 (97%)	364 (100%)	0	100	100
45	TE	364/376 (97%)	364 (100%)	0	100	100
45	TG	364/376 (97%)	364 (100%)	0	100	100
45	TI	364/376 (97%)	364 (100%)	0	100	100
45	TK	364/376 (97%)	364 (100%)	0	100	100
45	TM	364/376 (97%)	364 (100%)	0	100	100
45	UA	365/376 (97%)	365 (100%)	0	100	100
45	UC	365/376 (97%)	365 (100%)	0	100	100
45	UE	365/376 (97%)	365 (100%)	0	100	100
45	UG	365/376 (97%)	365 (100%)	0	100	100
45	UI	365/376 (97%)	365 (100%)	0	100	100
45	UK	365/376 (97%)	365 (100%)	0	100	100
45	UM	365/376 (97%)	365 (100%)	0	100	100
45	VA	367/376 (98%)	367 (100%)	0	100	100
45	VC	370/376 (98%)	370 (100%)	0	100	100
45	VE	367/376 (98%)	367 (100%)	0	100	100
45	VG	370/376 (98%)	370 (100%)	0	100	100
45	VI	367/376 (98%)	367 (100%)	0	100	100
45	VK	370/376 (98%)	370 (100%)	0	100	100
45	VM	367/376 (98%)	367 (100%)	0	100	100
45	WA	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	WC	370/376 (98%)	370 (100%)	0	100 100
45	WE	365/376 (97%)	365 (100%)	0	100 100
45	WG	370/376 (98%)	370 (100%)	0	100 100
45	WI	365/376 (97%)	365 (100%)	0	100 100
45	WK	370/376 (98%)	370 (100%)	0	100 100
45	WM	365/376 (97%)	365 (100%)	0	100 100
46	AB	365/376 (97%)	365 (100%)	0	100 100
46	AD	365/376 (97%)	365 (100%)	0	100 100
46	AF	365/376 (97%)	365 (100%)	0	100 100
46	AH	365/376 (97%)	365 (100%)	0	100 100
46	AJ	365/376 (97%)	364 (100%)	1 (0%)	86 85
46	AL	365/376 (97%)	364 (100%)	1 (0%)	86 85
46	AN	365/376 (97%)	365 (100%)	0	100 100
46	BB	365/376 (97%)	365 (100%)	0	100 100
46	BD	365/376 (97%)	365 (100%)	0	100 100
46	BF	365/376 (97%)	365 (100%)	0	100 100
46	BH	365/376 (97%)	365 (100%)	0	100 100
46	BJ	365/376 (97%)	365 (100%)	0	100 100
46	BL	365/376 (97%)	364 (100%)	1 (0%)	86 85
46	BN	365/376 (97%)	365 (100%)	0	100 100
46	CB	365/376 (97%)	364 (100%)	1 (0%)	86 85
46	CD	365/376 (97%)	365 (100%)	0	100 100
46	CF	365/376 (97%)	365 (100%)	0	100 100
46	CH	365/376 (97%)	365 (100%)	0	100 100
46	CJ	365/376 (97%)	365 (100%)	0	100 100
46	CL	365/376 (97%)	365 (100%)	0	100 100
46	CN	365/376 (97%)	365 (100%)	0	100 100
46	DB	365/376 (97%)	365 (100%)	0	100 100
46	DD	365/376 (97%)	365 (100%)	0	100 100
46	DF	365/376 (97%)	365 (100%)	0	100 100
46	DH	365/376 (97%)	365 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	DJ	365/376 (97%)	365 (100%)	0	100	100
46	DL	365/376 (97%)	365 (100%)	0	100	100
46	DN	365/376 (97%)	365 (100%)	0	100	100
46	EB	365/376 (97%)	365 (100%)	0	100	100
46	ED	365/376 (97%)	365 (100%)	0	100	100
46	EF	365/376 (97%)	365 (100%)	0	100	100
46	EH	365/376 (97%)	365 (100%)	0	100	100
46	EJ	365/376 (97%)	365 (100%)	0	100	100
46	EL	365/376 (97%)	365 (100%)	0	100	100
46	EN	365/376 (97%)	365 (100%)	0	100	100
46	FB	365/376 (97%)	365 (100%)	0	100	100
46	FD	365/376 (97%)	365 (100%)	0	100	100
46	FF	365/376 (97%)	365 (100%)	0	100	100
46	FH	365/376 (97%)	365 (100%)	0	100	100
46	FJ	365/376 (97%)	365 (100%)	0	100	100
46	FL	365/376 (97%)	365 (100%)	0	100	100
46	FN	365/376 (97%)	365 (100%)	0	100	100
46	GB	365/376 (97%)	364 (100%)	1 (0%)	86	85
46	GD	365/376 (97%)	365 (100%)	0	100	100
46	GF	365/376 (97%)	365 (100%)	0	100	100
46	GH	365/376 (97%)	365 (100%)	0	100	100
46	GJ	365/376 (97%)	365 (100%)	0	100	100
46	GL	365/376 (97%)	364 (100%)	1 (0%)	86	85
46	GN	365/376 (97%)	365 (100%)	0	100	100
46	HB	365/376 (97%)	365 (100%)	0	100	100
46	HD	365/376 (97%)	365 (100%)	0	100	100
46	HF	365/376 (97%)	365 (100%)	0	100	100
46	HH	365/376 (97%)	365 (100%)	0	100	100
46	HJ	365/376 (97%)	365 (100%)	0	100	100
46	HL	365/376 (97%)	365 (100%)	0	100	100
46	HN	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	IB	365/376 (97%)	364 (100%)	1 (0%)	86 85
46	ID	365/376 (97%)	365 (100%)	0	100 100
46	IF	365/376 (97%)	365 (100%)	0	100 100
46	IH	365/376 (97%)	365 (100%)	0	100 100
46	IJ	365/376 (97%)	363 (100%)	2 (0%)	81 82
46	IL	365/376 (97%)	365 (100%)	0	100 100
46	IN	365/376 (97%)	365 (100%)	0	100 100
46	JB	365/376 (97%)	365 (100%)	0	100 100
46	JD	365/376 (97%)	365 (100%)	0	100 100
46	JF	365/376 (97%)	365 (100%)	0	100 100
46	JH	365/376 (97%)	365 (100%)	0	100 100
46	JJ	365/376 (97%)	364 (100%)	1 (0%)	86 85
46	JL	365/376 (97%)	365 (100%)	0	100 100
46	JN	365/376 (97%)	365 (100%)	0	100 100
46	KB	365/376 (97%)	365 (100%)	0	100 100
46	KD	365/376 (97%)	365 (100%)	0	100 100
46	KF	365/376 (97%)	365 (100%)	0	100 100
46	KH	365/376 (97%)	365 (100%)	0	100 100
46	KJ	365/376 (97%)	365 (100%)	0	100 100
46	KL	365/376 (97%)	365 (100%)	0	100 100
46	KN	365/376 (97%)	365 (100%)	0	100 100
46	LB	365/376 (97%)	365 (100%)	0	100 100
46	LD	365/376 (97%)	365 (100%)	0	100 100
46	LF	365/376 (97%)	365 (100%)	0	100 100
46	LH	365/376 (97%)	364 (100%)	1 (0%)	86 85
46	LJ	365/376 (97%)	365 (100%)	0	100 100
46	LL	365/376 (97%)	364 (100%)	1 (0%)	86 85
46	LN	365/376 (97%)	364 (100%)	1 (0%)	86 85
46	MB	365/376 (97%)	365 (100%)	0	100 100
46	MD	365/376 (97%)	365 (100%)	0	100 100
46	MF	365/376 (97%)	365 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	MH	365/376 (97%)	365 (100%)	0	100	100
46	MJ	365/376 (97%)	365 (100%)	0	100	100
46	ML	365/376 (97%)	365 (100%)	0	100	100
46	MN	365/376 (97%)	365 (100%)	0	100	100
46	NB	359/376 (96%)	359 (100%)	0	100	100
46	ND	365/376 (97%)	365 (100%)	0	100	100
46	NF	359/376 (96%)	359 (100%)	0	100	100
46	NH	365/376 (97%)	365 (100%)	0	100	100
46	NJ	359/376 (96%)	359 (100%)	0	100	100
46	NL	365/376 (97%)	365 (100%)	0	100	100
46	NN	359/376 (96%)	359 (100%)	0	100	100
46	OB	365/376 (97%)	365 (100%)	0	100	100
46	OD	365/376 (97%)	365 (100%)	0	100	100
46	OF	365/376 (97%)	365 (100%)	0	100	100
46	OH	365/376 (97%)	365 (100%)	0	100	100
46	OJ	365/376 (97%)	365 (100%)	0	100	100
46	OL	365/376 (97%)	365 (100%)	0	100	100
46	ON	365/376 (97%)	365 (100%)	0	100	100
46	PB	365/376 (97%)	365 (100%)	0	100	100
46	PD	365/376 (97%)	365 (100%)	0	100	100
46	PF	365/376 (97%)	365 (100%)	0	100	100
46	PH	365/376 (97%)	365 (100%)	0	100	100
46	PJ	365/376 (97%)	365 (100%)	0	100	100
46	PL	365/376 (97%)	365 (100%)	0	100	100
46	PN	365/376 (97%)	365 (100%)	0	100	100
46	QB	365/376 (97%)	365 (100%)	0	100	100
46	QD	365/376 (97%)	365 (100%)	0	100	100
46	QF	365/376 (97%)	365 (100%)	0	100	100
46	QH	365/376 (97%)	365 (100%)	0	100	100
46	QJ	365/376 (97%)	365 (100%)	0	100	100
46	QL	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	QN	365/376 (97%)	365 (100%)	0	100	100
46	RB	365/376 (97%)	365 (100%)	0	100	100
46	RD	365/376 (97%)	365 (100%)	0	100	100
46	RF	365/376 (97%)	365 (100%)	0	100	100
46	RH	365/376 (97%)	365 (100%)	0	100	100
46	RJ	365/376 (97%)	365 (100%)	0	100	100
46	RL	365/376 (97%)	365 (100%)	0	100	100
46	RN	365/376 (97%)	365 (100%)	0	100	100
46	SB	365/376 (97%)	365 (100%)	0	100	100
46	SD	365/376 (97%)	365 (100%)	0	100	100
46	SF	365/376 (97%)	365 (100%)	0	100	100
46	SH	365/376 (97%)	365 (100%)	0	100	100
46	SJ	365/376 (97%)	365 (100%)	0	100	100
46	SL	365/376 (97%)	365 (100%)	0	100	100
46	SN	365/376 (97%)	365 (100%)	0	100	100
46	TB	365/376 (97%)	365 (100%)	0	100	100
46	TD	365/376 (97%)	365 (100%)	0	100	100
46	TF	365/376 (97%)	365 (100%)	0	100	100
46	TH	365/376 (97%)	365 (100%)	0	100	100
46	TJ	365/376 (97%)	365 (100%)	0	100	100
46	TL	365/376 (97%)	365 (100%)	0	100	100
46	TN	365/376 (97%)	365 (100%)	0	100	100
46	UB	365/376 (97%)	365 (100%)	0	100	100
46	UD	365/376 (97%)	365 (100%)	0	100	100
46	UF	365/376 (97%)	365 (100%)	0	100	100
46	UH	365/376 (97%)	365 (100%)	0	100	100
46	UJ	365/376 (97%)	365 (100%)	0	100	100
46	UL	365/376 (97%)	364 (100%)	1 (0%)	86	85
46	UN	365/376 (97%)	365 (100%)	0	100	100
46	VB	365/376 (97%)	365 (100%)	0	100	100
46	VD	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	VF	365/376 (97%)	365 (100%)	0	100	100
46	VH	365/376 (97%)	365 (100%)	0	100	100
46	VJ	365/376 (97%)	365 (100%)	0	100	100
46	VL	365/376 (97%)	365 (100%)	0	100	100
46	VN	365/376 (97%)	365 (100%)	0	100	100
46	WB	365/376 (97%)	365 (100%)	0	100	100
46	WD	365/376 (97%)	365 (100%)	0	100	100
46	WF	365/376 (97%)	365 (100%)	0	100	100
46	WH	365/376 (97%)	365 (100%)	0	100	100
46	WJ	365/376 (97%)	365 (100%)	0	100	100
46	WL	365/376 (97%)	365 (100%)	0	100	100
46	WN	365/376 (97%)	365 (100%)	0	100	100
All	All	142179/152289 (93%)	142139 (100%)	40 (0%)	100	100

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

Mol	Chain	Res	Type
46	JJ	332	ASN
45	NA	285	GLN
45	KI	128	ASN
45	LM	133	GLN
45	PG	133	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1774 such sidechains are listed below:

Mol	Chain	Res	Type
46	JL	329	GLN
45	DC	283	HIS
46	ND	99	ASN
46	WJ	424	GLN
45	UA	101	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 483 ligands modelled in this entry, 161 are monoatomic - leaving 322 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
49	GDP	UL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	SG	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	AA	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.60	8 (16%)
49	GDP	KB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
49	GDP	CB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	WC	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	NA	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	AM	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.61	9 (18%)
49	GDP	NB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	QC	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.62	9 (18%)
47	GTP	WM	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	SJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	8 (17%)
49	GDP	RD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
49	GDP	CH	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.80	7 (15%)
47	GTP	FE	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	HL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	BF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	IL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	GDP	QD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	FA	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.63	8 (16%)
47	GTP	SA	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.56	9 (18%)
49	GDP	DH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	EK	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.58	8 (16%)
47	GTP	LC	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.59	8 (16%)
49	GDP	EL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
49	GDP	TH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
49	GDP	HD	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	BD	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.72	7 (15%)
49	GDP	QN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	ON	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	HK	501	48	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
49	GDP	DL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	TB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	SF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	CM	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	KE	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	LH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	EI	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	PK	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.62	9 (18%)
47	GTP	JC	501	48	33,34,34	0.96	2 (6%)	50,54,54	1.58	8 (16%)
47	GTP	NC	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
47	GTP	UA	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	SB	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.80	7 (15%)
49	GDP	VD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.81	7 (15%)
47	GTP	WK	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
47	GTP	WA	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.61	8 (16%)
47	GTP	VM	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	SL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.79	7 (15%)
49	GDP	CL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	EG	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	QA	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	FF	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.73	7 (15%)
47	GTP	BC	502	48	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	GDP	TJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	SH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	8 (17%)
49	GDP	BH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	8 (17%)
49	GDP	MN	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	RM	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.56	8 (16%)
47	GTP	RE	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.60	8 (16%)
49	GDP	WB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	RA	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.56	9 (18%)
49	GDP	SD	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	QM	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	OK	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)
47	GTP	KM	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
49	GDP	NF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	SC	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.56	8 (16%)
49	GDP	GF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
49	GDP	EB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	EC	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	VK	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	DA	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.57	9 (18%)
47	GTP	KG	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	MM	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.60	8 (16%)
49	GDP	PJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	EJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	KN	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.72	6 (13%)
49	GDP	VB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	IA	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	UB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	BA	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	JJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
49	GDP	WJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	8 (17%)
49	GDP	UH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	PA	501	48	33,34,34	0.96	2 (6%)	50,54,54	1.58	9 (18%)
49	GDP	UF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	QL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	IF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	GDP	CF	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	7 (15%)
47	GTP	IG	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.59	10 (20%)
49	GDP	DJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	WD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	KA	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
47	GTP	UI	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.61	9 (18%)
49	GDP	IJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
49	GDP	JB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
49	GDP	GD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
47	GTP	CI	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.61	10 (20%)
47	GTP	CK	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	RI	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.58	8 (16%)
49	GDP	AJ	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.81	9 (20%)
47	GTP	BM	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.62	9 (18%)
47	GTP	GA	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	GJ	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	JH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	6 (13%)
49	GDP	TF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	NG	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.59	8 (16%)
47	GTP	JE	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	AF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
49	GDP	QB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	NM	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	JM	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	NJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	HI	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.61	8 (16%)
47	GTP	HG	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.62	9 (18%)
47	GTP	QE	501	48	33,34,34	0.97	1 (3%)	50,54,54	1.63	8 (16%)
49	GDP	JN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	SN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	ND	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	FL	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	HN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	JL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
47	GTP	OI	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.56	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	GTP	MG	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	MI	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	VL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
49	GDP	LL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	TM	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	SM	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	AE	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	RF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	MK	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	LJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	VE	501	48	33,34,34	0.95	2 (6%)	50,54,54	1.62	8 (16%)
49	GDP	CD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	SI	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	IC	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	NH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	NI	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	8 (16%)
47	GTP	CC	501	48	33,34,34	0.96	2 (6%)	50,54,54	1.63	9 (18%)
47	GTP	UM	501	48	33,34,34	0.97	2 (6%)	50,54,54	1.63	9 (18%)
47	GTP	QG	501	48	33,34,34	1.00	2 (6%)	50,54,54	1.61	9 (18%)
47	GTP	AG	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.61	9 (18%)
47	GTP	IK	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.61	9 (18%)
49	GDP	KH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	8 (17%)
49	GDP	OB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	PE	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.61	8 (16%)
49	GDP	PB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	PI	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.58	8 (16%)
49	GDP	CJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	OD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	DG	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	EE	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	GH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	8 (17%)
49	GDP	PD	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	JK	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	TE	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	VN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	GDP	AH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	NN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	BB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	NE	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.56	8 (16%)
47	GTP	RC	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.62	9 (18%)
49	GDP	PH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	WI	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.61	8 (16%)
49	GDP	HH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	LB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	WF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
47	GTP	HA	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	AL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	BL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	DD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
47	GTP	NK	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	PM	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	WL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	DK	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.61	9 (18%)
49	GDP	LD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	FH	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	7 (15%)
49	GDP	FN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	OH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	LM	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.55	9 (18%)
49	GDP	UJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	FD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	LI	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.57	8 (16%)
49	GDP	FJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	QK	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.59	8 (16%)
47	GTP	RG	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.62	8 (16%)
47	GTP	FI	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.60	8 (16%)
47	GTP	ME	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.61	9 (18%)
47	GTP	LK	501	48	33,34,34	0.91	2 (6%)	50,54,54	1.60	8 (16%)
49	GDP	EF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	SE	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.56	8 (16%)
49	GDP	PL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	GTP	QI	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.61	9 (18%)
49	GDP	QF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	TK	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	MF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	AI	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.61	9 (18%)
47	GTP	LA	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	ID	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
47	GTP	KK	501	48	33,34,34	0.88	1 (3%)	50,54,54	1.57	8 (16%)
47	GTP	KC	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	UN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	FK	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.55	9 (18%)
47	GTP	CG	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.61	8 (16%)
47	GTP	CE	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	IN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	7 (15%)
49	GDP	VF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	EM	501	48	33,34,34	0.98	2 (6%)	50,54,54	1.59	8 (16%)
49	GDP	QH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	IM	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	BE	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.60	8 (16%)
47	GTP	HM	501	48	33,34,34	0.97	2 (6%)	50,54,54	1.58	9 (18%)
47	GTP	OG	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)
49	GDP	OL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	UG	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	KF	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	6 (13%)
47	GTP	CA	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	QJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
47	GTP	OM	501	48	33,34,34	0.98	2 (6%)	50,54,54	1.58	8 (16%)
49	GDP	KL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
49	GDP	AD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	MB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	AN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	VC	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.63	8 (16%)
49	GDP	NL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	HB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	MD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	GTP	IE	501	48	33,34,34	0.94	2 (6%)	50,54,54	1.63	9 (18%)
47	GTP	AC	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	VI	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
49	GDP	GL	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
49	GDP	IB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	DE	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	II	501	48	33,34,34	0.92	2 (6%)	50,54,54	1.57	9 (18%)
47	GTP	DC	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	KI	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	PN	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	UC	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	ED	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	TN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	EH	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	DI	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.60	8 (16%)
47	GTP	JA	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	RN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	RB	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.82	7 (15%)
49	GDP	DB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	FG	501	48	33,34,34	0.88	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	MH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	LF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
47	GTP	FM	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	HC	501	48	33,34,34	0.88	1 (3%)	50,54,54	1.60	8 (16%)
47	GTP	TC	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
47	GTP	EA	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	TA	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	KJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	5 (11%)
49	GDP	CN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	VJ	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	DF	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	WE	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	RL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	GI	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	WH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	GDP	AB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	7 (15%)
49	GDP	GB	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	SK	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.56	8 (16%)
47	GTP	BI	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	LN	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	MC	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	GN	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	OF	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	MA	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.60	8 (16%)
47	GTP	VG	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	TI	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.54	9 (18%)
49	GDP	BN	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.79	7 (15%)
49	GDP	RH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	LG	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.57	8 (16%)
49	GDP	UD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	VA	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	OJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	JG	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	FC	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
47	GTP	UK	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	MJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	IH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
49	GDP	HJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
49	GDP	VH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	RJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	TD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
49	GDP	BJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	GC	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	GM	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.56	9 (18%)
47	GTP	AK	501	48	33,34,34	0.95	2 (6%)	50,54,54	1.59	8 (16%)
47	GTP	LE	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.60	8 (16%)
47	GTP	RK	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.63	9 (18%)
49	GDP	DN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	PG	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	OF	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	GTP	OC	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.59	8 (16%)
49	GDP	ML	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	WG	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	GK	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
47	GTP	HE	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.63	8 (16%)
49	GDP	FB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	KD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
47	GTP	GG	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.59	8 (16%)
49	GDP	HF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	DM	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)
47	GTP	BG	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.61	9 (18%)
47	GTP	UE	501	48	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	JF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	PD	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	JD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
49	GDP	PF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	BK	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	JI	501	48	33,34,34	0.87	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	OA	501	48	33,34,34	0.97	1 (3%)	50,54,54	1.60	8 (16%)
49	GDP	TL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	WN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
49	GDP	EN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
47	GTP	GE	501	48	33,34,34	0.89	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	TG	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.53	8 (16%)

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
49	GDP	UL	501	-	-	0/16/32/32	0/3/3/3
47	GTP	SG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	AA	501	48	-	7/22/38/38	0/3/3/3
49	GDP	KB	501	-	-	0/16/32/32	0/3/3/3
49	GDP	CB	501	-	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	WC	501	48	-	7/22/38/38	0/3/3/3
47	GTP	NA	501	48	-	8/22/38/38	0/3/3/3
47	GTP	AM	501	48	-	8/22/38/38	0/3/3/3
49	GDP	NB	501	-	-	1/16/32/32	0/3/3/3
47	GTP	QC	501	48	-	5/22/38/38	0/3/3/3
47	GTP	WM	501	48	-	8/22/38/38	0/3/3/3
49	GDP	SJ	501	-	-	0/16/32/32	0/3/3/3
49	GDP	RD	501	-	-	0/16/32/32	0/3/3/3
49	GDP	CH	501	-	-	1/16/32/32	0/3/3/3
47	GTP	FE	501	48	-	9/22/38/38	0/3/3/3
49	GDP	HL	501	-	-	1/16/32/32	0/3/3/3
49	GDP	BF	501	-	-	1/16/32/32	0/3/3/3
49	GDP	IL	501	-	-	0/16/32/32	0/3/3/3
49	GDP	QD	501	-	-	0/16/32/32	0/3/3/3
47	GTP	FA	501	48	-	8/22/38/38	0/3/3/3
47	GTP	SA	501	48	-	7/22/38/38	0/3/3/3
49	GDP	DH	501	-	-	0/16/32/32	0/3/3/3
47	GTP	EK	501	48	-	7/22/38/38	0/3/3/3
47	GTP	LC	501	48	-	5/22/38/38	0/3/3/3
49	GDP	EL	501	-	-	0/16/32/32	0/3/3/3
49	GDP	TH	501	-	-	1/16/32/32	0/3/3/3
49	GDP	HD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	BD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	QN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	ON	501	-	-	0/16/32/32	0/3/3/3
47	GTP	HK	501	48	-	8/22/38/38	0/3/3/3
49	GDP	DL	501	-	-	0/16/32/32	0/3/3/3
49	GDP	TB	501	-	-	1/16/32/32	0/3/3/3
49	GDP	SF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	CM	501	48	-	7/22/38/38	0/3/3/3
47	GTP	KE	501	48	-	6/22/38/38	0/3/3/3
49	GDP	LH	501	-	-	3/16/32/32	0/3/3/3
47	GTP	EI	501	48	-	7/22/38/38	0/3/3/3
47	GTP	PK	501	48	-	6/22/38/38	0/3/3/3
47	GTP	JC	501	48	-	5/22/38/38	0/3/3/3
47	GTP	NC	501	48	-	5/22/38/38	0/3/3/3
47	GTP	UA	501	48	-	8/22/38/38	0/3/3/3
49	GDP	SB	501	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	GDP	VD	501	-	-	1/16/32/32	0/3/3/3
47	GTP	WK	501	48	-	8/22/38/38	0/3/3/3
47	GTP	WA	501	48	-	6/22/38/38	0/3/3/3
47	GTP	VM	501	48	-	8/22/38/38	0/3/3/3
49	GDP	SL	501	-	-	2/16/32/32	0/3/3/3
49	GDP	CL	501	-	-	0/16/32/32	0/3/3/3
47	GTP	EG	501	48	-	7/22/38/38	0/3/3/3
47	GTP	QA	501	48	-	8/22/38/38	0/3/3/3
49	GDP	FF	501	-	-	0/16/32/32	0/3/3/3
47	GTP	BC	502	48	-	9/22/38/38	0/3/3/3
49	GDP	TJ	501	-	-	2/16/32/32	0/3/3/3
49	GDP	SH	501	-	-	1/16/32/32	0/3/3/3
49	GDP	BH	501	-	-	0/16/32/32	0/3/3/3
49	GDP	MN	501	-	-	0/16/32/32	0/3/3/3
47	GTP	RM	501	48	-	9/22/38/38	0/3/3/3
47	GTP	RE	501	48	-	8/22/38/38	0/3/3/3
49	GDP	WB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	RA	501	48	-	8/22/38/38	0/3/3/3
49	GDP	SD	501	-	-	2/16/32/32	0/3/3/3
47	GTP	QM	501	48	-	8/22/38/38	0/3/3/3
47	GTP	OK	501	48	-	5/22/38/38	0/3/3/3
47	GTP	KM	501	48	-	6/22/38/38	0/3/3/3
49	GDP	NF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	SC	501	48	-	7/22/38/38	0/3/3/3
49	GDP	GF	501	-	-	1/16/32/32	0/3/3/3
49	GDP	EB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	EC	501	48	-	7/22/38/38	0/3/3/3
47	GTP	VK	501	48	-	9/22/38/38	0/3/3/3
47	GTP	DA	501	-	-	8/22/38/38	0/3/3/3
47	GTP	KG	501	48	-	7/22/38/38	0/3/3/3
47	GTP	MM	501	48	-	6/22/38/38	0/3/3/3
49	GDP	PJ	501	-	-	0/16/32/32	0/3/3/3
49	GDP	EJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	KN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	VB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	IA	501	48	-	8/22/38/38	0/3/3/3
49	GDP	UB	501	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	BA	501	48	-	7/22/38/38	0/3/3/3
49	GDP	JJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	WJ	501	-	-	2/16/32/32	0/3/3/3
49	GDP	UH	501	-	-	0/16/32/32	0/3/3/3
47	GTP	PA	501	48	-	8/22/38/38	0/3/3/3
49	GDP	UF	501	-	-	1/16/32/32	0/3/3/3
49	GDP	QL	501	-	-	0/16/32/32	0/3/3/3
49	GDP	IF	501	-	-	0/16/32/32	0/3/3/3
49	GDP	CF	501	-	-	0/16/32/32	0/3/3/3
47	GTP	IG	501	48	-	8/22/38/38	0/3/3/3
49	GDP	DJ	501	-	-	0/16/32/32	0/3/3/3
49	GDP	WD	501	-	-	0/16/32/32	0/3/3/3
47	GTP	KA	501	48	-	8/22/38/38	0/3/3/3
47	GTP	UI	501	48	-	8/22/38/38	0/3/3/3
49	GDP	IJ	501	-	-	0/16/32/32	0/3/3/3
49	GDP	JB	501	-	-	1/16/32/32	0/3/3/3
49	GDP	GD	501	-	-	1/16/32/32	0/3/3/3
47	GTP	CI	501	48	-	4/22/38/38	0/3/3/3
47	GTP	CK	501	48	-	7/22/38/38	0/3/3/3
47	GTP	RI	501	48	-	7/22/38/38	0/3/3/3
49	GDP	AJ	501	-	-	1/16/32/32	0/3/3/3
47	GTP	BM	501	48	-	7/22/38/38	0/3/3/3
47	GTP	GA	501	48	-	8/22/38/38	0/3/3/3
49	GDP	GJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	JH	501	-	-	1/16/32/32	0/3/3/3
49	GDP	TF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	NG	501	48	-	7/22/38/38	0/3/3/3
47	GTP	JE	501	48	-	7/22/38/38	0/3/3/3
49	GDP	AF	501	-	-	1/16/32/32	0/3/3/3
49	GDP	QB	501	-	-	1/16/32/32	0/3/3/3
47	GTP	NM	501	48	-	5/22/38/38	0/3/3/3
47	GTP	JM	501	48	-	8/22/38/38	0/3/3/3
49	GDP	NJ	501	-	-	1/16/32/32	0/3/3/3
47	GTP	HI	501	48	-	9/22/38/38	0/3/3/3
47	GTP	HG	501	48	-	9/22/38/38	0/3/3/3
47	GTP	QE	501	48	-	7/22/38/38	0/3/3/3
49	GDP	JN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	SN	501	-	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	GDP	ND	502	-	-	1/16/32/32	0/3/3/3
49	GDP	FL	502	-	-	1/16/32/32	0/3/3/3
49	GDP	HN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	JL	501	-	-	1/16/32/32	0/3/3/3
47	GTP	OI	501	48	-	5/22/38/38	0/3/3/3
47	GTP	MG	501	48	-	7/22/38/38	0/3/3/3
47	GTP	MI	501	48	-	7/22/38/38	0/3/3/3
49	GDP	VL	501	-	-	0/16/32/32	0/3/3/3
49	GDP	LL	501	-	-	3/16/32/32	0/3/3/3
47	GTP	TM	501	48	-	8/22/38/38	0/3/3/3
47	GTP	SM	501	48	-	8/22/38/38	0/3/3/3
47	GTP	AE	501	48	-	9/22/38/38	0/3/3/3
49	GDP	RF	501	-	-	2/16/32/32	0/3/3/3
47	GTP	MK	501	48	-	7/22/38/38	0/3/3/3
49	GDP	LJ	501	-	-	2/16/32/32	0/3/3/3
47	GTP	VE	501	48	-	7/22/38/38	0/3/3/3
49	GDP	CD	501	-	-	1/16/32/32	0/3/3/3
47	GTP	SI	501	48	-	7/22/38/38	0/3/3/3
47	GTP	IC	501	48	-	9/22/38/38	0/3/3/3
49	GDP	NH	501	-	-	0/16/32/32	0/3/3/3
47	GTP	NI	501	48	-	5/22/38/38	0/3/3/3
47	GTP	CC	501	48	-	5/22/38/38	0/3/3/3
47	GTP	UM	501	48	-	8/22/38/38	0/3/3/3
47	GTP	QG	501	48	-	5/22/38/38	0/3/3/3
47	GTP	AG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	IK	501	48	-	8/22/38/38	0/3/3/3
49	GDP	KH	501	-	-	0/16/32/32	0/3/3/3
49	GDP	OB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	PE	501	48	-	7/22/38/38	0/3/3/3
49	GDP	PB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	PI	501	48	-	6/22/38/38	0/3/3/3
49	GDP	CJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	OD	501	-	-	0/16/32/32	0/3/3/3
47	GTP	DG	501	48	-	7/22/38/38	0/3/3/3
47	GTP	EE	501	48	-	8/22/38/38	0/3/3/3
49	GDP	GH	501	-	-	0/16/32/32	0/3/3/3
49	GDP	PD	502	-	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	JK	501	48	-	9/22/38/38	0/3/3/3
47	GTP	TE	501	48	-	8/22/38/38	0/3/3/3
49	GDP	VN	501	-	-	1/16/32/32	0/3/3/3
49	GDP	AH	501	-	-	0/16/32/32	0/3/3/3
49	GDP	NN	501	-	-	1/16/32/32	0/3/3/3
49	GDP	BB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	NE	501	48	-	7/22/38/38	0/3/3/3
47	GTP	RC	501	48	-	8/22/38/38	0/3/3/3
49	GDP	PH	501	-	-	0/16/32/32	0/3/3/3
47	GTP	WI	501	48	-	7/22/38/38	0/3/3/3
49	GDP	HH	501	-	-	0/16/32/32	0/3/3/3
49	GDP	LB	501	-	-	0/16/32/32	0/3/3/3
49	GDP	WF	501	-	-	0/16/32/32	0/3/3/3
47	GTP	HA	501	48	-	7/22/38/38	0/3/3/3
49	GDP	AL	501	-	-	1/16/32/32	0/3/3/3
49	GDP	BL	501	-	-	0/16/32/32	0/3/3/3
49	GDP	DD	501	-	-	1/16/32/32	0/3/3/3
47	GTP	NK	501	48	-	6/22/38/38	0/3/3/3
47	GTP	PM	501	48	-	7/22/38/38	0/3/3/3
49	GDP	WL	501	-	-	1/16/32/32	0/3/3/3
47	GTP	DK	501	48	-	7/22/38/38	0/3/3/3
49	GDP	LD	501	-	-	3/16/32/32	0/3/3/3
49	GDP	FH	501	-	-	1/16/32/32	0/3/3/3
49	GDP	FN	501	-	-	1/16/32/32	0/3/3/3
49	GDP	OH	501	-	-	1/16/32/32	0/3/3/3
47	GTP	LM	501	48	-	7/22/38/38	0/3/3/3
49	GDP	UJ	501	-	-	0/16/32/32	0/3/3/3
49	GDP	FD	501	-	-	1/16/32/32	0/3/3/3
47	GTP	LI	501	48	-	8/22/38/38	0/3/3/3
49	GDP	FJ	501	-	-	3/16/32/32	0/3/3/3
47	GTP	QK	501	48	-	9/22/38/38	0/3/3/3
47	GTP	RG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	FI	501	48	-	8/22/38/38	0/3/3/3
47	GTP	ME	501	48	-	8/22/38/38	0/3/3/3
47	GTP	LK	501	48	-	9/22/38/38	0/3/3/3
49	GDP	EF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	SE	501	48	-	8/22/38/38	0/3/3/3
49	GDP	PL	501	-	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	QI	501	48	-	8/22/38/38	0/3/3/3
49	GDP	QF	501	-	-	0/16/32/32	0/3/3/3
47	GTP	TK	501	48	-	8/22/38/38	0/3/3/3
49	GDP	MF	501	-	-	0/16/32/32	0/3/3/3
47	GTP	AI	501	48	-	7/22/38/38	0/3/3/3
47	GTP	LA	501	48	-	8/22/38/38	0/3/3/3
49	GDP	ID	501	-	-	1/16/32/32	0/3/3/3
47	GTP	KK	501	48	-	6/22/38/38	0/3/3/3
47	GTP	KC	501	48	-	6/22/38/38	0/3/3/3
49	GDP	UN	501	-	-	1/16/32/32	0/3/3/3
47	GTP	FK	501	48	-	8/22/38/38	0/3/3/3
47	GTP	CG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	CE	501	48	-	8/22/38/38	0/3/3/3
49	GDP	IN	501	-	-	1/16/32/32	0/3/3/3
49	GDP	VF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	EM	501	48	-	9/22/38/38	0/3/3/3
49	GDP	QH	501	-	-	0/16/32/32	0/3/3/3
47	GTP	IM	501	48	-	8/22/38/38	0/3/3/3
47	GTP	BE	501	48	-	9/22/38/38	0/3/3/3
47	GTP	HM	501	48	-	8/22/38/38	0/3/3/3
47	GTP	OG	501	48	-	8/22/38/38	0/3/3/3
49	GDP	OL	501	-	-	0/16/32/32	0/3/3/3
47	GTP	UG	501	48	-	8/22/38/38	0/3/3/3
49	GDP	KF	501	-	-	0/16/32/32	0/3/3/3
47	GTP	CA	501	48	-	9/22/38/38	0/3/3/3
49	GDP	QJ	501	-	-	0/16/32/32	0/3/3/3
47	GTP	OM	501	48	-	4/22/38/38	0/3/3/3
49	GDP	KL	501	-	-	1/16/32/32	0/3/3/3
49	GDP	AD	501	-	-	0/16/32/32	0/3/3/3
49	GDP	MB	501	-	-	3/16/32/32	0/3/3/3
49	GDP	AN	501	-	-	1/16/32/32	0/3/3/3
47	GTP	VC	501	48	-	9/22/38/38	0/3/3/3
49	GDP	NL	501	-	-	0/16/32/32	0/3/3/3
49	GDP	HB	501	-	-	0/16/32/32	0/3/3/3
49	GDP	MD	501	-	-	3/16/32/32	0/3/3/3
47	GTP	IE	501	48	-	8/22/38/38	0/3/3/3
47	GTP	AC	501	48	-	8/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	VI	501	48	-	8/22/38/38	0/3/3/3
49	GDP	GL	502	-	-	1/16/32/32	0/3/3/3
49	GDP	IB	501	-	-	1/16/32/32	0/3/3/3
47	GTP	DE	501	48	-	7/22/38/38	0/3/3/3
47	GTP	II	501	48	-	8/22/38/38	0/3/3/3
47	GTP	DC	501	48	-	8/22/38/38	0/3/3/3
47	GTP	KI	501	48	-	7/22/38/38	0/3/3/3
49	GDP	PN	502	-	-	0/16/32/32	0/3/3/3
47	GTP	UC	501	48	-	6/22/38/38	0/3/3/3
49	GDP	ED	501	-	-	0/16/32/32	0/3/3/3
49	GDP	TN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	EH	501	-	-	1/16/32/32	0/3/3/3
47	GTP	DI	501	48	-	8/22/38/38	0/3/3/3
47	GTP	JA	501	48	-	7/22/38/38	0/3/3/3
49	GDP	RN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	RB	501	-	-	0/16/32/32	0/3/3/3
49	GDP	DB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	FG	501	48	-	8/22/38/38	0/3/3/3
49	GDP	MH	501	-	-	1/16/32/32	0/3/3/3
49	GDP	LF	501	-	-	2/16/32/32	0/3/3/3
47	GTP	FM	501	48	-	8/22/38/38	0/3/3/3
47	GTP	HC	501	48	-	7/22/38/38	0/3/3/3
47	GTP	TC	501	48	-	8/22/38/38	0/3/3/3
47	GTP	EA	501	48	-	8/22/38/38	0/3/3/3
47	GTP	TA	501	48	-	8/22/38/38	0/3/3/3
49	GDP	KJ	501	-	-	0/16/32/32	0/3/3/3
49	GDP	CN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	VJ	501	-	-	0/16/32/32	0/3/3/3
49	GDP	DF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	WE	501	48	-	8/22/38/38	0/3/3/3
49	GDP	RL	501	-	-	0/16/32/32	0/3/3/3
47	GTP	GI	501	48	-	9/22/38/38	0/3/3/3
49	GDP	WH	501	-	-	1/16/32/32	0/3/3/3
49	GDP	AB	501	-	-	2/16/32/32	0/3/3/3
49	GDP	GB	502	-	-	0/16/32/32	0/3/3/3
47	GTP	SK	501	48	-	8/22/38/38	0/3/3/3
47	GTP	BI	501	48	-	8/22/38/38	0/3/3/3
49	GDP	LN	501	-	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	MC	501	48	-	8/22/38/38	0/3/3/3
49	GDP	GN	502	-	-	0/16/32/32	0/3/3/3
49	GDP	OF	502	-	-	0/16/32/32	0/3/3/3
47	GTP	MA	501	48	-	9/22/38/38	0/3/3/3
47	GTP	VG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	TI	501	48	-	7/22/38/38	0/3/3/3
49	GDP	BN	501	-	-	3/16/32/32	0/3/3/3
49	GDP	RH	501	-	-	0/16/32/32	0/3/3/3
47	GTP	LG	501	48	-	5/22/38/38	0/3/3/3
49	GDP	UD	501	-	-	1/16/32/32	0/3/3/3
47	GTP	VA	501	48	-	7/22/38/38	0/3/3/3
49	GDP	OJ	501	-	-	0/16/32/32	0/3/3/3
47	GTP	JG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	FC	501	48	-	8/22/38/38	0/3/3/3
47	GTP	UK	501	48	-	7/22/38/38	0/3/3/3
49	GDP	MJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	IH	501	-	-	0/16/32/32	0/3/3/3
49	GDP	HJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	VH	501	-	-	1/16/32/32	0/3/3/3
49	GDP	RJ	501	-	-	3/16/32/32	0/3/3/3
49	GDP	TD	501	-	-	3/16/32/32	0/3/3/3
49	GDP	BJ	501	-	-	0/16/32/32	0/3/3/3
47	GTP	GC	501	48	-	8/22/38/38	0/3/3/3
47	GTP	GM	501	48	-	9/22/38/38	0/3/3/3
47	GTP	AK	501	48	-	7/22/38/38	0/3/3/3
47	GTP	LE	501	48	-	8/22/38/38	0/3/3/3
47	GTP	RK	501	48	-	8/22/38/38	0/3/3/3
49	GDP	DN	501	-	-	0/16/32/32	0/3/3/3
47	GTP	PG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	OF	501	48	-	6/22/38/38	0/3/3/3
47	GTP	OC	501	48	-	7/22/38/38	0/3/3/3
49	GDP	ML	501	-	-	1/16/32/32	0/3/3/3
47	GTP	WG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	GK	501	48	-	8/22/38/38	0/3/3/3
47	GTP	HE	501	48	-	8/22/38/38	0/3/3/3
49	GDP	FB	501	-	-	0/16/32/32	0/3/3/3
49	GDP	KD	501	-	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	GG	501	48	-	8/22/38/38	0/3/3/3
49	GDP	HF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	DM	501	48	-	7/22/38/38	0/3/3/3
47	GTP	BG	501	48	-	9/22/38/38	0/3/3/3
47	GTP	UE	501	48	-	8/22/38/38	0/3/3/3
49	GDP	JF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	PD	501	48	-	9/22/38/38	0/3/3/3
49	GDP	JD	501	-	-	2/16/32/32	0/3/3/3
49	GDP	PF	501	-	-	0/16/32/32	0/3/3/3
47	GTP	BK	501	48	-	9/22/38/38	0/3/3/3
47	GTP	JI	501	48	-	7/22/38/38	0/3/3/3
47	GTP	OA	501	48	-	5/22/38/38	0/3/3/3
49	GDP	TL	501	-	-	3/16/32/32	0/3/3/3
49	GDP	WN	501	-	-	1/16/32/32	0/3/3/3
49	GDP	EN	501	-	-	1/16/32/32	0/3/3/3
47	GTP	GE	501	48	-	7/22/38/38	0/3/3/3
47	GTP	TG	501	48	-	7/22/38/38	0/3/3/3

The worst 5 of 658 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	TN	501	GDP	C5-C4	3.20	1.47	1.38
49	BB	501	GDP	C5-C4	3.19	1.47	1.38
49	PB	501	GDP	C5-C4	3.19	1.47	1.38
49	EB	501	GDP	C5-C4	3.19	1.47	1.38
49	SB	501	GDP	C5-C4	3.19	1.47	1.38

The worst 5 of 2519 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	VD	501	GDP	C5-C4-N3	-6.41	118.19	128.39
49	KH	501	GDP	C5-C4-N3	-6.40	118.20	128.39
49	RB	501	GDP	C5-C4-N3	-6.40	118.21	128.39
49	ID	501	GDP	C5-C4-N3	-6.29	118.38	128.39
49	RJ	501	GDP	C5-C4-N3	-6.27	118.42	128.39

There are no chirality outliers.

5 of 1310 torsion outliers are listed below:

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

There are no ring outliers.

251 monomers are involved in 487 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	UL	501	GDP	2	0
47	AA	501	GTP	3	0
49	CB	501	GDP	2	0
47	NA	501	GTP	3	0
47	AM	501	GTP	2	0
49	NB	501	GDP	1	0
47	QC	501	GTP	3	0
47	WM	501	GTP	1	0
49	SJ	501	GDP	1	0
49	CH	501	GDP	1	0
47	FE	501	GTP	1	0
49	HL	501	GDP	1	0
49	BF	501	GDP	4	0
49	IL	501	GDP	4	0
49	QD	501	GDP	1	0
47	FA	501	GTP	3	0
47	SA	501	GTP	2	0
49	DH	501	GDP	2	0
47	EK	501	GTP	3	0
47	LC	501	GTP	3	0
49	EL	501	GDP	3	0
49	TH	501	GDP	1	0
49	HD	501	GDP	1	0
49	BD	501	GDP	2	0
49	QN	501	GDP	1	0
49	ON	501	GDP	2	0
49	DL	501	GDP	1	0
49	SF	501	GDP	1	0
47	CM	501	GTP	1	0
47	KE	501	GTP	2	0
47	EI	501	GTP	1	0
47	PK	501	GTP	4	0
47	JC	501	GTP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	UA	501	GTP	2	0
49	SB	501	GDP	1	0
49	VD	501	GDP	1	0
47	WK	501	GTP	2	0
47	WA	501	GTP	3	0
47	VM	501	GTP	2	0
47	EG	501	GTP	2	0
47	QA	501	GTP	2	0
49	FF	501	GDP	2	0
49	TJ	501	GDP	1	0
49	BH	501	GDP	2	0
47	RM	501	GTP	2	0
47	RE	501	GTP	3	0
47	RA	501	GTP	2	0
47	QM	501	GTP	2	0
47	OK	501	GTP	1	0
47	KM	501	GTP	3	0
47	SC	501	GTP	2	0
49	GF	501	GDP	1	0
47	EC	501	GTP	3	0
47	VK	501	GTP	1	0
47	DA	501	GTP	2	0
47	KG	501	GTP	2	0
47	MM	501	GTP	4	0
49	PJ	501	GDP	1	0
49	VB	501	GDP	1	0
47	IA	501	GTP	1	0
47	BA	501	GTP	1	0
49	JJ	501	GDP	3	0
49	UH	501	GDP	1	0
47	PA	501	GTP	2	0
49	UF	501	GDP	5	0
49	QL	501	GDP	1	0
49	IF	501	GDP	1	0
49	CF	501	GDP	6	0
47	IG	501	GTP	2	0
49	DJ	501	GDP	2	0
49	WD	501	GDP	3	0
47	KA	501	GTP	2	0
47	UI	501	GTP	2	0
49	IJ	501	GDP	3	0
49	GD	501	GDP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	CI	501	GTP	2	0
47	CK	501	GTP	1	0
47	RI	501	GTP	1	0
49	AJ	501	GDP	2	0
47	BM	501	GTP	2	0
49	GJ	501	GDP	1	0
49	JH	501	GDP	1	0
49	TF	501	GDP	1	0
47	NG	501	GTP	1	0
49	AF	501	GDP	1	0
49	QB	501	GDP	1	0
47	NM	501	GTP	2	0
49	NJ	501	GDP	1	0
47	HG	501	GTP	2	0
47	QE	501	GTP	5	0
49	JN	501	GDP	1	0
49	SN	501	GDP	1	0
49	FL	502	GDP	2	0
49	HN	501	GDP	1	0
49	JL	501	GDP	1	0
47	OI	501	GTP	3	0
49	VL	501	GDP	3	0
49	LL	501	GDP	1	0
47	TM	501	GTP	2	0
47	SM	501	GTP	1	0
49	LJ	501	GDP	1	0
47	VE	501	GTP	4	0
49	CD	501	GDP	2	0
47	SI	501	GTP	2	0
47	CC	501	GTP	1	0
47	UM	501	GTP	1	0
47	QG	501	GTP	5	0
47	AG	501	GTP	1	0
47	IK	501	GTP	3	0
49	KH	501	GDP	1	0
49	OB	501	GDP	2	0
47	PE	501	GTP	1	0
49	PB	501	GDP	1	0
47	PI	501	GTP	4	0
49	CJ	501	GDP	4	0
49	OD	501	GDP	2	0
47	DG	501	GTP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	EE	501	GTP	1	0
47	JK	501	GTP	2	0
47	TE	501	GTP	1	0
49	VN	501	GDP	2	0
49	AH	501	GDP	2	0
47	NE	501	GTP	1	0
47	RC	501	GTP	3	0
49	PH	501	GDP	2	0
47	WI	501	GTP	3	0
49	HH	501	GDP	2	0
49	WF	501	GDP	1	0
47	HA	501	GTP	1	0
49	AL	501	GDP	1	0
49	BL	501	GDP	2	0
49	DD	501	GDP	2	0
47	NK	501	GTP	1	0
47	PM	501	GTP	2	0
49	WL	501	GDP	2	0
47	DK	501	GTP	3	0
49	FH	501	GDP	4	0
49	FN	501	GDP	1	0
47	LM	501	GTP	1	0
49	UJ	501	GDP	3	0
47	LI	501	GTP	1	0
49	FJ	501	GDP	1	0
47	QK	501	GTP	2	0
47	RG	501	GTP	2	0
47	ME	501	GTP	1	0
47	LK	501	GTP	3	0
49	EF	501	GDP	1	0
47	SE	501	GTP	2	0
47	QI	501	GTP	3	0
49	QF	501	GDP	6	0
47	TK	501	GTP	2	0
49	MF	501	GDP	2	0
47	AI	501	GTP	1	0
47	LA	501	GTP	1	0
47	KC	501	GTP	2	0
49	UN	501	GDP	1	0
47	FK	501	GTP	1	0
47	CG	501	GTP	2	0
47	CE	501	GTP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	IN	501	GDP	3	0
49	VF	501	GDP	2	0
47	EM	501	GTP	2	0
49	QH	501	GDP	1	0
47	IM	501	GTP	3	0
47	BE	501	GTP	4	0
47	HM	501	GTP	1	0
47	OG	501	GTP	4	0
49	OL	501	GDP	1	0
47	UG	501	GTP	1	0
49	KF	501	GDP	1	0
47	CA	501	GTP	2	0
49	QJ	501	GDP	3	0
47	OM	501	GTP	1	0
49	AN	501	GDP	1	0
47	VC	501	GTP	2	0
49	HB	501	GDP	1	0
47	IE	501	GTP	3	0
47	AC	501	GTP	1	0
49	GL	502	GDP	3	0
49	IB	501	GDP	1	0
47	DE	501	GTP	2	0
47	DC	501	GTP	3	0
47	KI	501	GTP	1	0
49	PN	502	GDP	3	0
47	UC	501	GTP	1	0
49	ED	501	GDP	1	0
49	TN	501	GDP	1	0
49	EH	501	GDP	4	0
47	DI	501	GTP	4	0
47	JA	501	GTP	1	0
49	RN	501	GDP	1	0
49	RB	501	GDP	1	0
47	FG	501	GTP	1	0
49	MH	501	GDP	1	0
47	FM	501	GTP	2	0
47	TC	501	GTP	3	0
47	EA	501	GTP	2	0
47	TA	501	GTP	2	0
49	VJ	501	GDP	4	0
49	DF	501	GDP	1	0
47	WE	501	GTP	1	0

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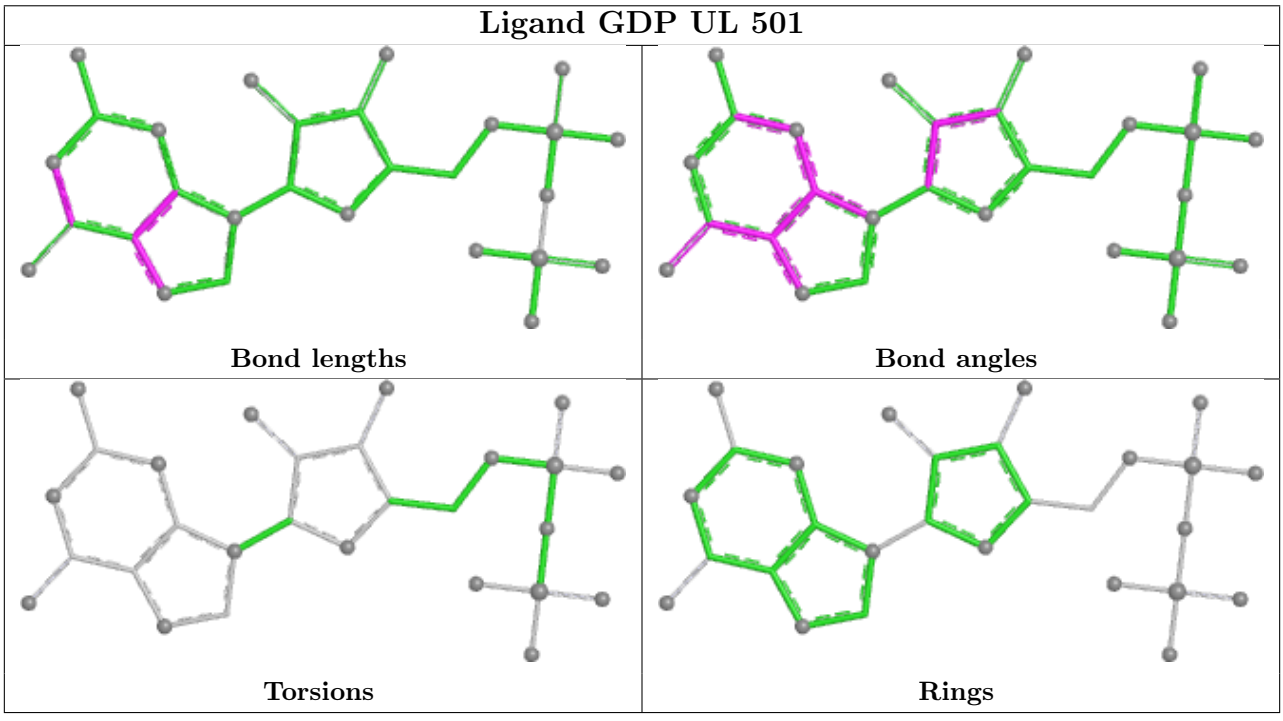
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	RL	501	GDP	1	0
47	GI	501	GTP	1	0
49	WH	501	GDP	2	0
47	SK	501	GTP	4	0
47	BI	501	GTP	3	0
49	LN	501	GDP	2	0
47	MC	501	GTP	1	0
49	GN	502	GDP	1	0
49	OF	502	GDP	3	0
47	VG	501	GTP	4	0
47	TI	501	GTP	1	0
49	RH	501	GDP	1	0
47	LG	501	GTP	2	0
49	UD	501	GDP	2	0
47	VA	501	GTP	3	0
49	OJ	501	GDP	2	0
47	JG	501	GTP	2	0
47	FC	501	GTP	2	0
49	MJ	501	GDP	3	0
49	IH	501	GDP	3	0
49	HJ	501	GDP	2	0
49	VH	501	GDP	2	0
49	RJ	501	GDP	3	0
49	TD	501	GDP	1	0
49	BJ	501	GDP	2	0
47	GC	501	GTP	1	0
47	GM	501	GTP	2	0
47	AK	501	GTP	1	0
47	RK	501	GTP	3	0
49	DN	501	GDP	1	0
47	PG	501	GTP	4	0
47	OF	501	GTP	4	0
47	OC	501	GTP	1	0
47	WG	501	GTP	1	0
47	GK	501	GTP	1	0
47	HE	501	GTP	2	0
47	GG	501	GTP	1	0
49	HF	501	GDP	2	0
47	DM	501	GTP	2	0
47	BG	501	GTP	1	0
47	UE	501	GTP	3	0
49	JF	501	GDP	1	0

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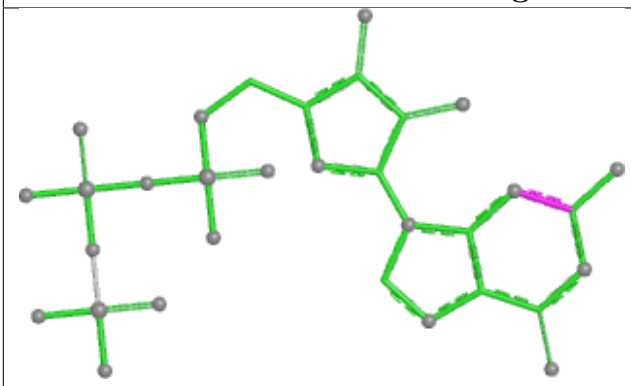
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	PD	501	GTP	3	0
49	JD	501	GDP	1	0
47	BK	501	GTP	1	0
47	JI	501	GTP	1	0
49	TL	501	GDP	1	0
49	EN	501	GDP	5	0
47	GE	501	GTP	1	0
47	TG	501	GTP	1	0

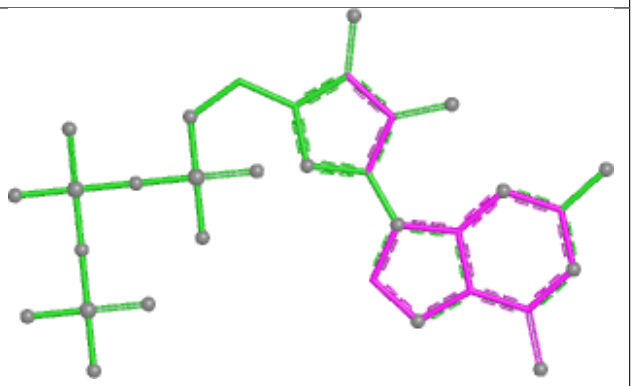
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



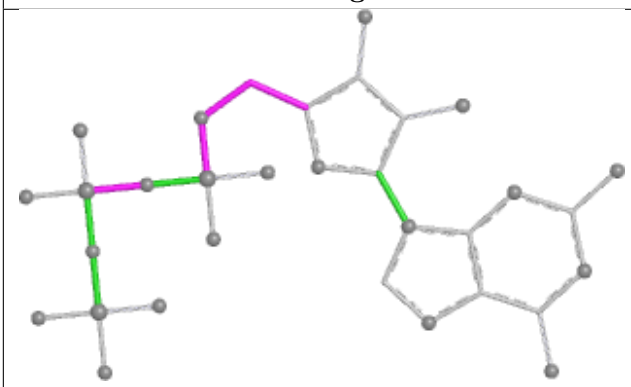
Ligand GTP SG 501



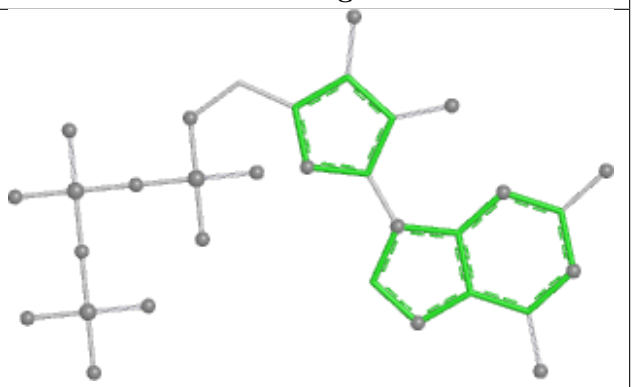
Bond lengths



Bond angles

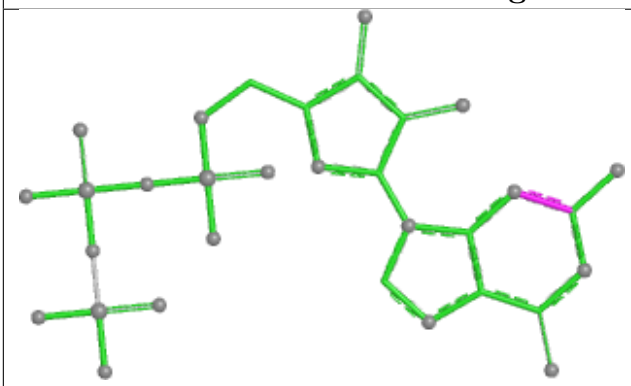


Torsions

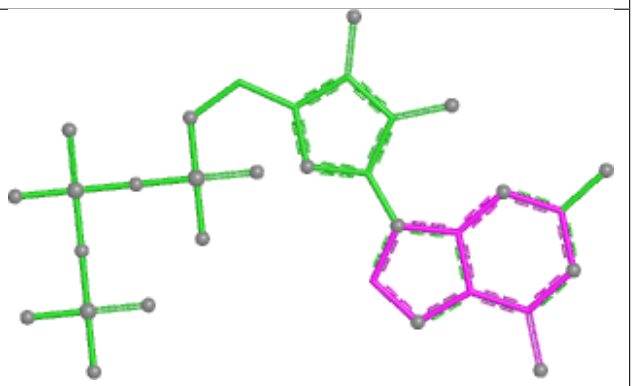


Rings

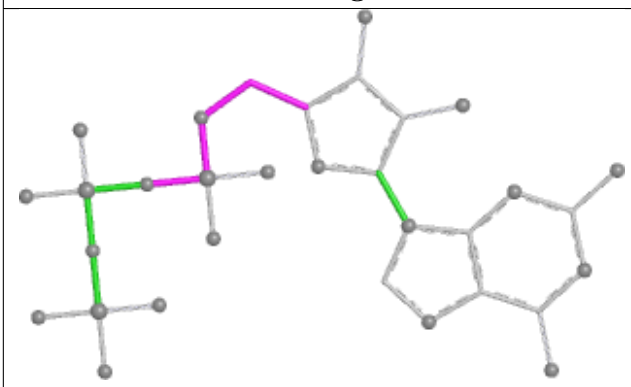
Ligand GTP AA 501



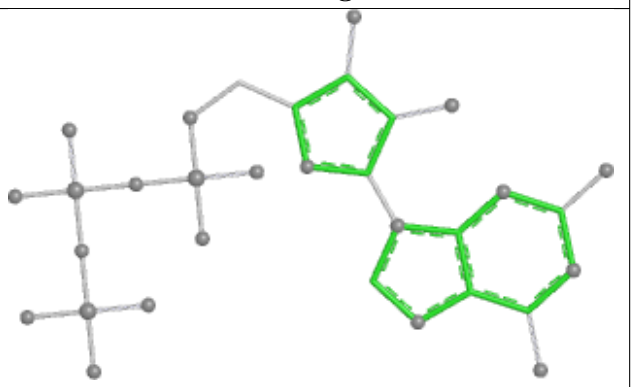
Bond lengths



Bond angles

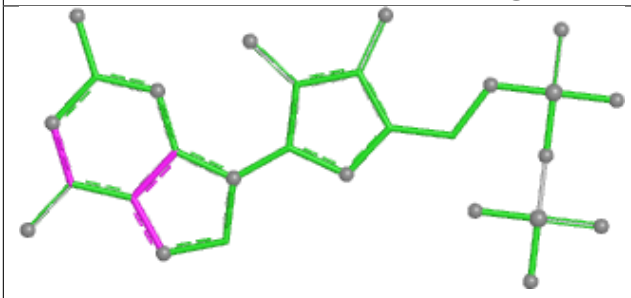


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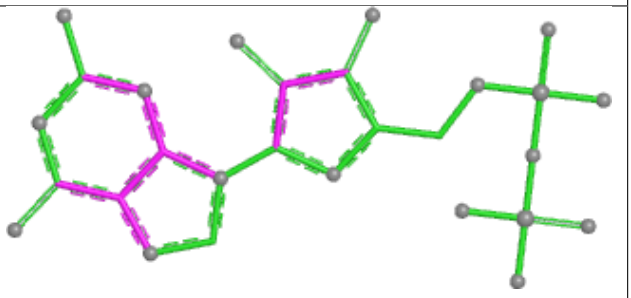


Rings

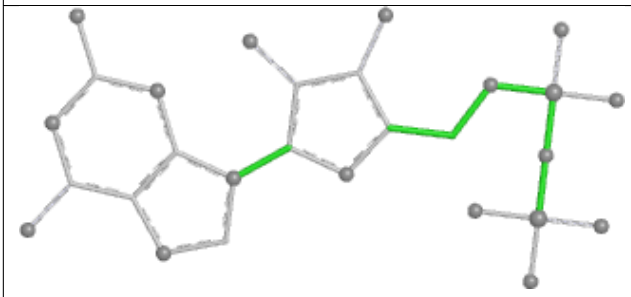
Ligand GDP KB 501



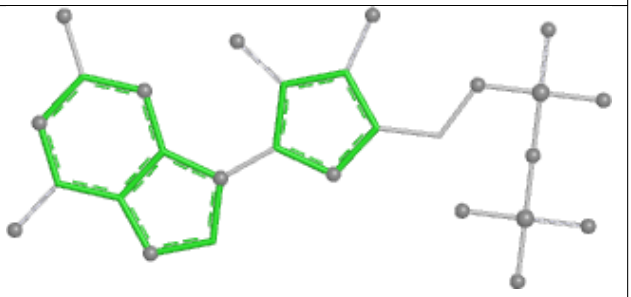
Bond lengths



Bond angles

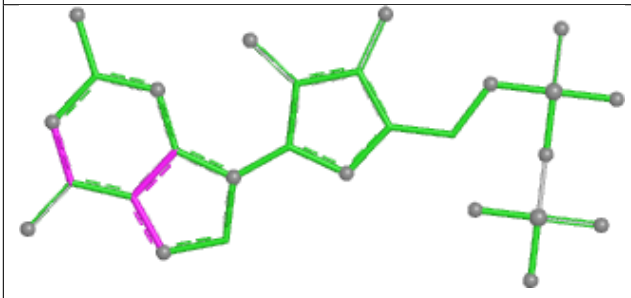


Torsions

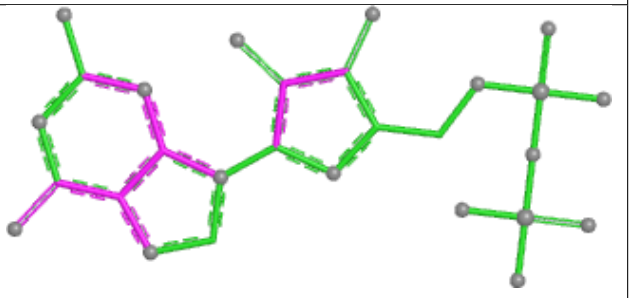


Rings

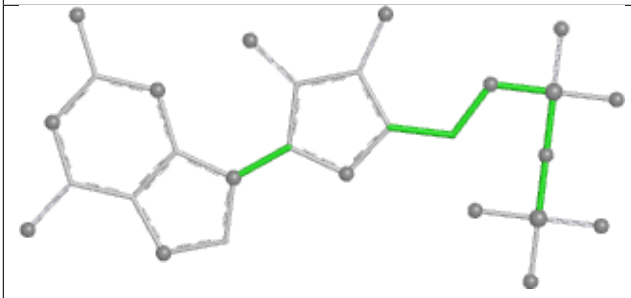
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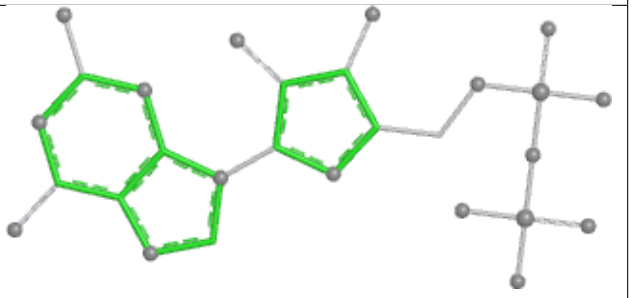
Bond lengths



Bond angles

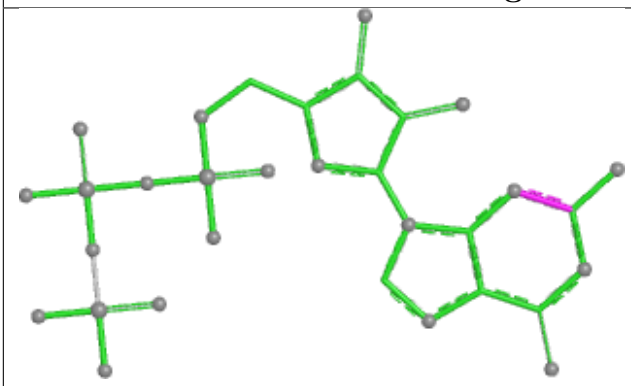


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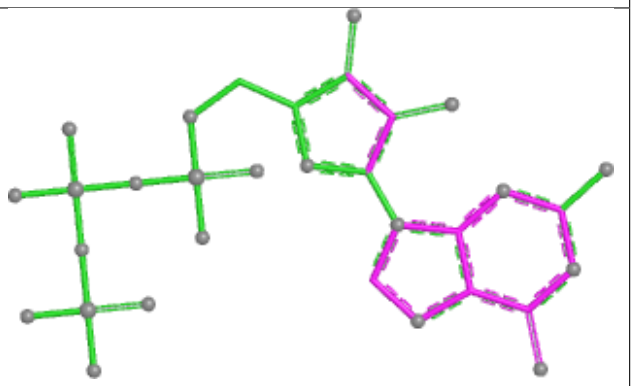


Rings

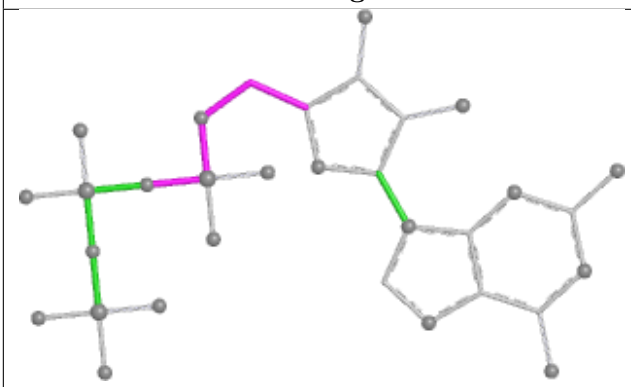
Ligand GTP WC 501



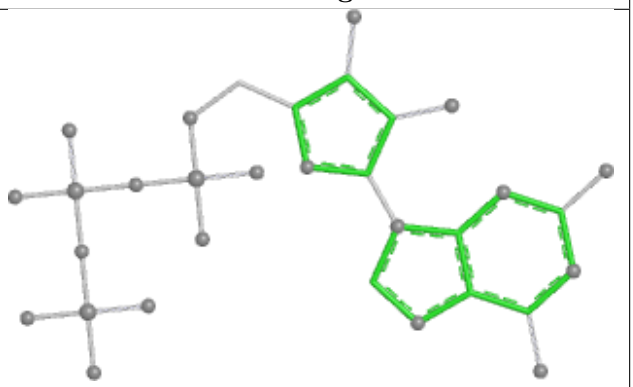
Bond lengths



Bond angles

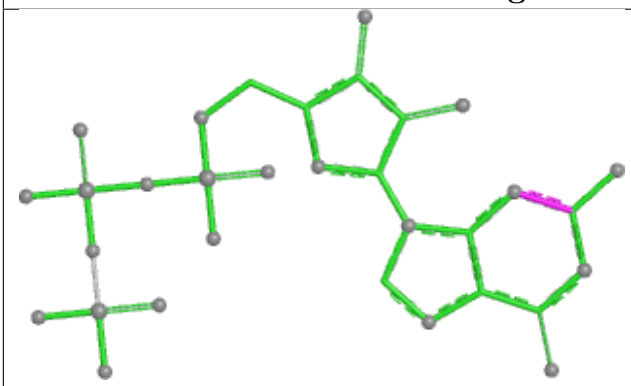


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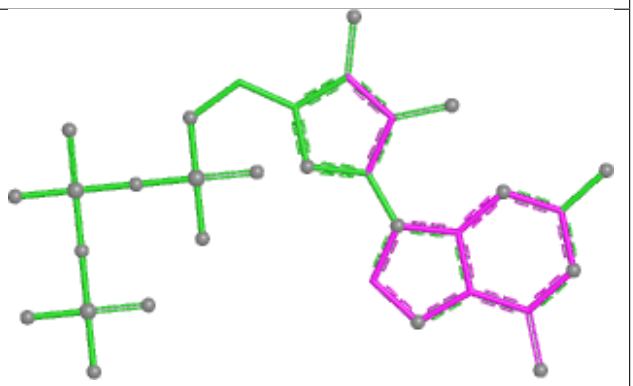


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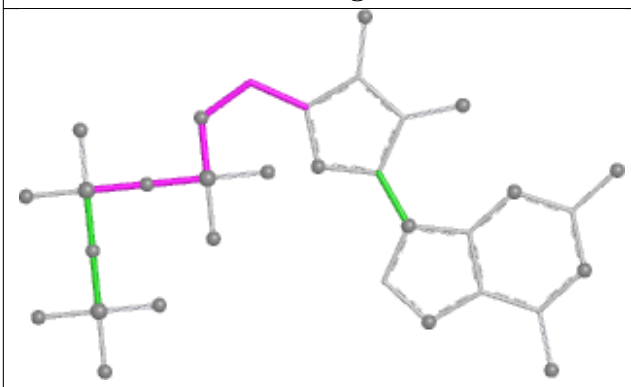
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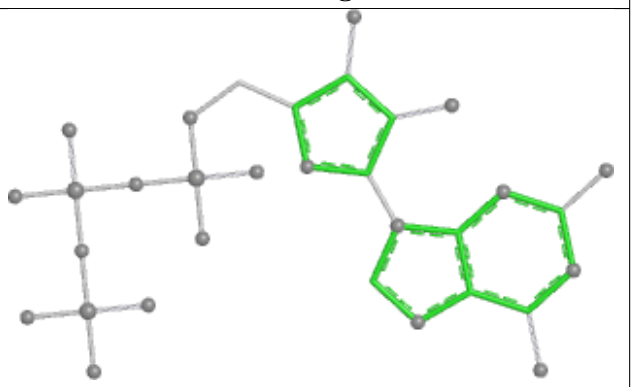
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Bond angles

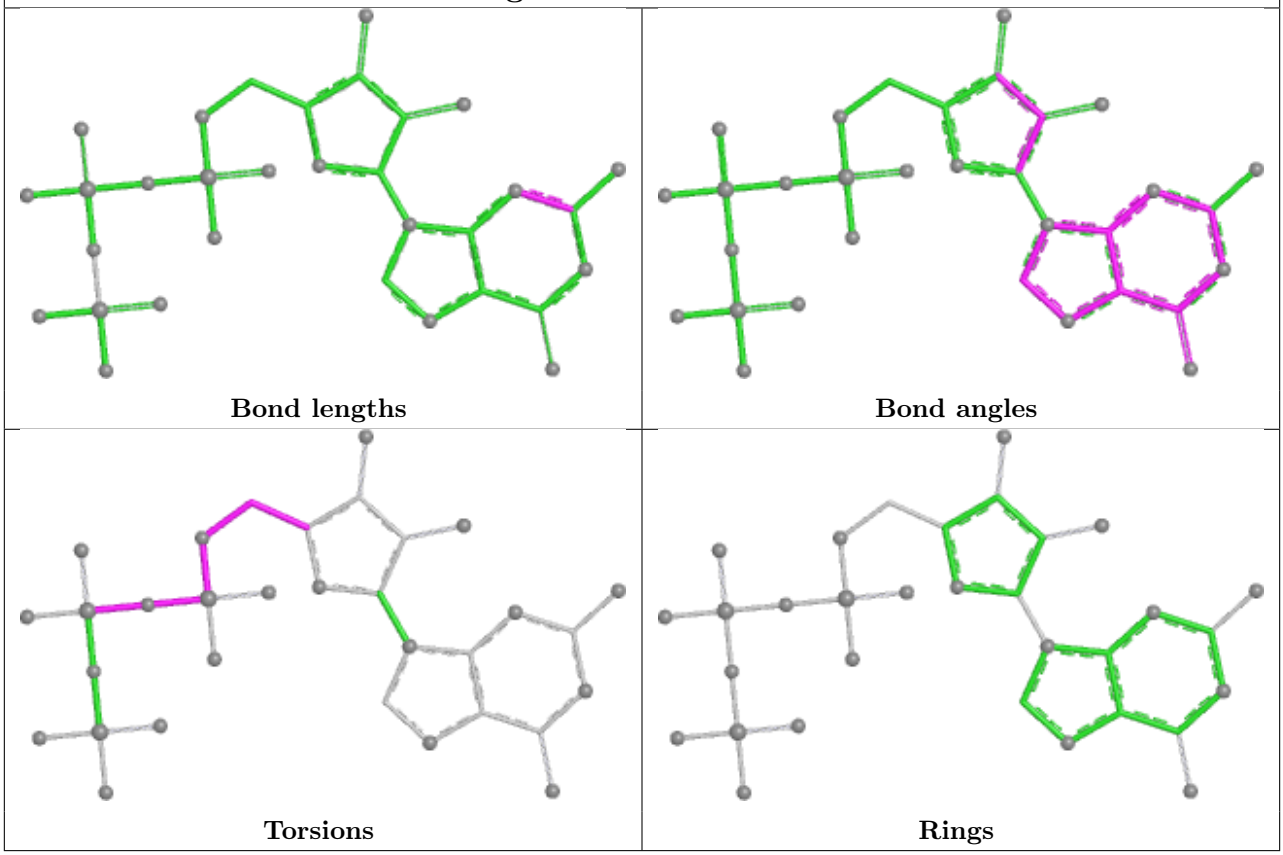


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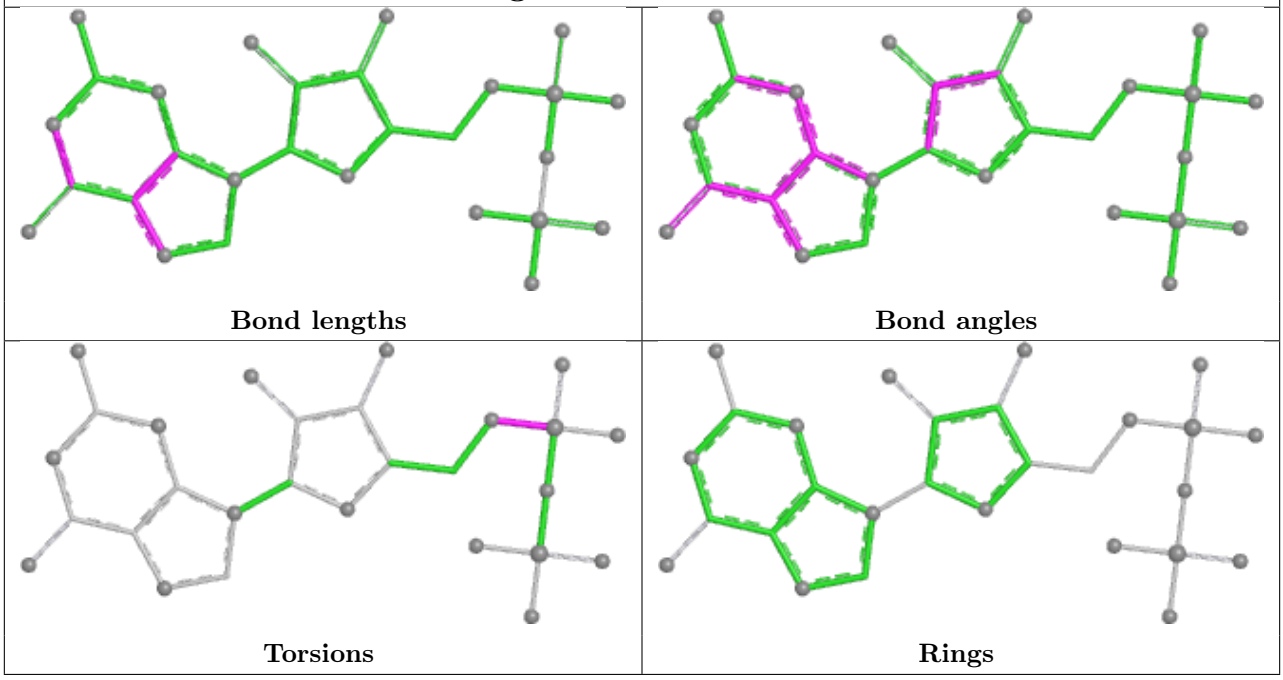


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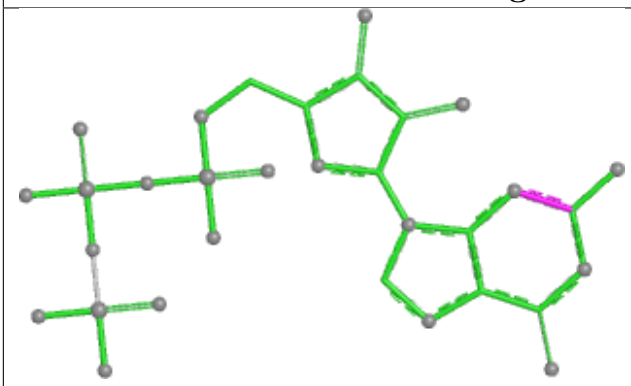
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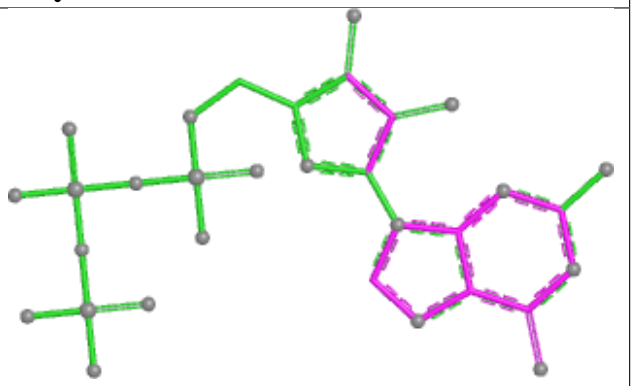
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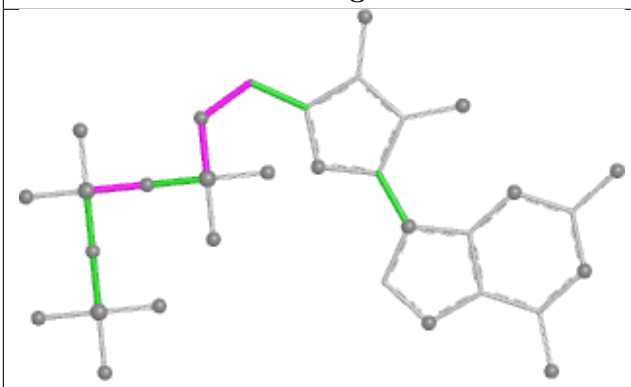
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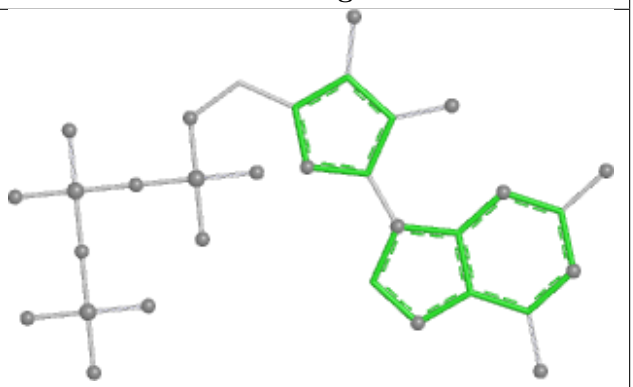
Bond lengths



Bond angles

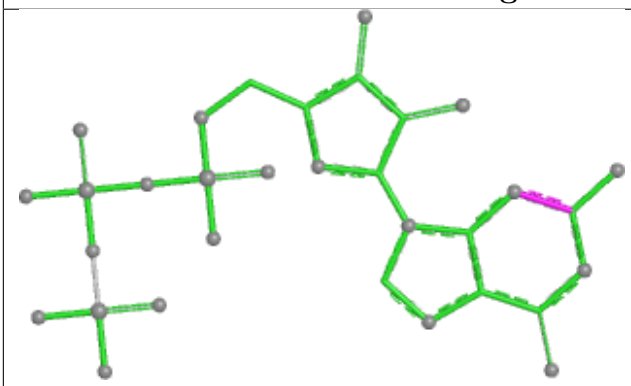


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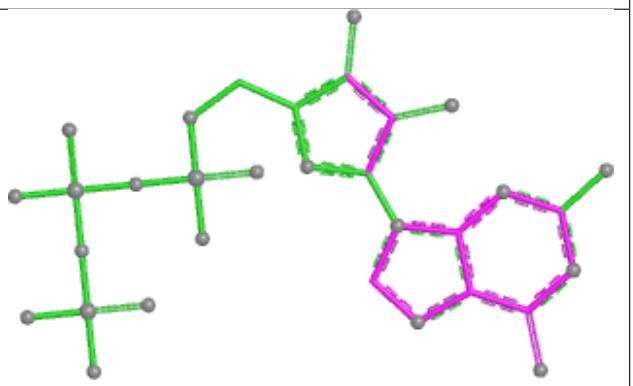


Rings

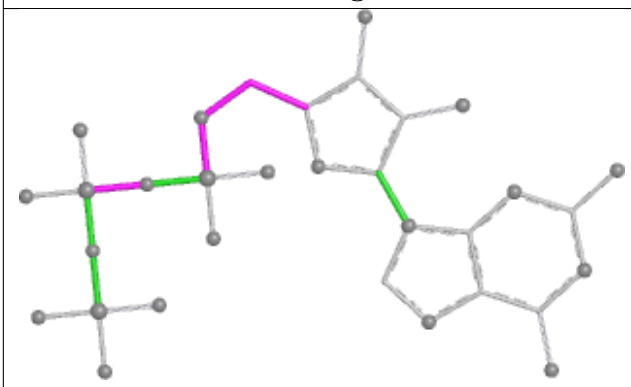
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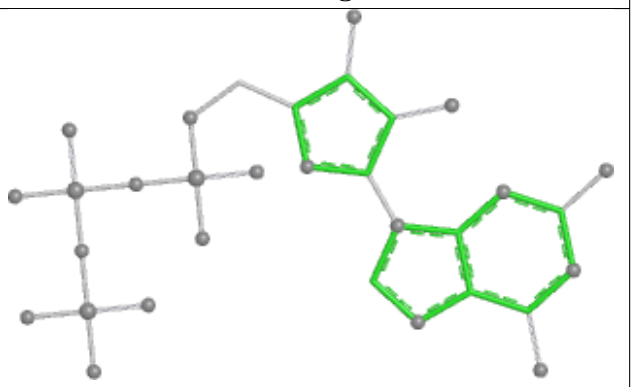
Bond lengths



Bond angles

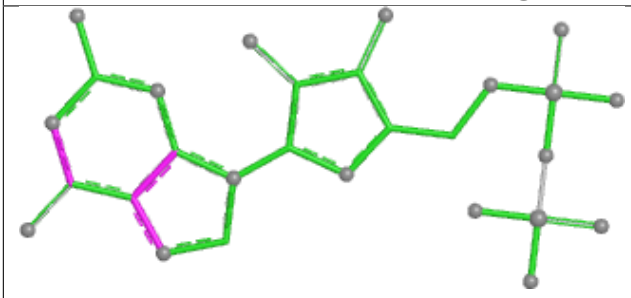


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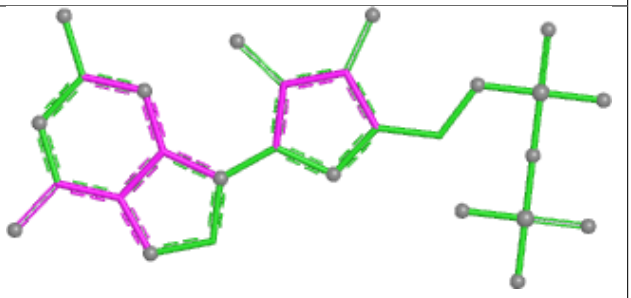


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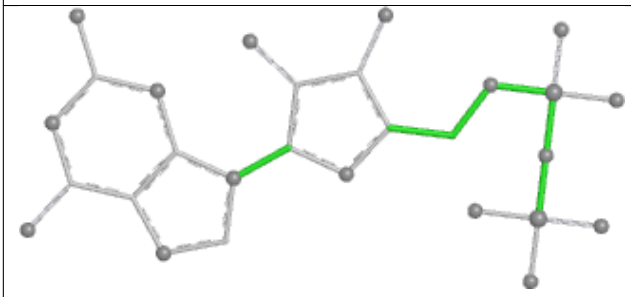
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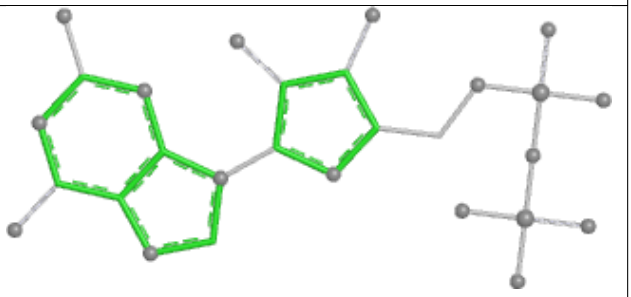
Bond lengths



Bond angles

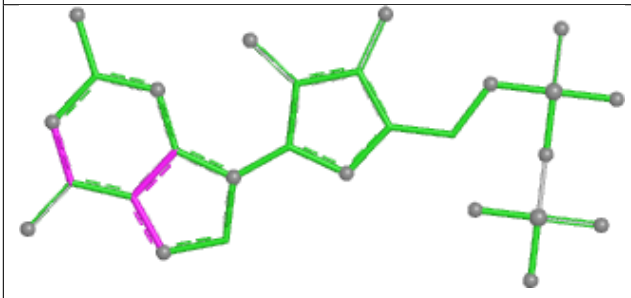


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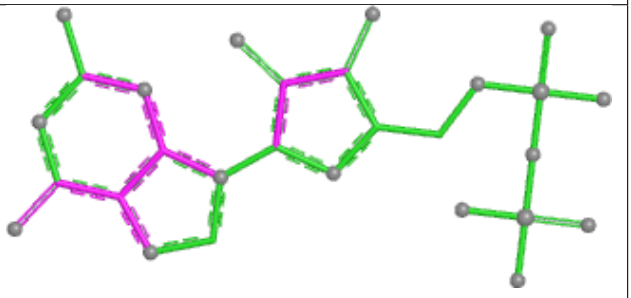


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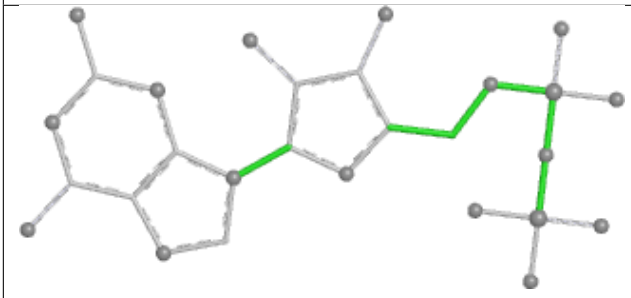
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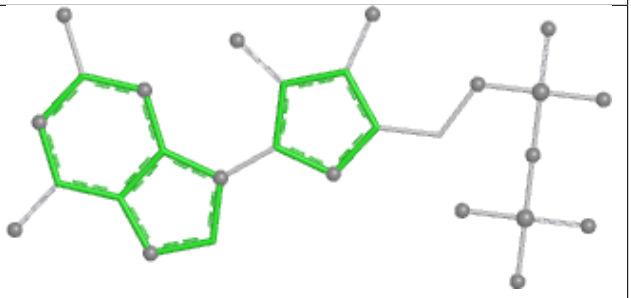
Bond lengths



Bond angles

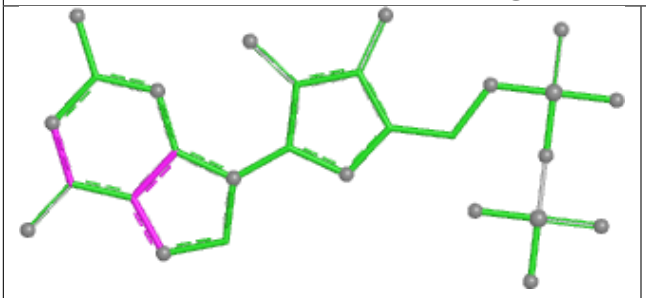


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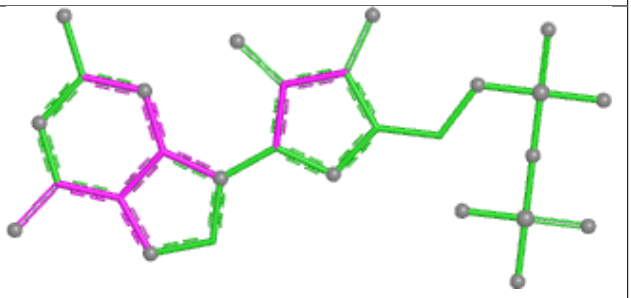


Rings

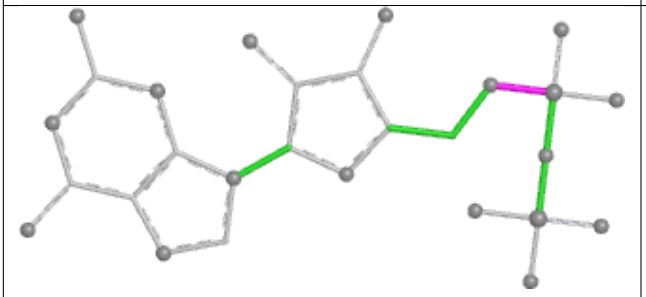
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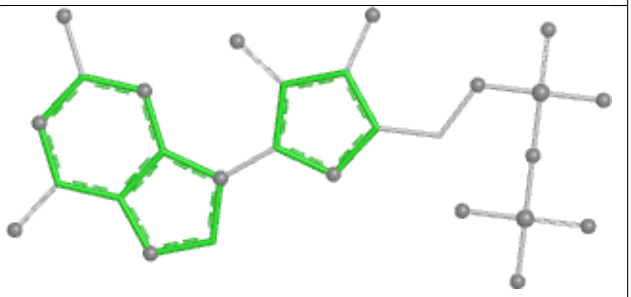
Bond lengths



Bond angles

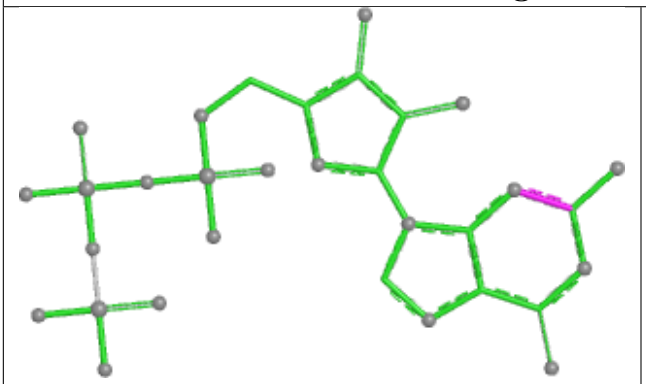


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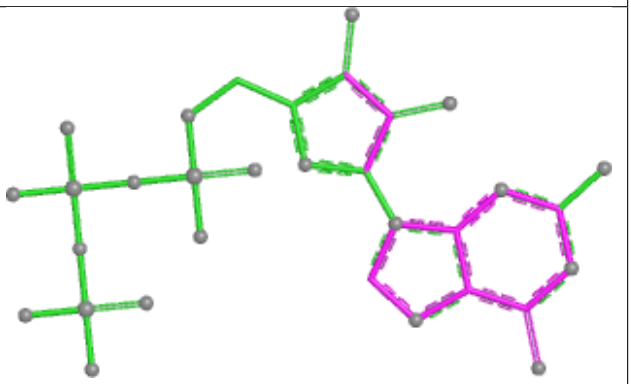


Rings

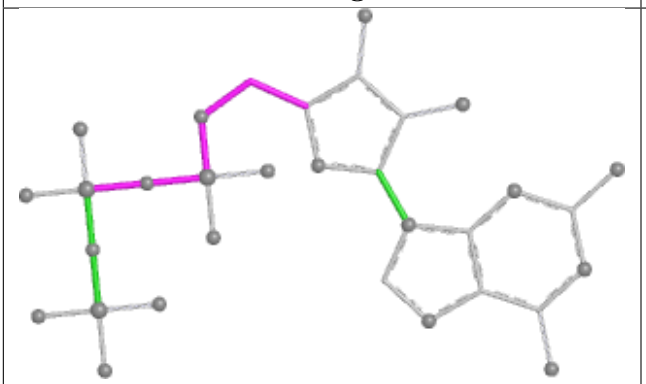
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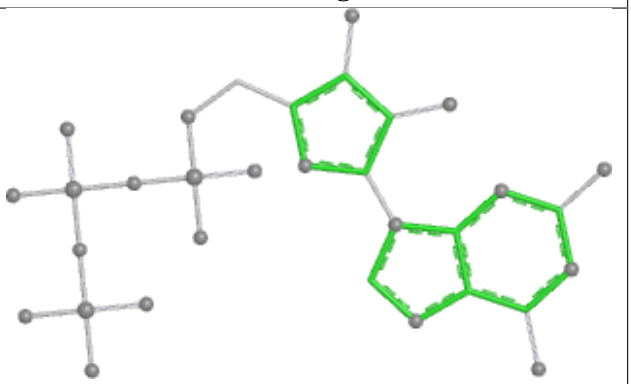
Bond lengths



Bond angles

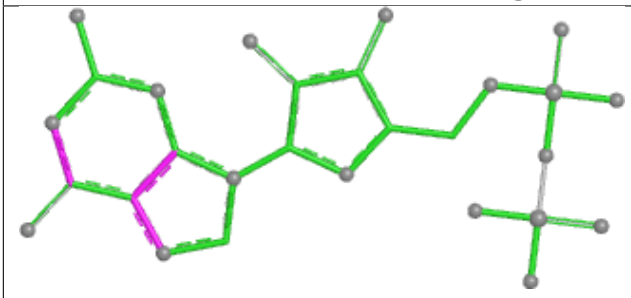


Torsions

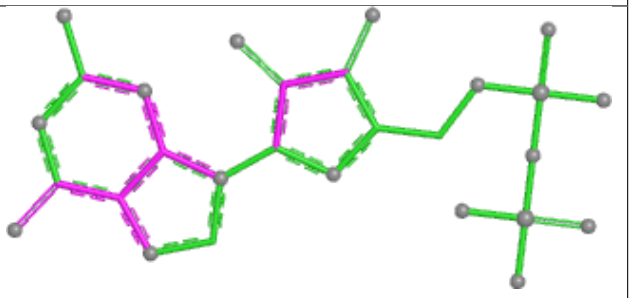


Rings

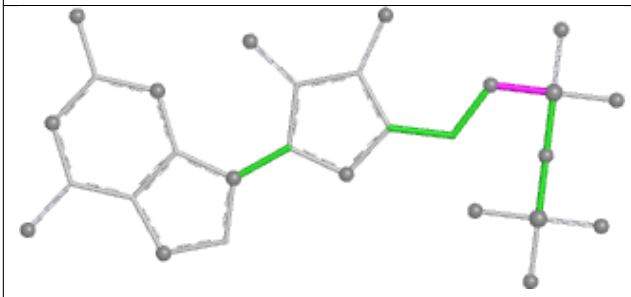
Ligand GDP HL 501



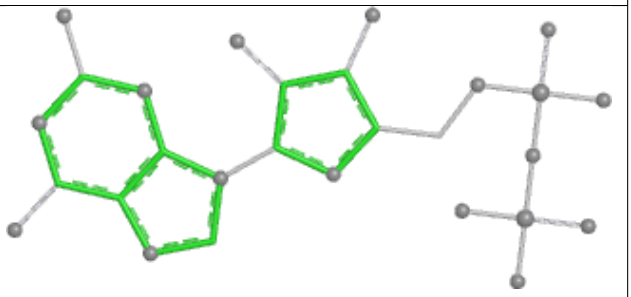
Bond lengths



Bond angles

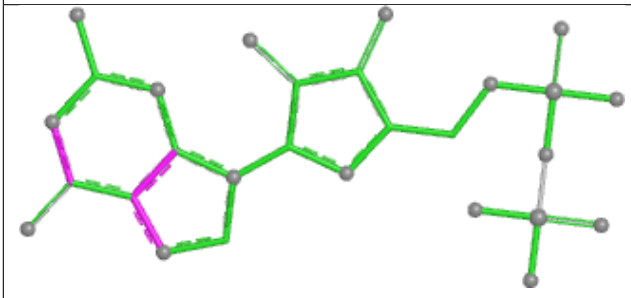


Torsions

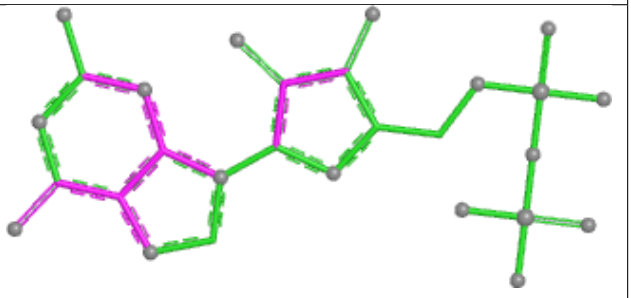


Rings

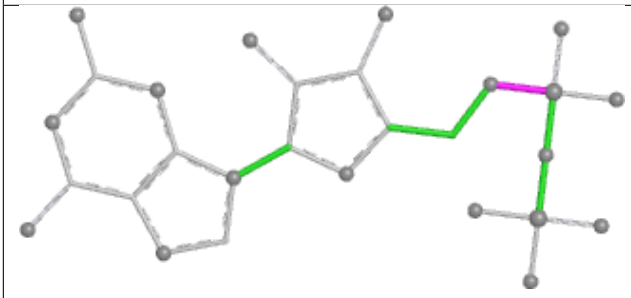
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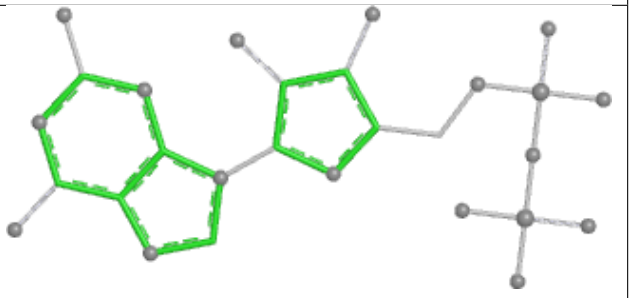
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Bond angles

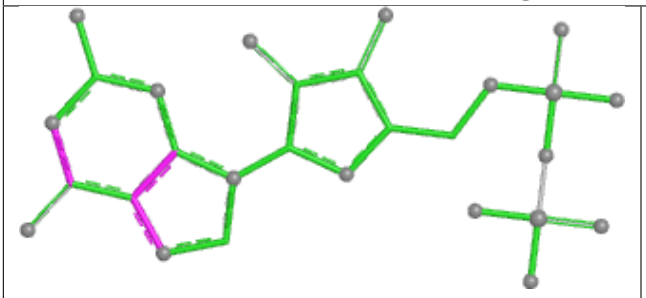


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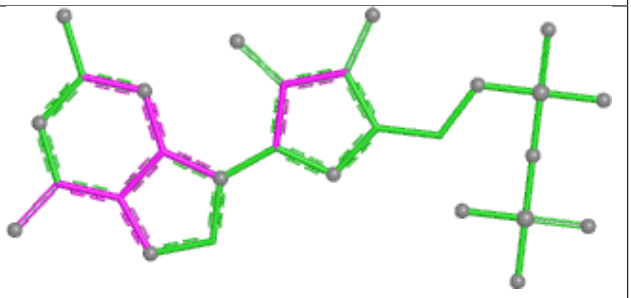


Rings

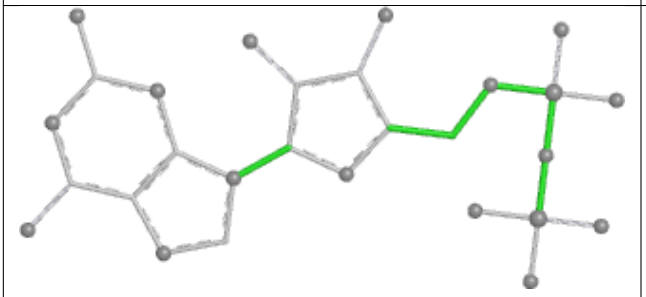
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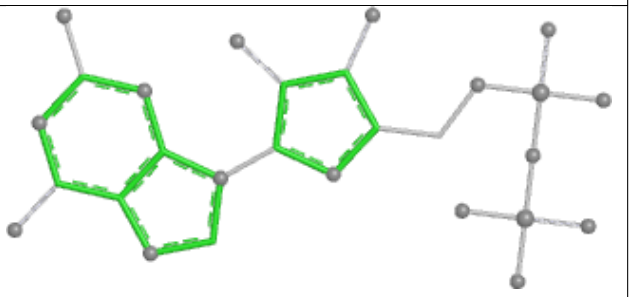
Bond lengths



Bond angles

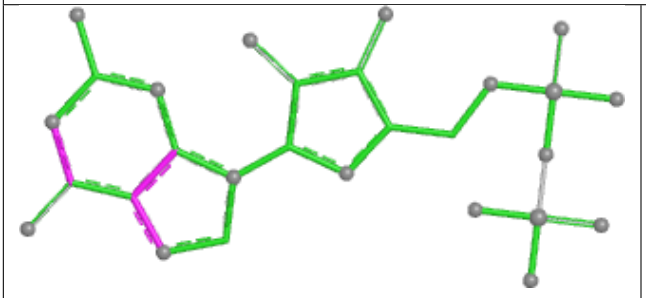


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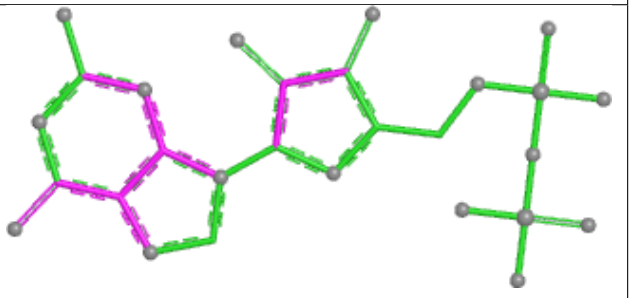


Rings

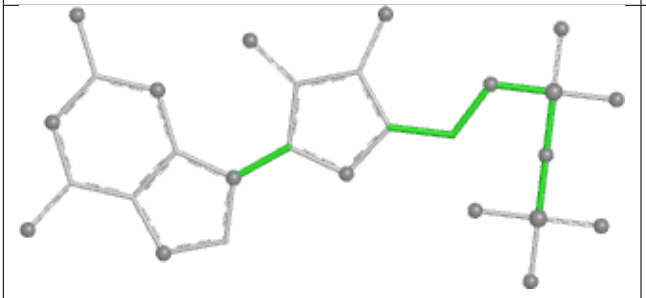
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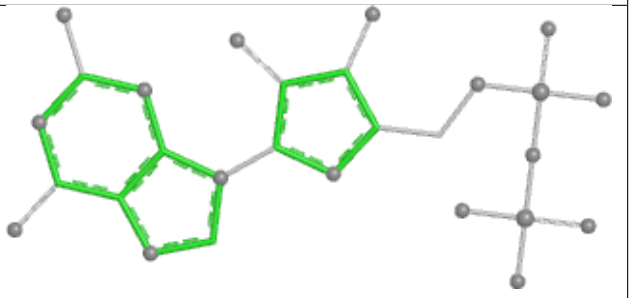
Bond lengths



Bond angles

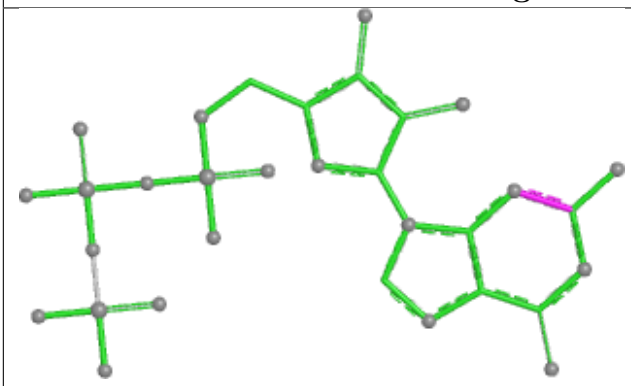


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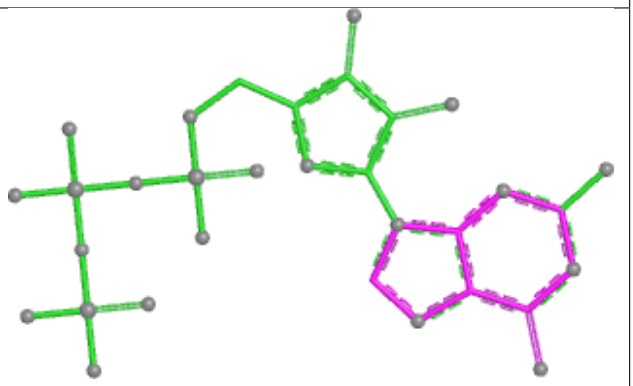


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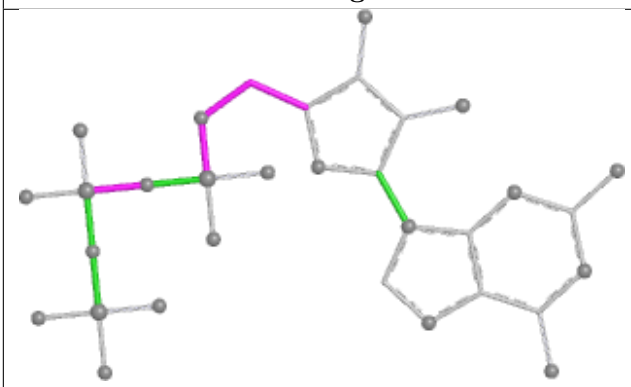
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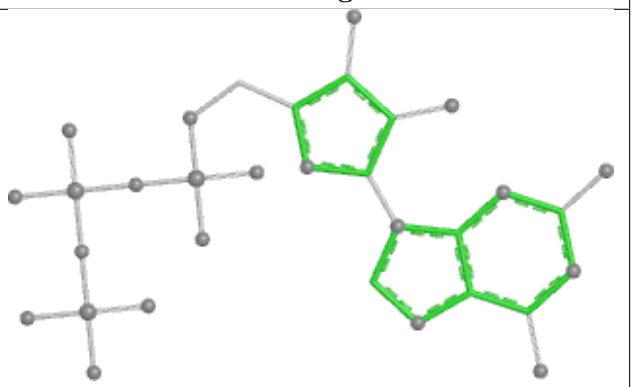
Bond lengths



Bond angles

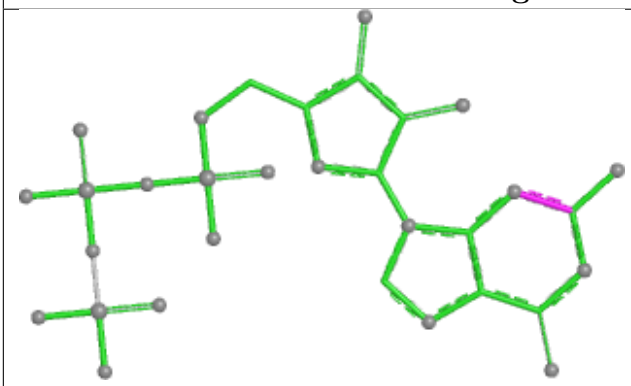


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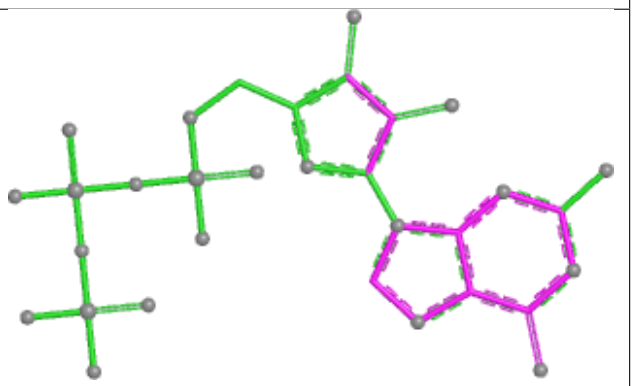


Rings

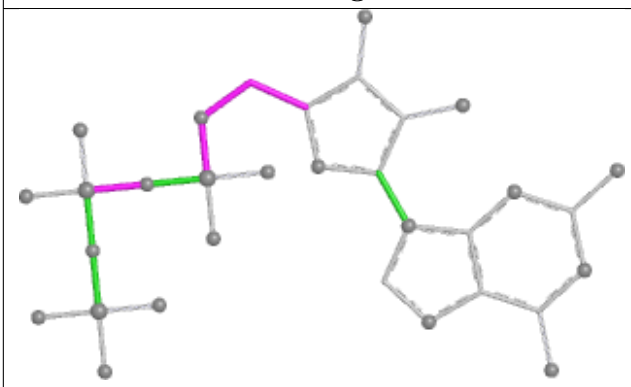
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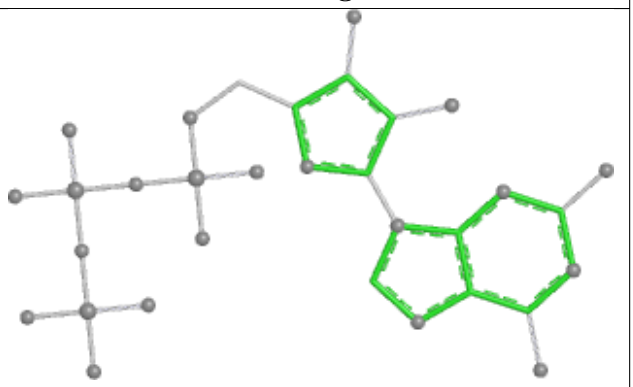
Bond lengths



Bond angles

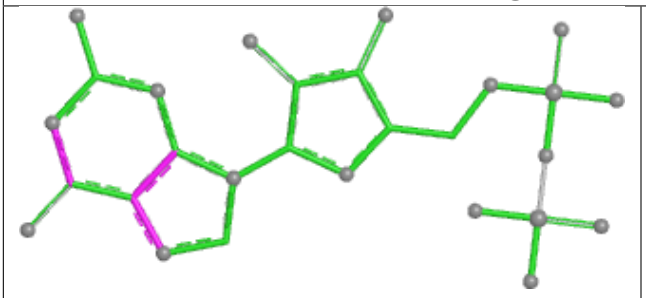


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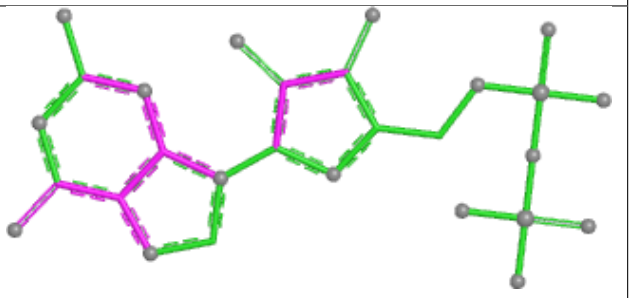


Rings

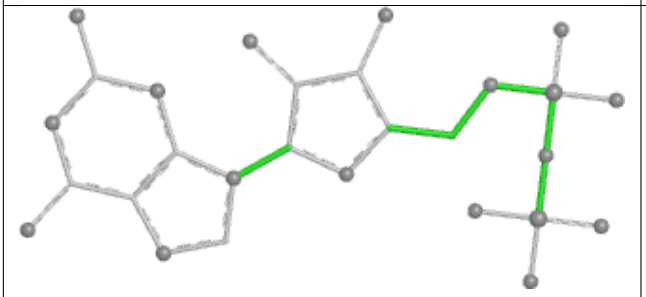
Ligand GDP DH 501



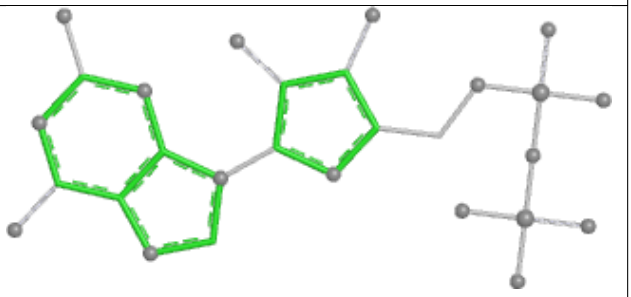
Bond lengths



Bond angles

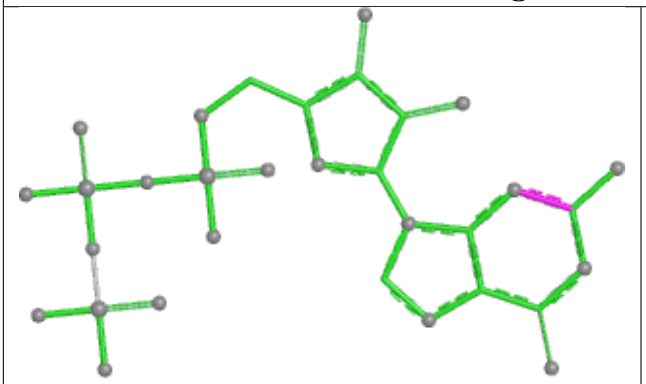


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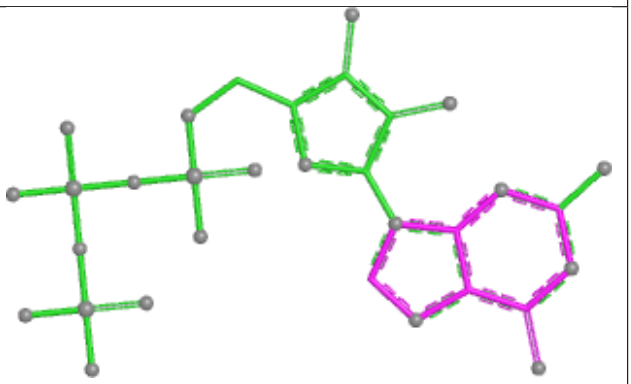


Rings

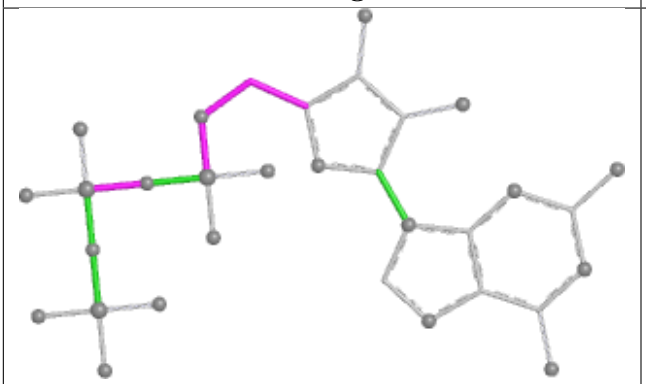
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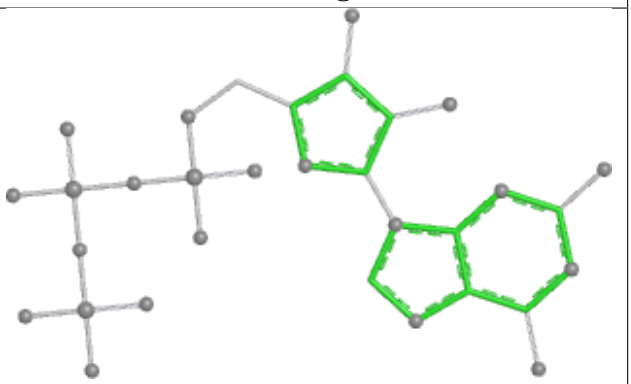
Bond lengths



Bond angles

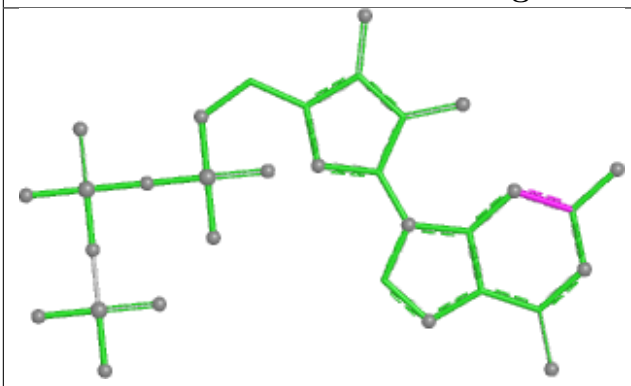


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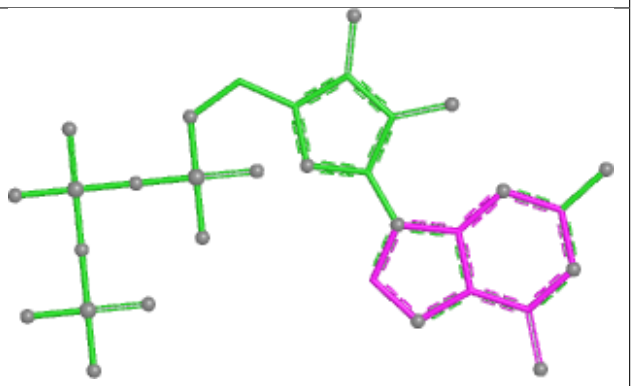


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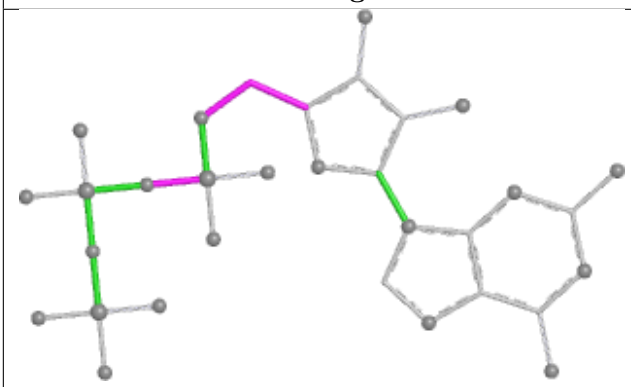
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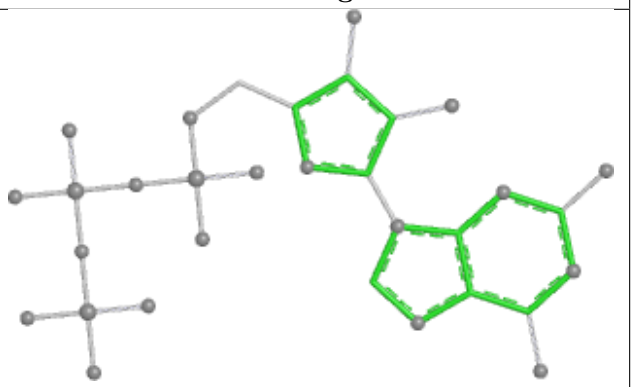
Bond lengths



Bond angles

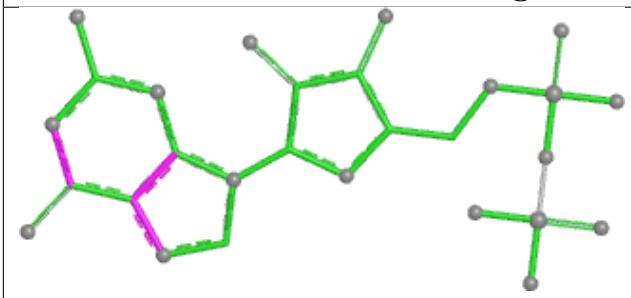


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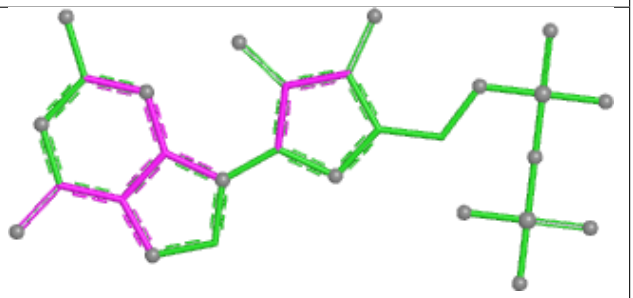


Rings

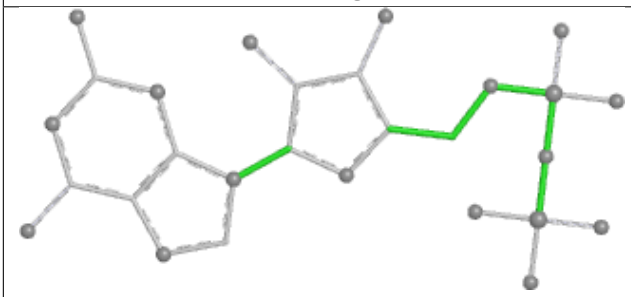
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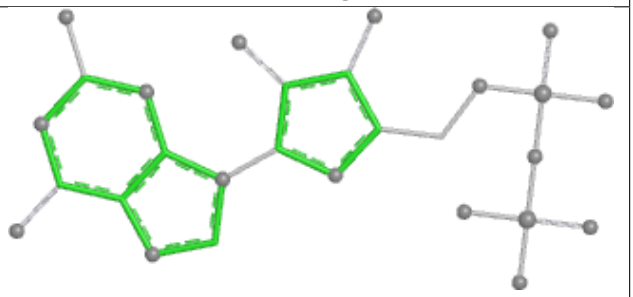
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Bond angles

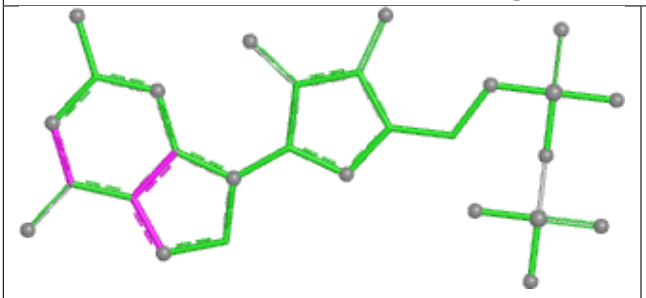


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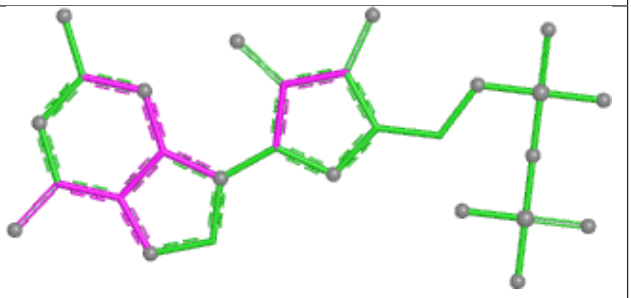


Rings

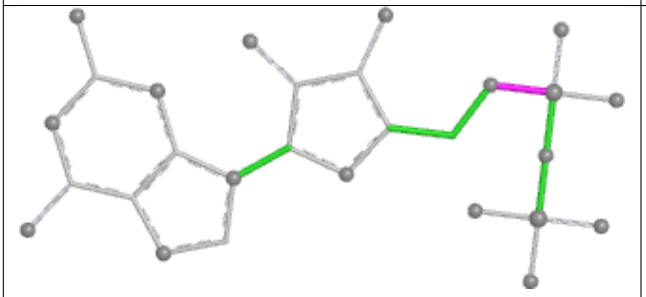
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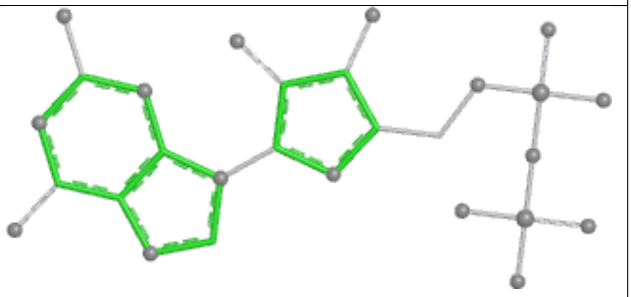
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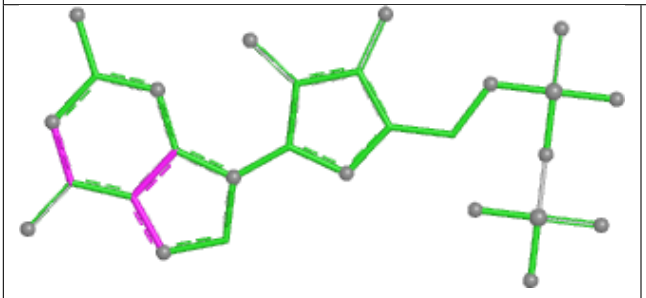


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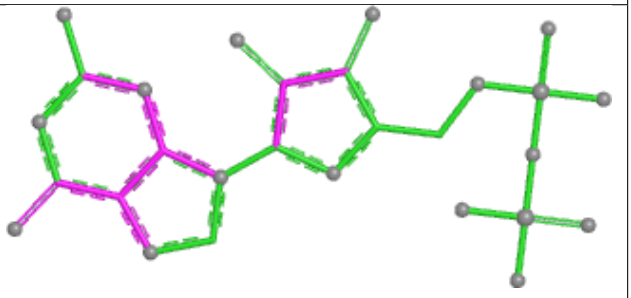


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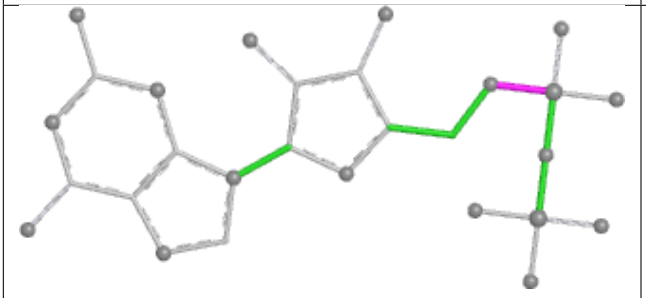
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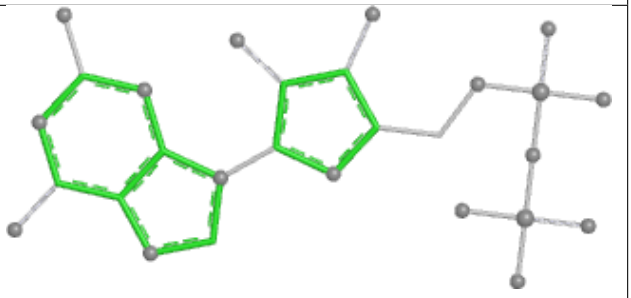
Bond lengths



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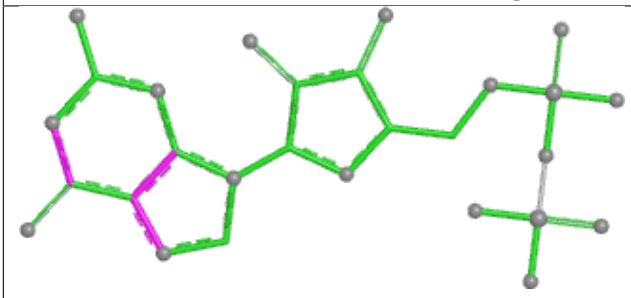


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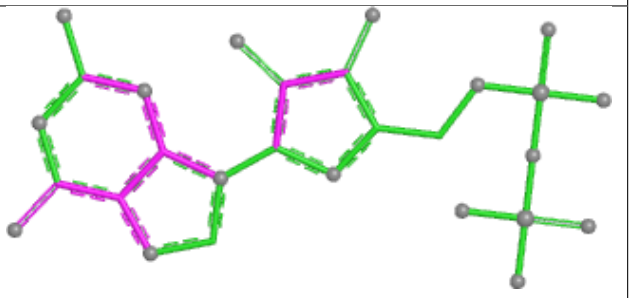


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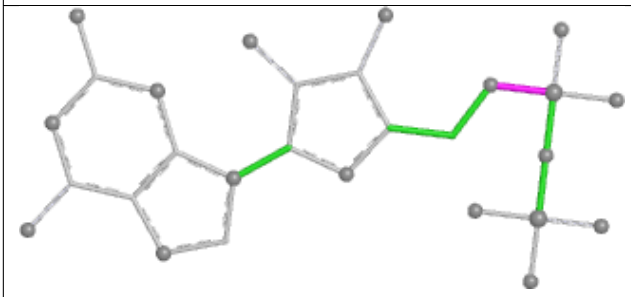
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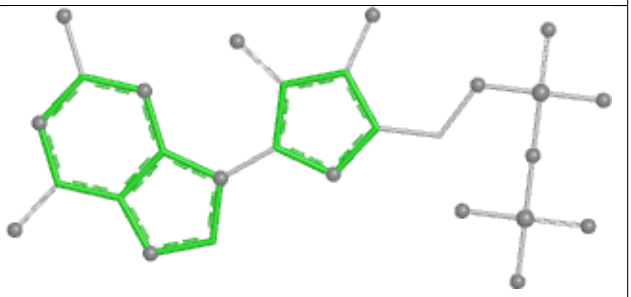
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Bond angles

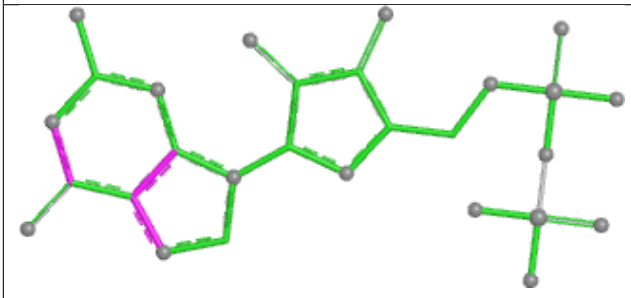


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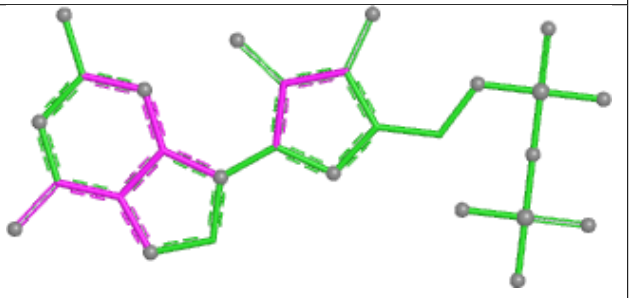


Rings

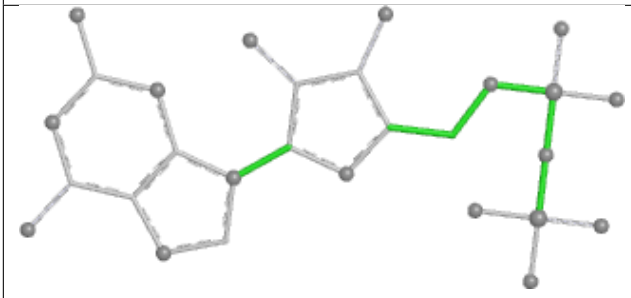
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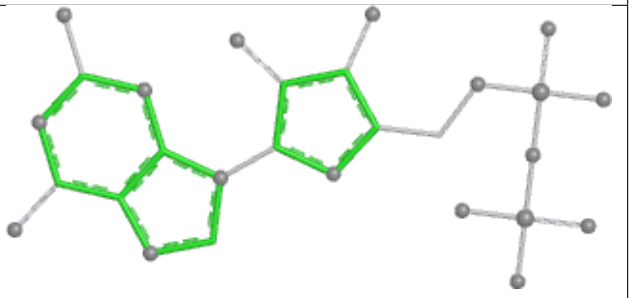
Bond lengths



Bond angles

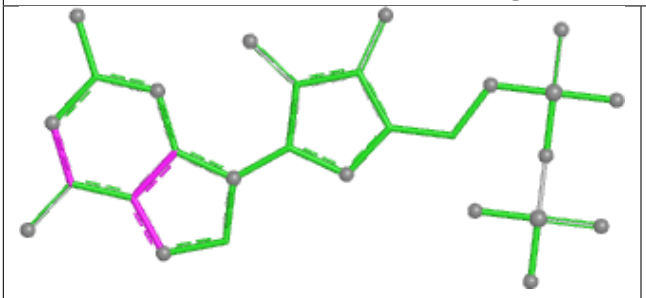


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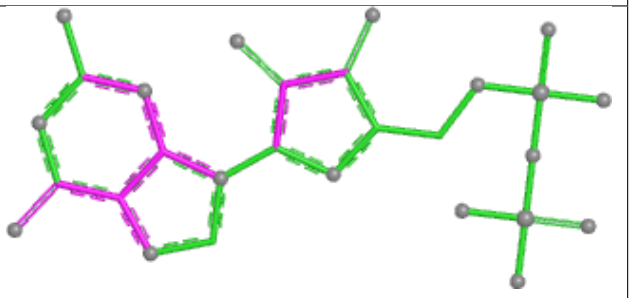


Rings

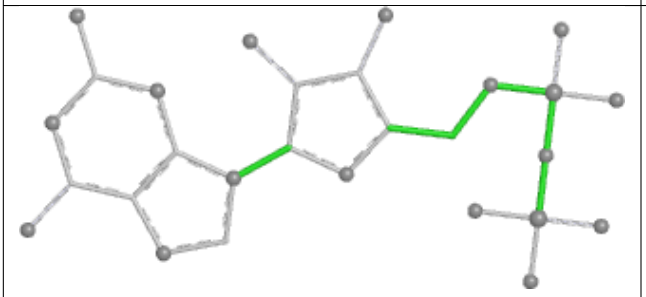
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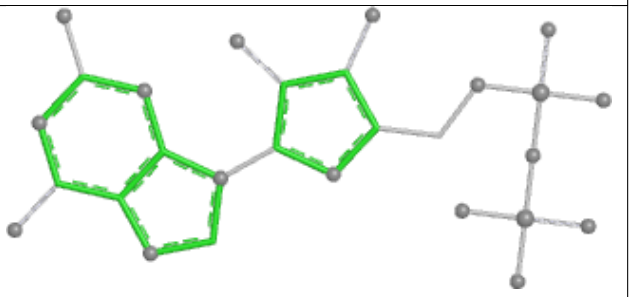
Bond lengths



Bond angles

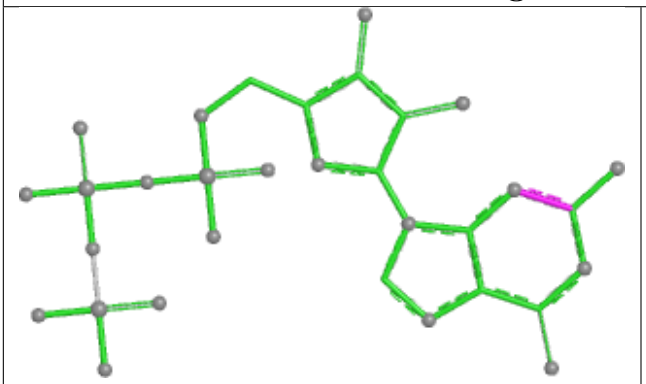


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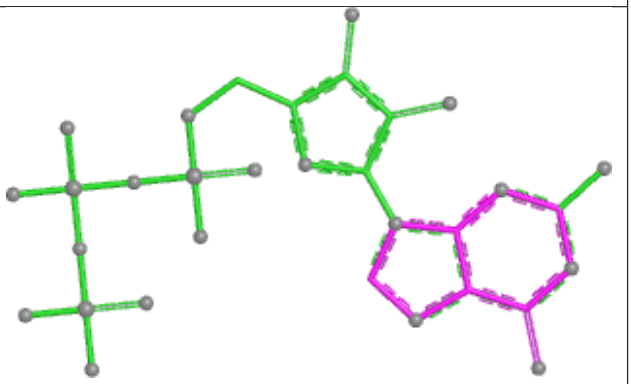


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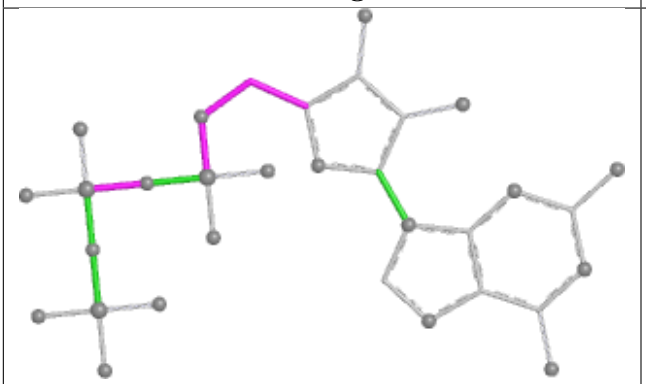
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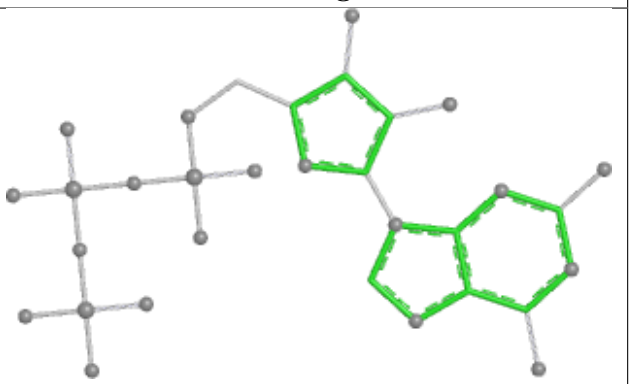
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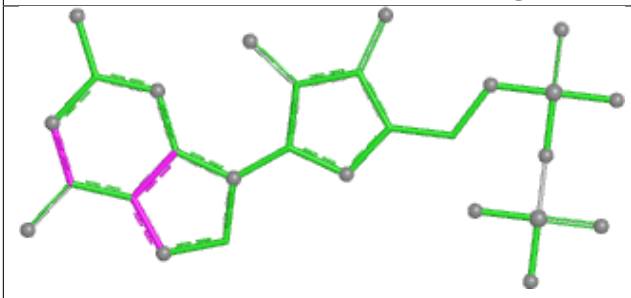


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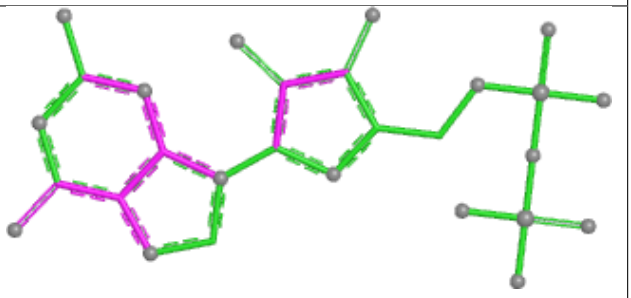


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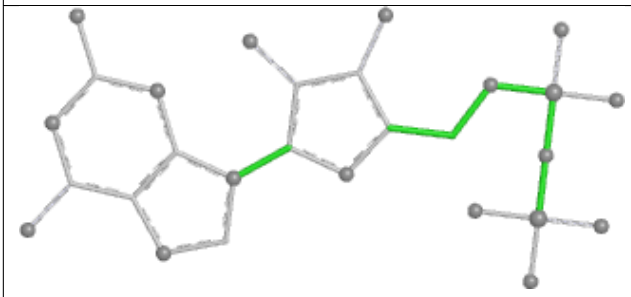
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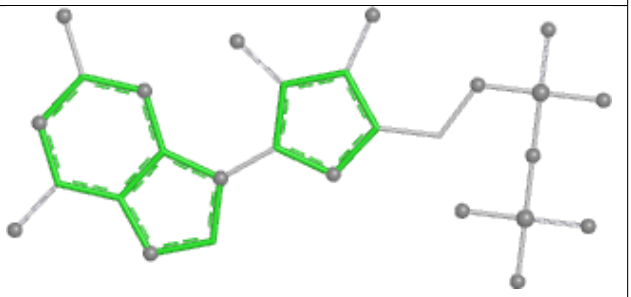
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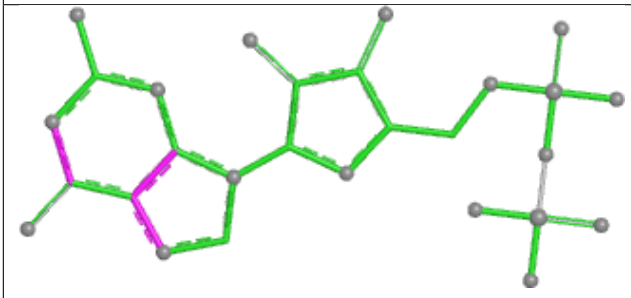


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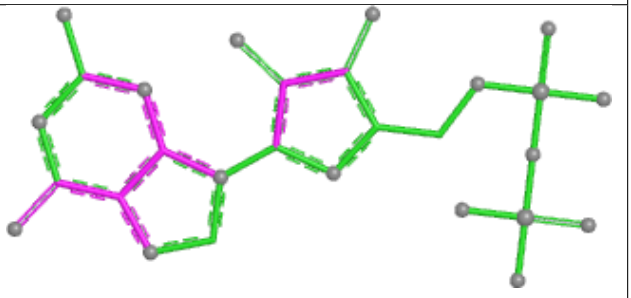


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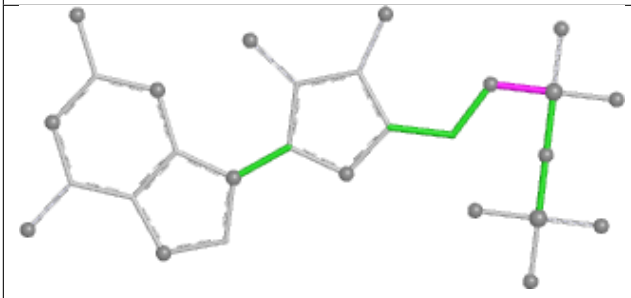
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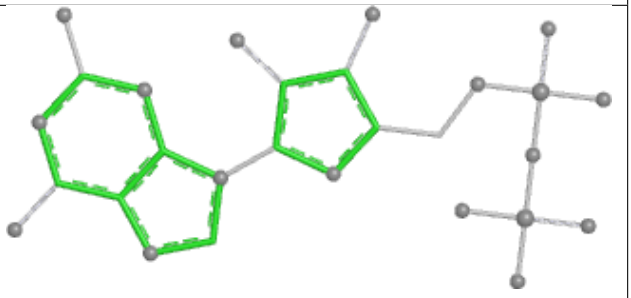
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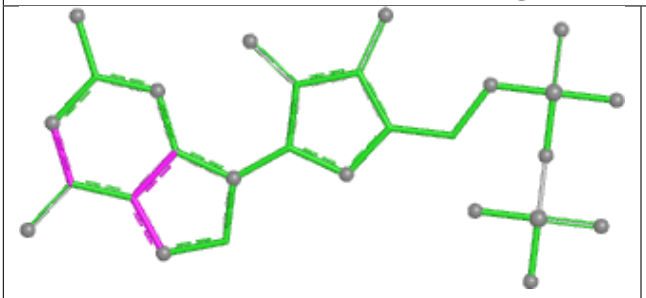


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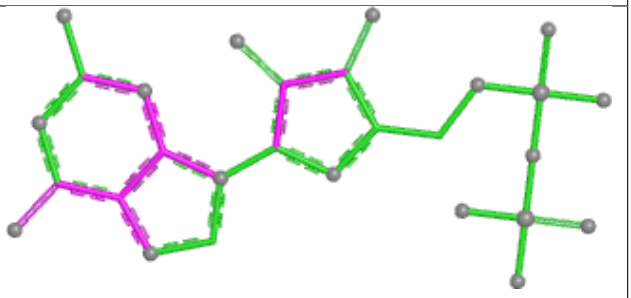


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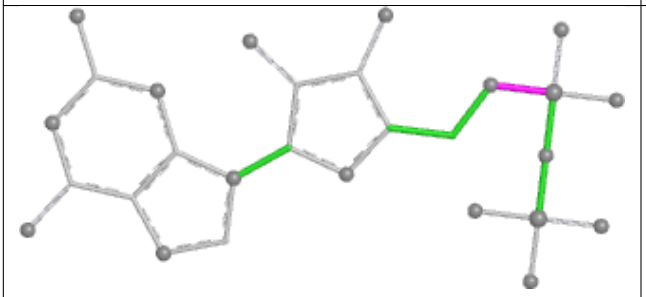
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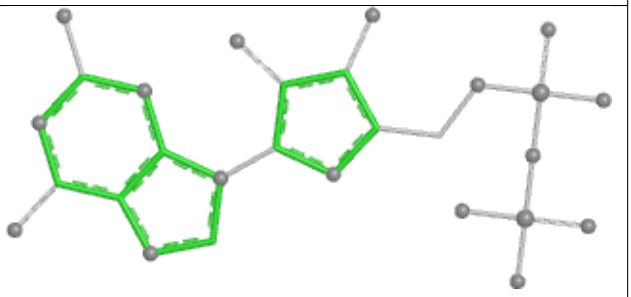
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Bond angles

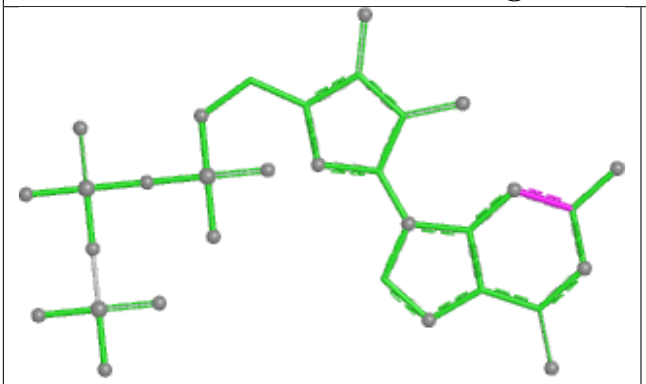


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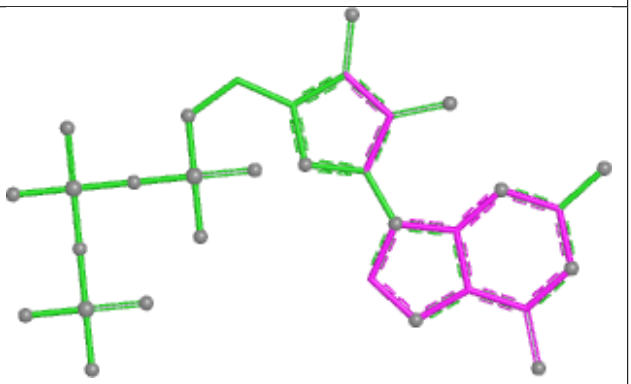


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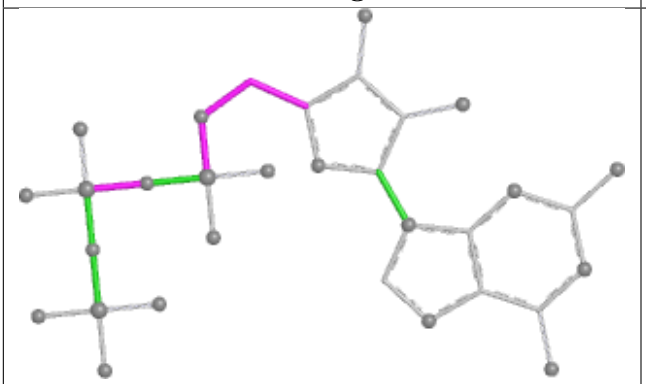
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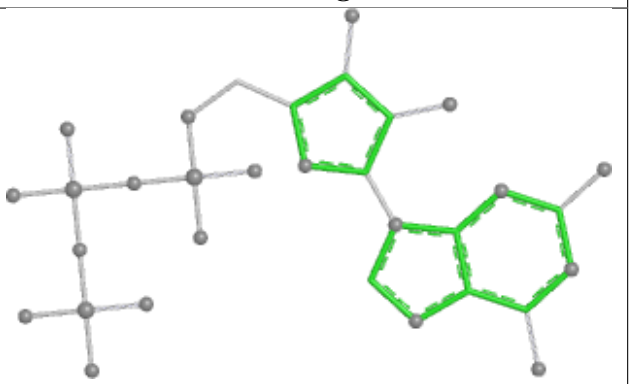
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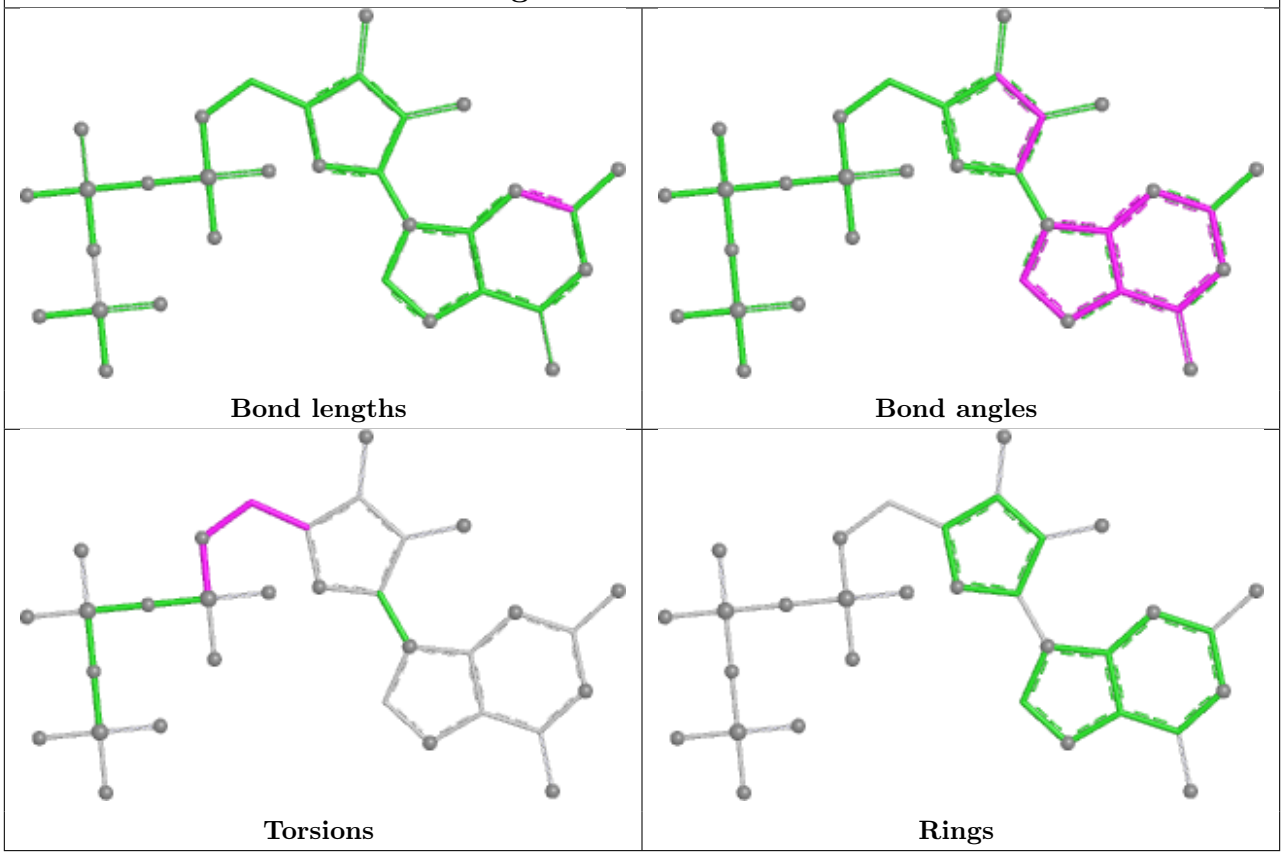


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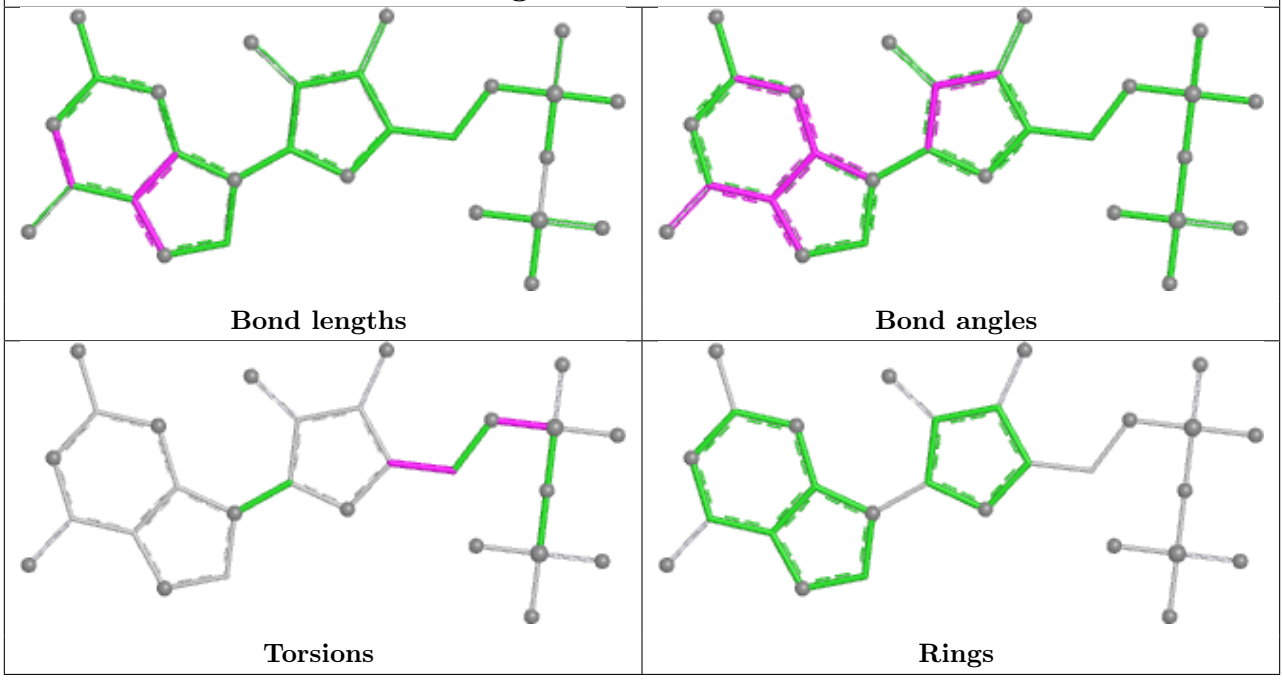


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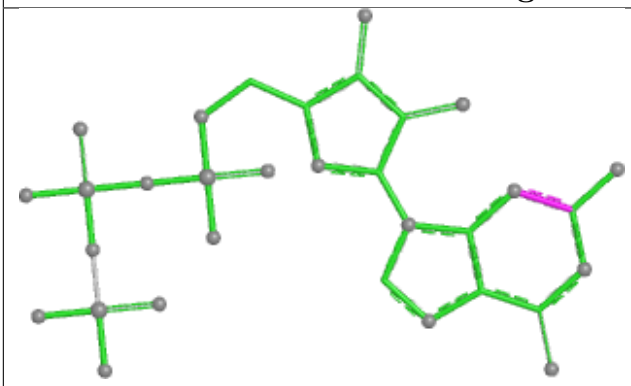
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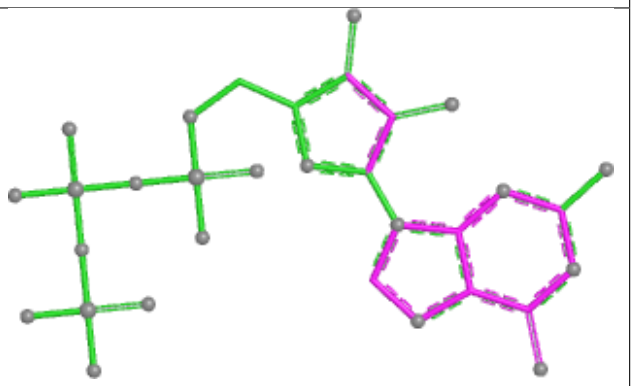
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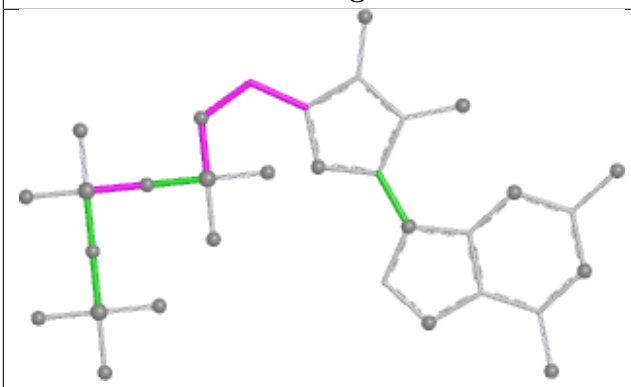
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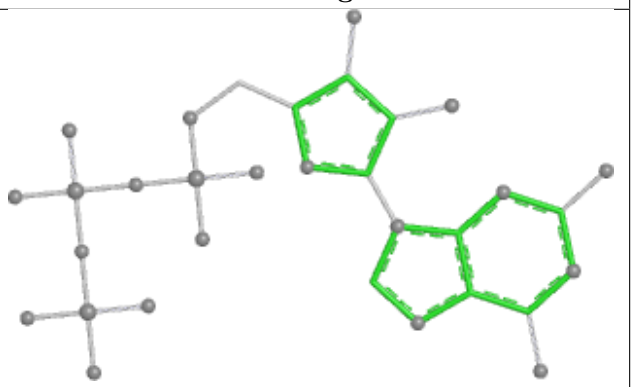
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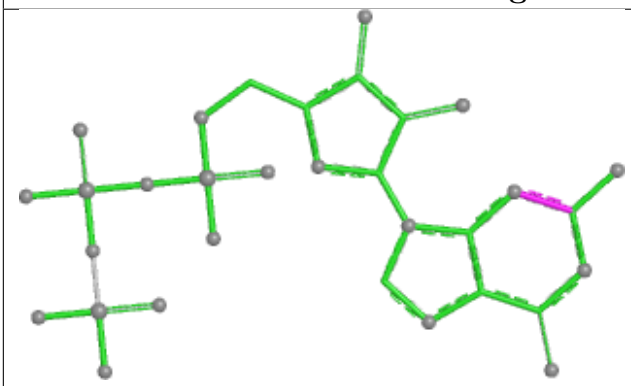


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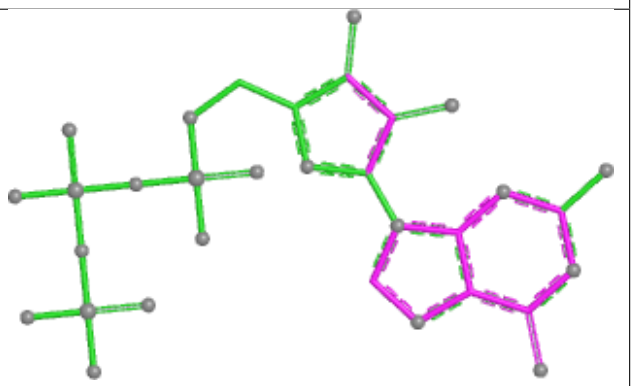


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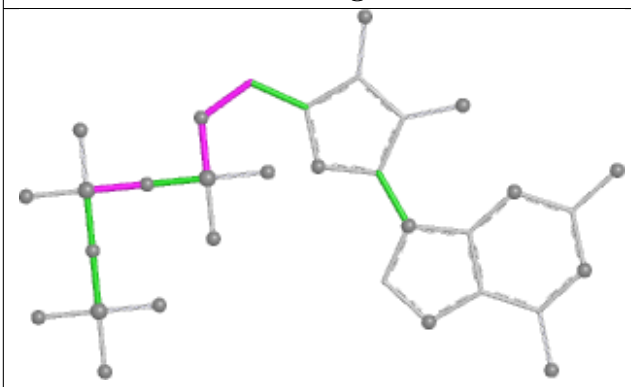
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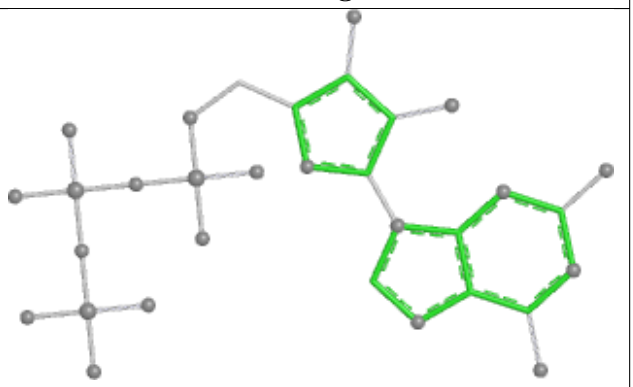
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Bond angles

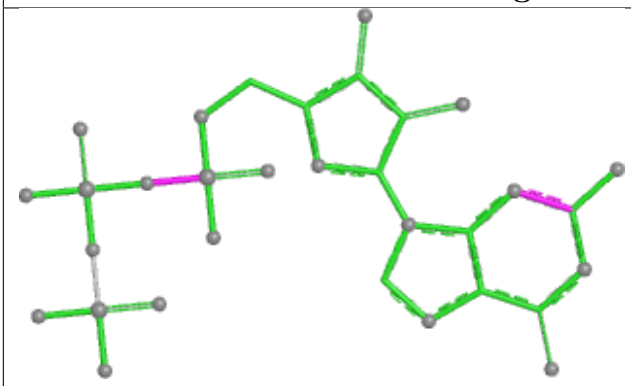


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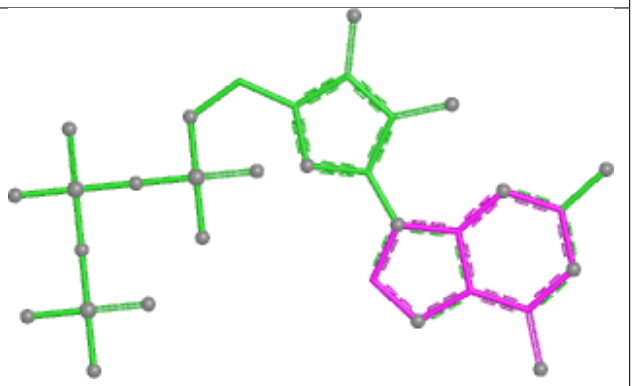


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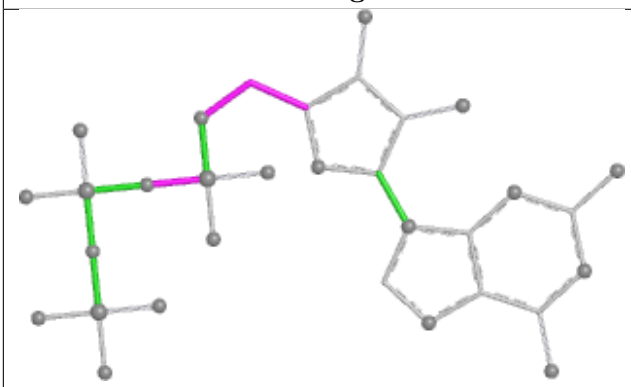
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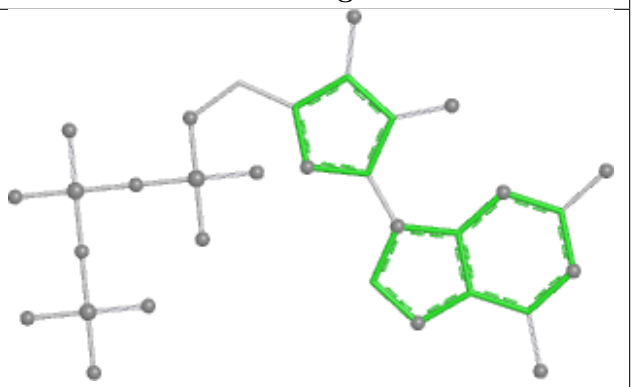
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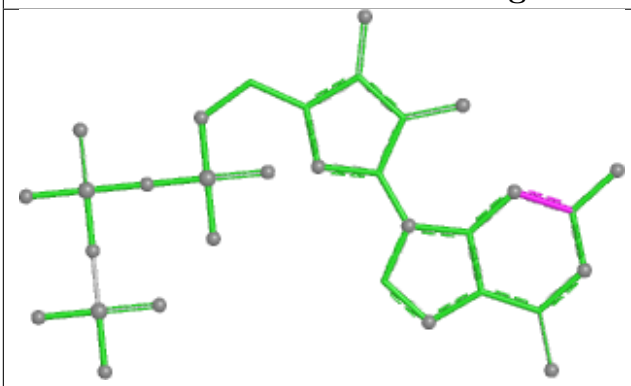


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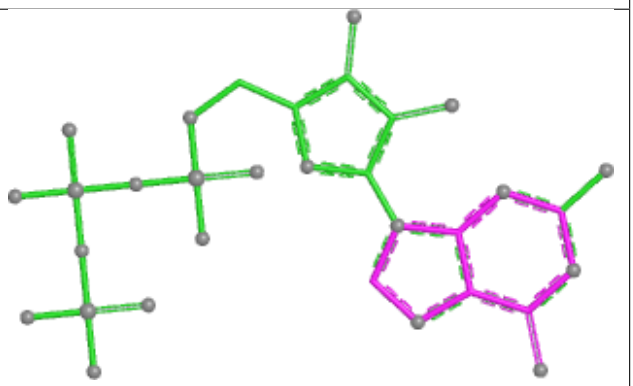


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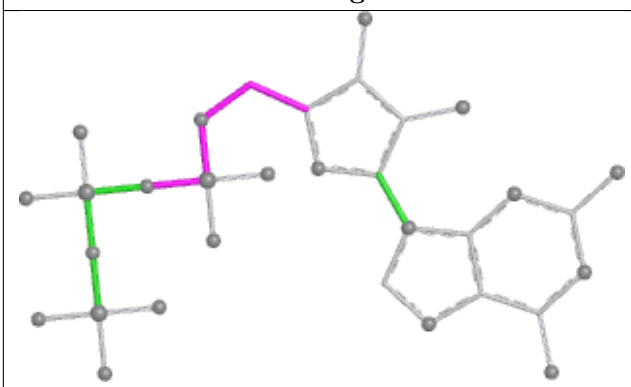
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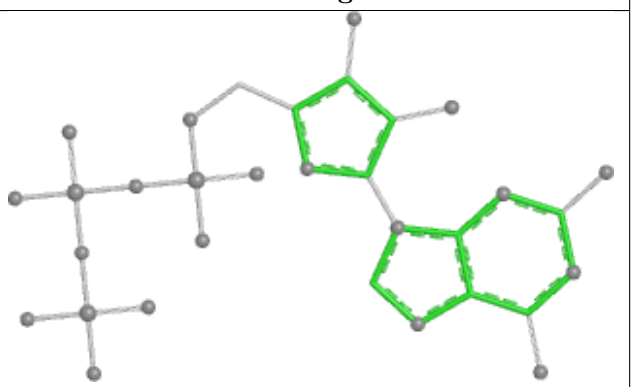
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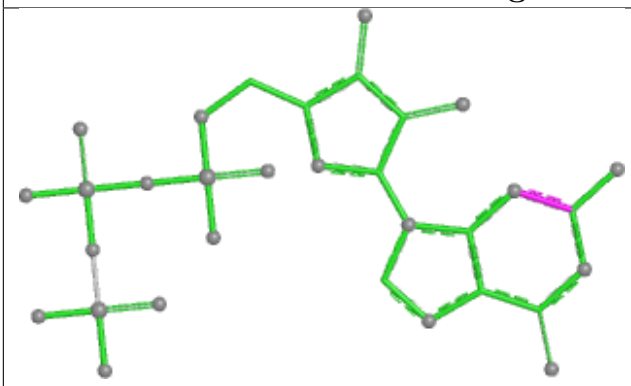


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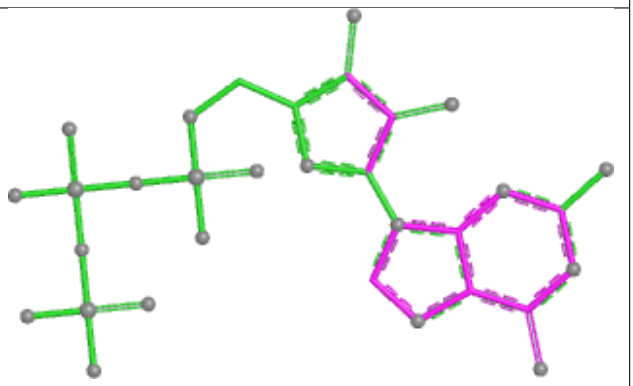


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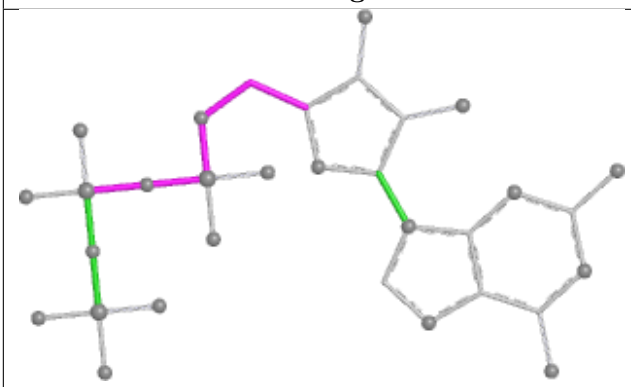
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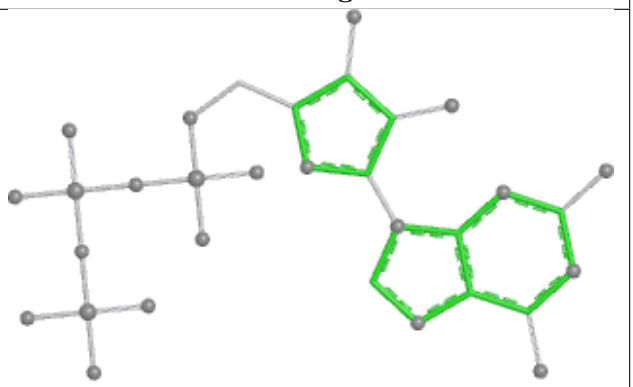
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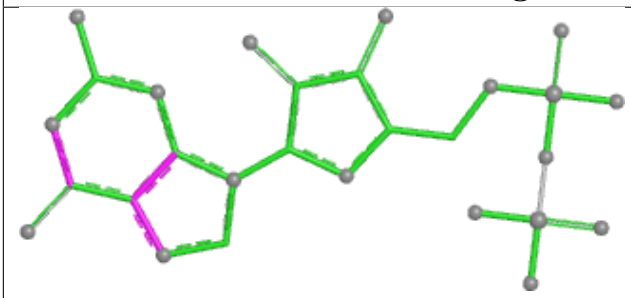


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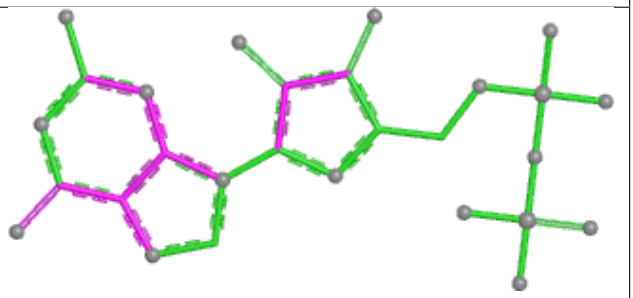


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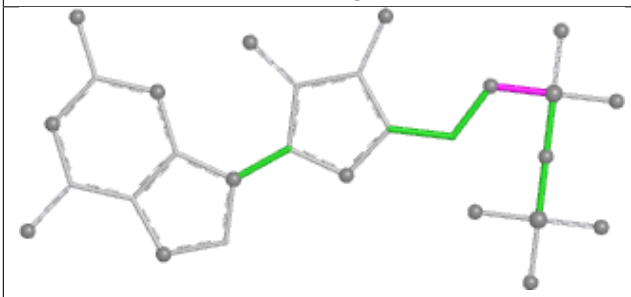
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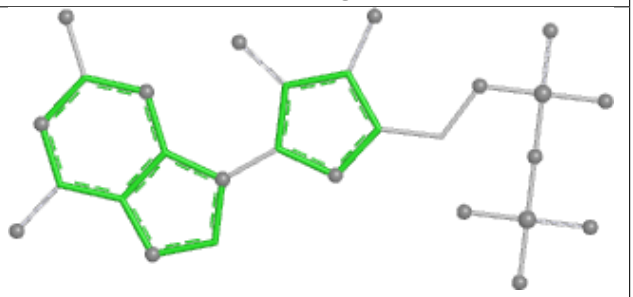
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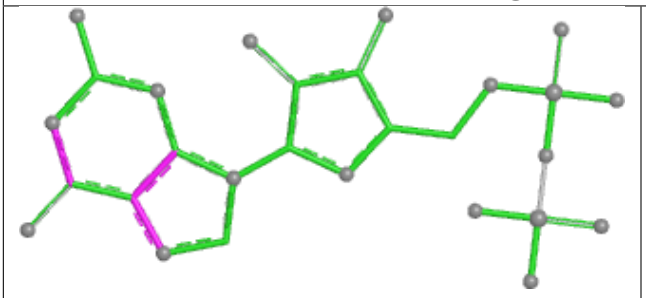


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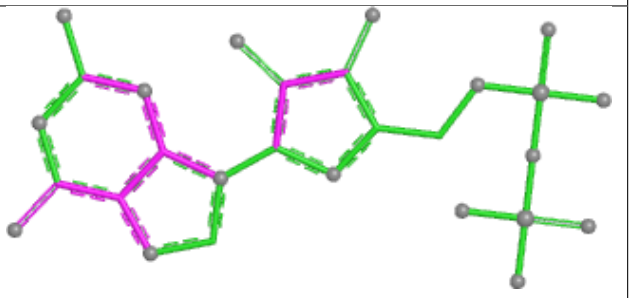


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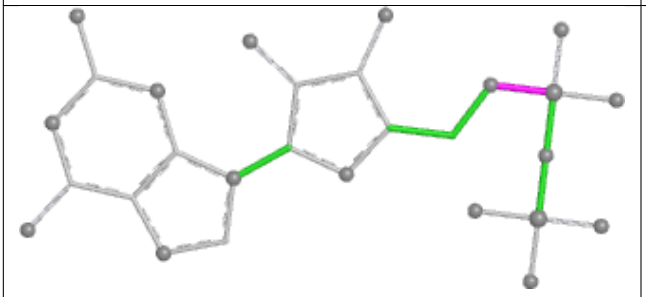
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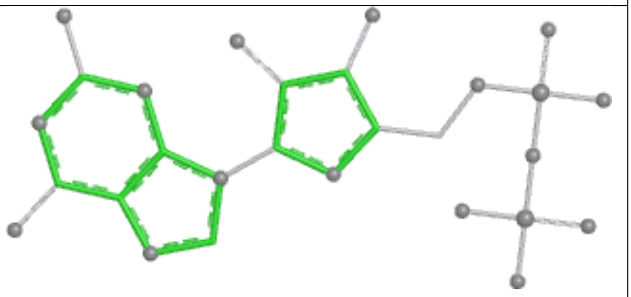
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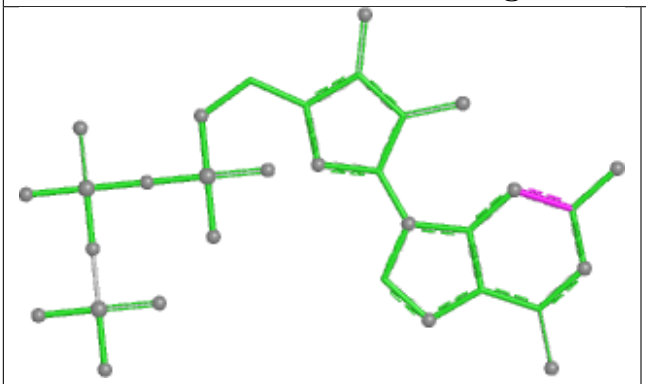


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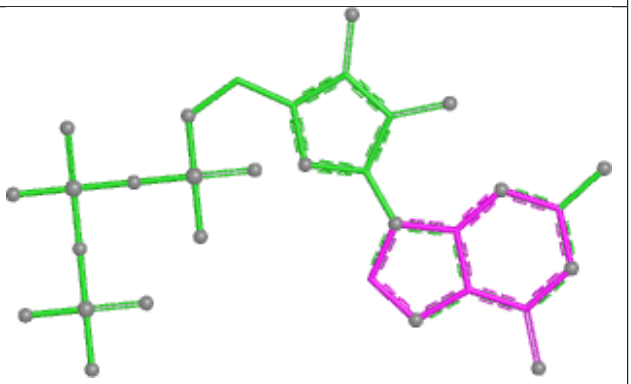


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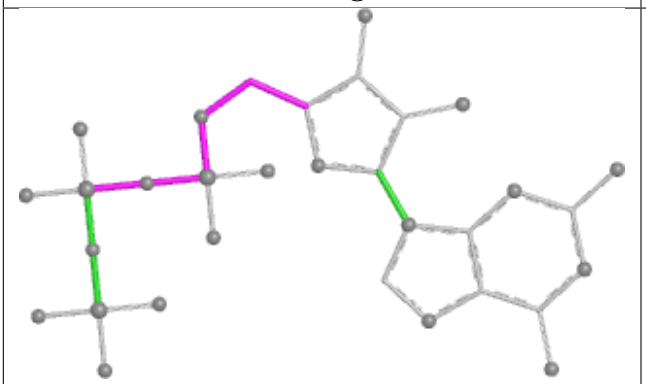
Ligand GTP WK 501



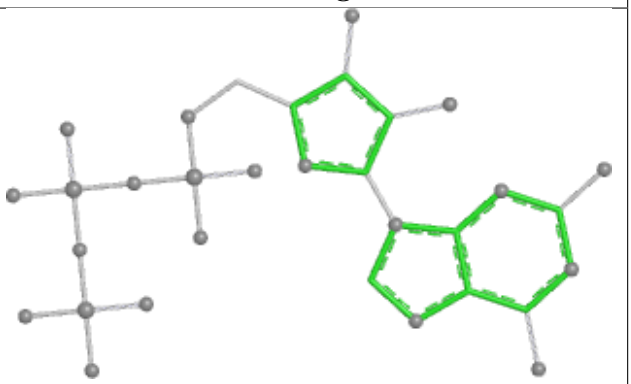
Bond lengths



Bond angles

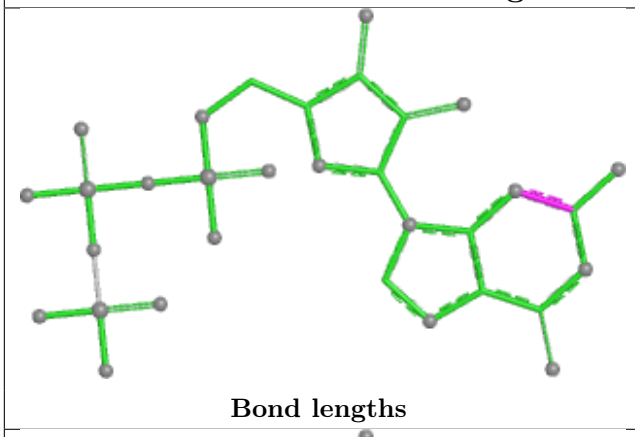


Torsions

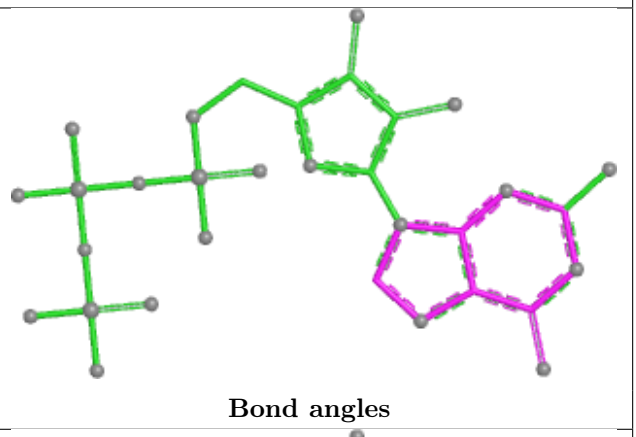


Rings

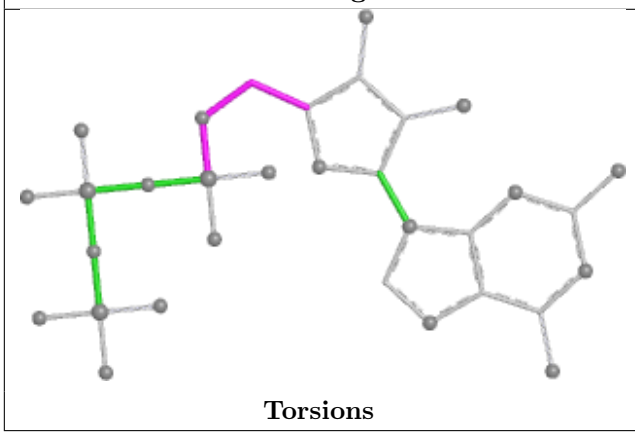
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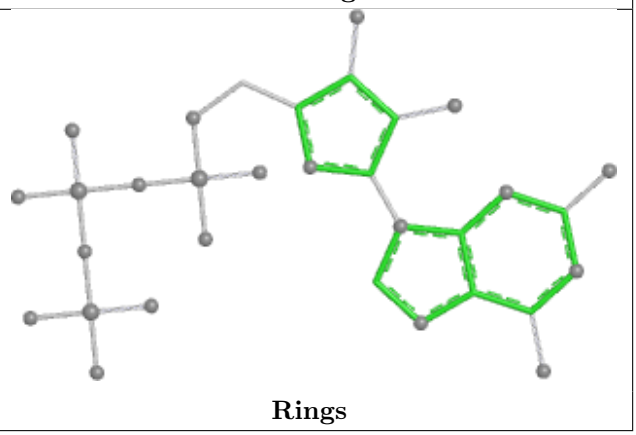
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Bond angles

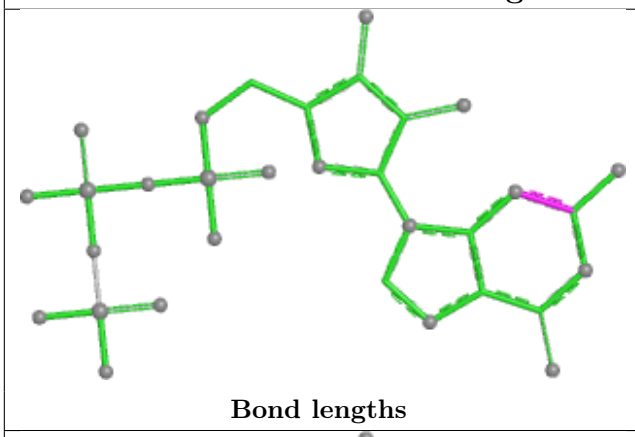


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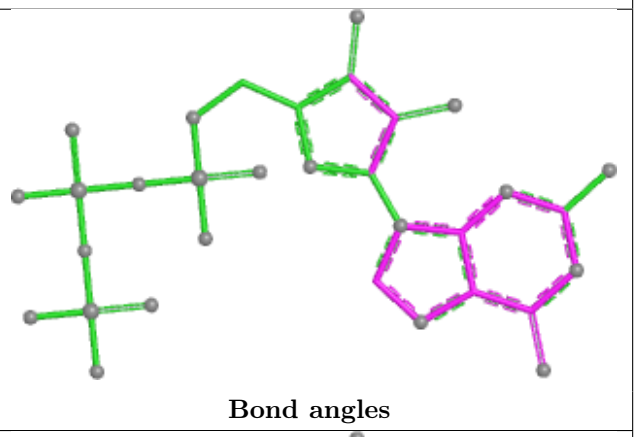


Rings

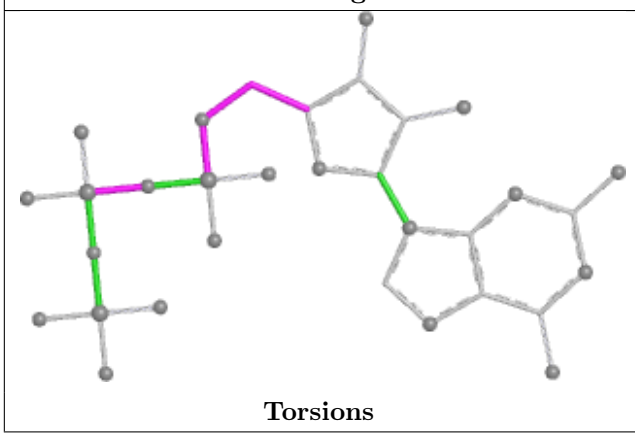
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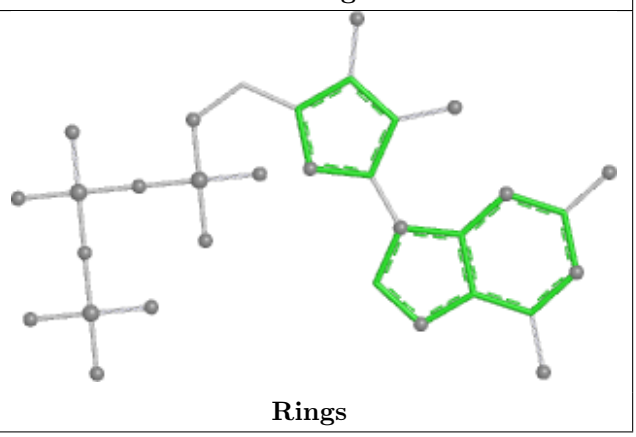
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Bond angles

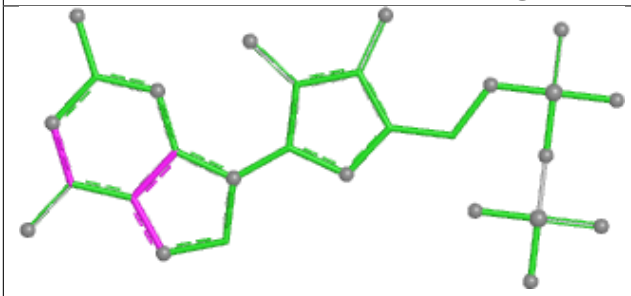


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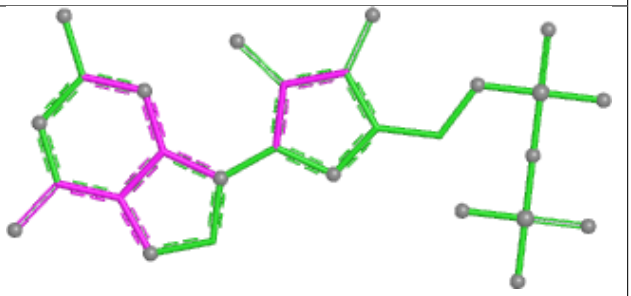


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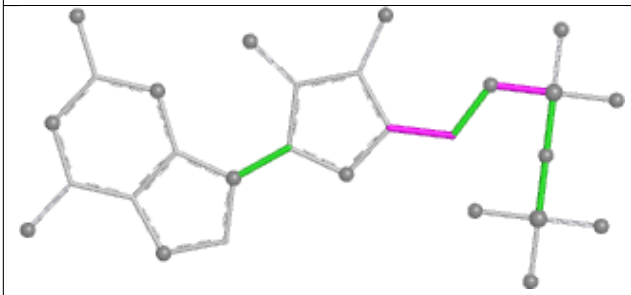
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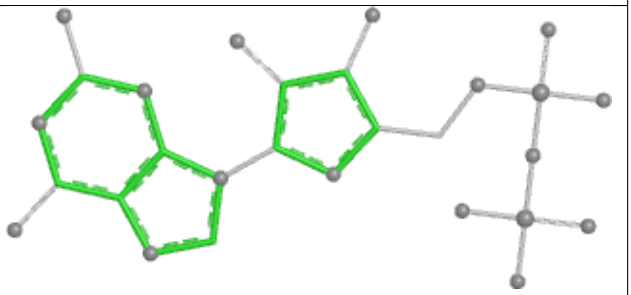
Bond lengths



Bond angles

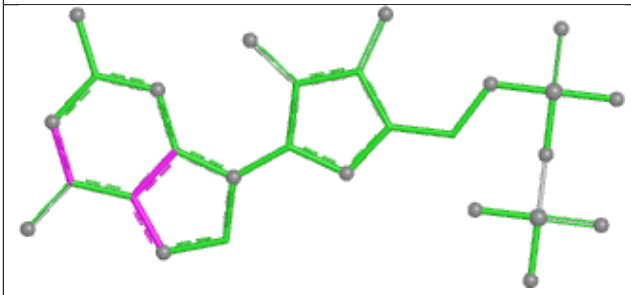


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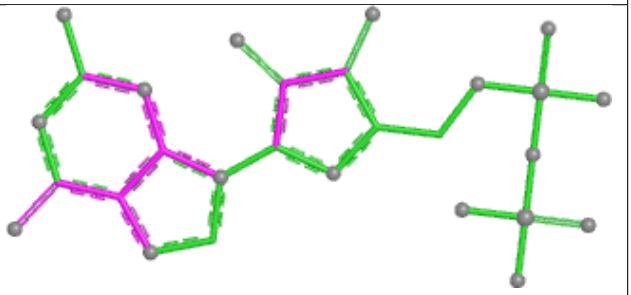


Rings

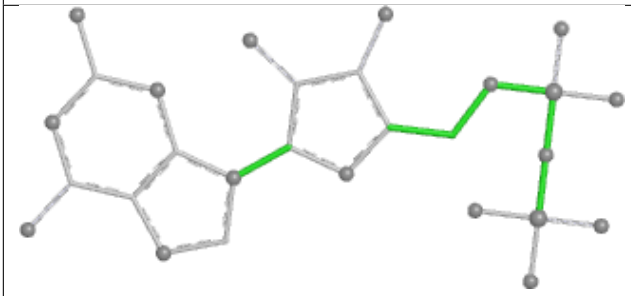
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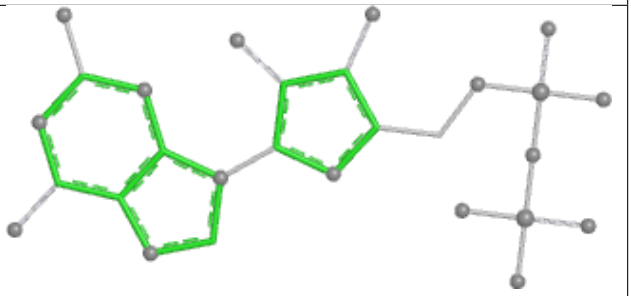
Bond lengths



Bond angles

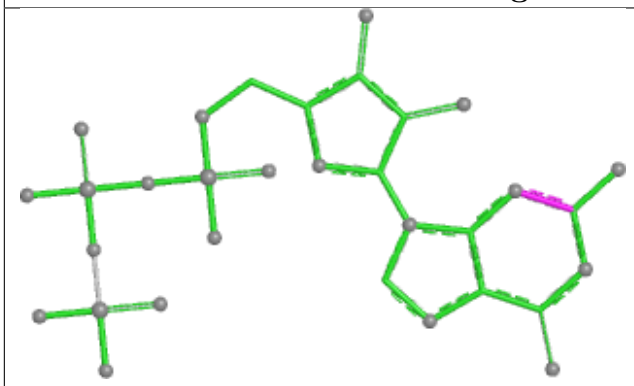


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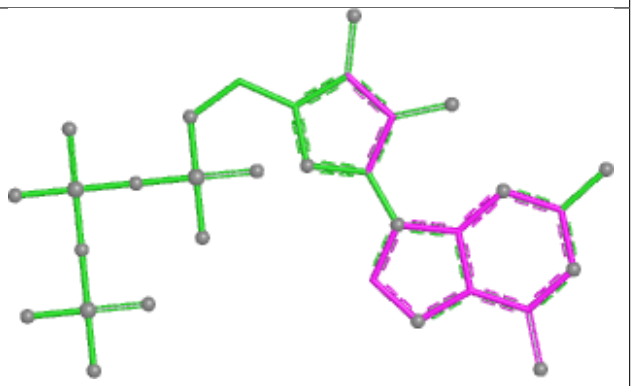


Rings

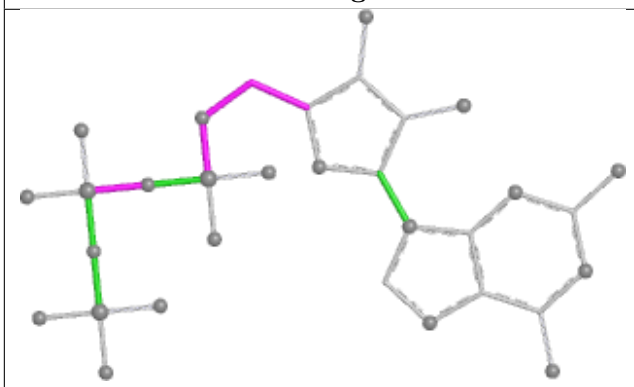
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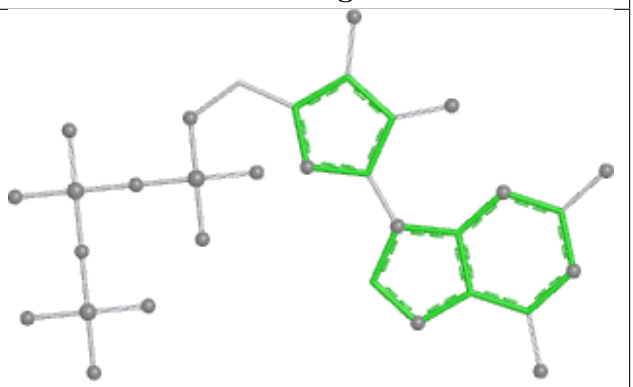
Bond lengths



Bond angles

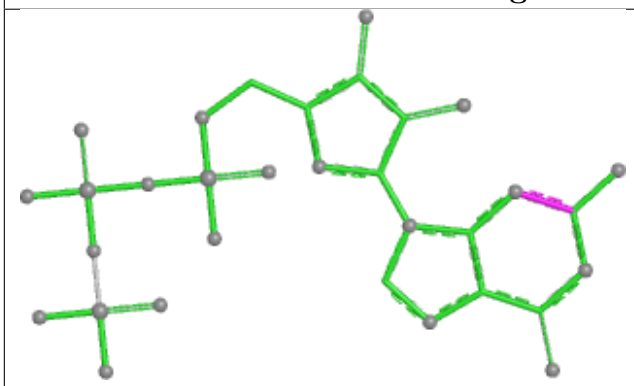


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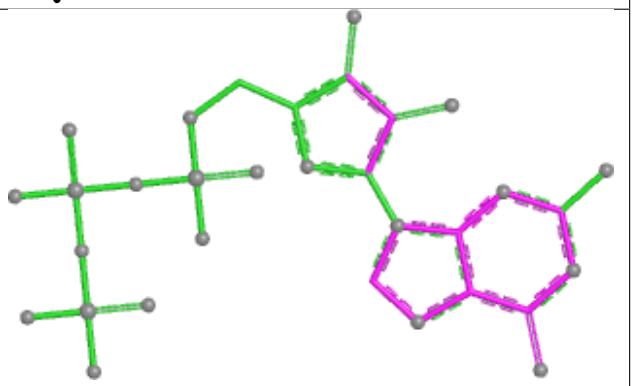


Rings

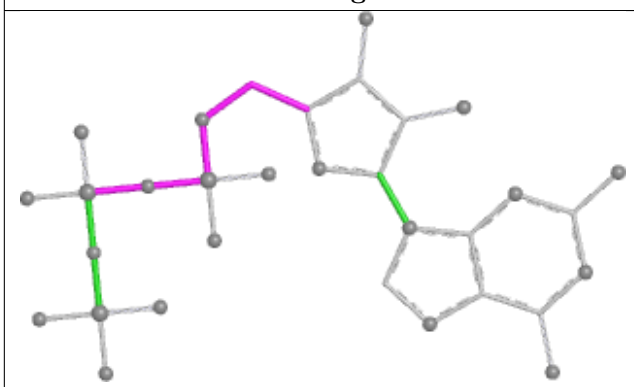
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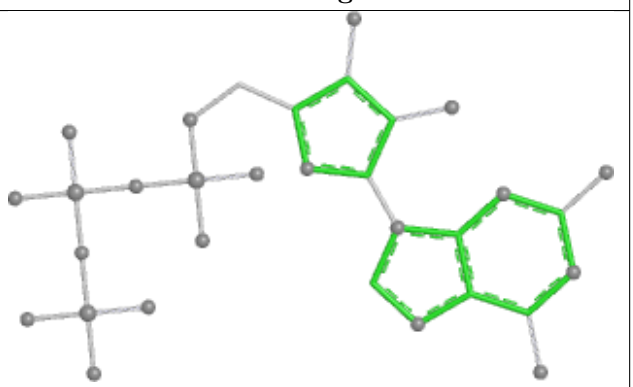
Bond lengths



Bond angles

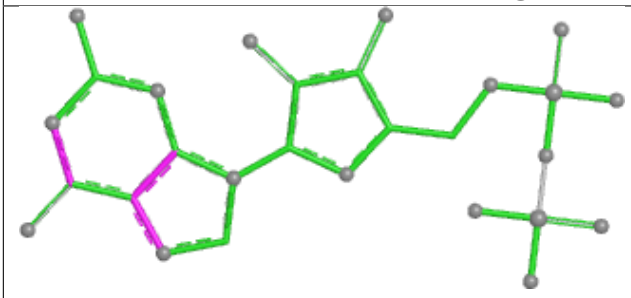


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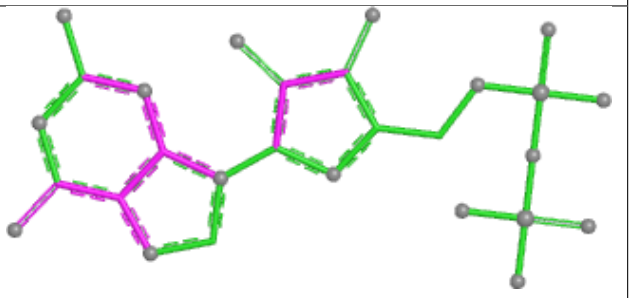


Rings

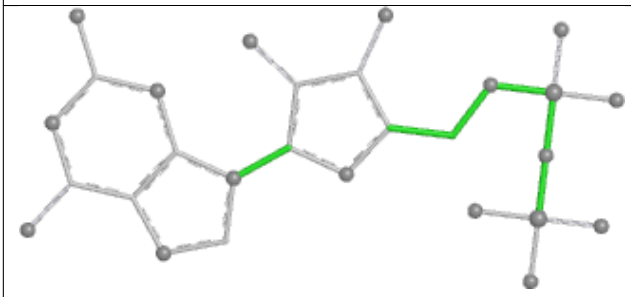
Ligand GDP FF 501



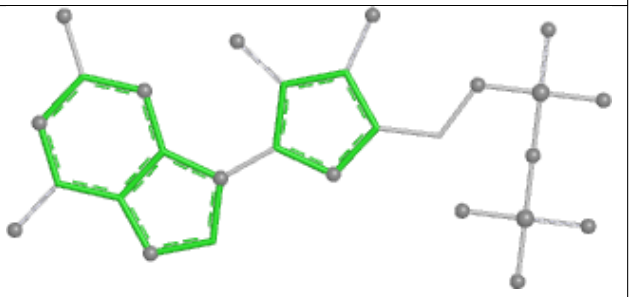
Bond lengths



Bond angles

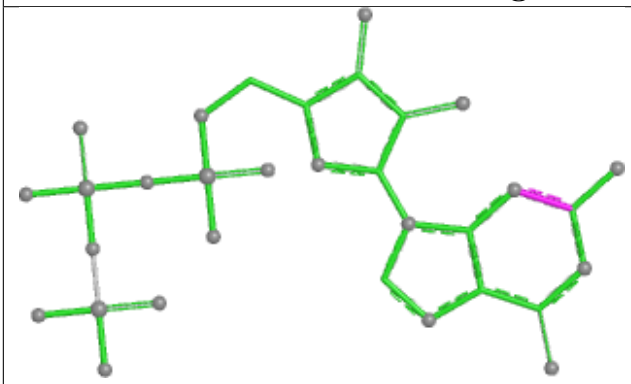


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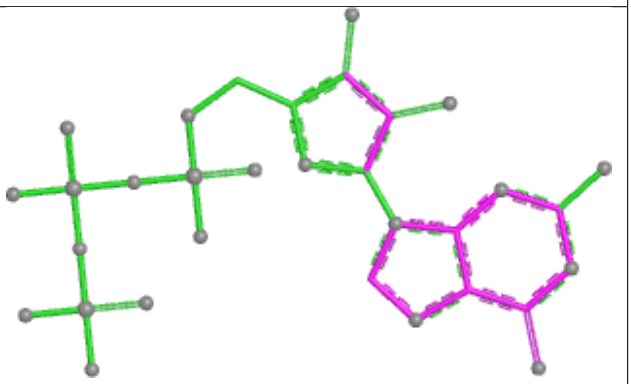


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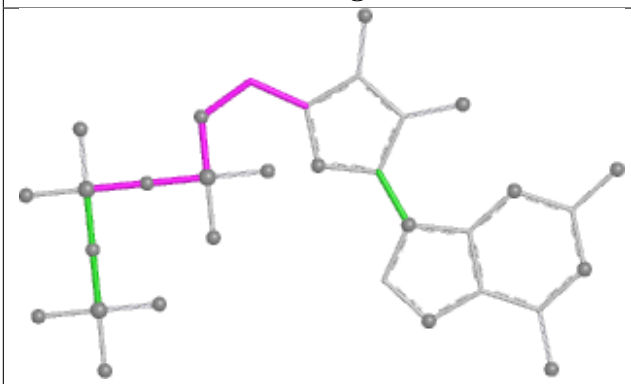
Ligand GTP BC 502



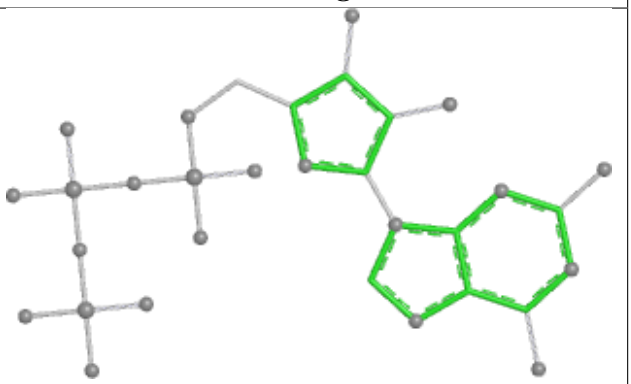
Bond lengths



Bond angles

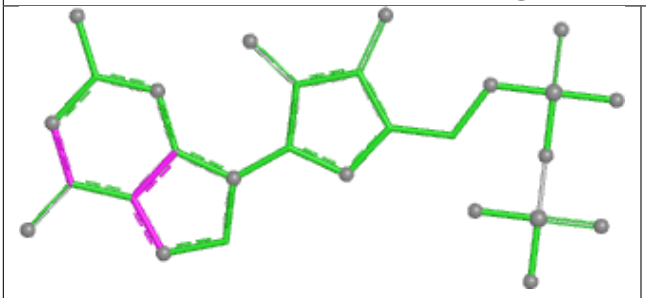


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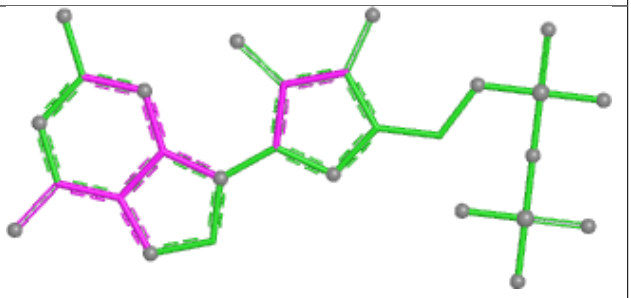


Rings

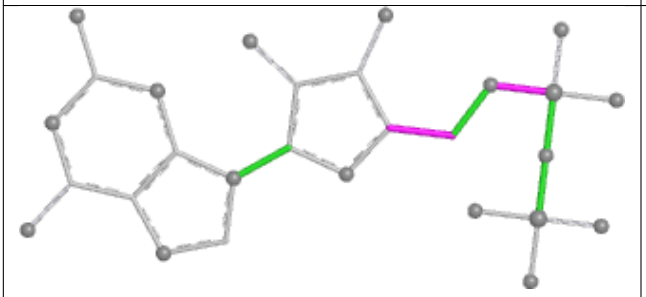
Ligand GDP TJ 501



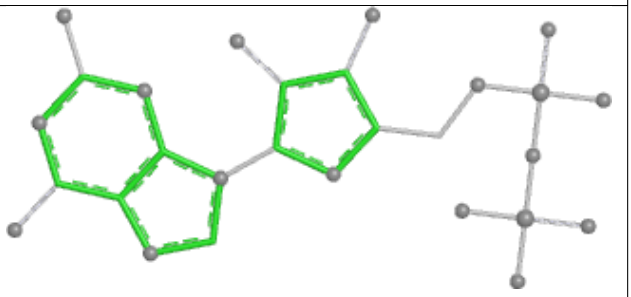
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Bond angles

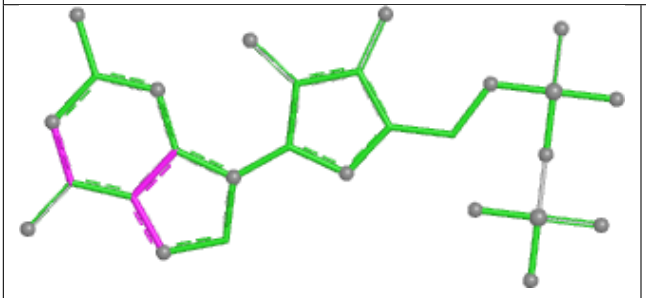


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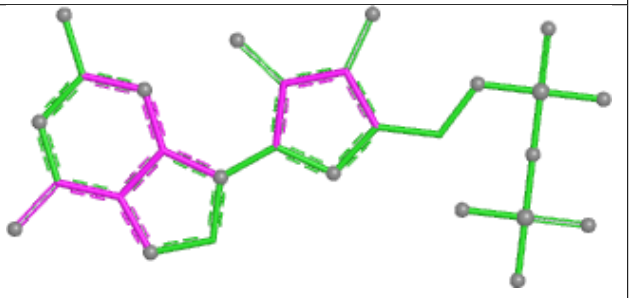


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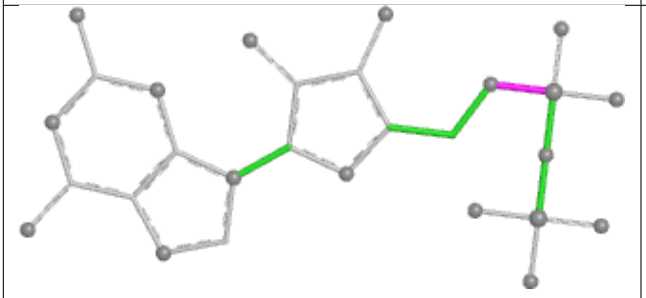
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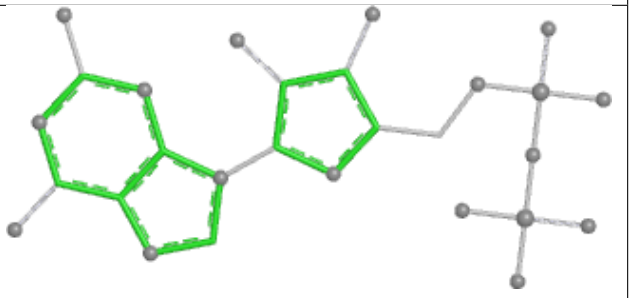
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Bond angles

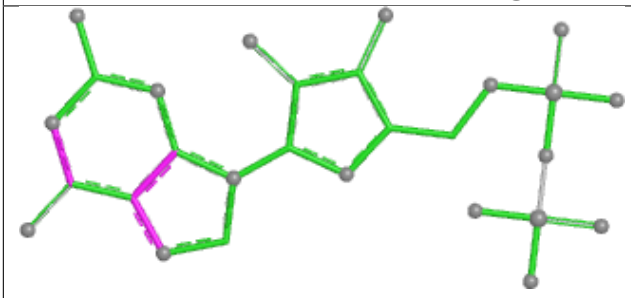


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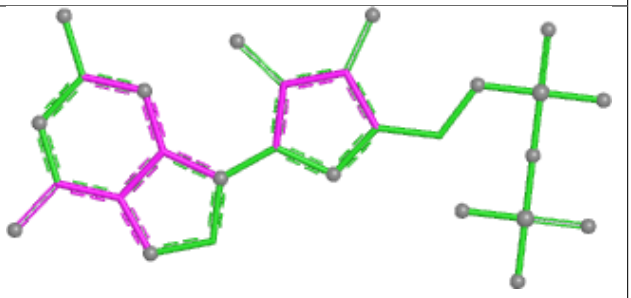


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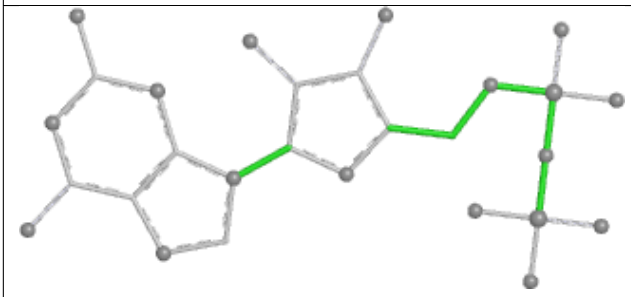
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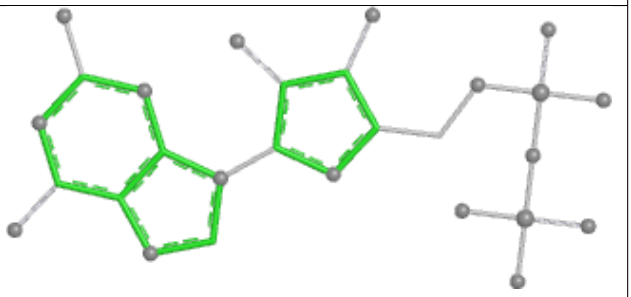
Bond lengths



Bond angles

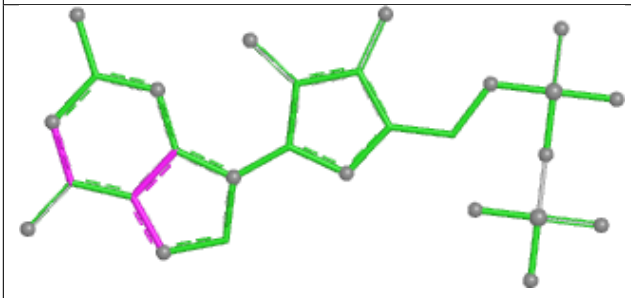


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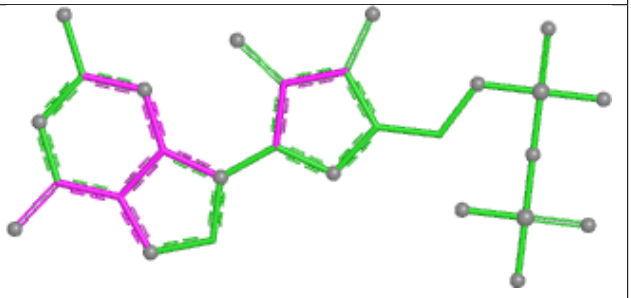


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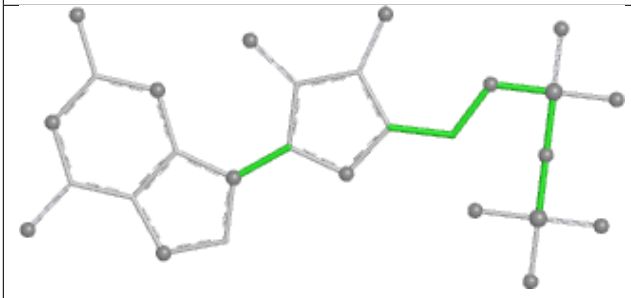
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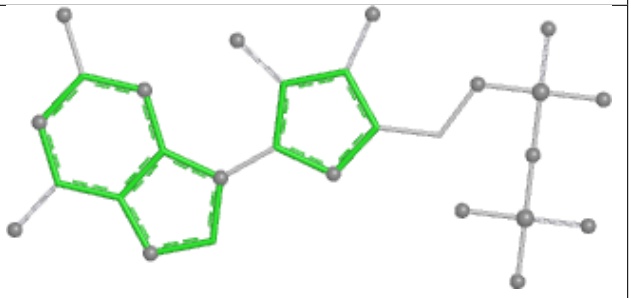
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Bond angles

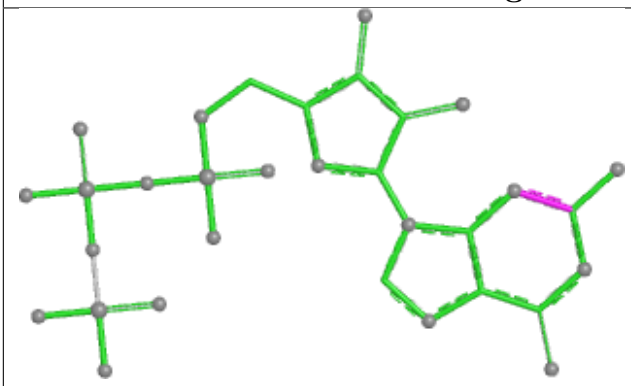


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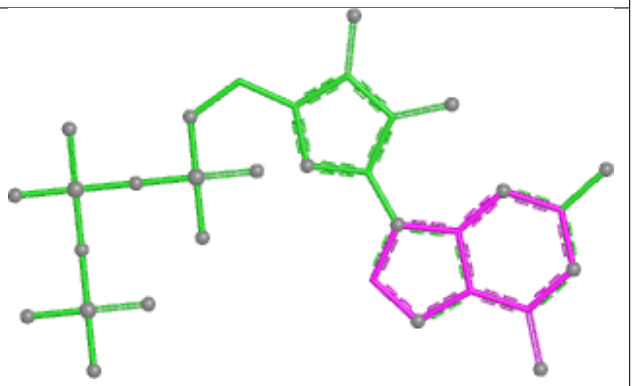


Rings

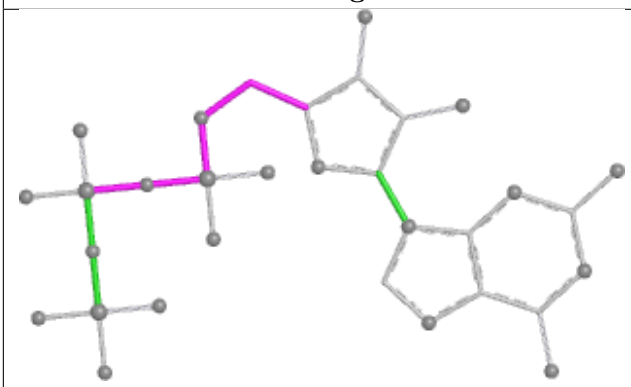
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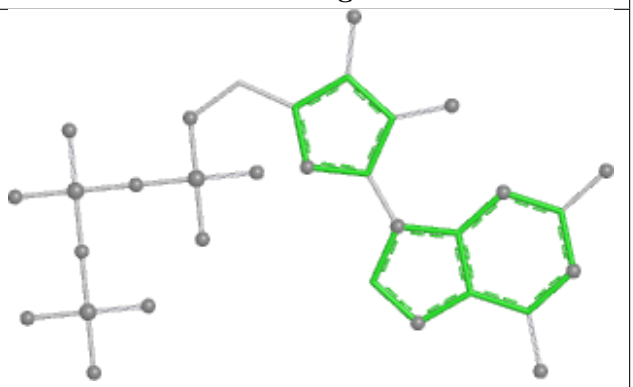
Bond lengths



Bond angles

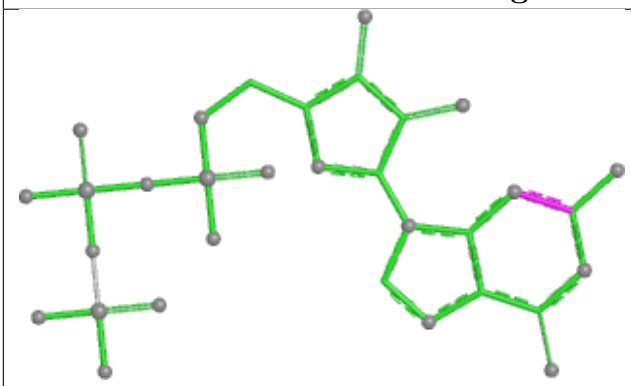


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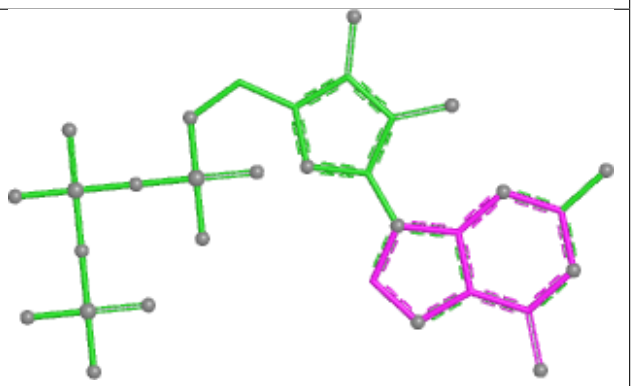


Rings

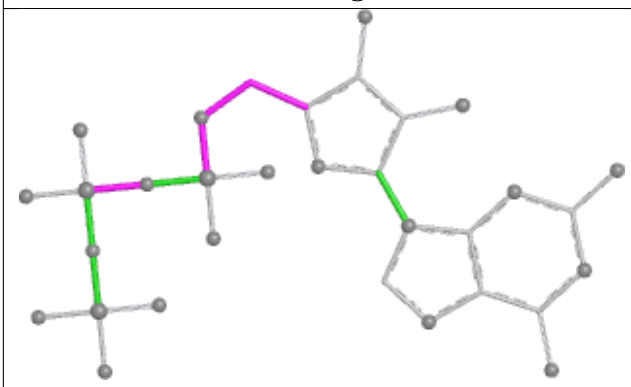
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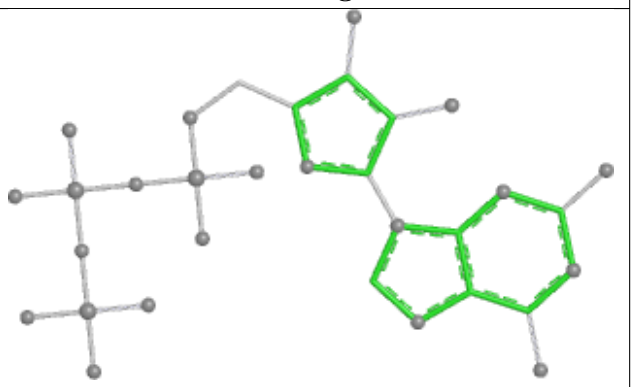
Bond lengths



Bond angles

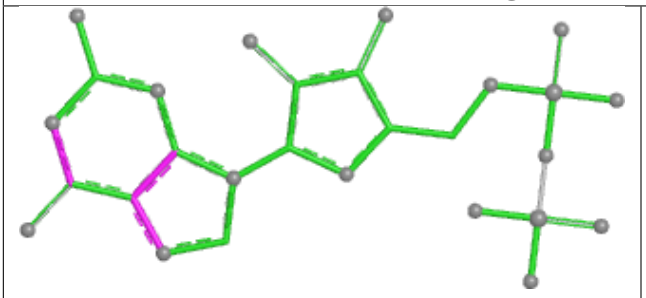


Torsions

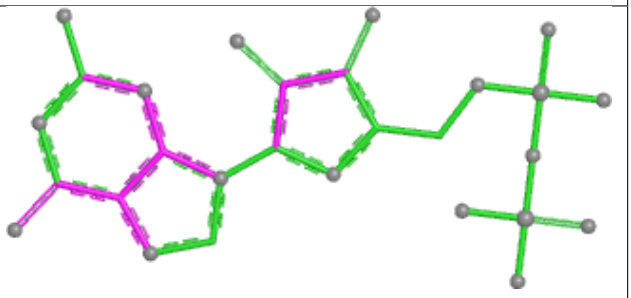


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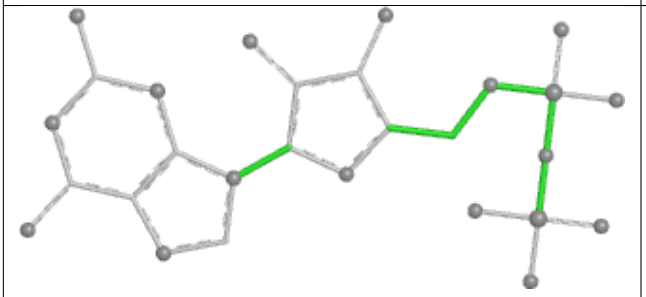
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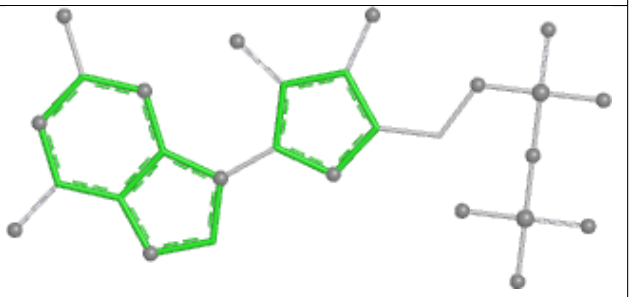
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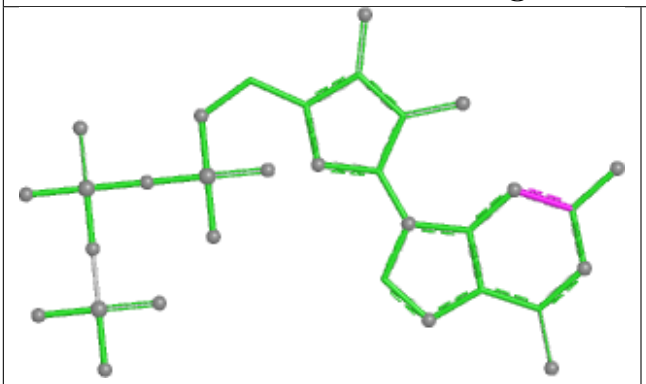


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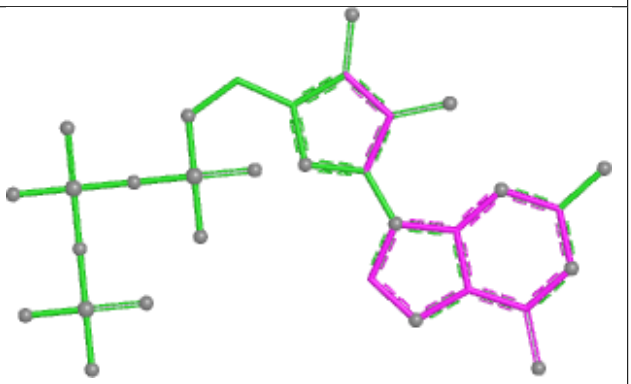


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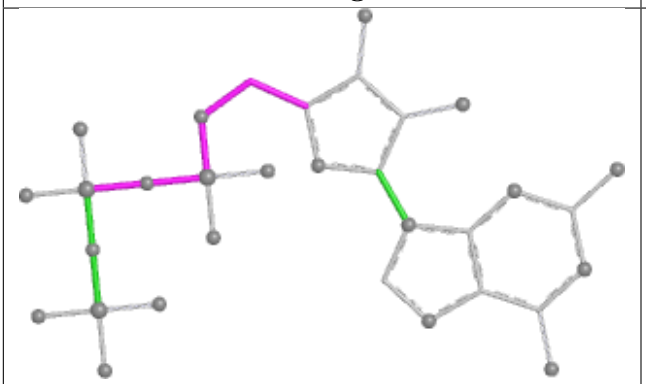
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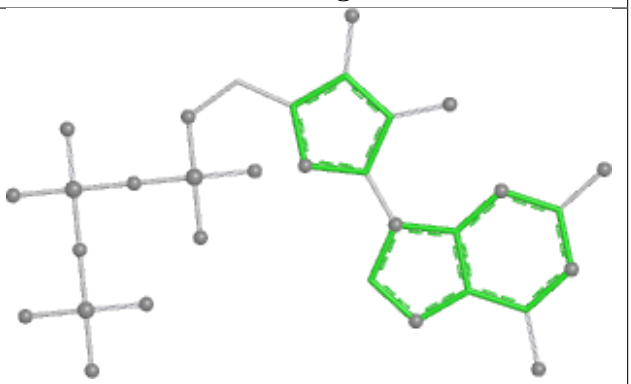
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Bond angles

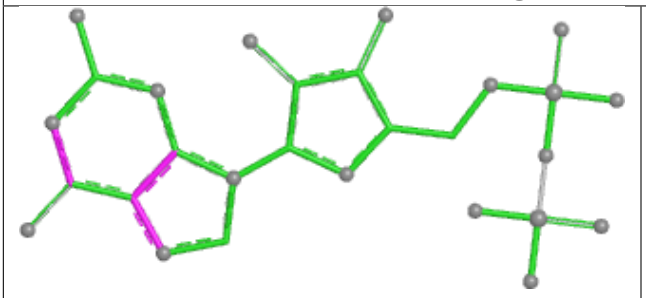


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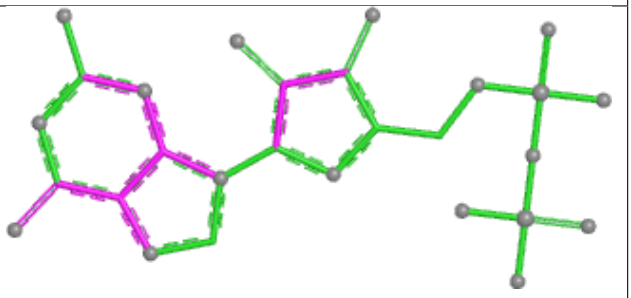


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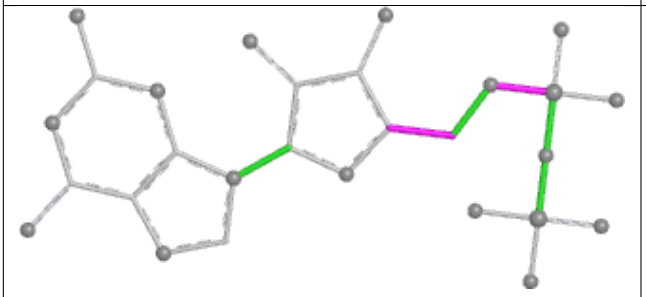
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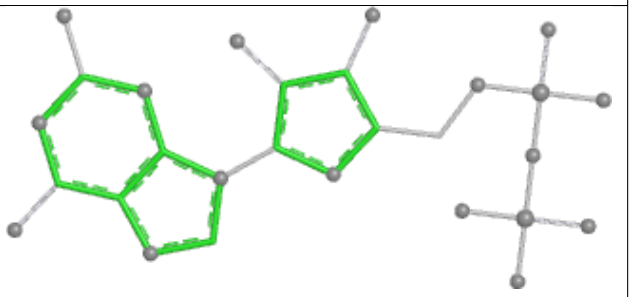
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Bond angles

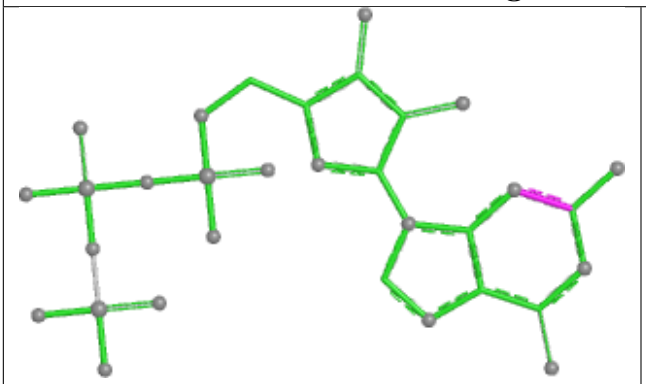


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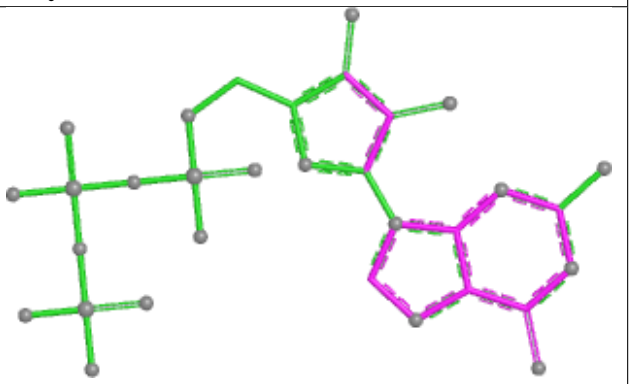


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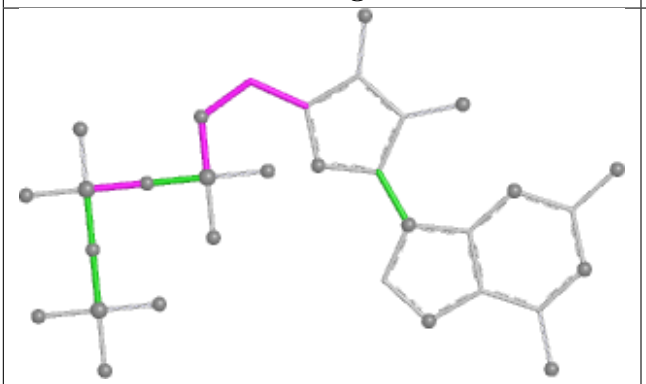
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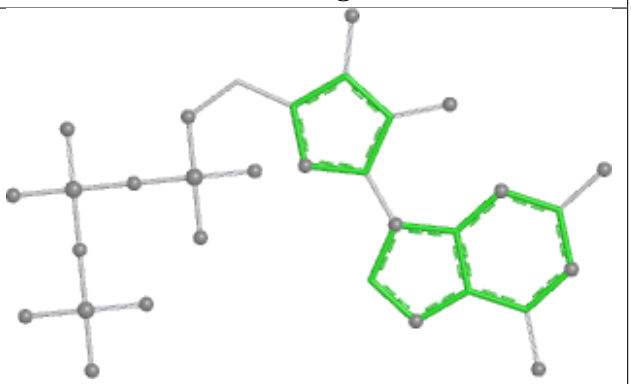
Bond lengths



Bond angles

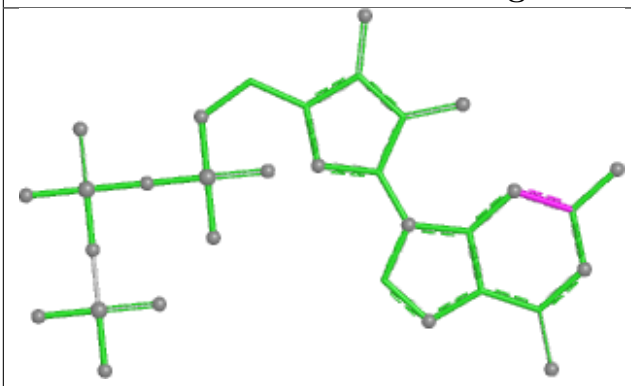


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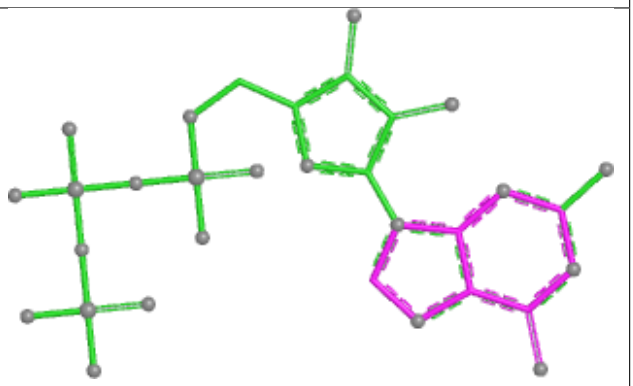


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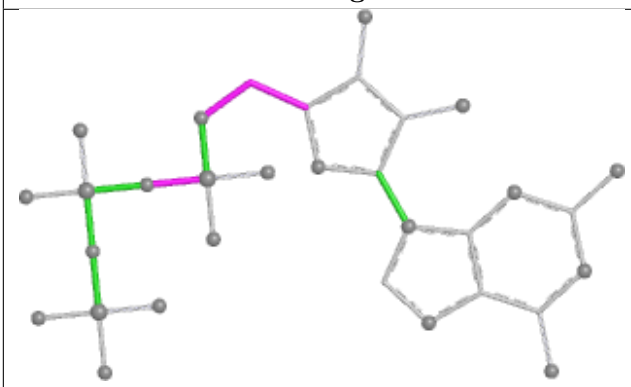
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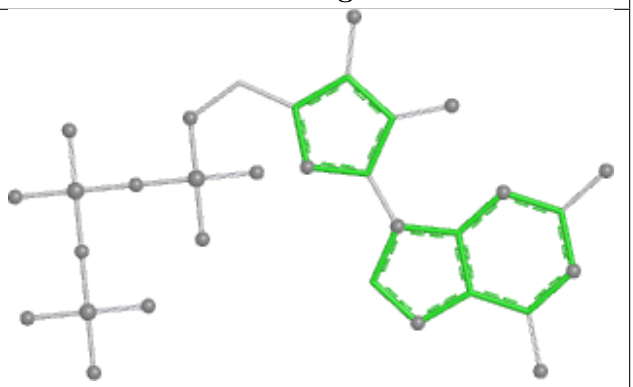
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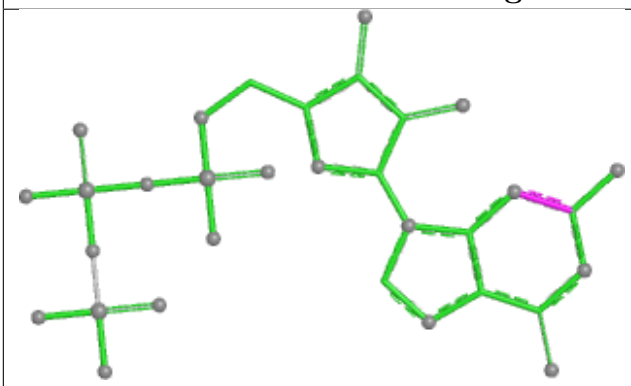


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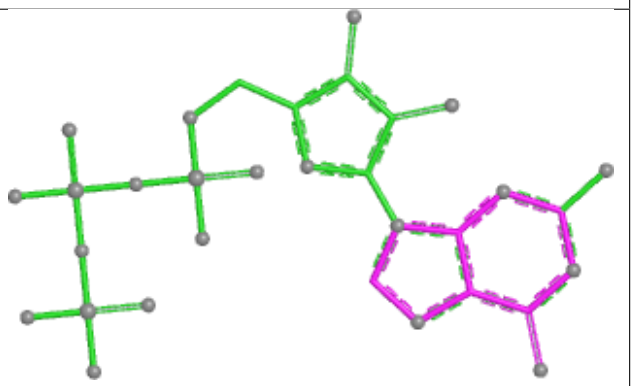


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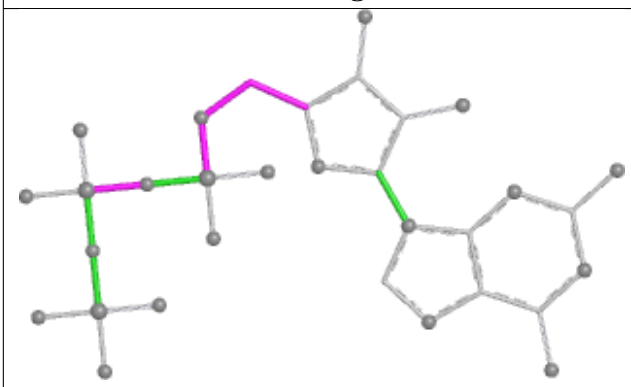
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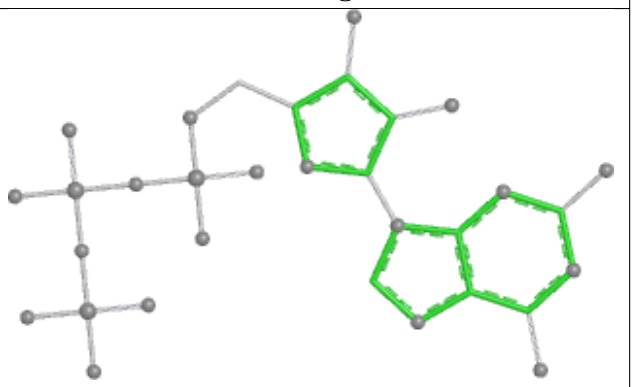
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Bond angles

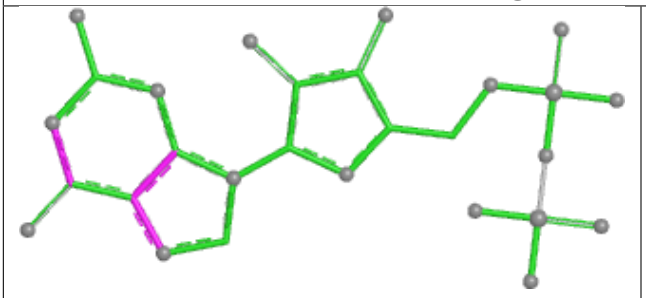


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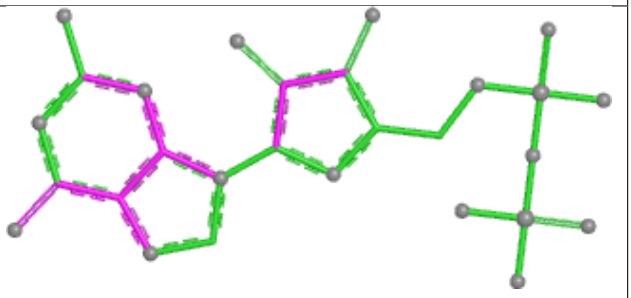


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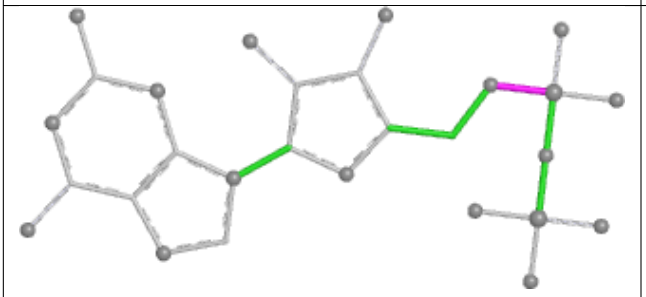
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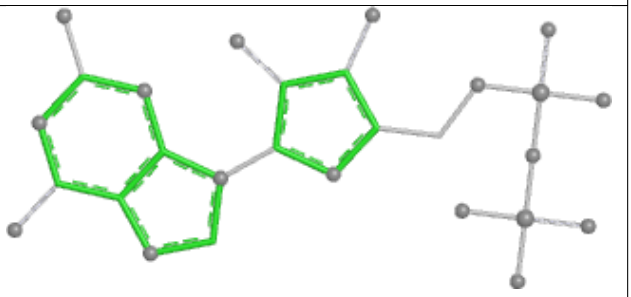
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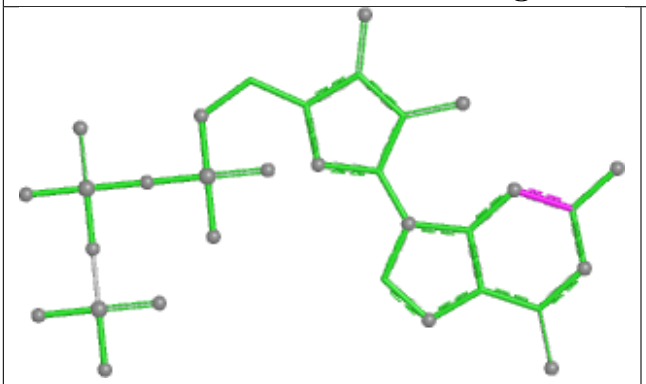


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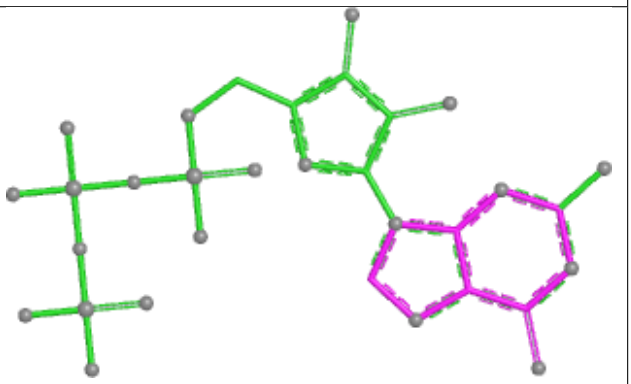


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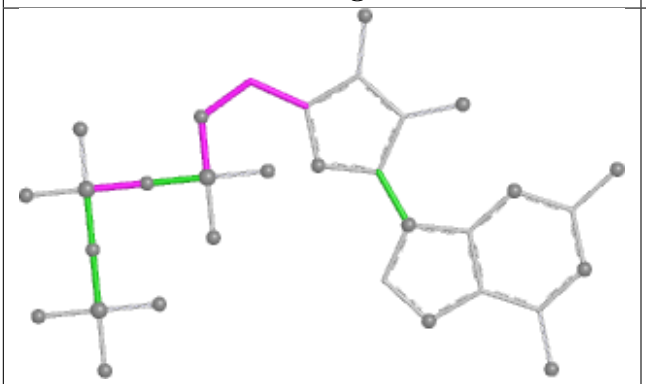
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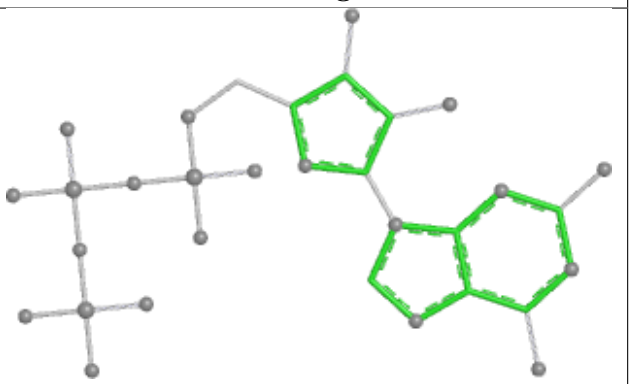
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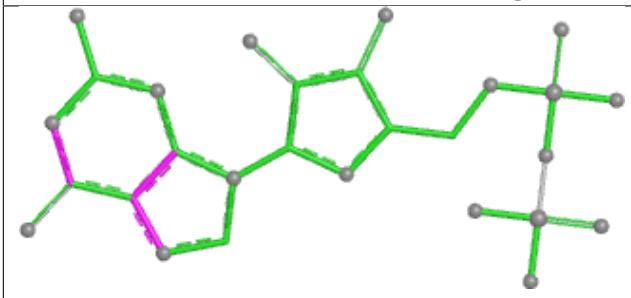


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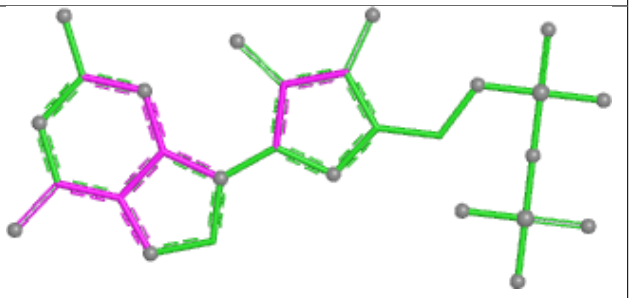


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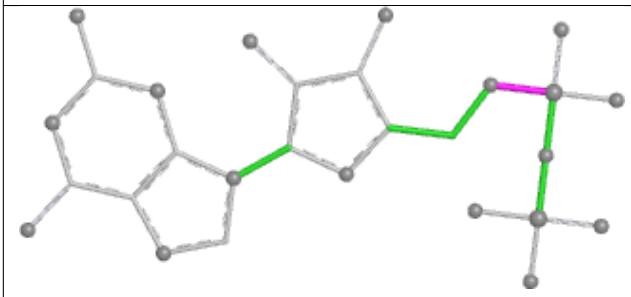
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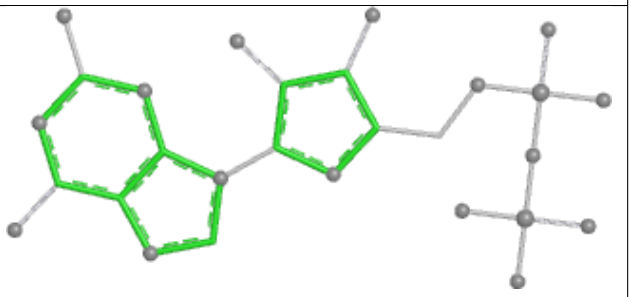
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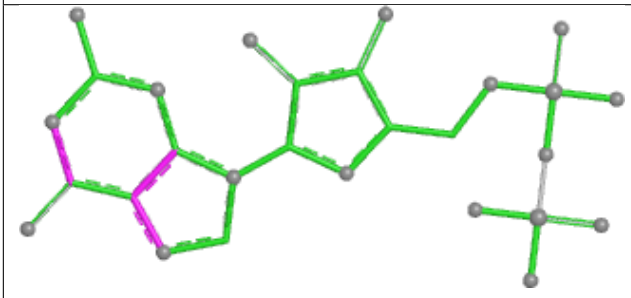


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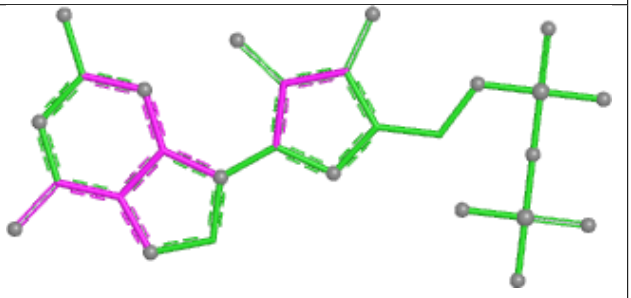


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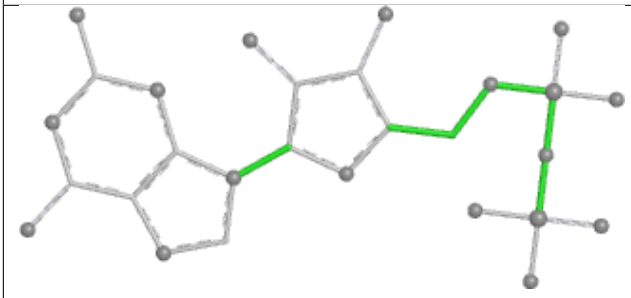
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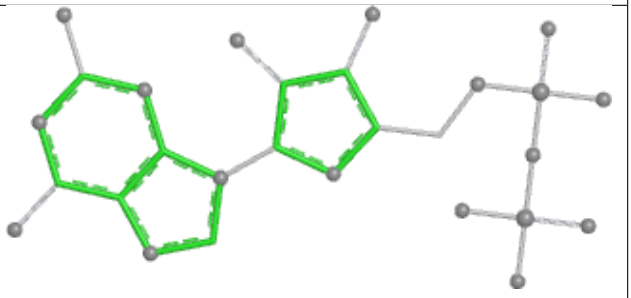
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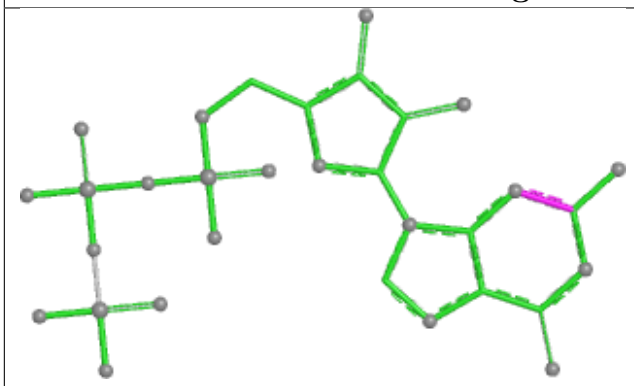


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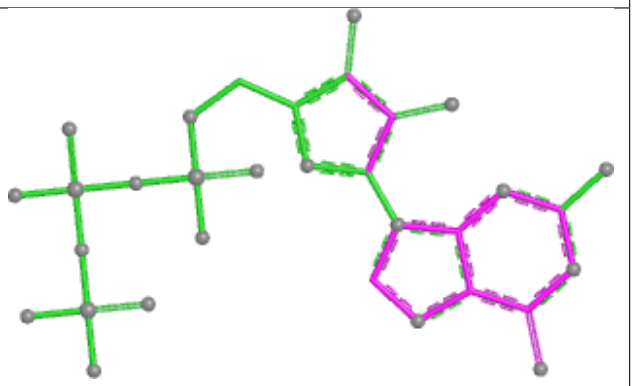


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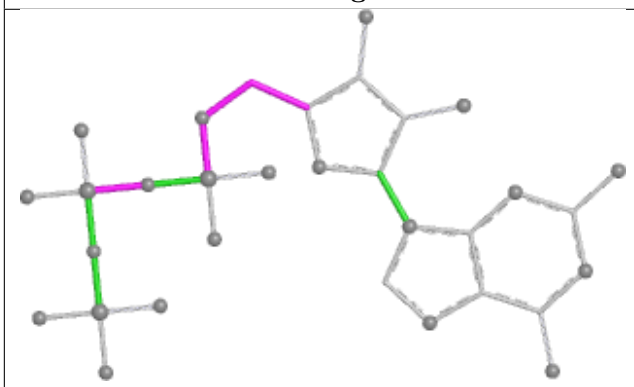
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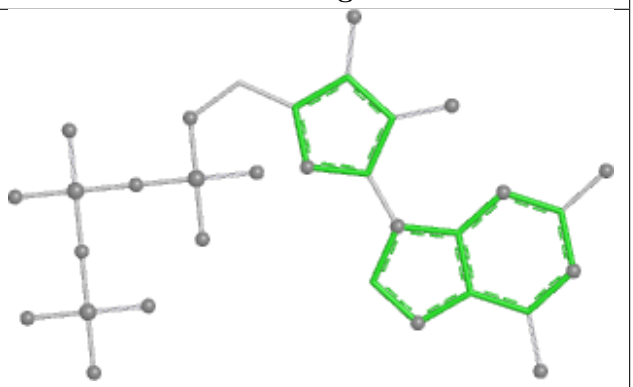
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Bond angles

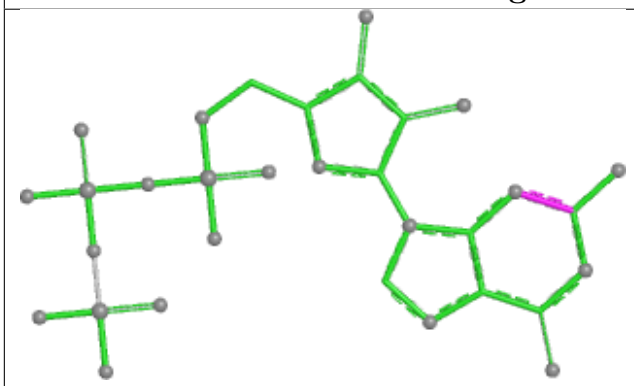


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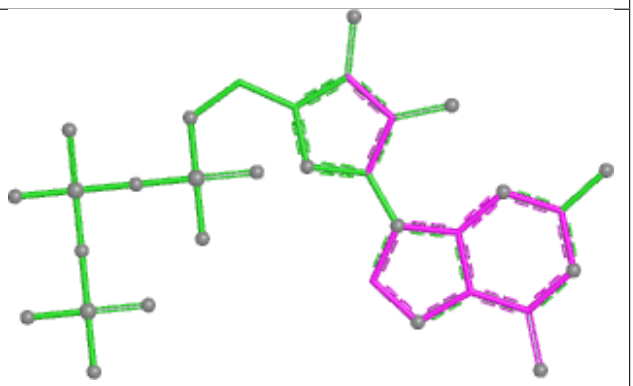


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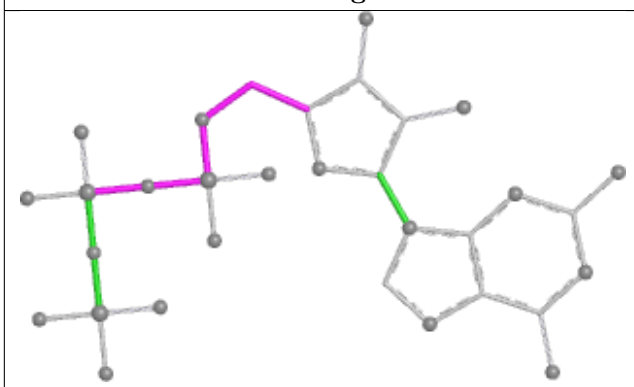
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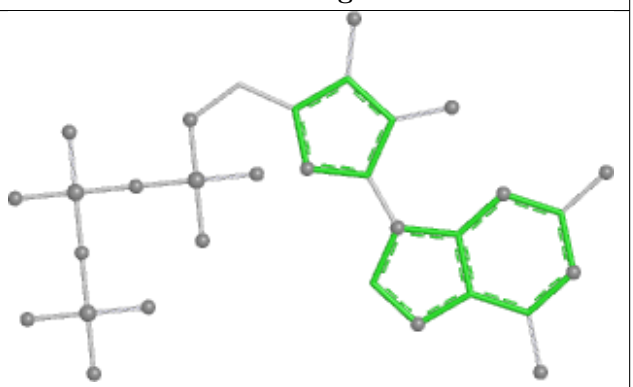
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Bond angles

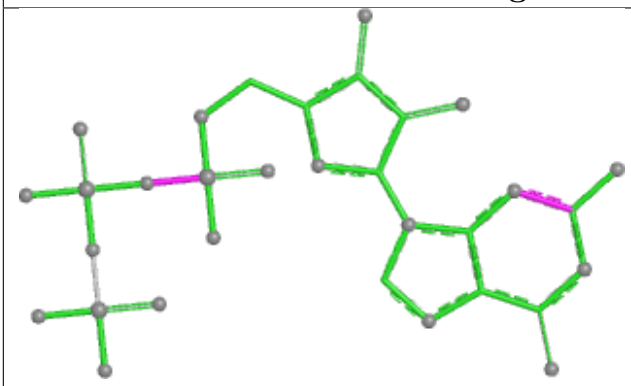


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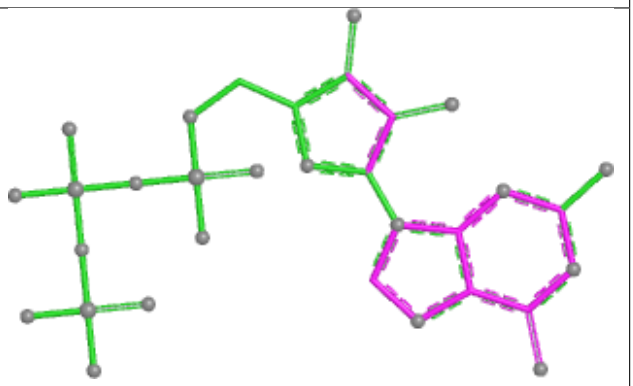


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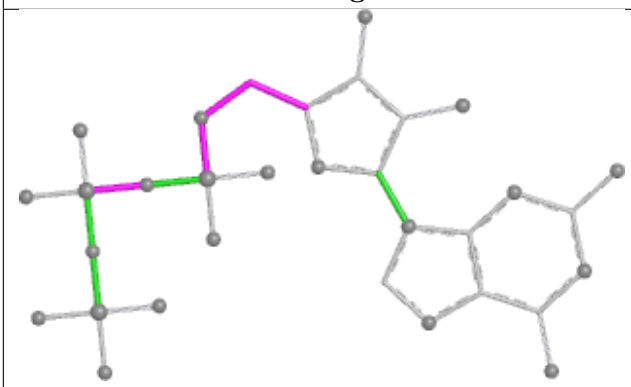
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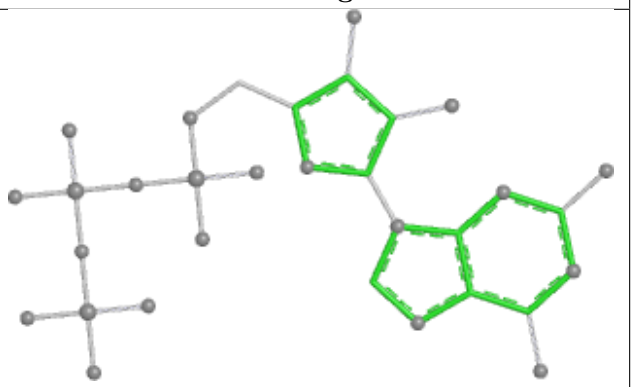
Bond lengths



Bond angles

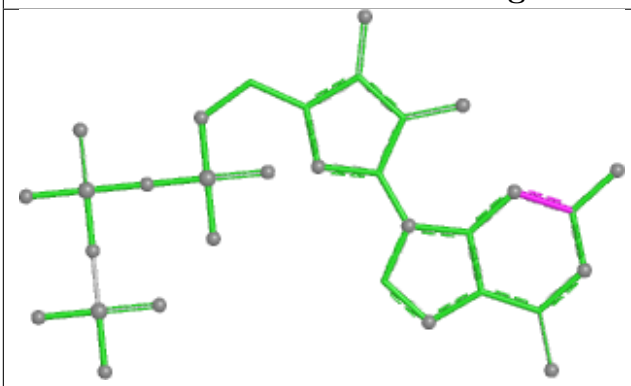


Torsions

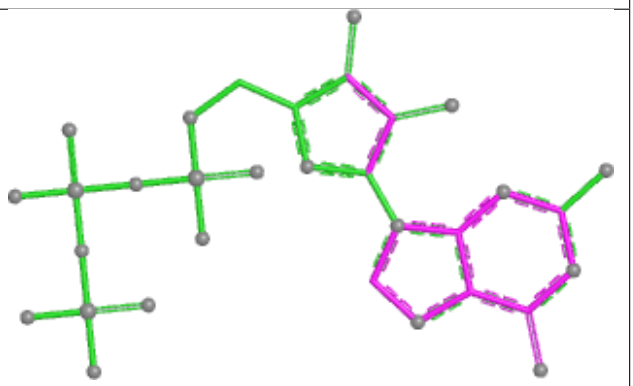


Rings

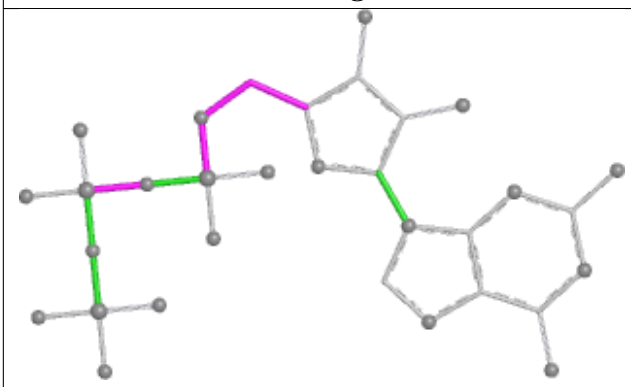
Ligand GTP KG 501



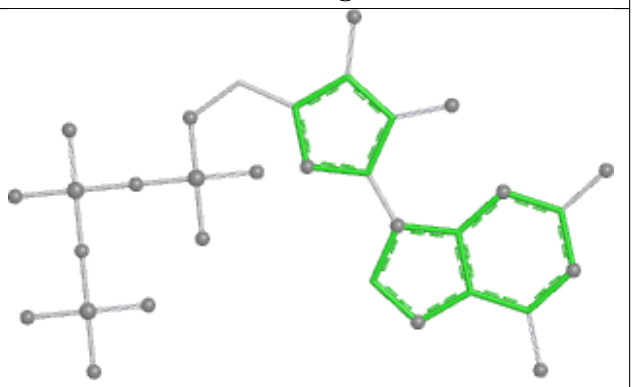
Bond lengths



Bond angles

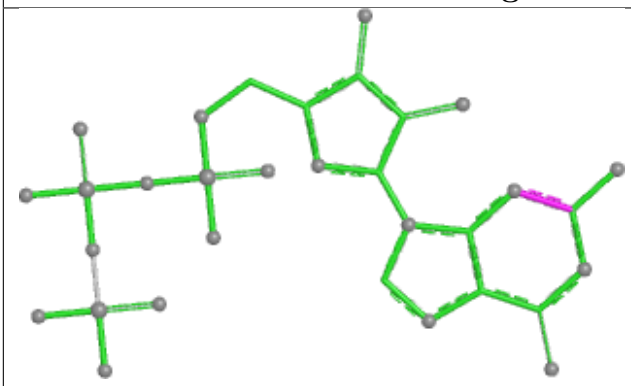


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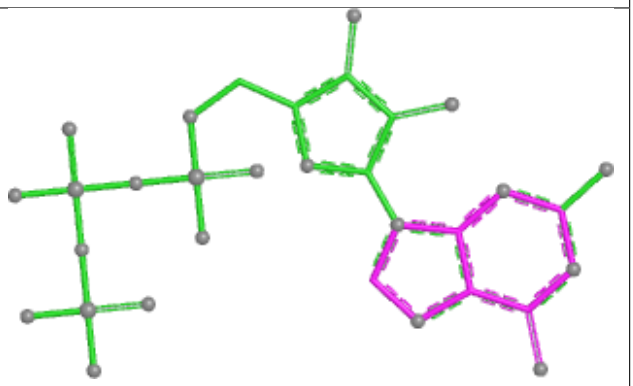


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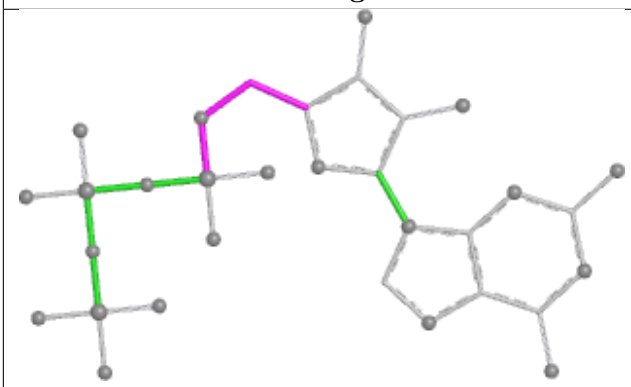
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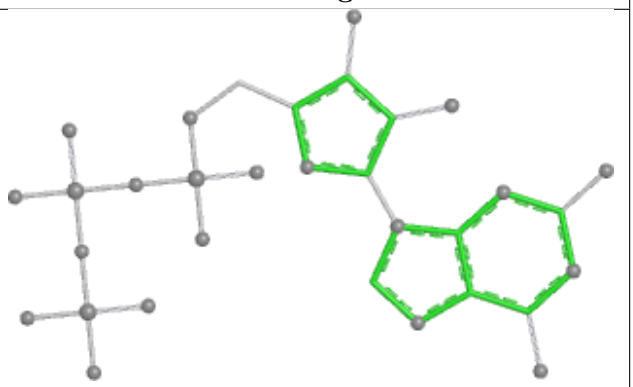
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Bond angles

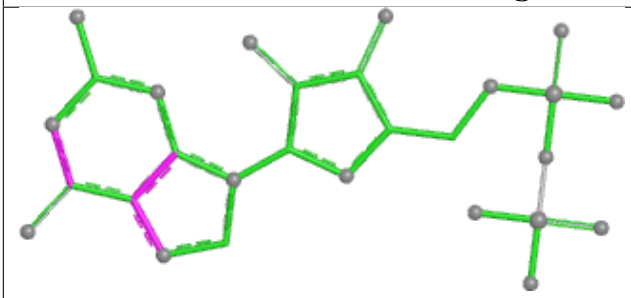


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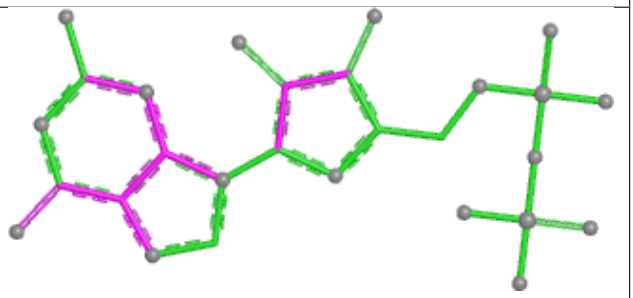


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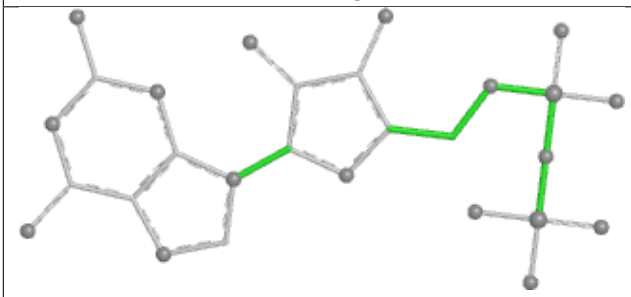
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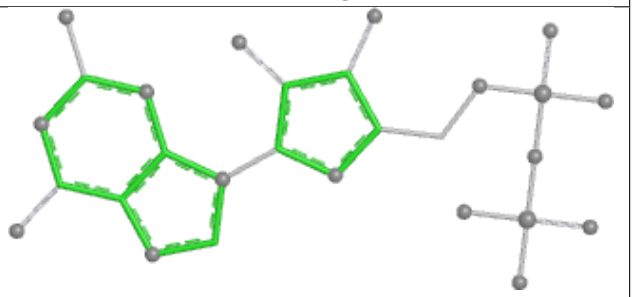
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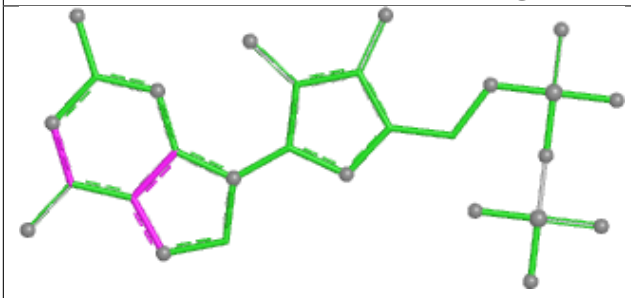


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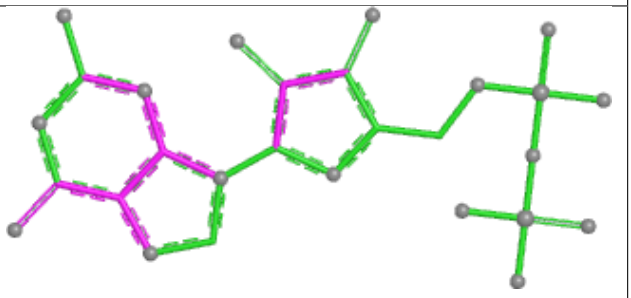


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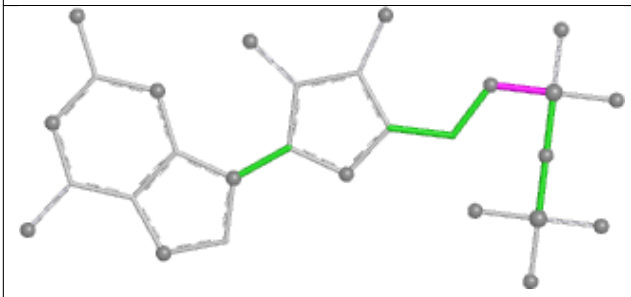
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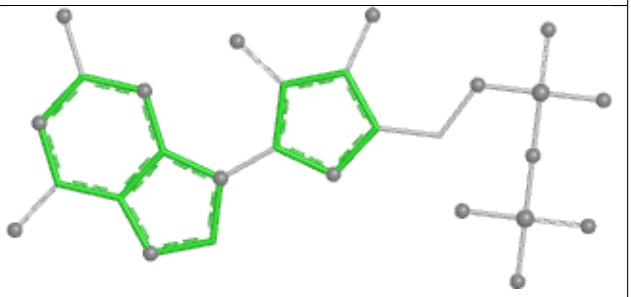
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Bond angles

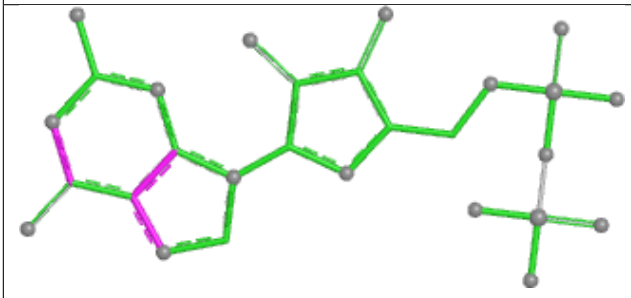


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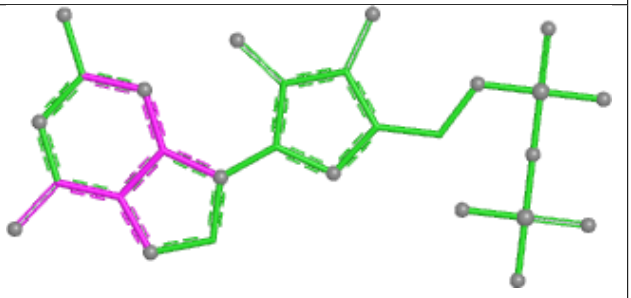


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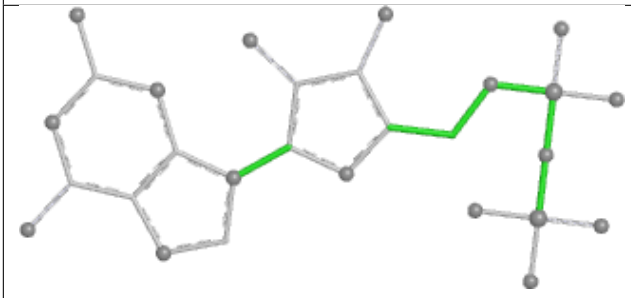
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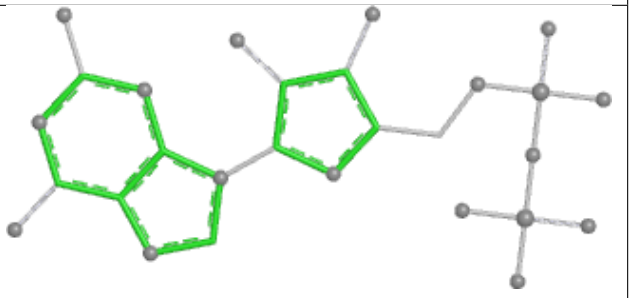
Bond lengths



Bond angles

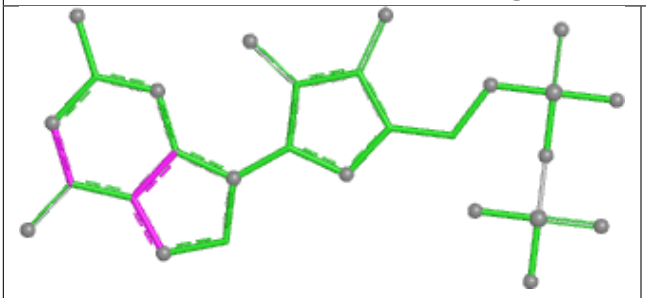


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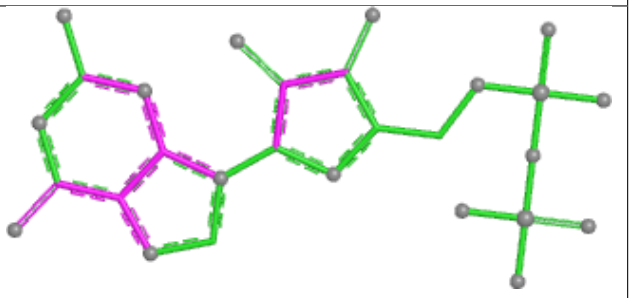


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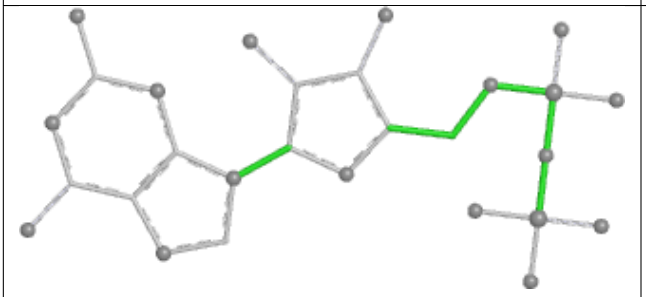
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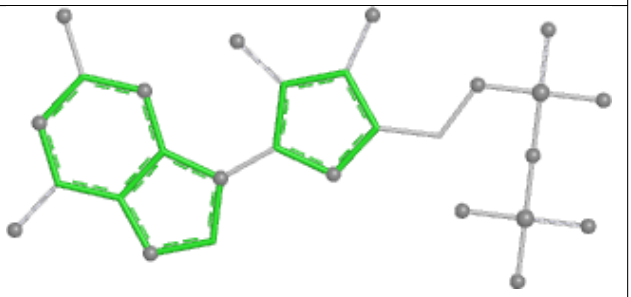
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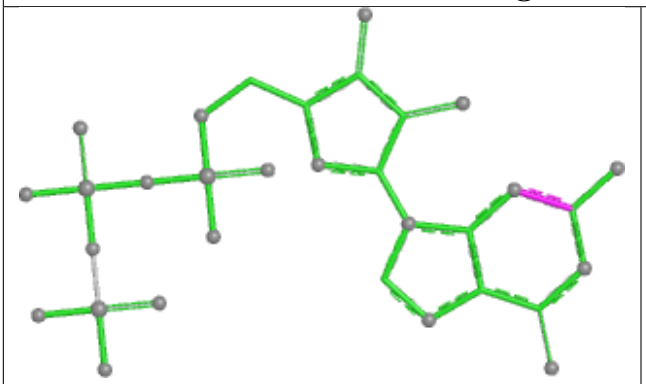


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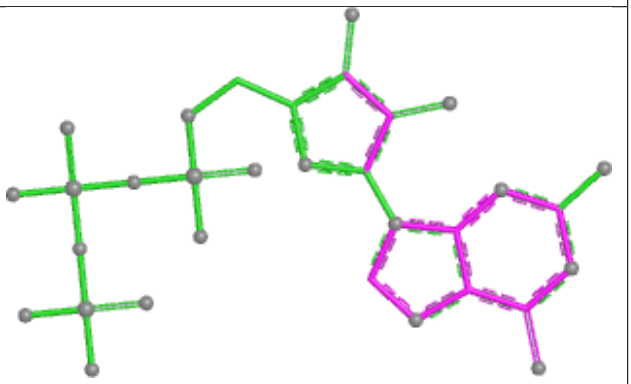


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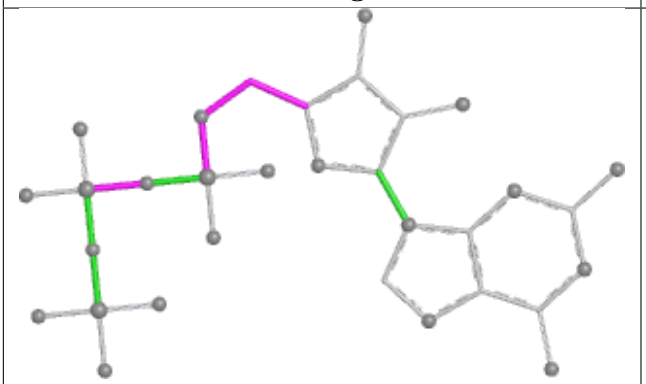
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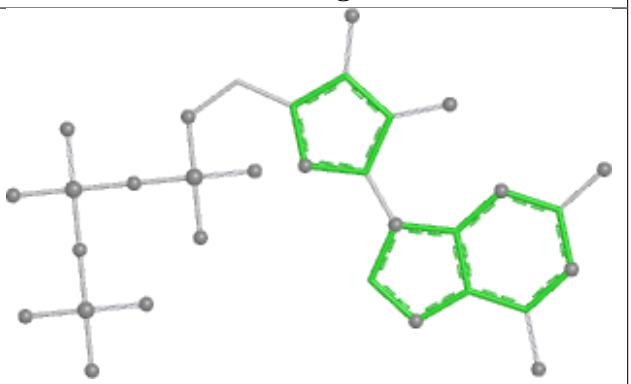
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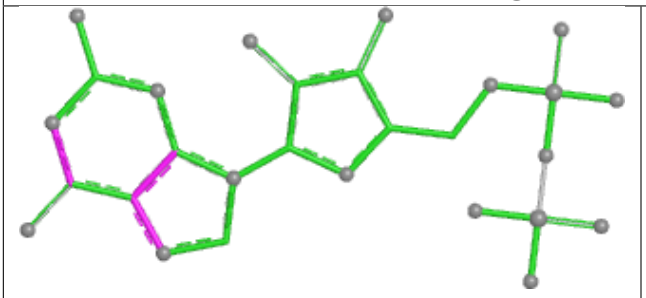


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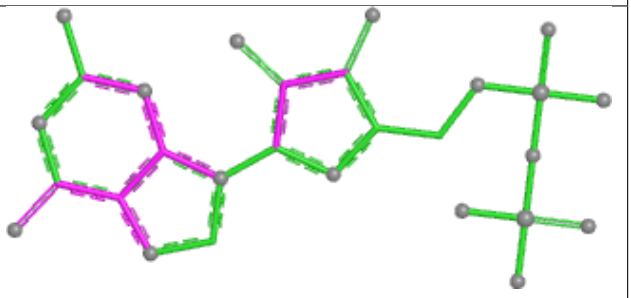


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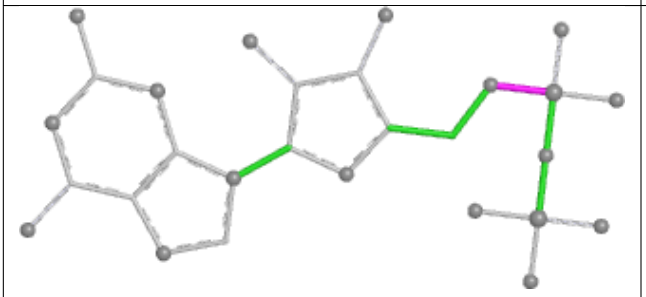
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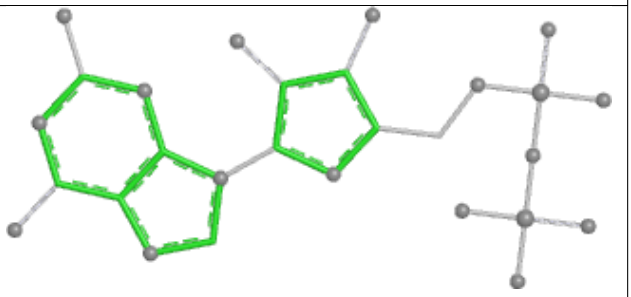
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Bond angles

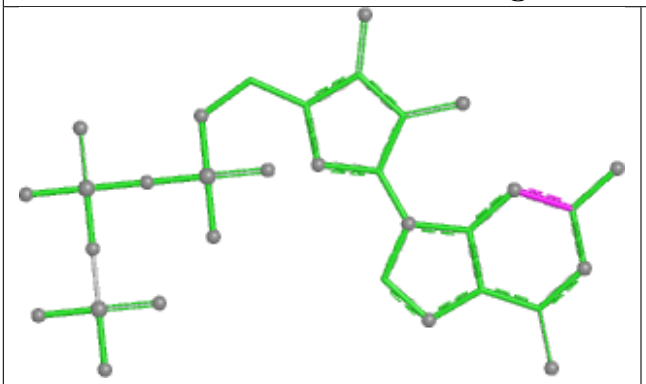


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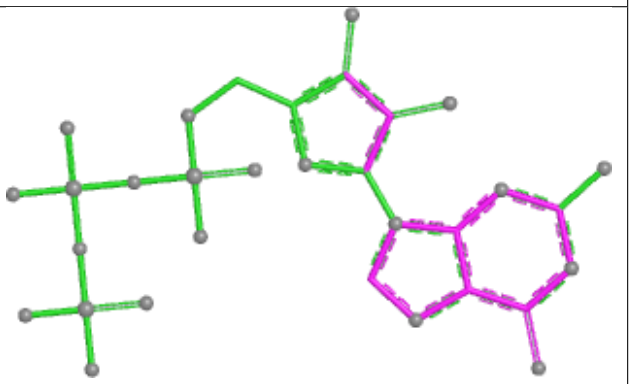


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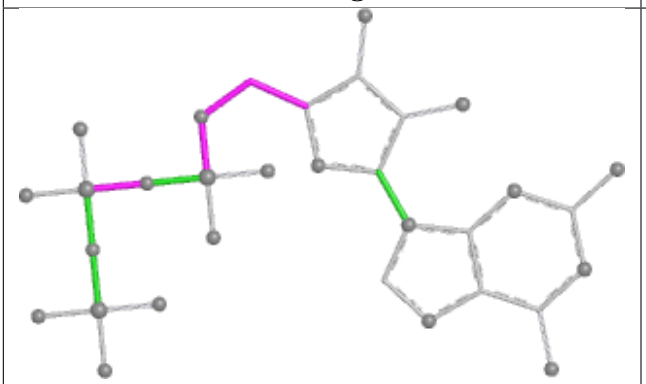
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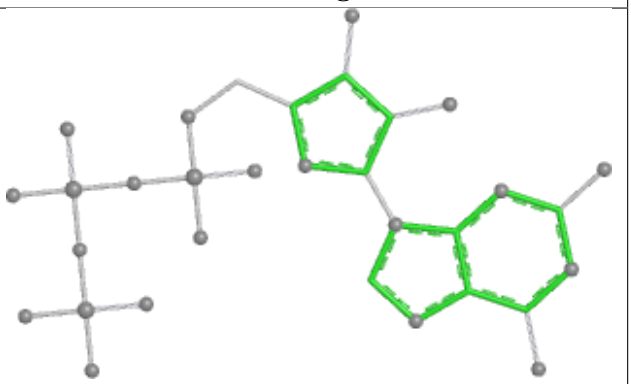
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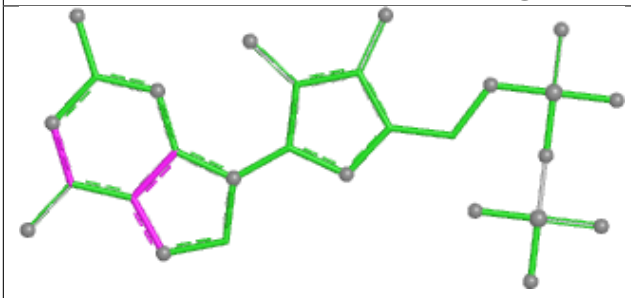


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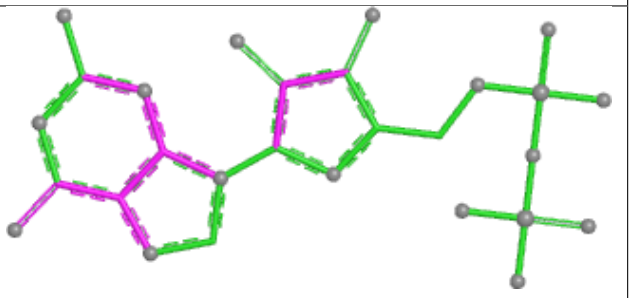


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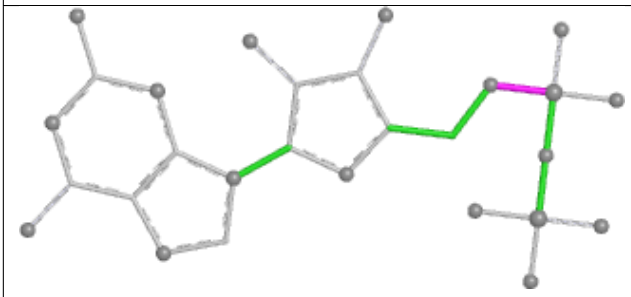
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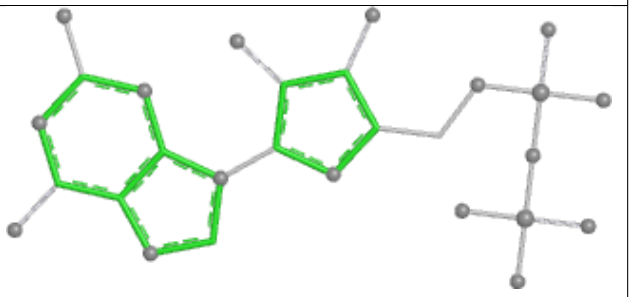
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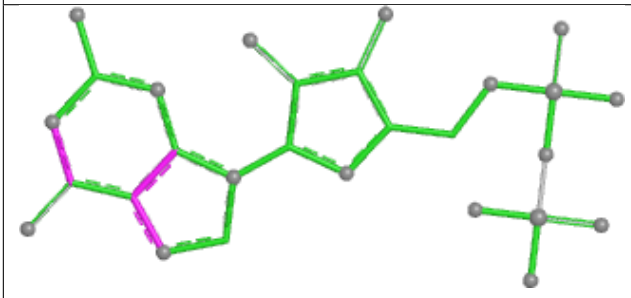


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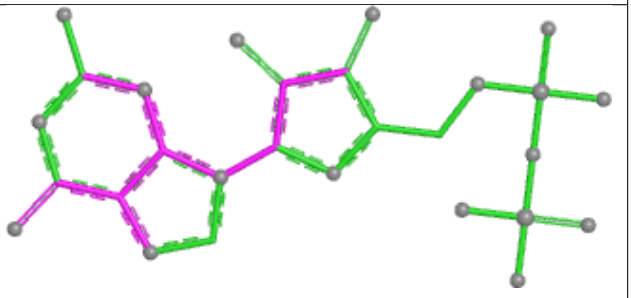


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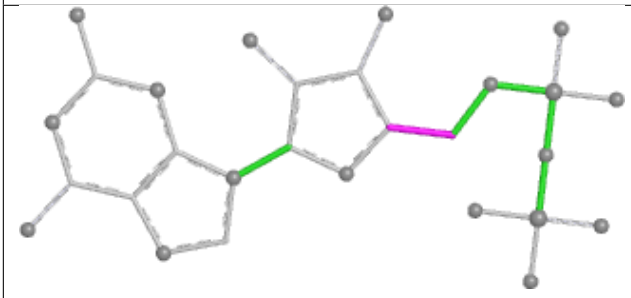
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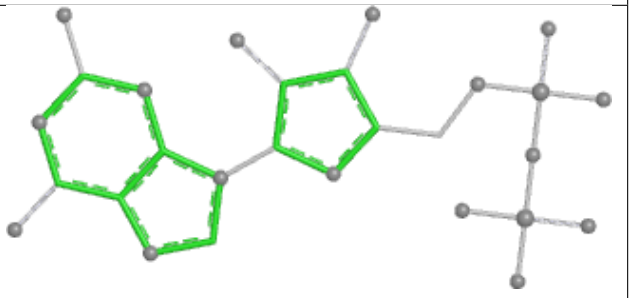
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Bond angles

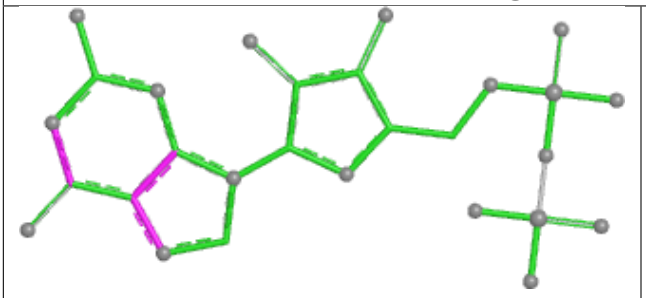


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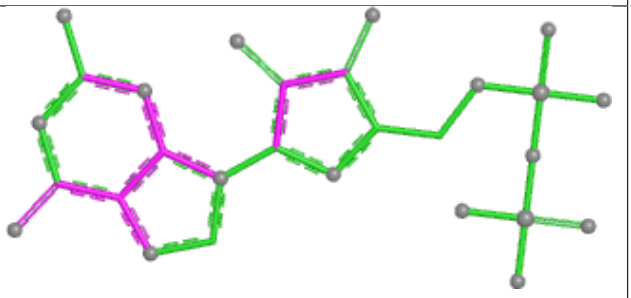


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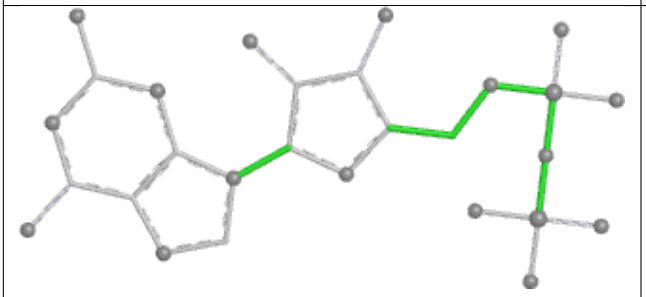
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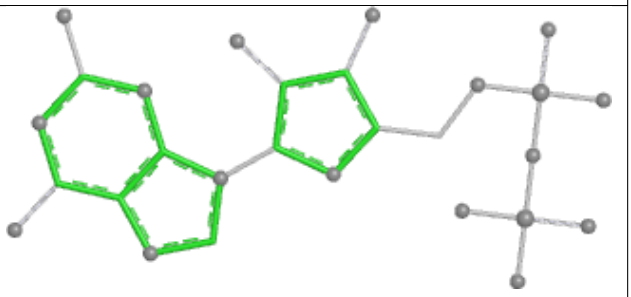
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Bond angles

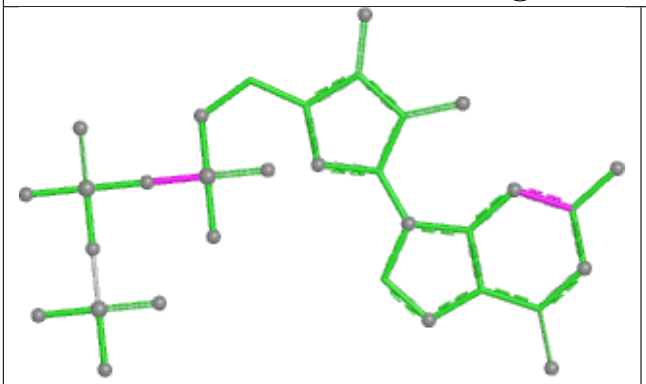


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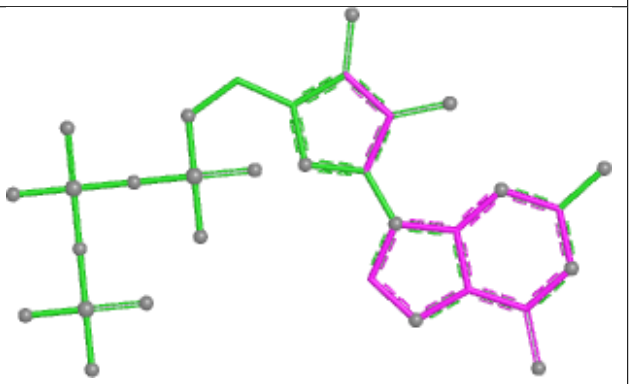


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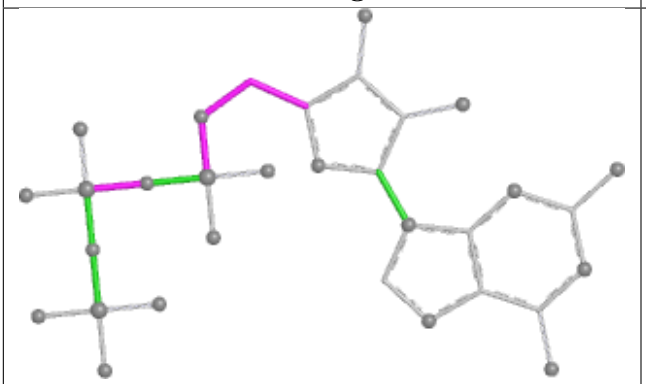
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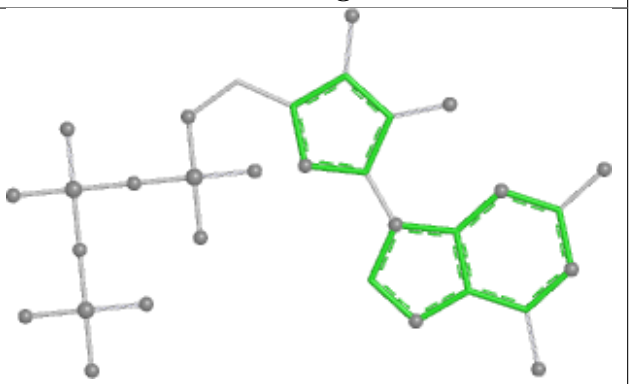
Bond lengths



Bond angles

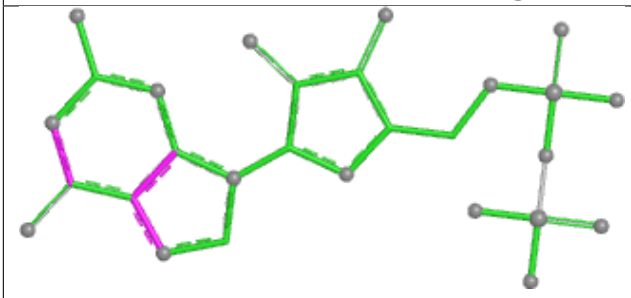


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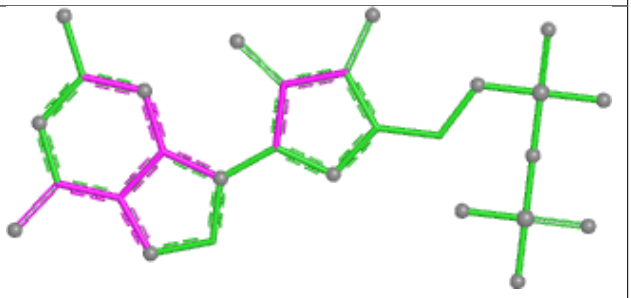


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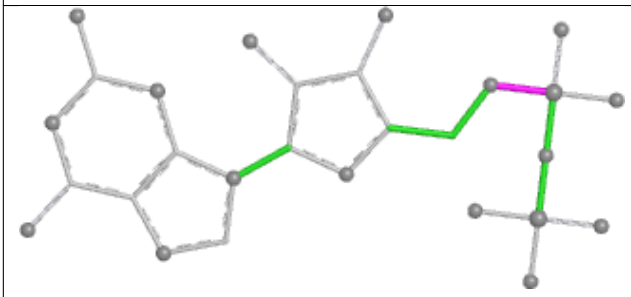
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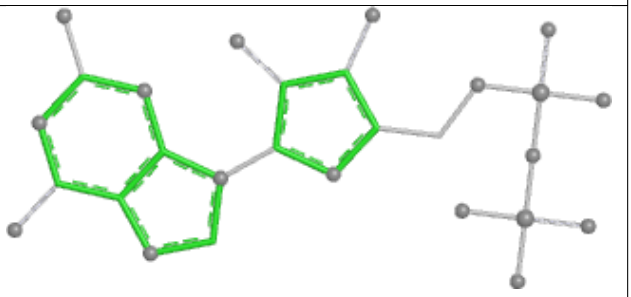
Bond lengths



Bond angles

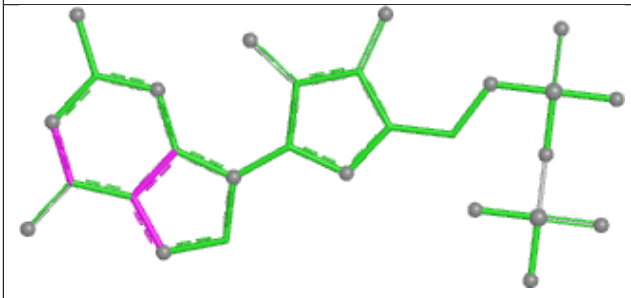


Torsions

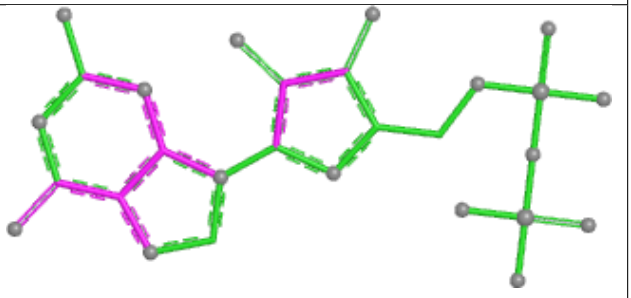


Rings

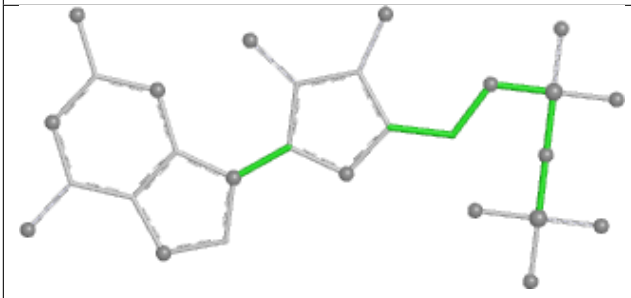
Ligand GDP QL 501



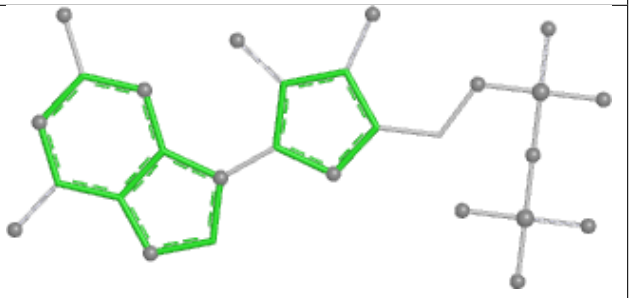
Bond lengths



Bond angles

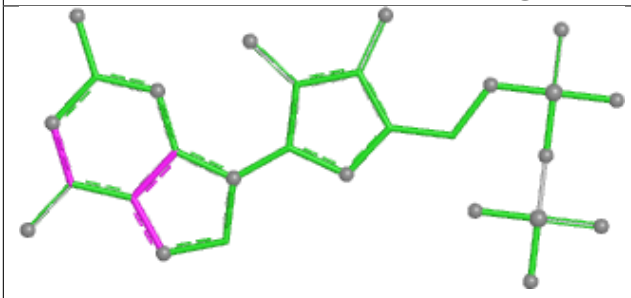


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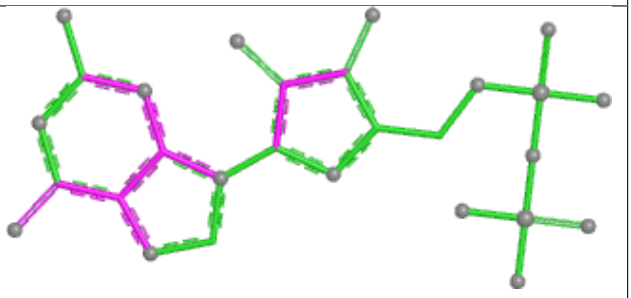


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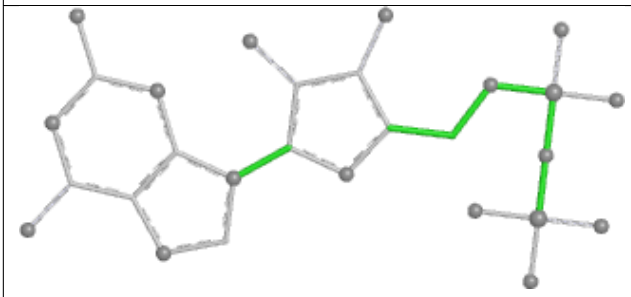
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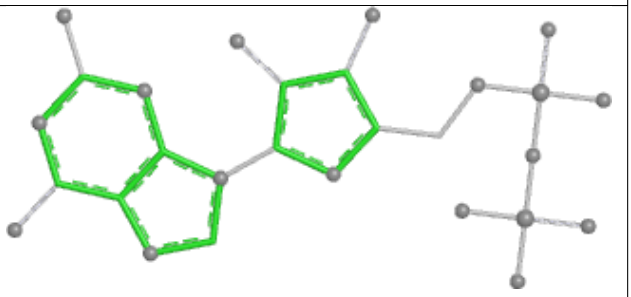
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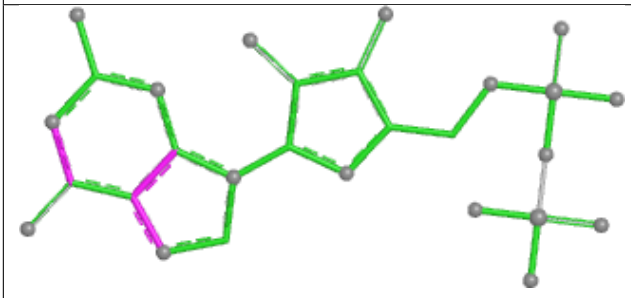


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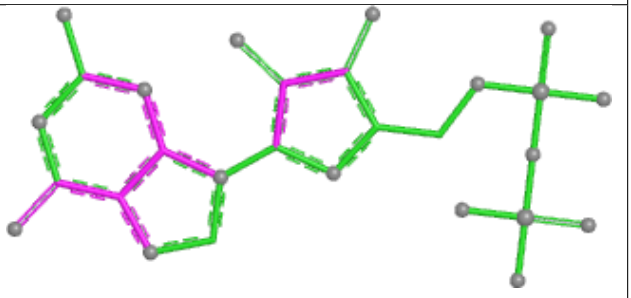


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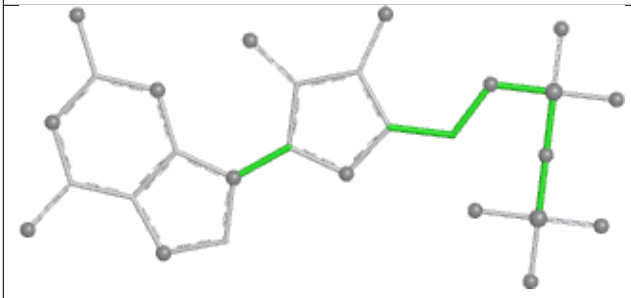
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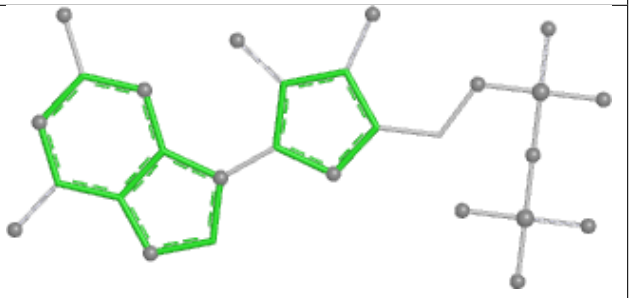
Bond lengths



Bond angles

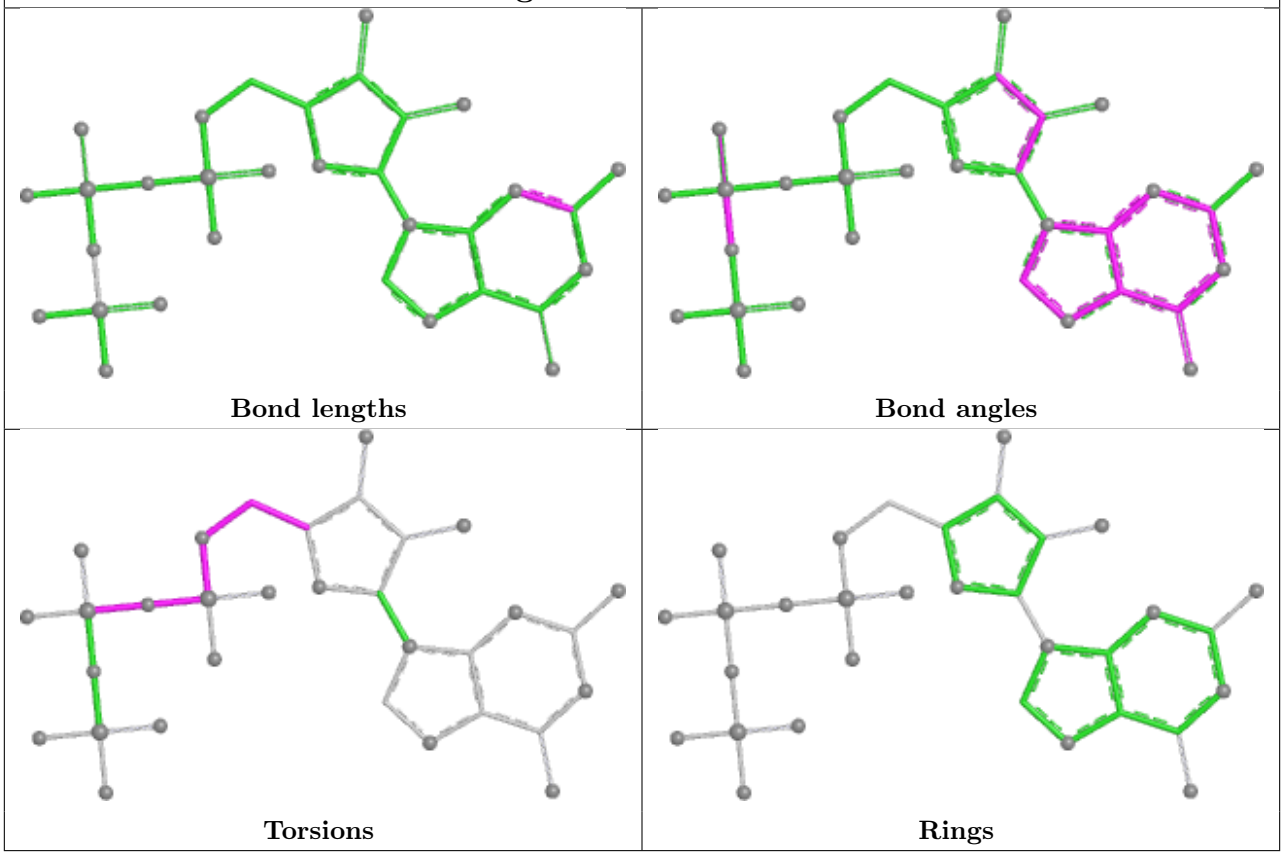


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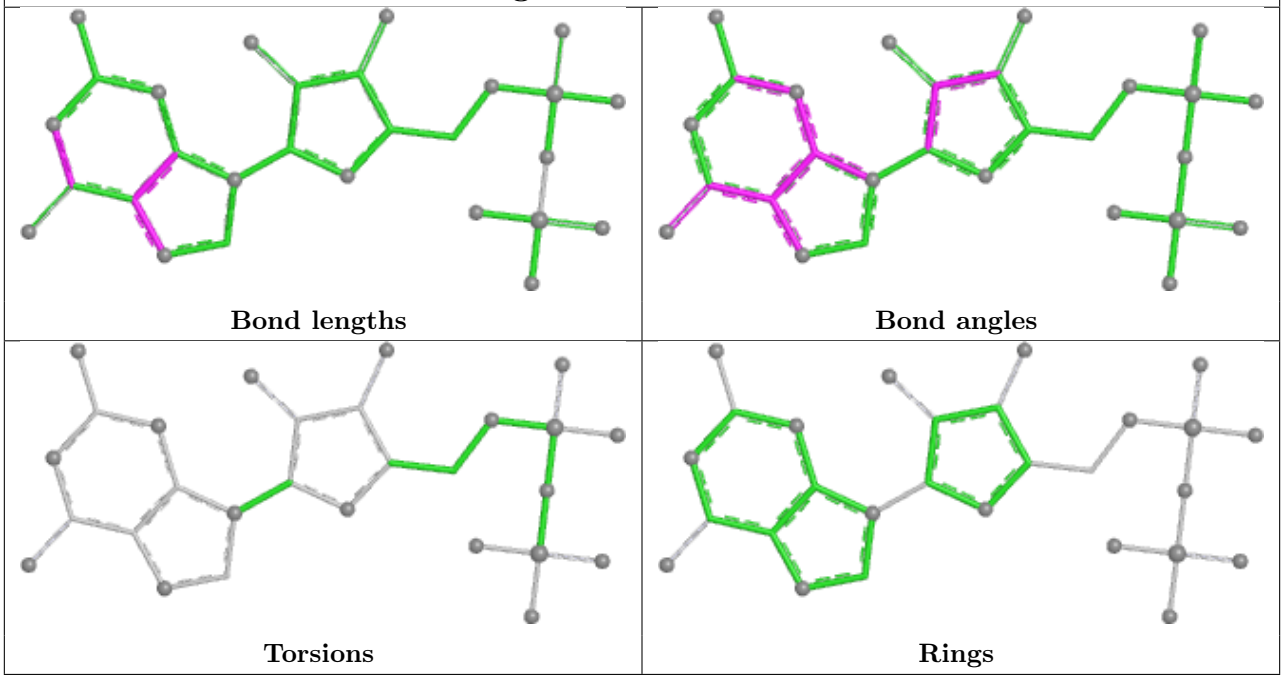


Rings

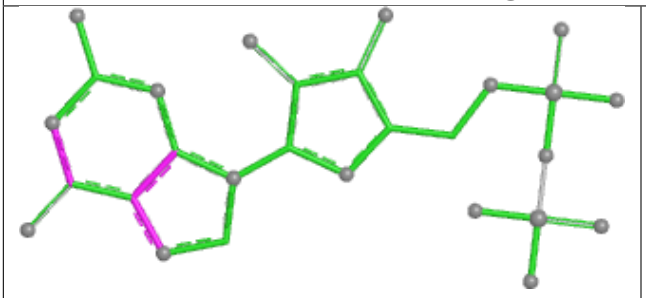
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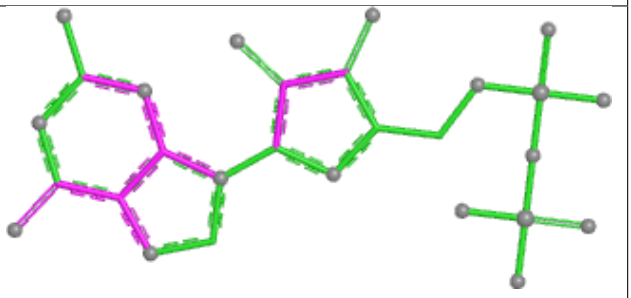
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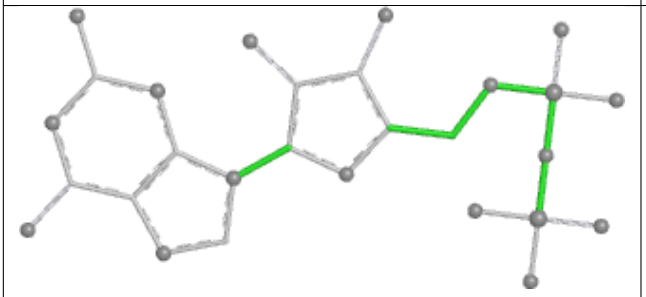
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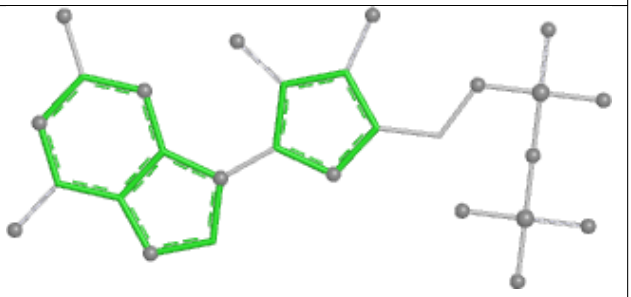
Bond lengths



Bond angles

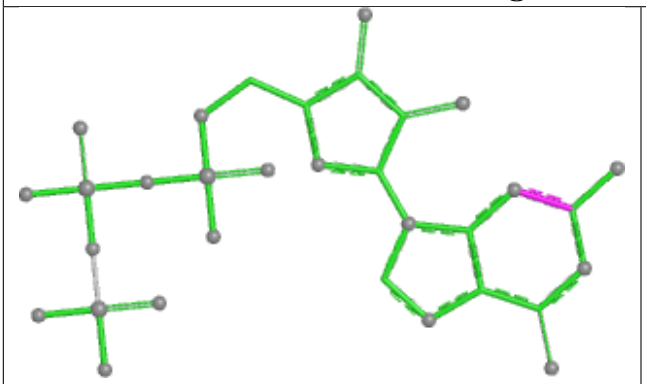


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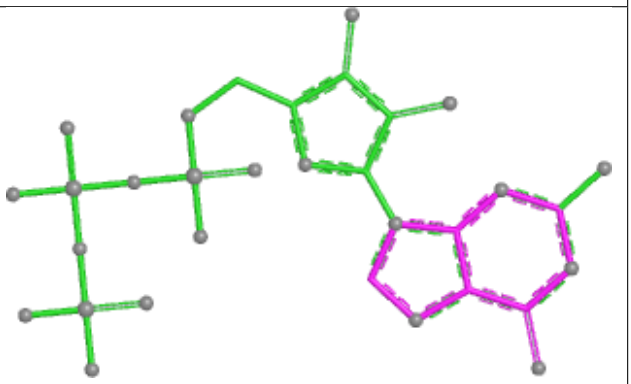


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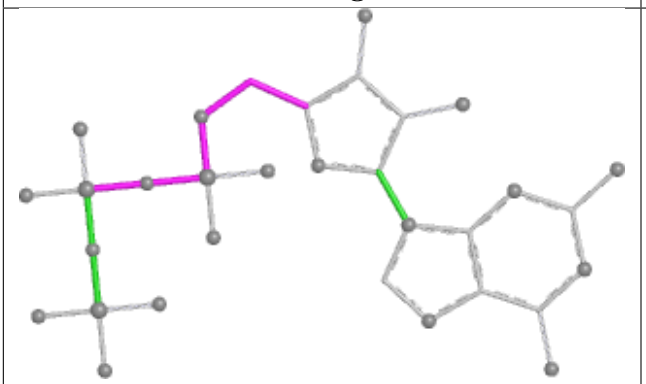
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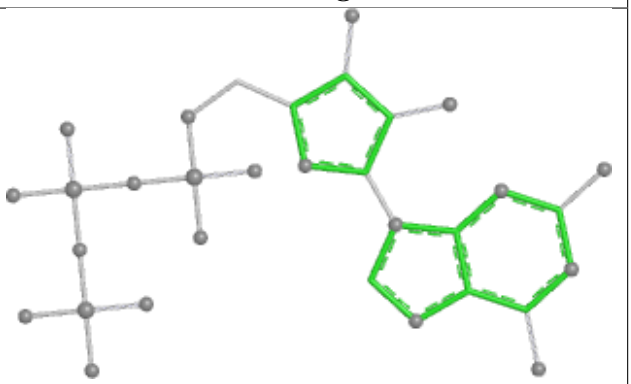
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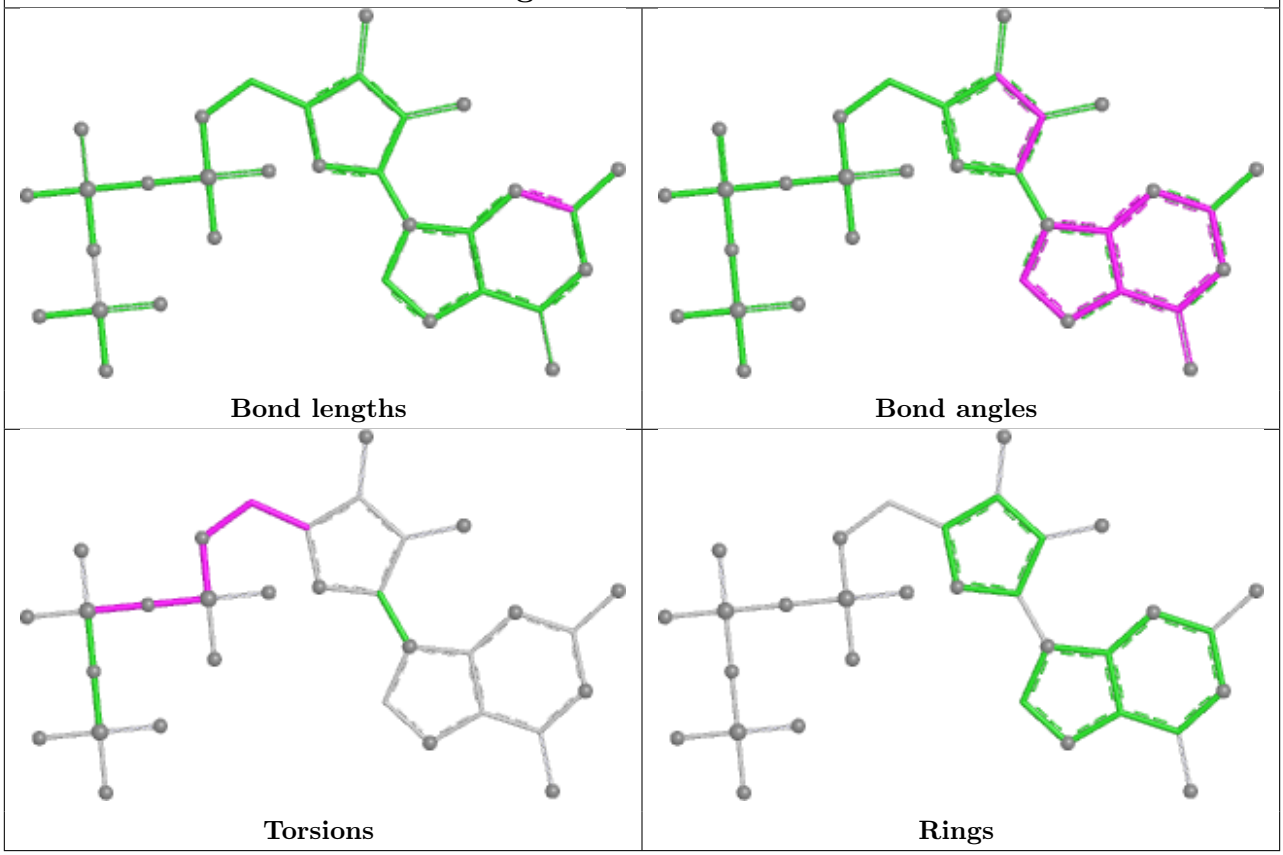


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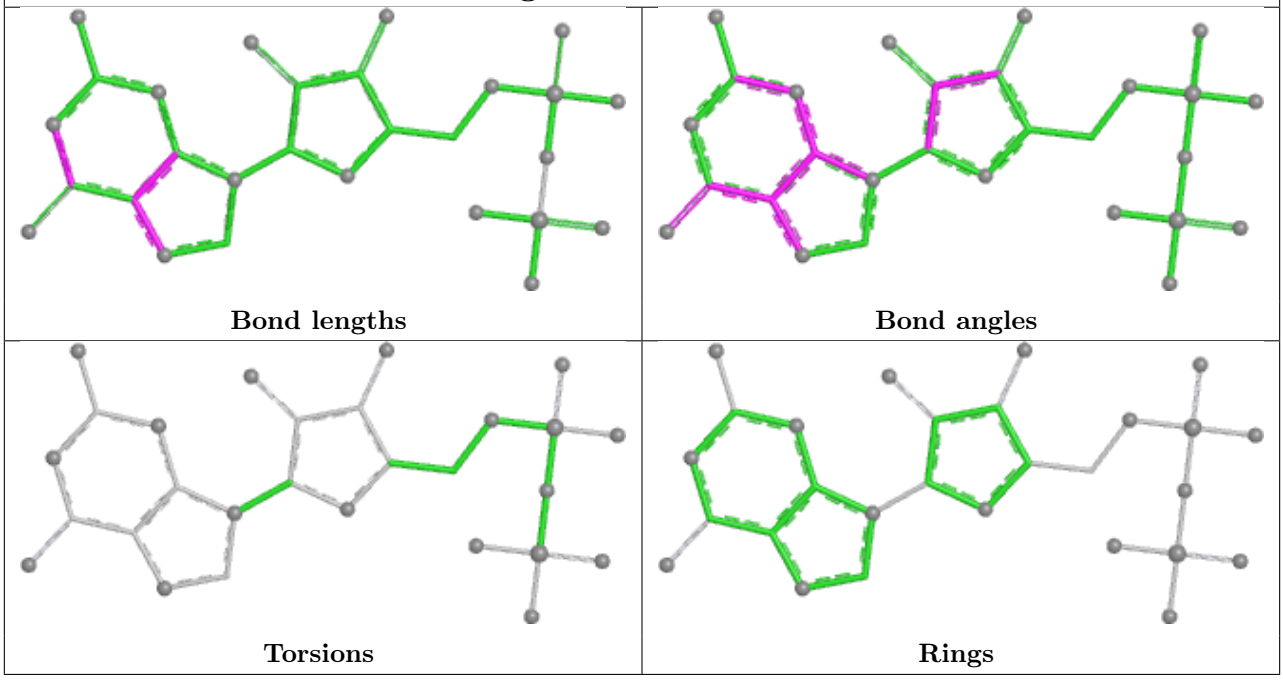


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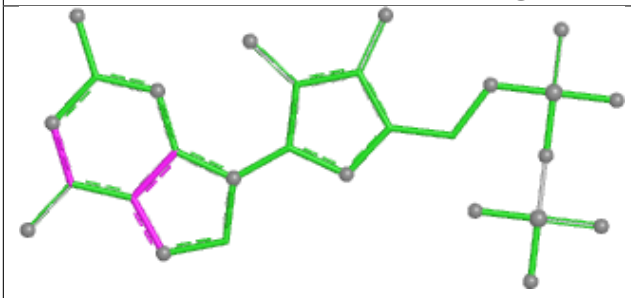
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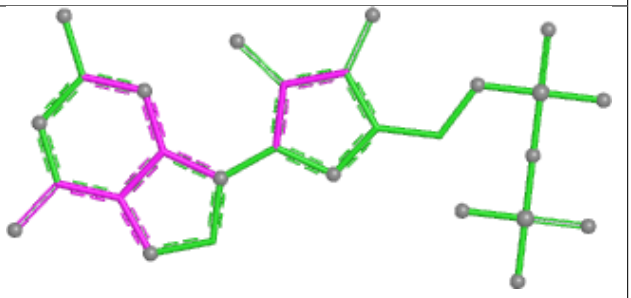
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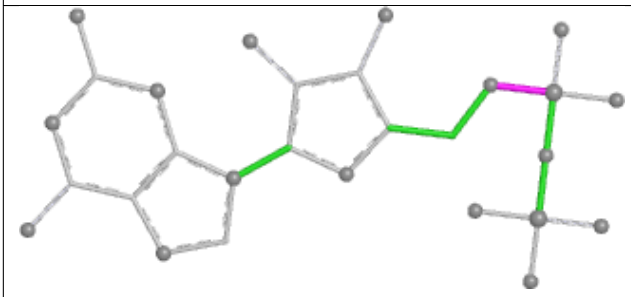
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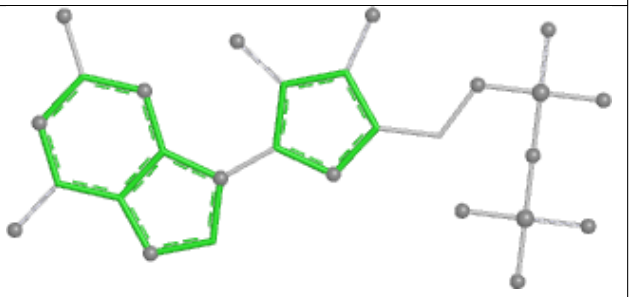
Bond lengths



Bond angles

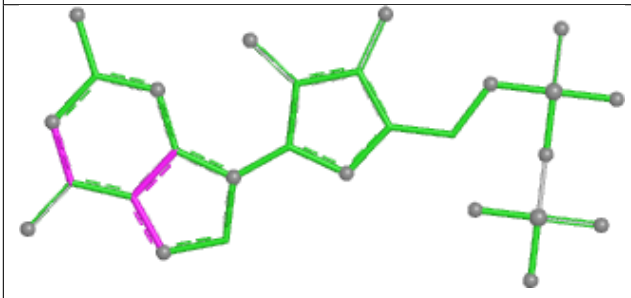


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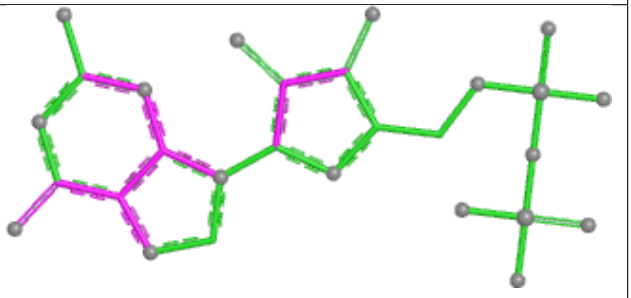


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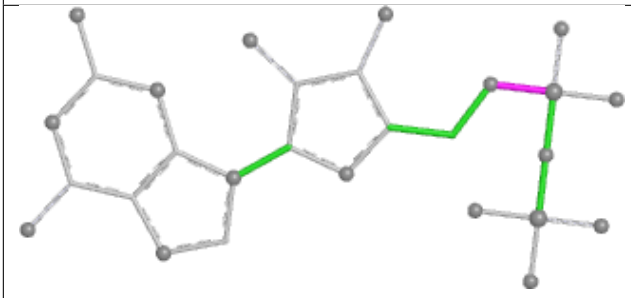
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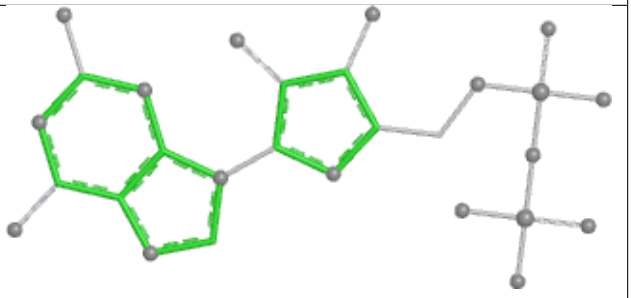
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Bond angles

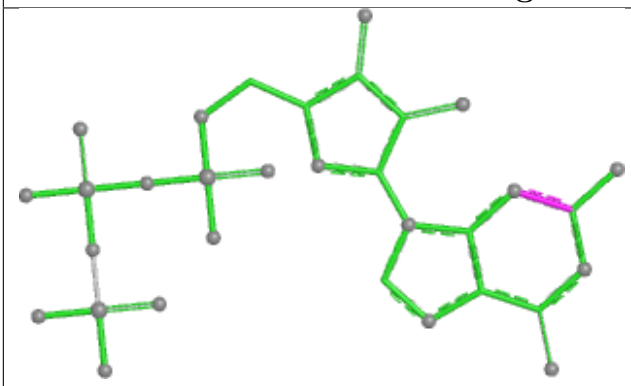


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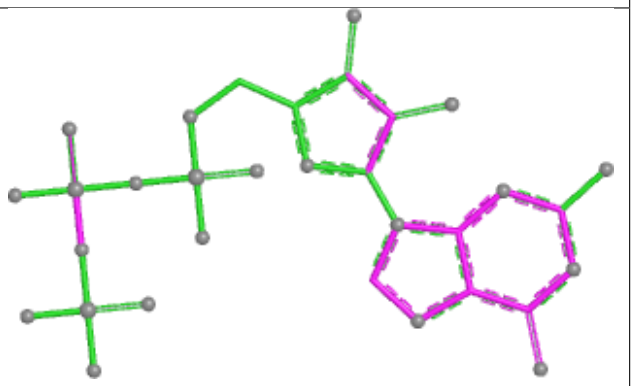


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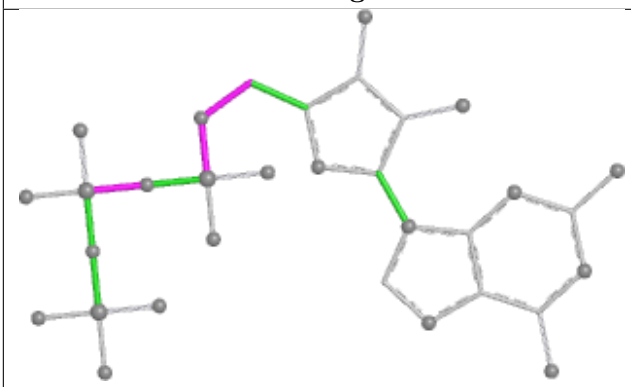
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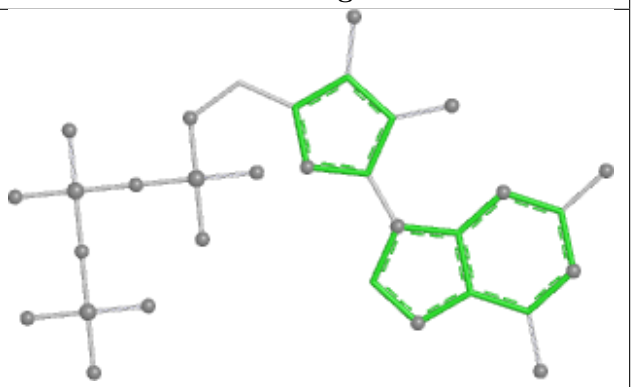
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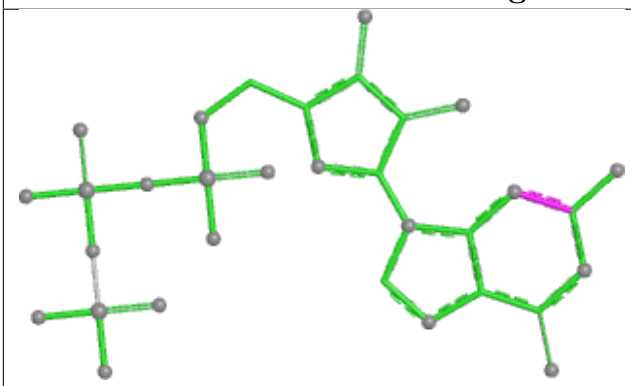


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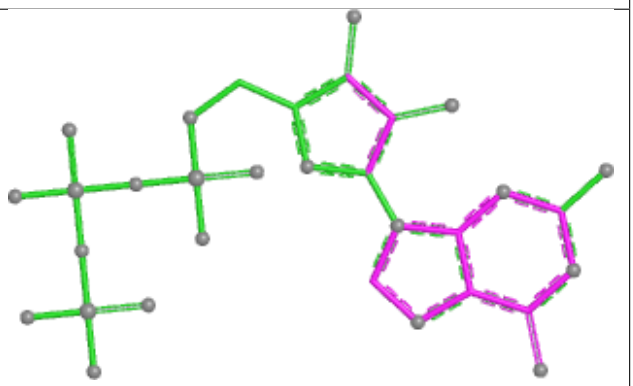


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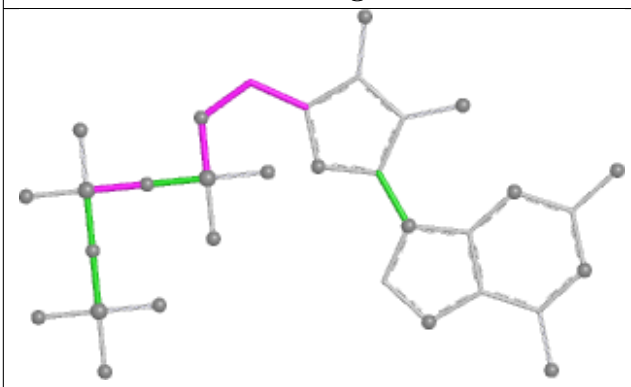
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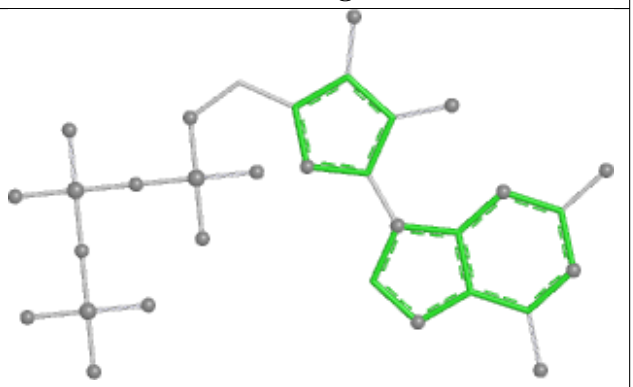
Bond lengths



Bond angles

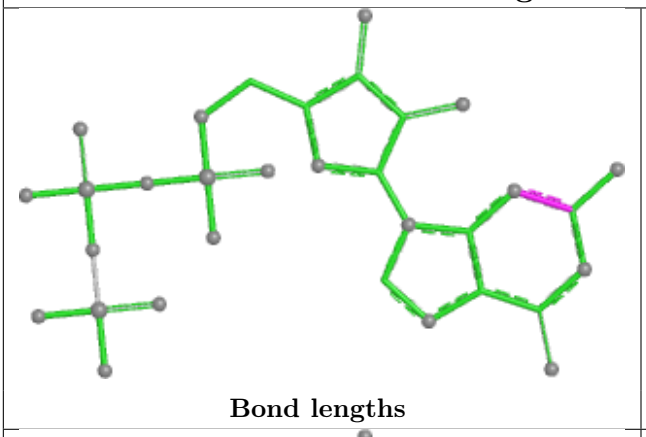


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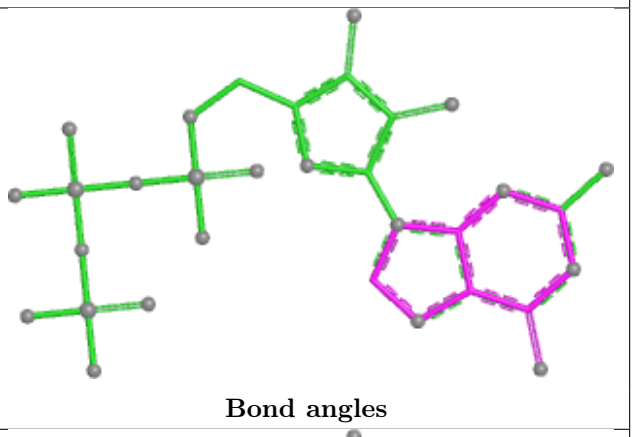


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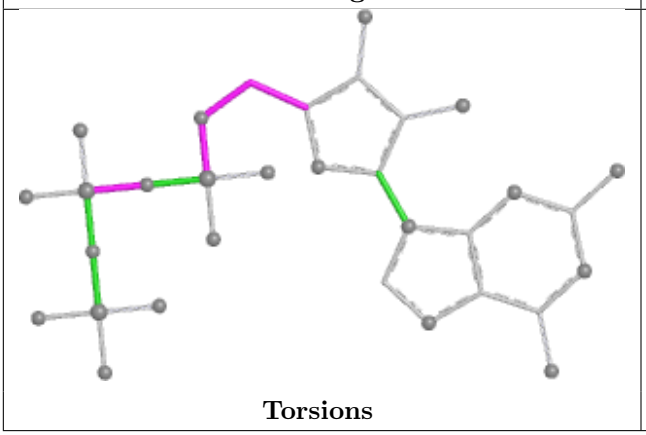
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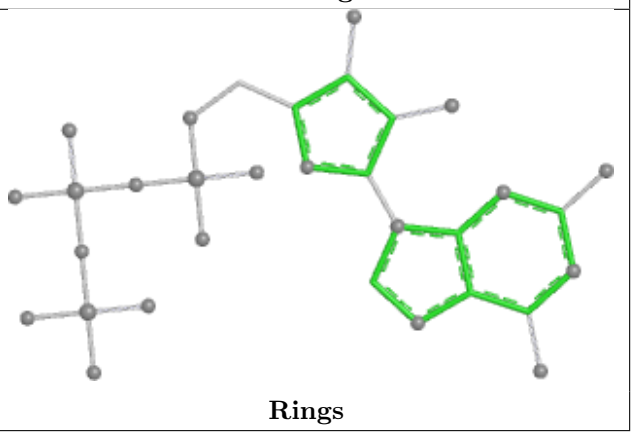
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Bond angles

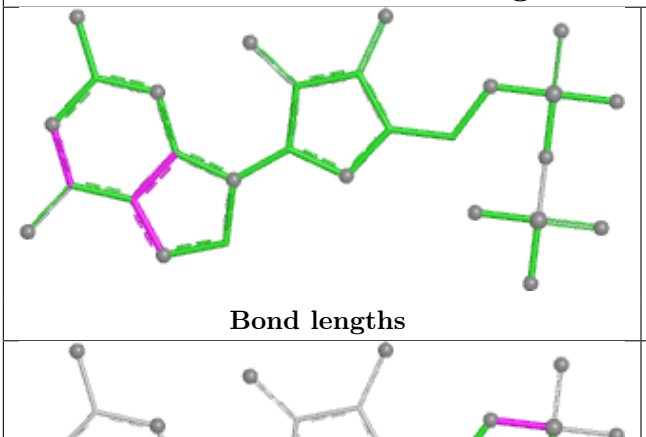


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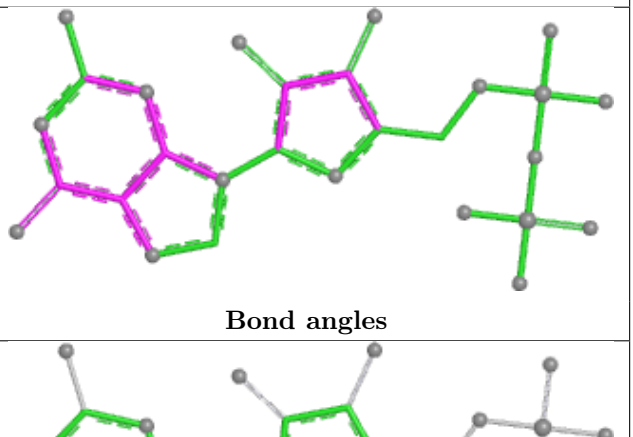


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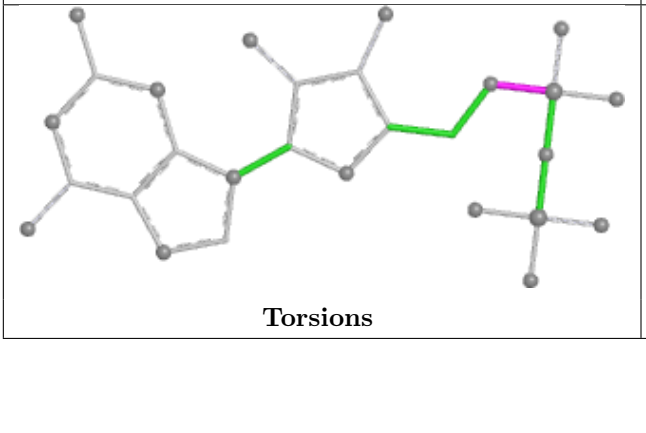
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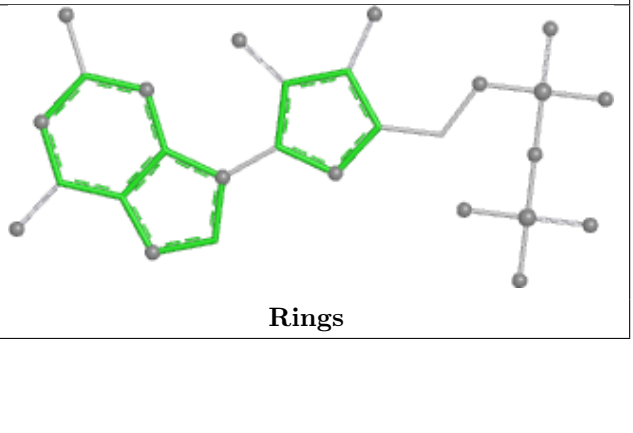
Bond lengths



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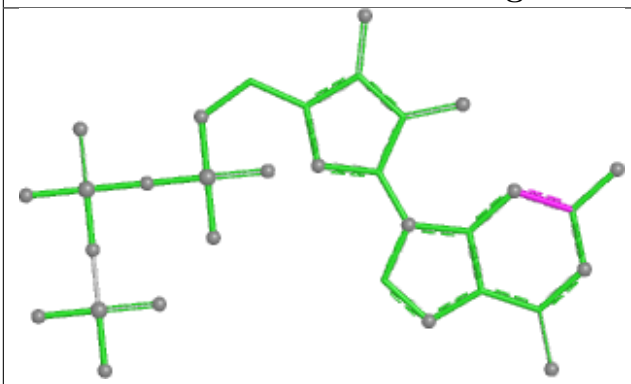


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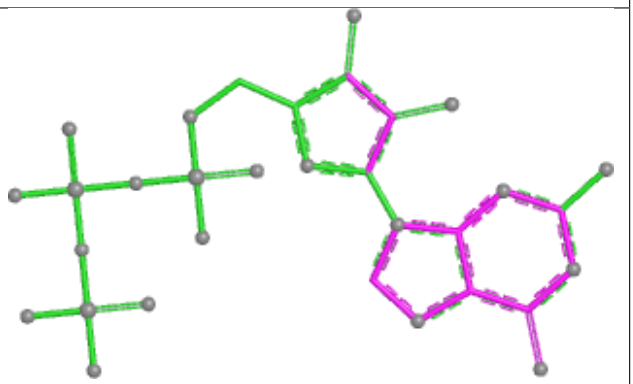


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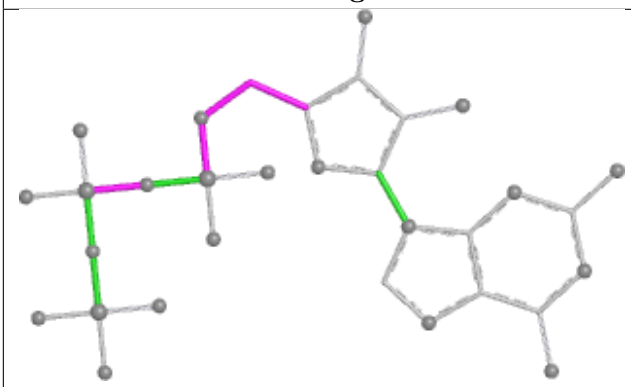
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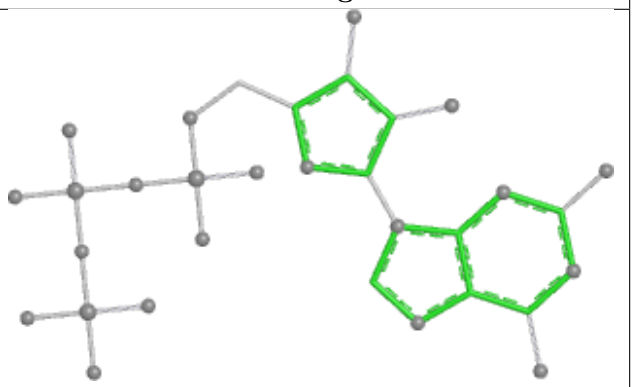
Bond lengths



Bond angles

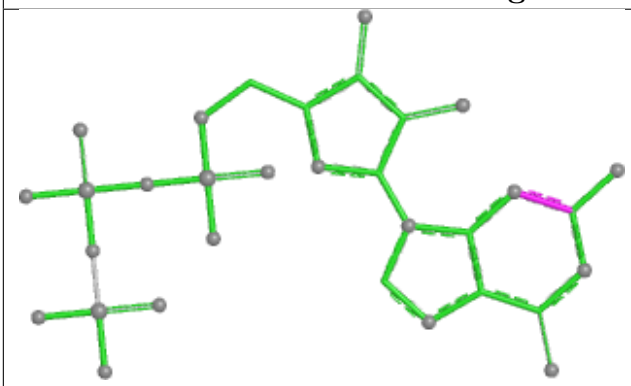


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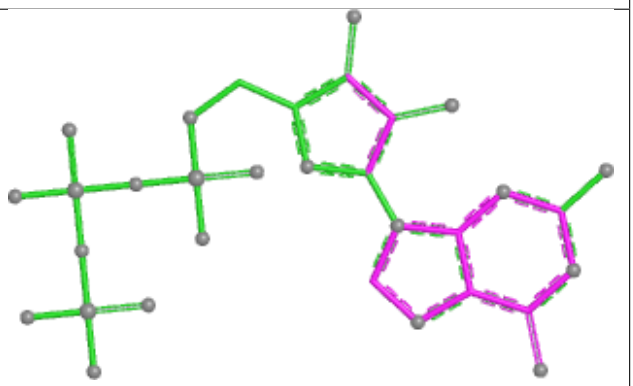


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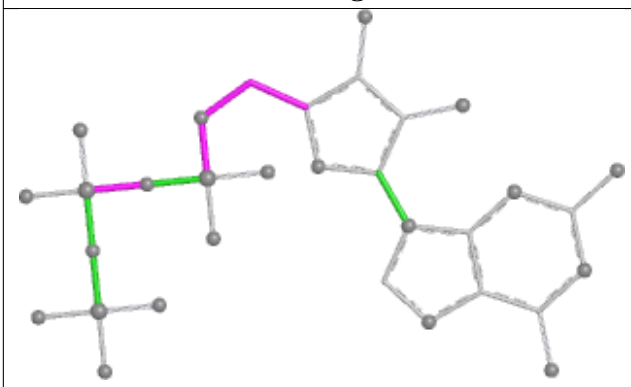
Ligand GTP GA 501



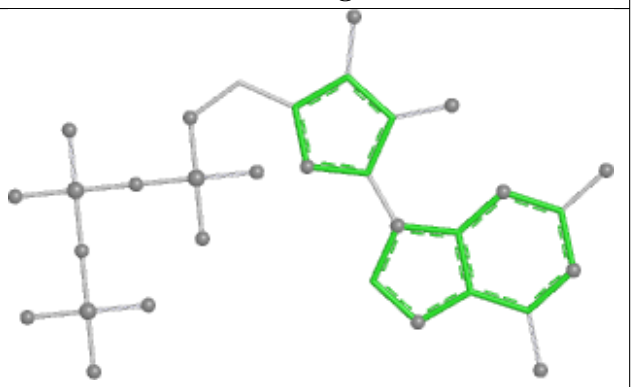
Bond lengths



Bond angles

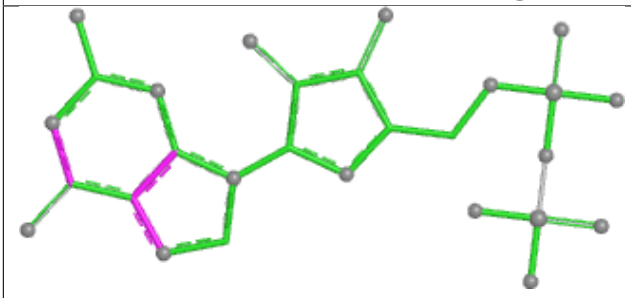


Torsions

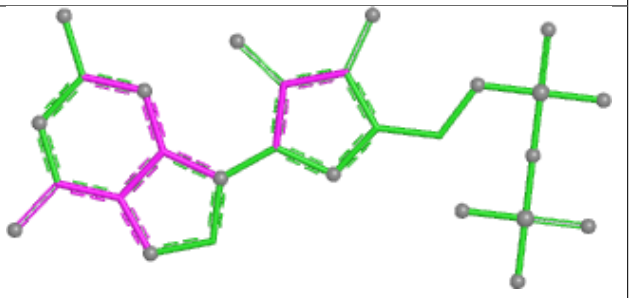


Rings

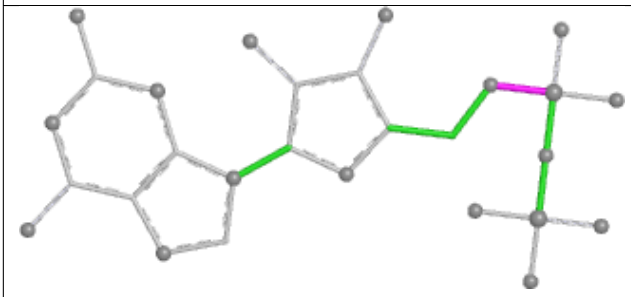
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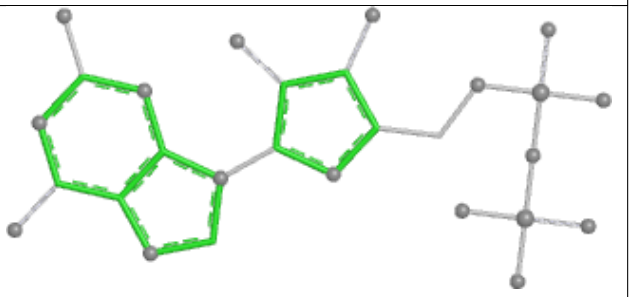
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Bond angles

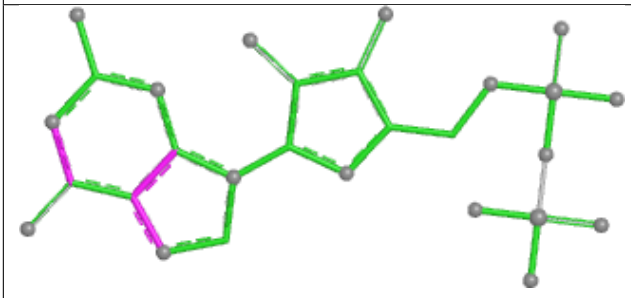


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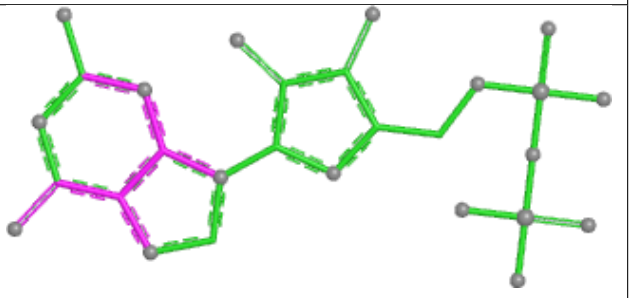


Rings

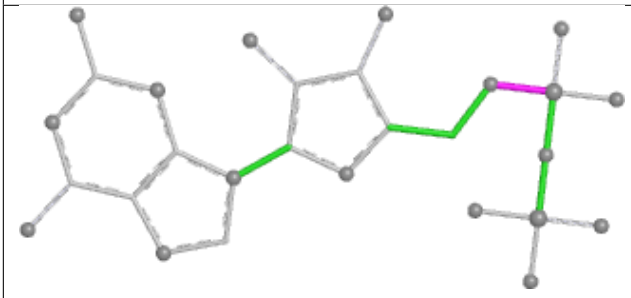
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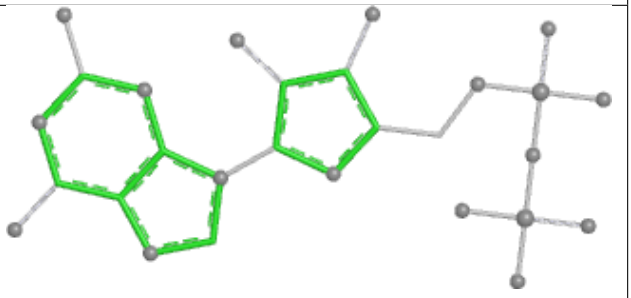
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Bond angles

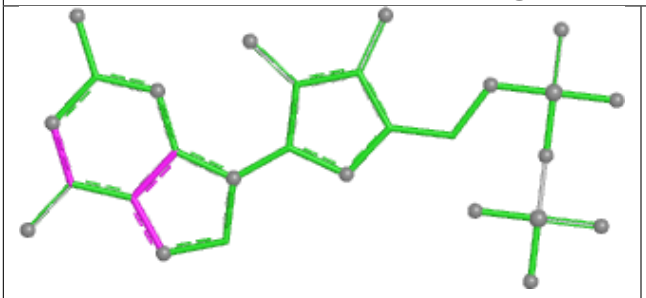


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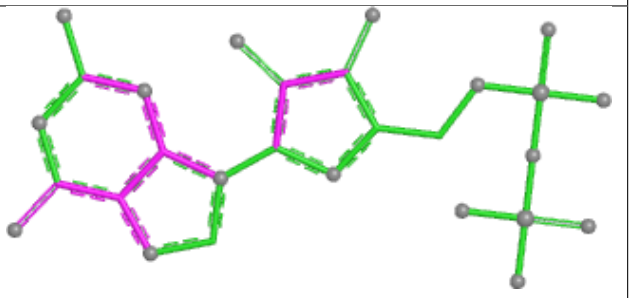


Rings

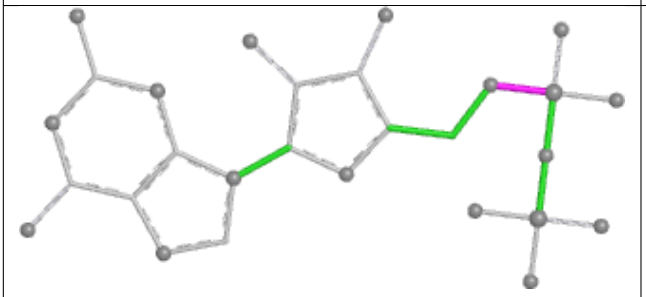
Ligand GDP TF 501



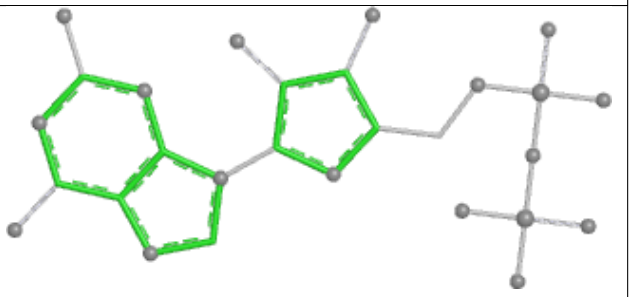
Bond lengths



Bond angles

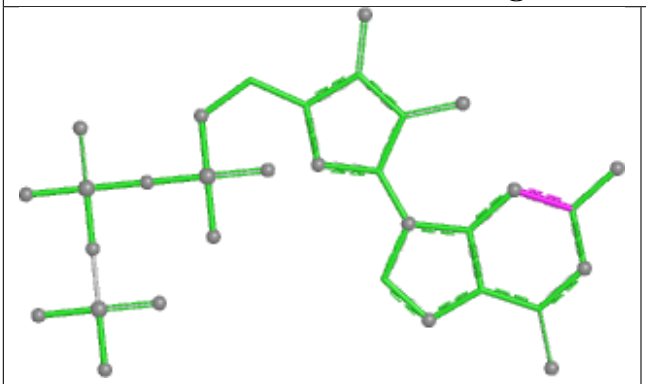


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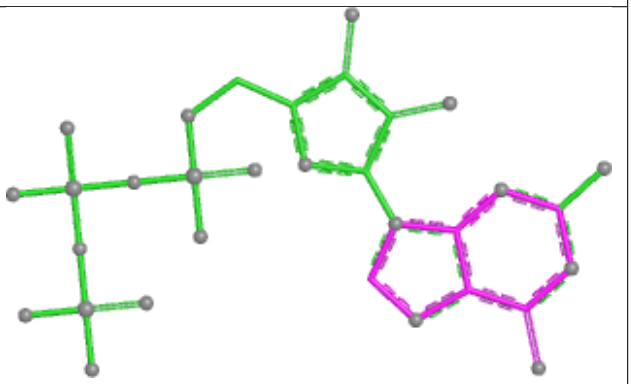


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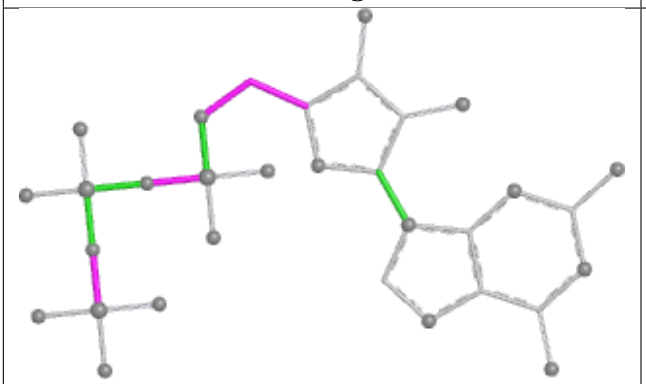
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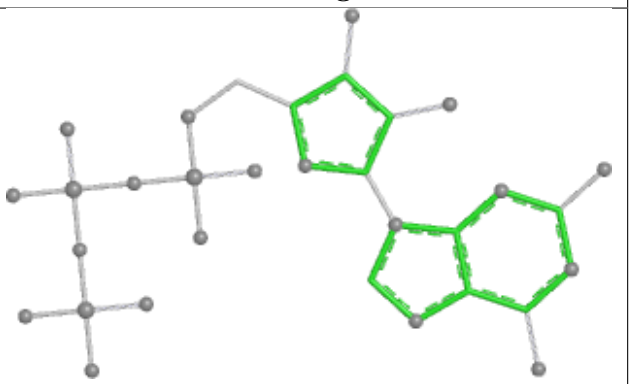
Bond lengths



Bond angles

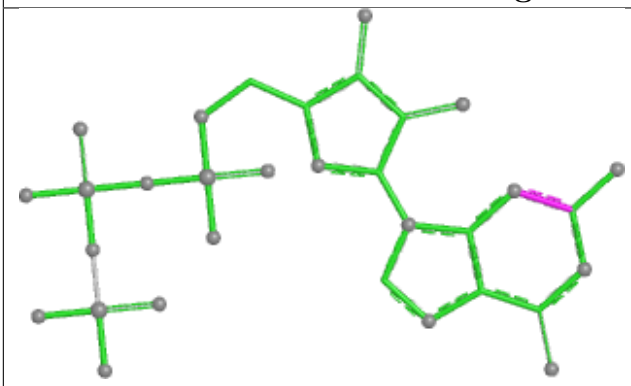


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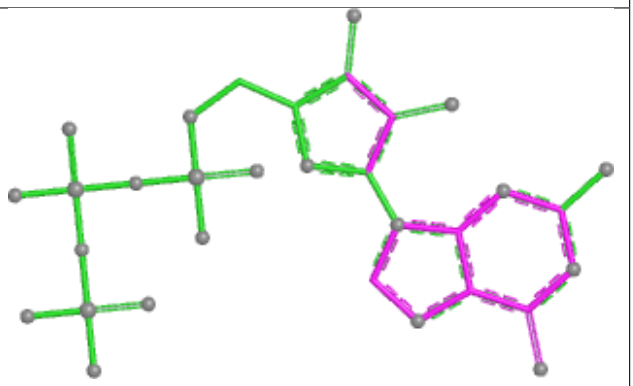


Rings

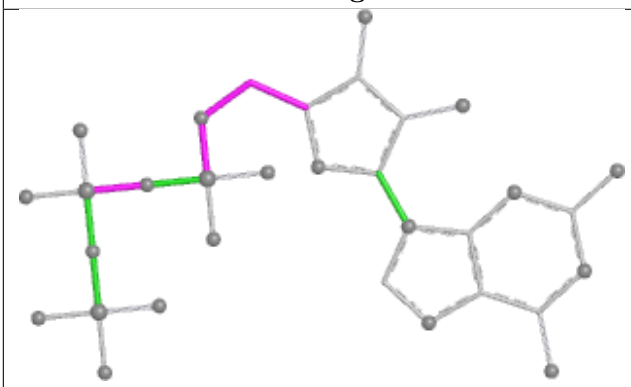
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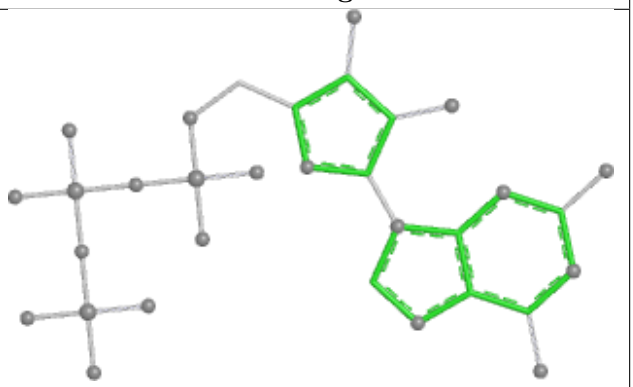
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Bond angles

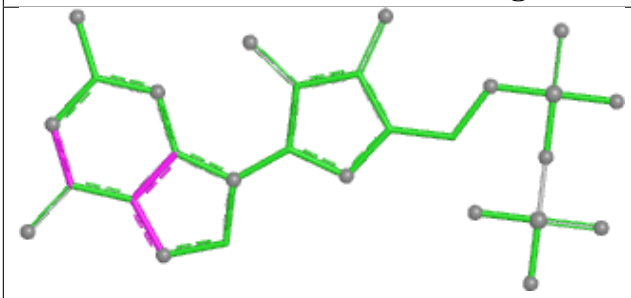


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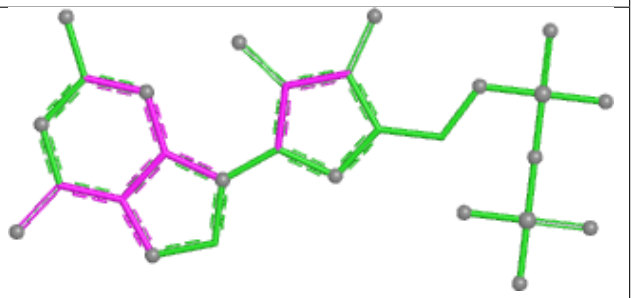


Rings

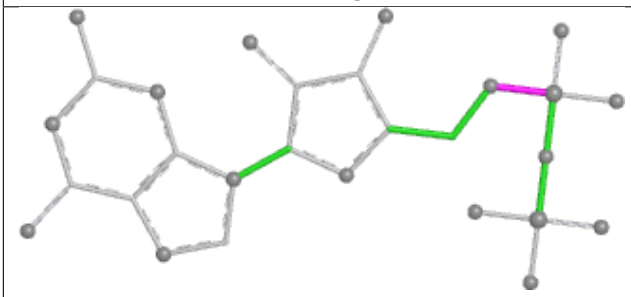
Ligand GDP AF 501



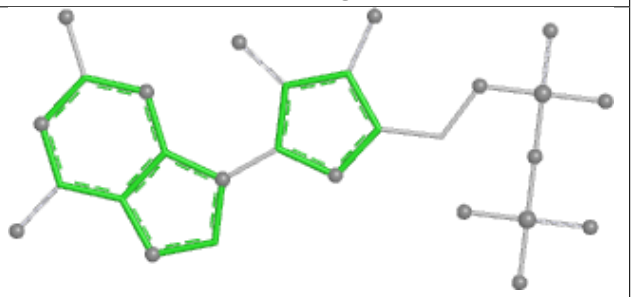
Bond lengths



Bond angles

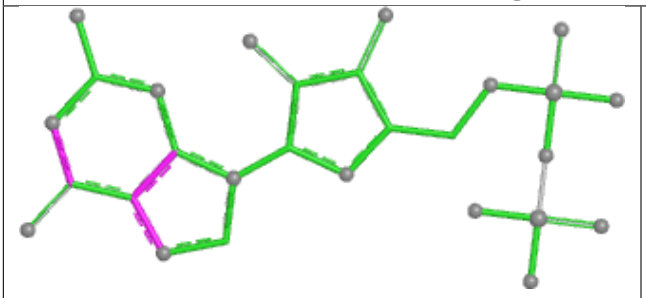


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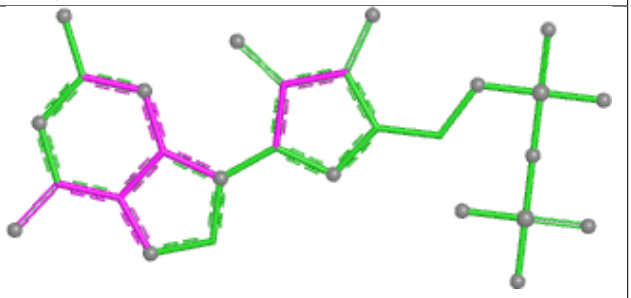


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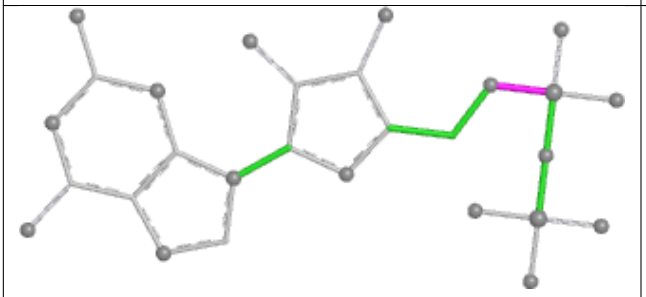
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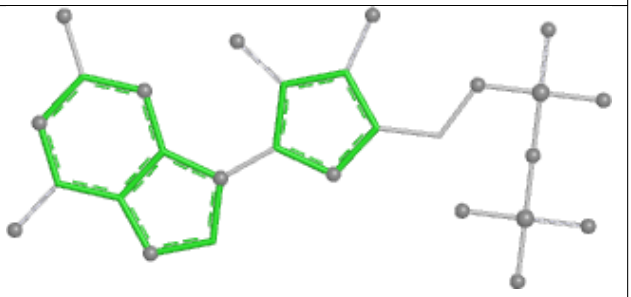
Bond lengths



Bond angles

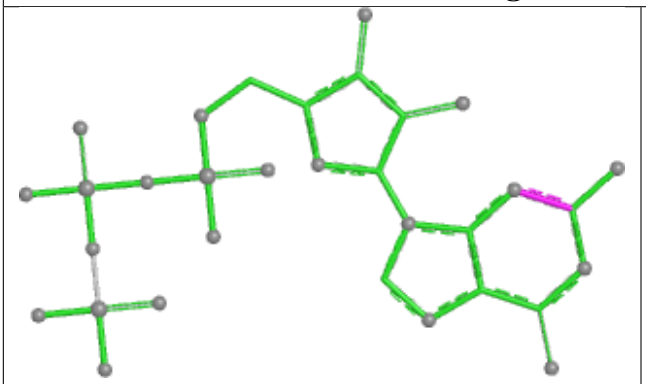


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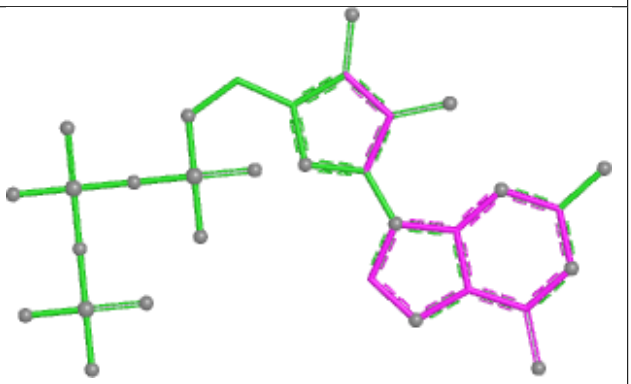


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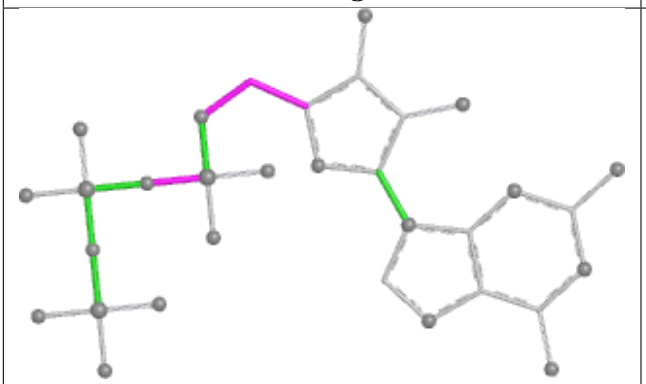
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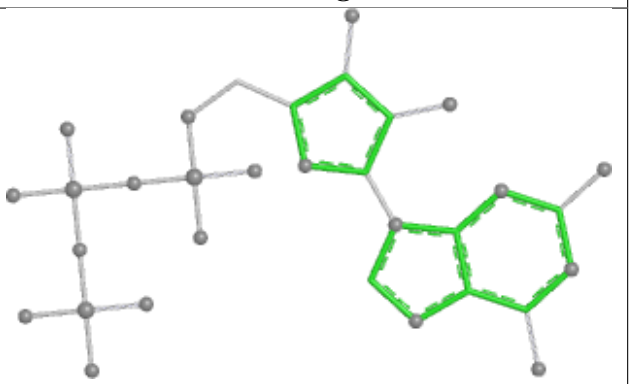
Bond lengths



Bond angles

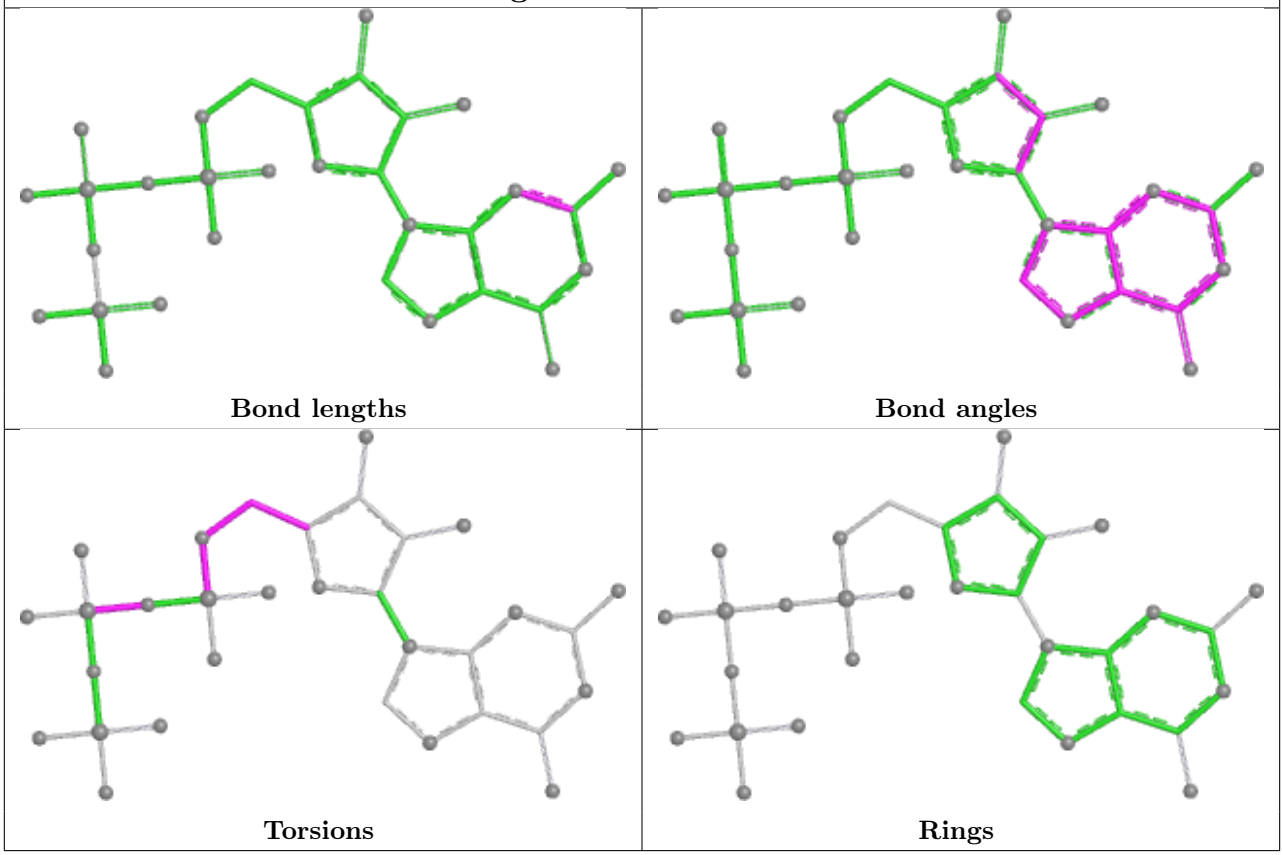


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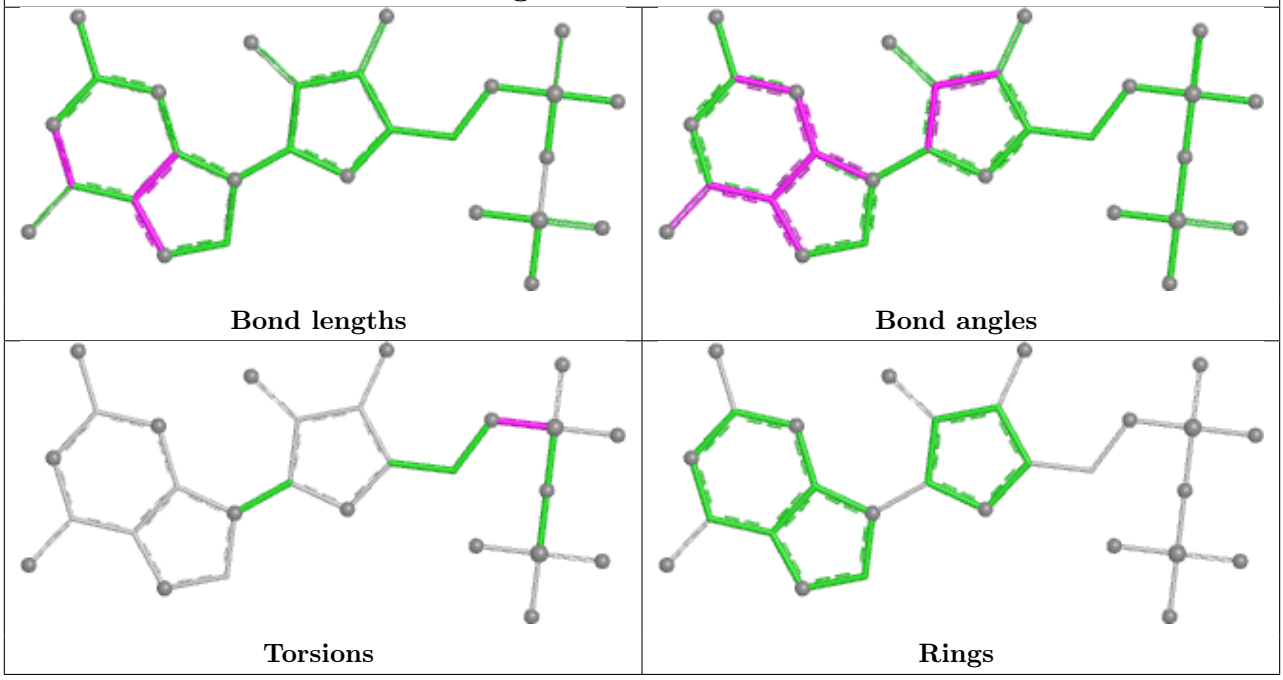


Rings

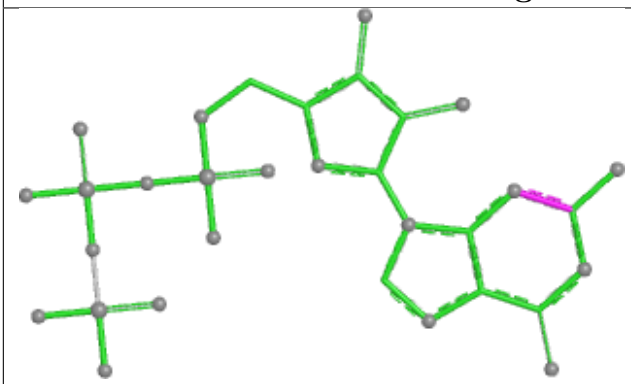
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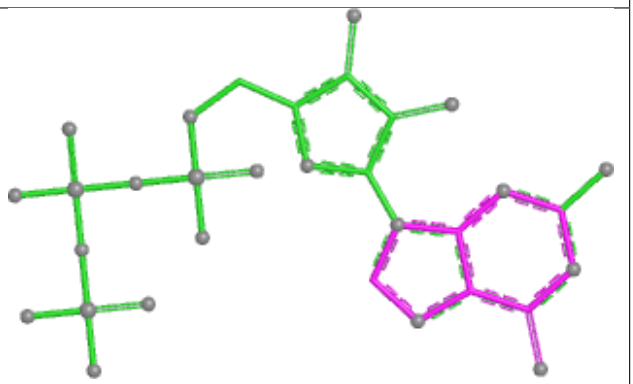
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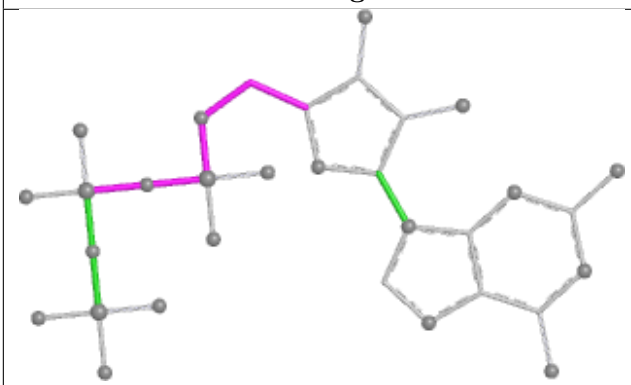
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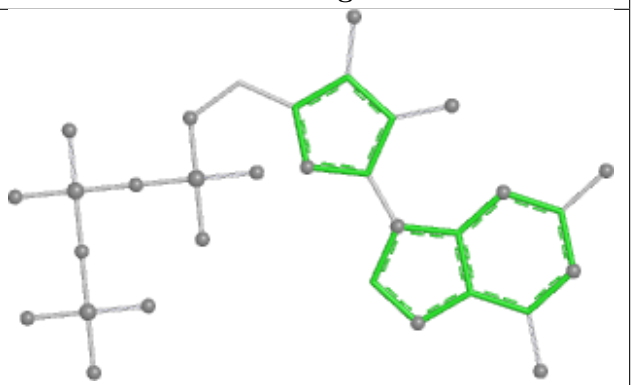
Bond lengths



Bond angles

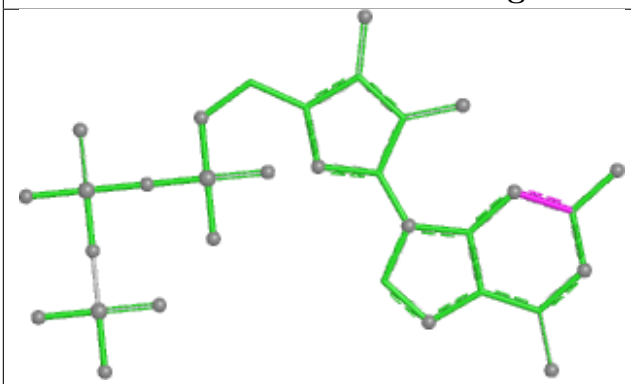


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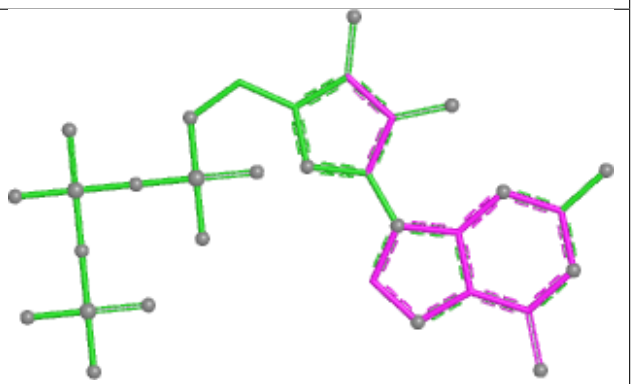


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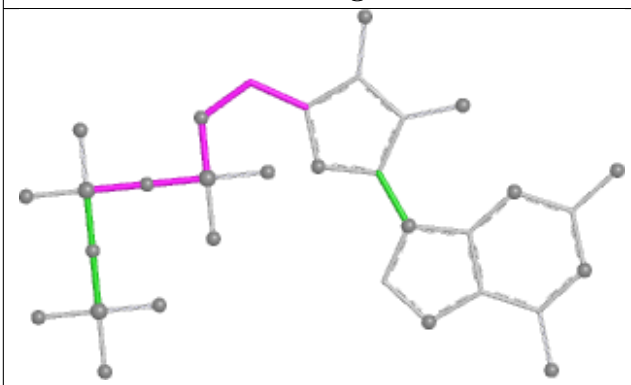
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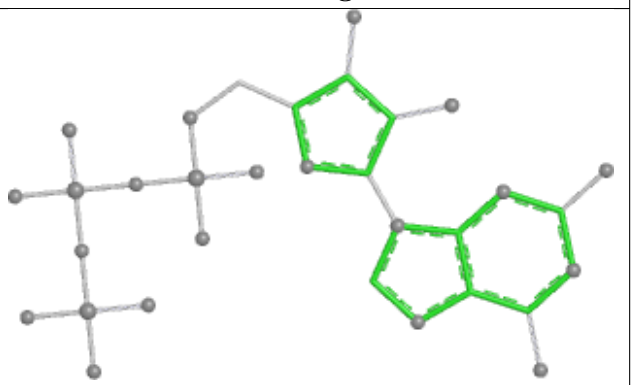
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Bond angles

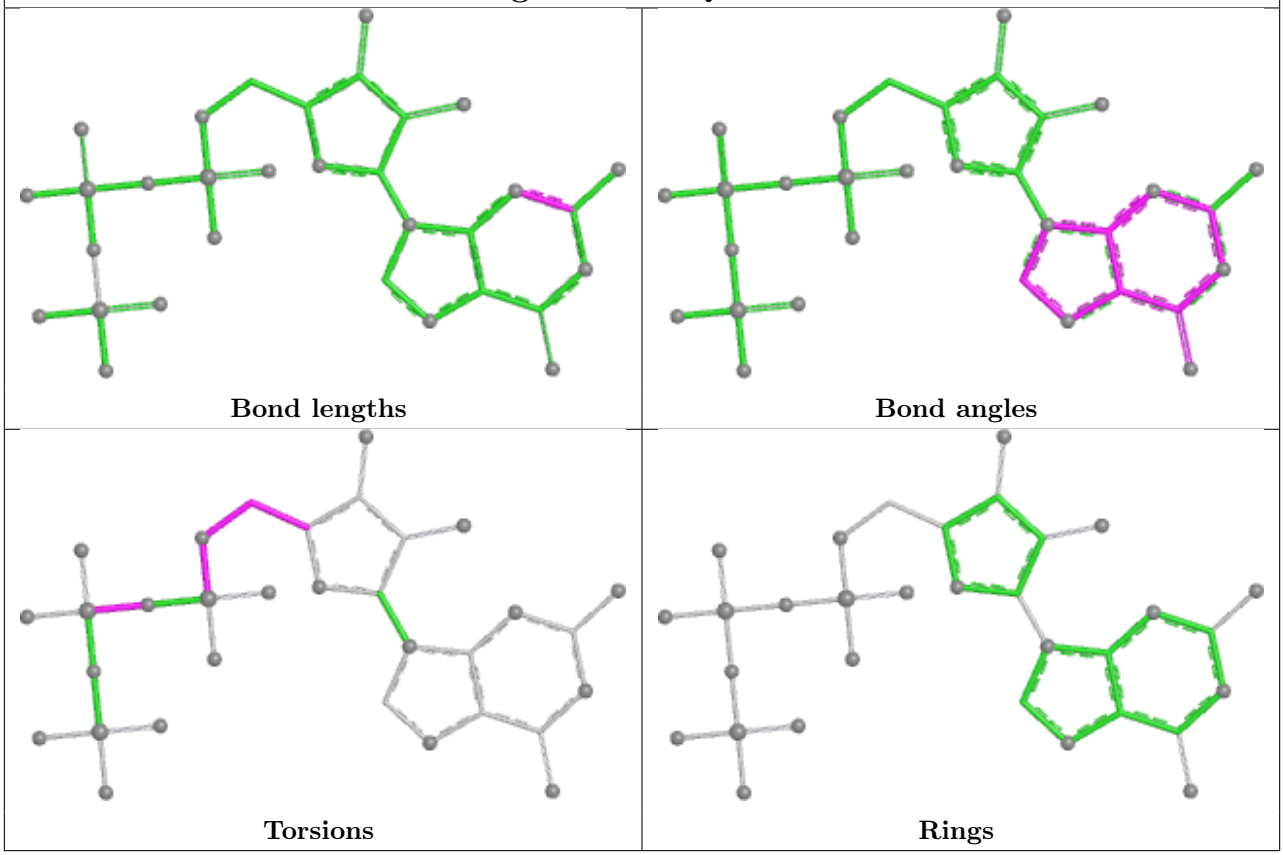


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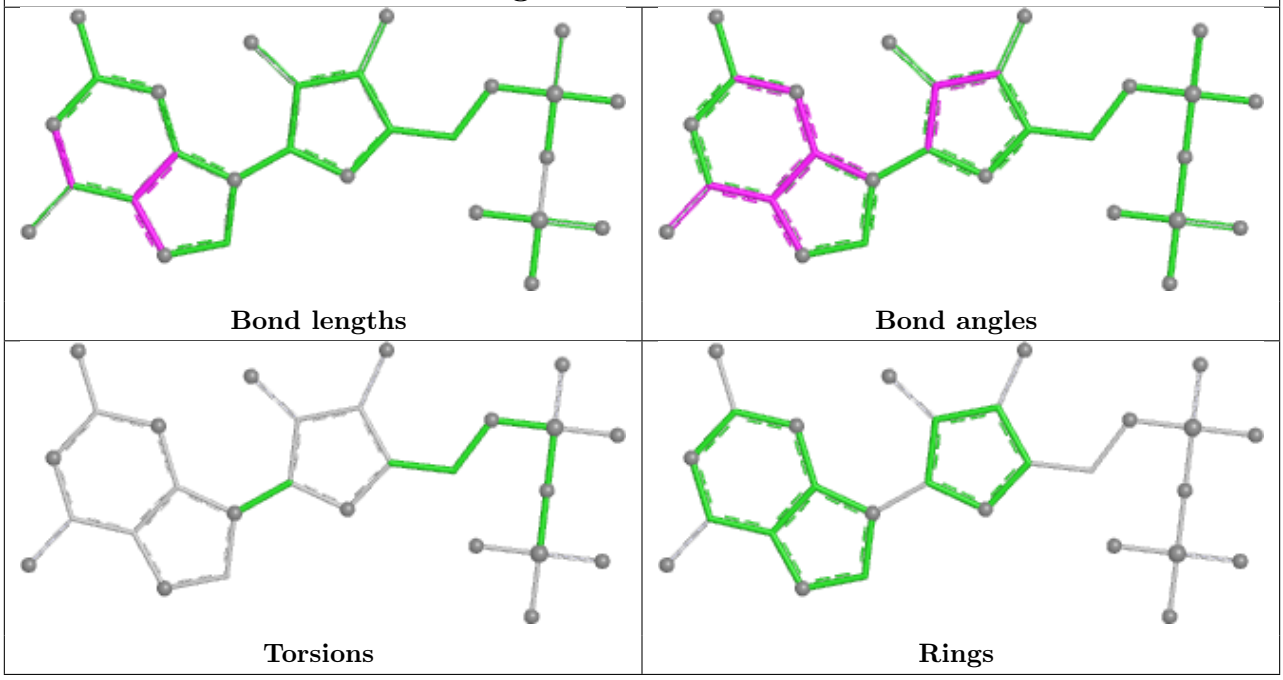


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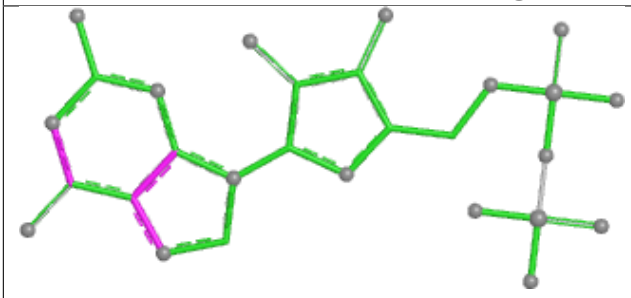
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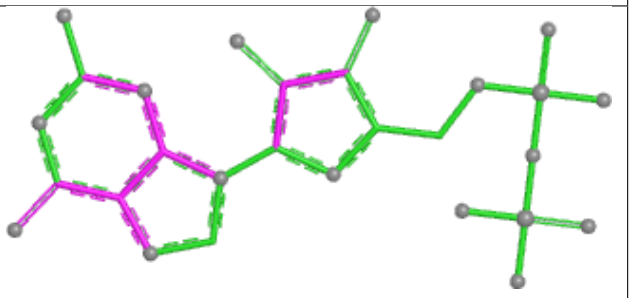
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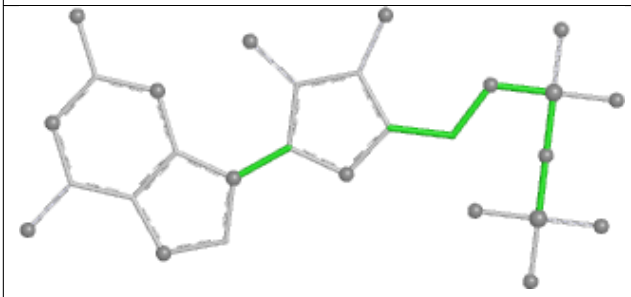
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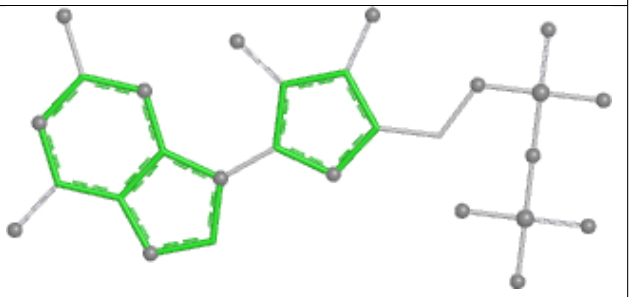
Bond lengths



Bond angles

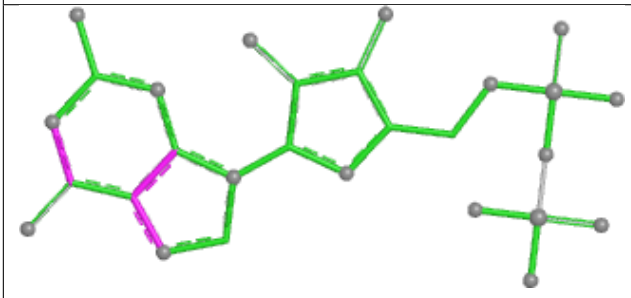


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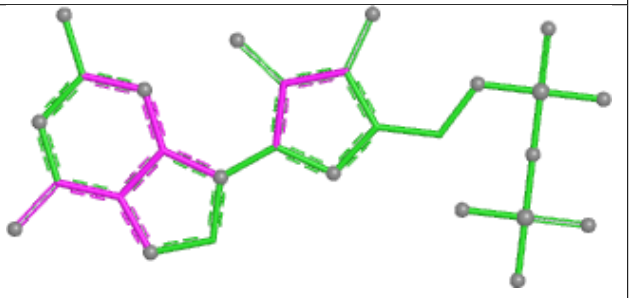


Rings

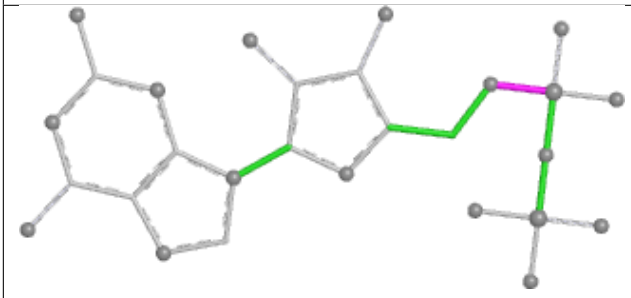
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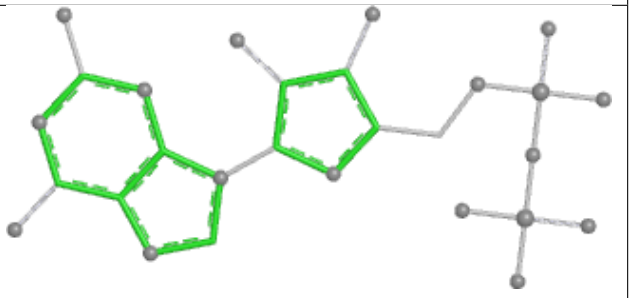
Bond lengths



Bond angles

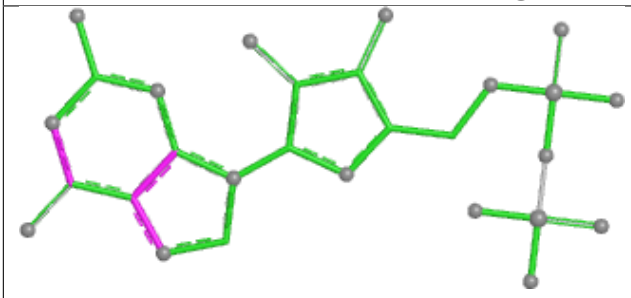


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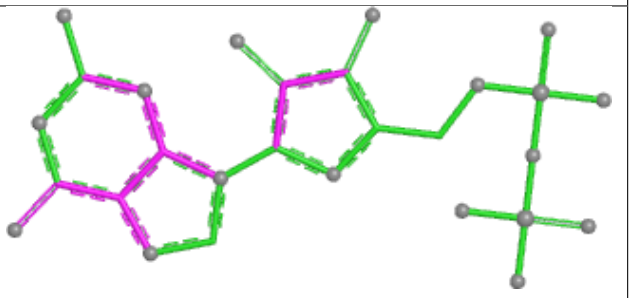


Rings

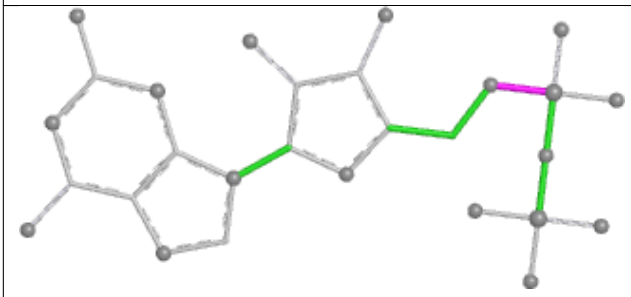
Ligand GDP FL 502



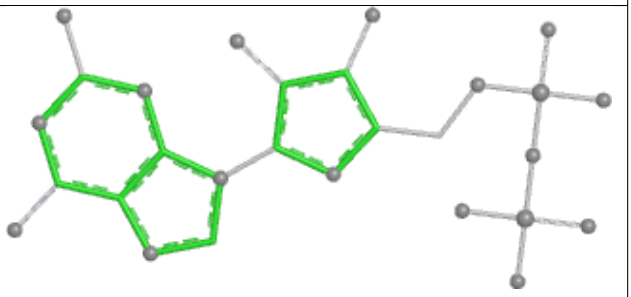
Bond lengths



Bond angles

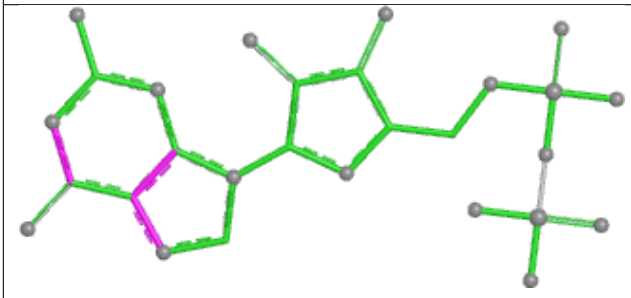


Torsions

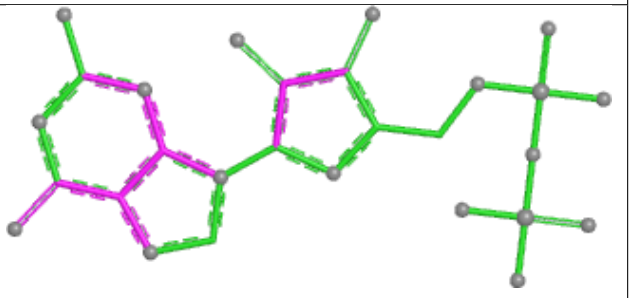


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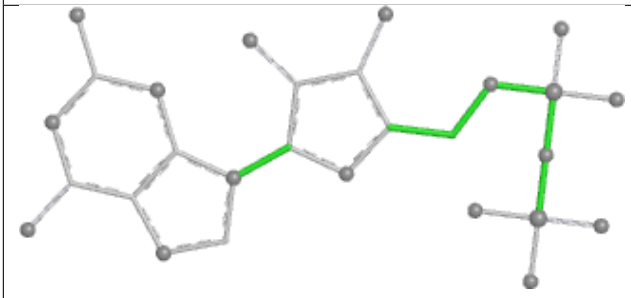
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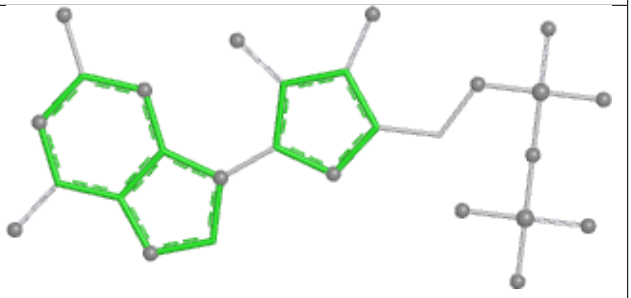
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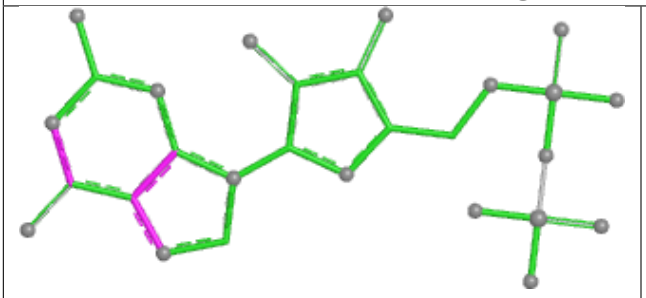


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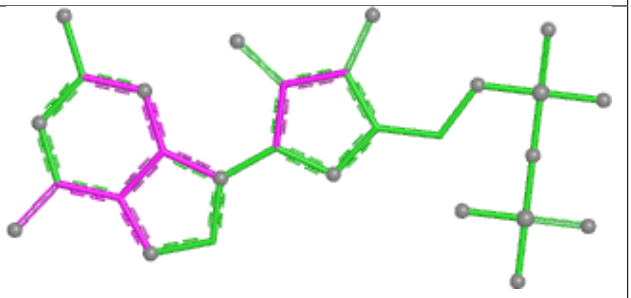


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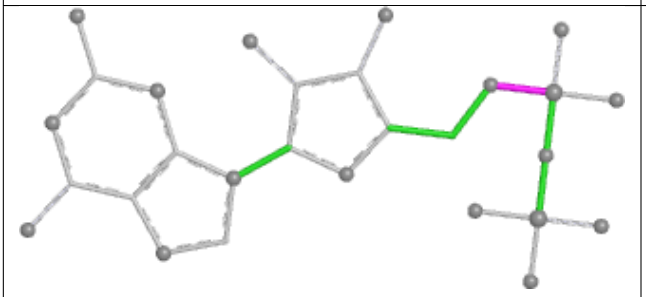
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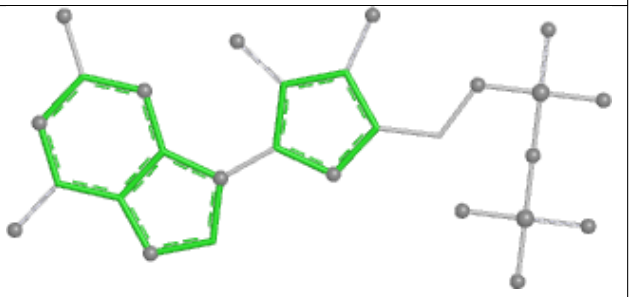
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Bond angles

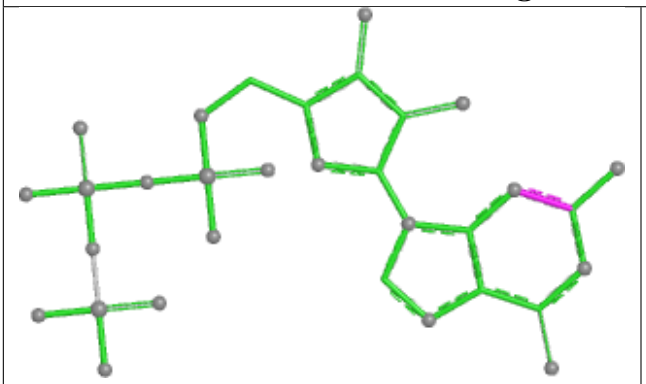


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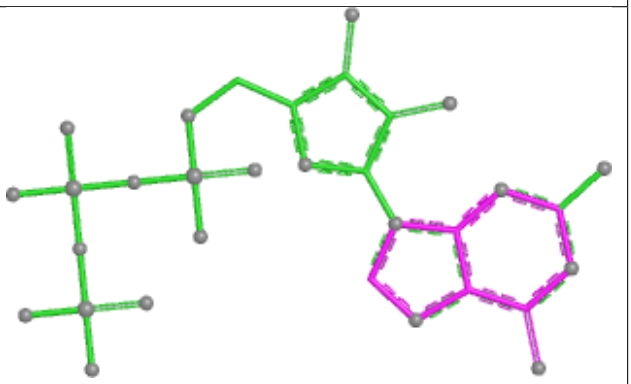


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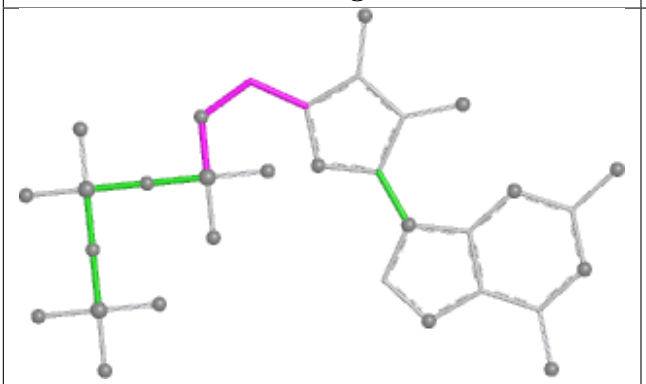
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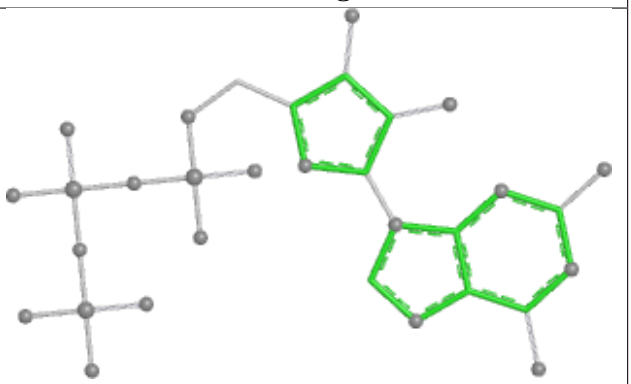
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Bond angles

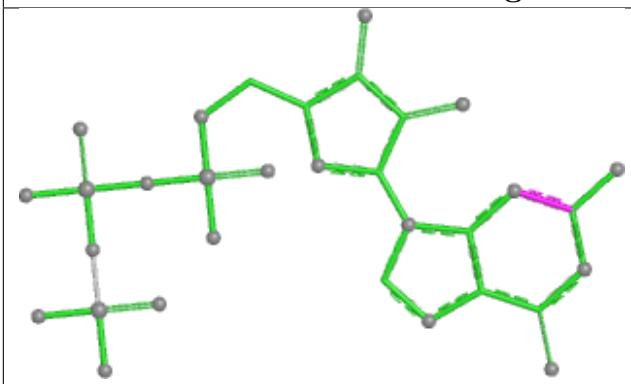


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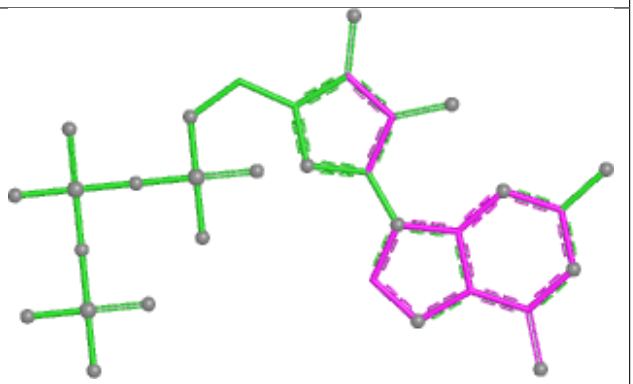


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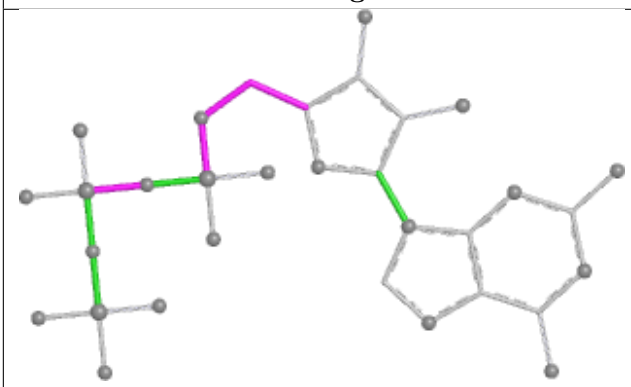
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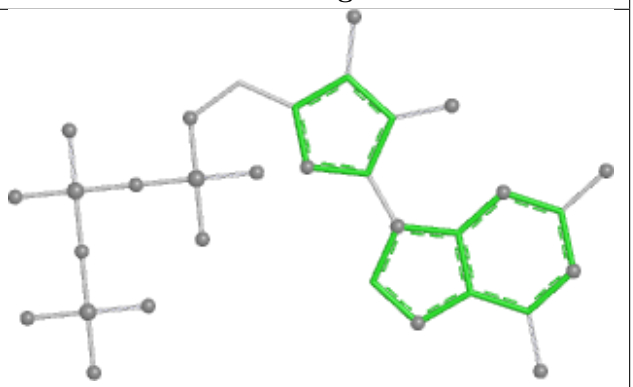
Bond lengths



Bond angles

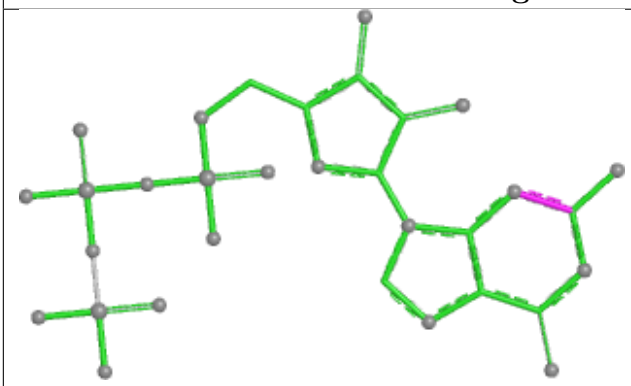


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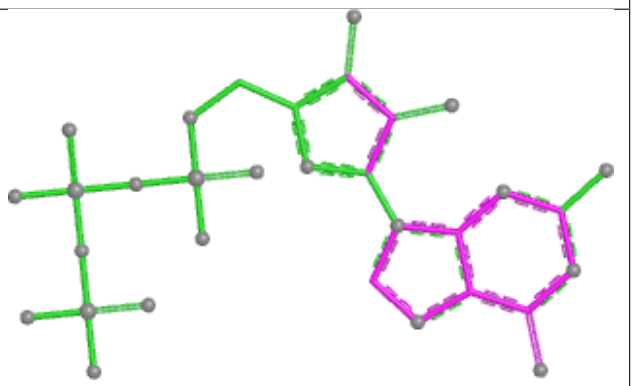


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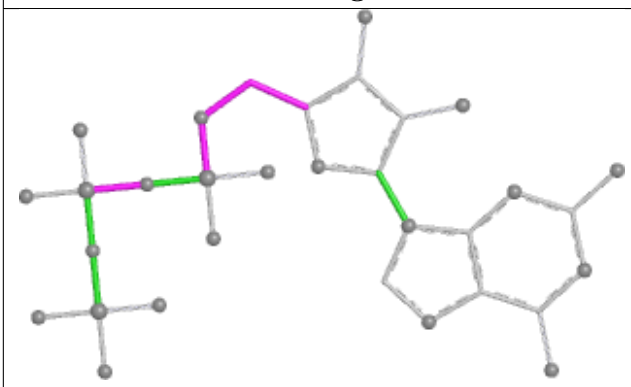
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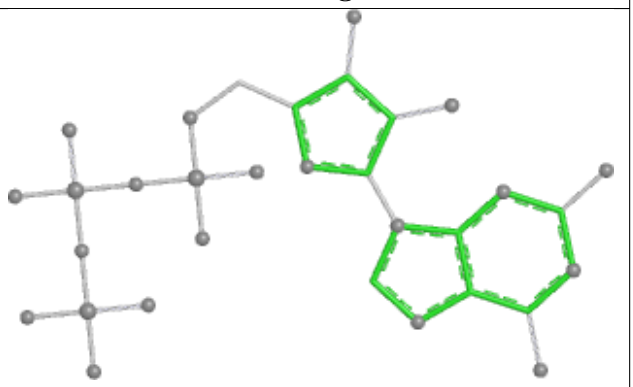
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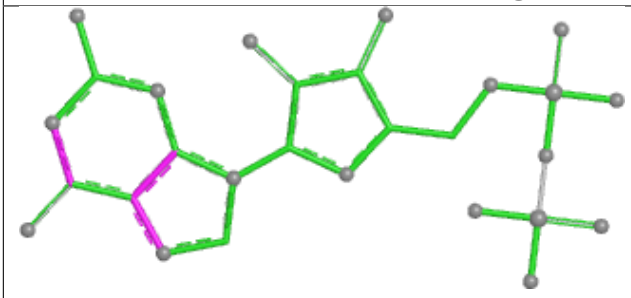


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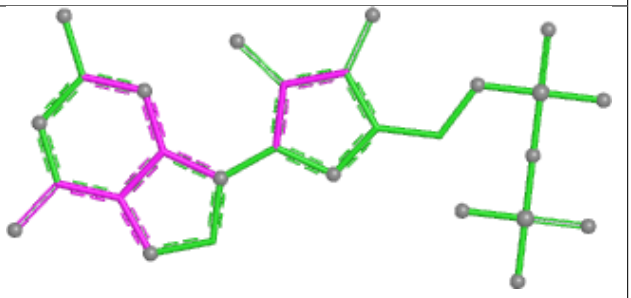


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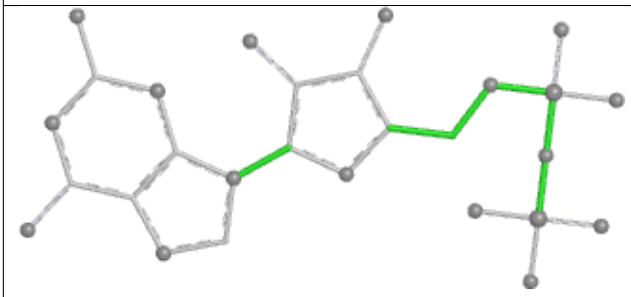
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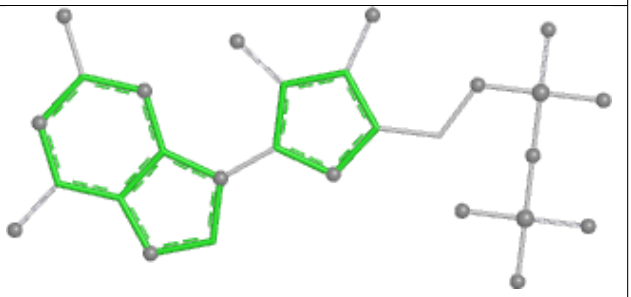
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Bond angles

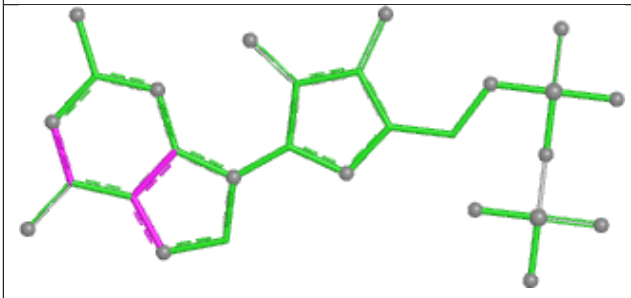


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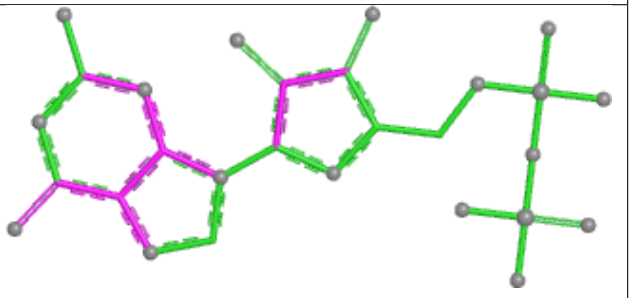


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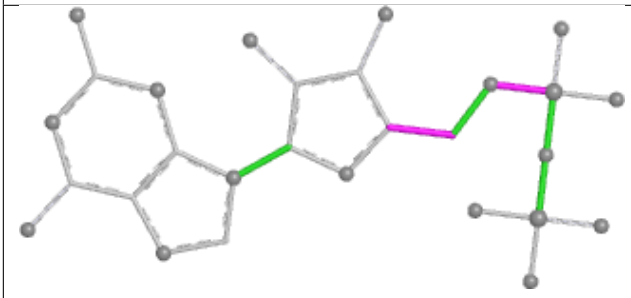
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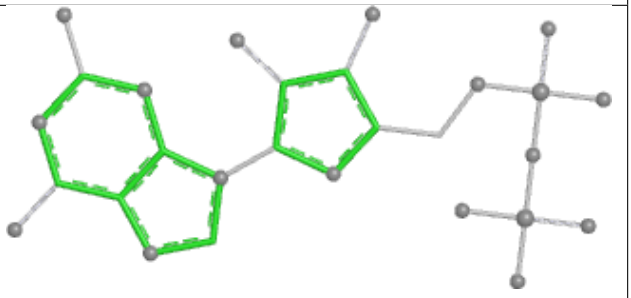
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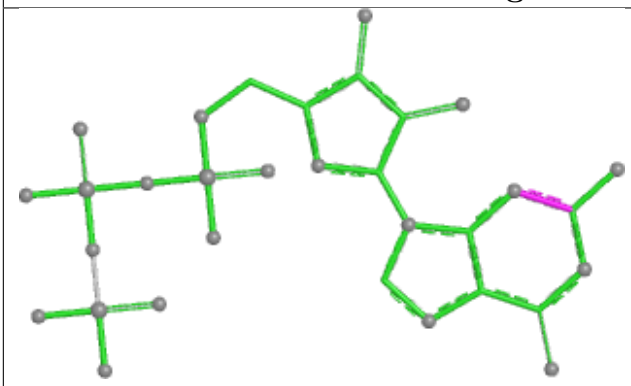


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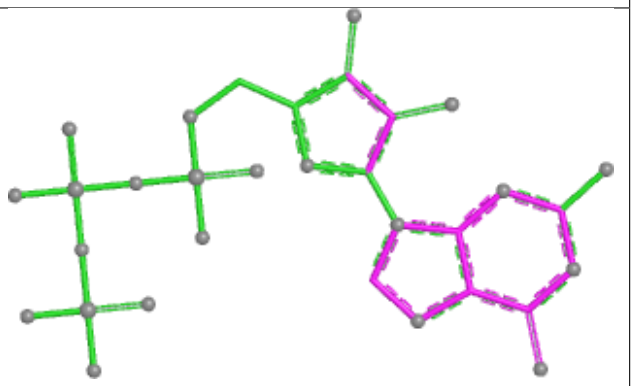


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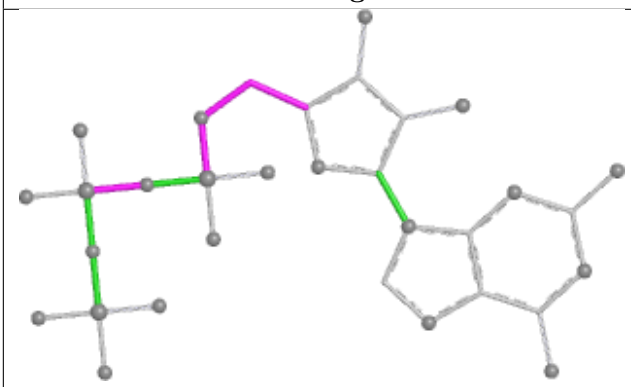
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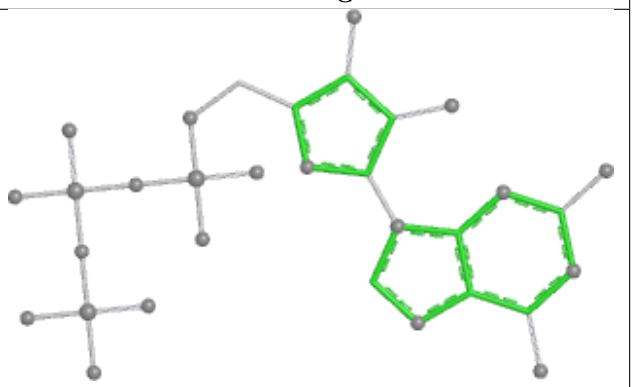
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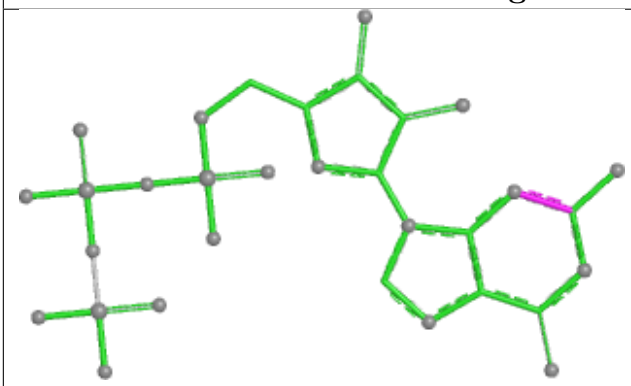


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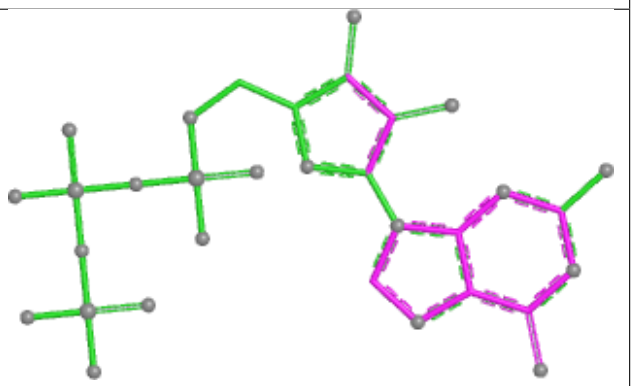


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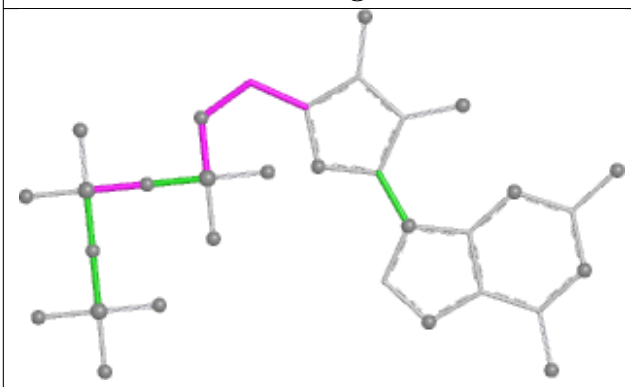
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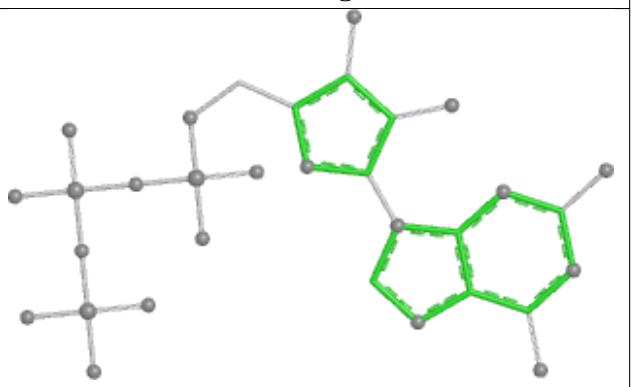
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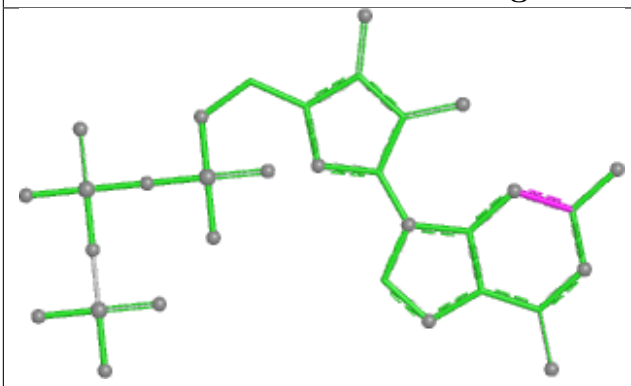


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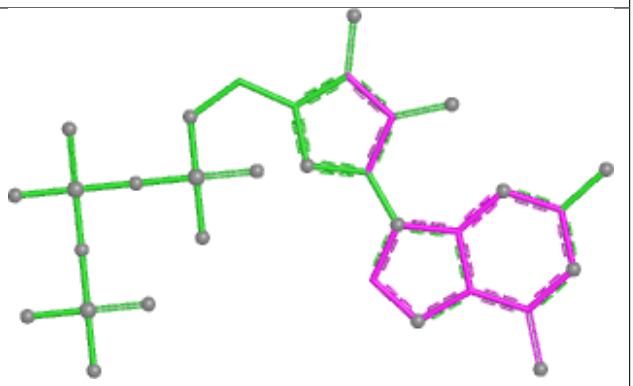


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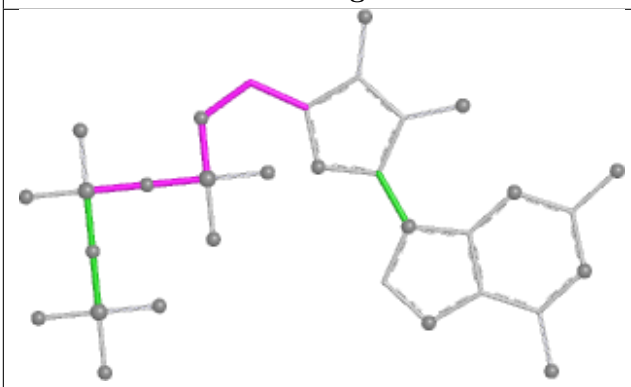
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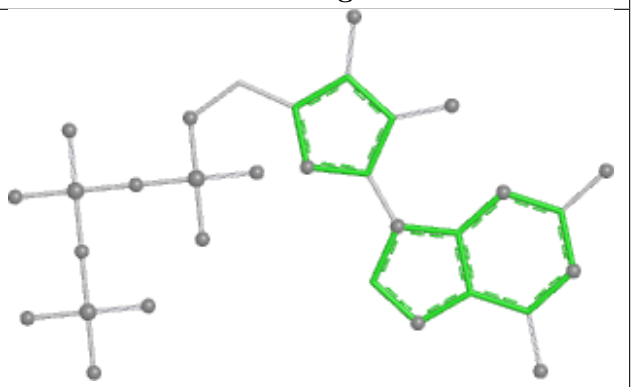
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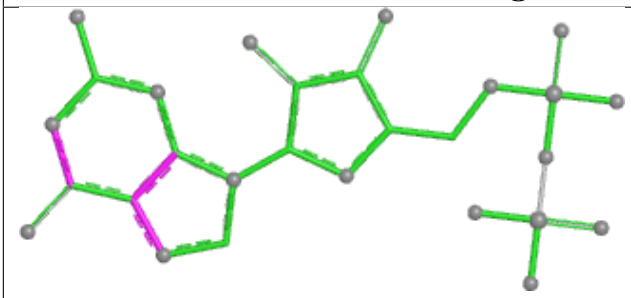


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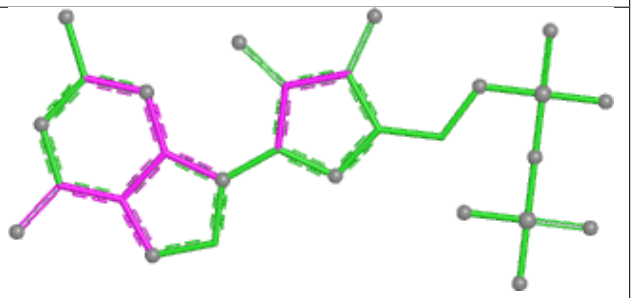


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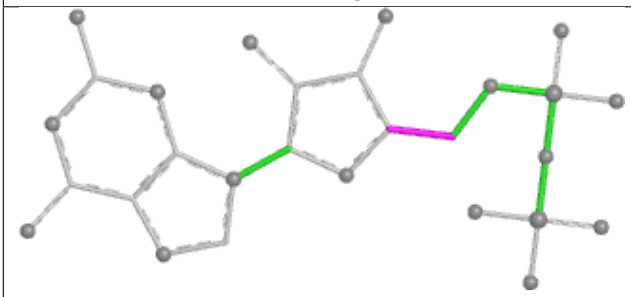
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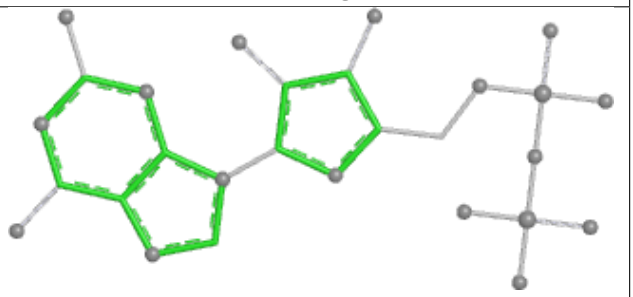
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Bond angles

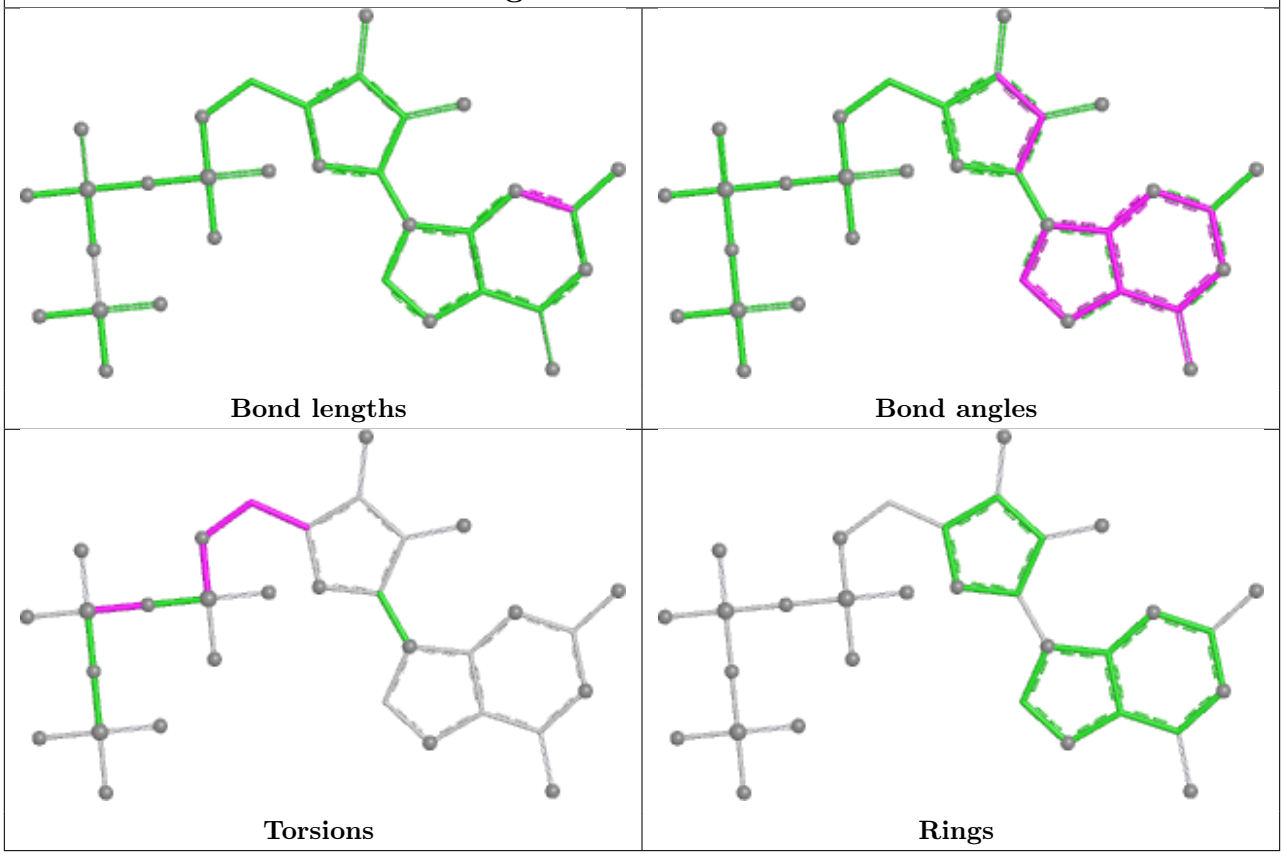


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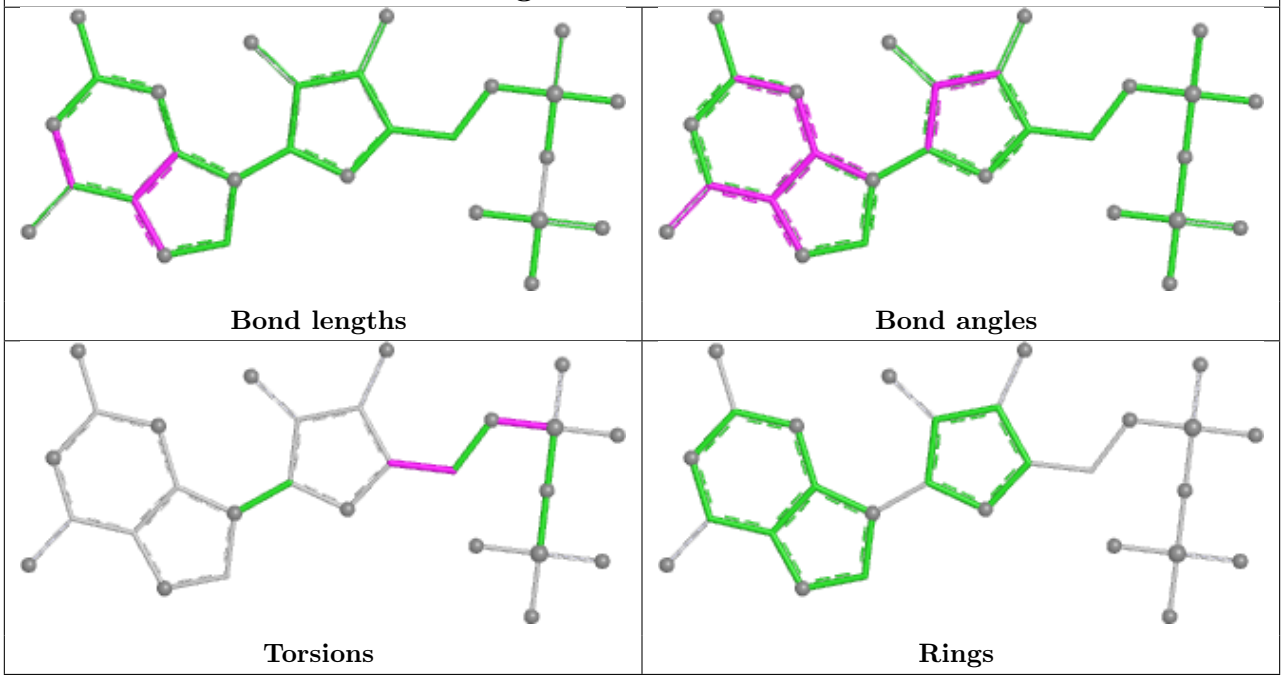


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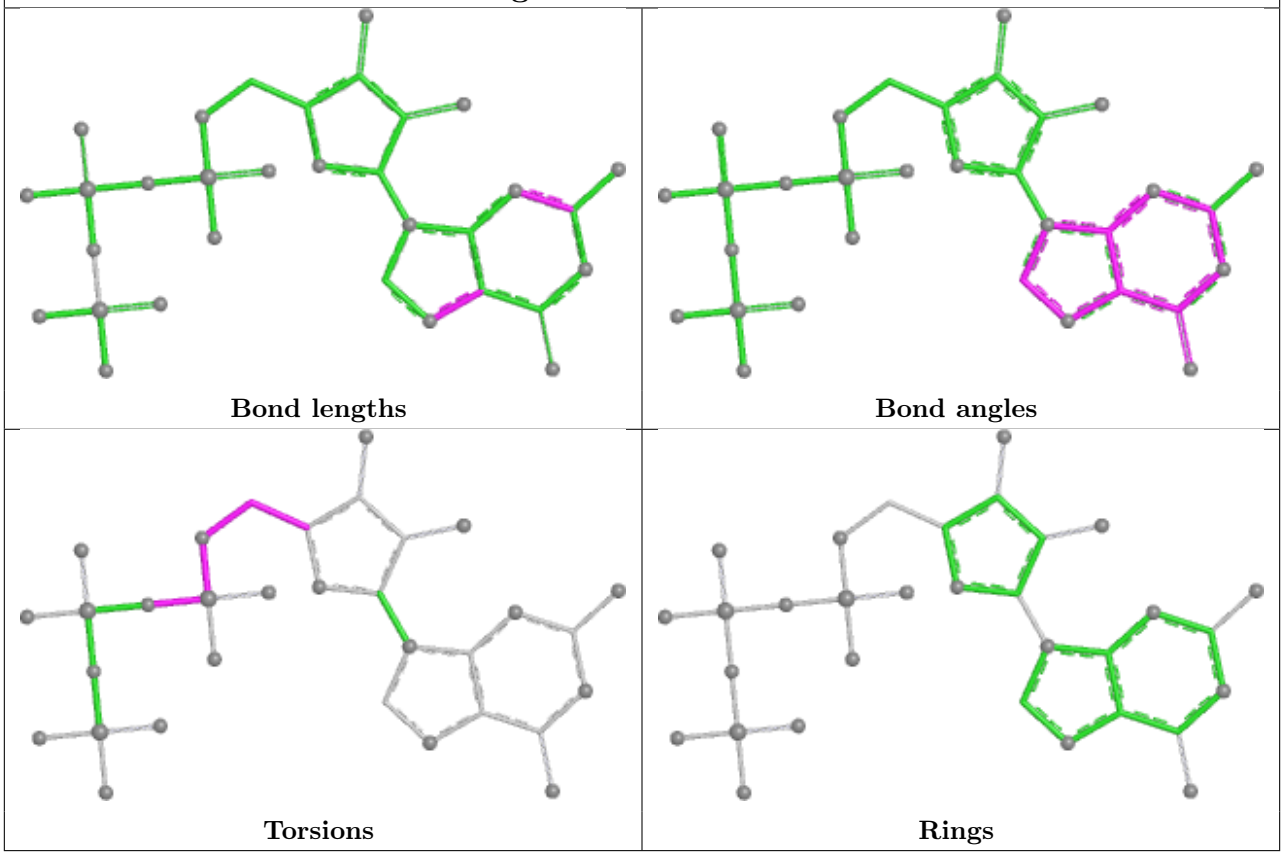
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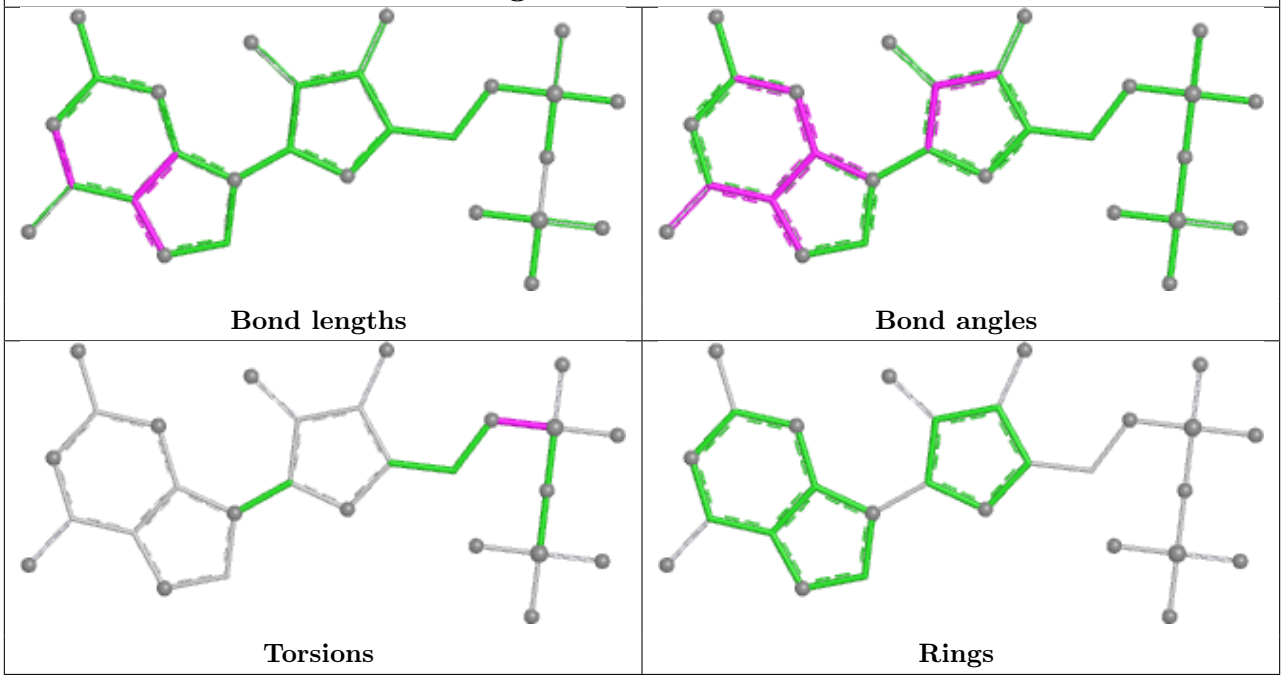
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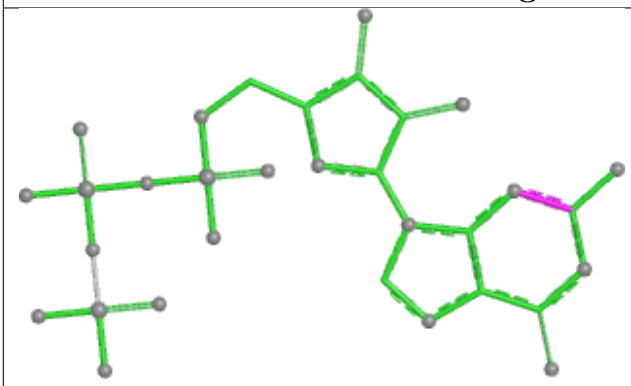
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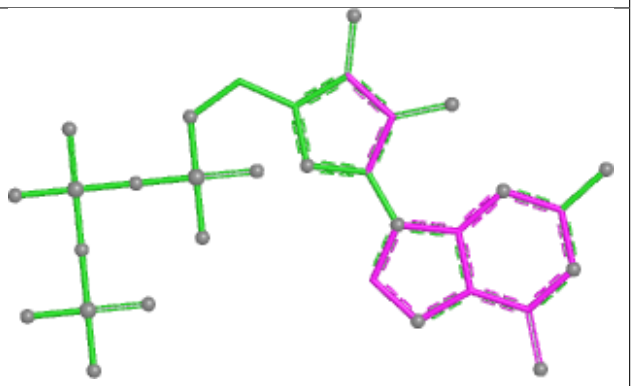
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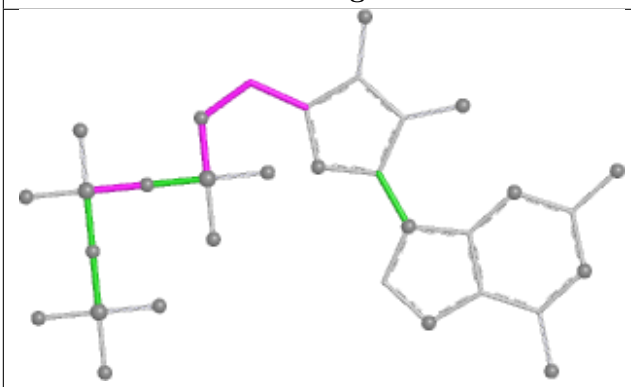
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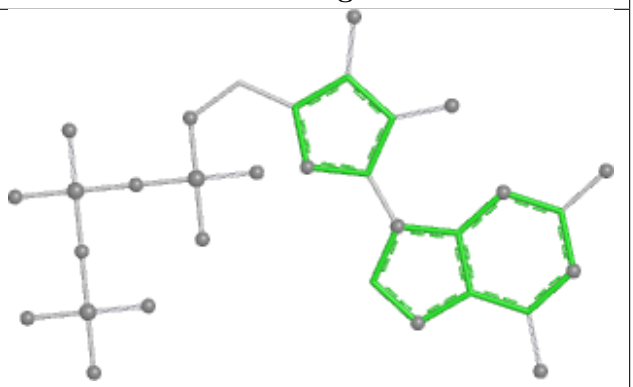
Bond lengths



Bond angles

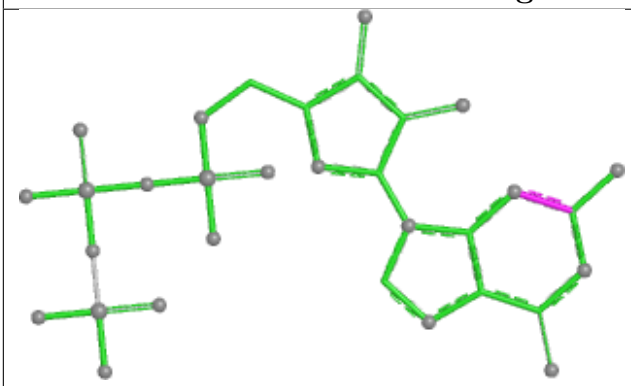


Torsions

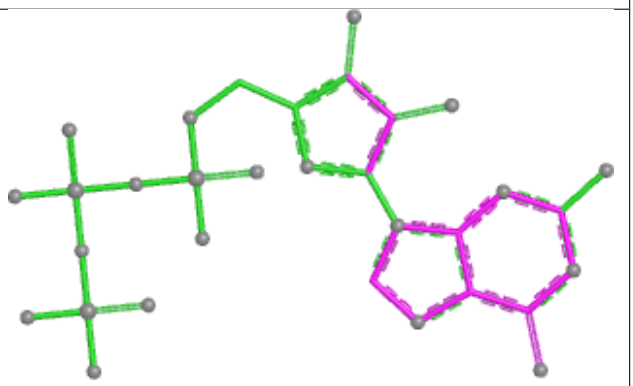


Rings

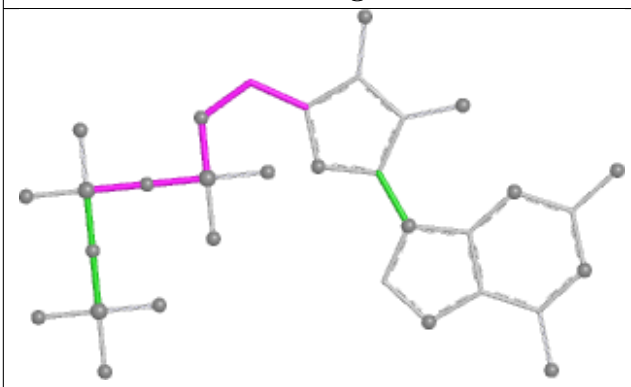
Ligand GTP IC 501



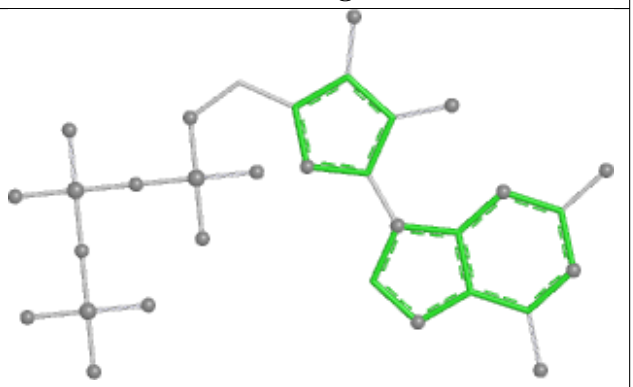
Bond lengths



Bond angles

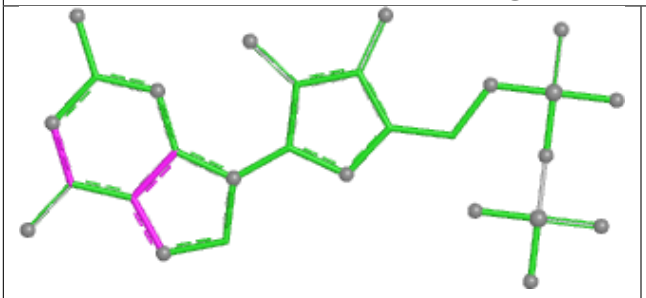


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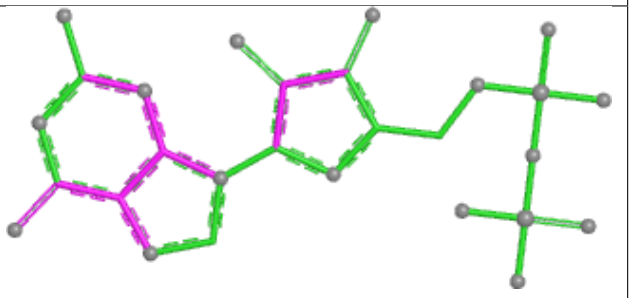


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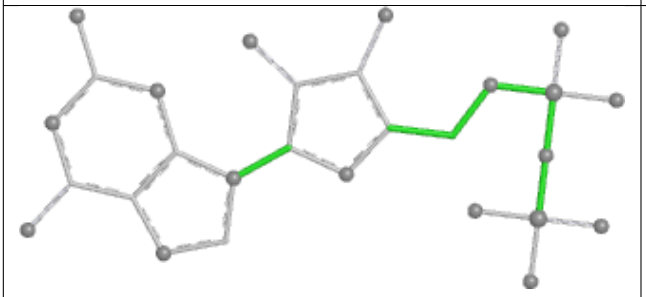
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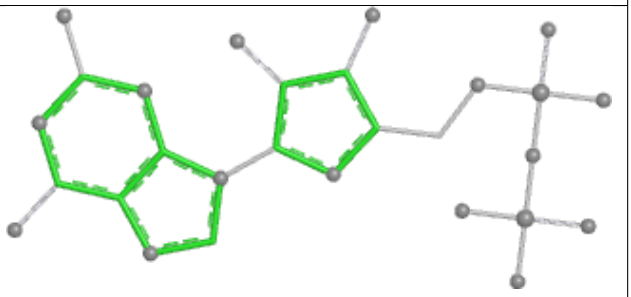
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Bond angles

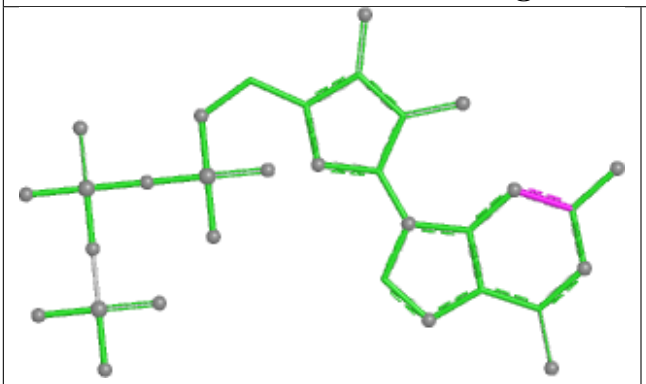


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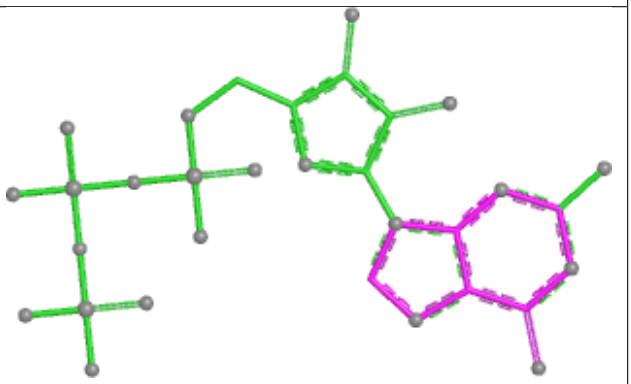


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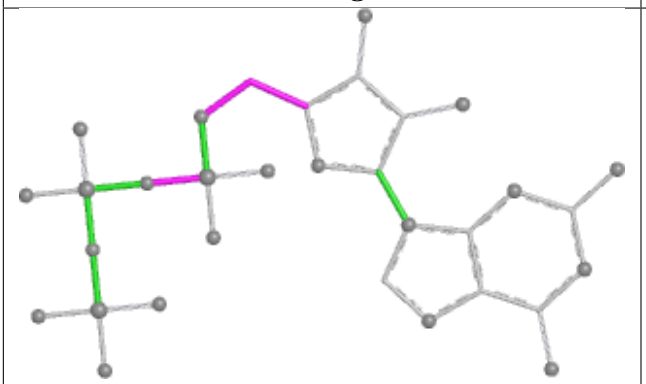
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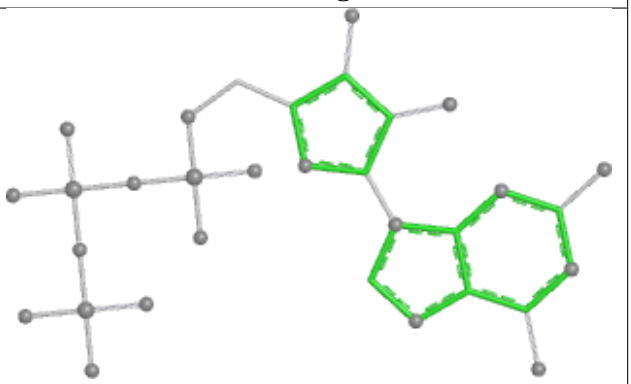
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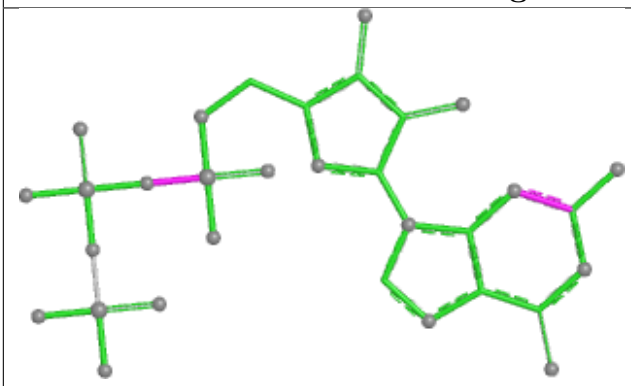


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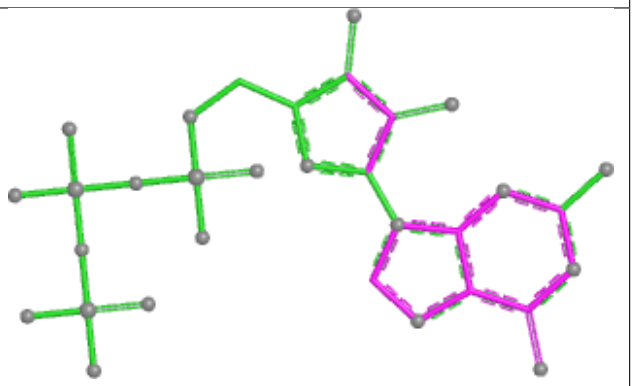


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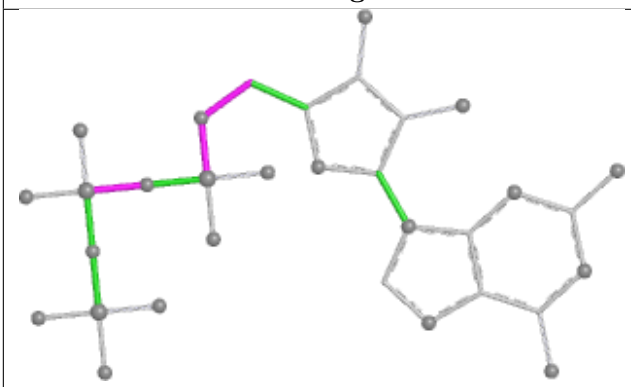
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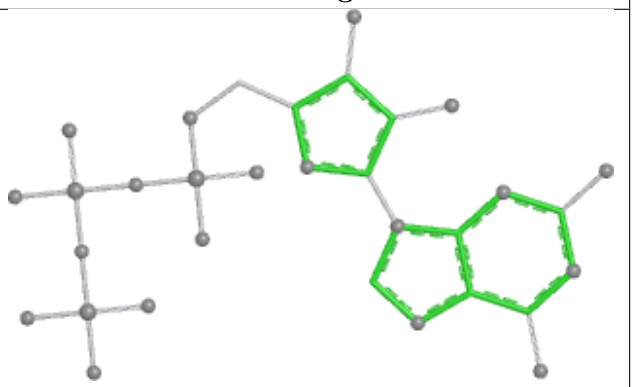
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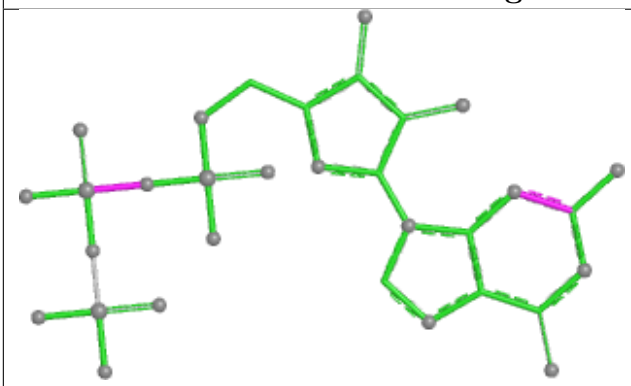


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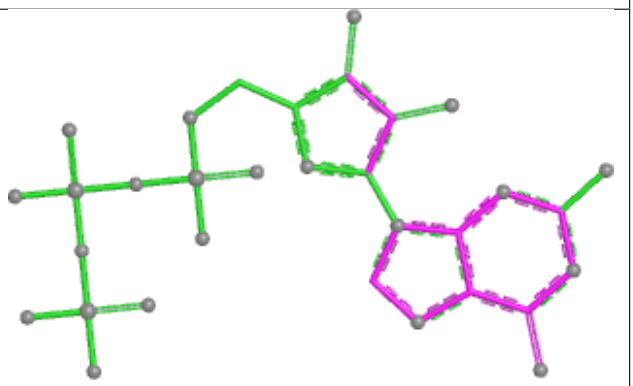


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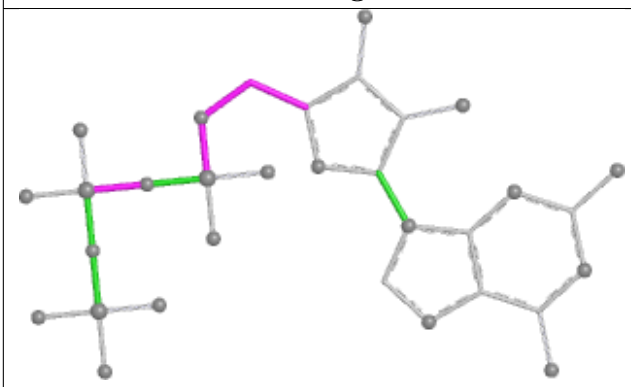
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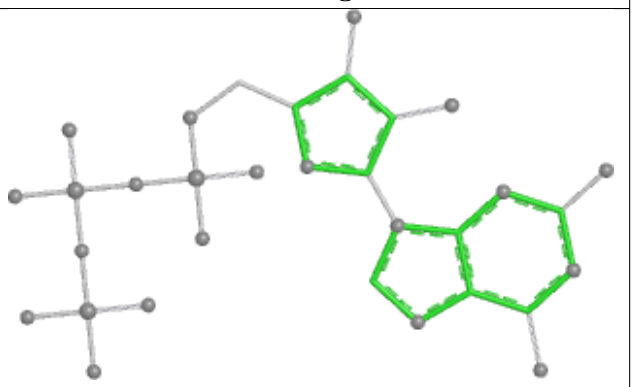
Bond lengths



Bond angles

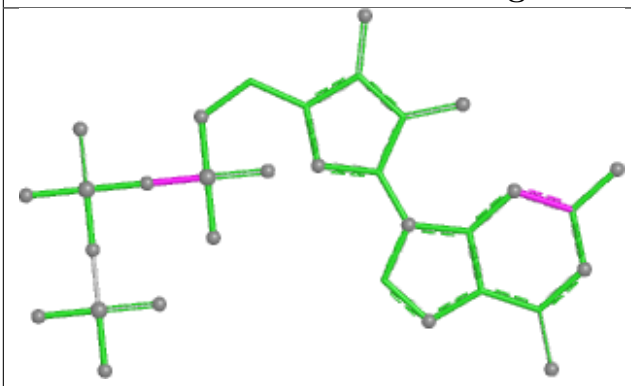


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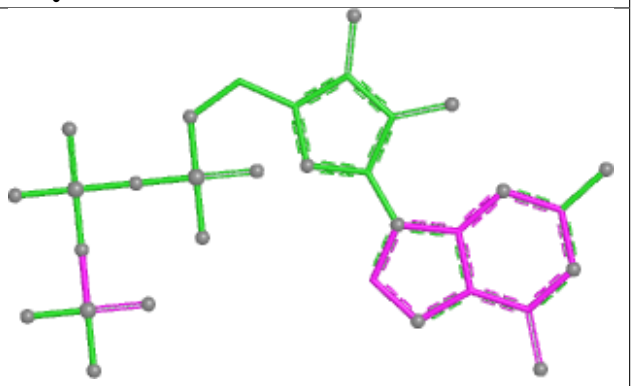


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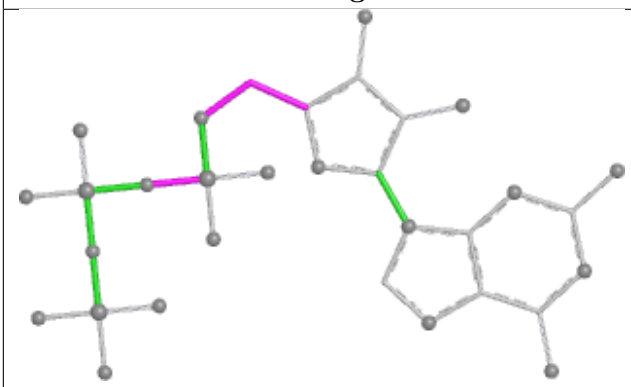
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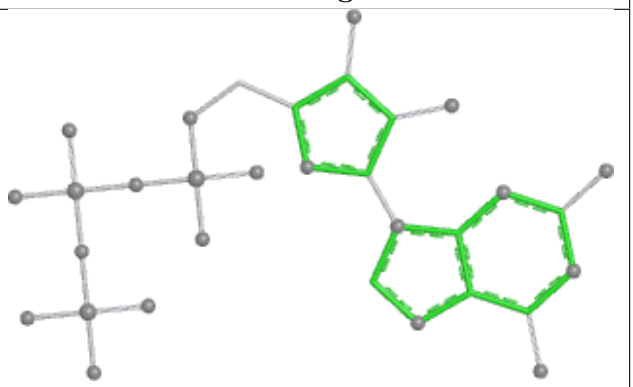
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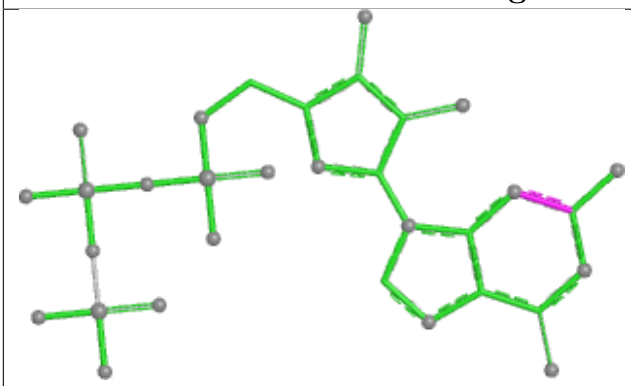


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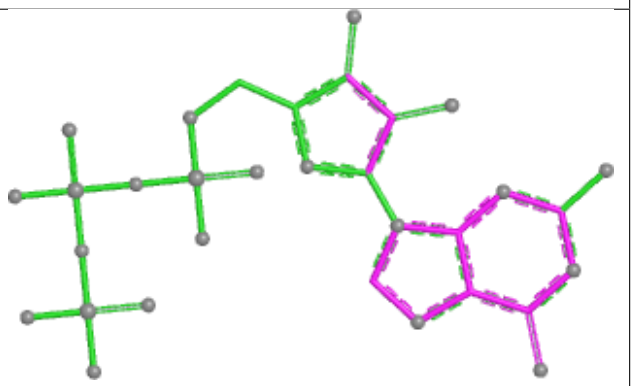


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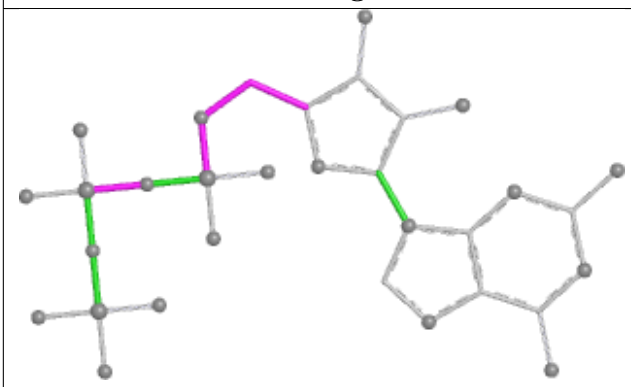
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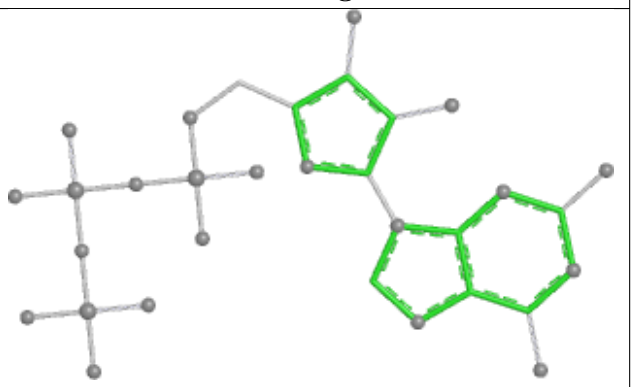
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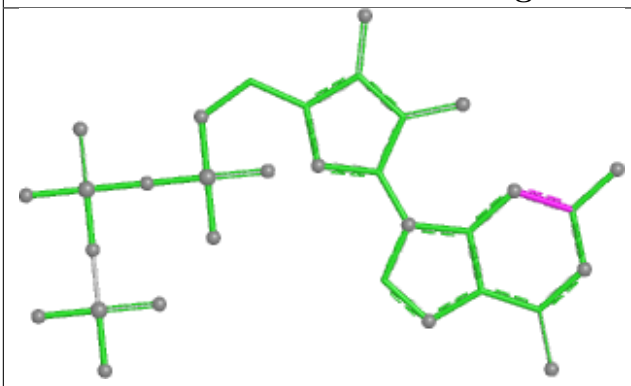


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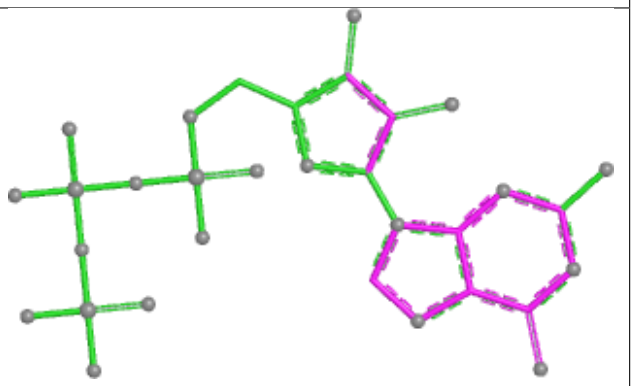


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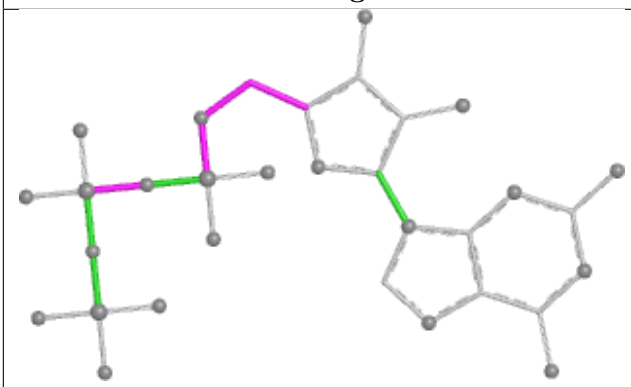
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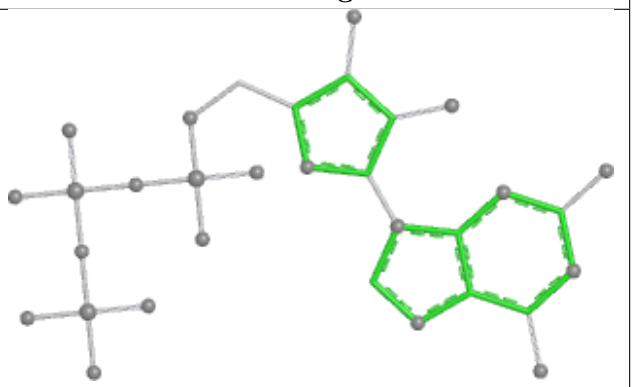
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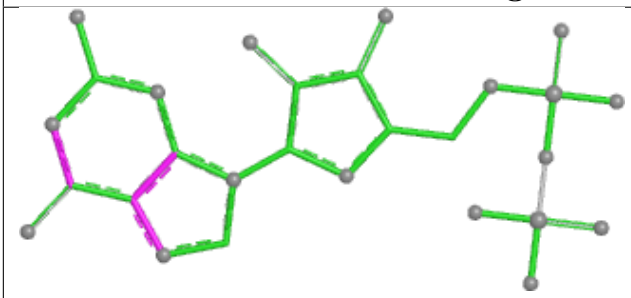


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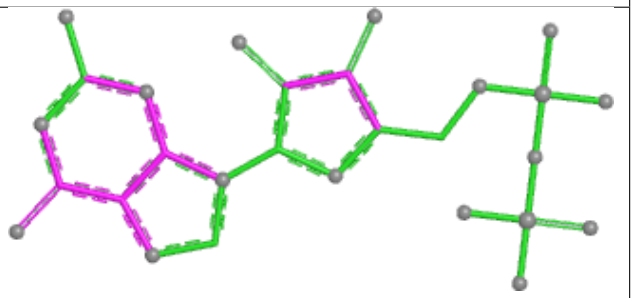


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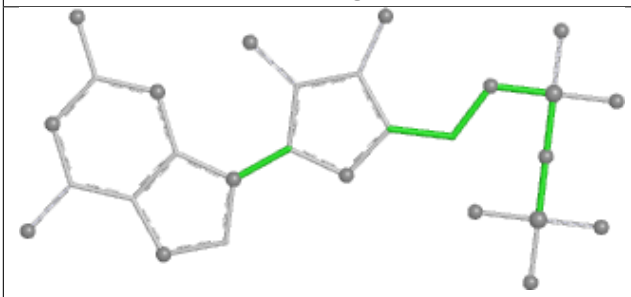
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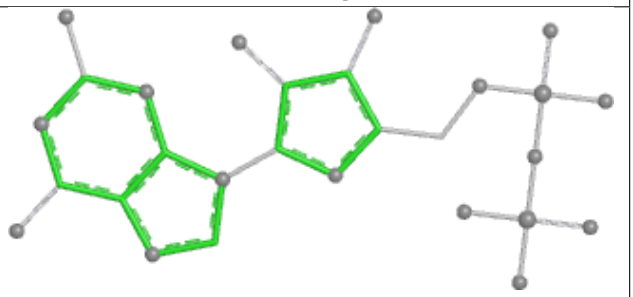
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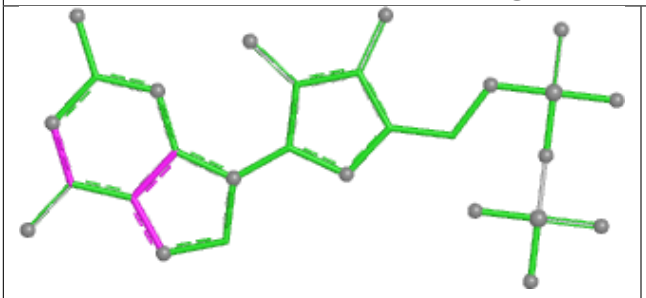


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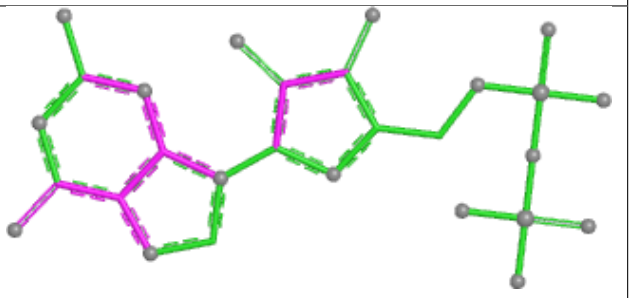


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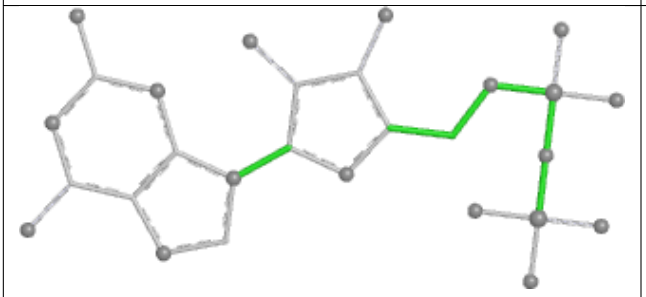
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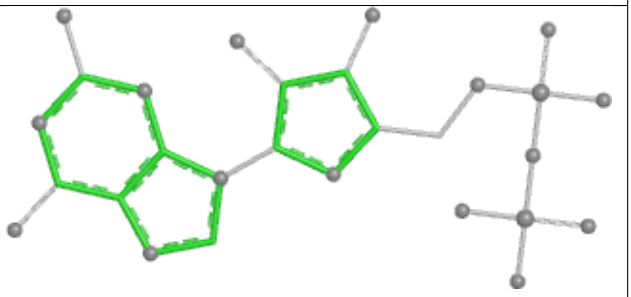
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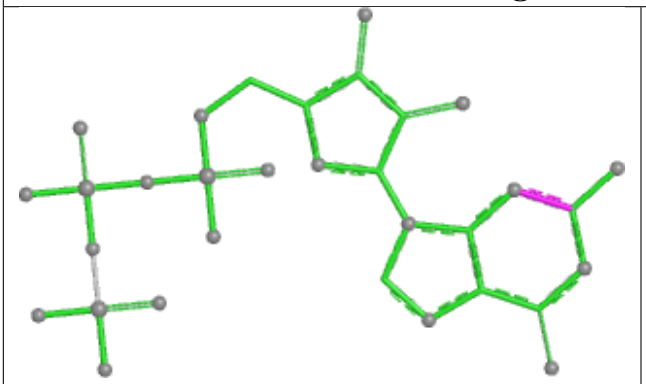


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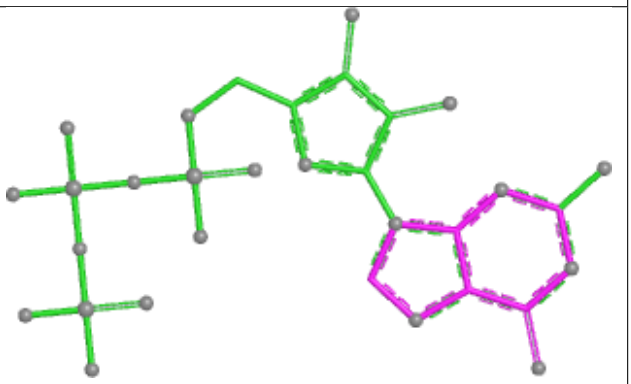


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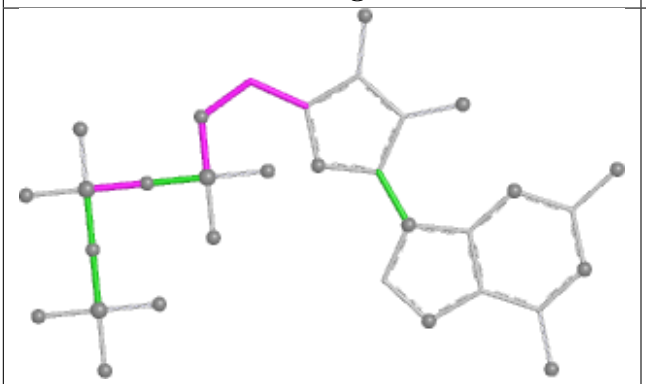
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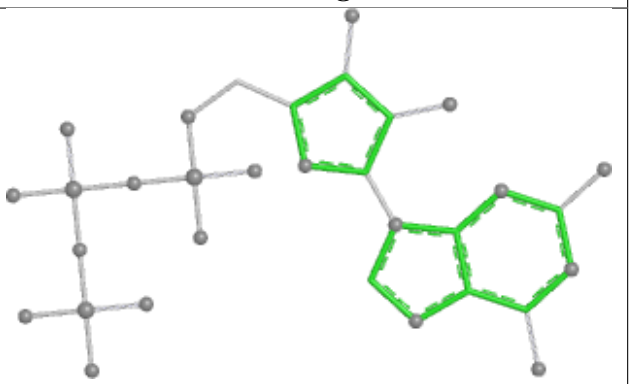
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Bond angles

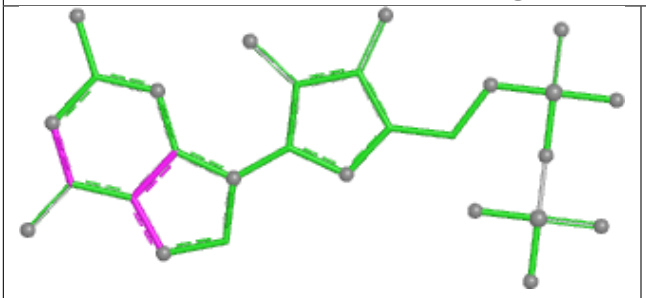


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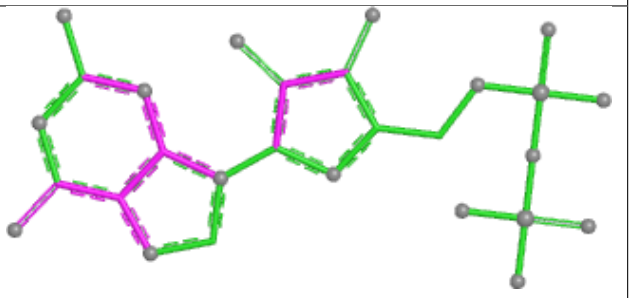


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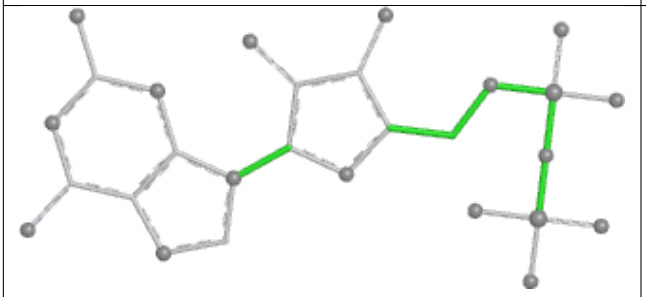
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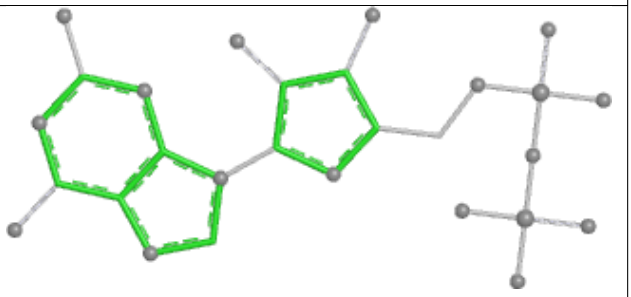
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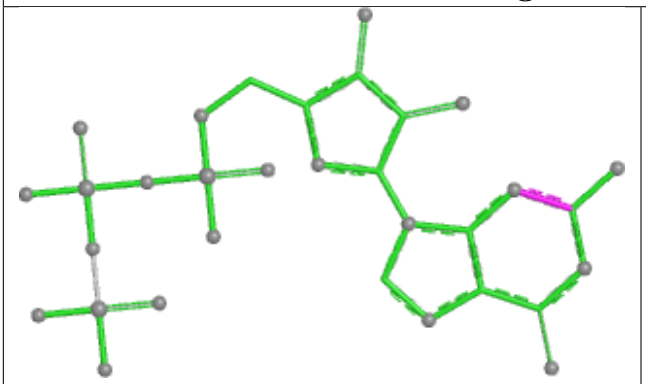


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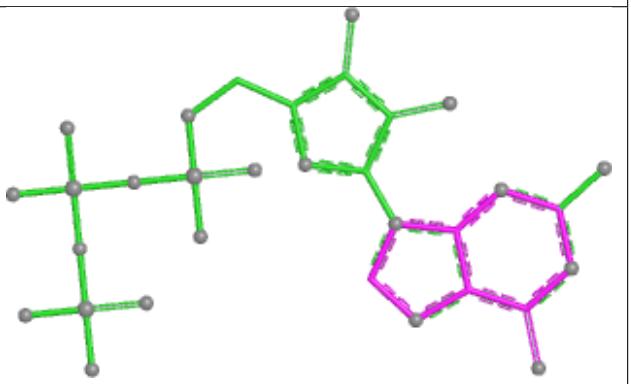


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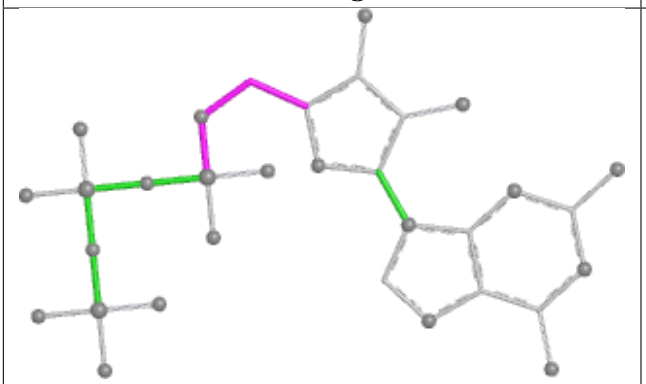
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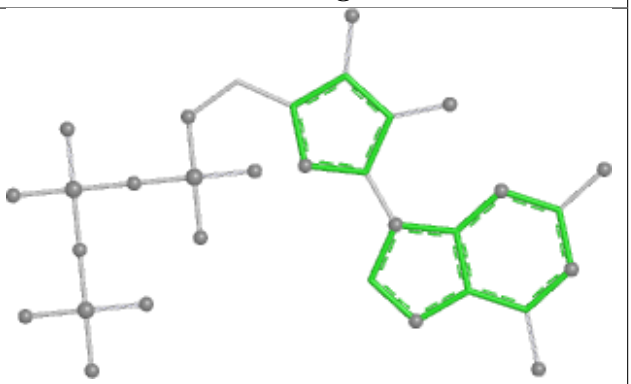
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Bond angles

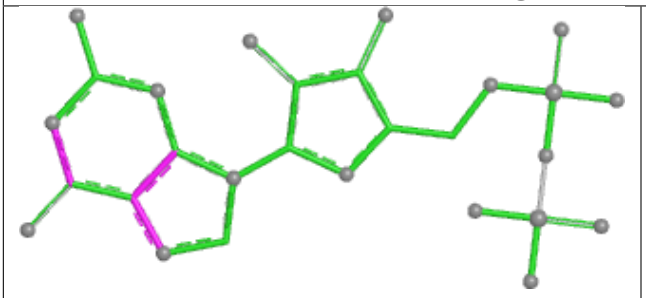


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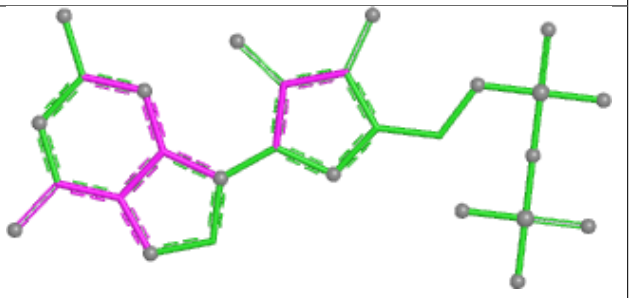


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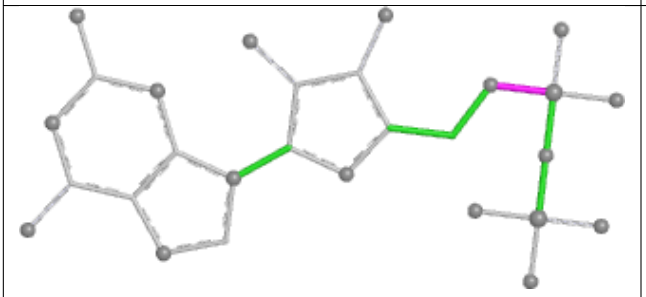
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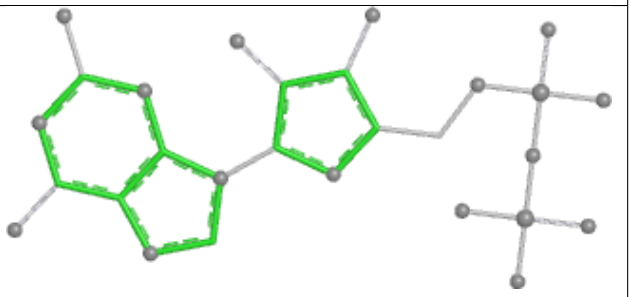
Bond lengths



Bond angles

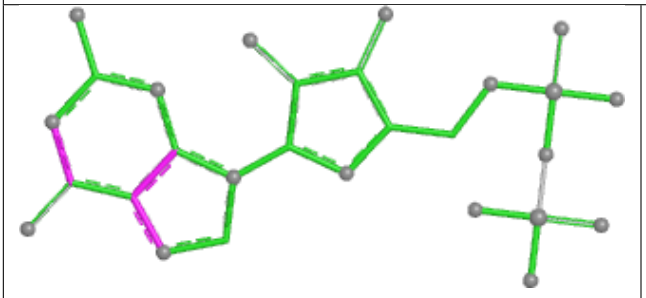


Torsions

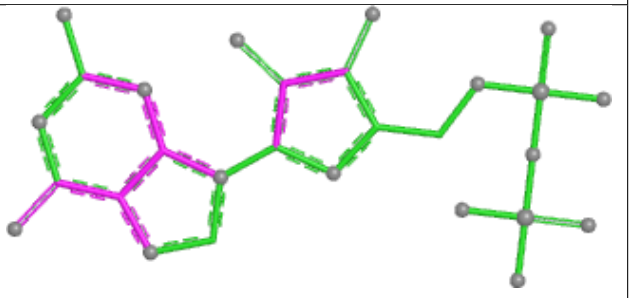


Rings

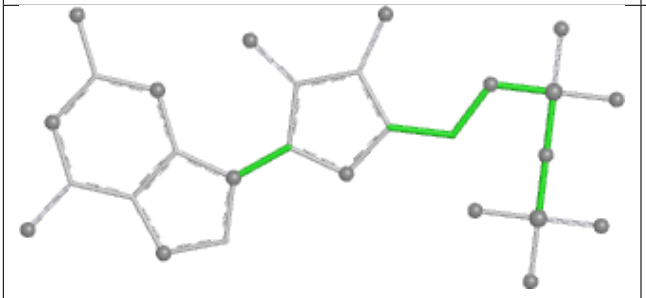
Ligand GDP OD 501



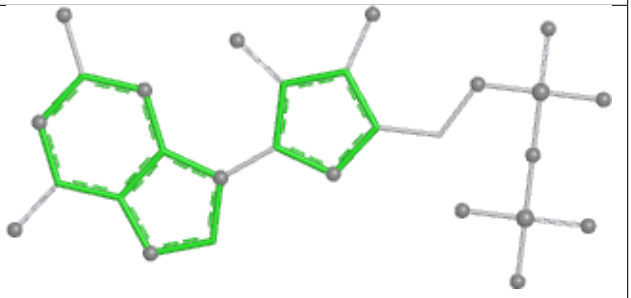
Bond lengths



Bond angles

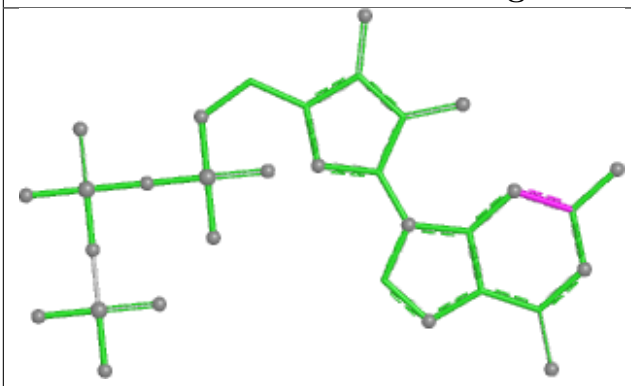


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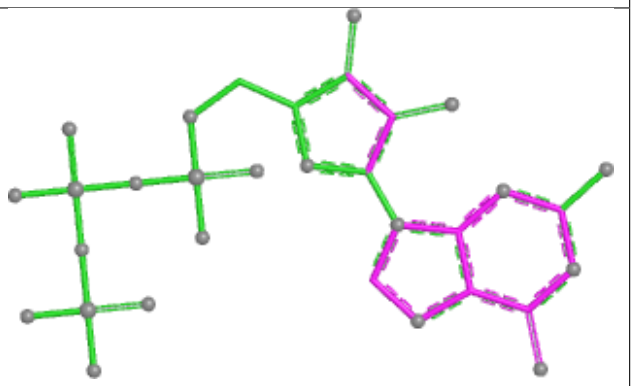


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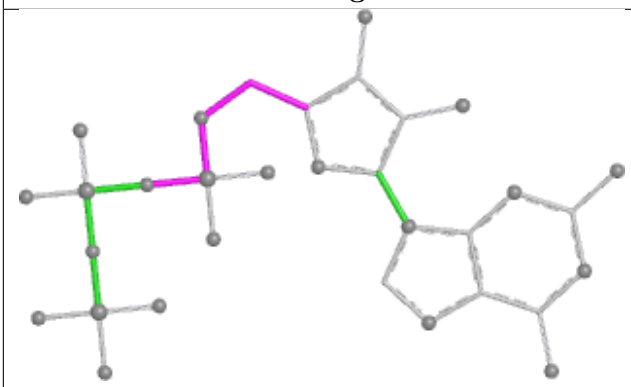
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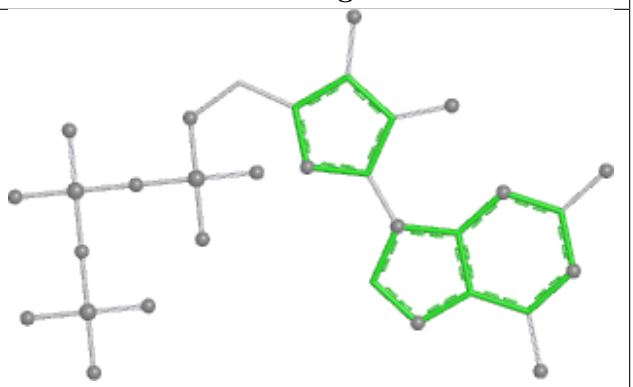
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Bond angles

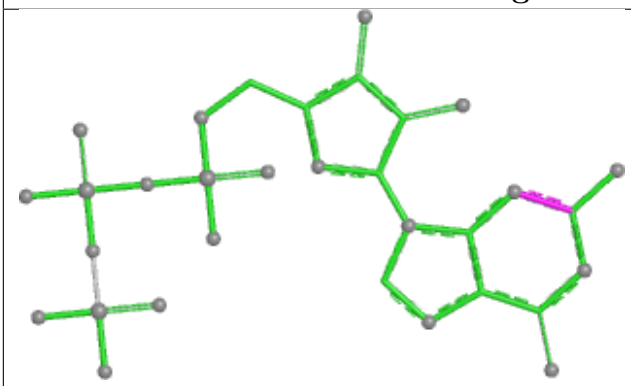


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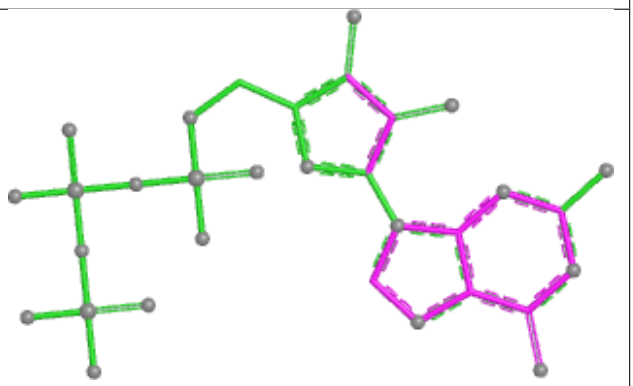


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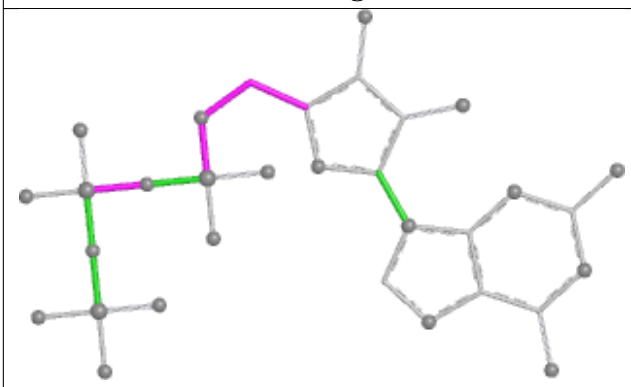
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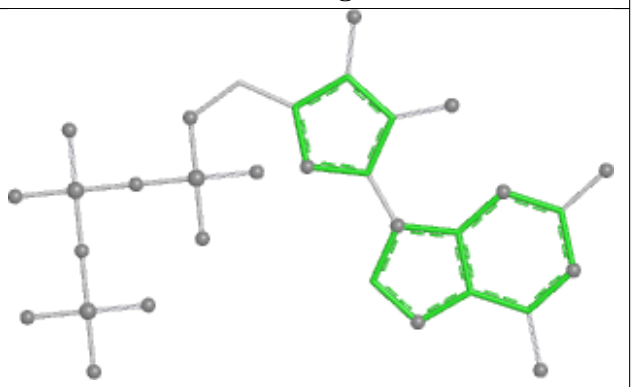
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Bond angles

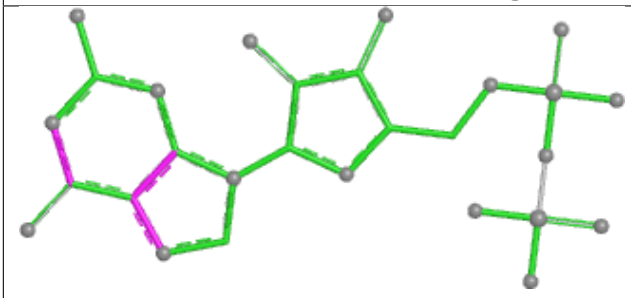


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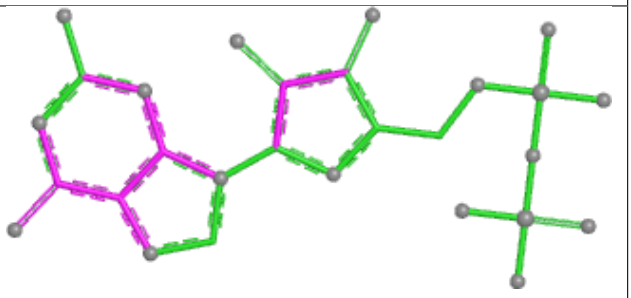


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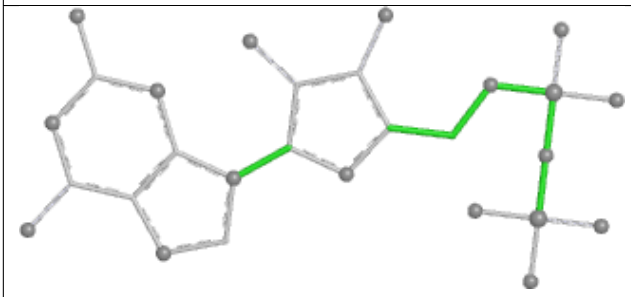
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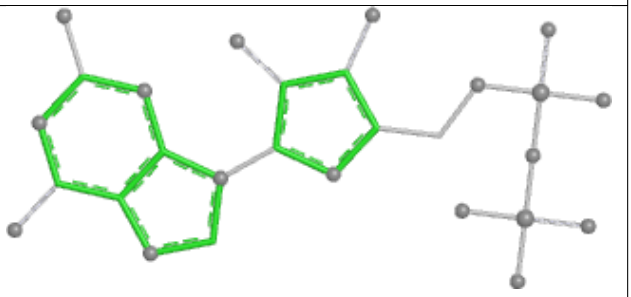
Bond lengths



Bond angles

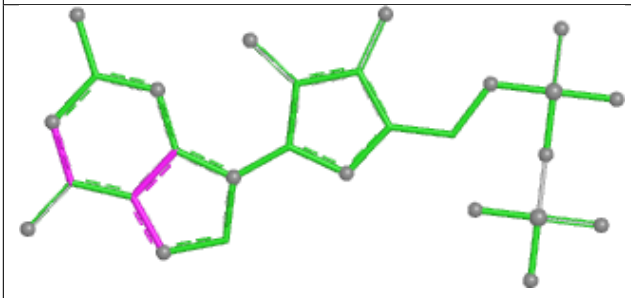


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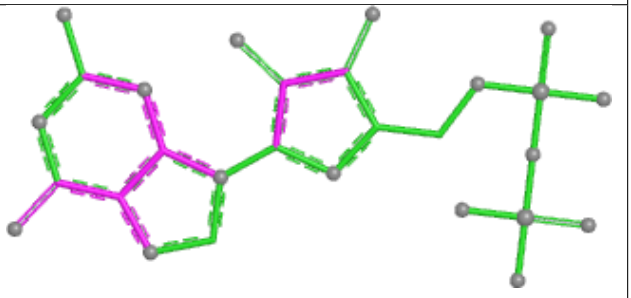


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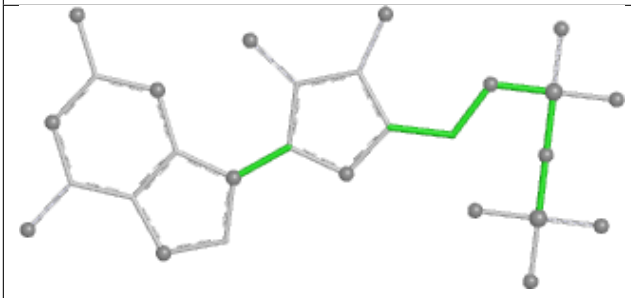
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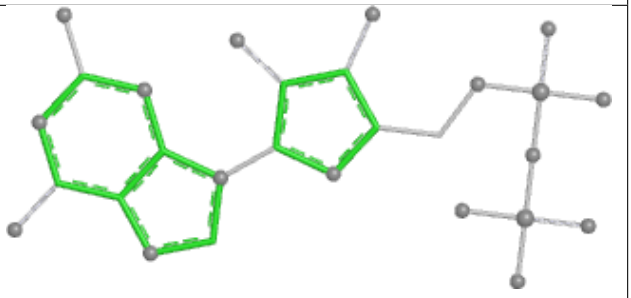
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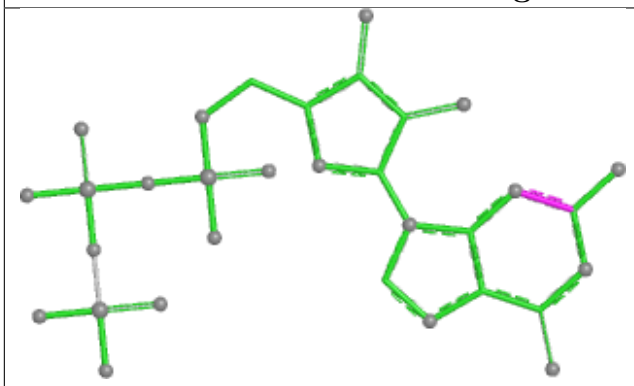


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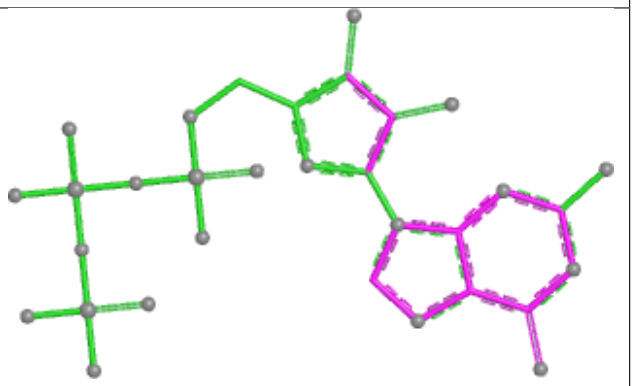


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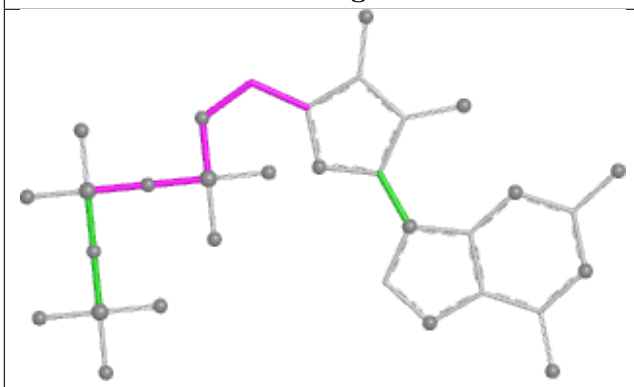
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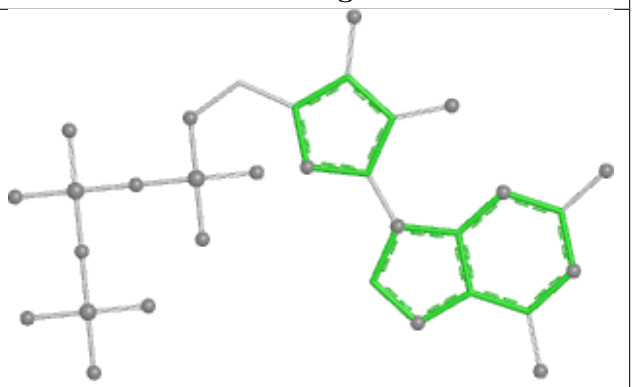
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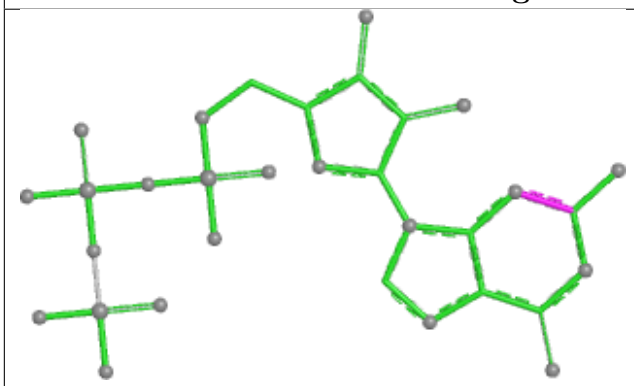


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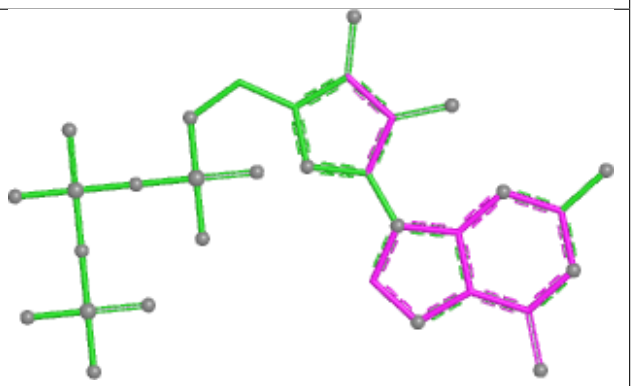


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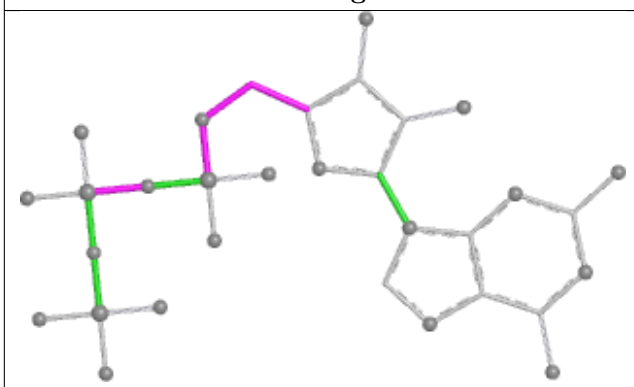
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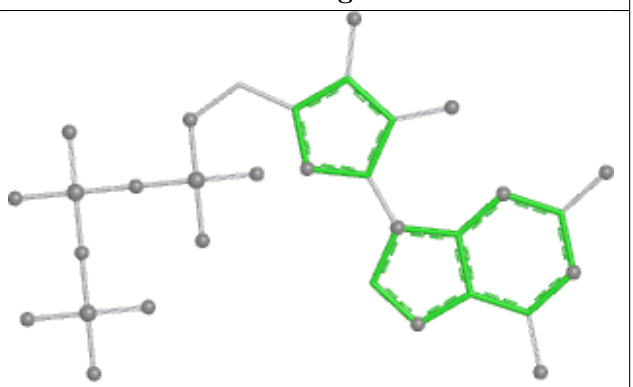
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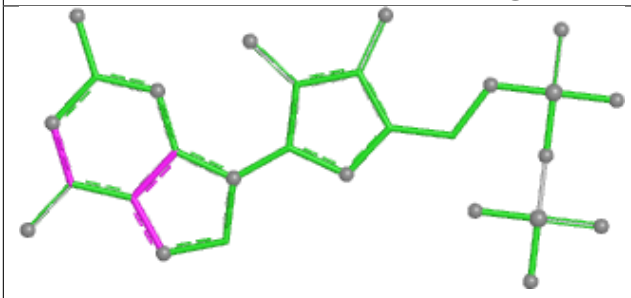


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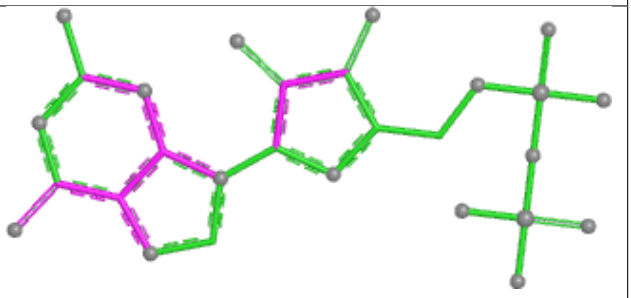


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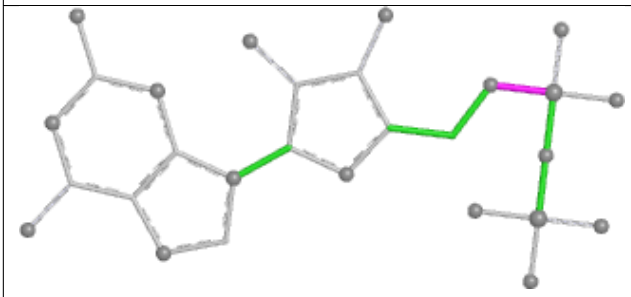
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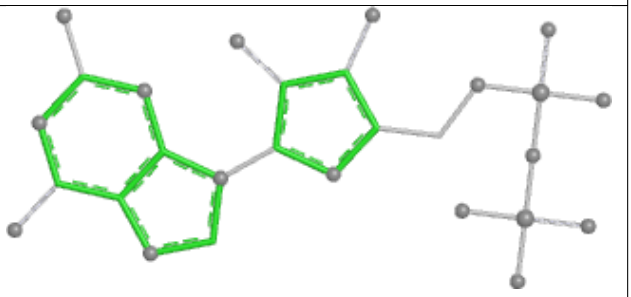
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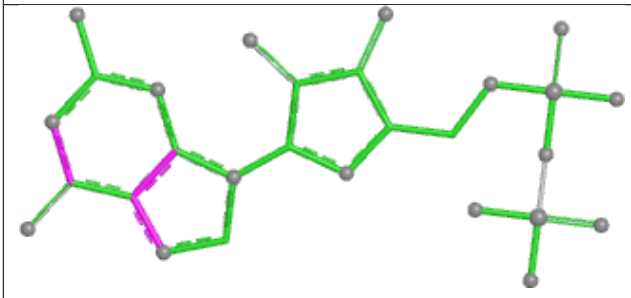


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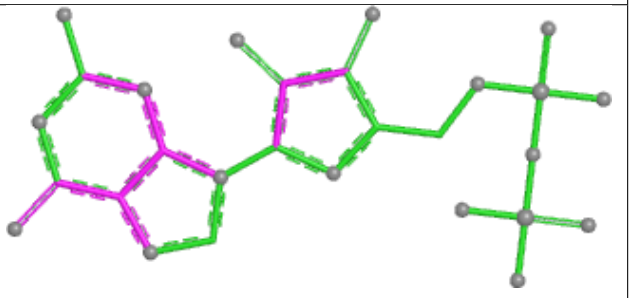


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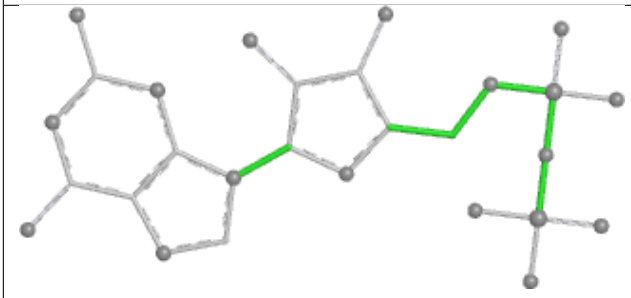
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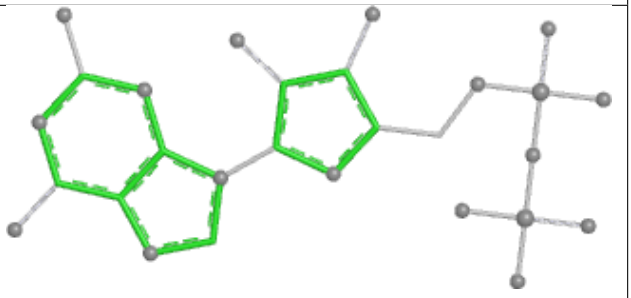
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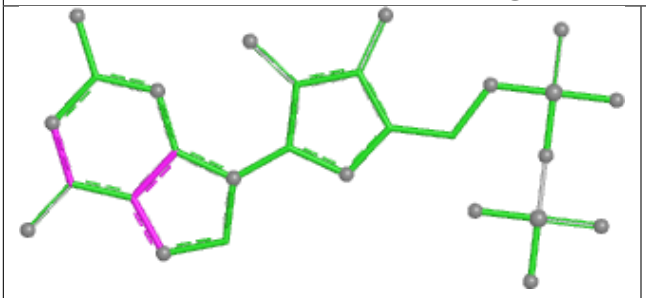


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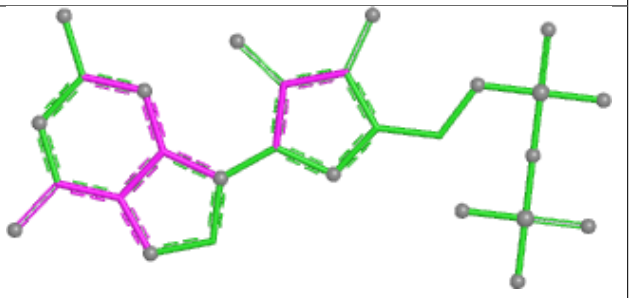


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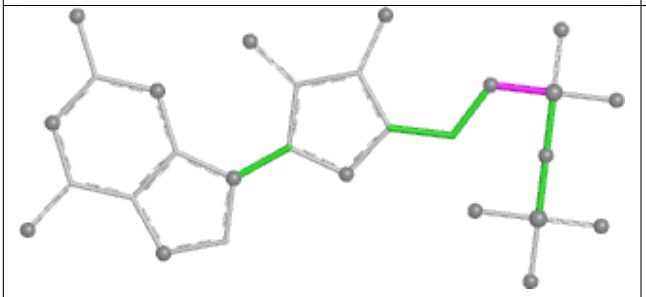
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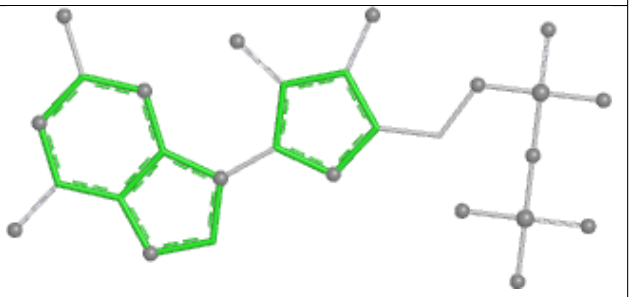
Bond lengths



Bond angles

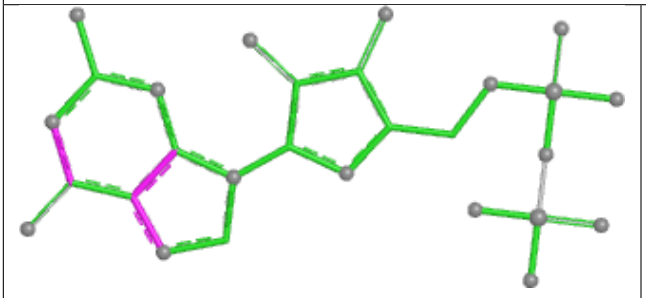


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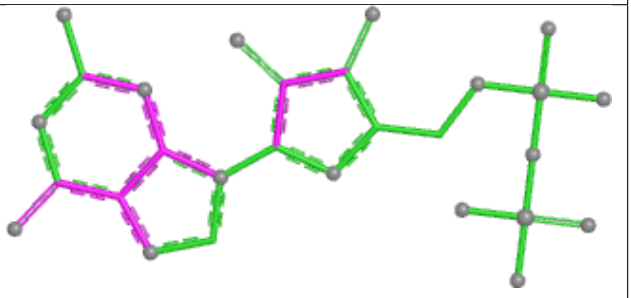


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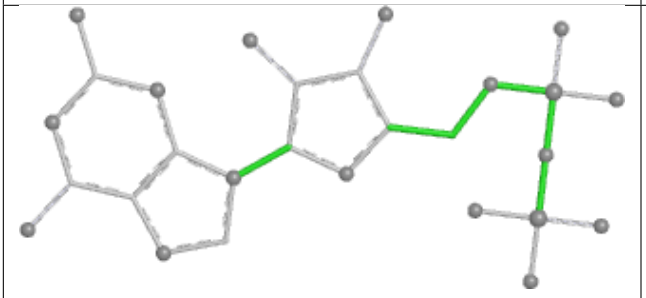
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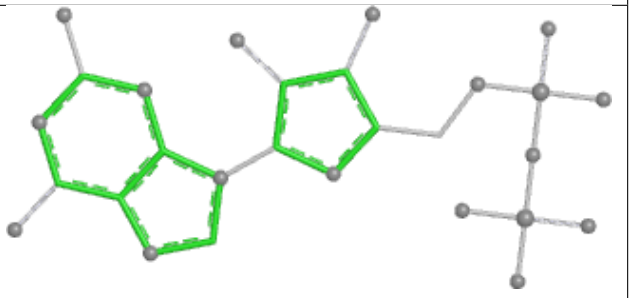
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Bond angles

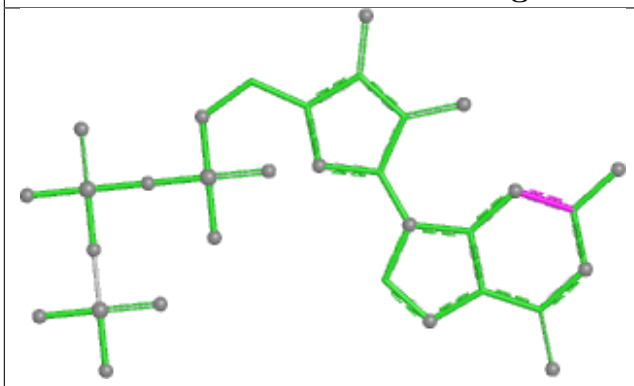


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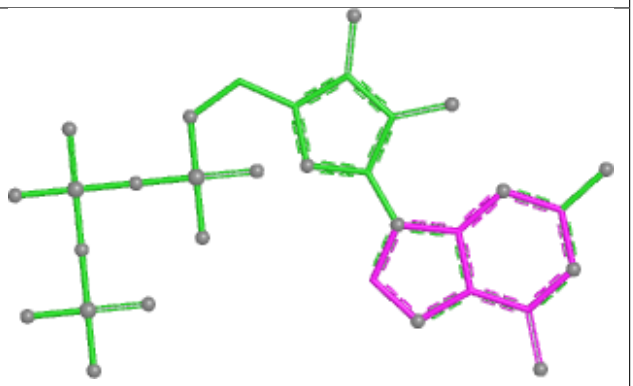


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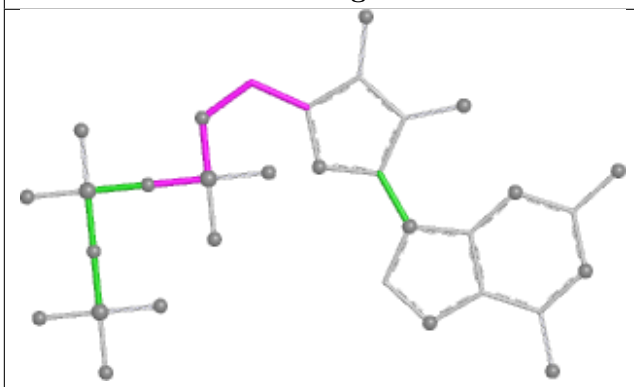
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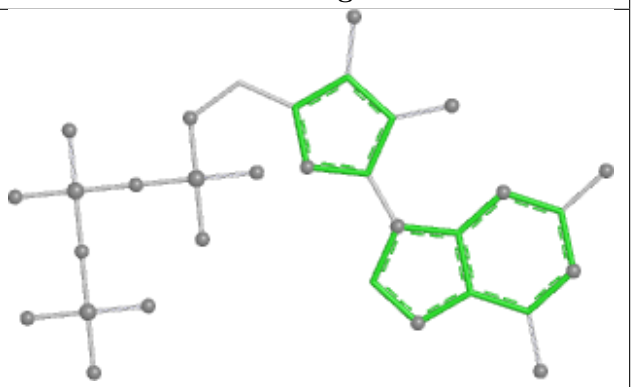
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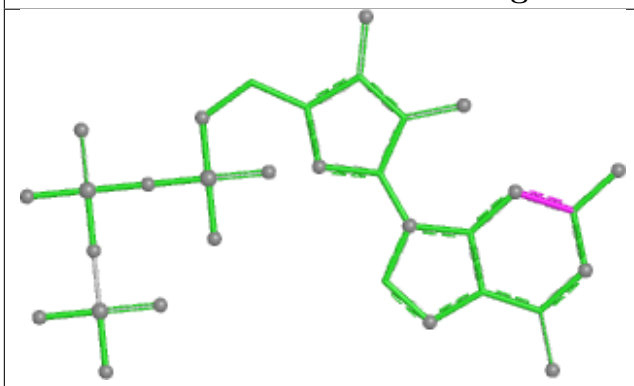


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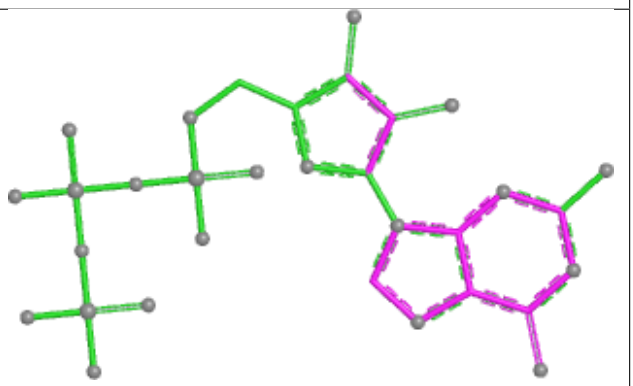


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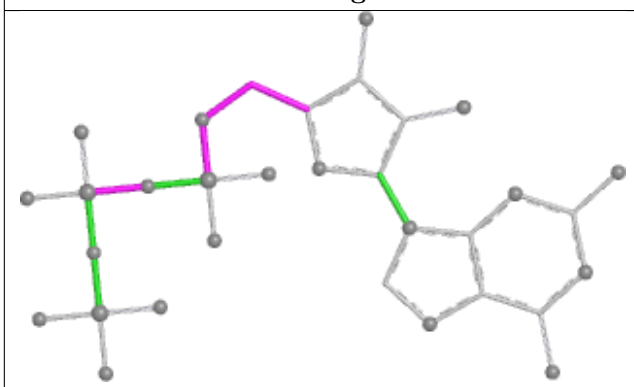
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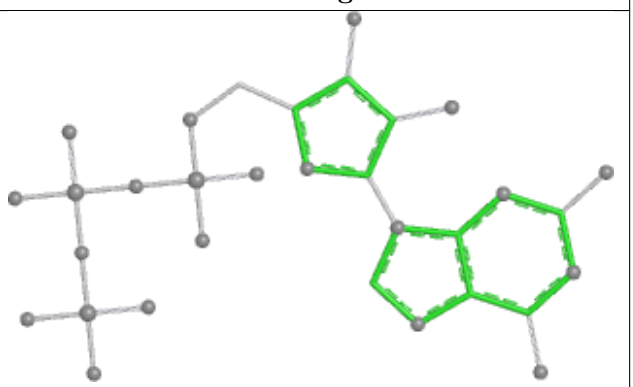
Bond lengths



Bond angles

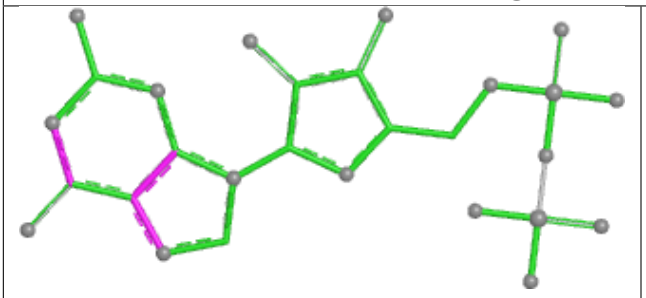


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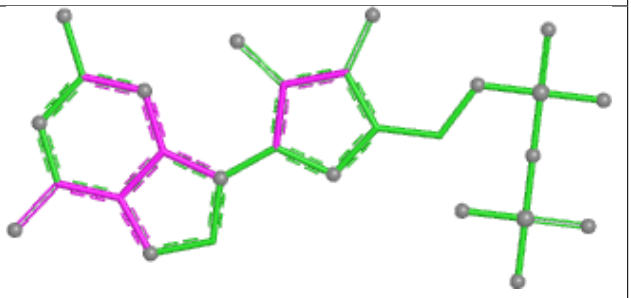


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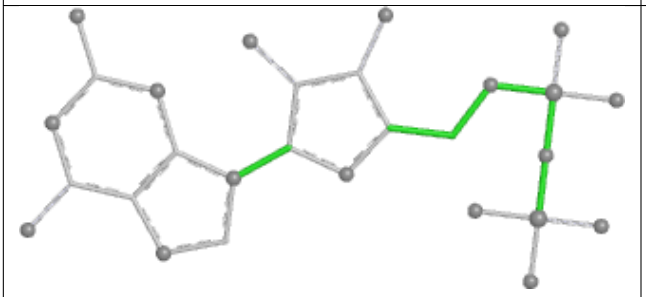
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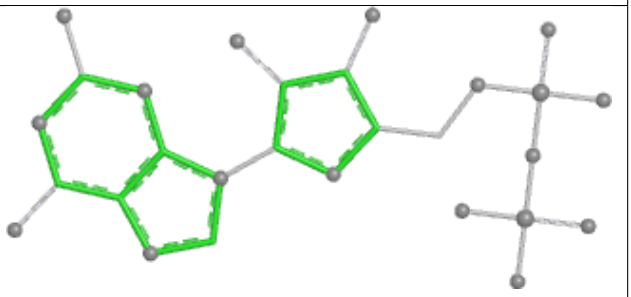
Bond lengths



Bond angles

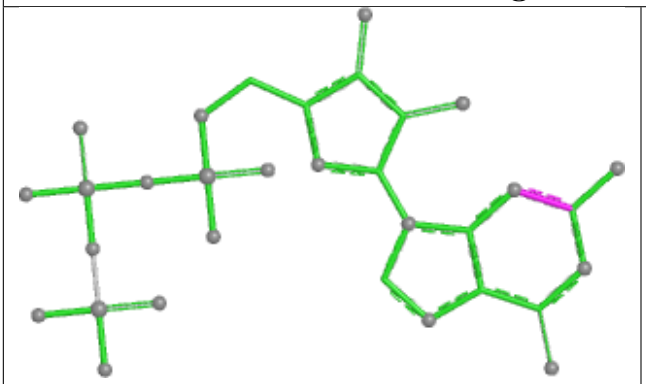


Torsions

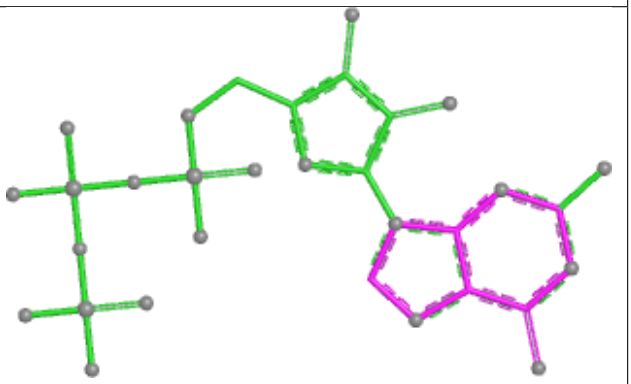


Rings

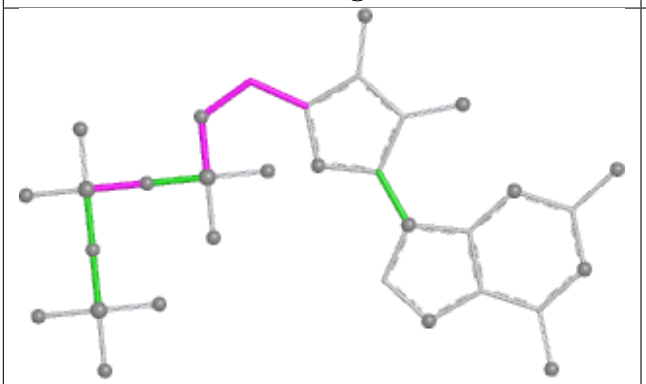
Ligand GTP WI 501



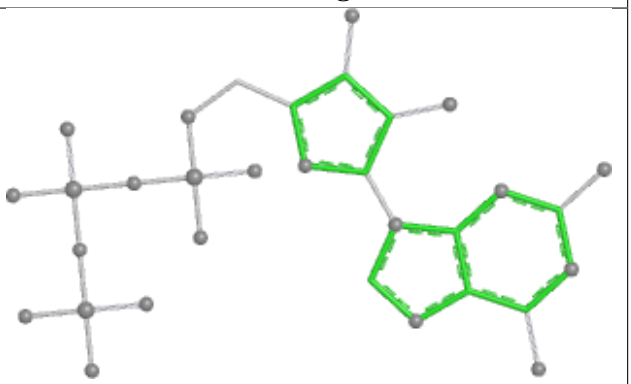
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Bond angles

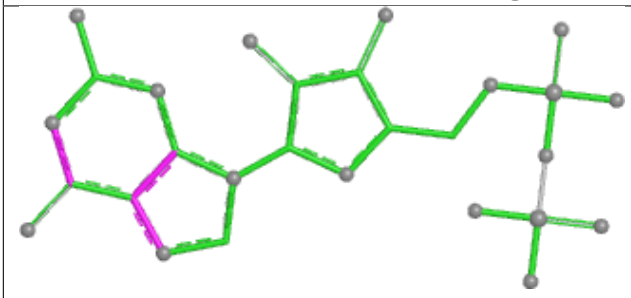


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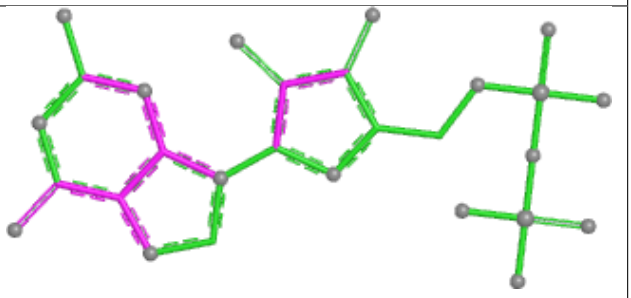


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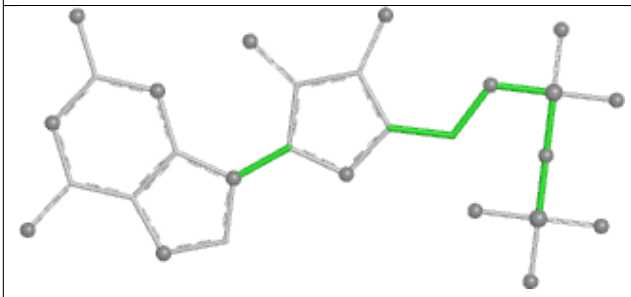
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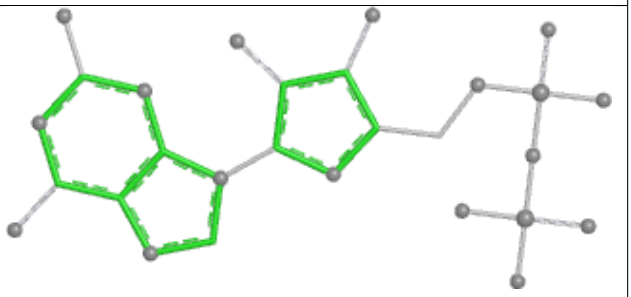
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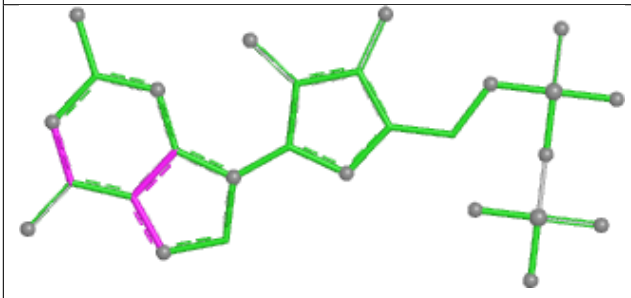


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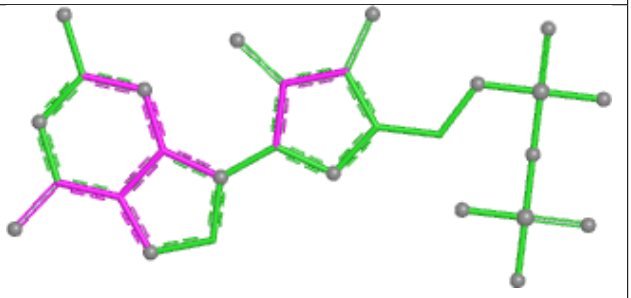


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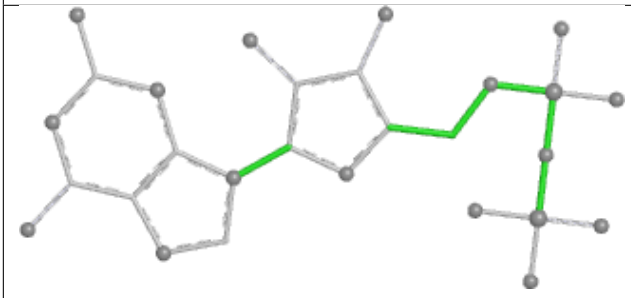
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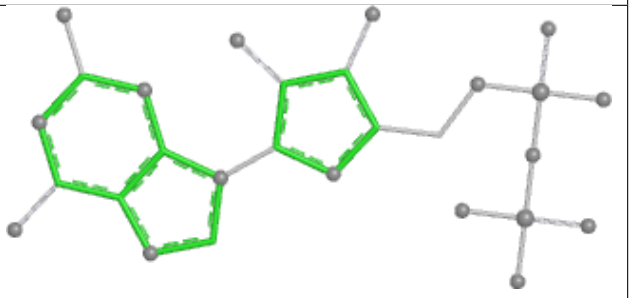
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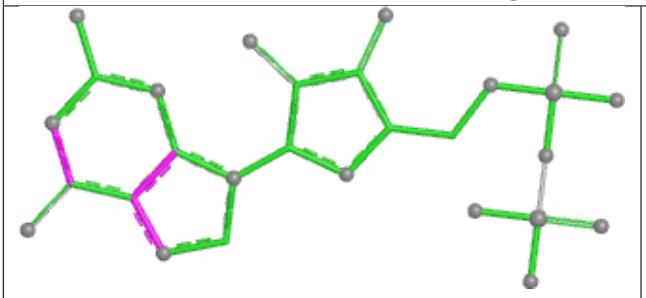


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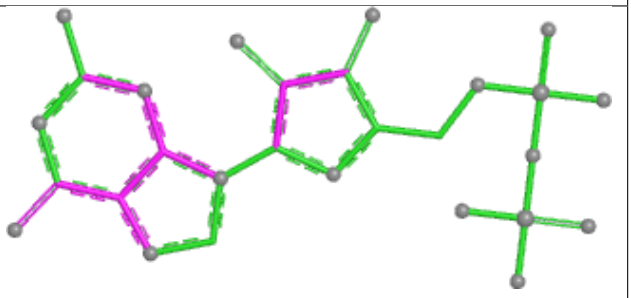


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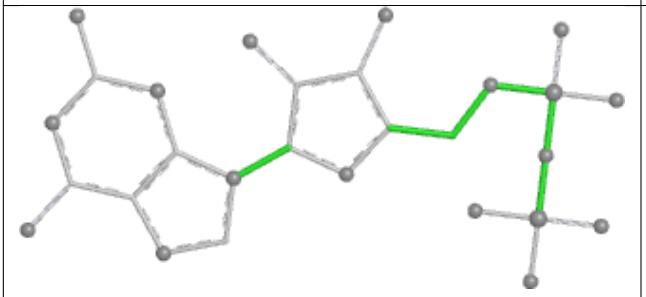
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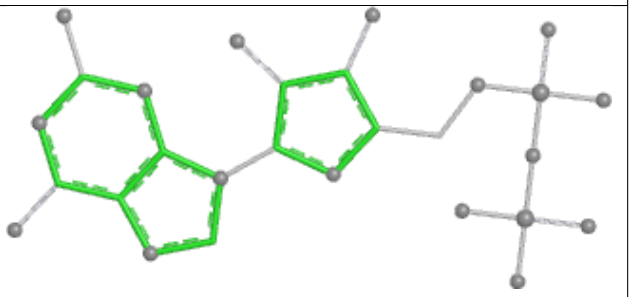
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Bond angles

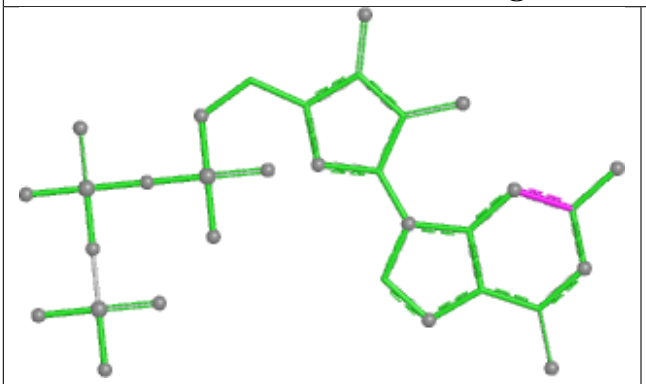


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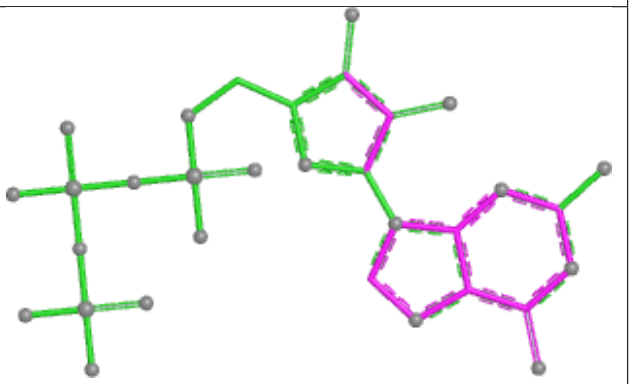


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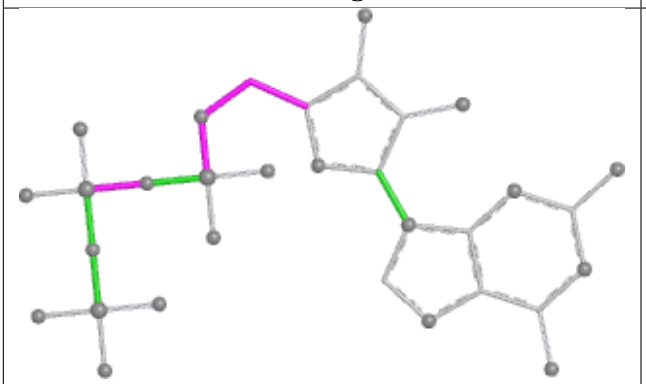
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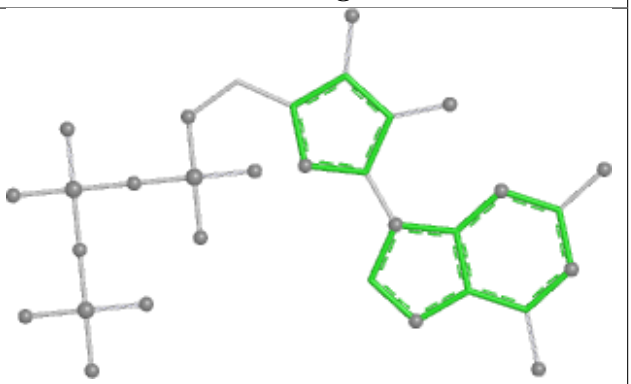
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Bond angles

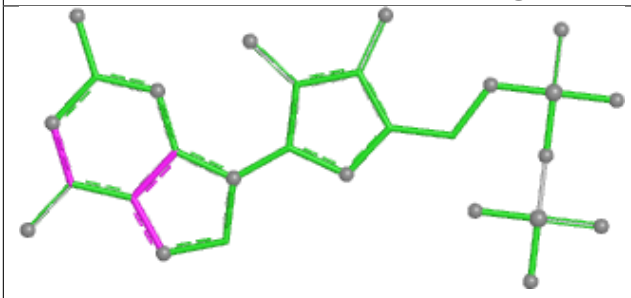


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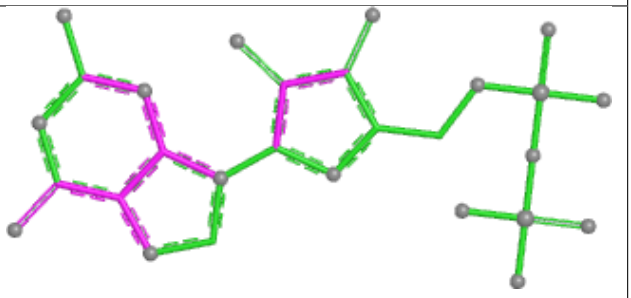


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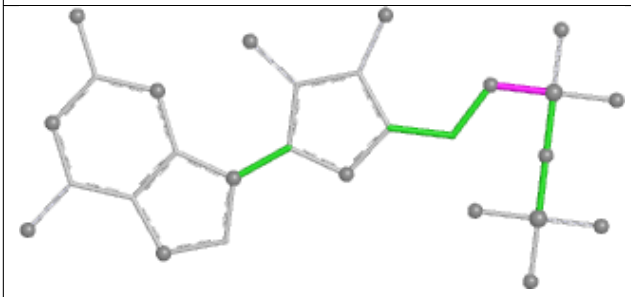
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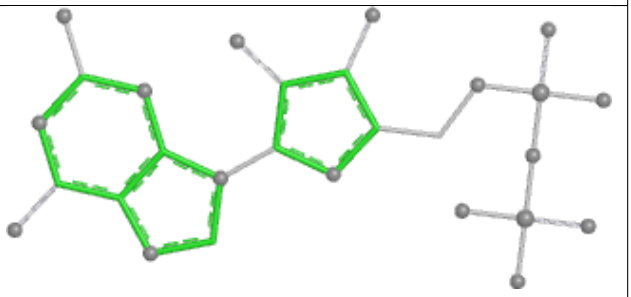
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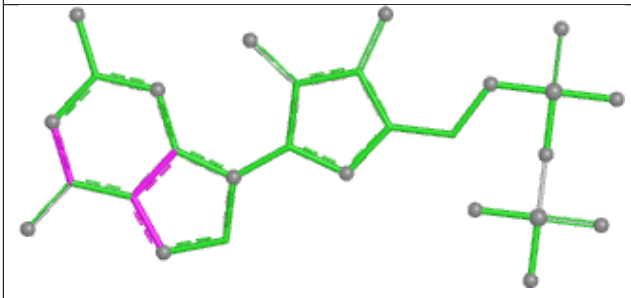


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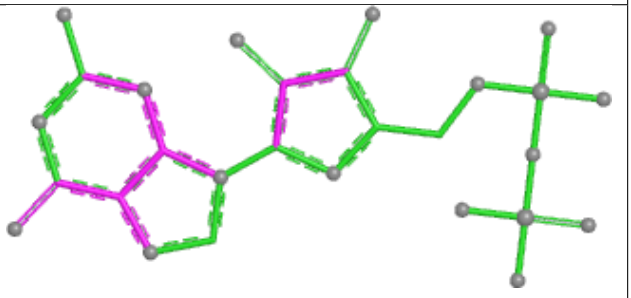


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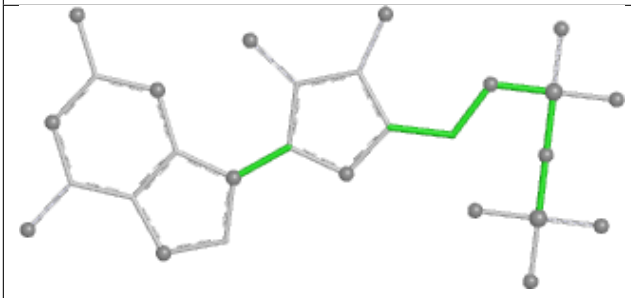
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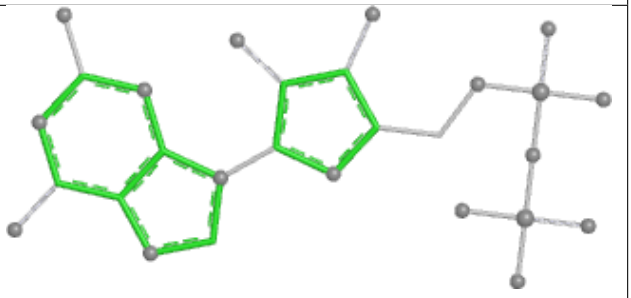
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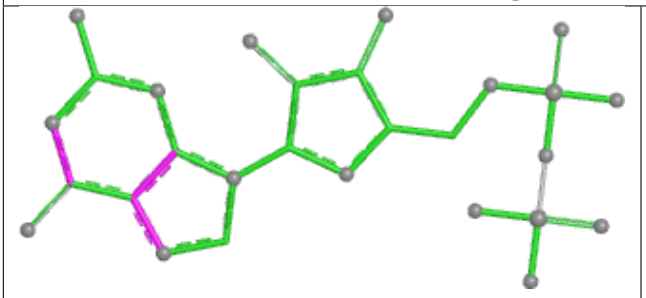


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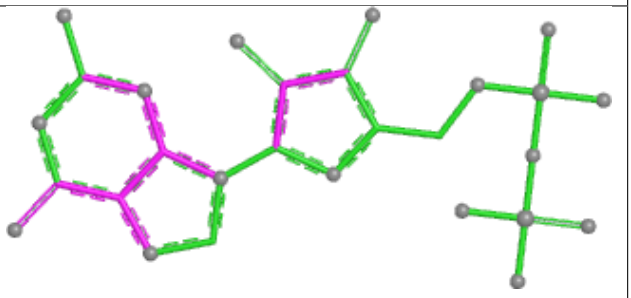


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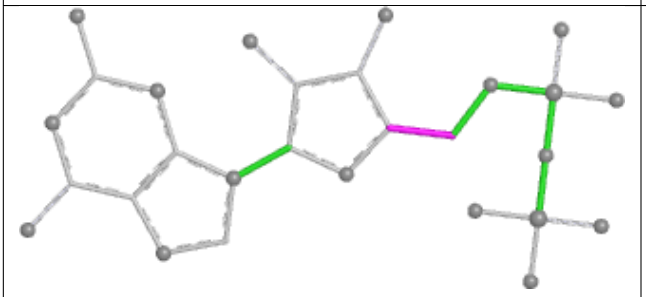
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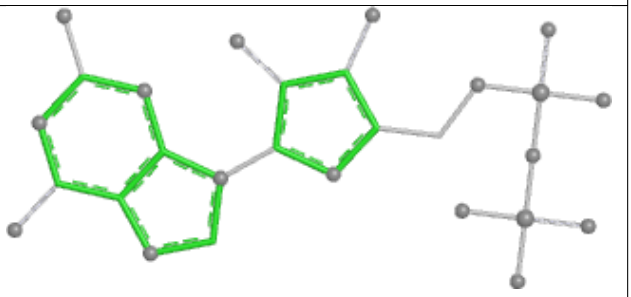
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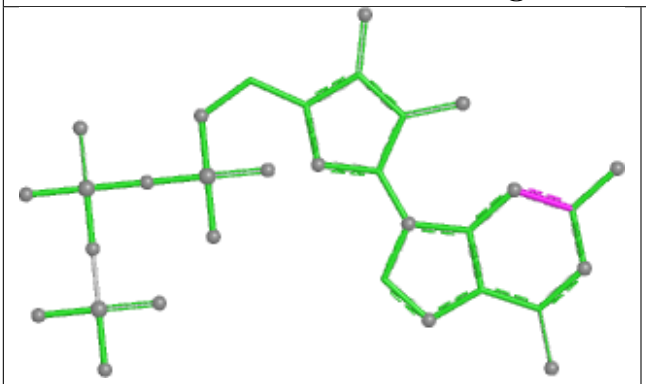


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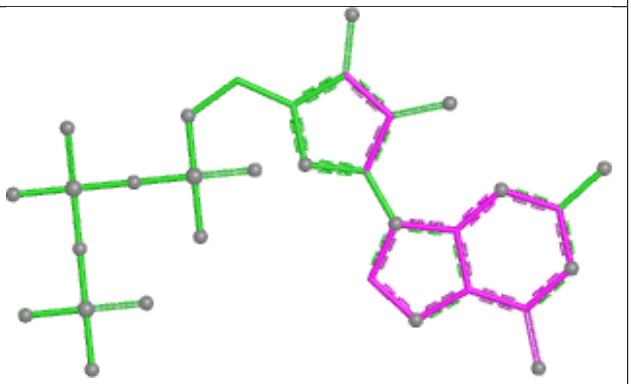


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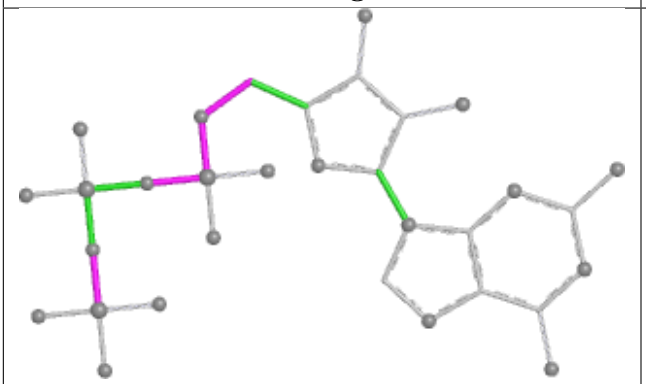
Ligand GTP NK 501



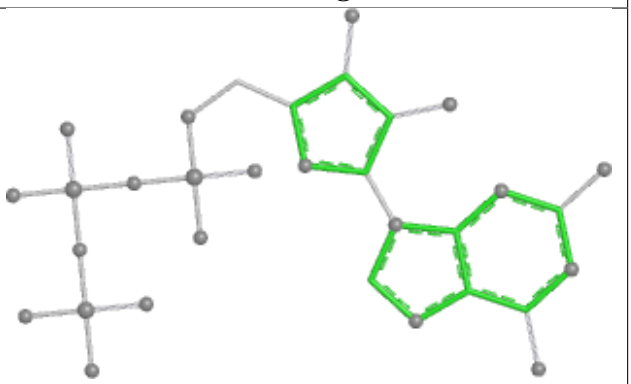
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Bond angles

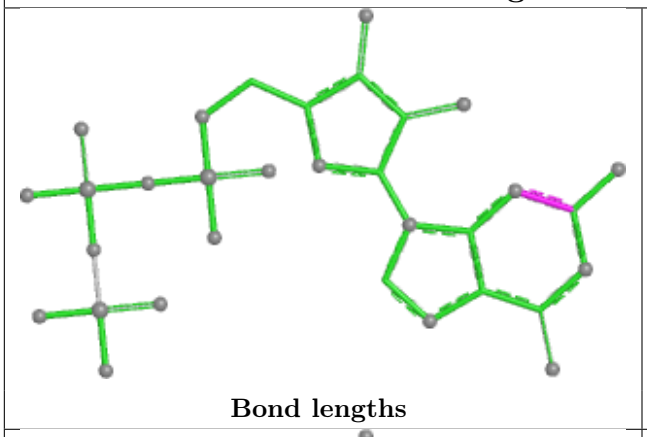


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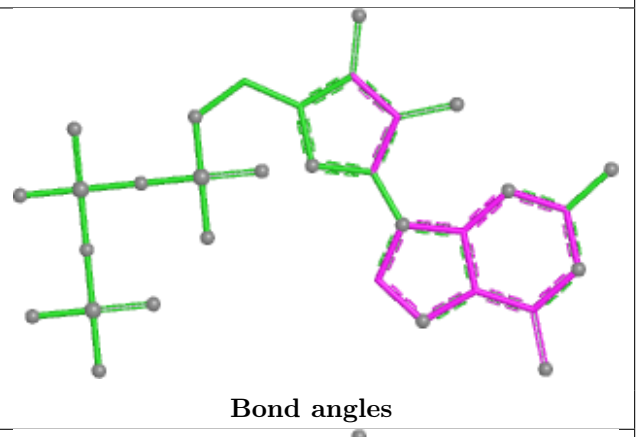


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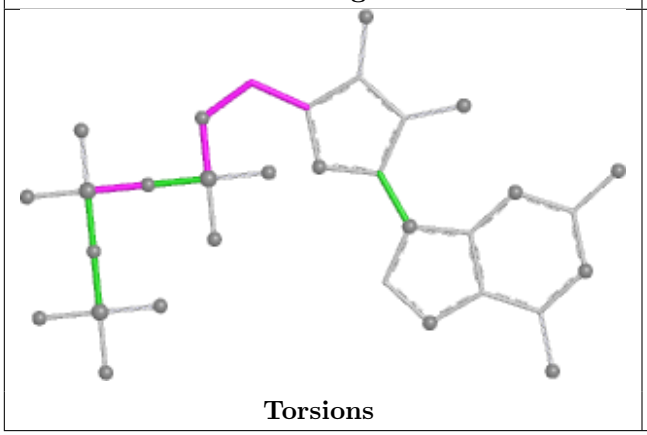
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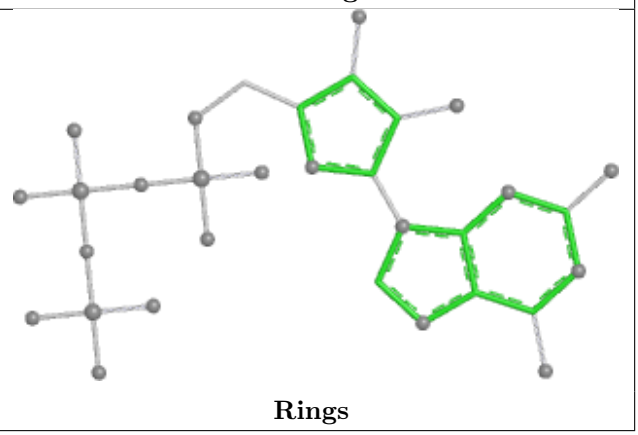
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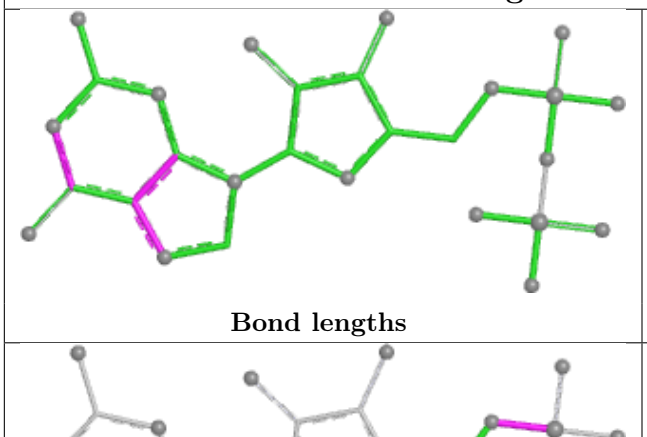


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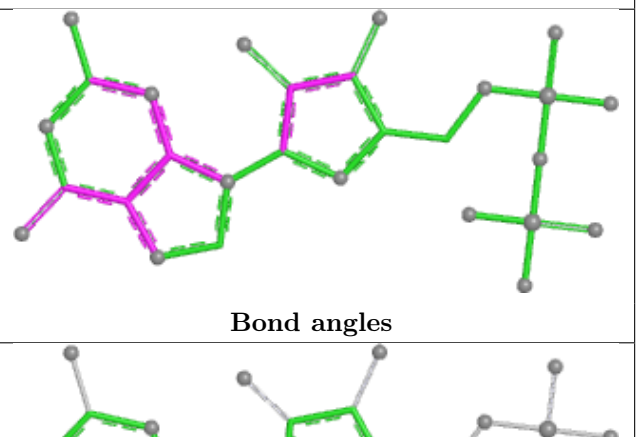


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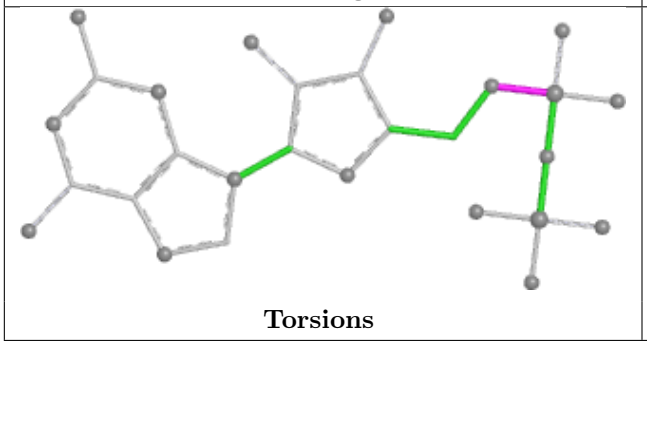
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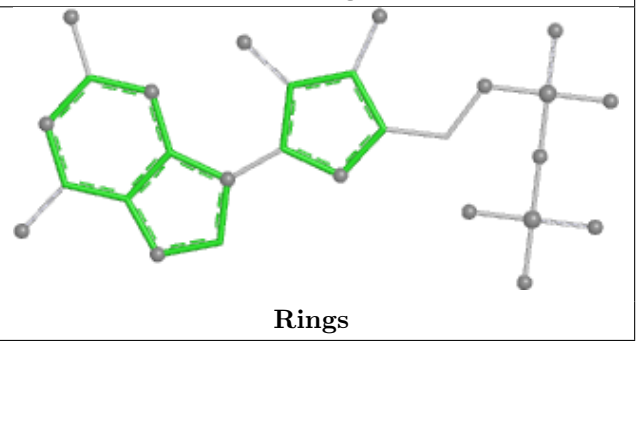
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Bond angles

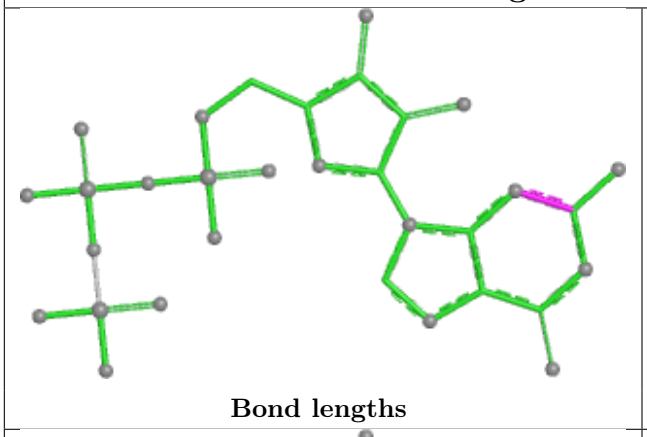


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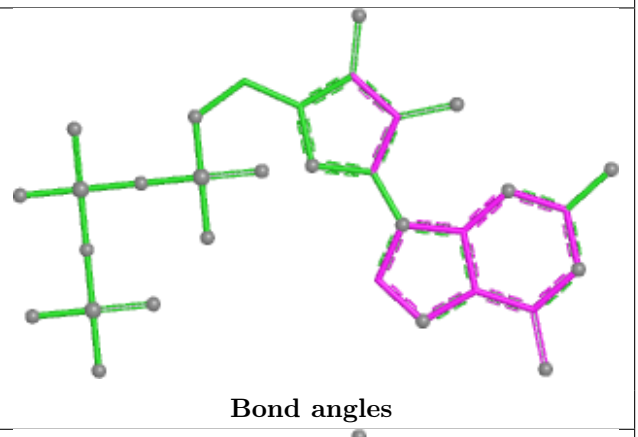


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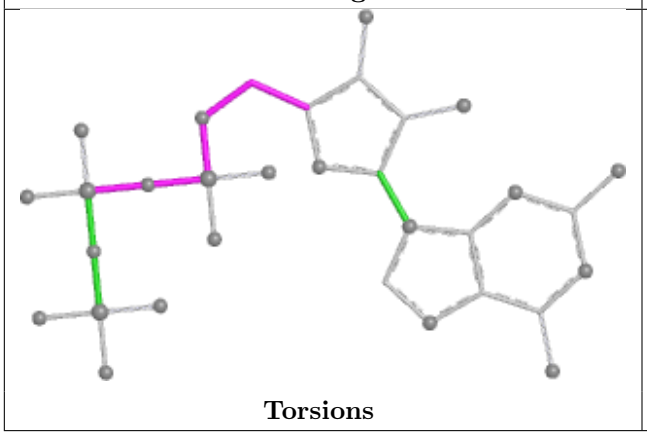
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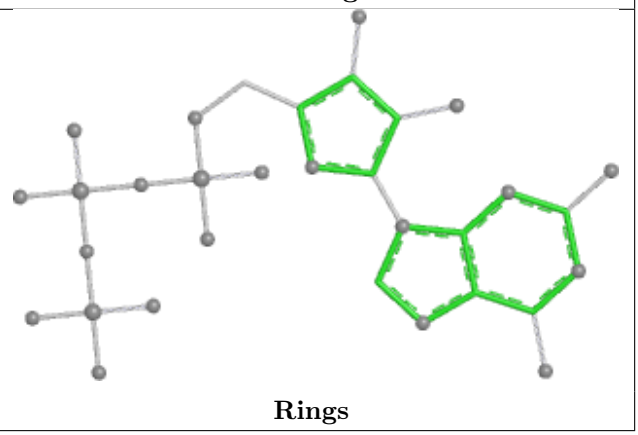
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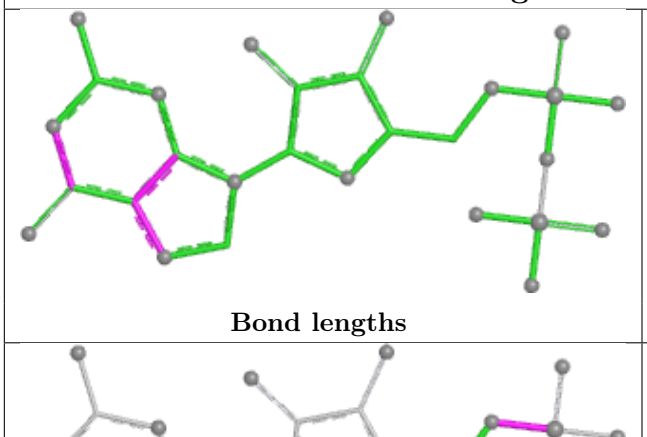


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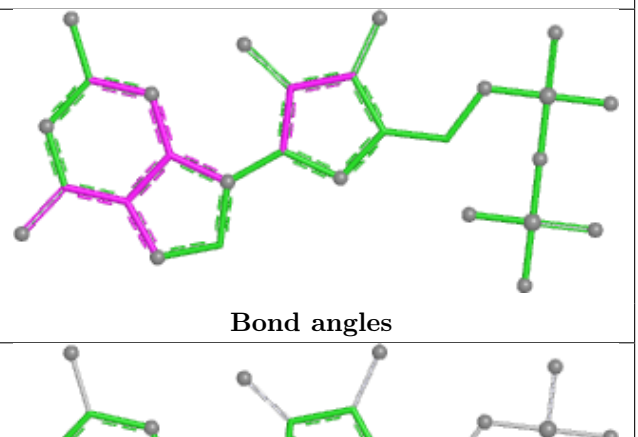


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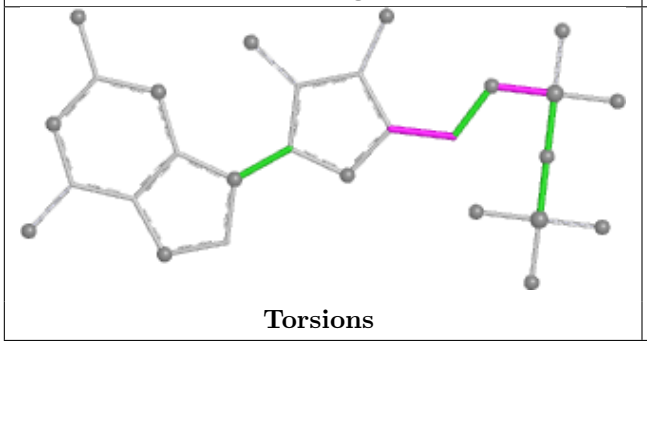
Ligand GDP LD 501



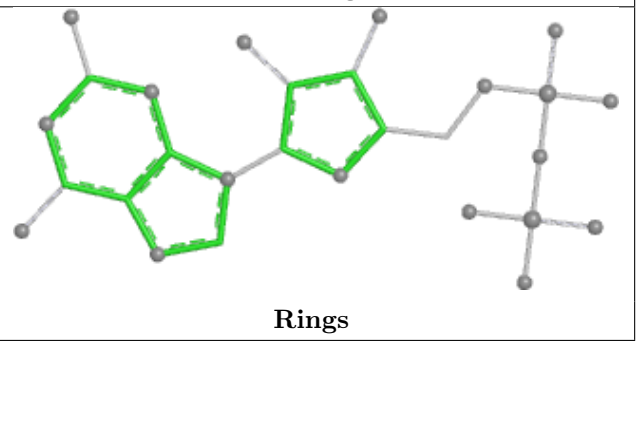
Bond lengths



Bond angles

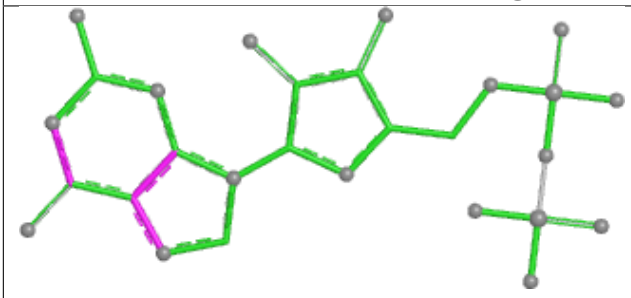


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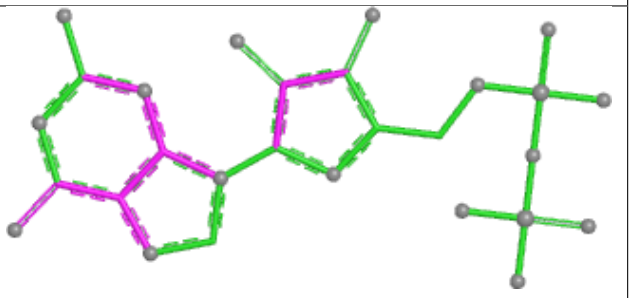


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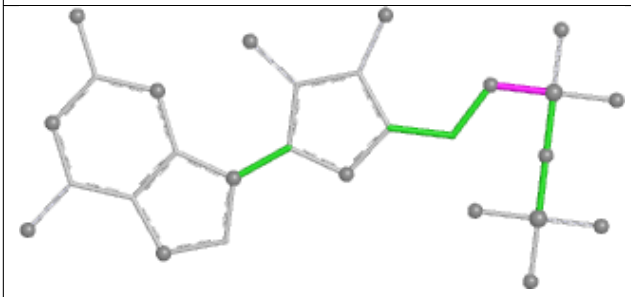
Ligand GDP FH 501



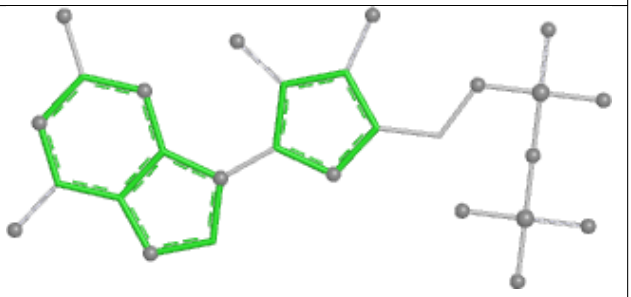
Bond lengths



Bond angles

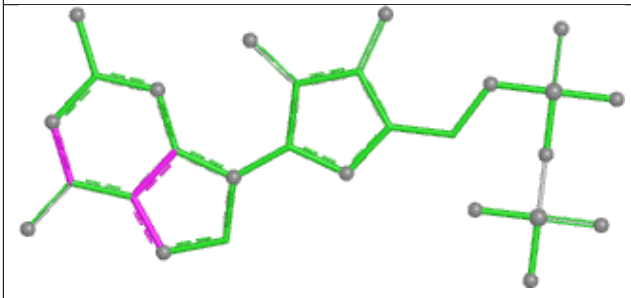


Torsions

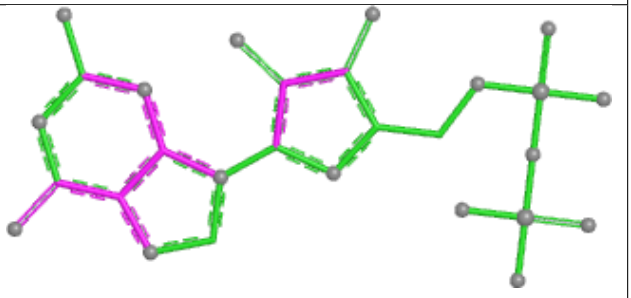


Rings

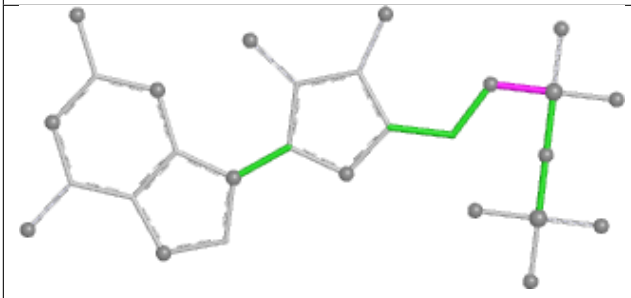
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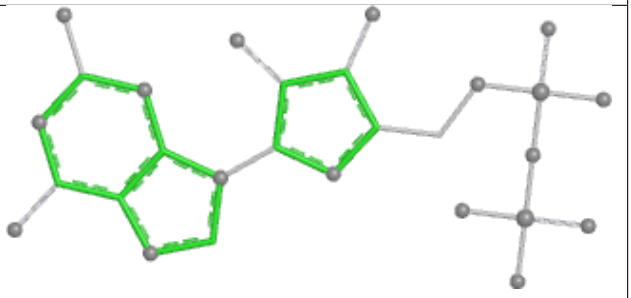
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Bond angles

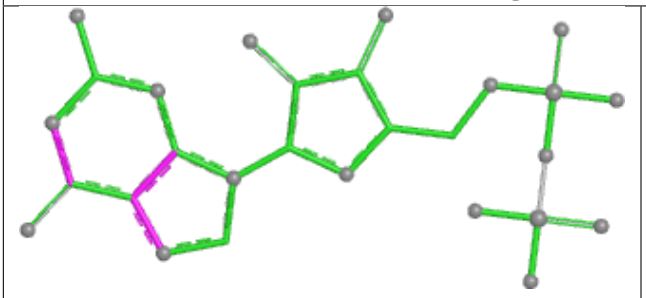


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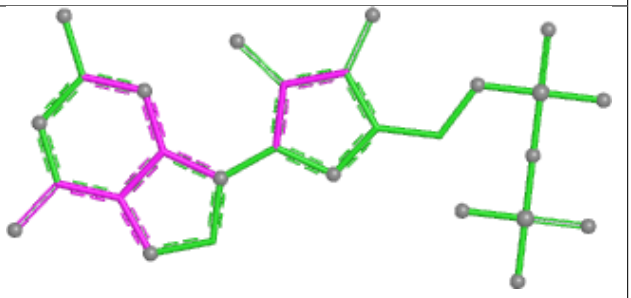


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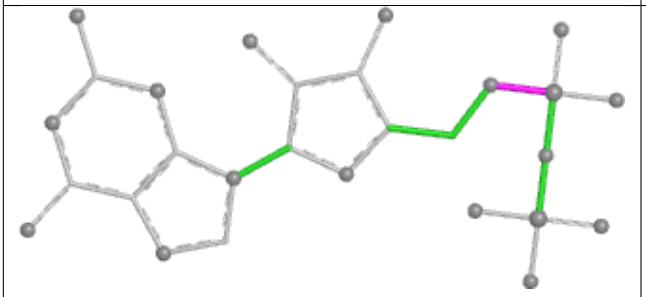
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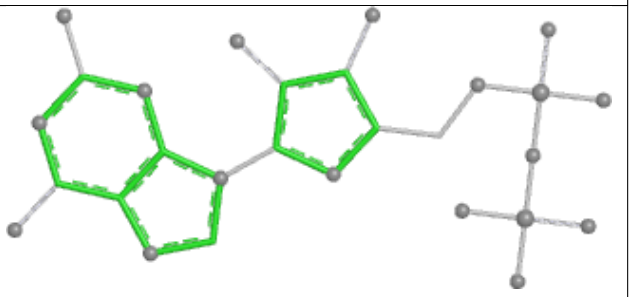
Bond lengths



Bond angles

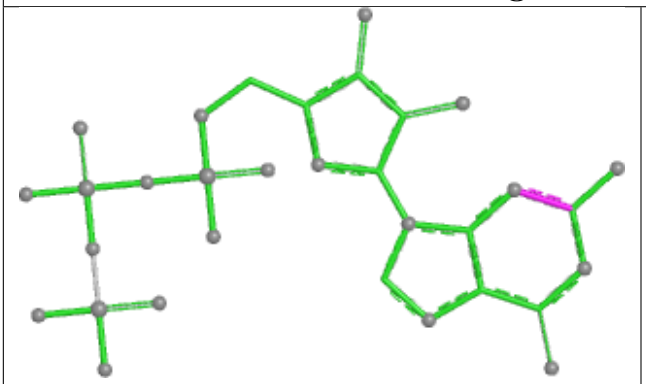


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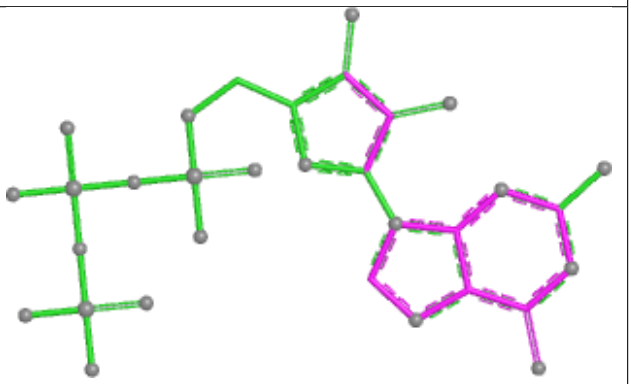


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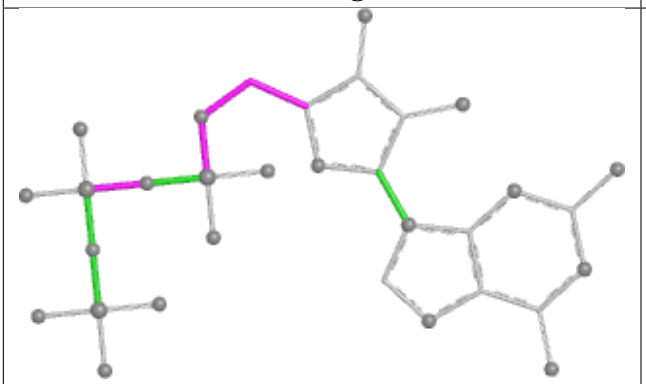
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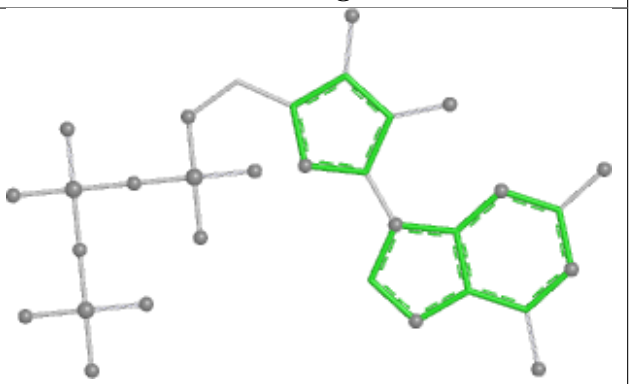
Bond lengths



Bond angles

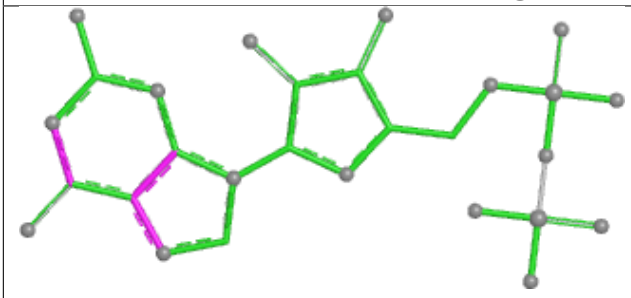


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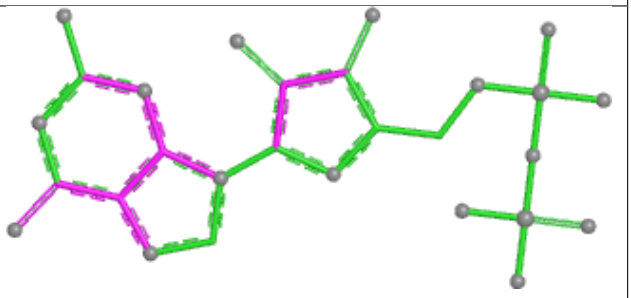


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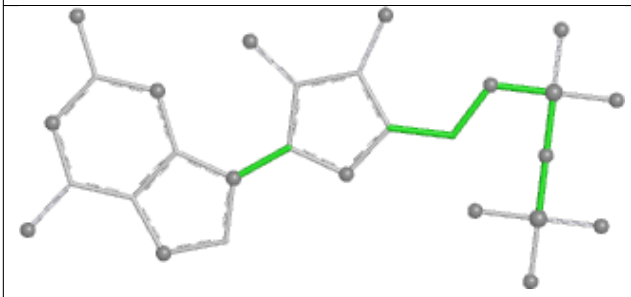
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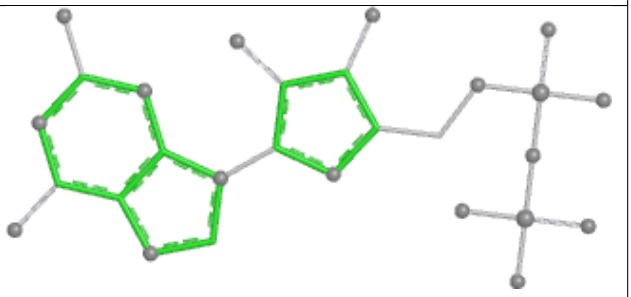
Bond lengths



Bond angles

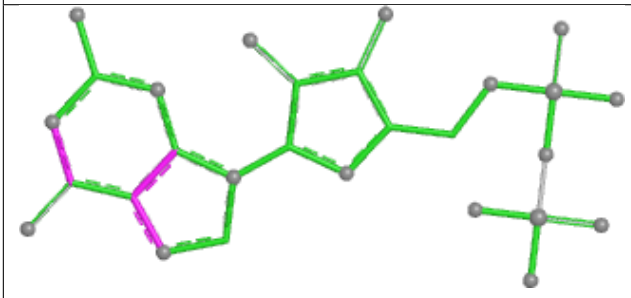


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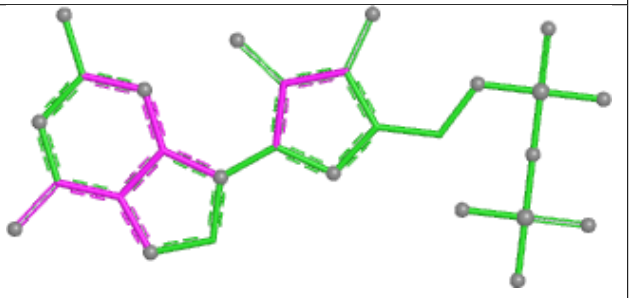


Rings

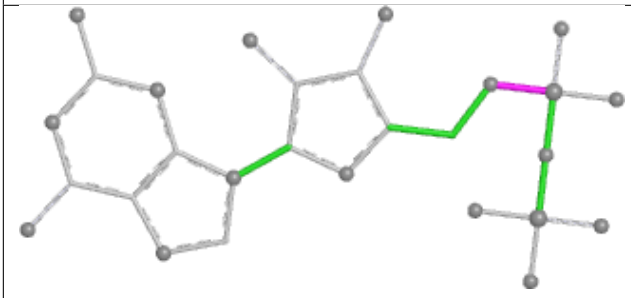
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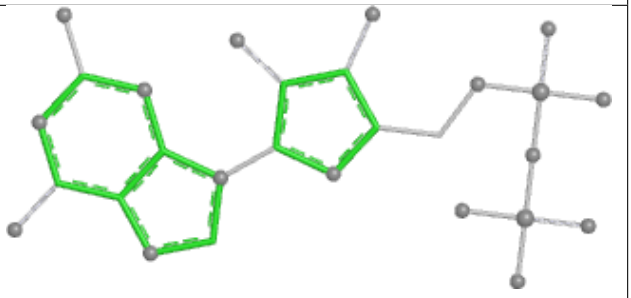
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Bond angles

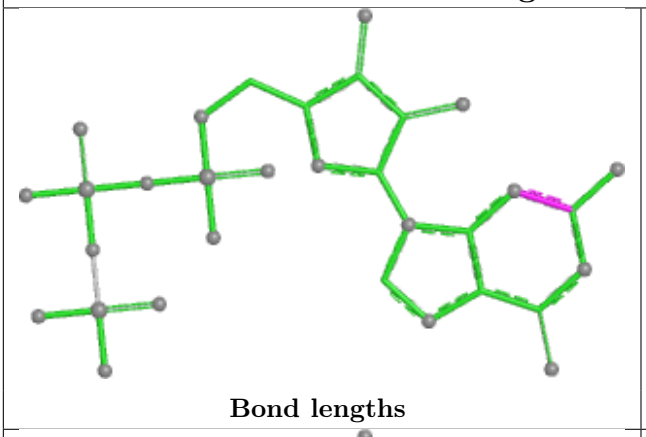


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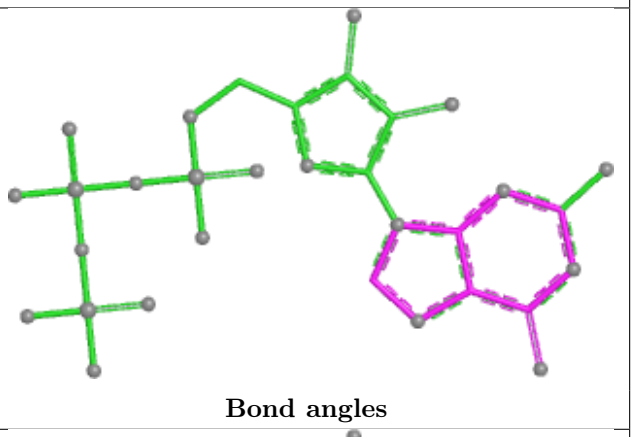


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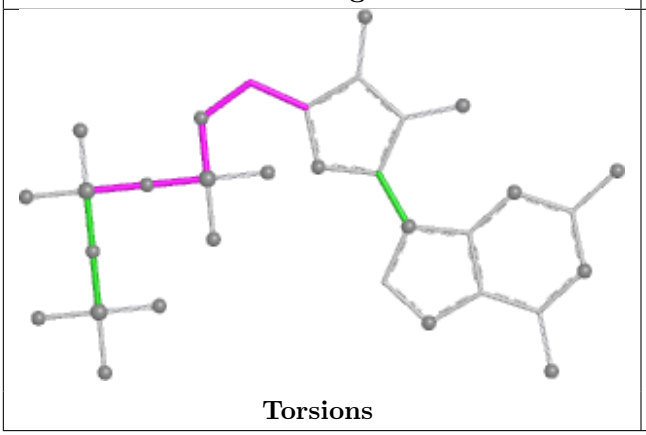
Ligand GTP LI 501



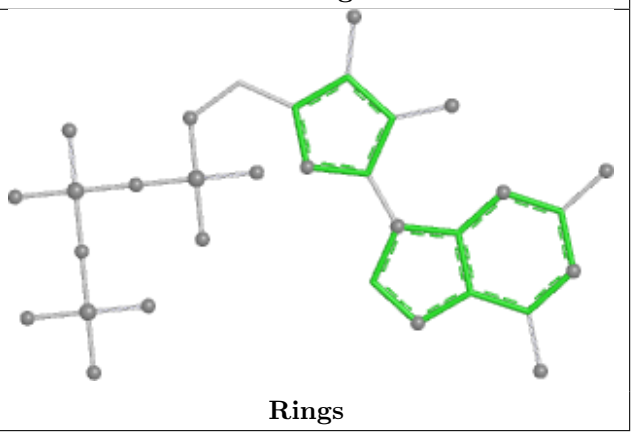
Bond lengths



Bond angles

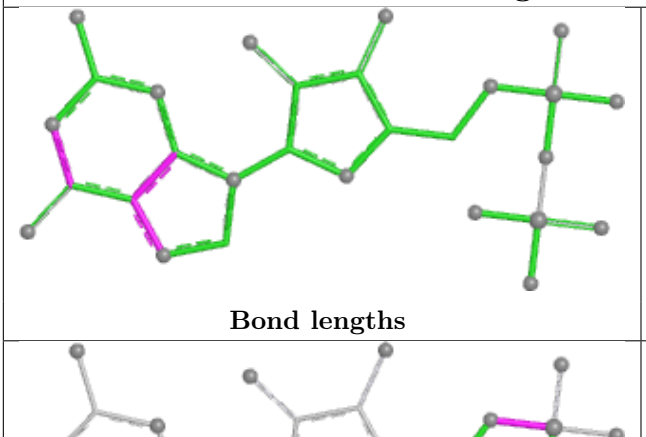


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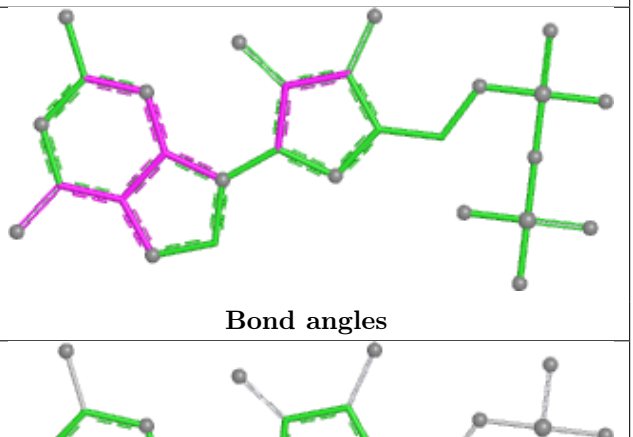


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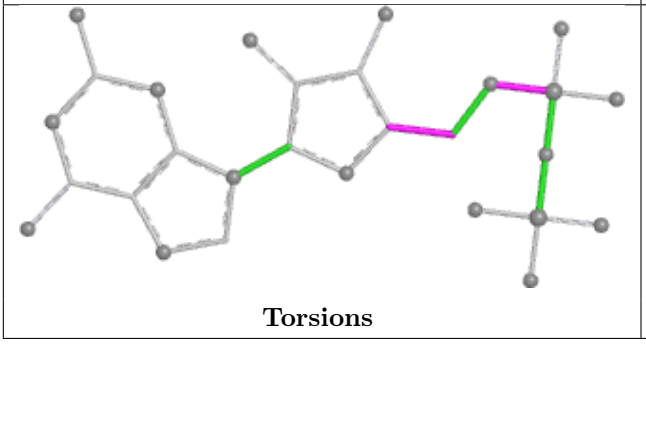
Ligand GDP FJ 501



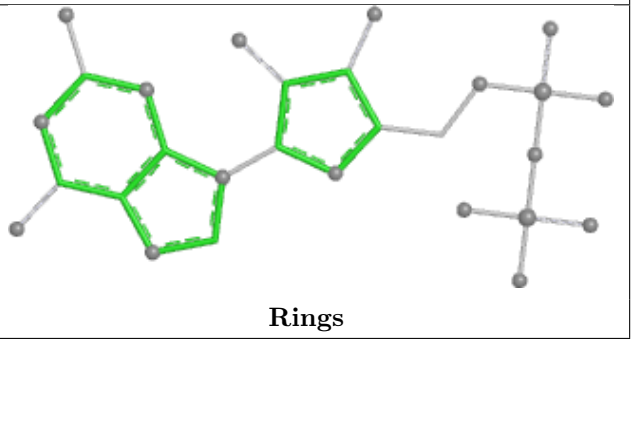
Bond lengths



Bond angles

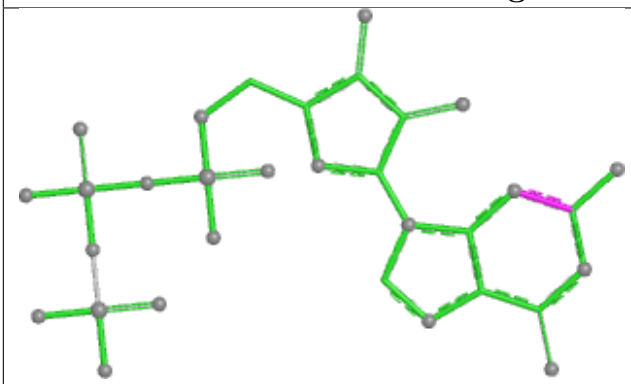


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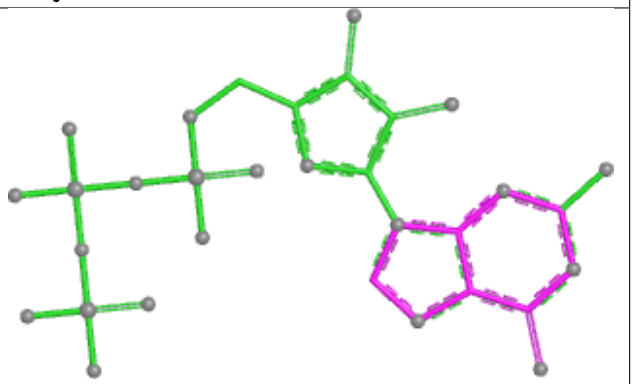


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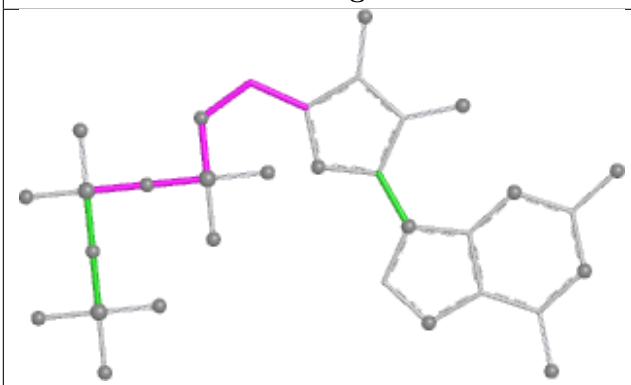
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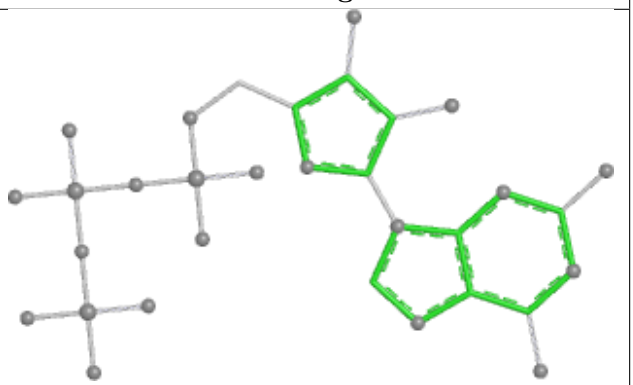
Bond lengths



Bond angles

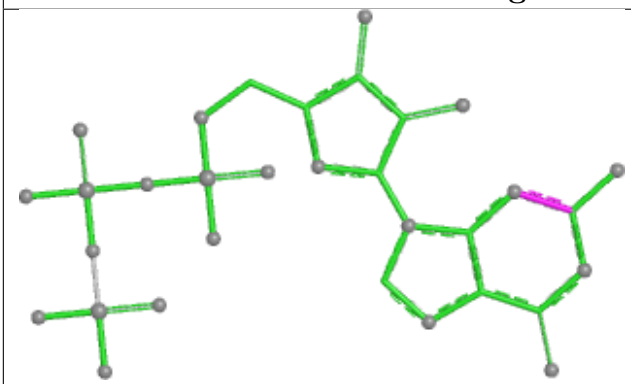


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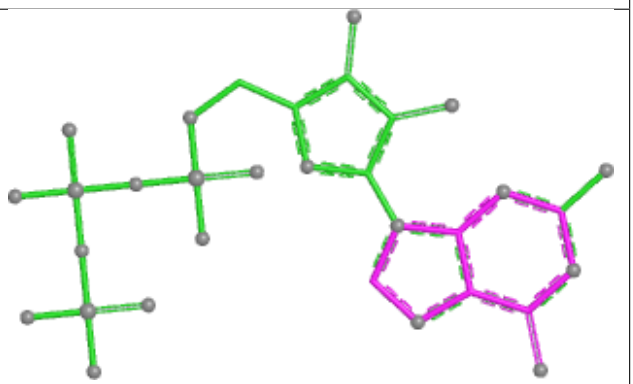


Rings

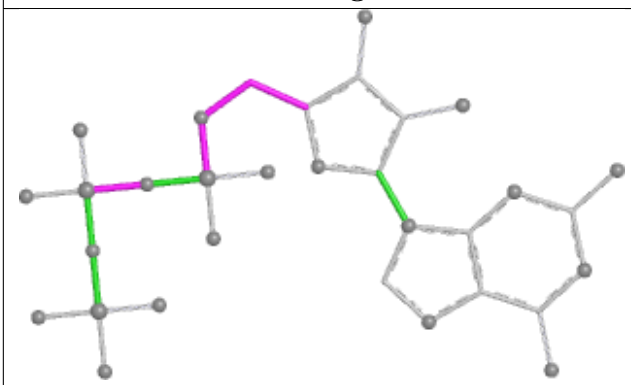
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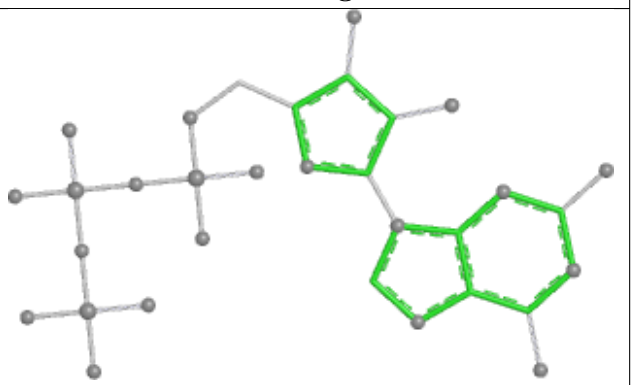
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Bond angles

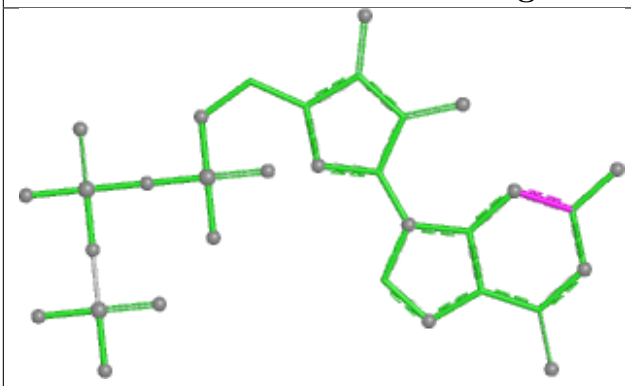


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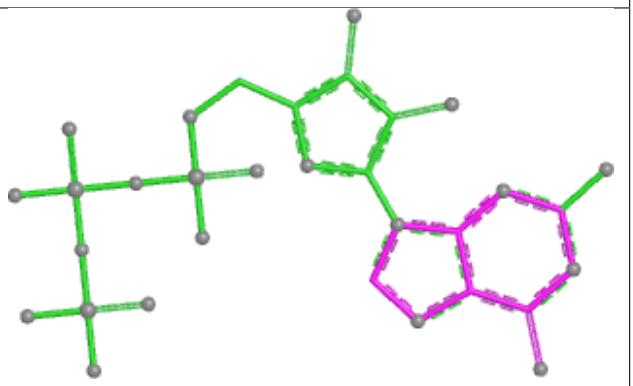


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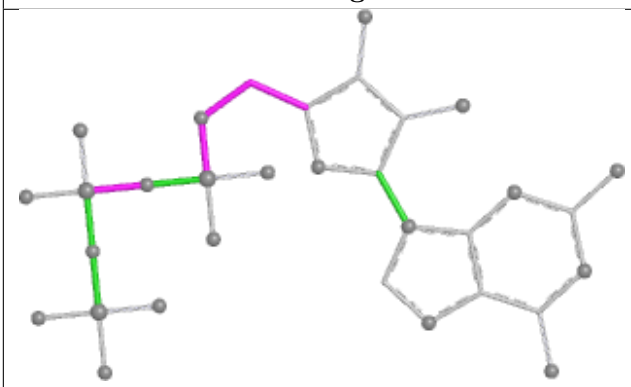
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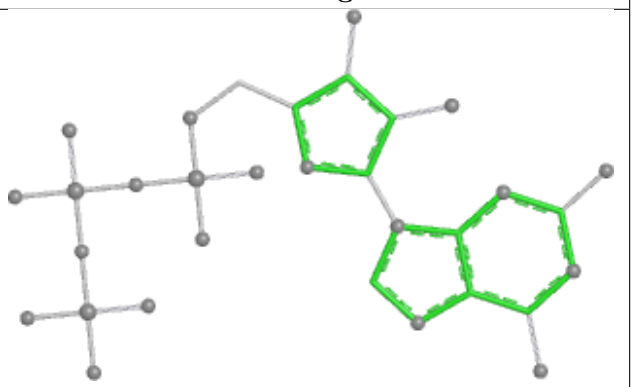
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Bond angles

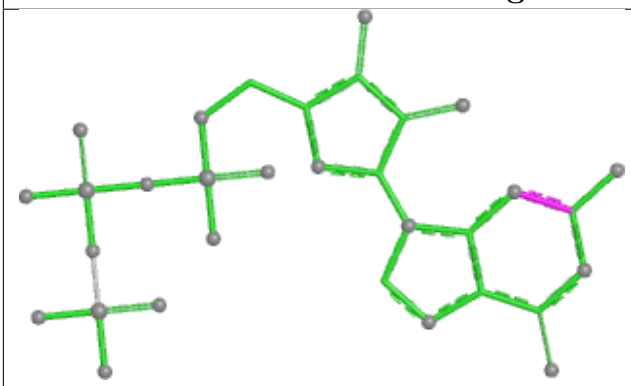


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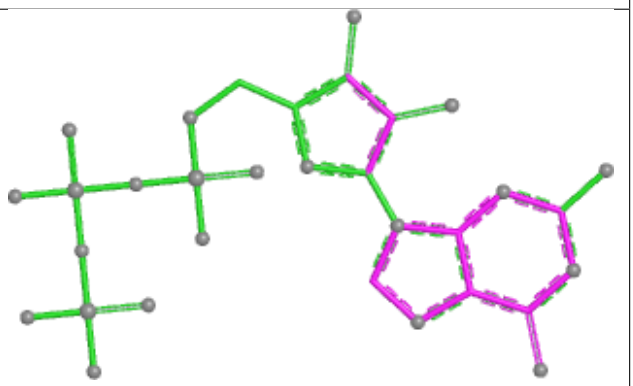


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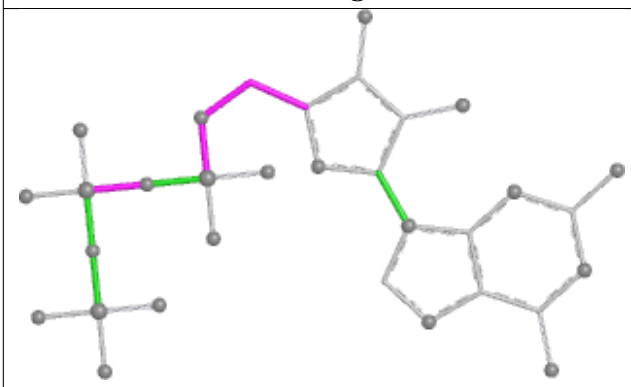
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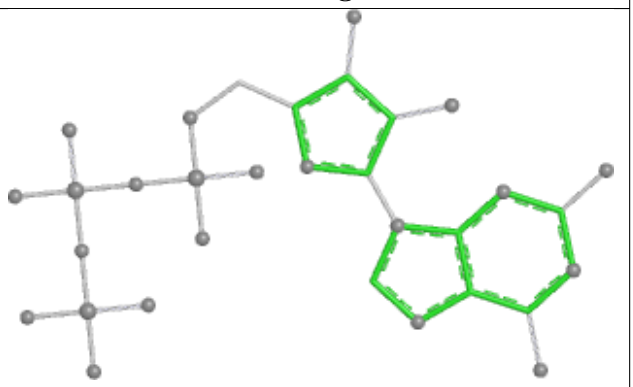
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Bond angles

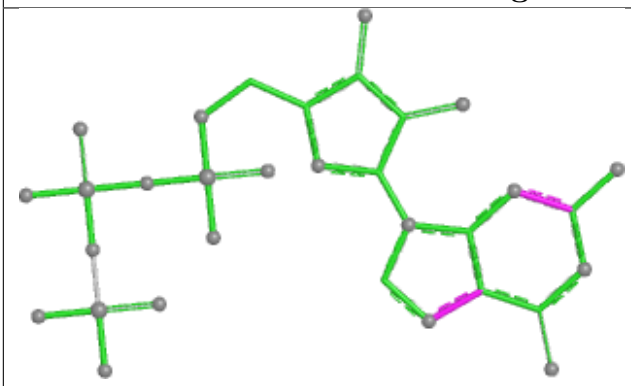


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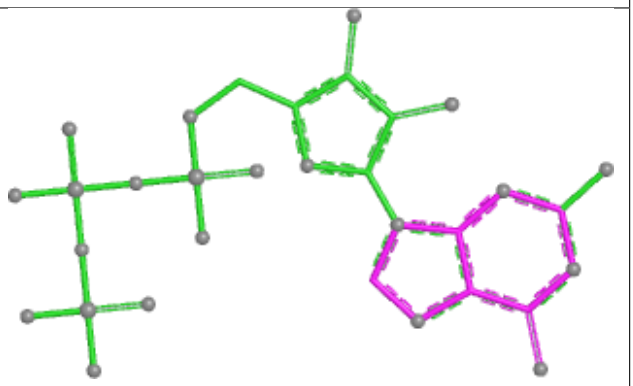


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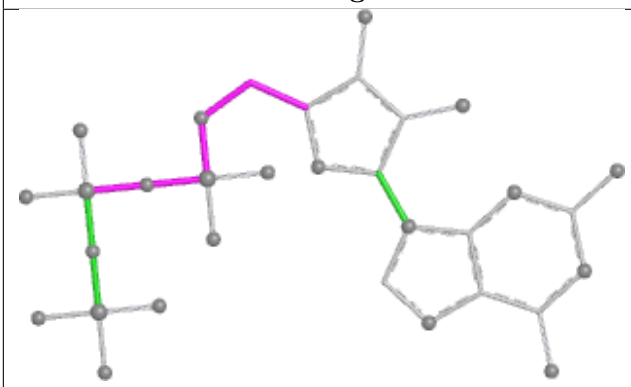
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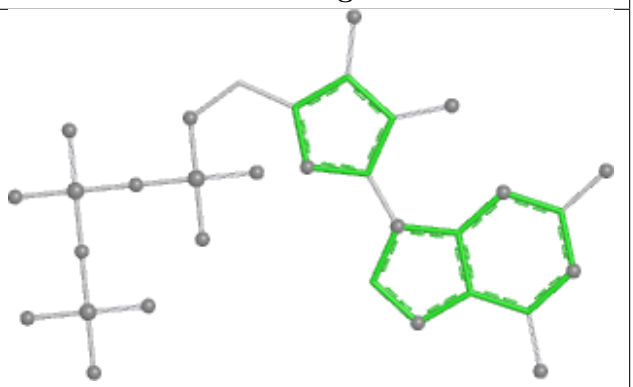
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Bond angles

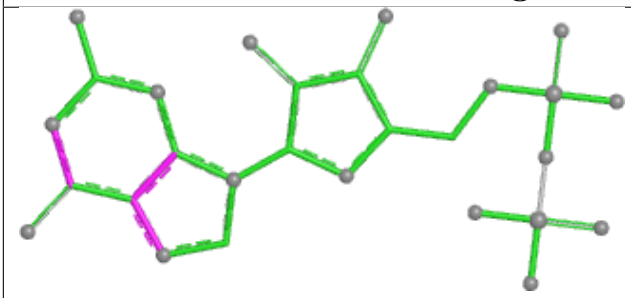


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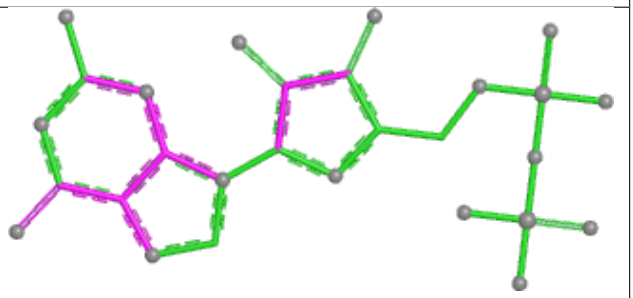


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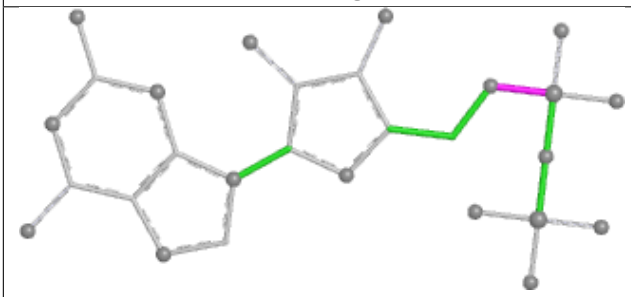
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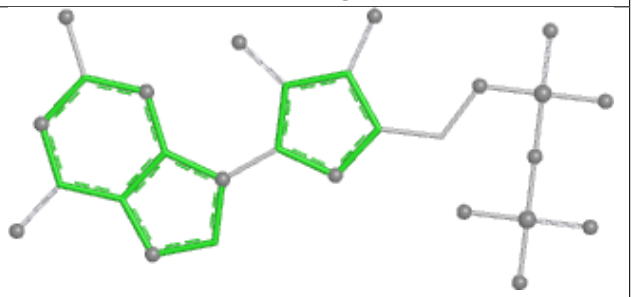
Bond lengths



Bond angles

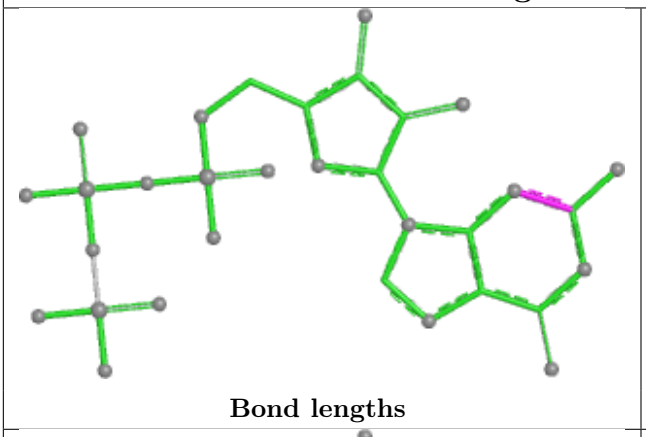


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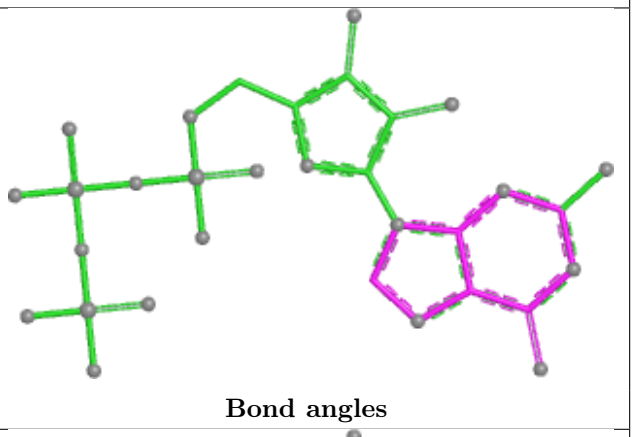


Rings

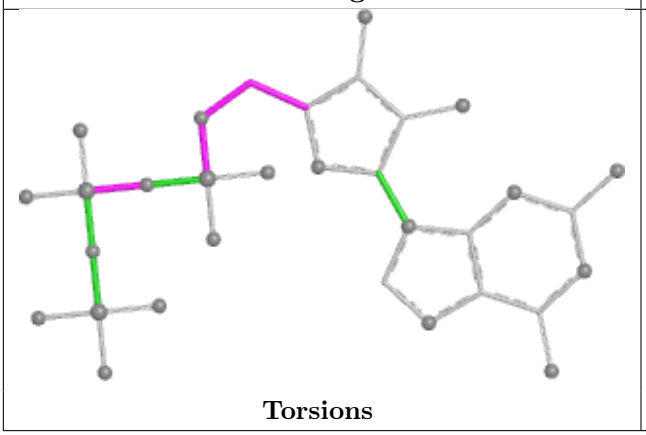
Ligand GTP SE 501



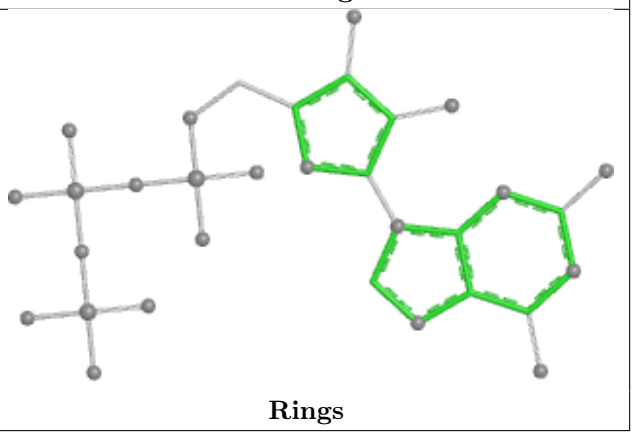
Bond lengths



Bond angles

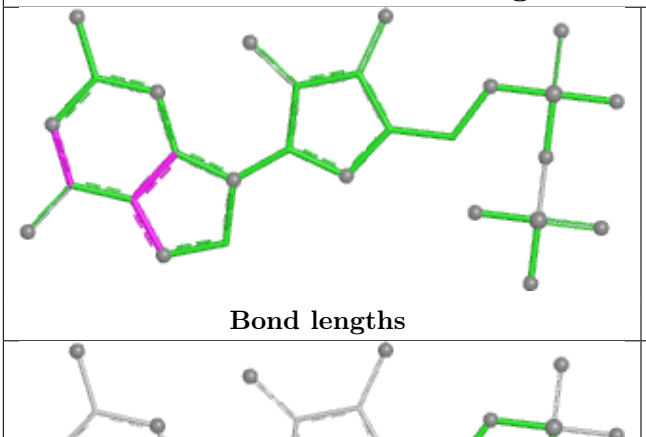


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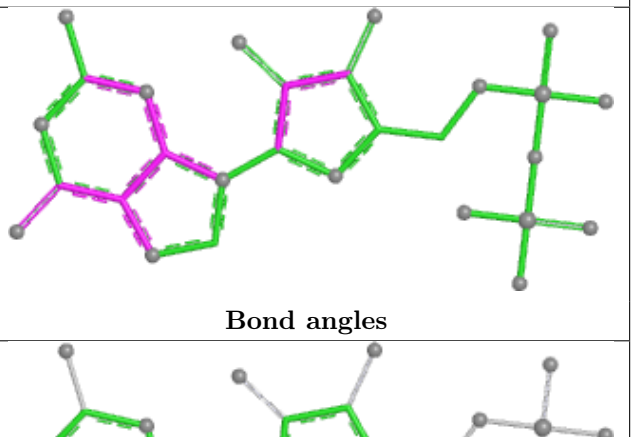


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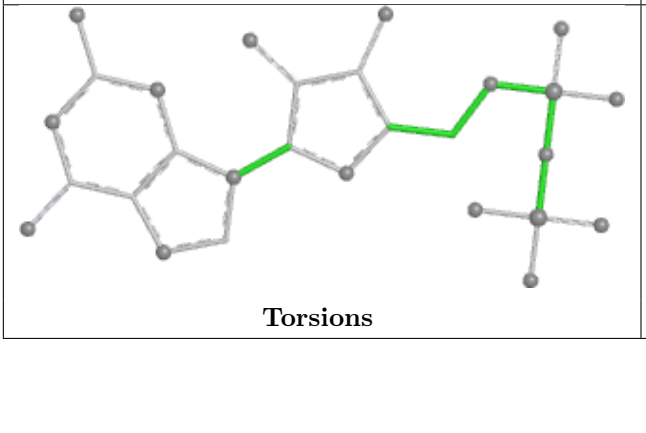
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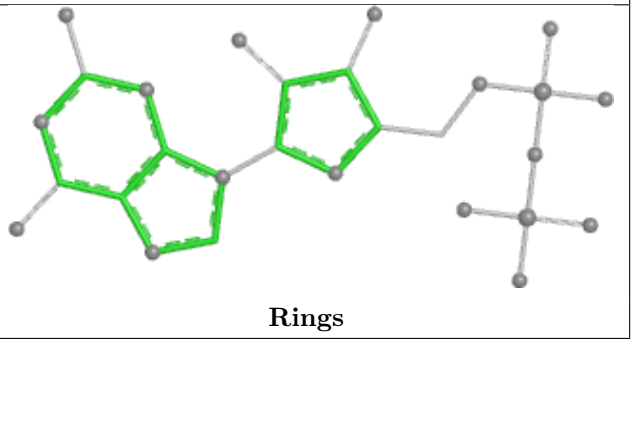
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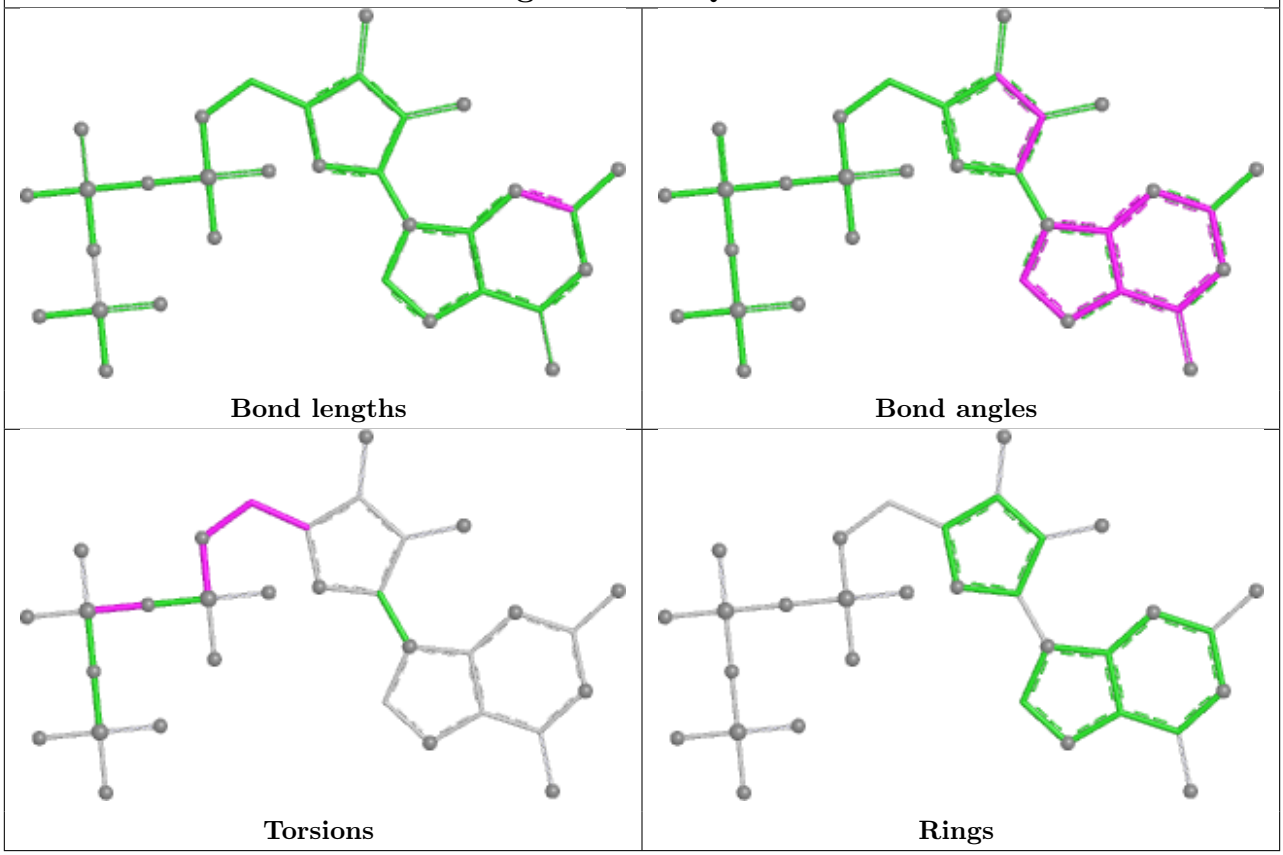


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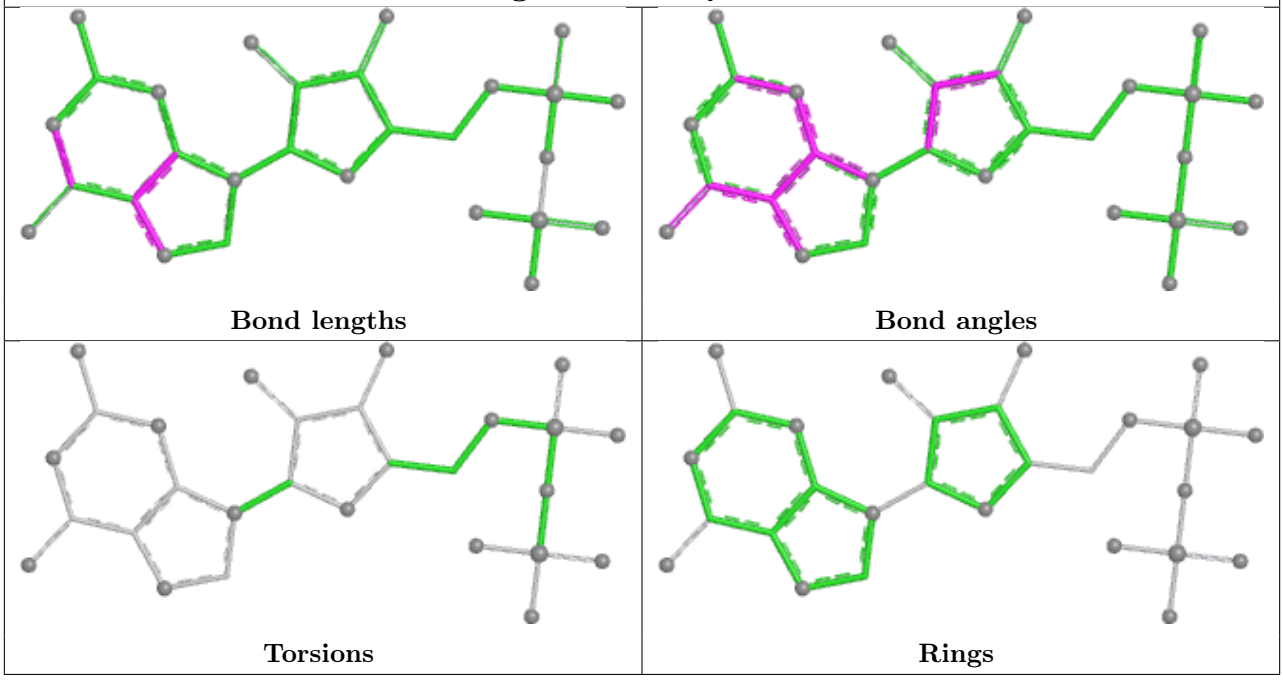


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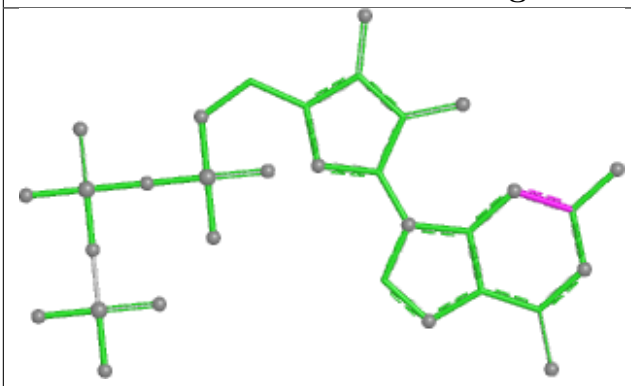
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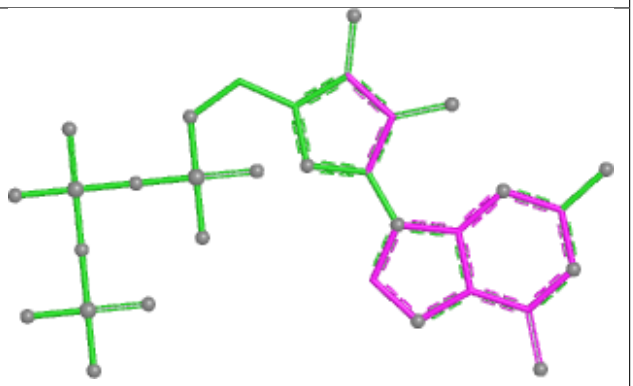
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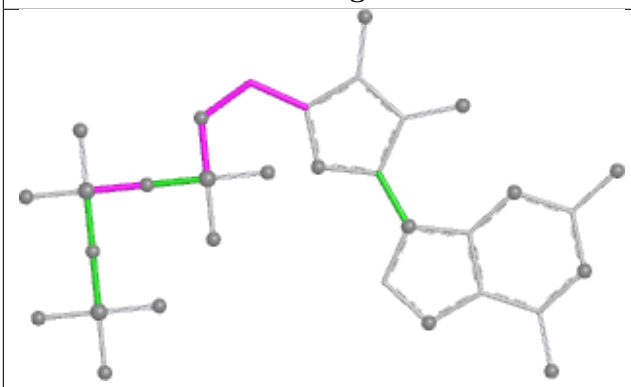
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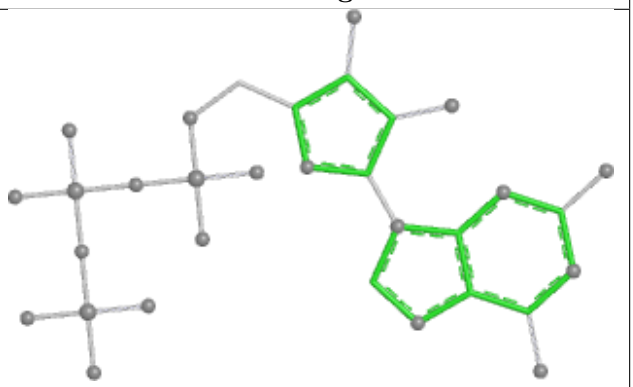
Bond lengths



Bond angles

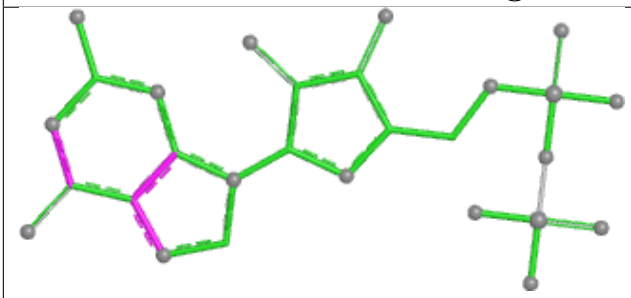


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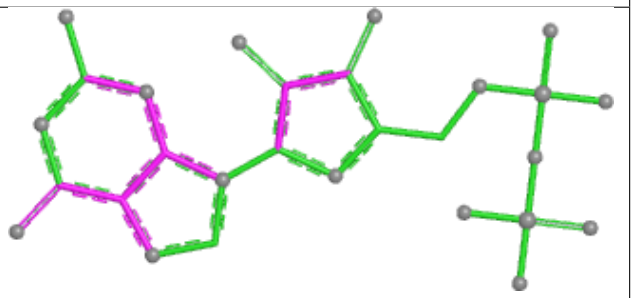


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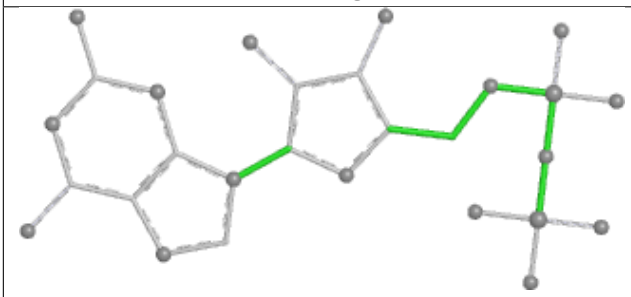
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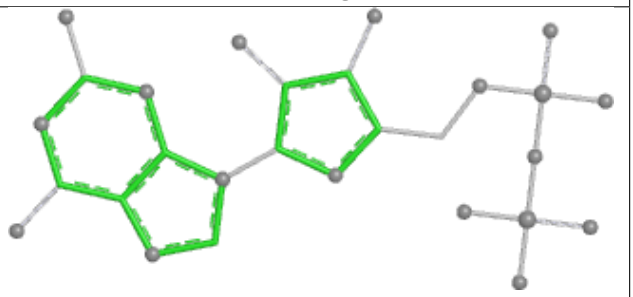
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Bond angles

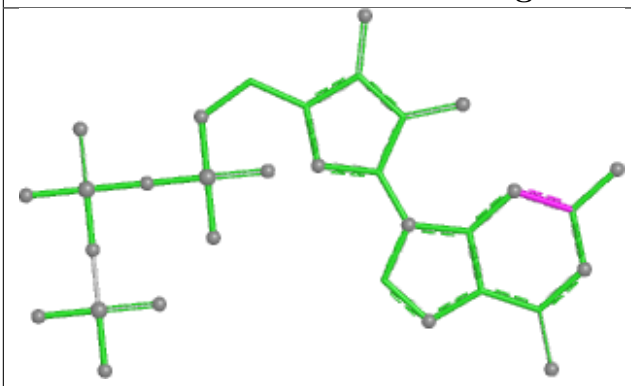


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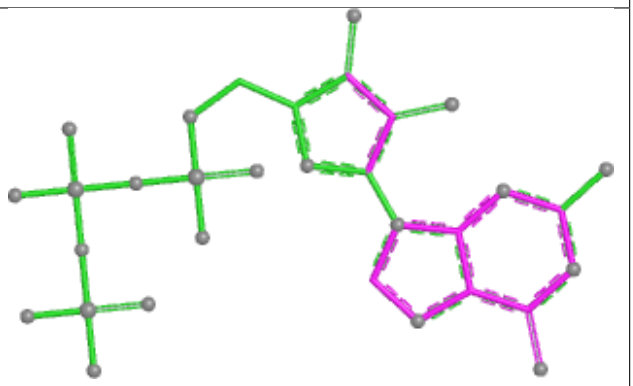


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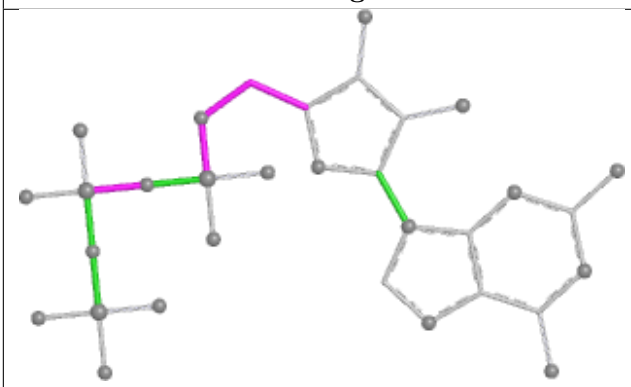
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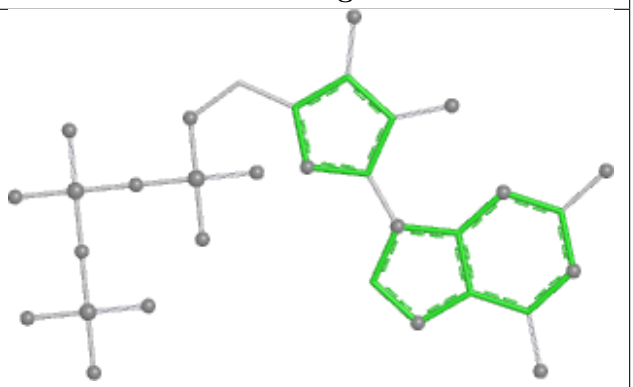
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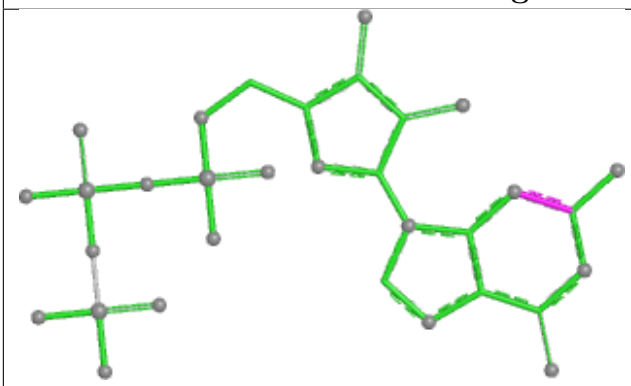


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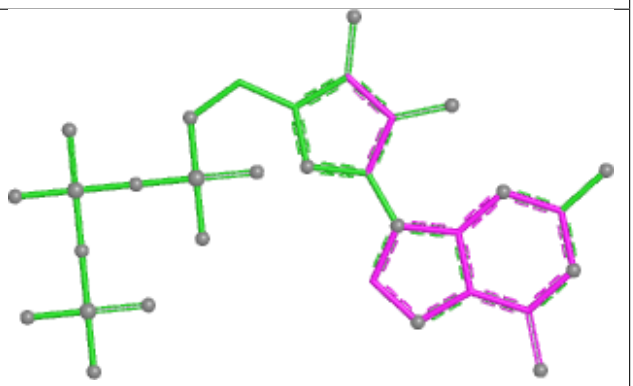


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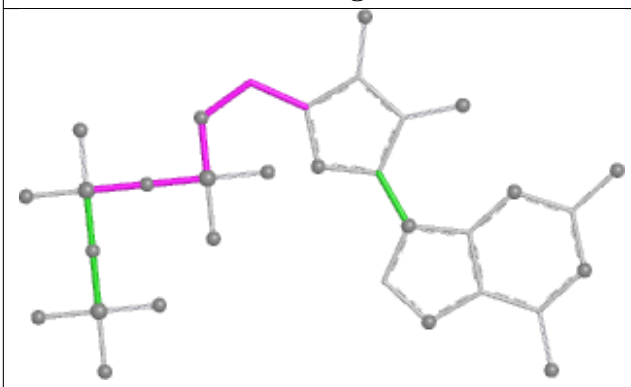
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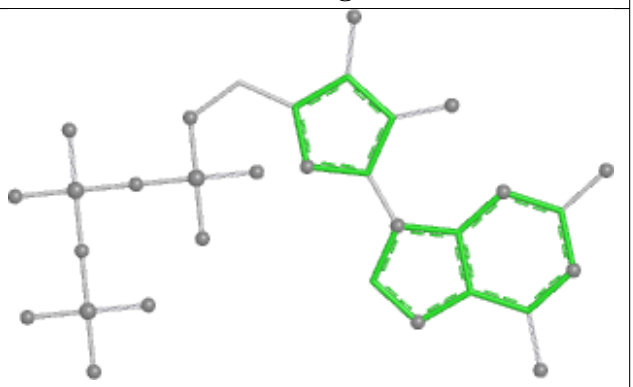
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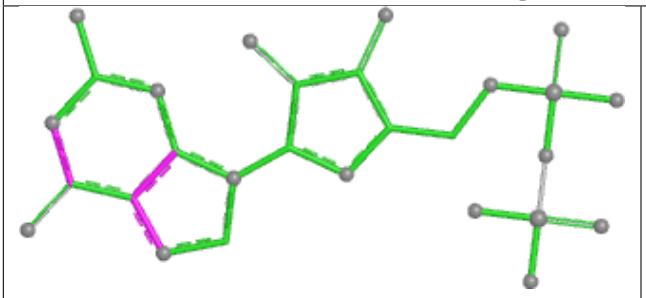


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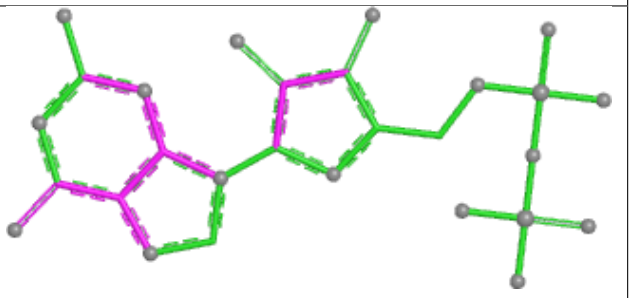


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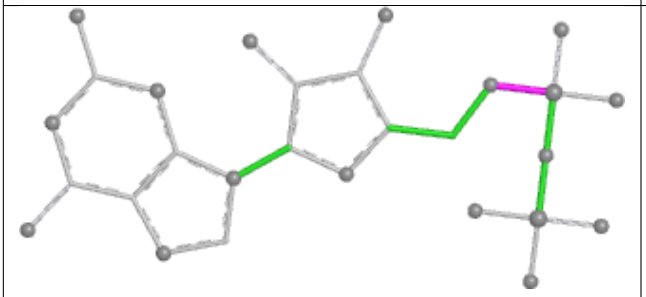
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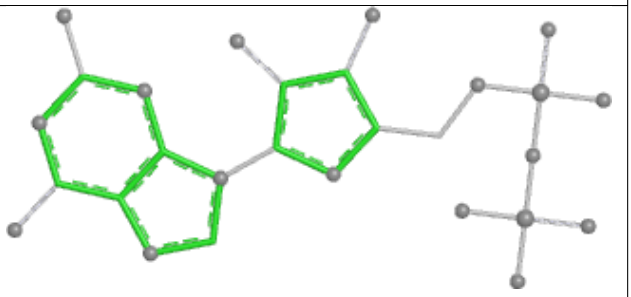
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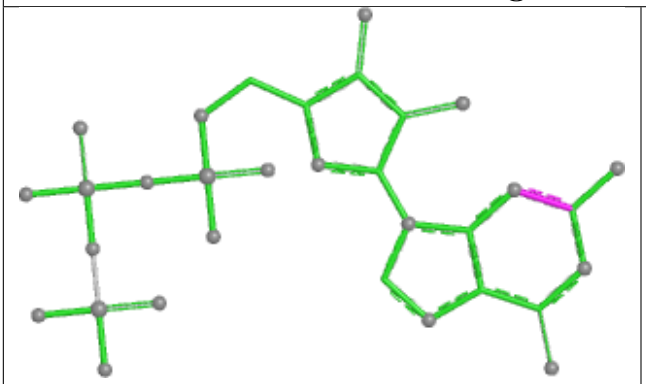


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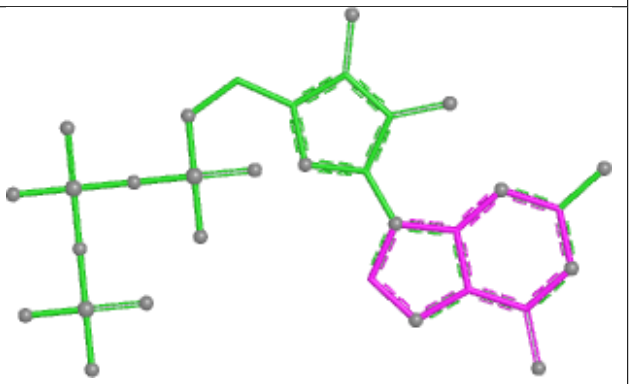


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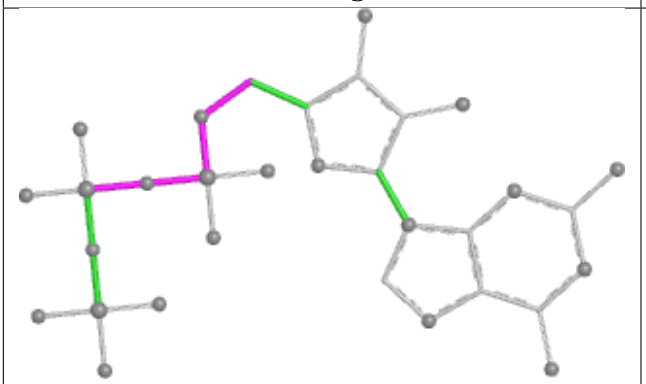
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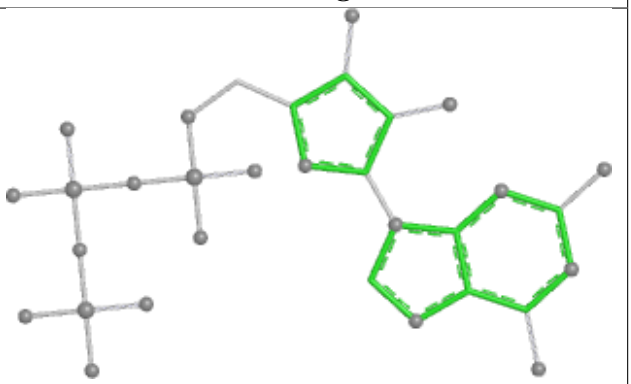
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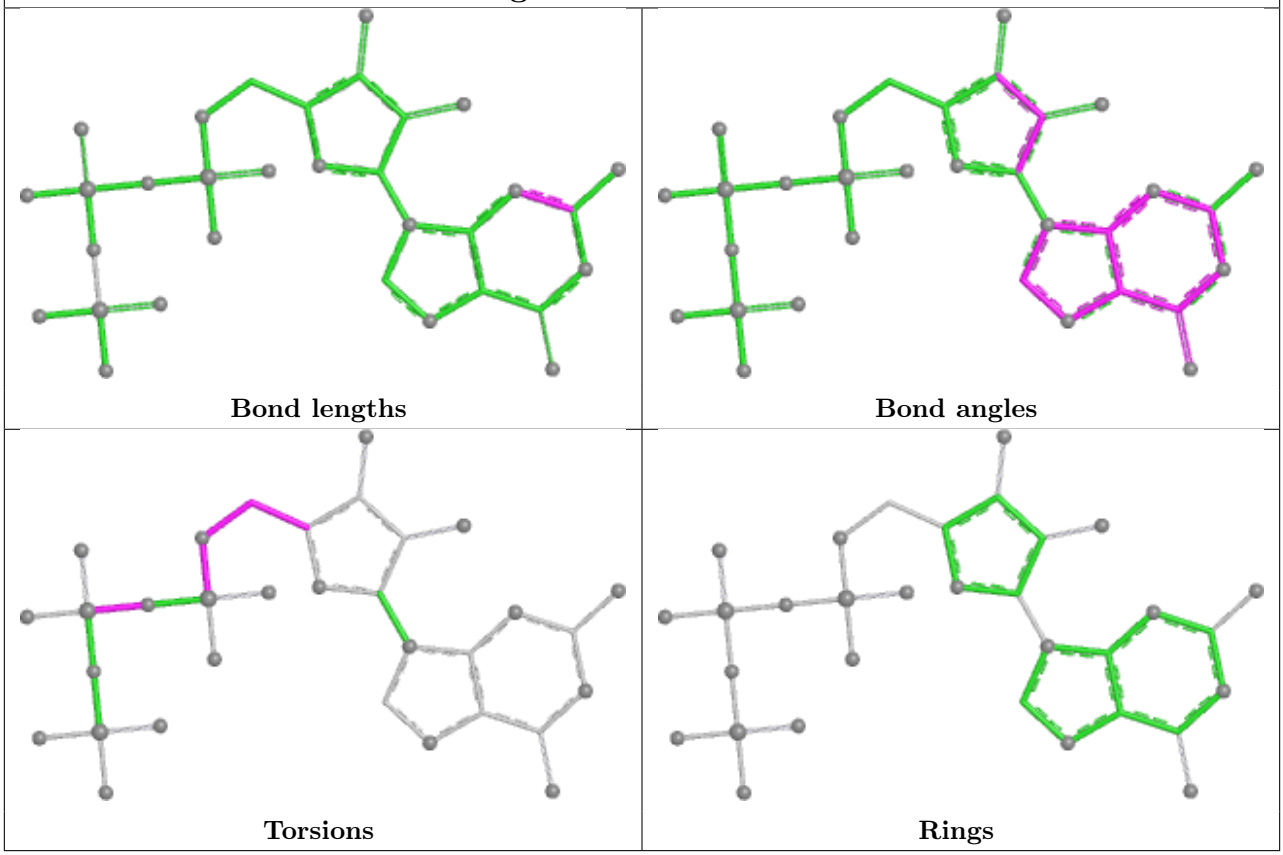


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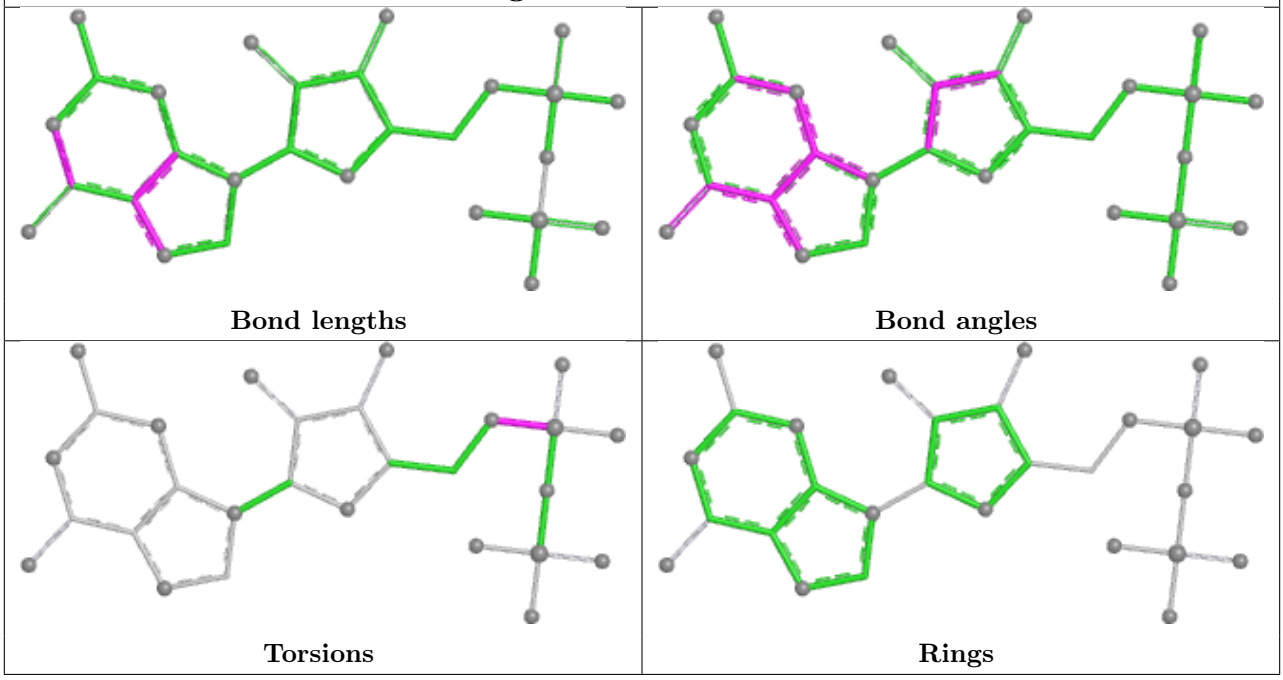


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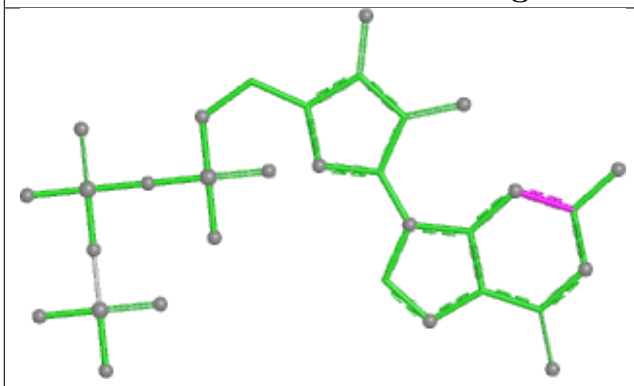
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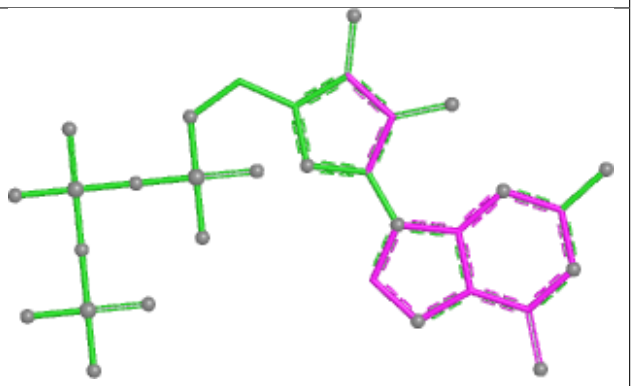
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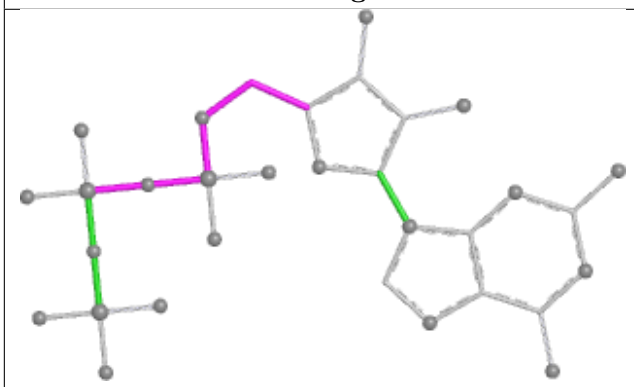
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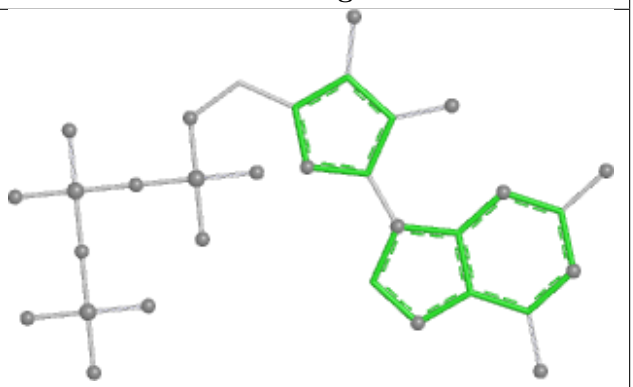
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Bond angles

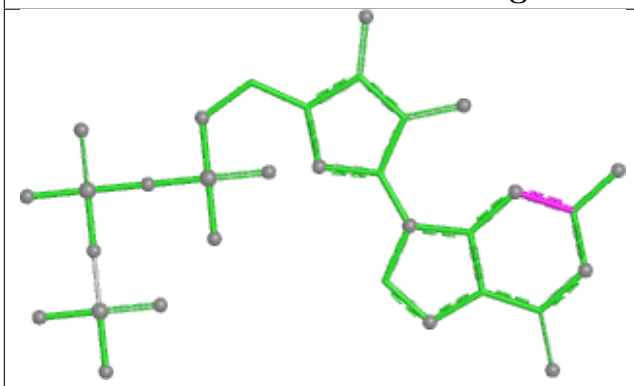


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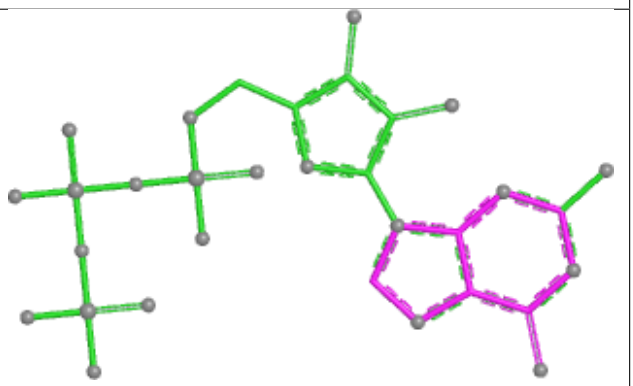


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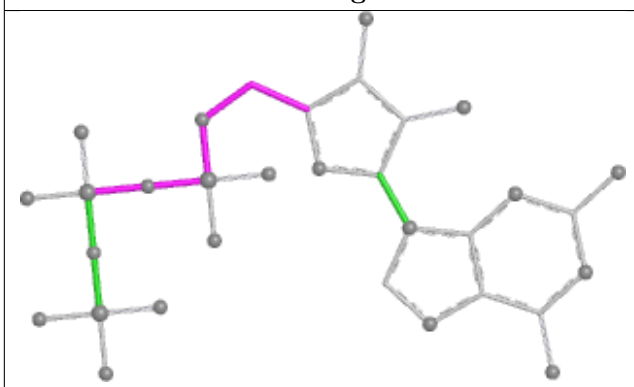
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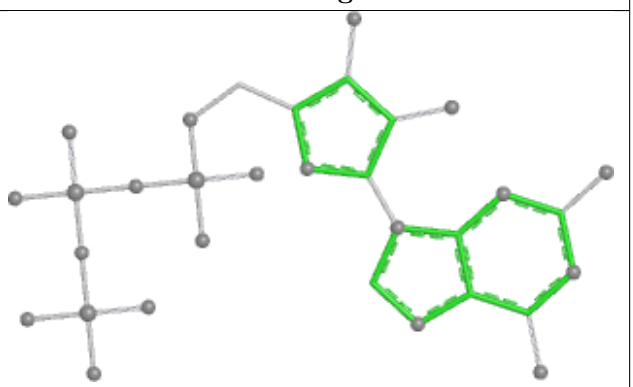
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Bond angles

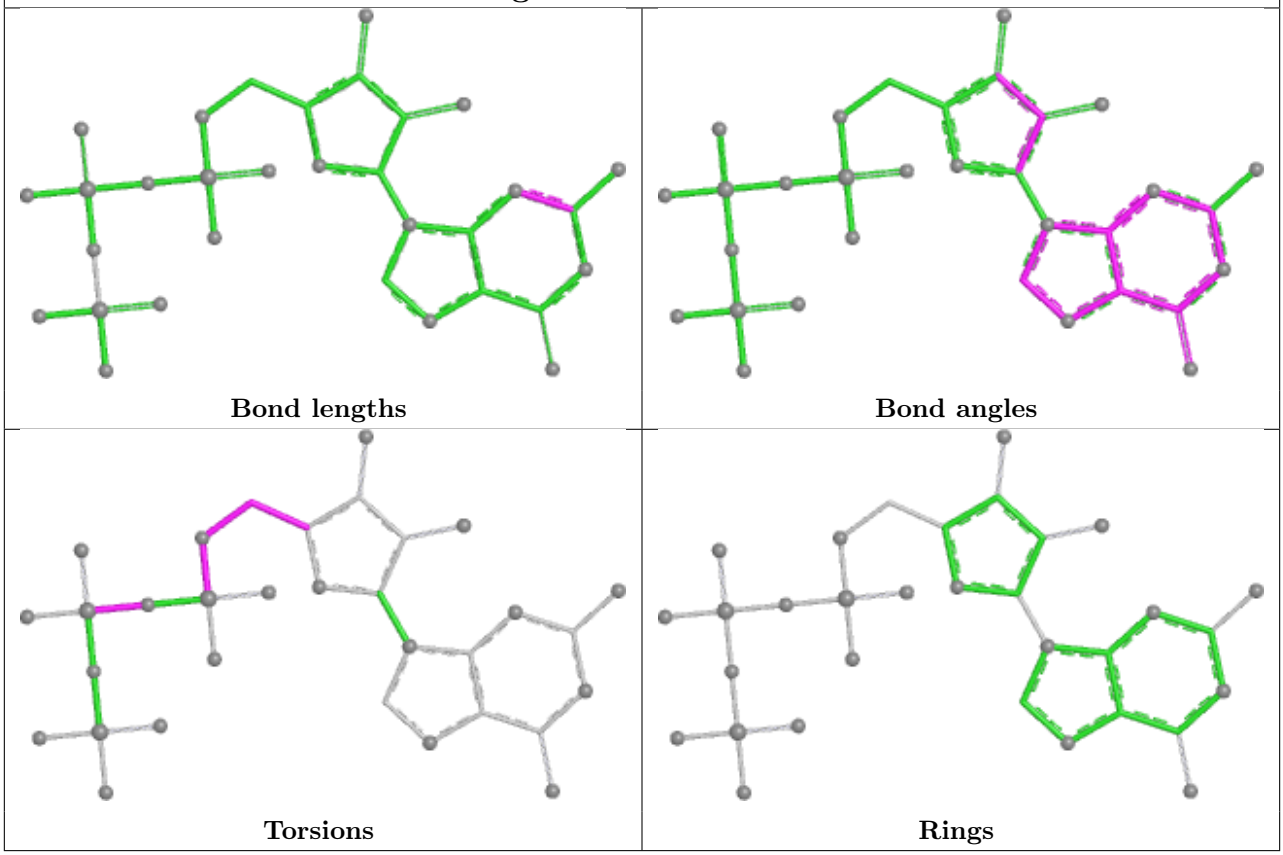


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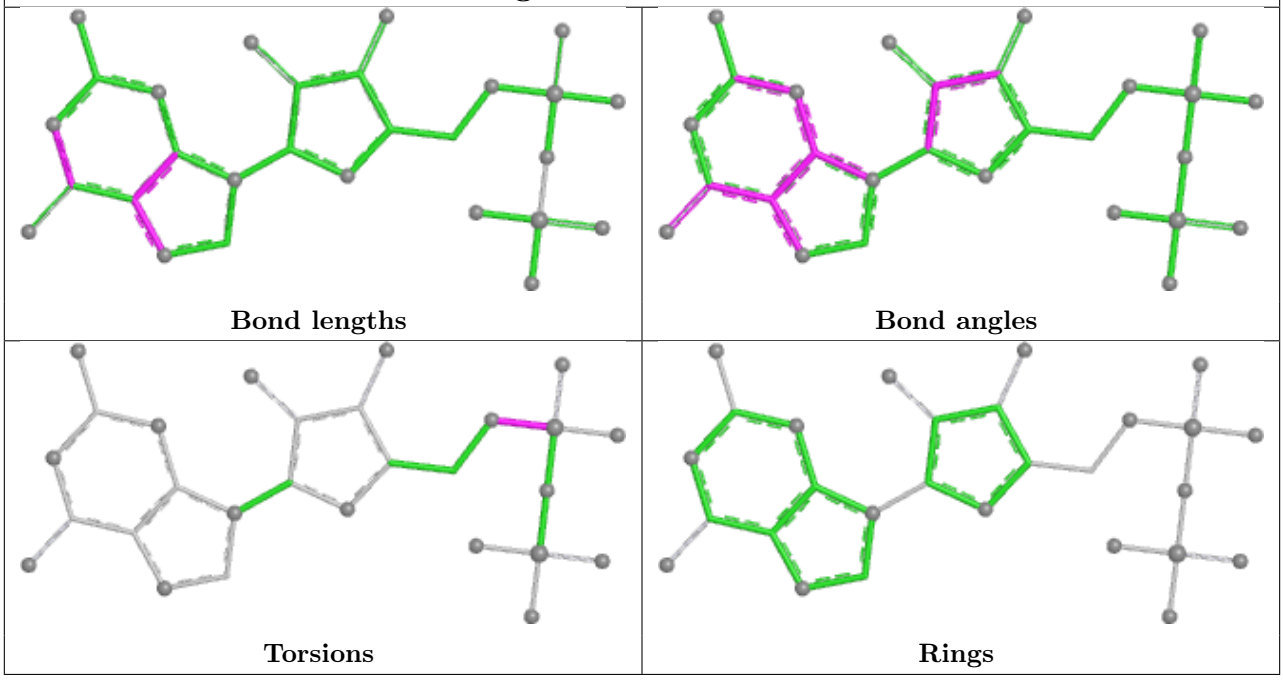


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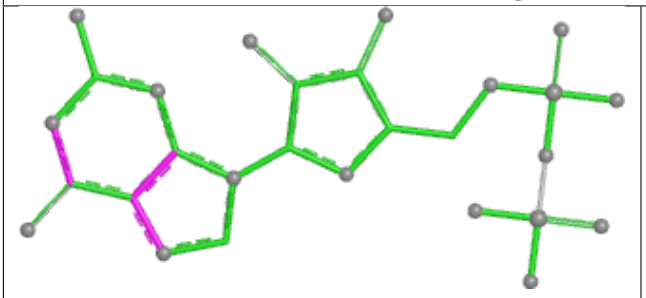
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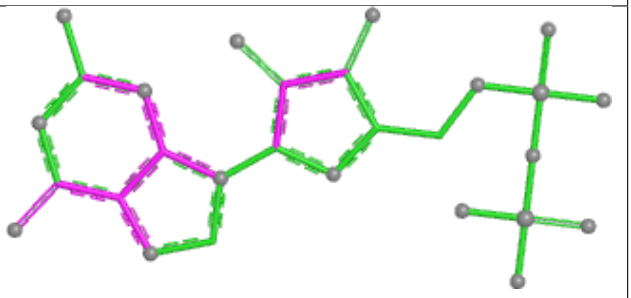
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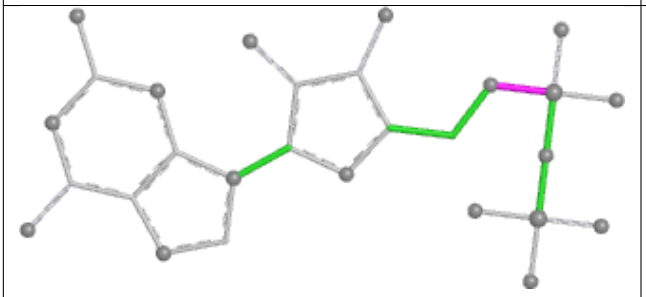
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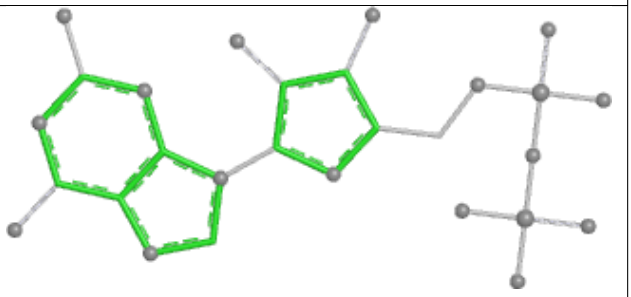
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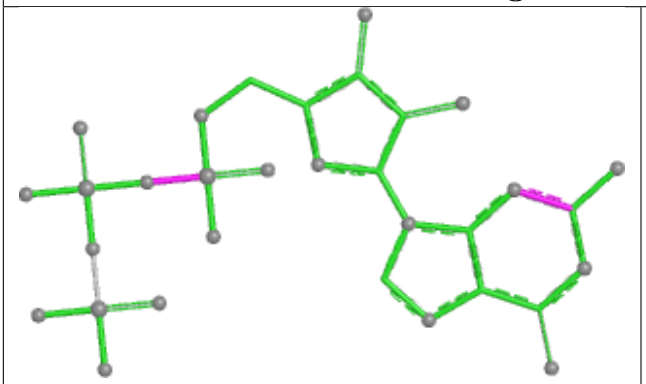


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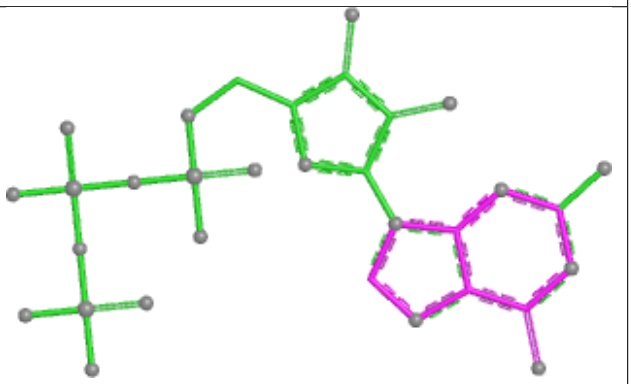


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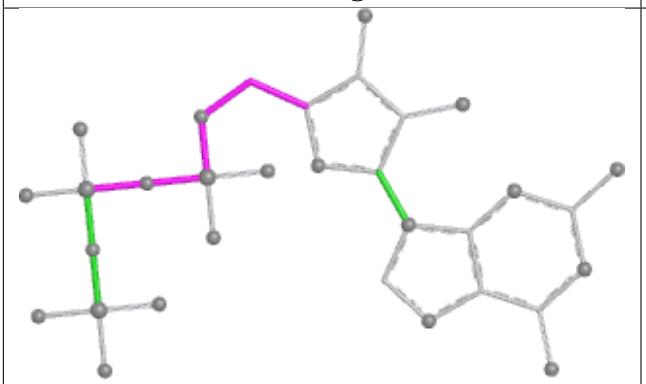
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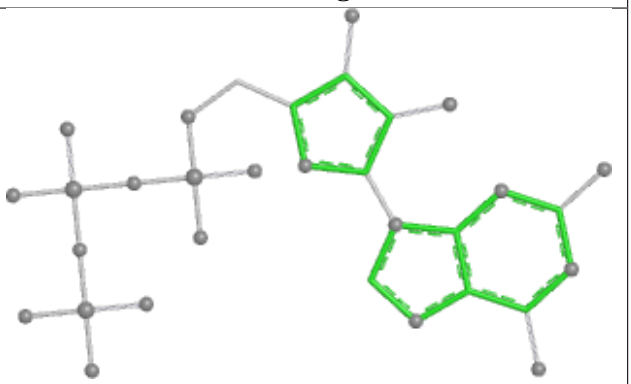
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Bond angles

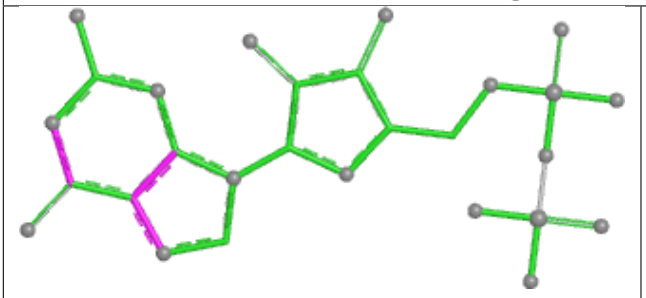


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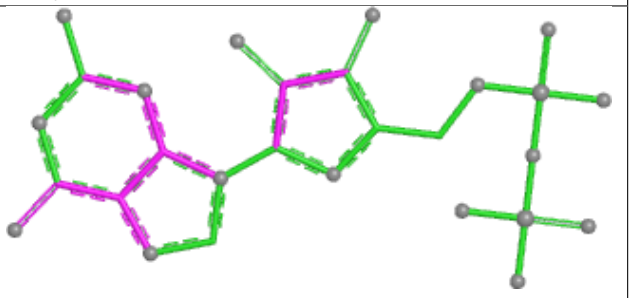


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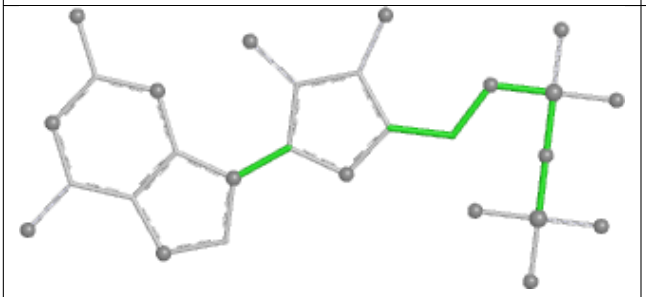
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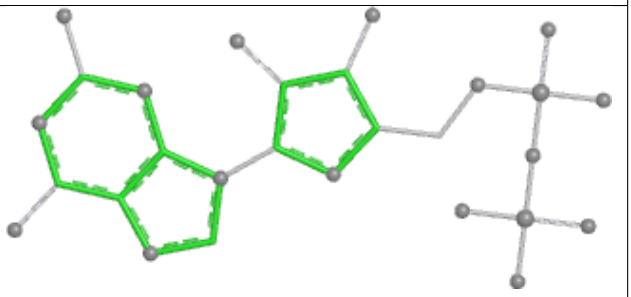
Bond lengths



Bond angles

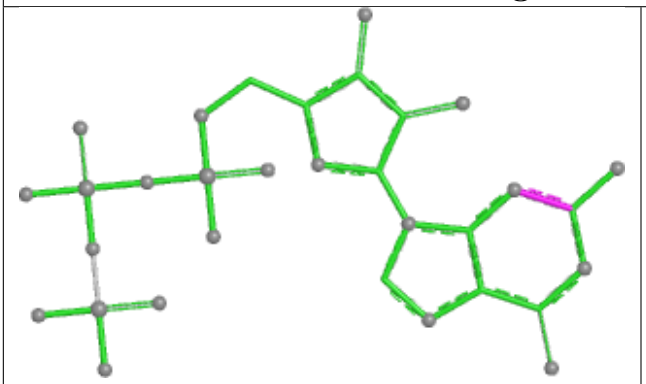


Torsions

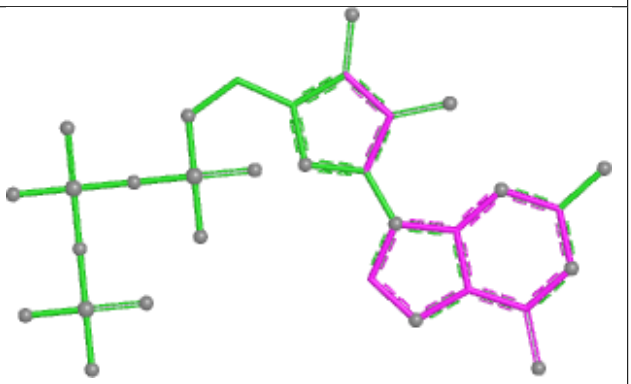


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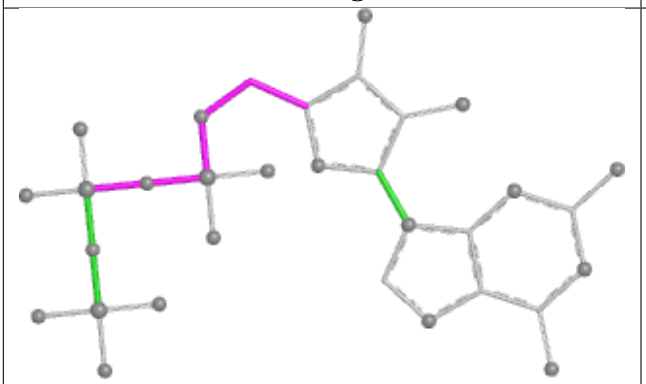
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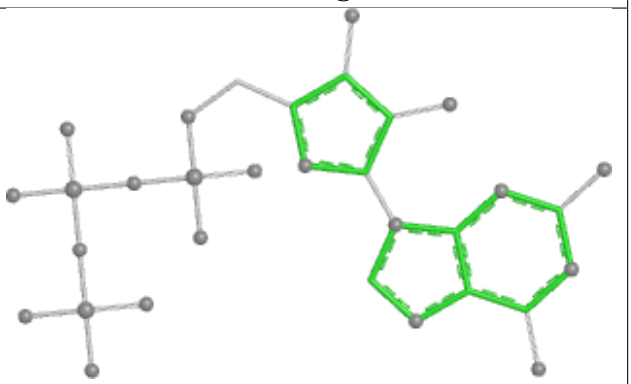
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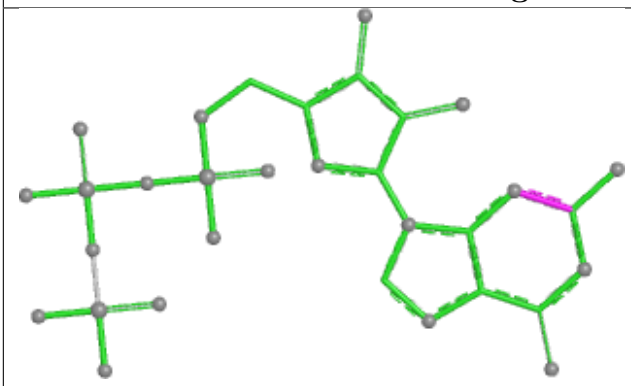


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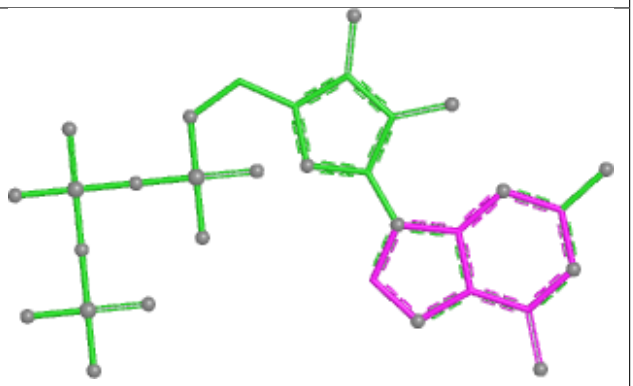


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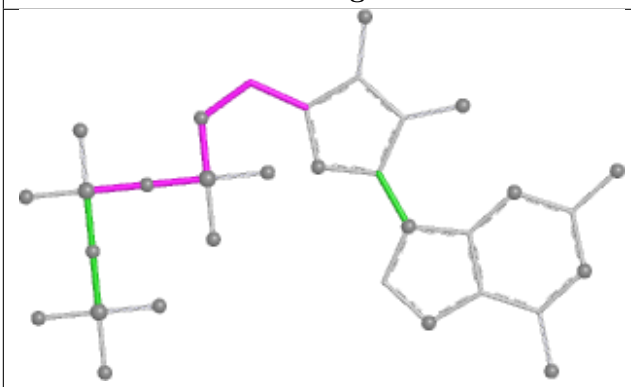
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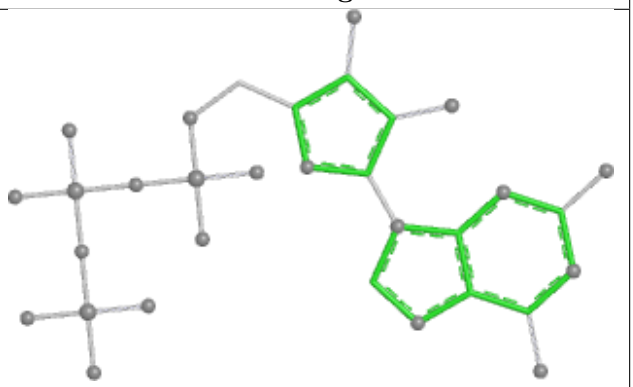
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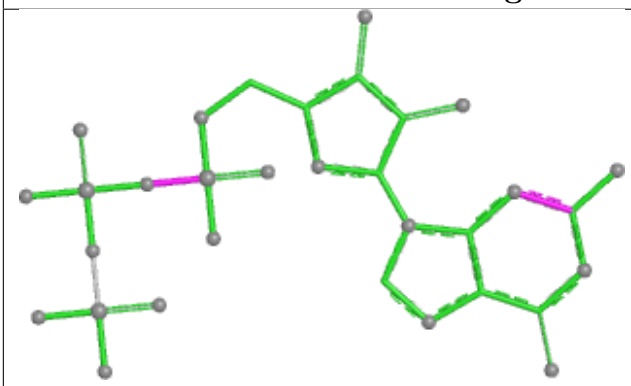


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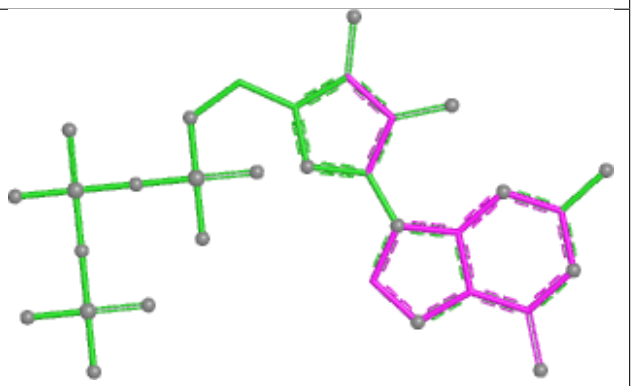


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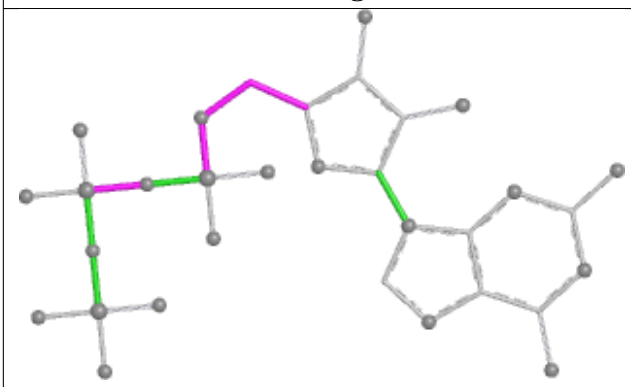
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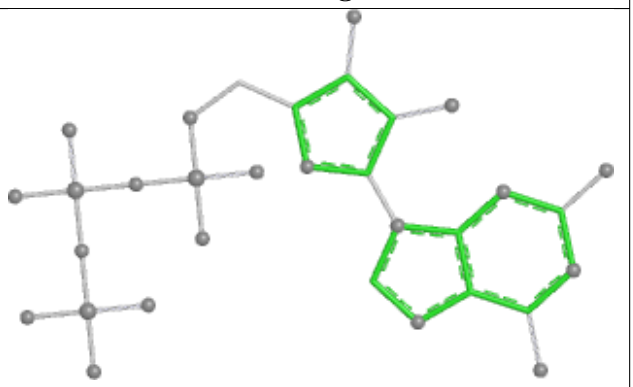
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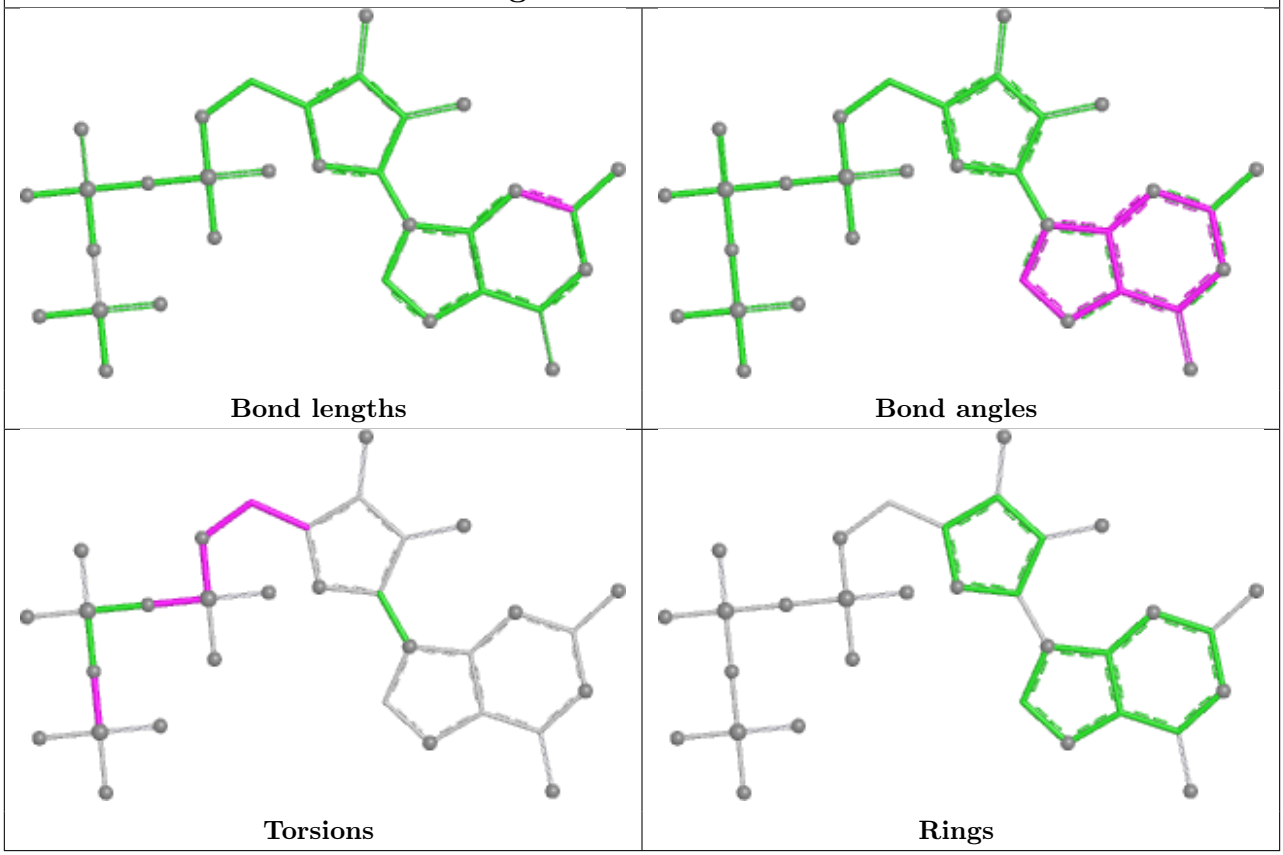


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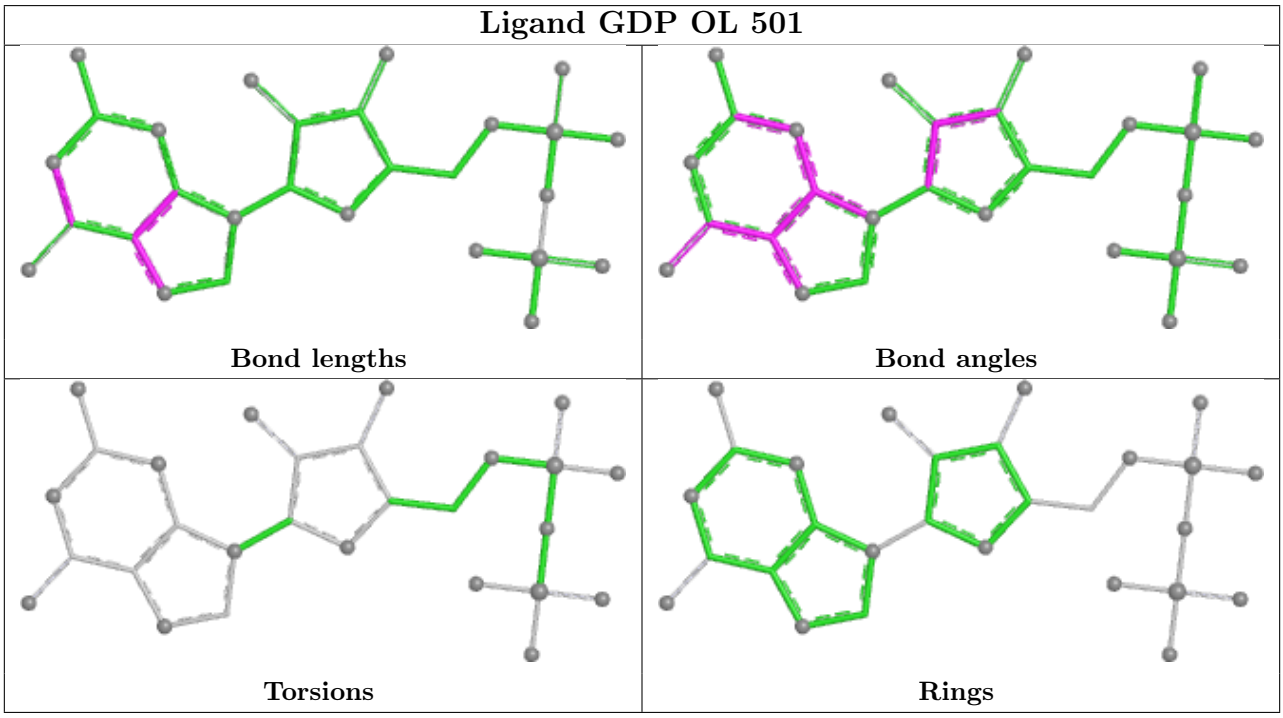


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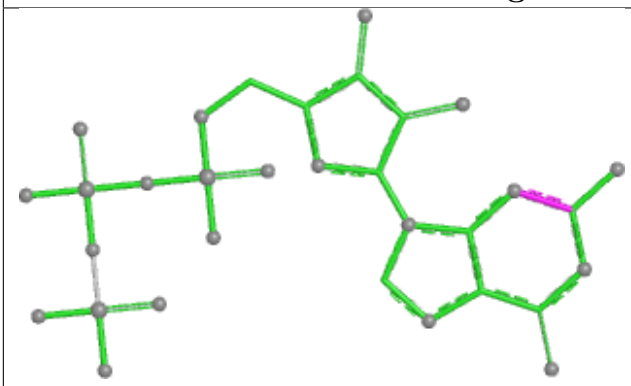
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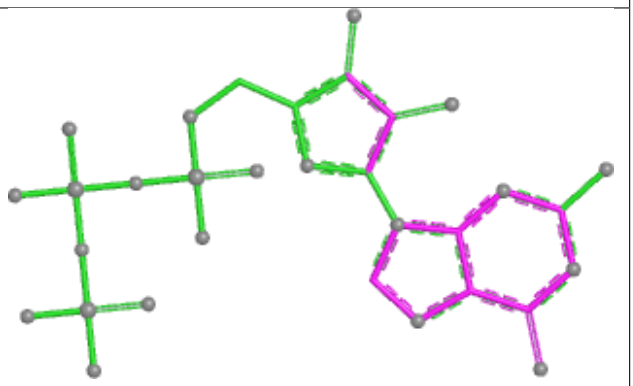
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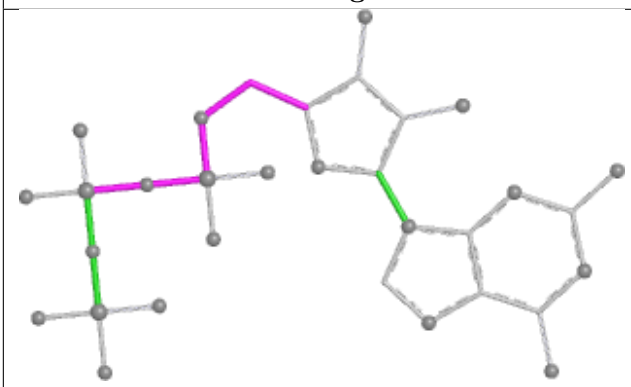
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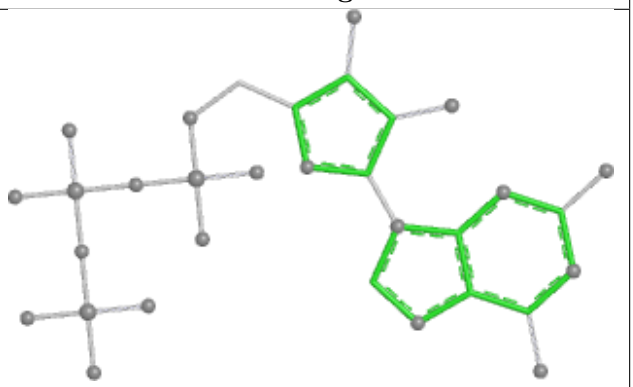
Bond lengths



Bond angles

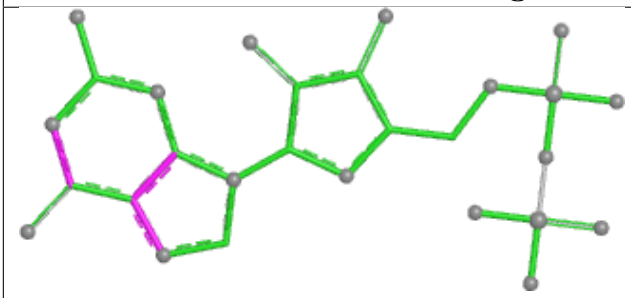


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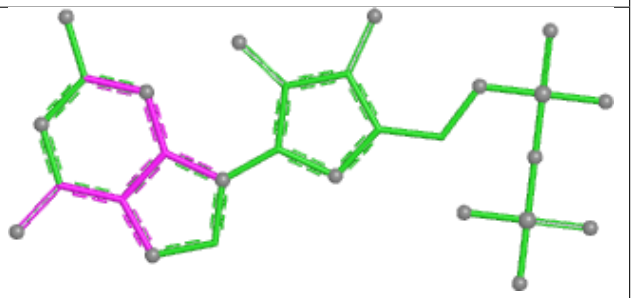


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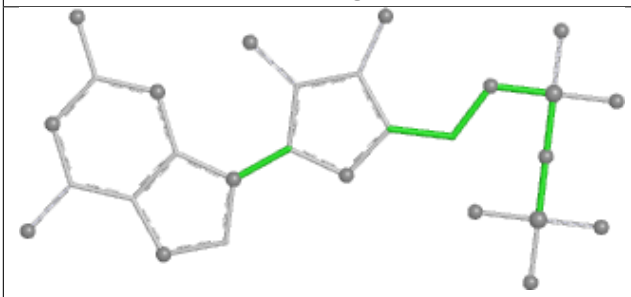
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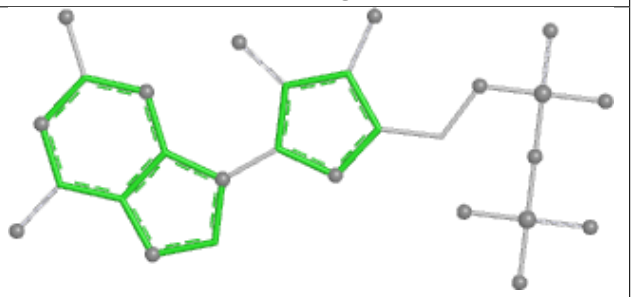
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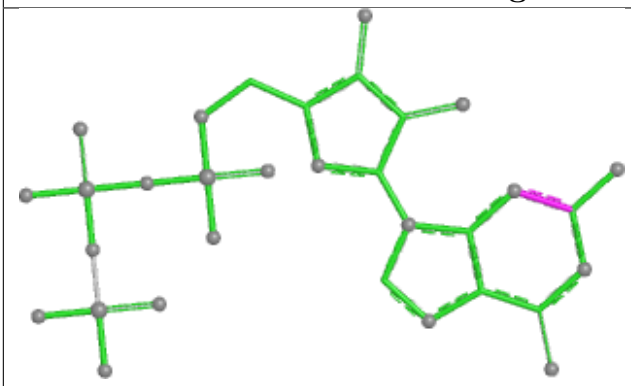


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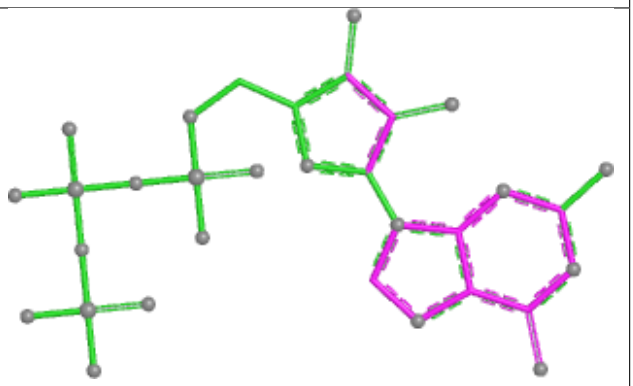


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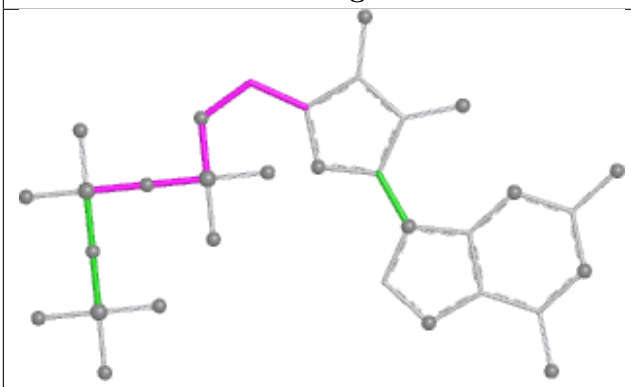
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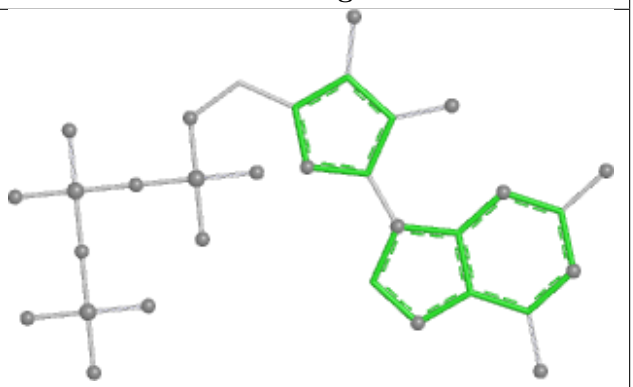
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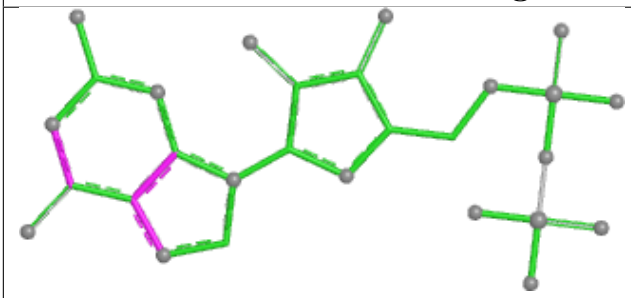


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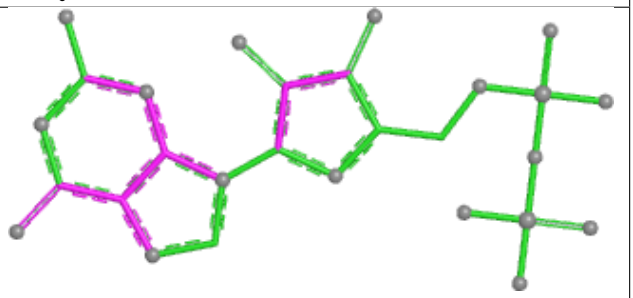


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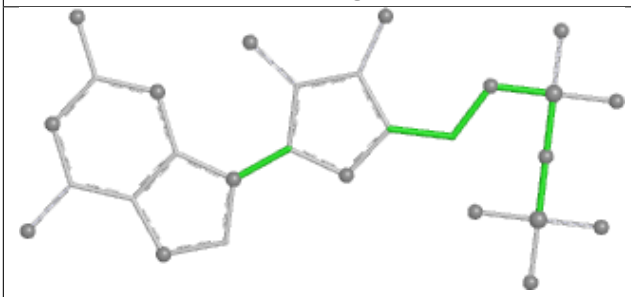
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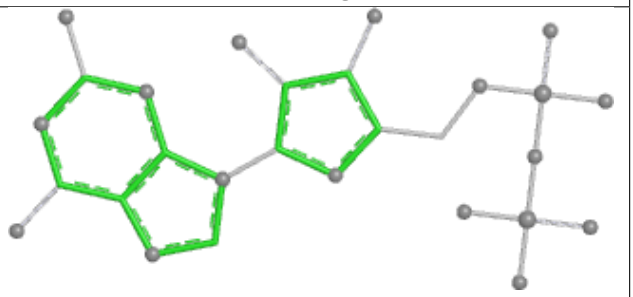
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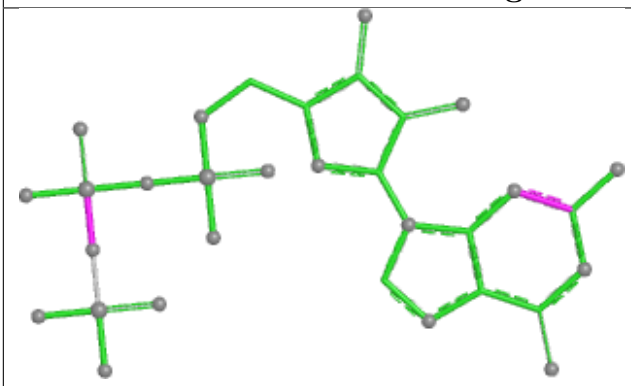


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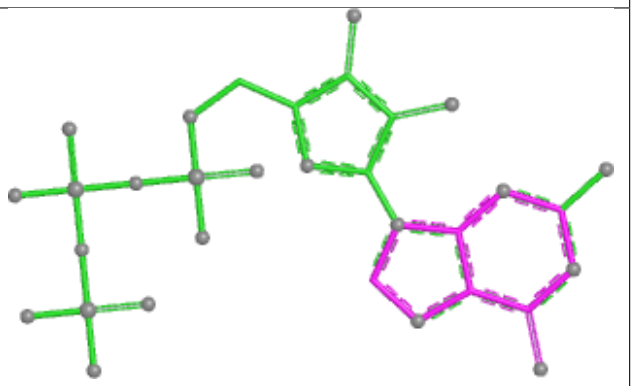


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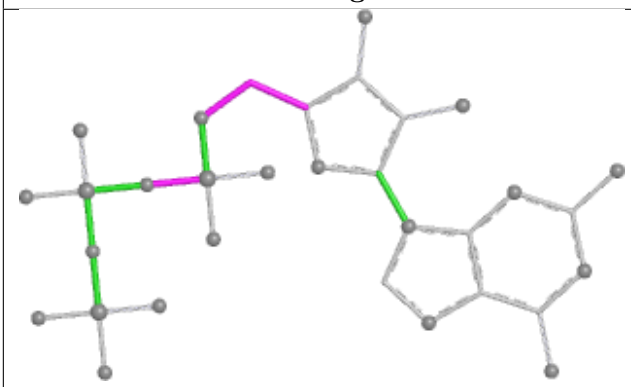
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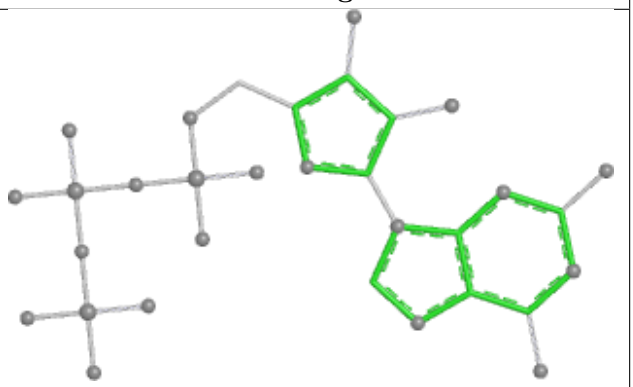
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Bond angles

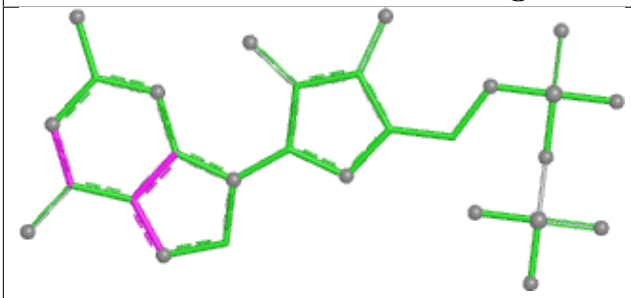


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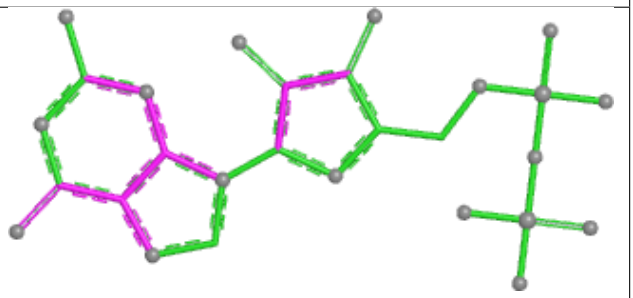


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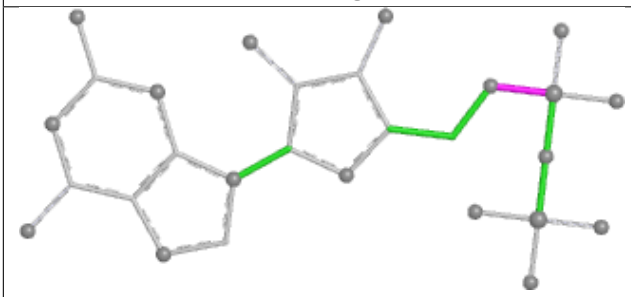
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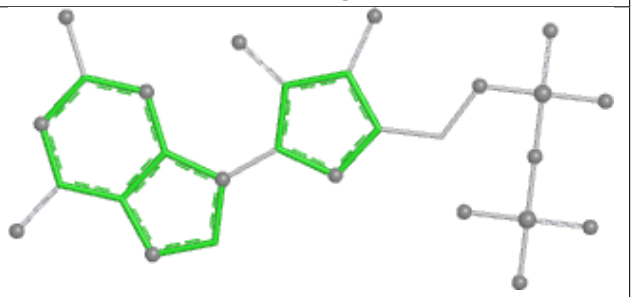
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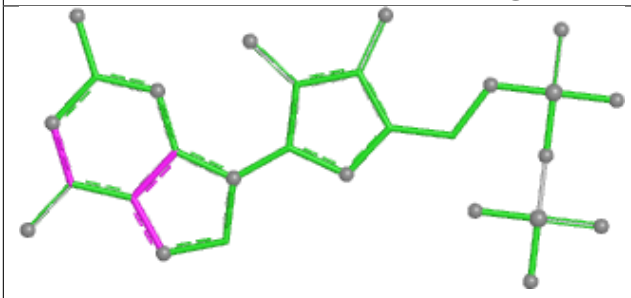


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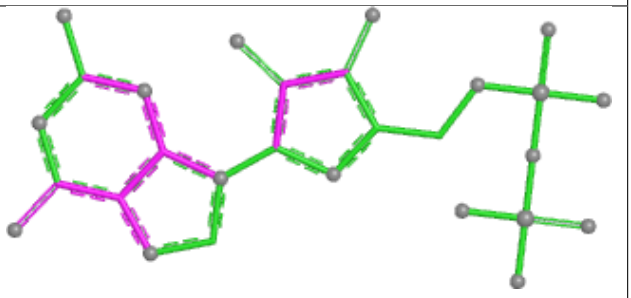


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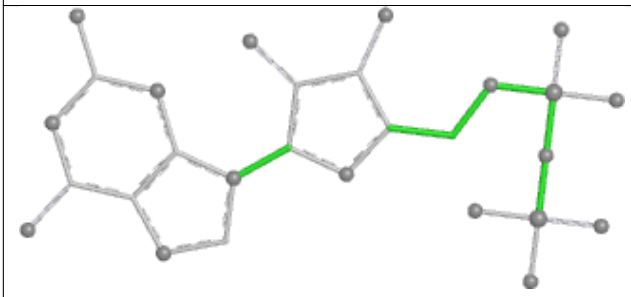
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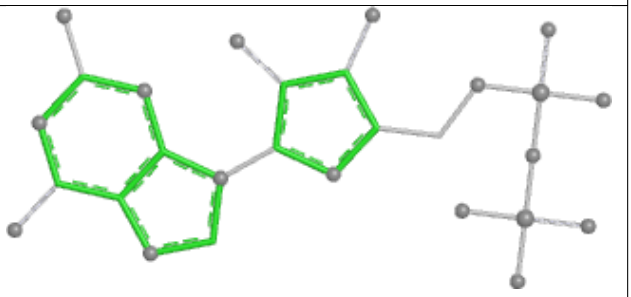
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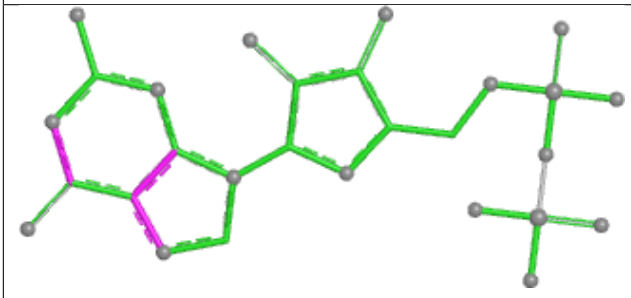


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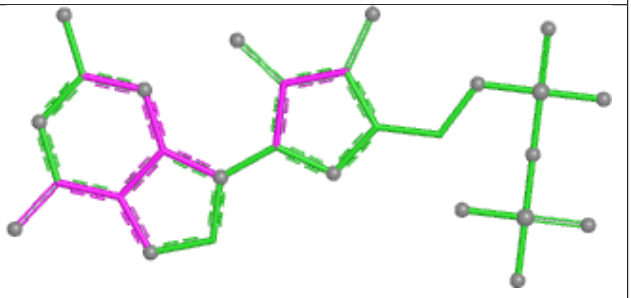


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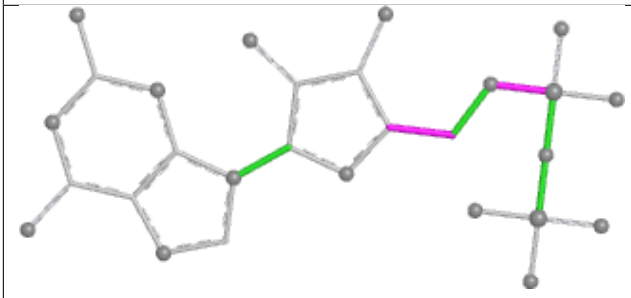
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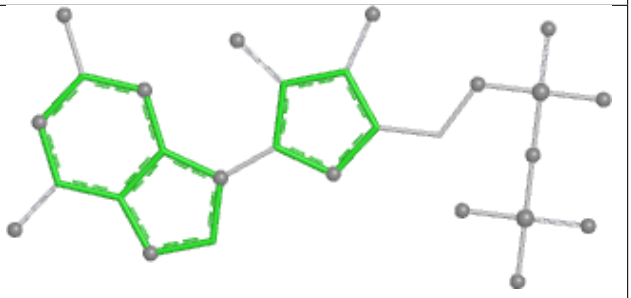
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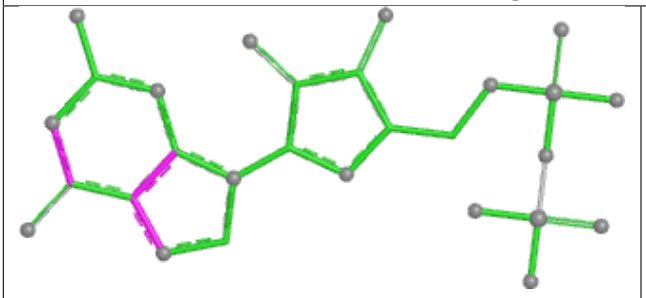


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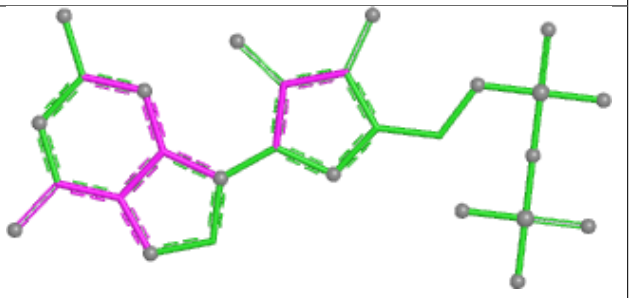


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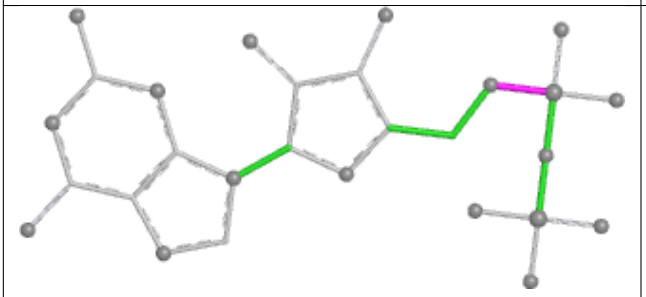
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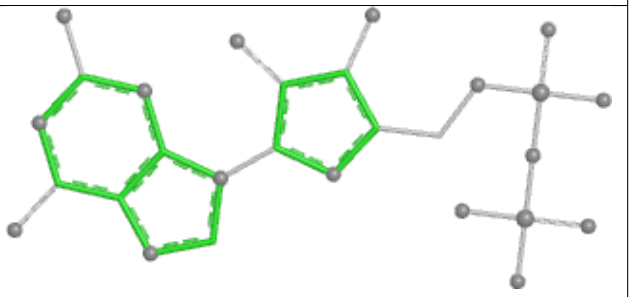
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Bond angles

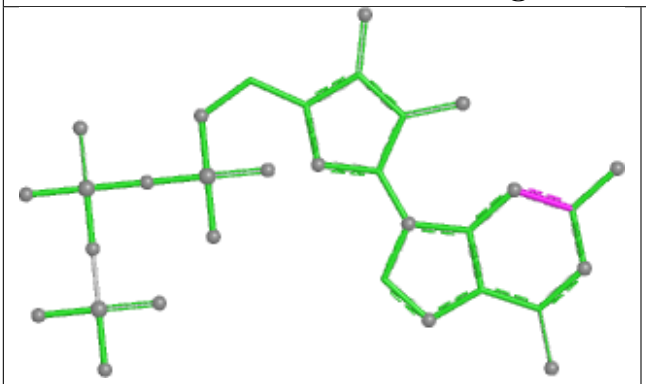


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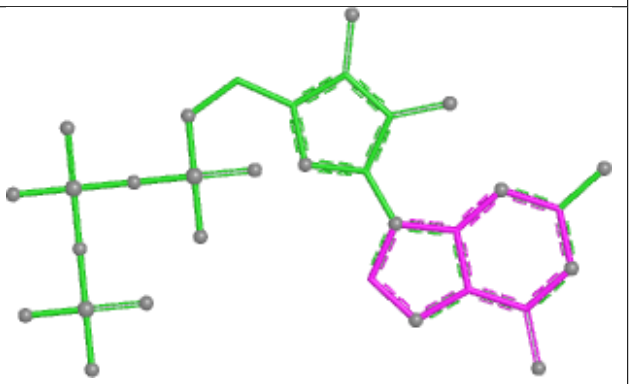


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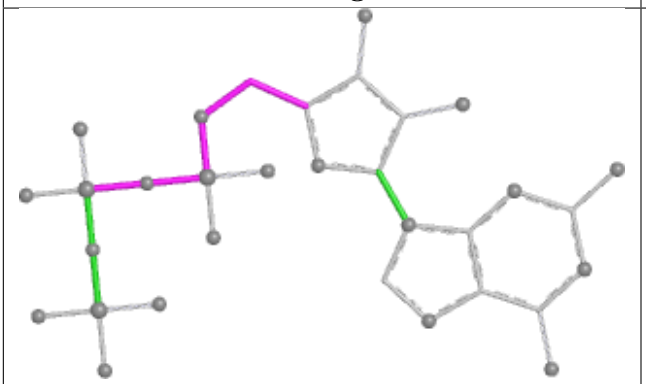
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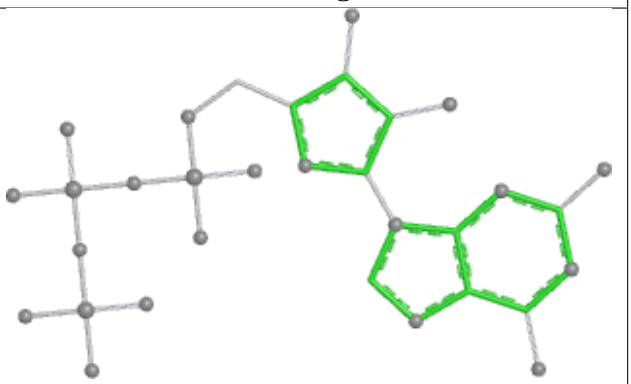
Bond lengths



Bond angles

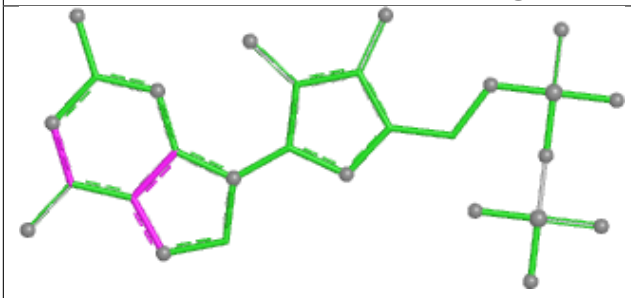


Torsions

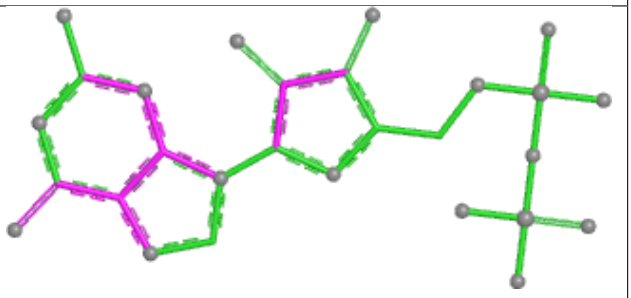


Rings

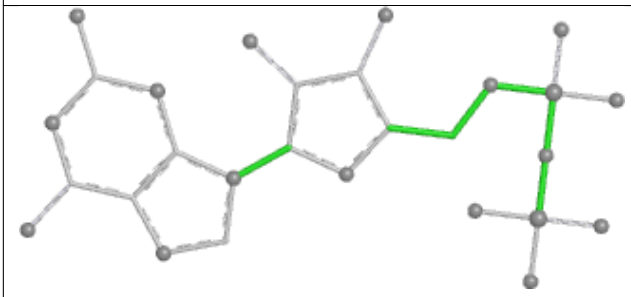
Ligand GDP NL 501



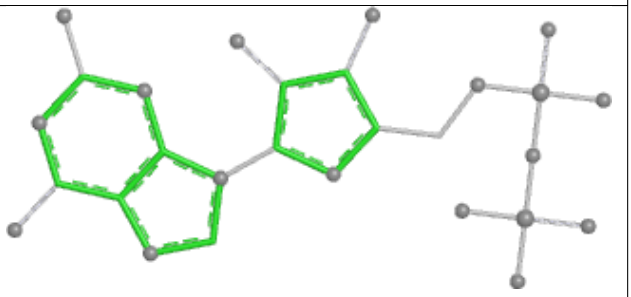
Bond lengths



Bond angles

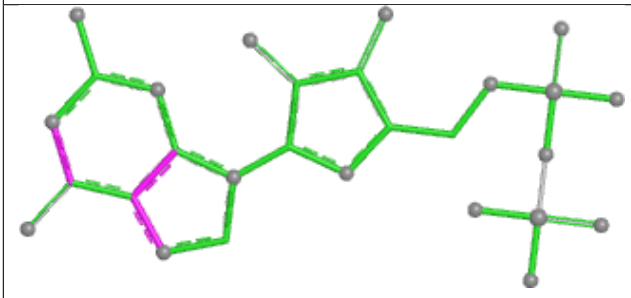


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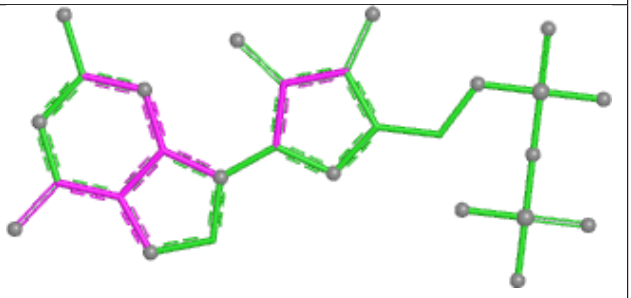


Rings

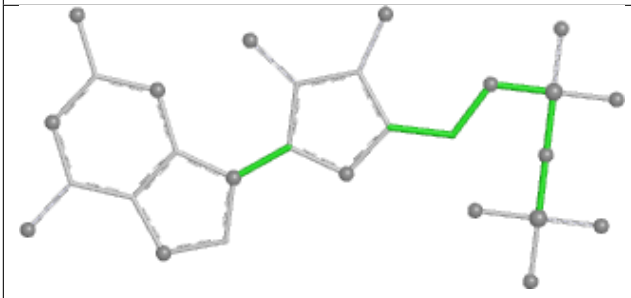
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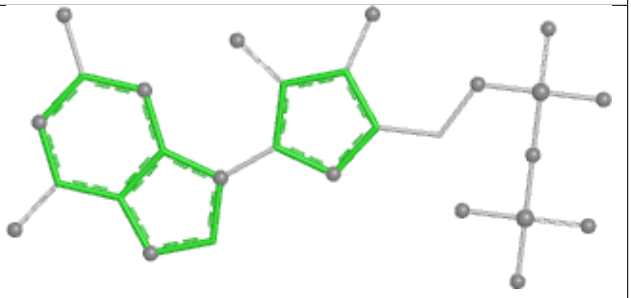
Bond lengths



Bond angles

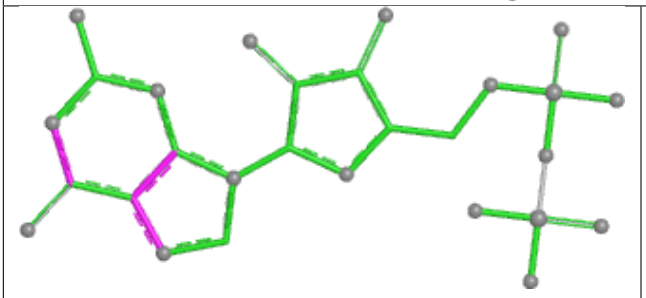


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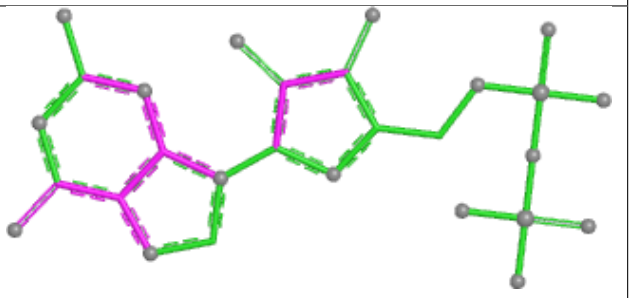


Rings

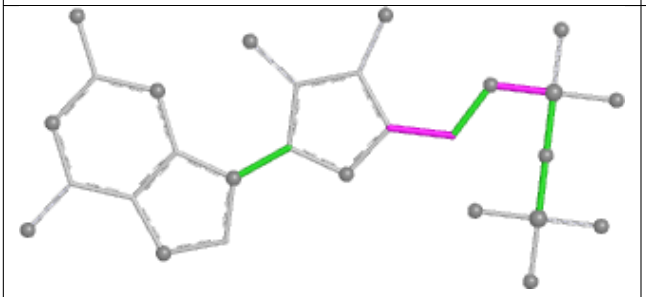
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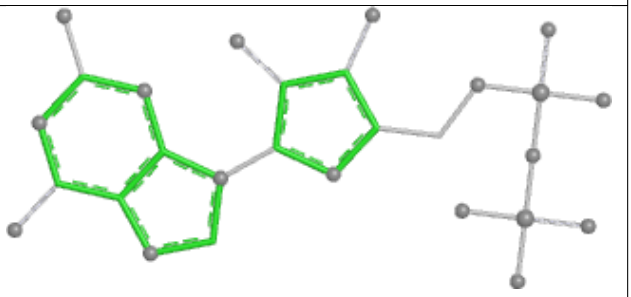
Bond lengths



Bond angles

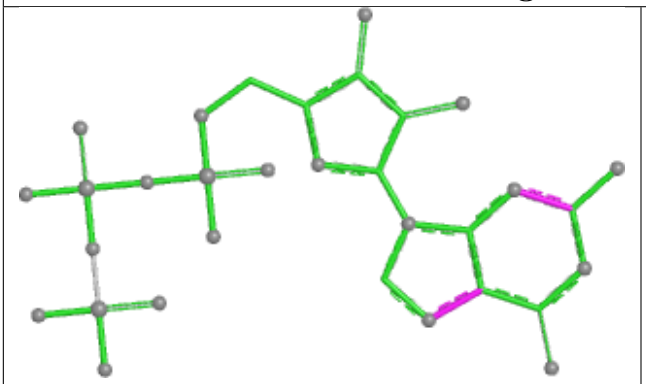


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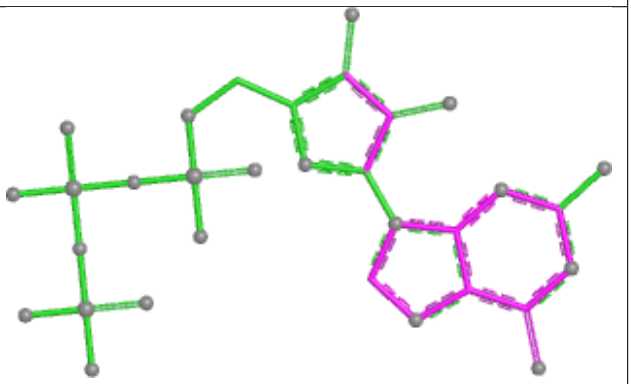


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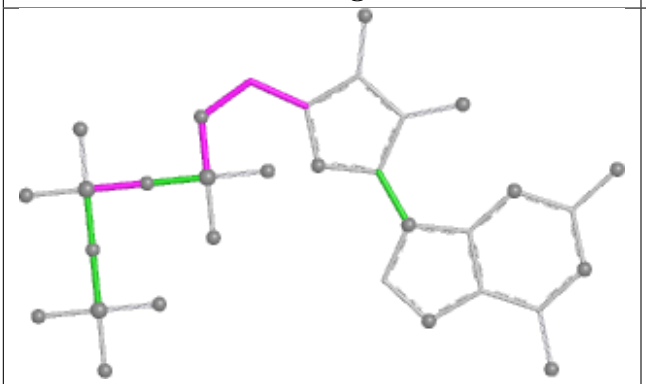
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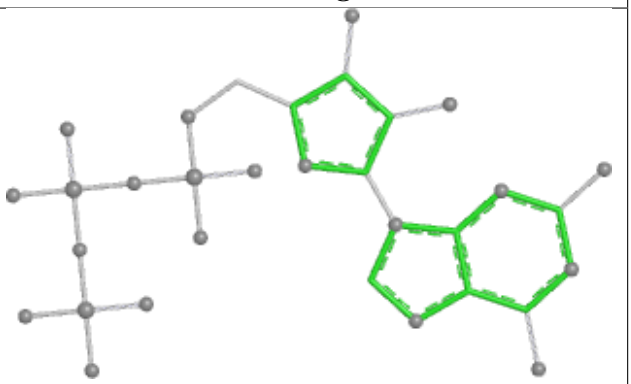
Bond lengths



Bond angles

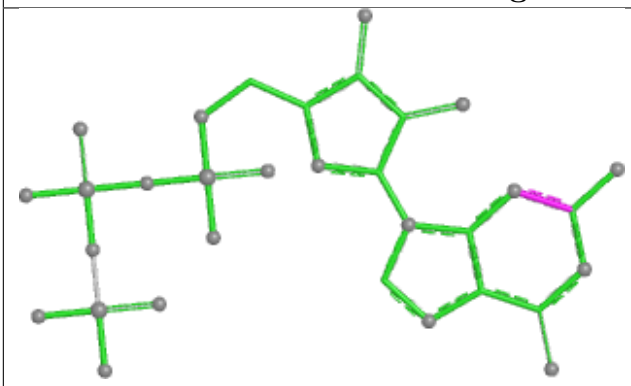


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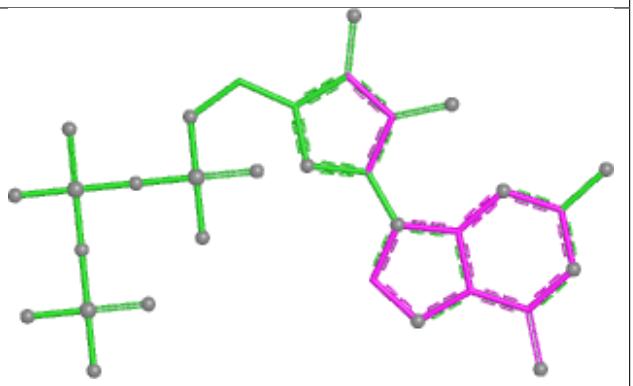


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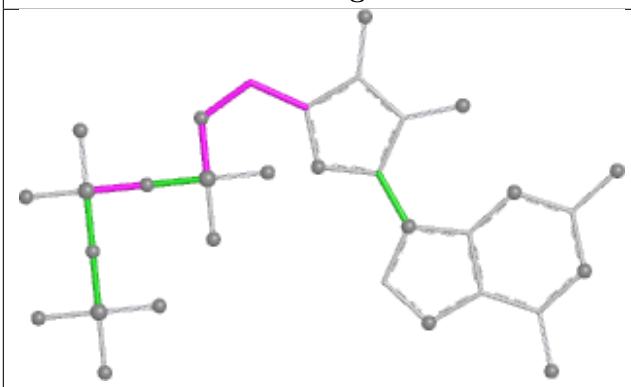
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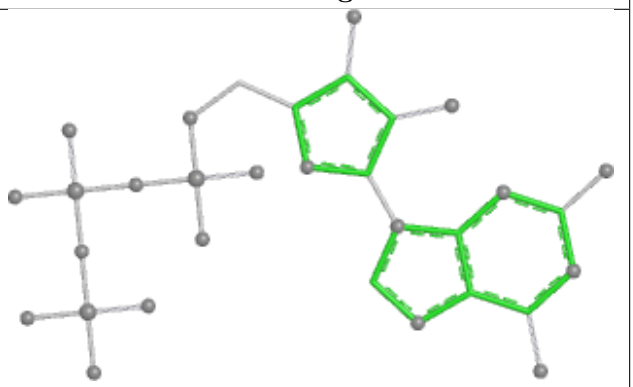
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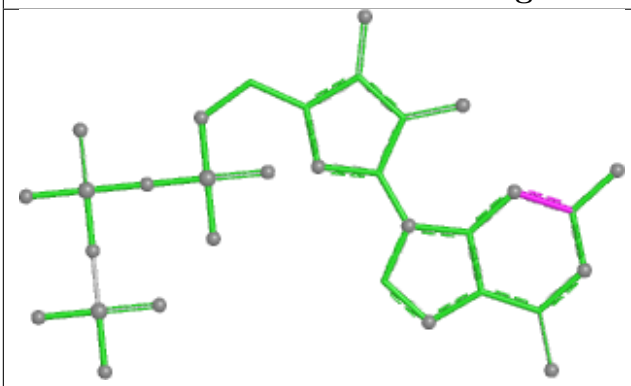


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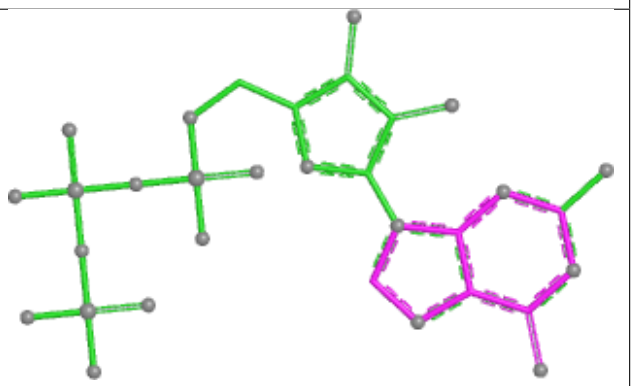


Rings

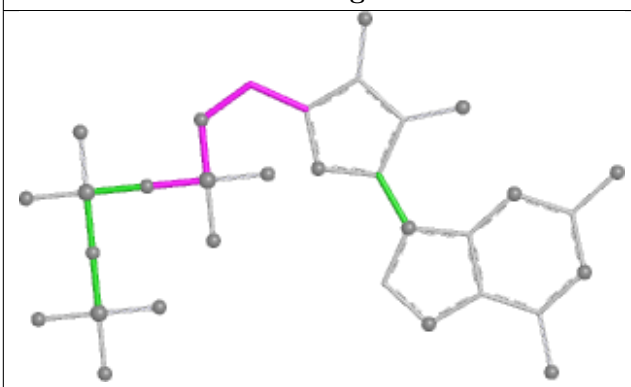
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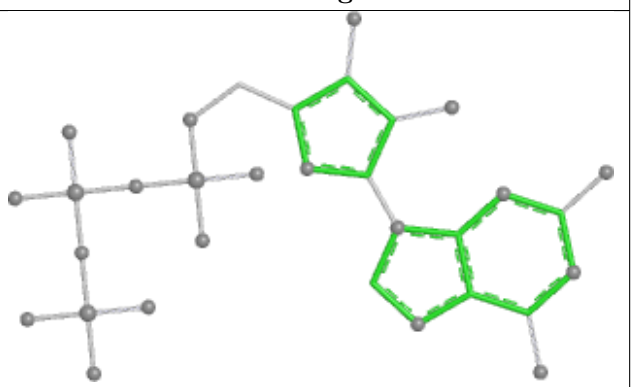
Bond lengths



Bond angles

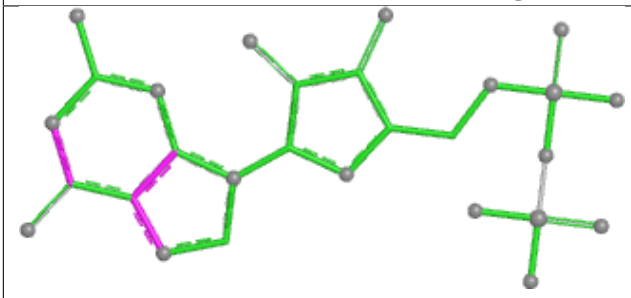


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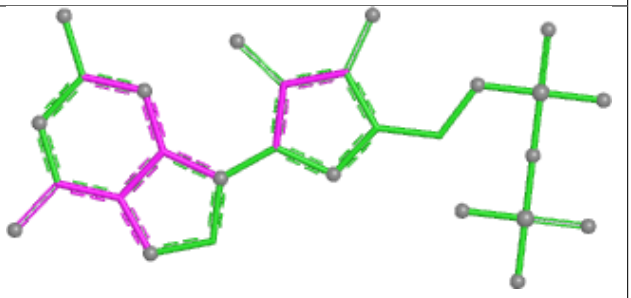


Rings

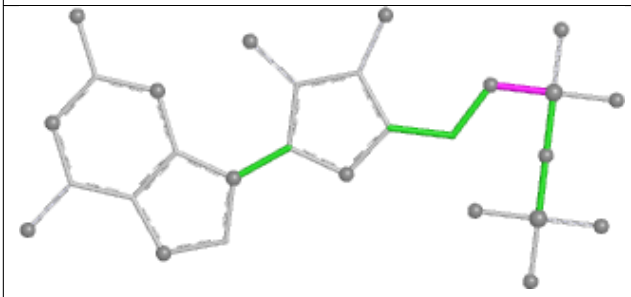
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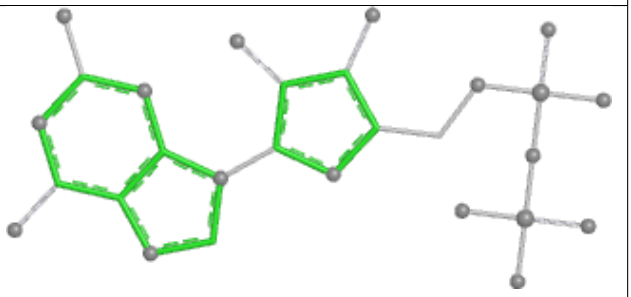
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Bond angles

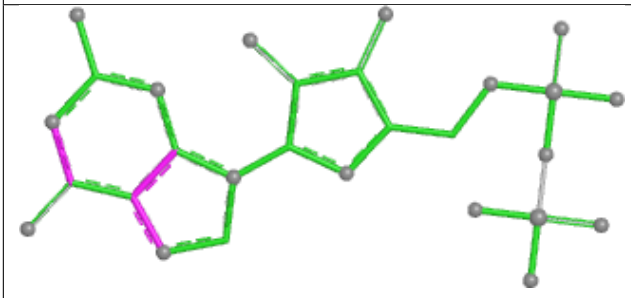


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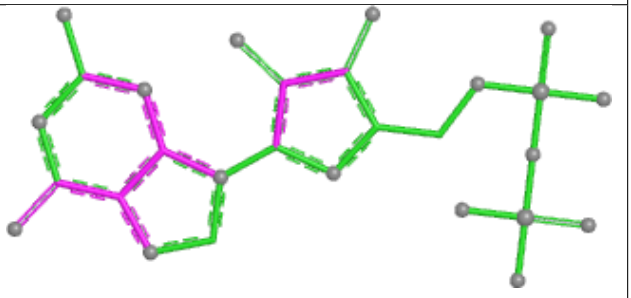


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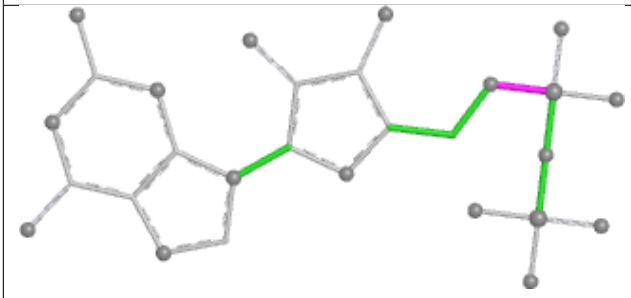
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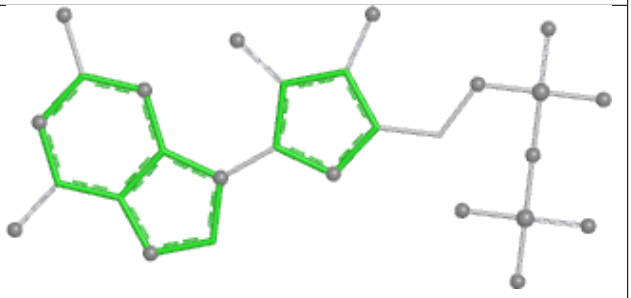
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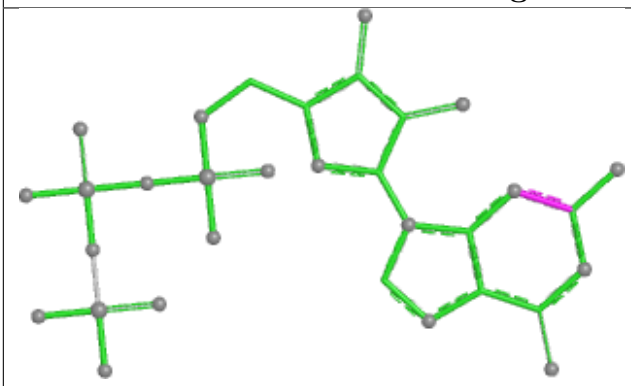


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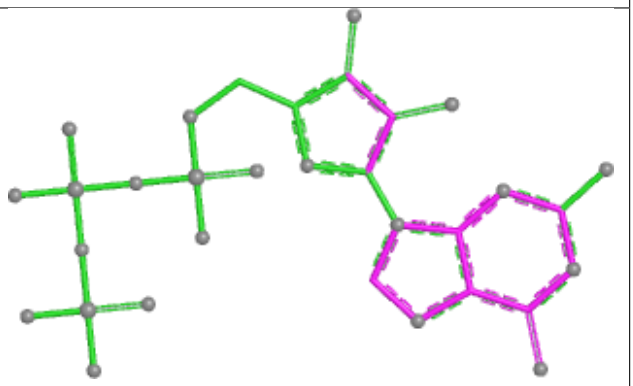


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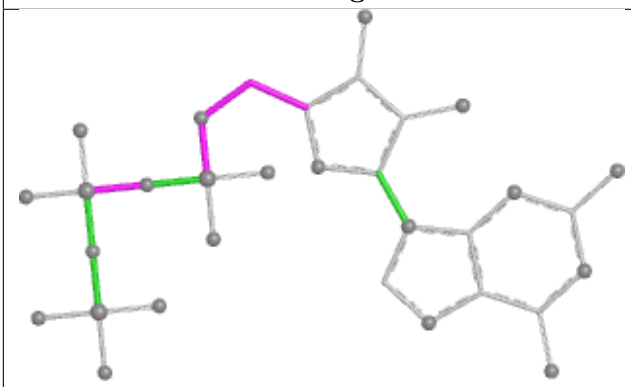
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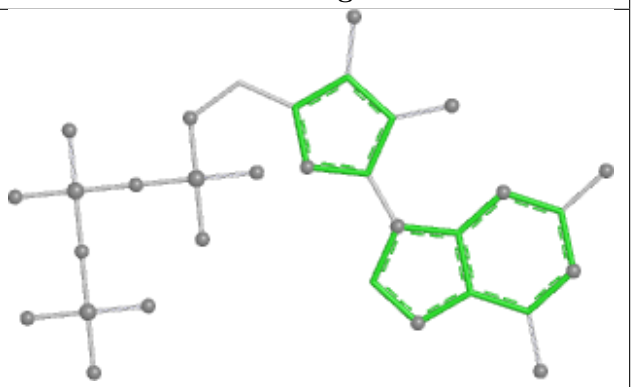
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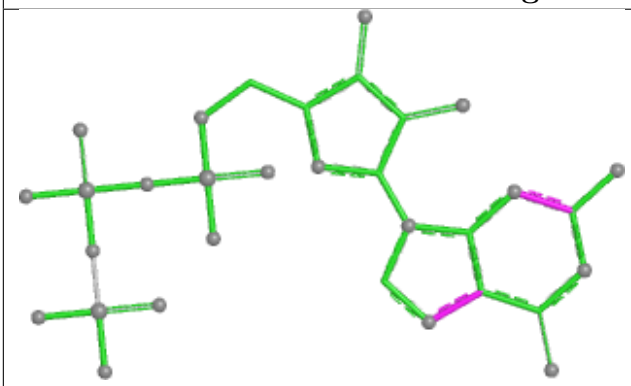


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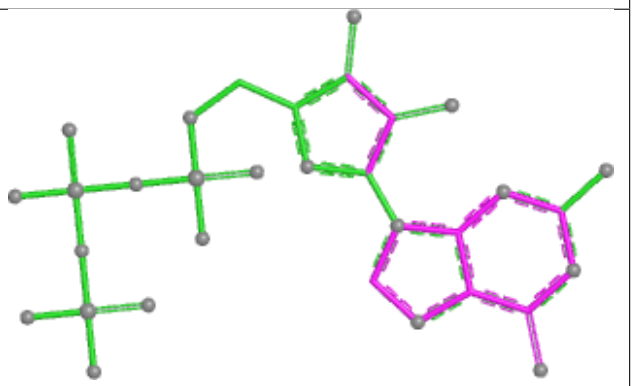


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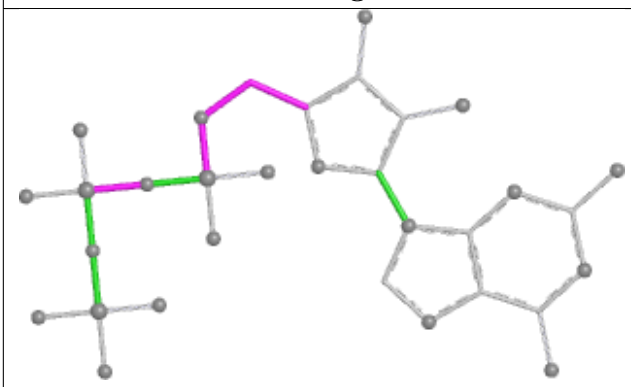
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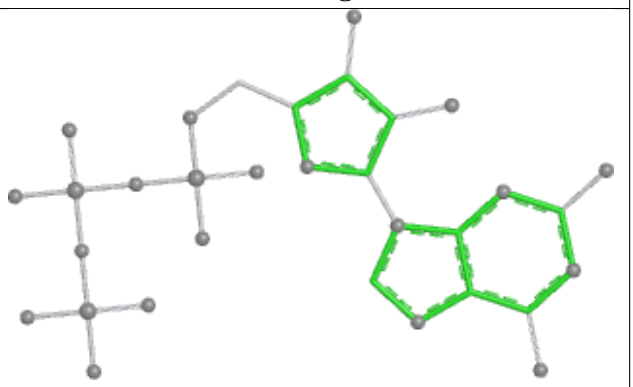
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Bond angles

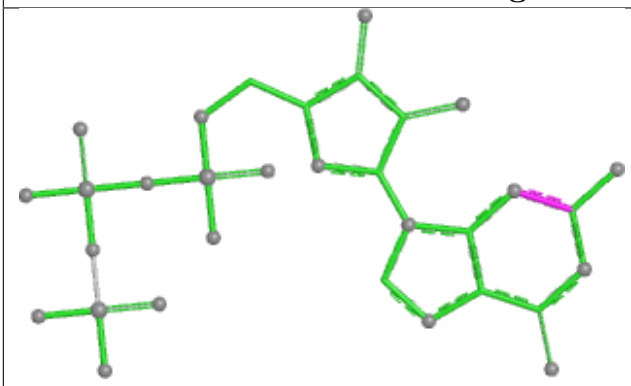


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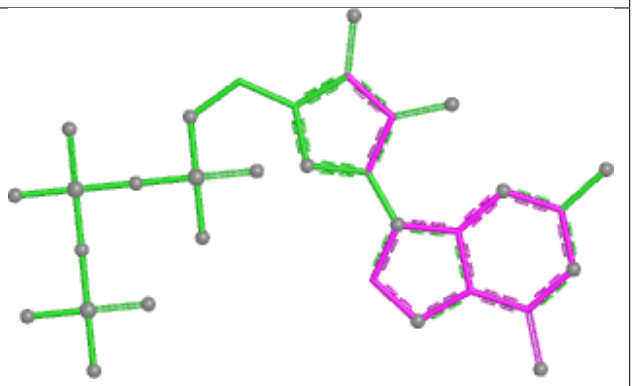


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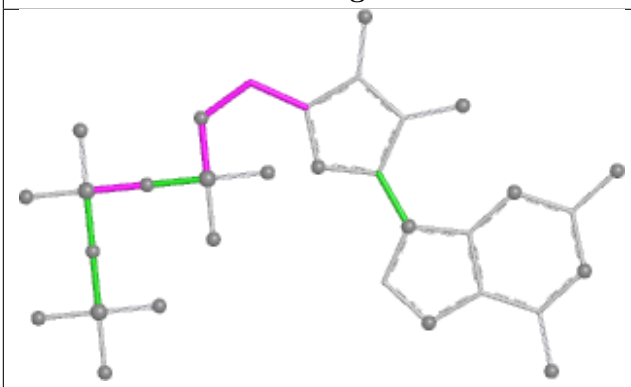
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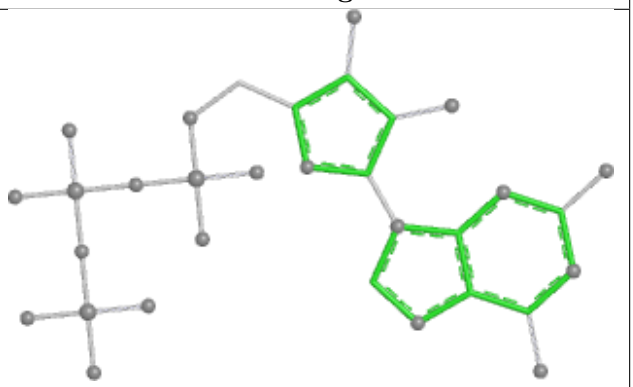
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Bond angles

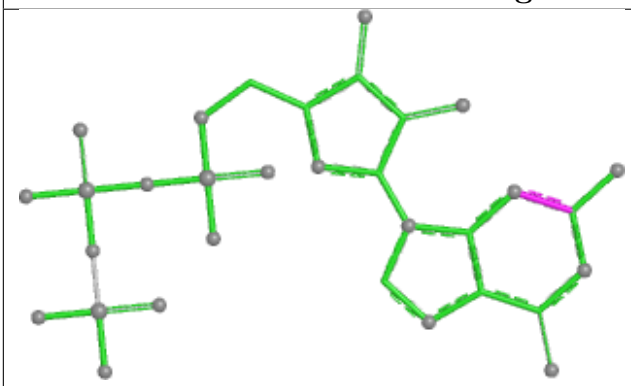


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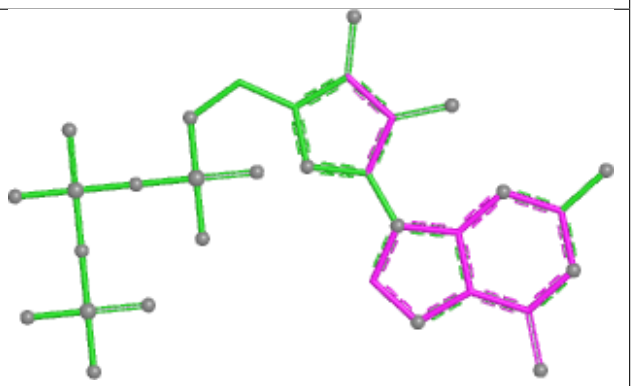


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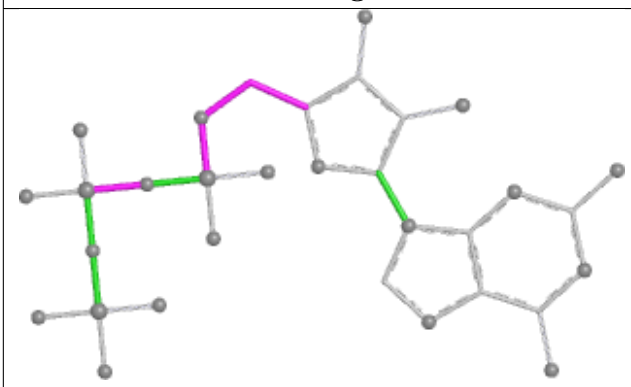
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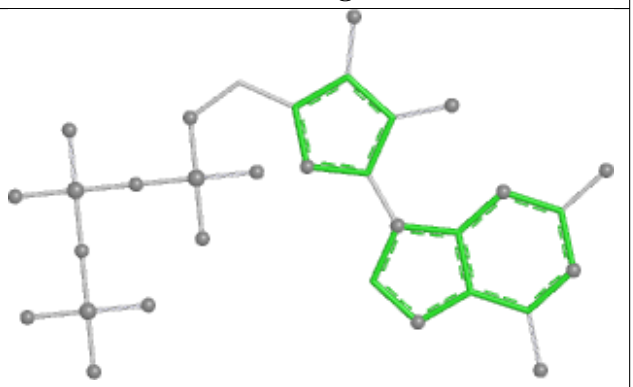
Bond lengths



Bond angles

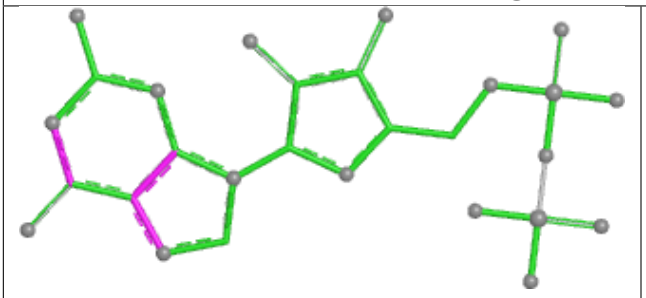


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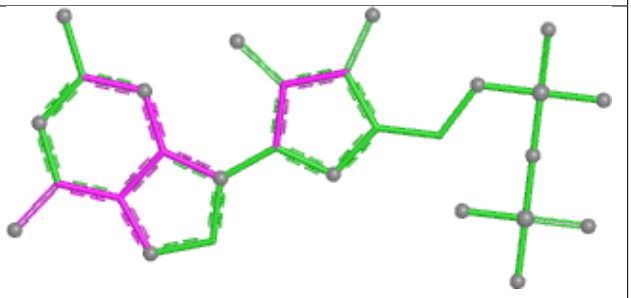


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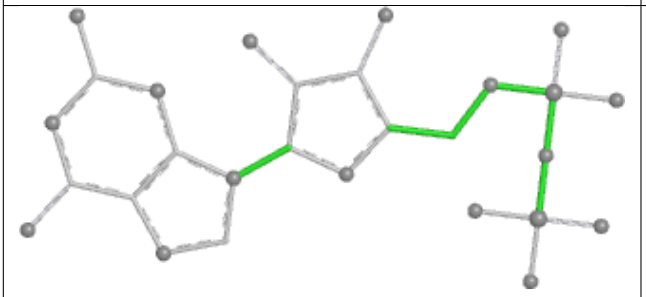
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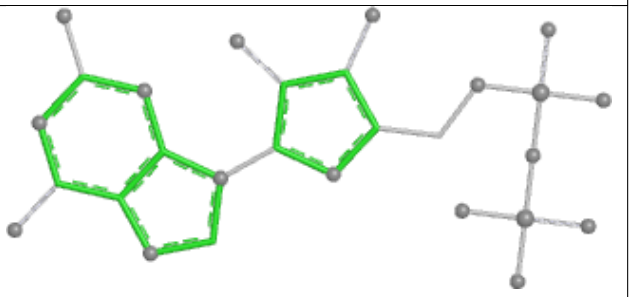
Bond lengths



Bond angles

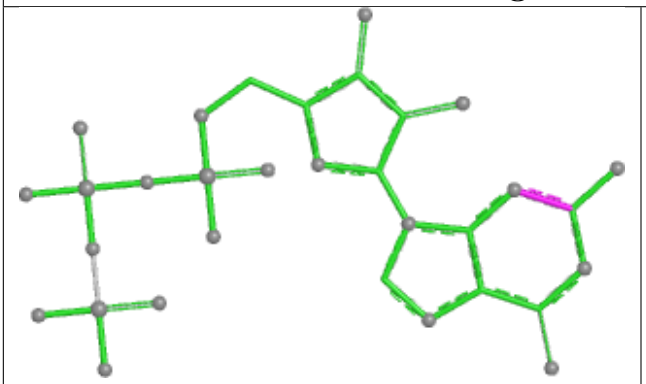


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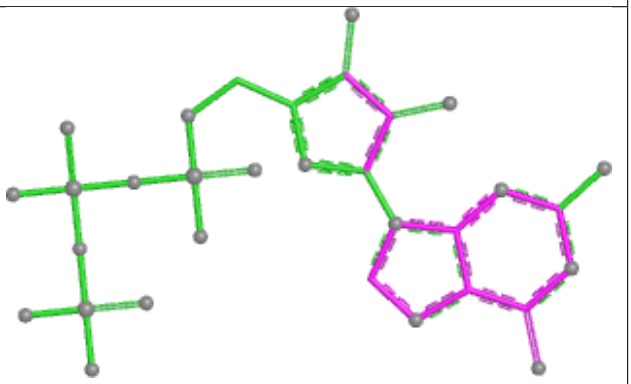


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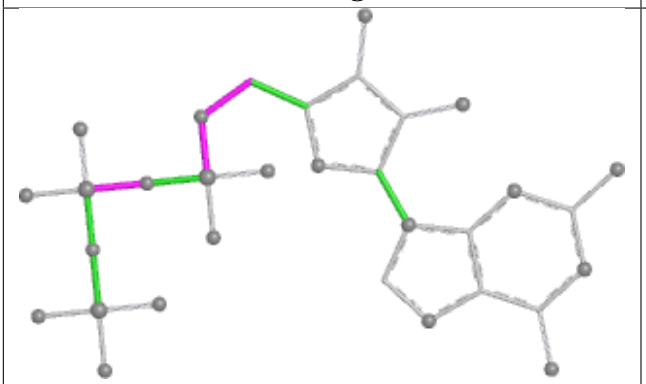
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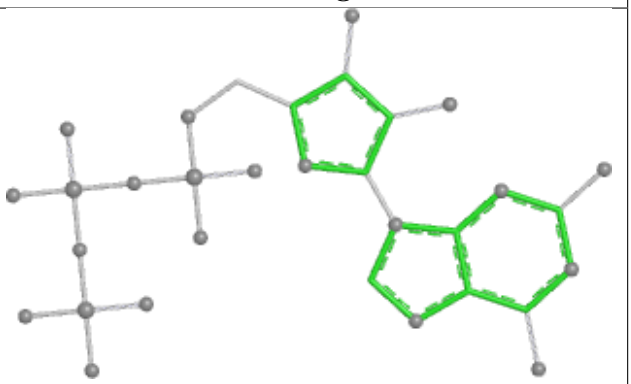
Bond lengths



Bond angles

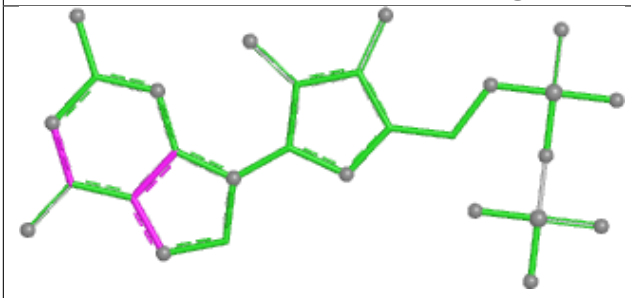


Torsions

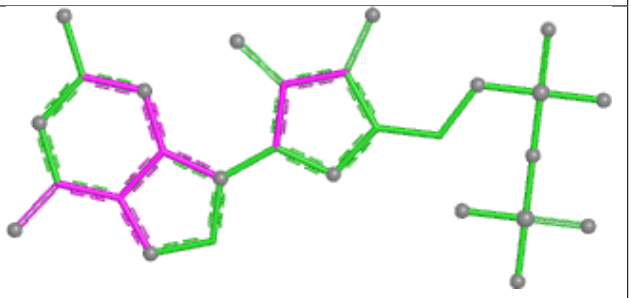


Rings

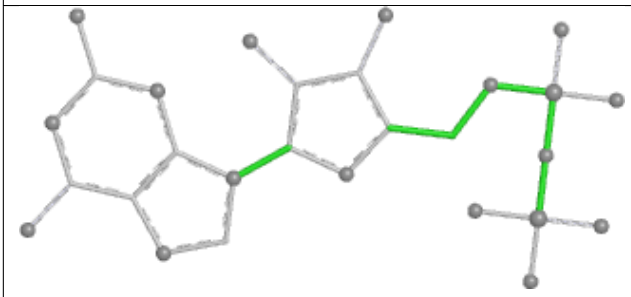
Ligand GDP ED 501



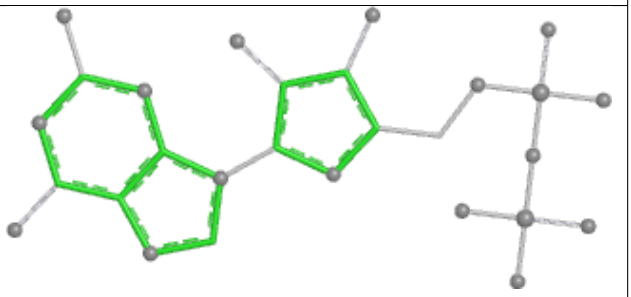
Bond lengths



Bond angles

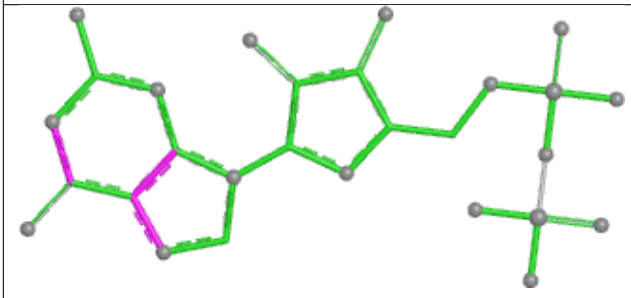


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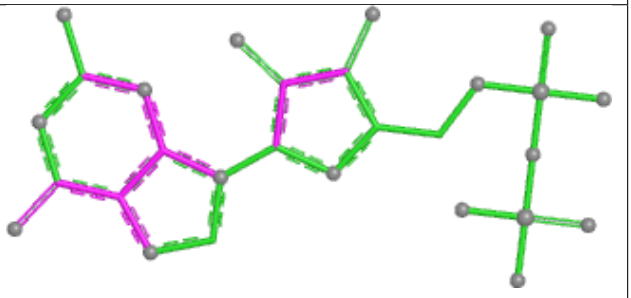


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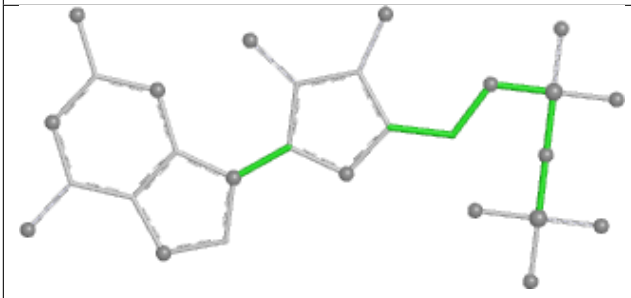
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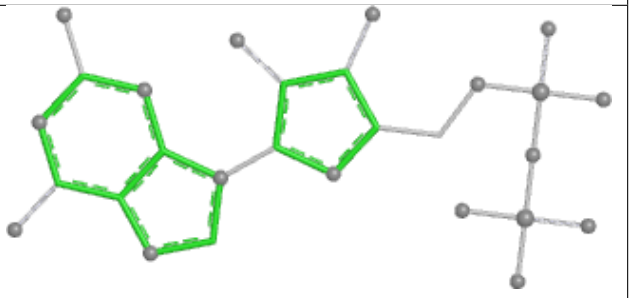
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Bond angles

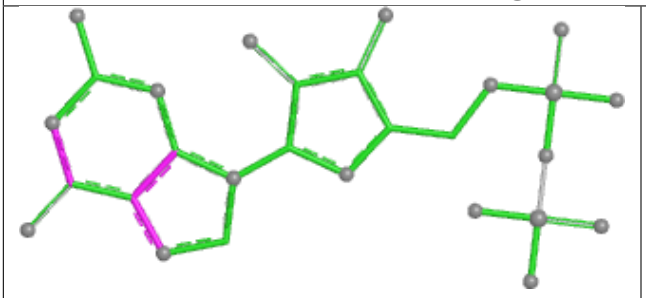


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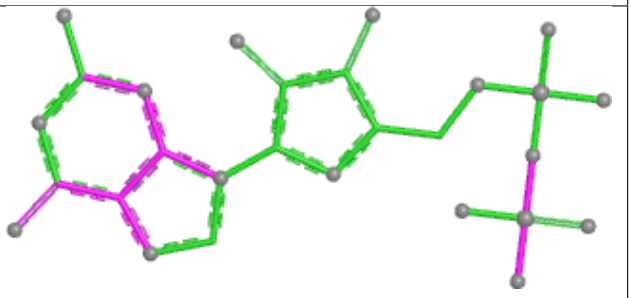


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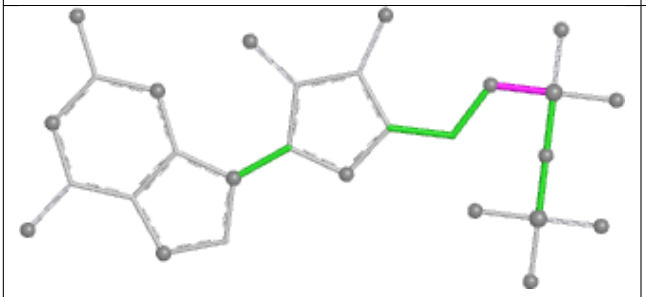
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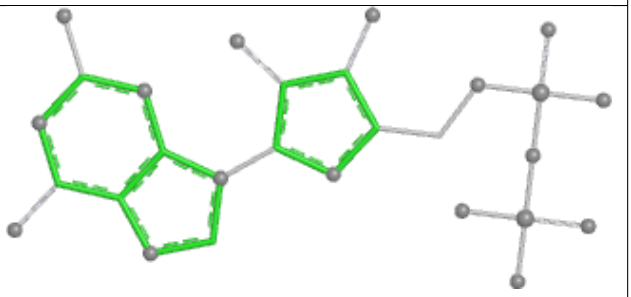
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Bond angles

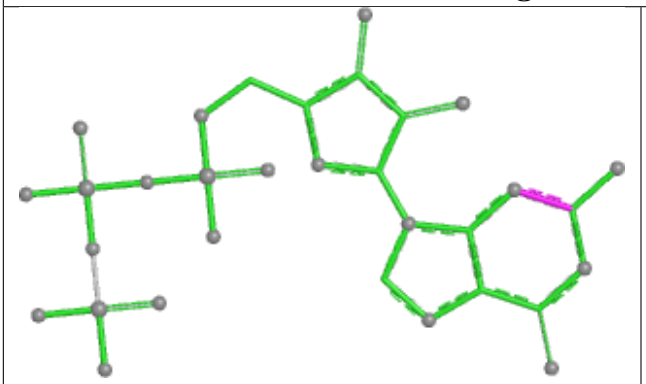


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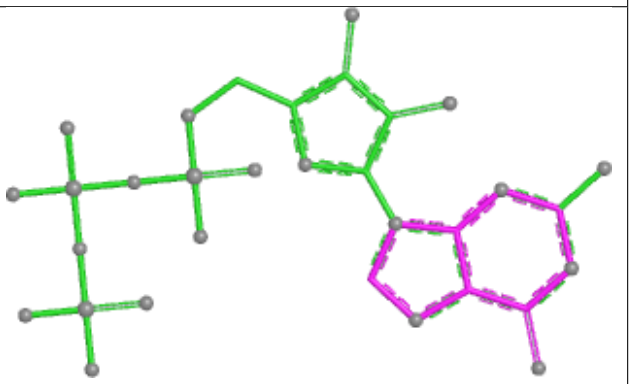


Rings

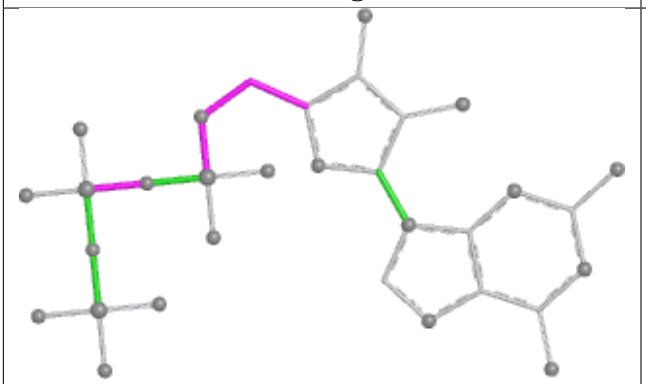
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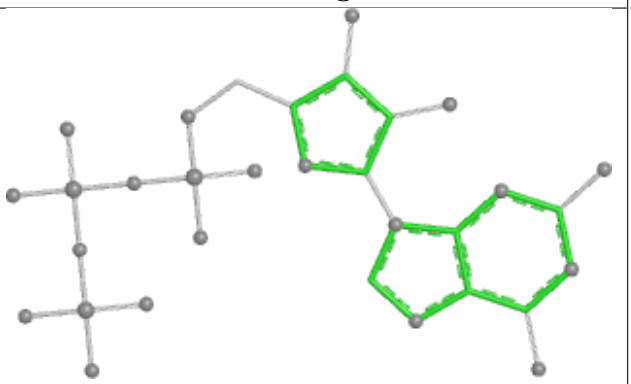
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Bond angles

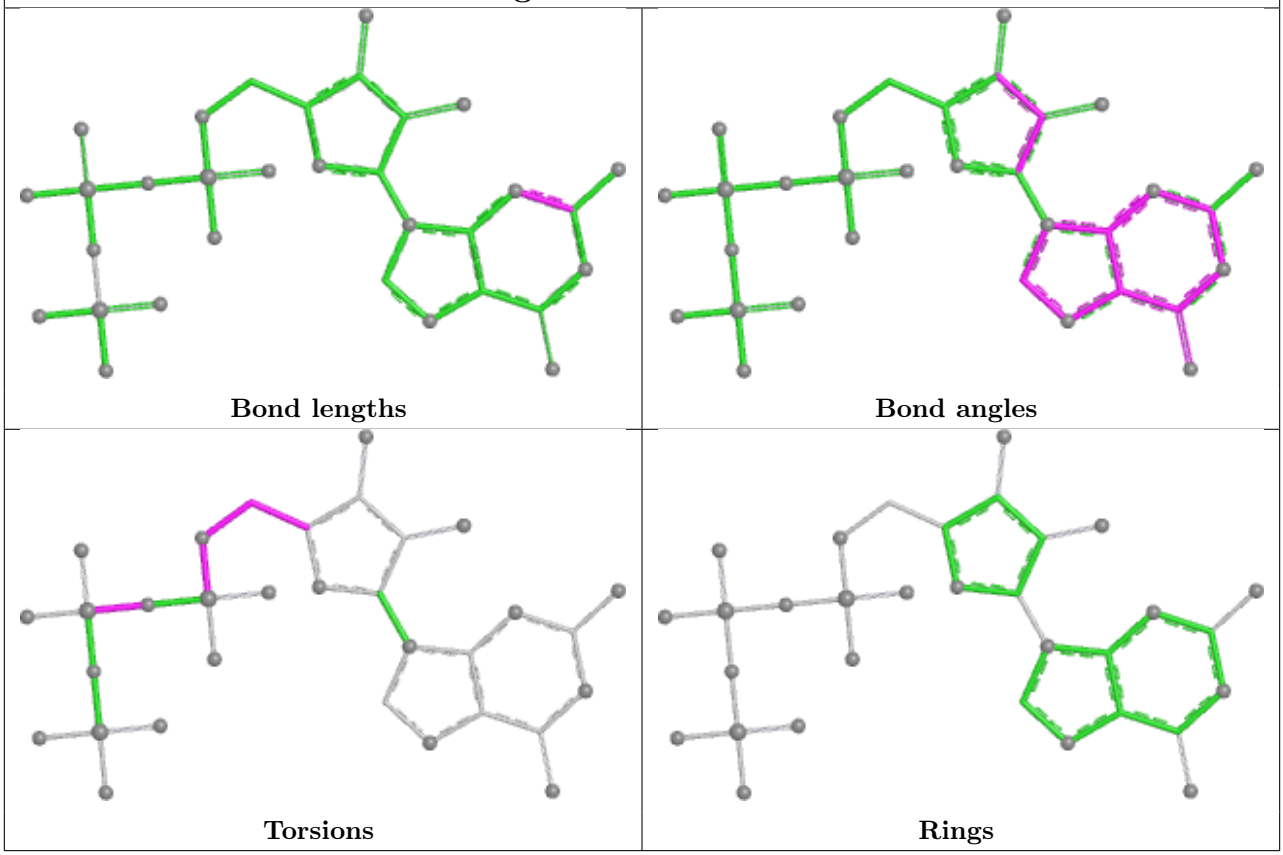


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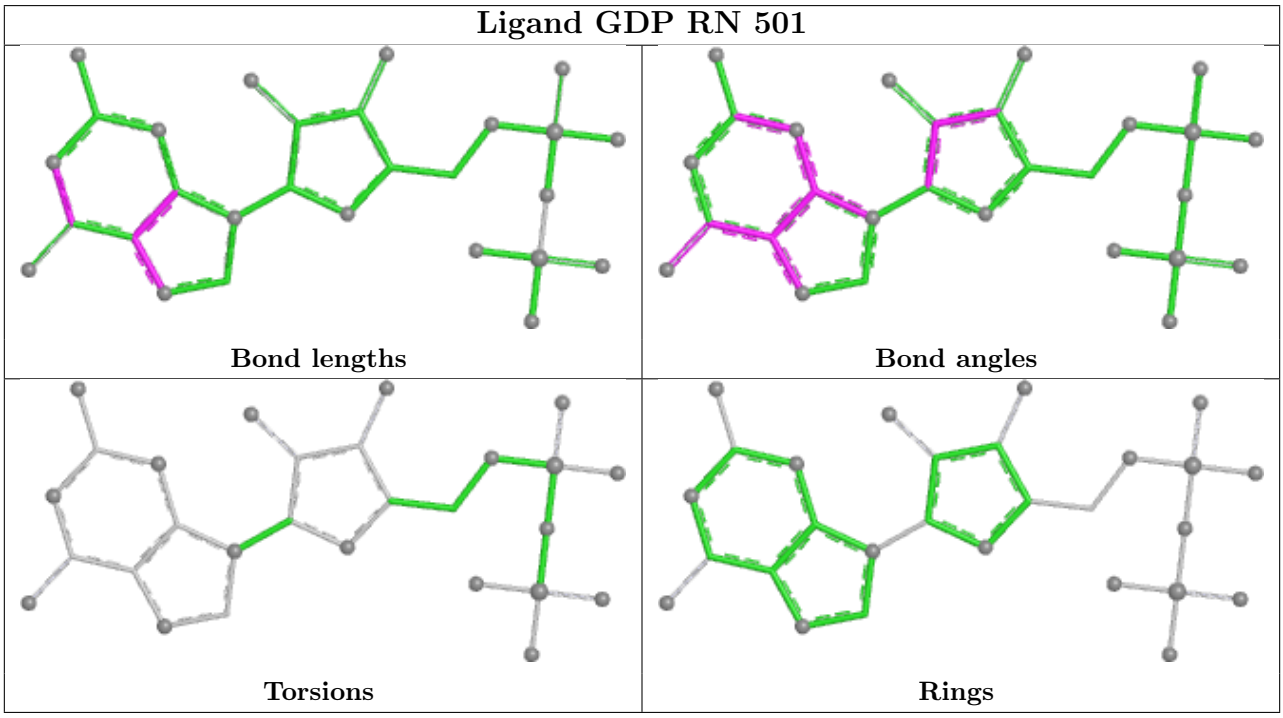


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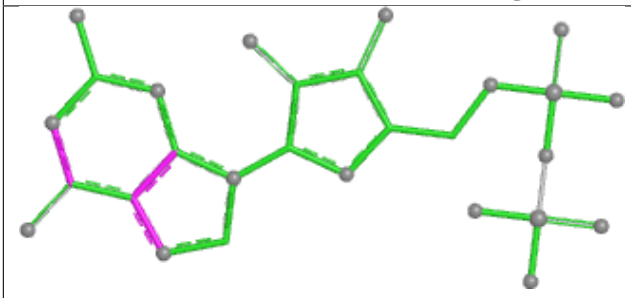
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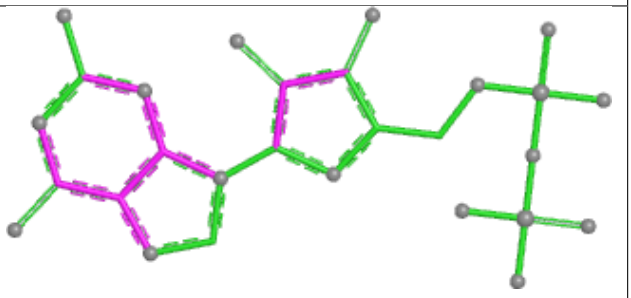
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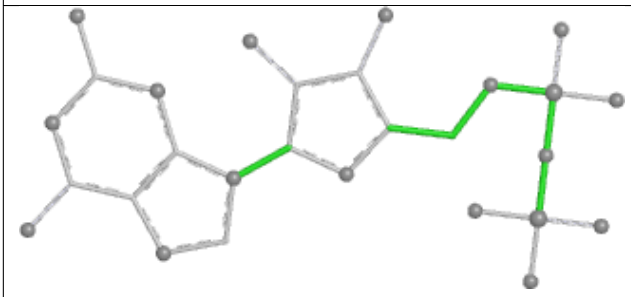
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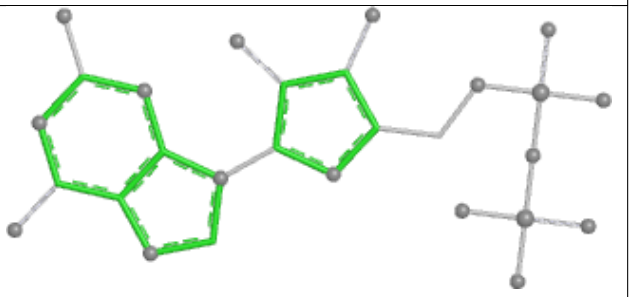
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Bond angles

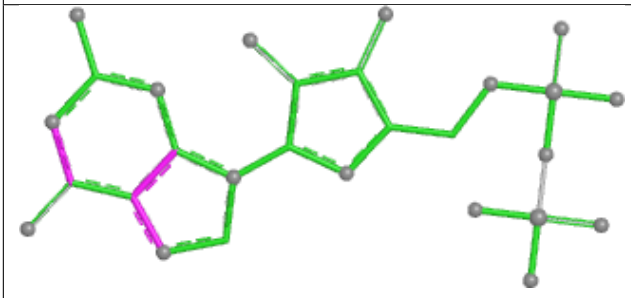


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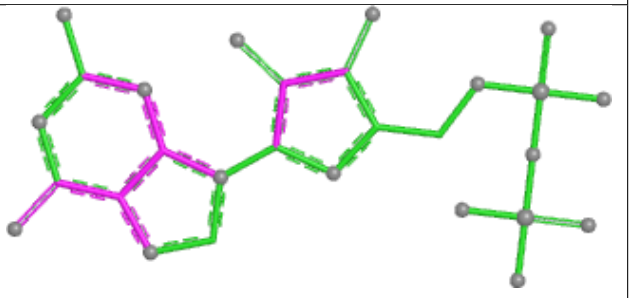


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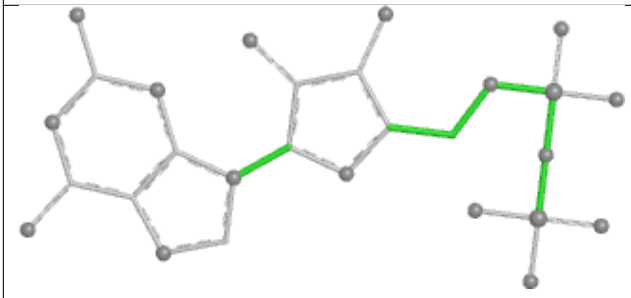
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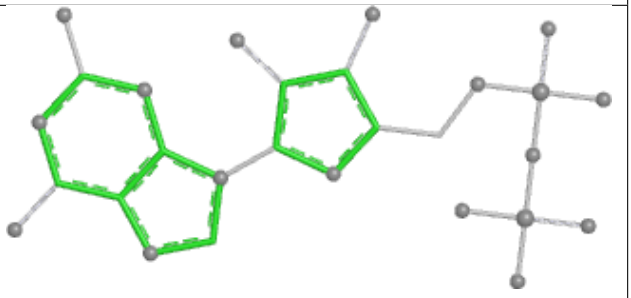
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Bond angles

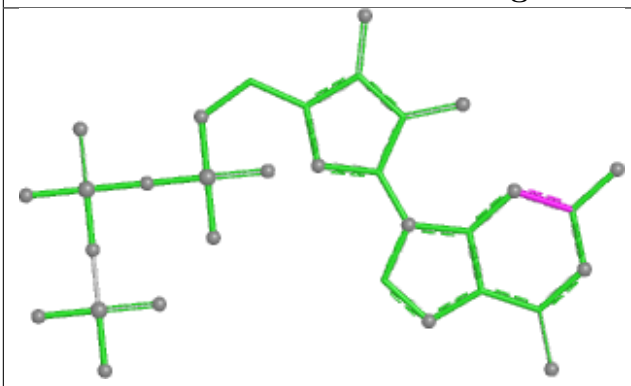


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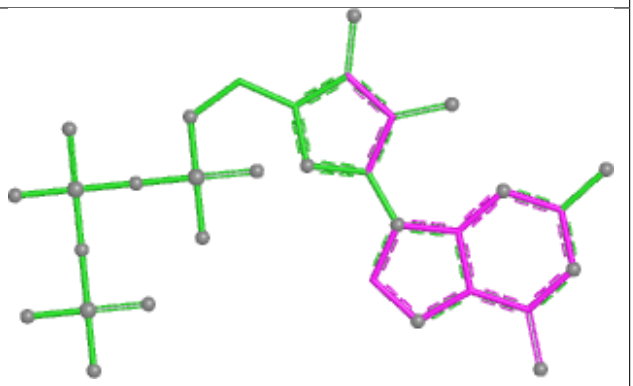


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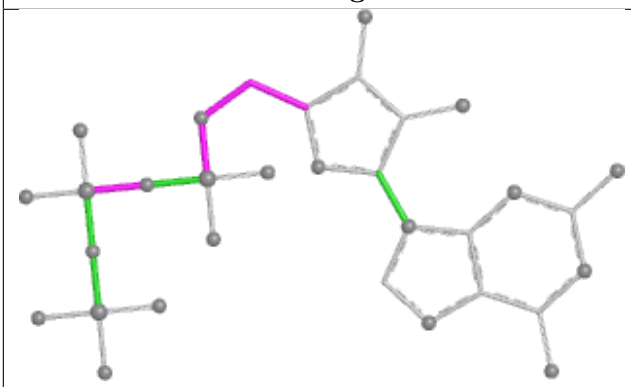
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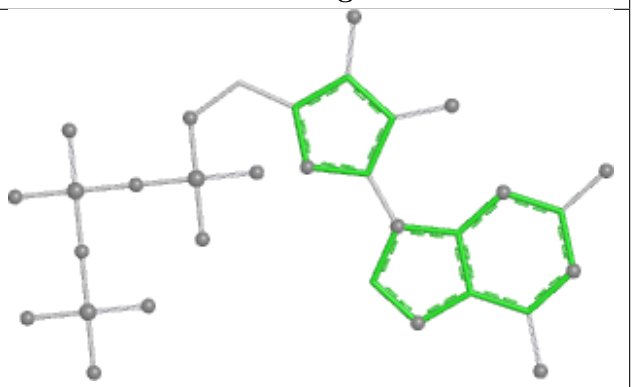
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Bond angles

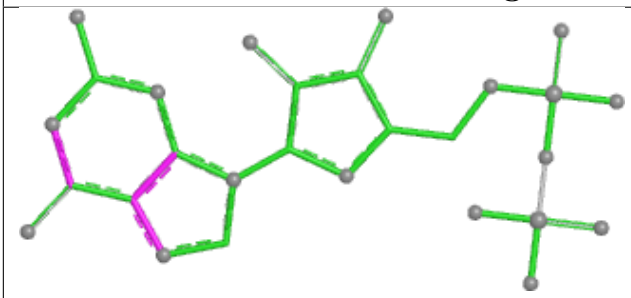


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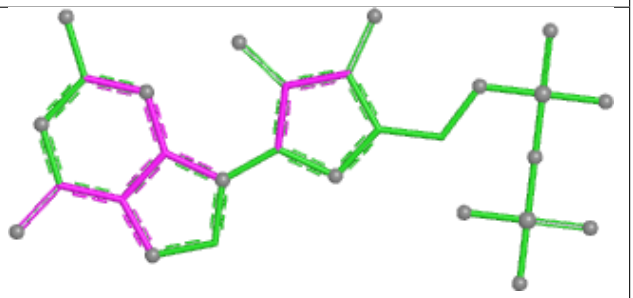


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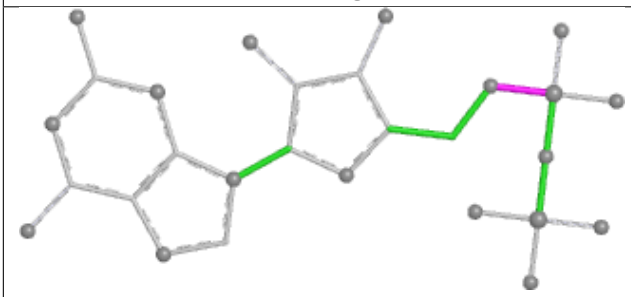
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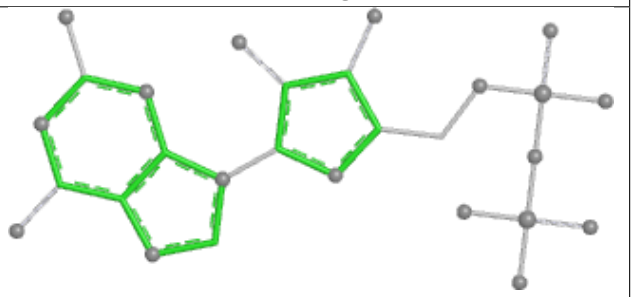
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Bond angles

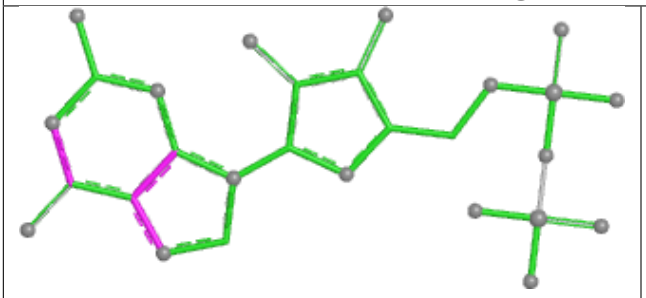


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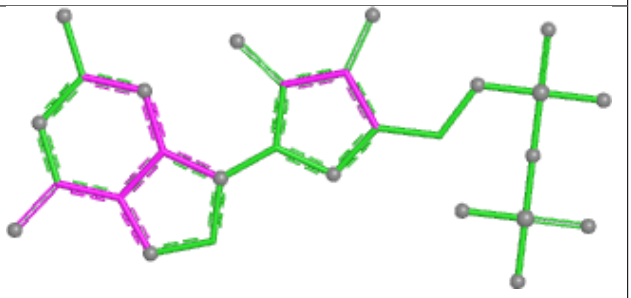


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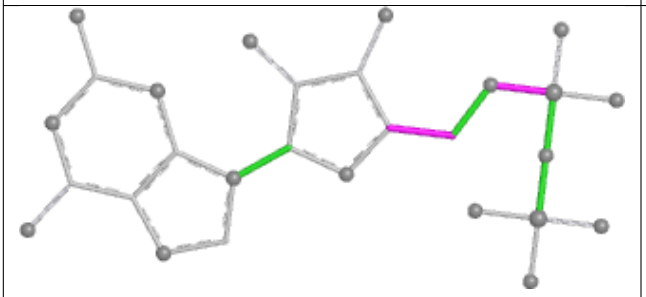
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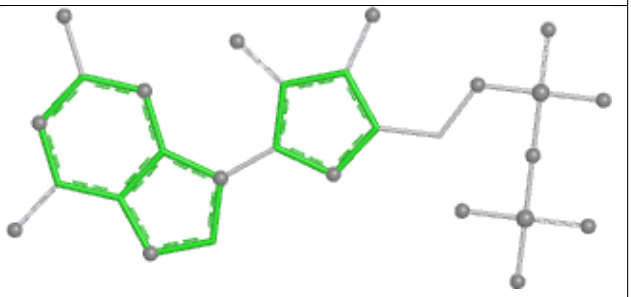
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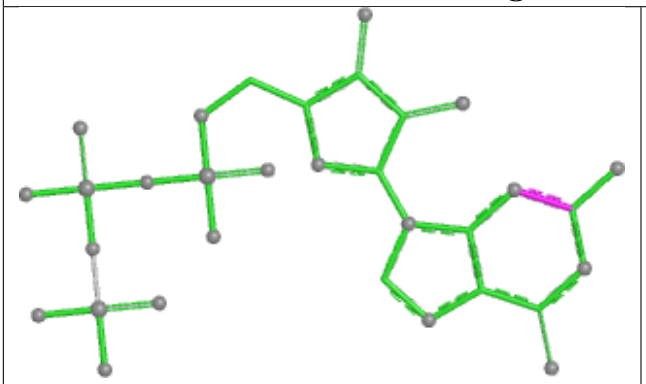


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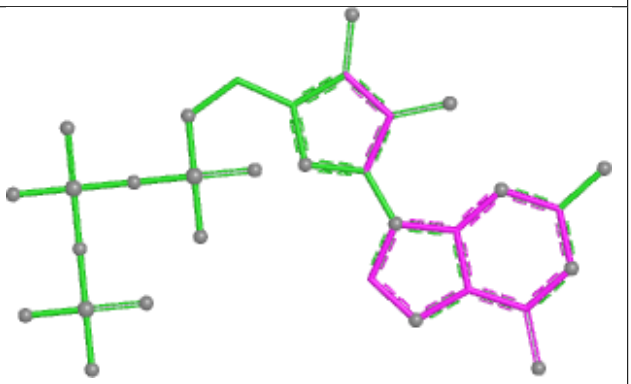


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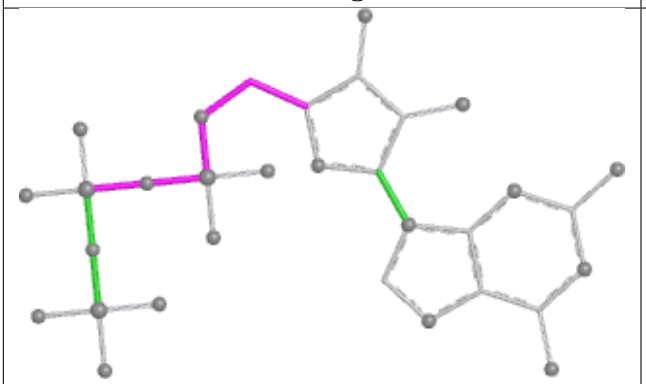
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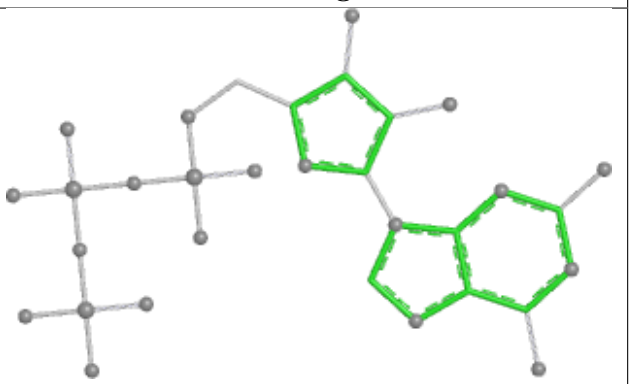
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Bond angles

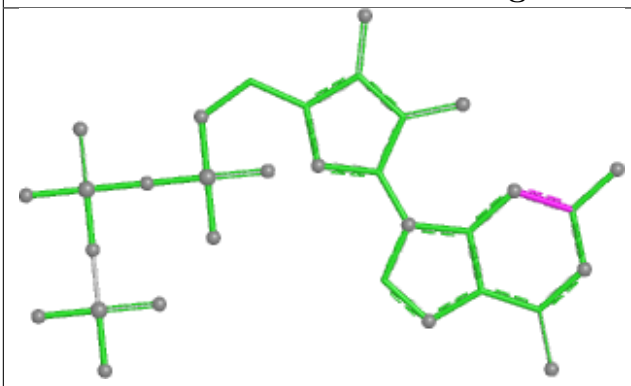


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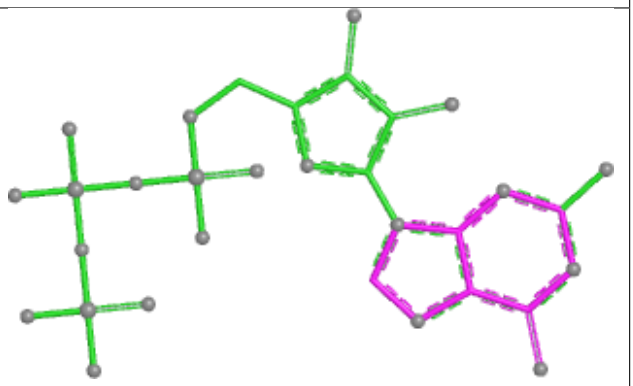


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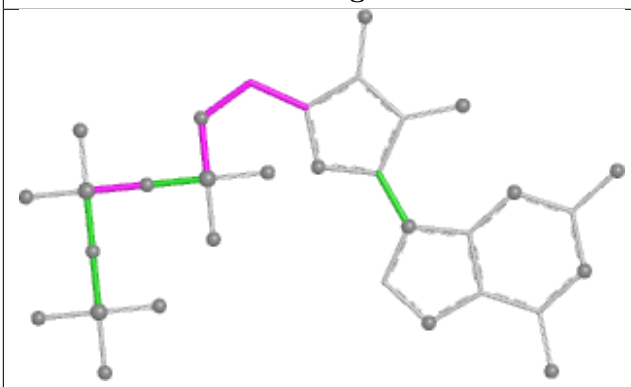
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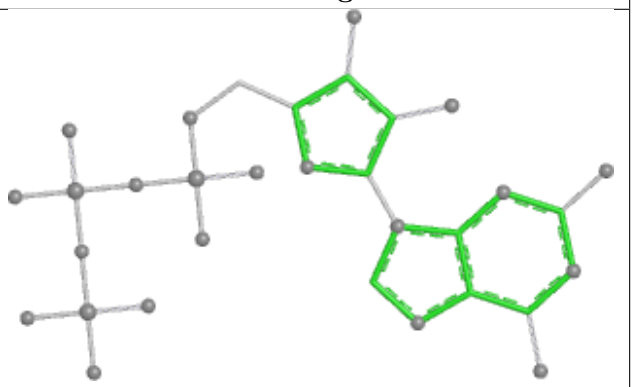
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Bond angles

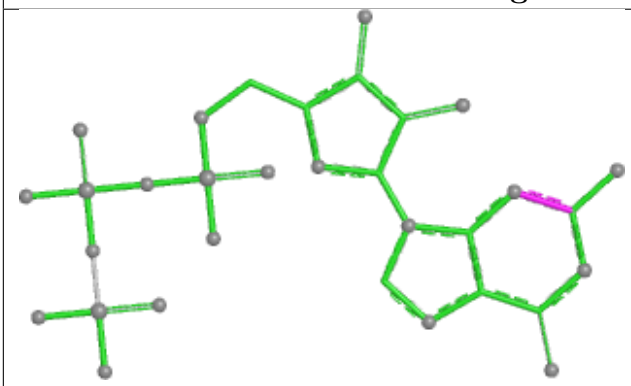


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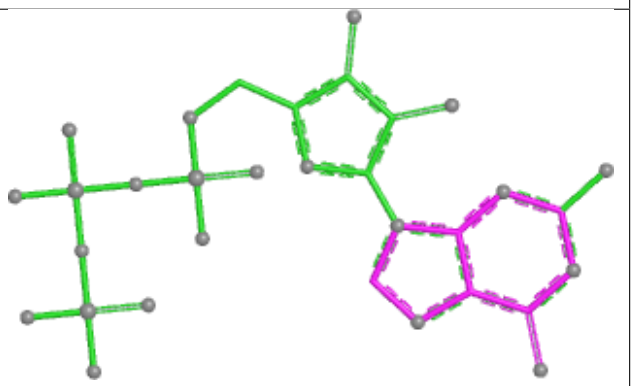


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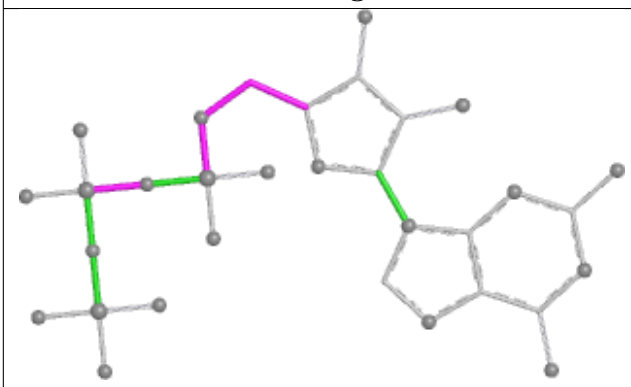
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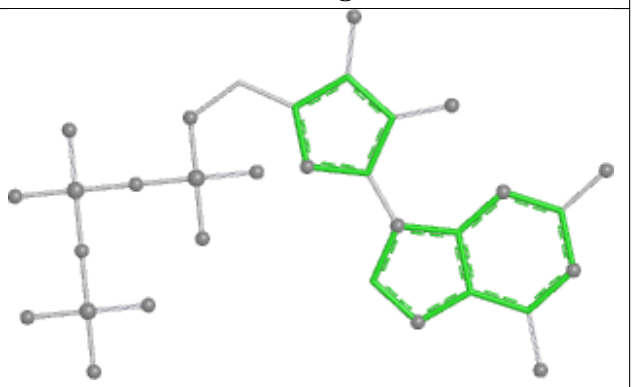
Bond lengths



Bond angles

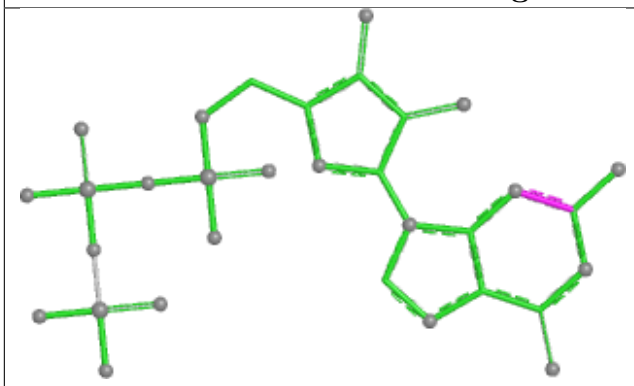


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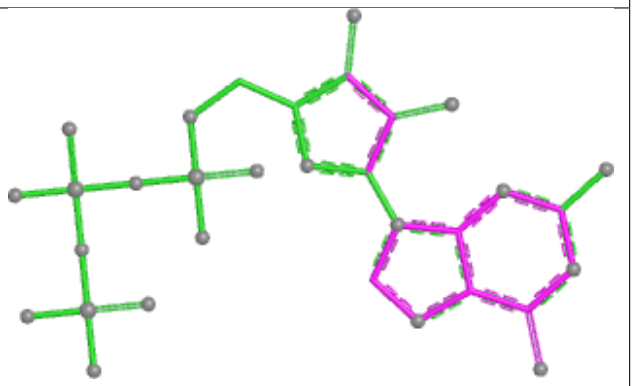


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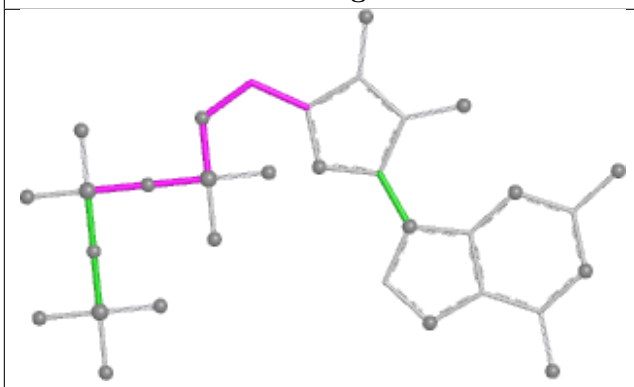
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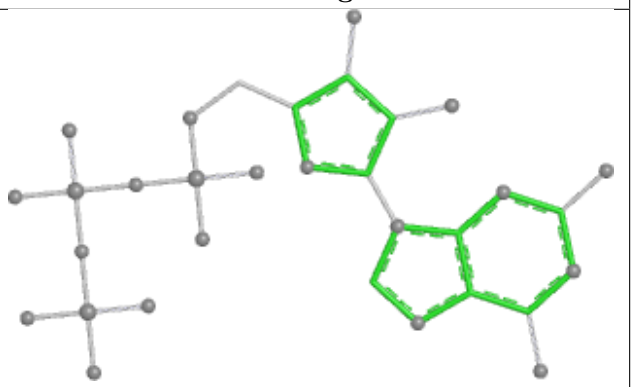
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Bond angles

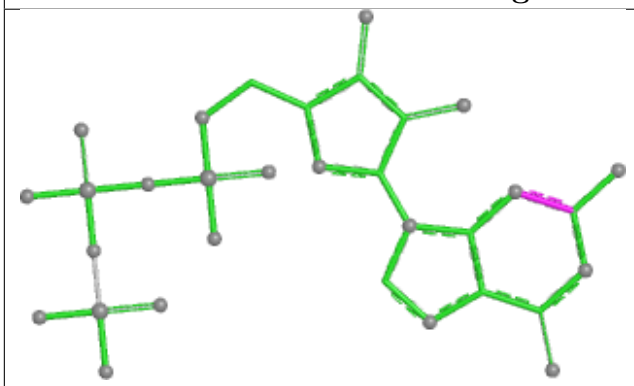


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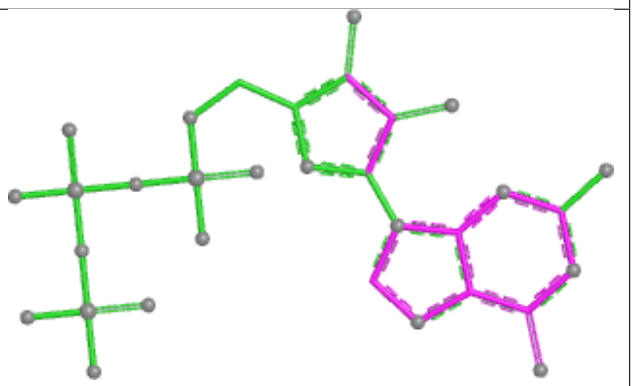


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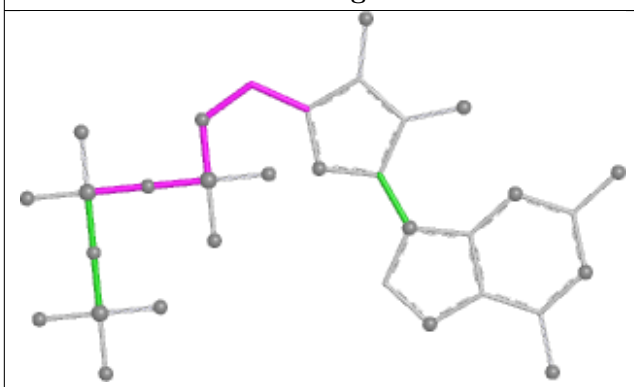
Ligand GTP TA 501



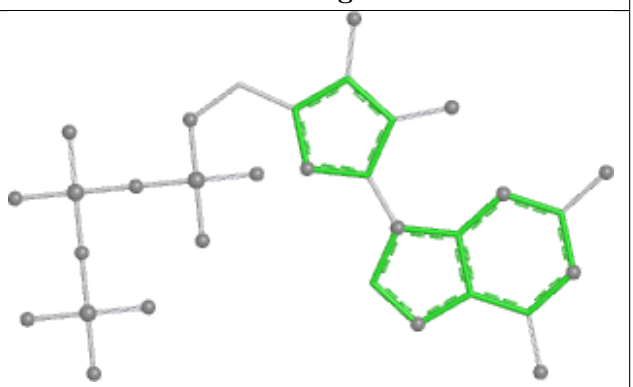
Bond lengths



Bond angles

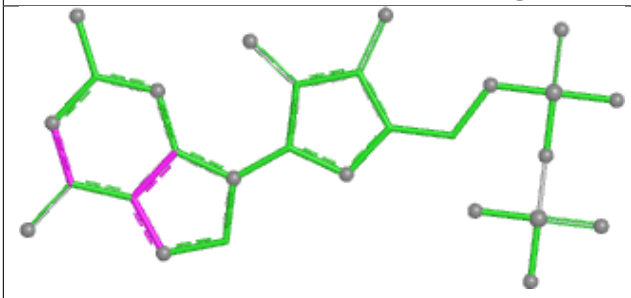


Torsions

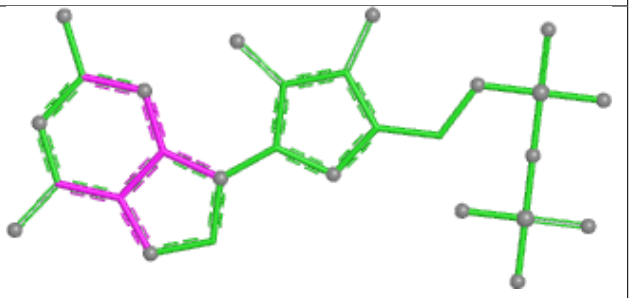


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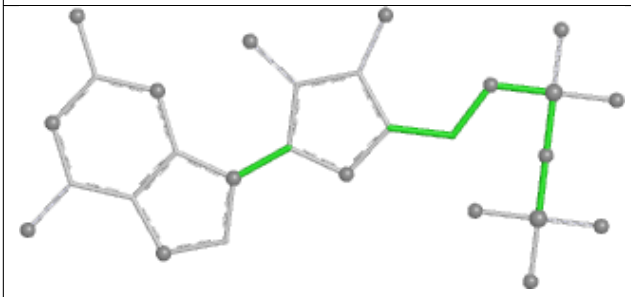
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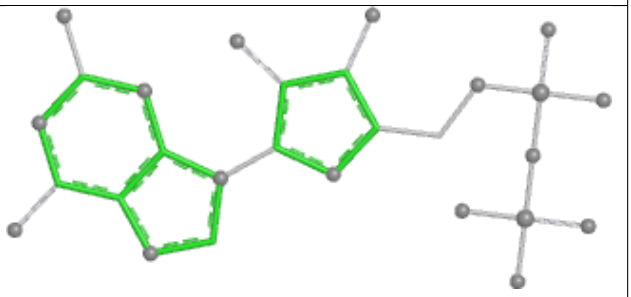
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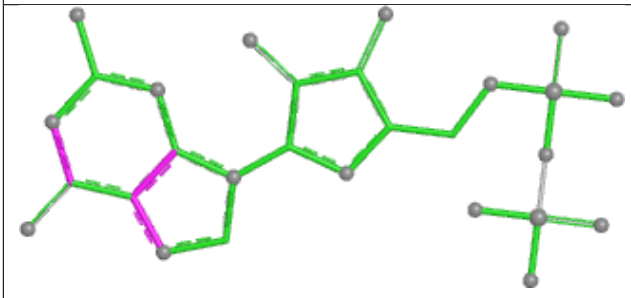


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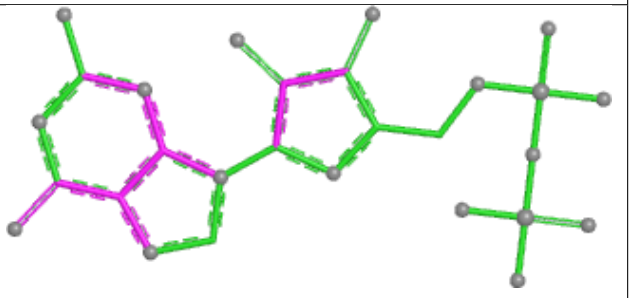


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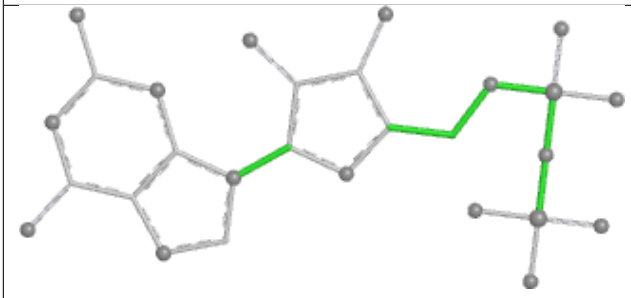
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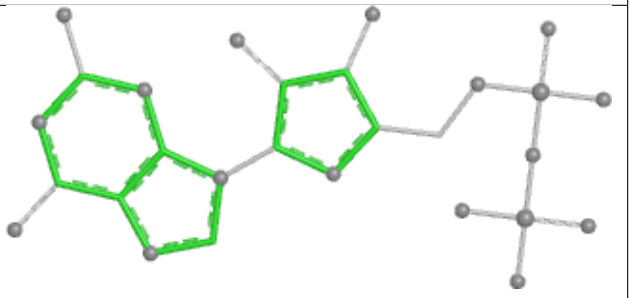
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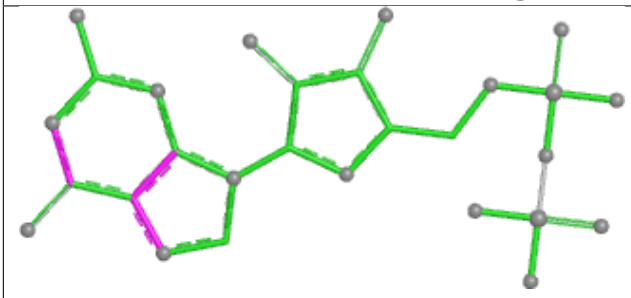


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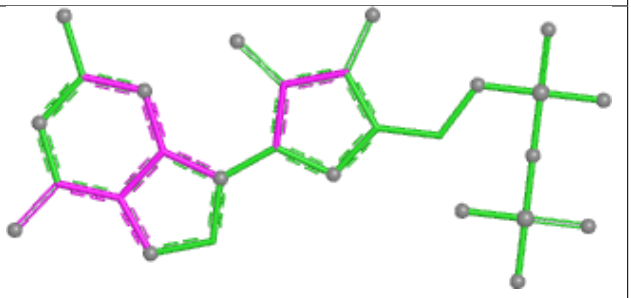


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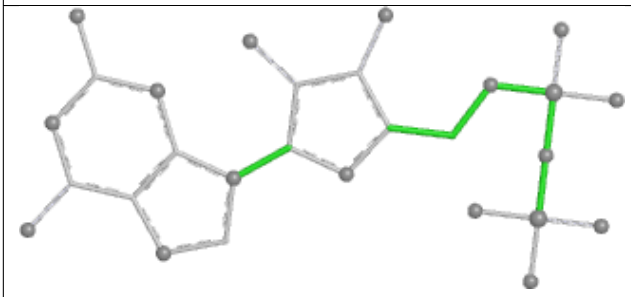
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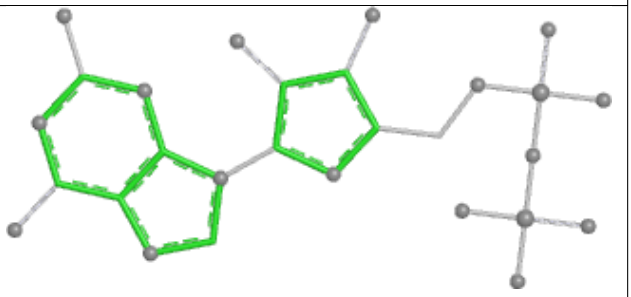
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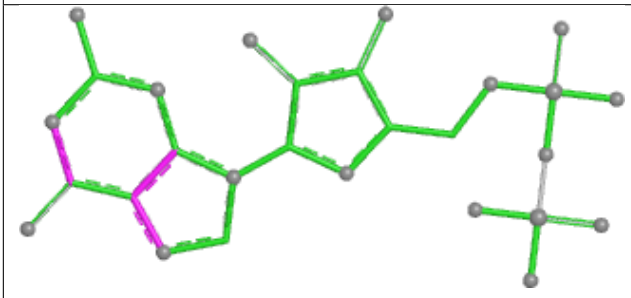


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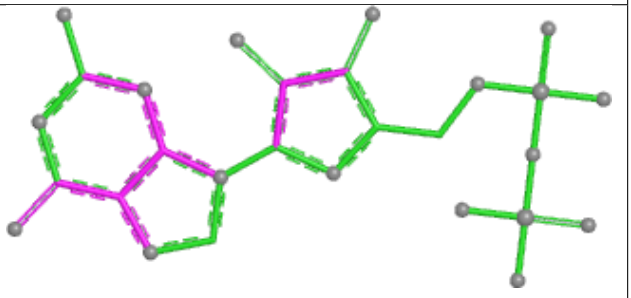


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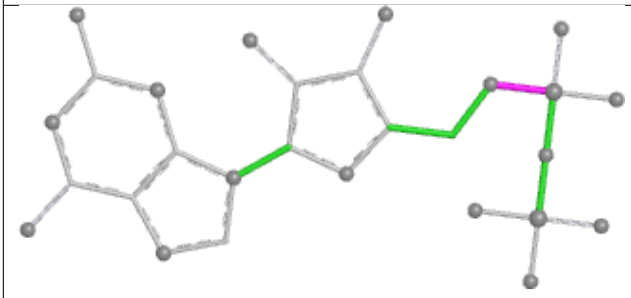
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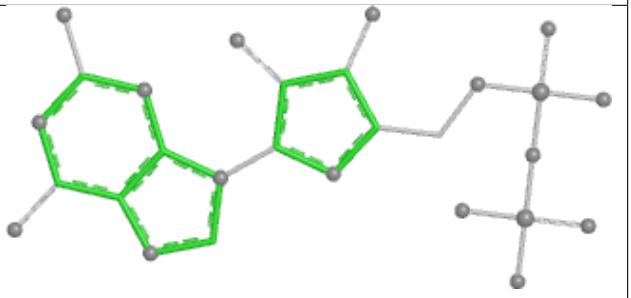
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Bond angles

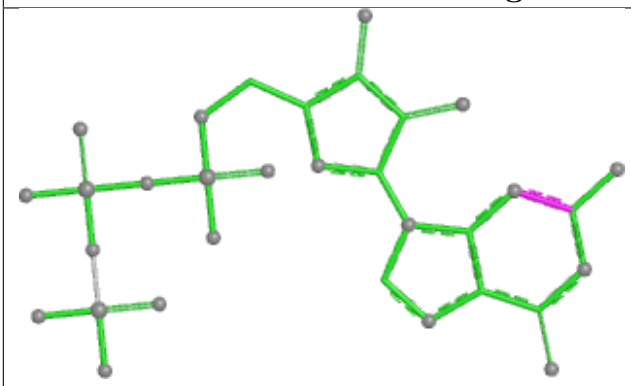


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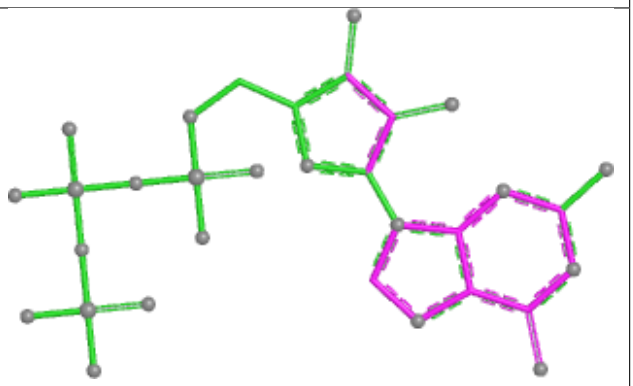


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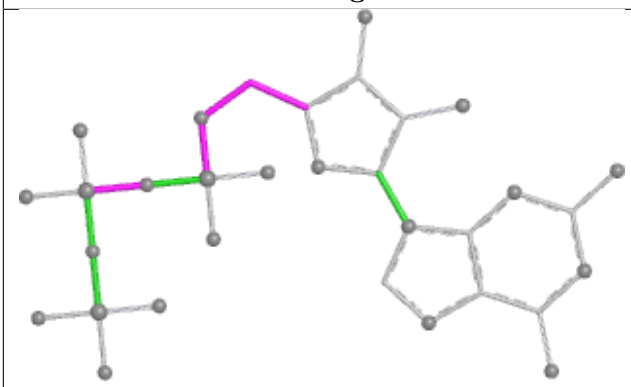
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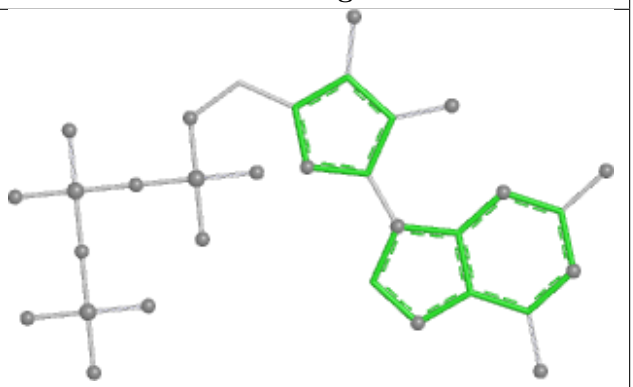
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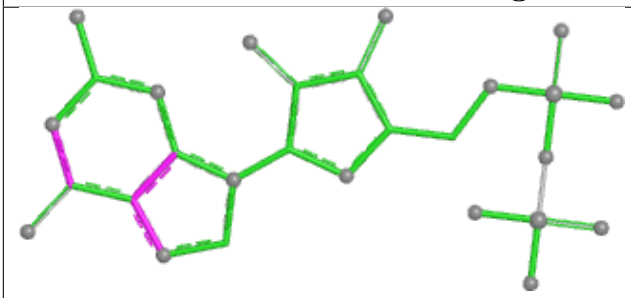


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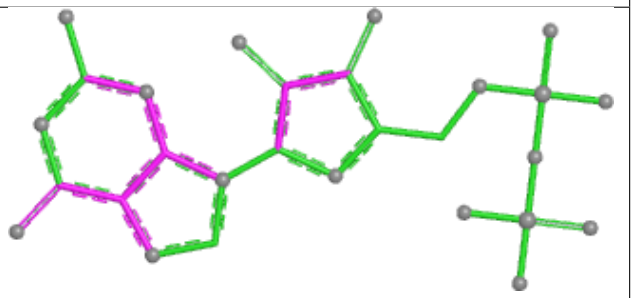


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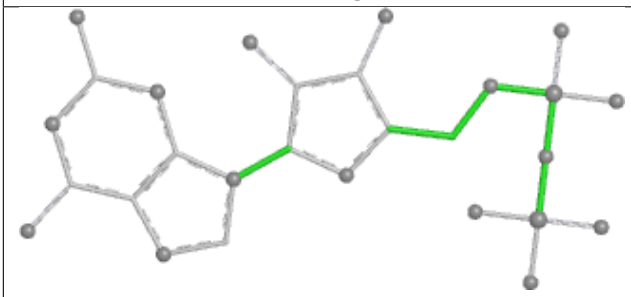
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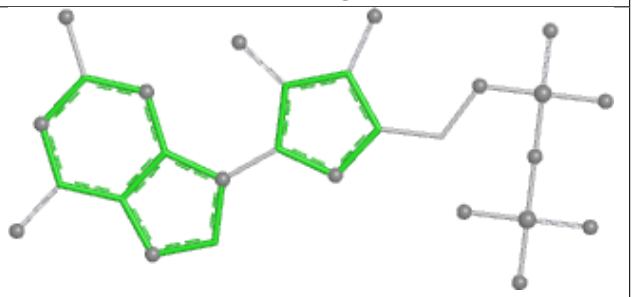
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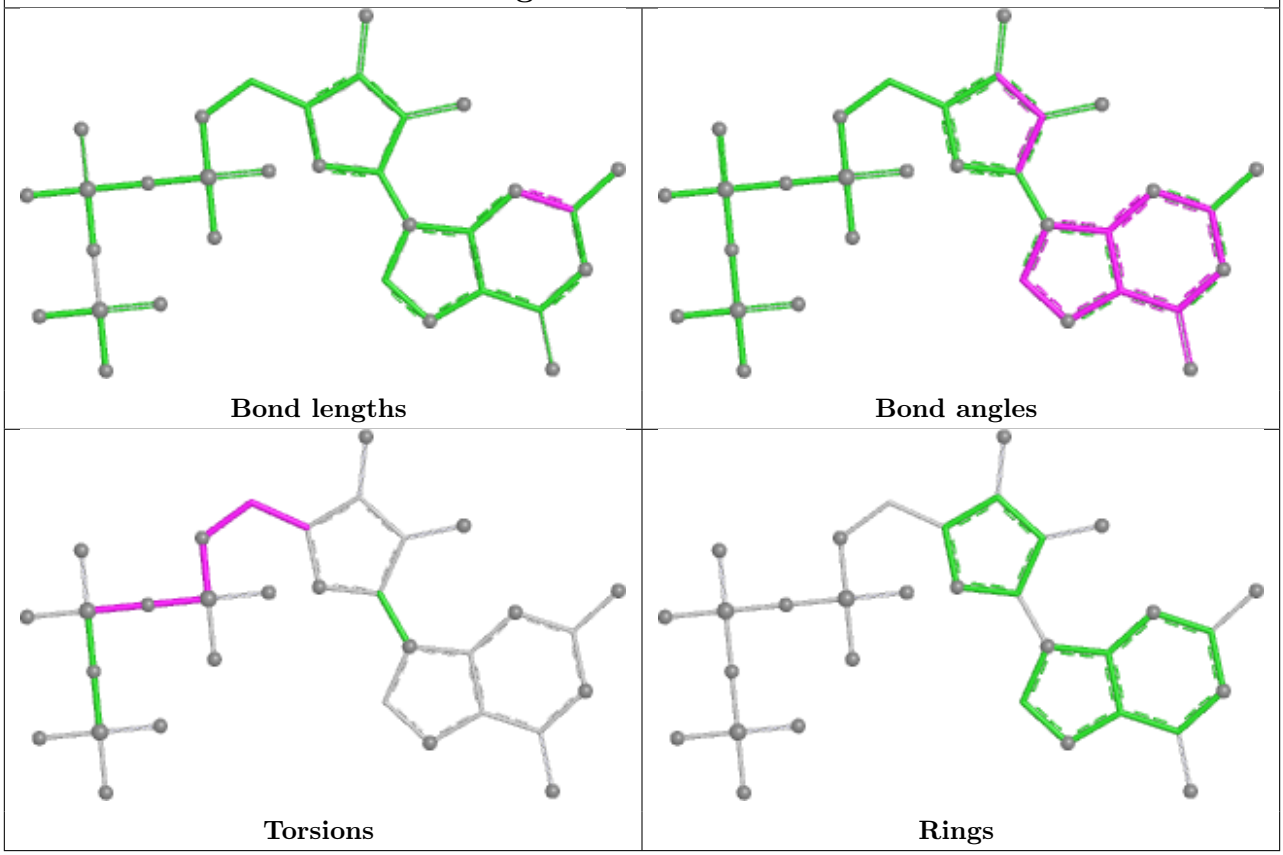


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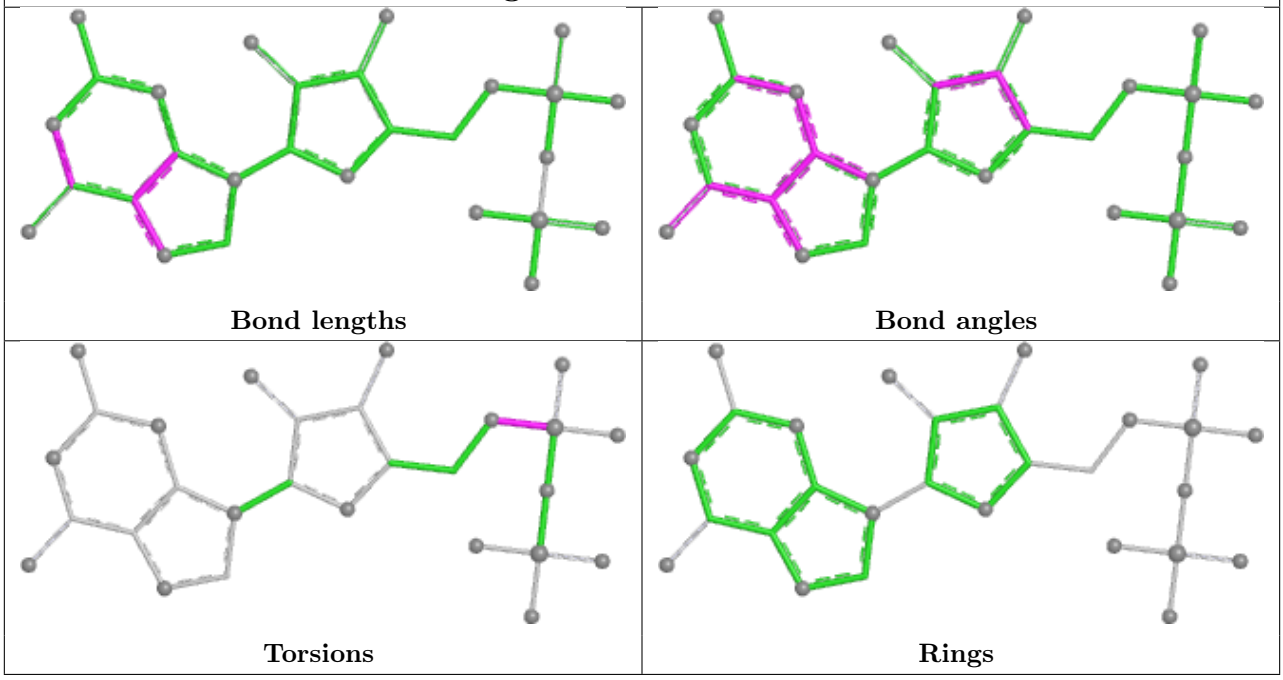


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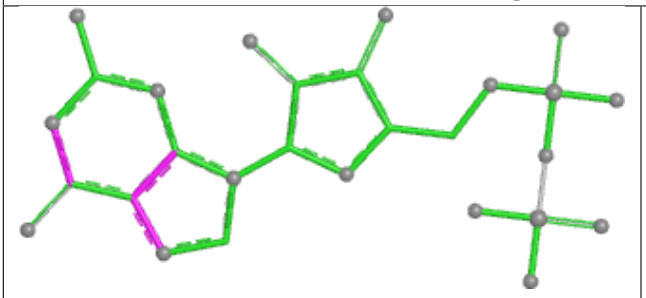
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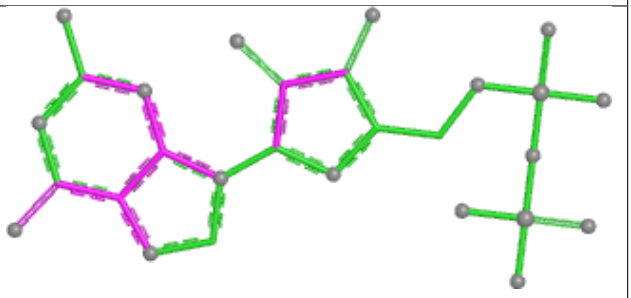
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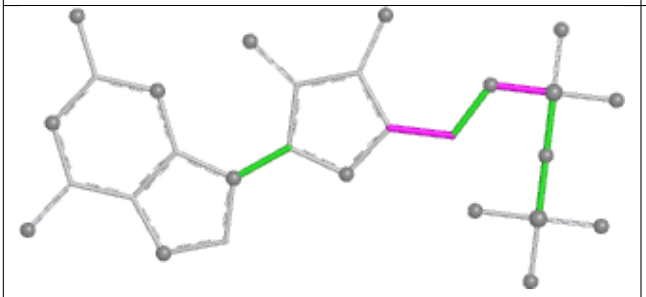
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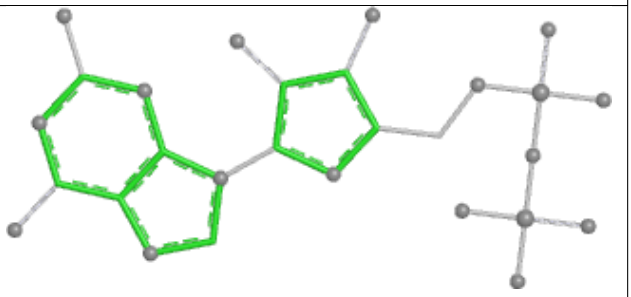
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Bond angles

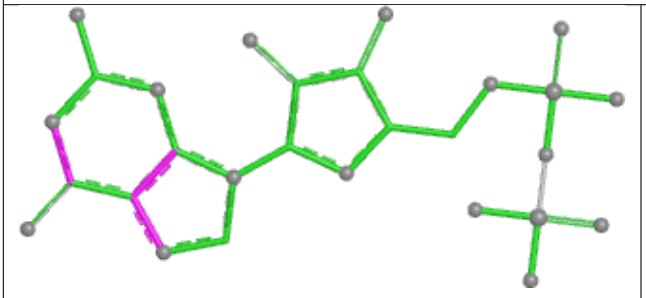


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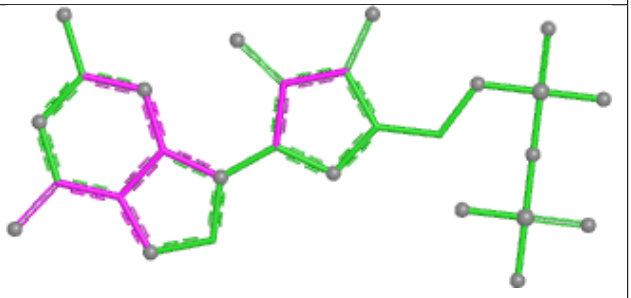


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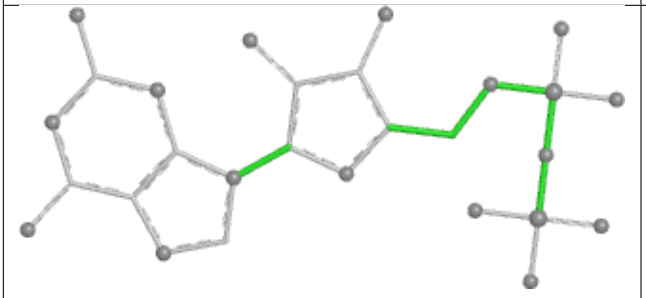
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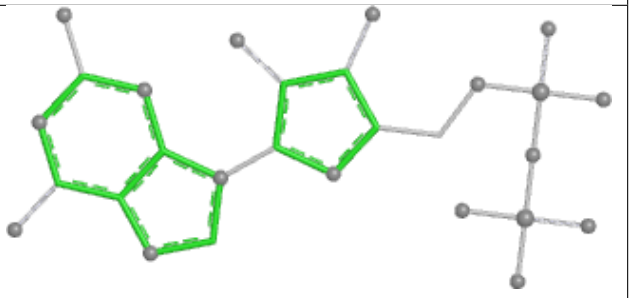
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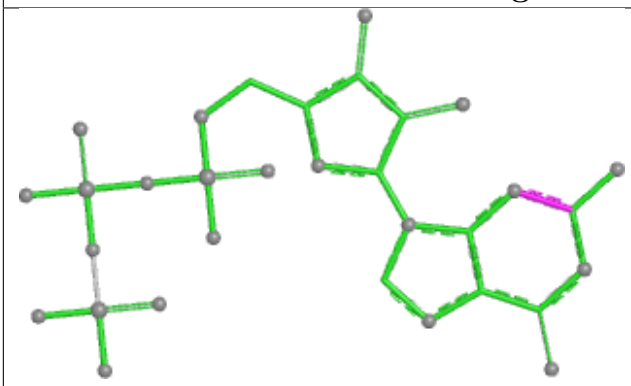


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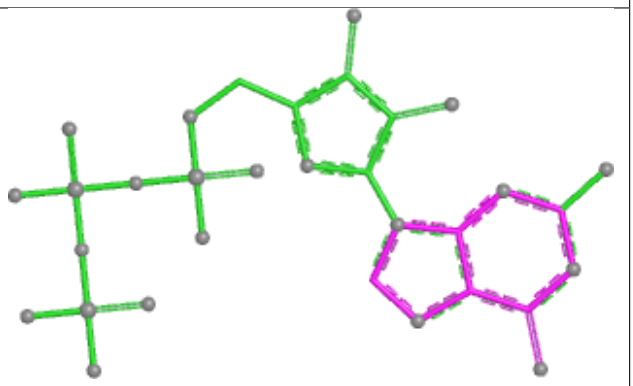


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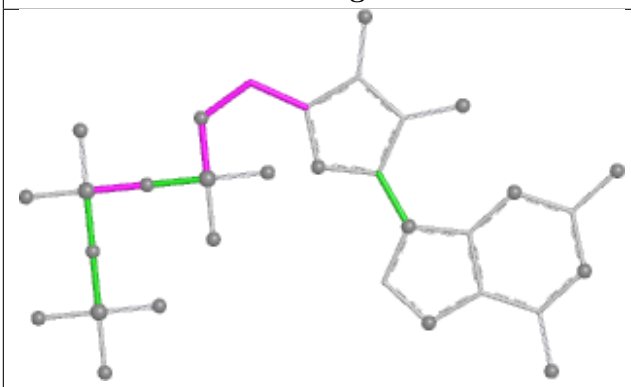
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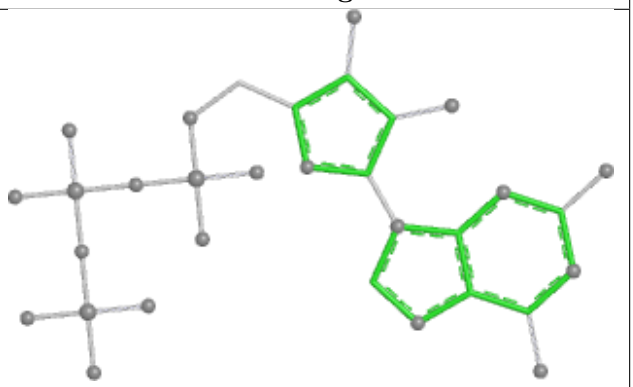
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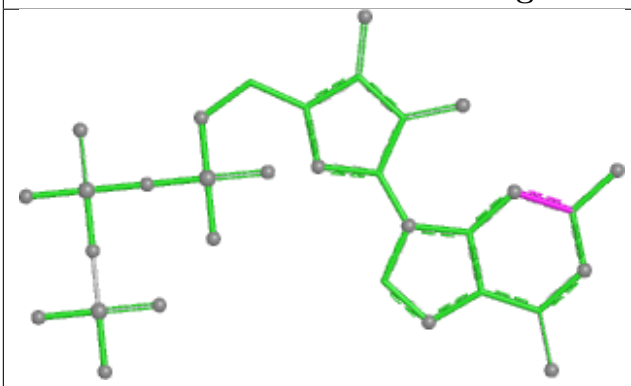


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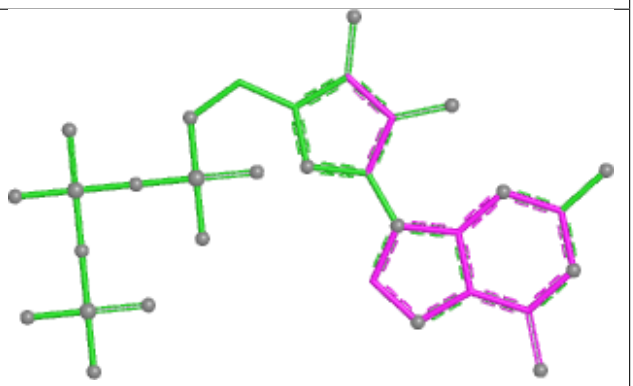


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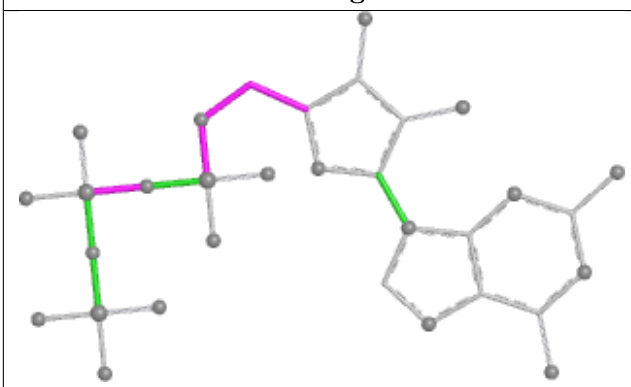
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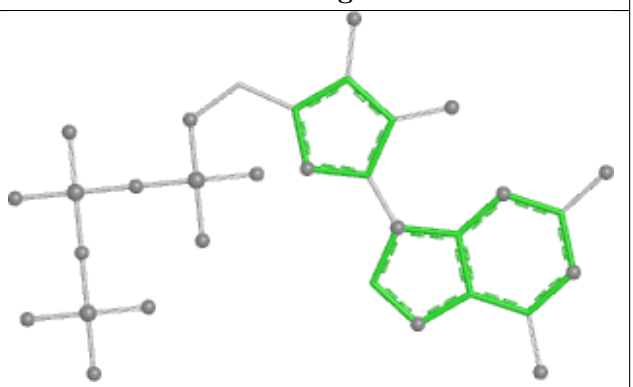
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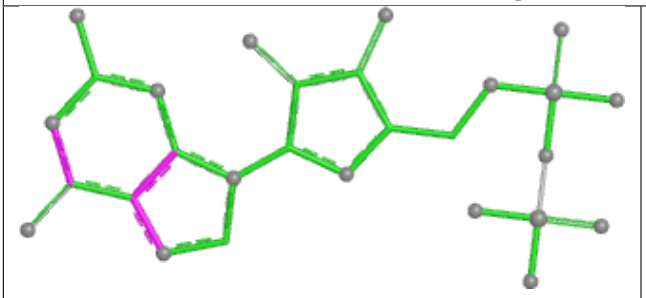


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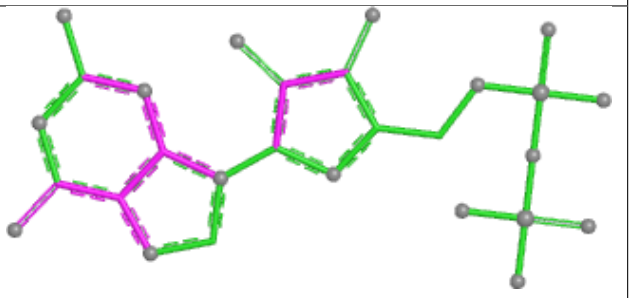


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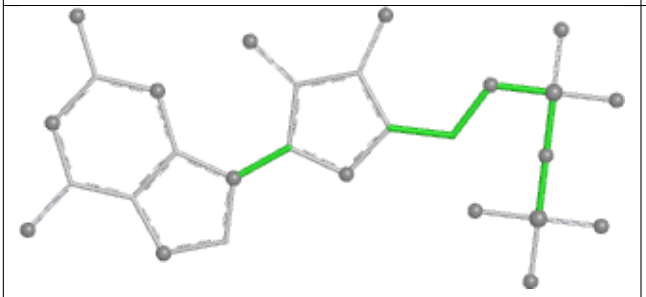
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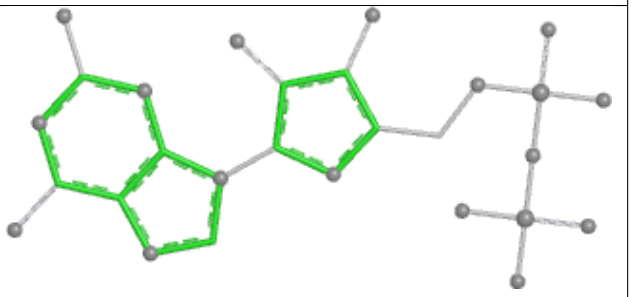
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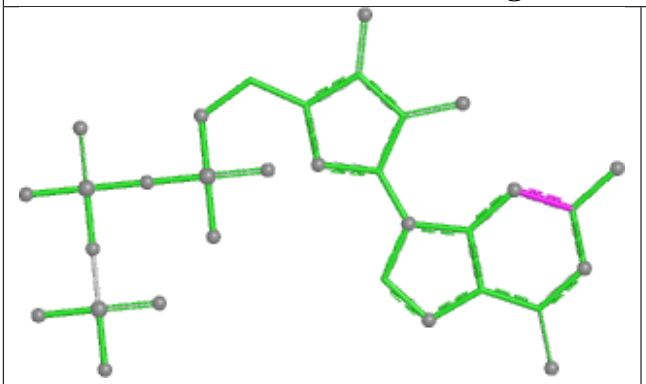


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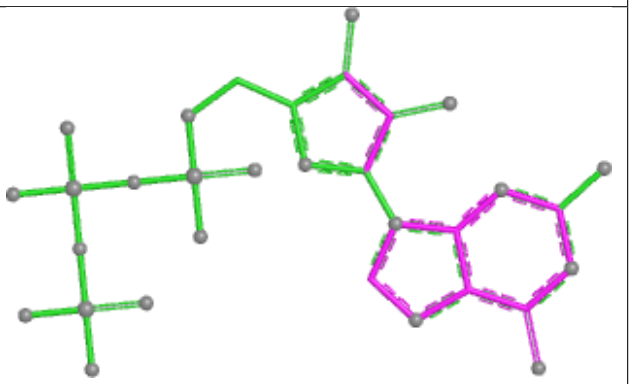


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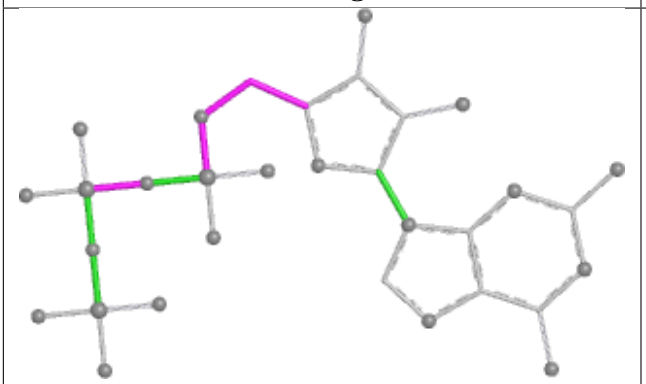
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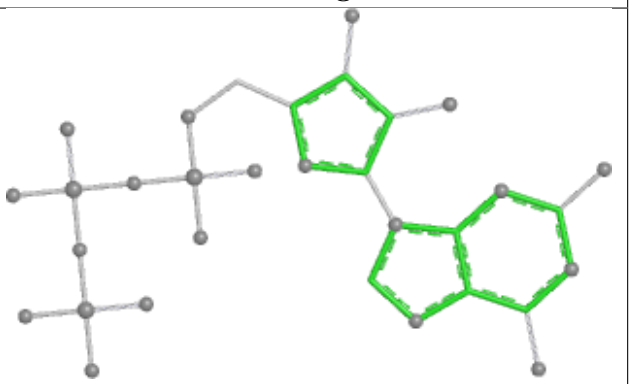
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Bond angles

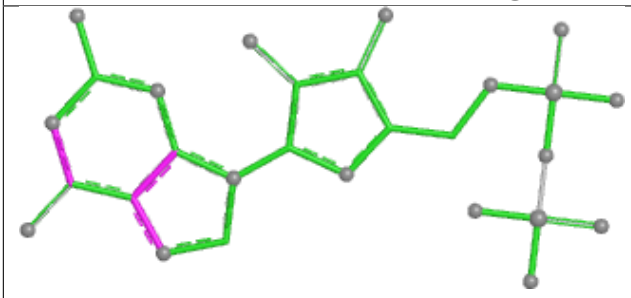


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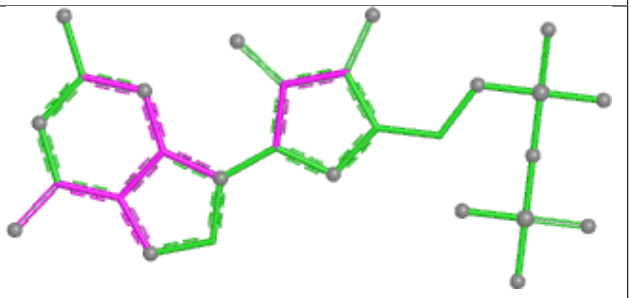


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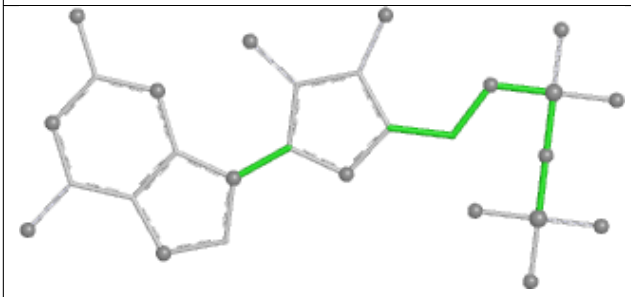
Ligand GDP GN 502



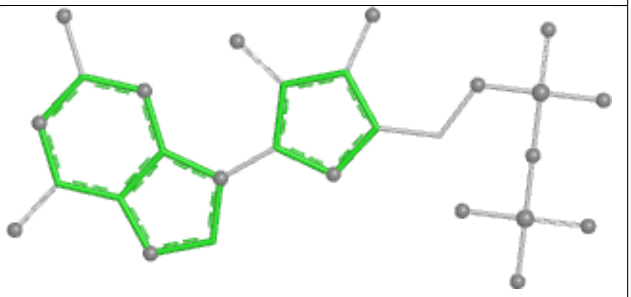
Bond lengths



Bond angles

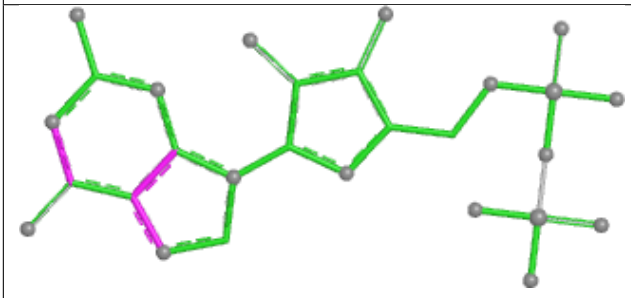


Torsions

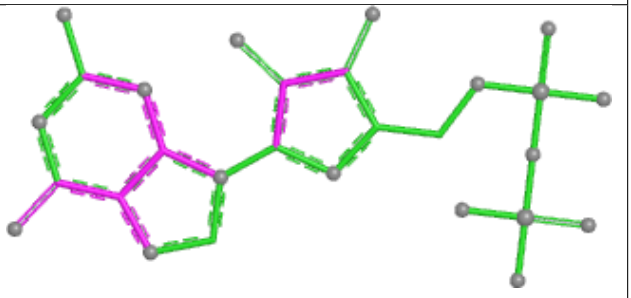


Rings

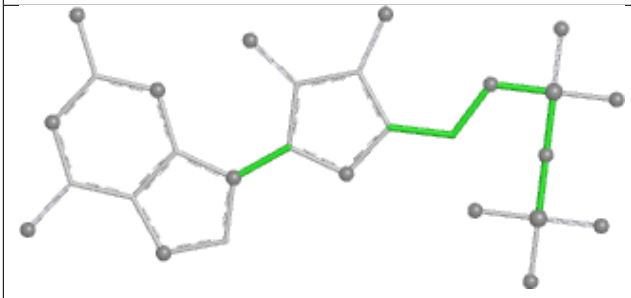
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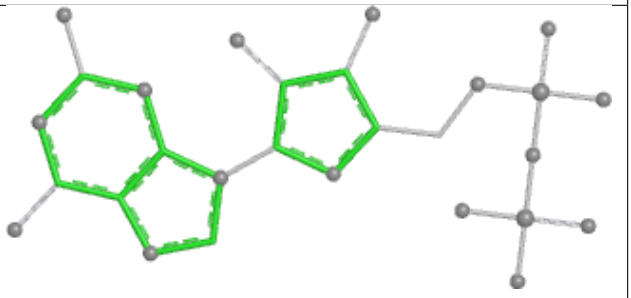
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Bond angles

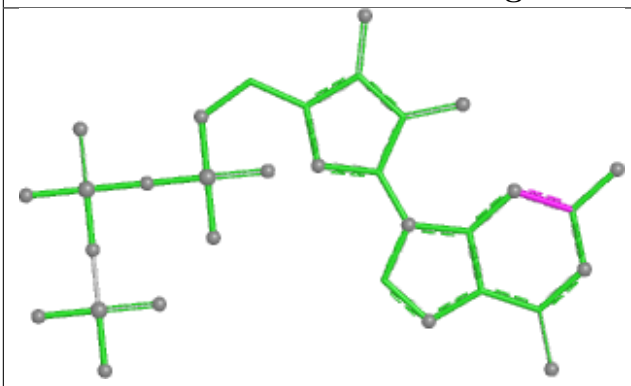


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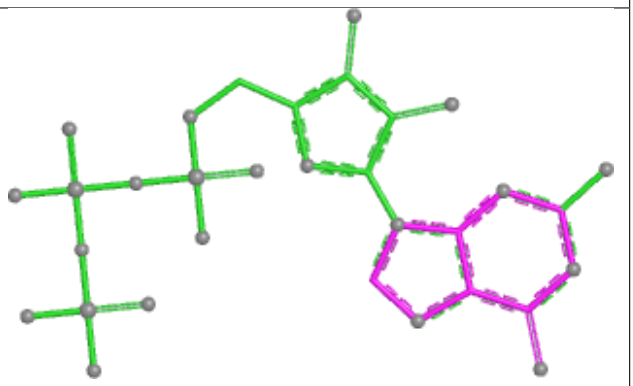


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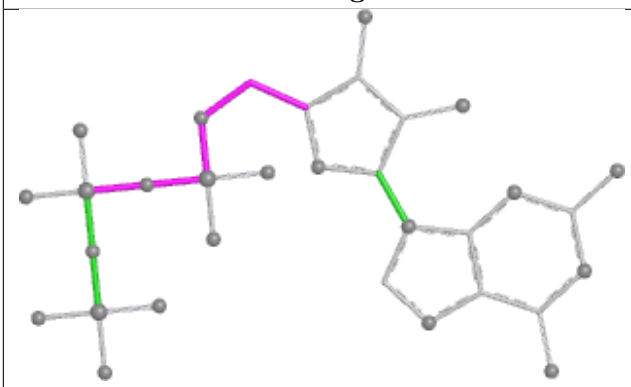
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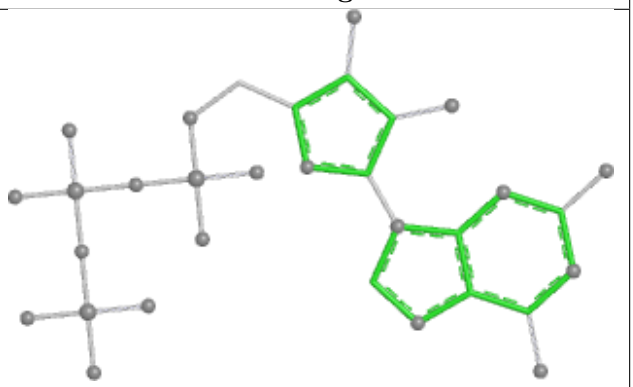
Bond lengths



Bond angles

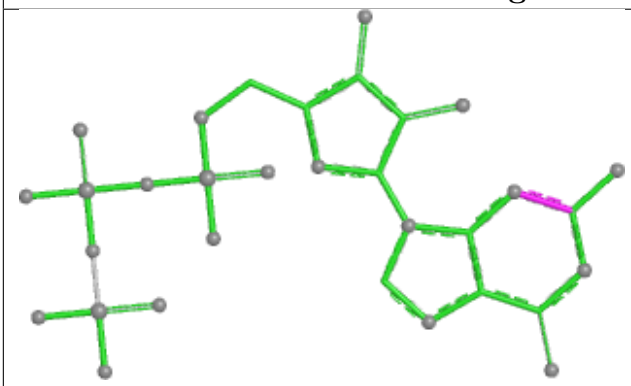


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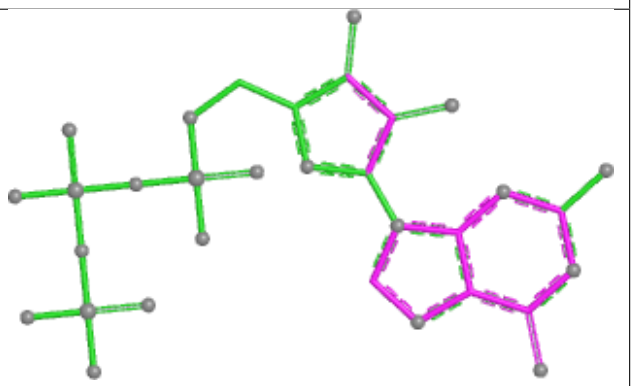


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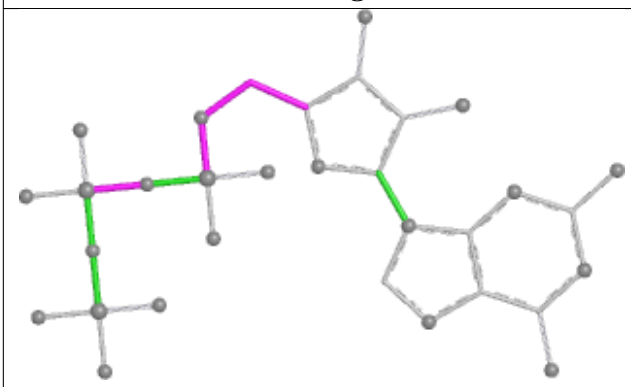
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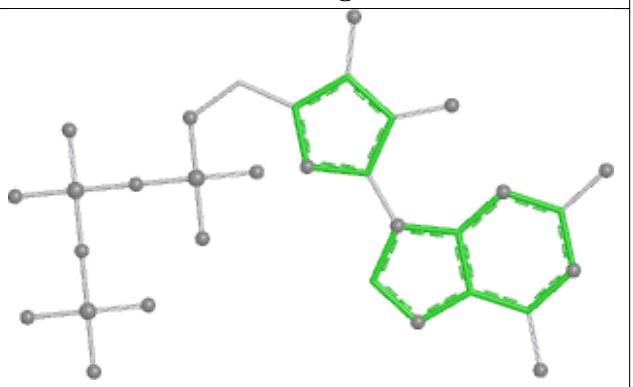
Bond lengths



Bond angles

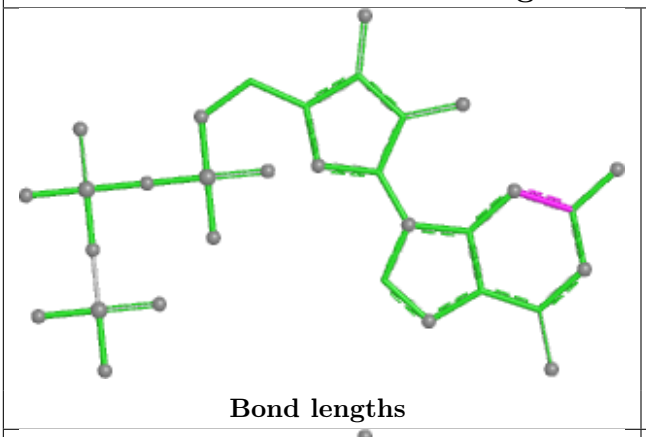


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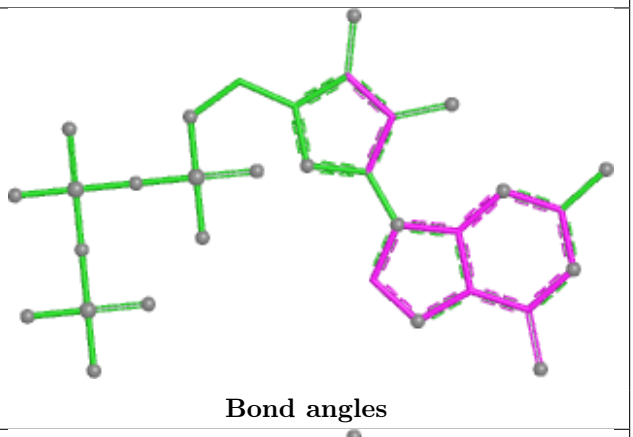


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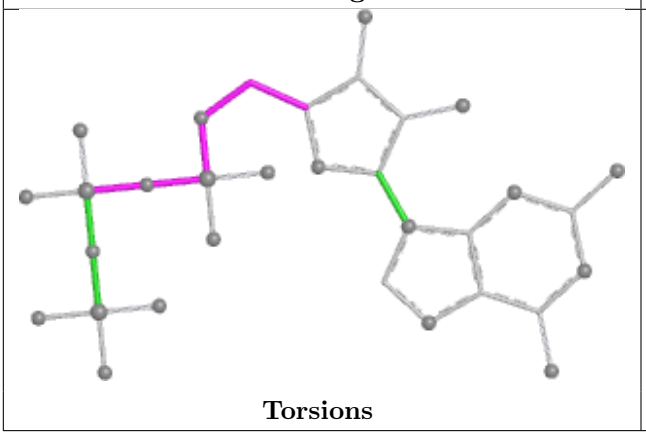
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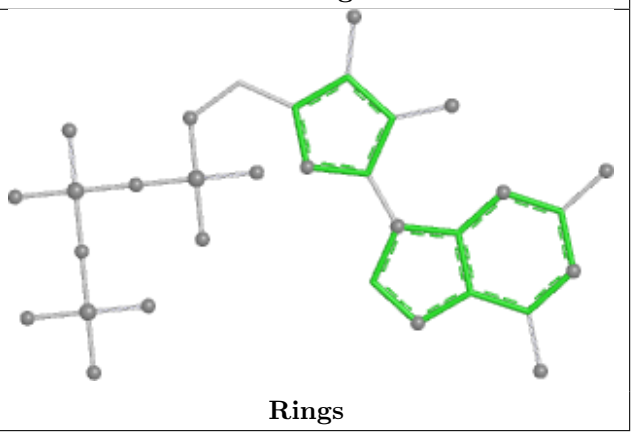
Bond lengths



Bond angles

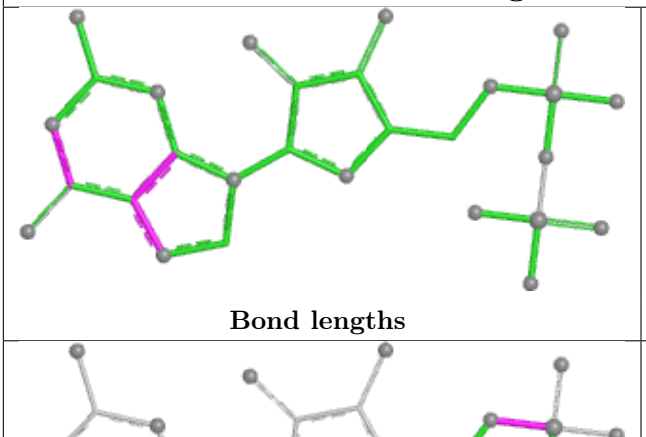


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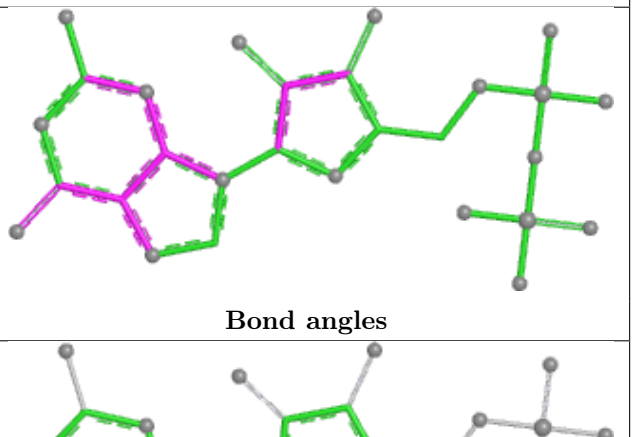


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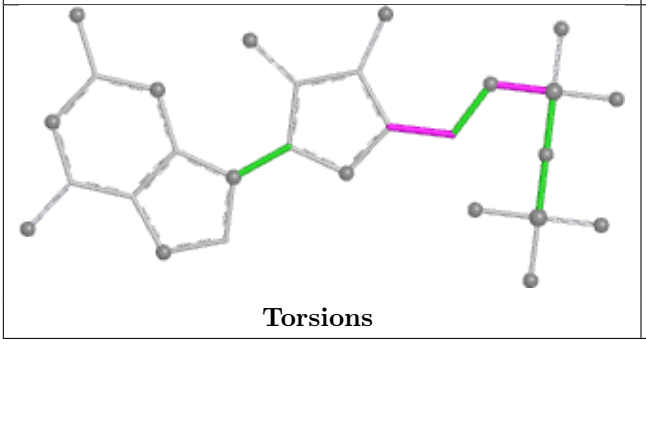
Ligand GDP BN 501



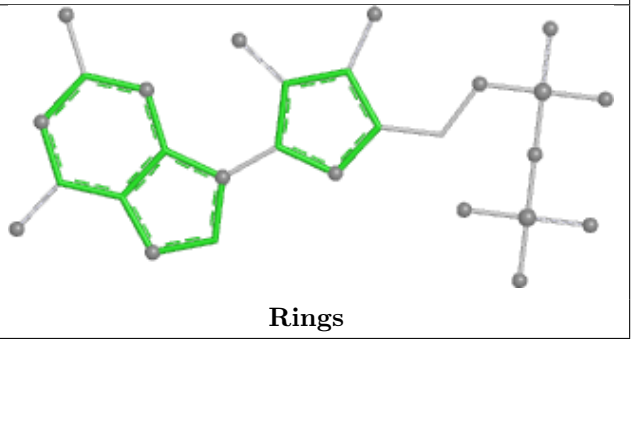
Bond lengths



Bond angles

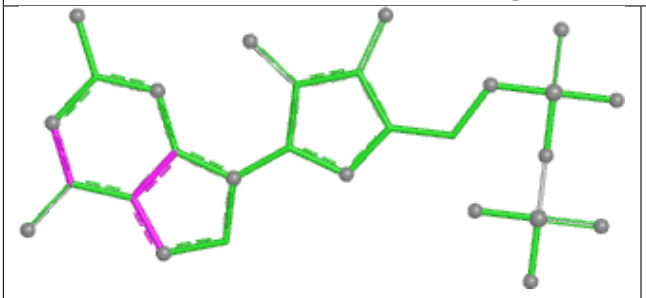


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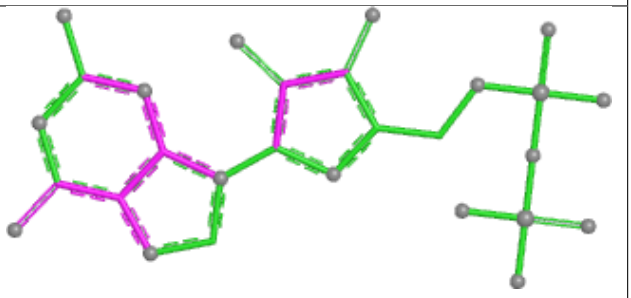


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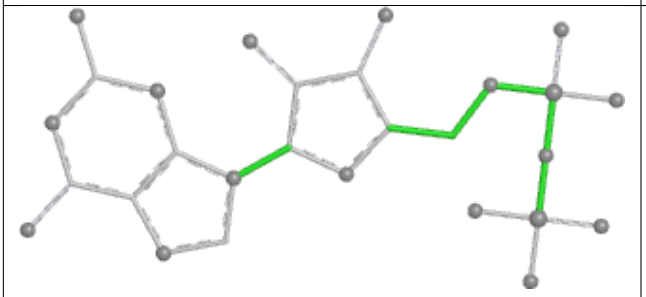
Ligand GDP RH 501



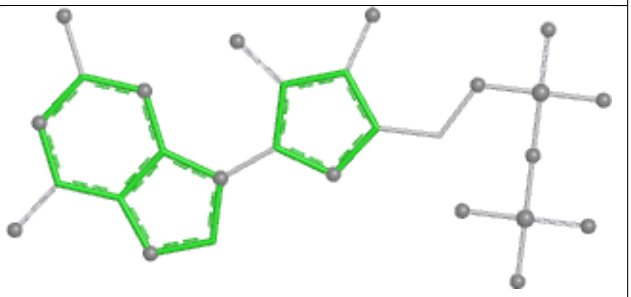
Bond lengths



Bond angles

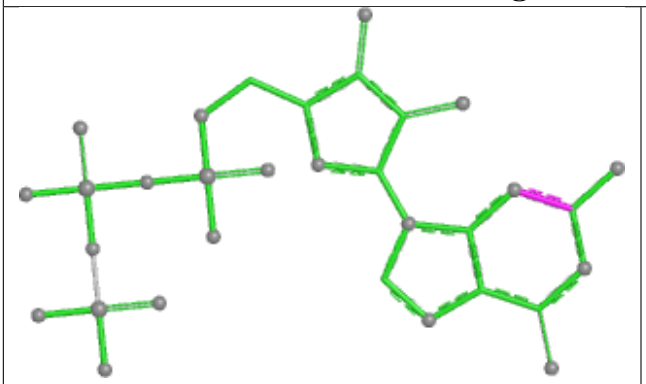


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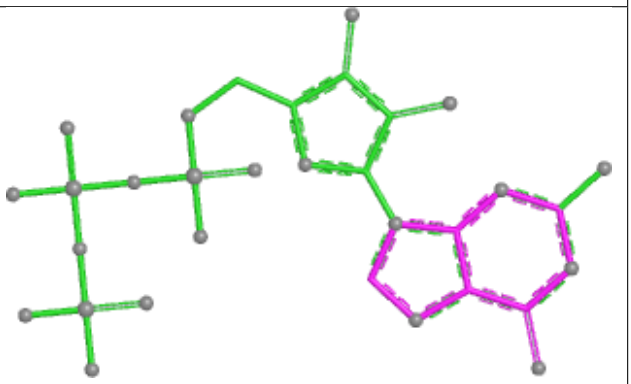


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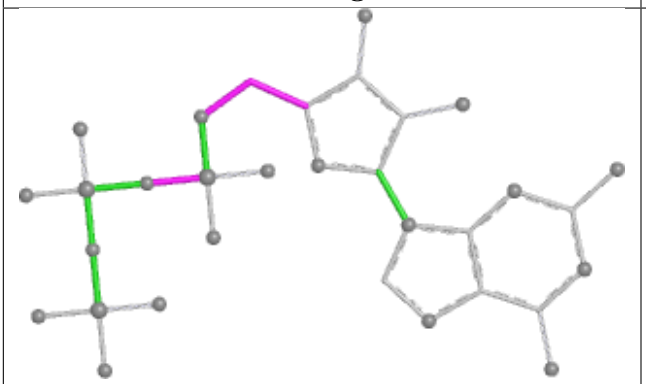
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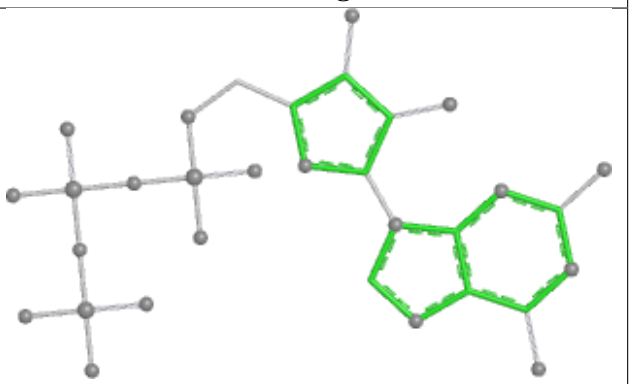
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Bond angles

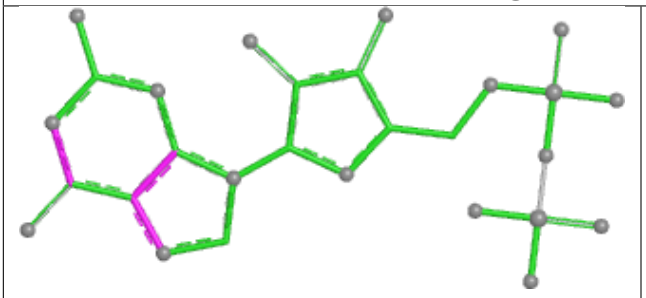


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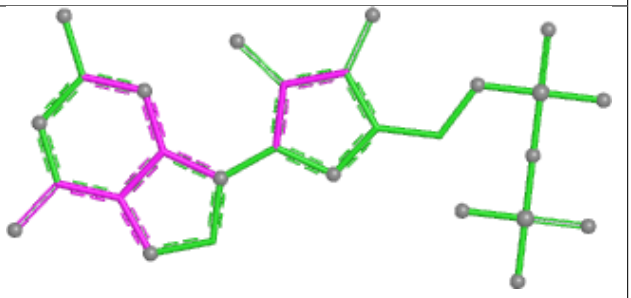


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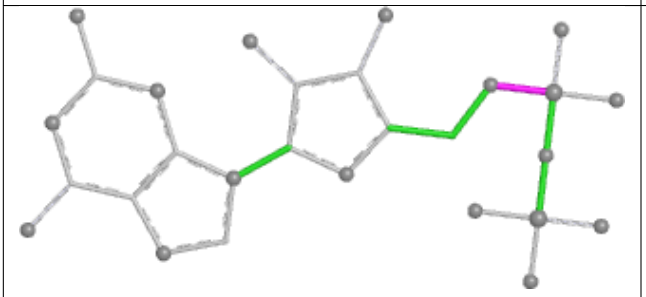
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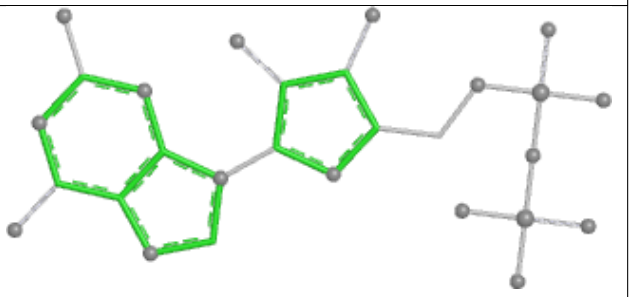
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Bond angles

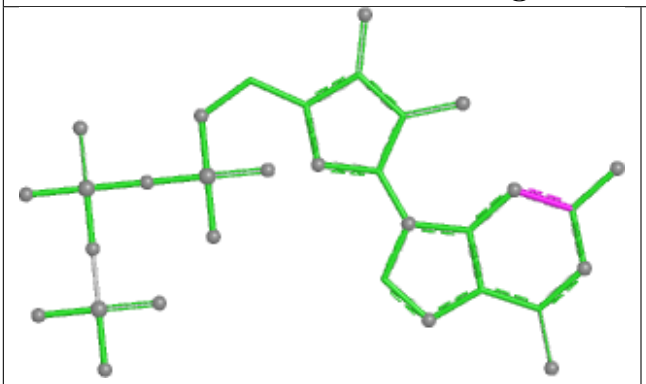


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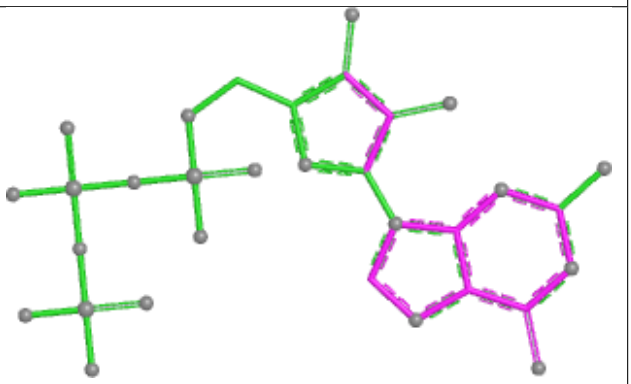


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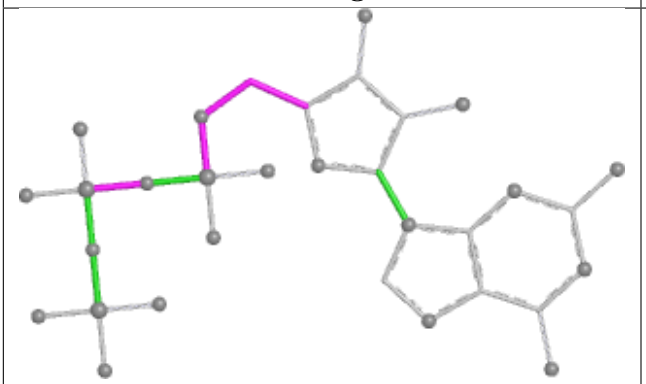
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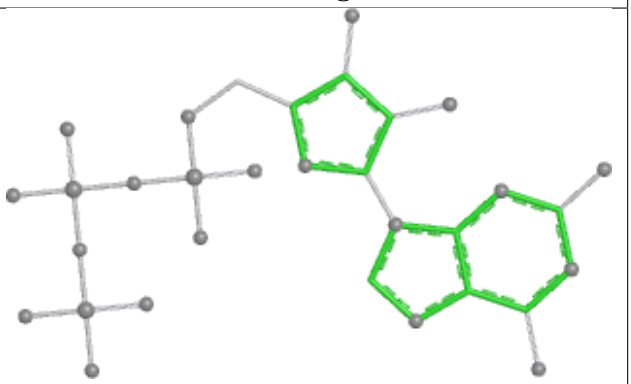
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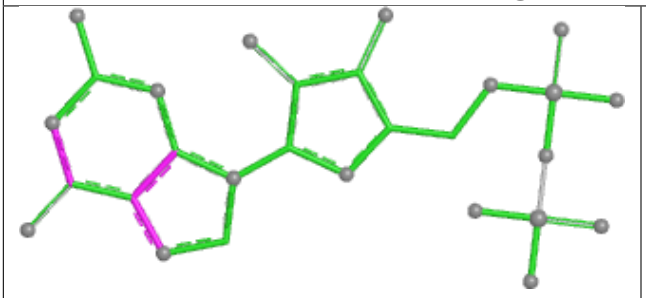


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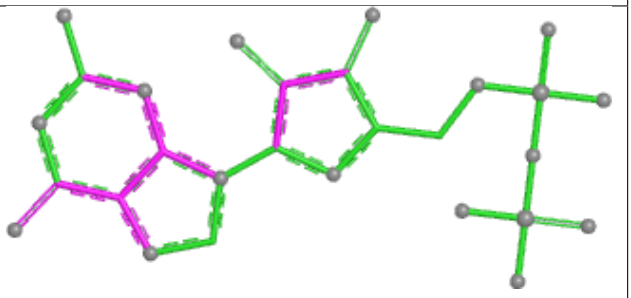


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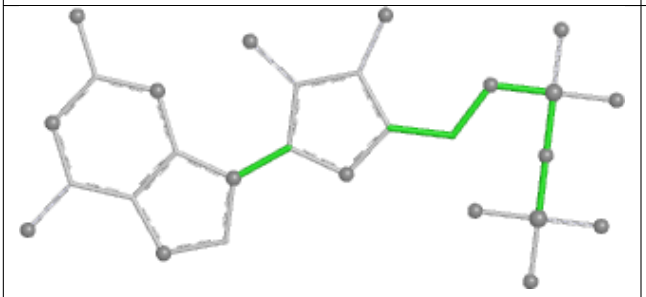
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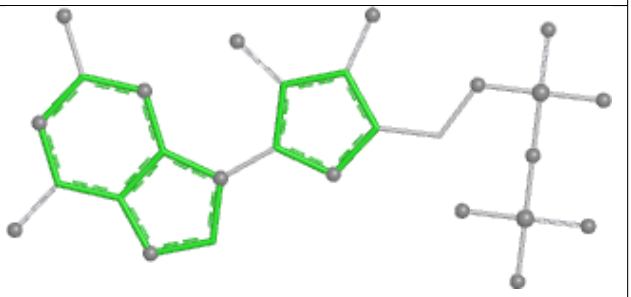
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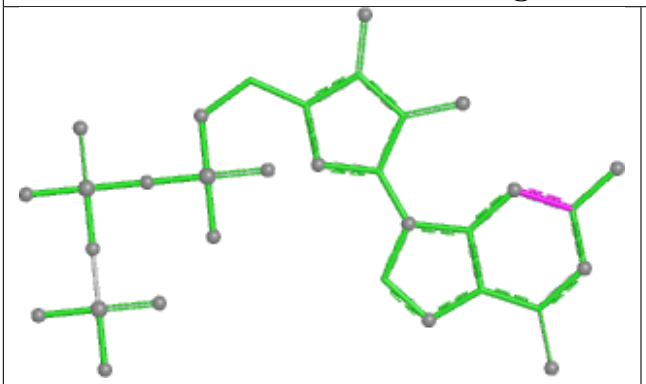


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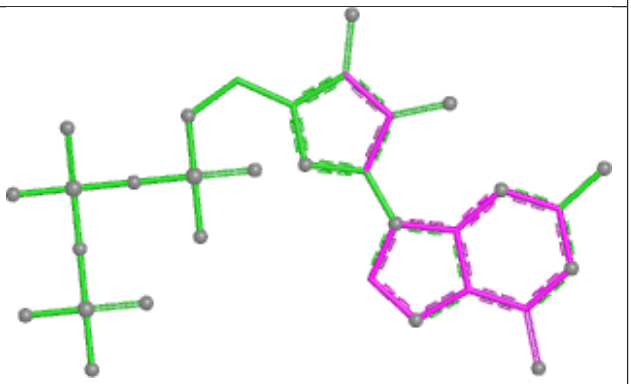


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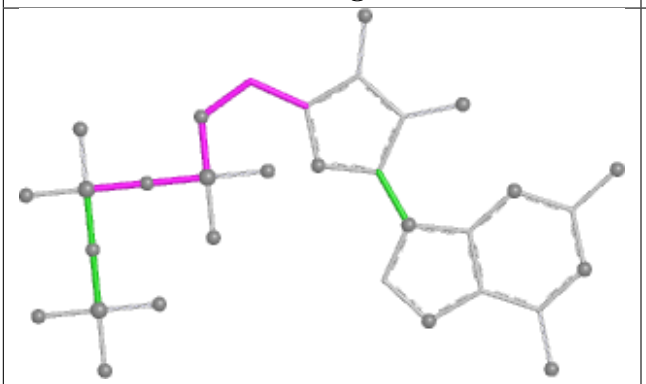
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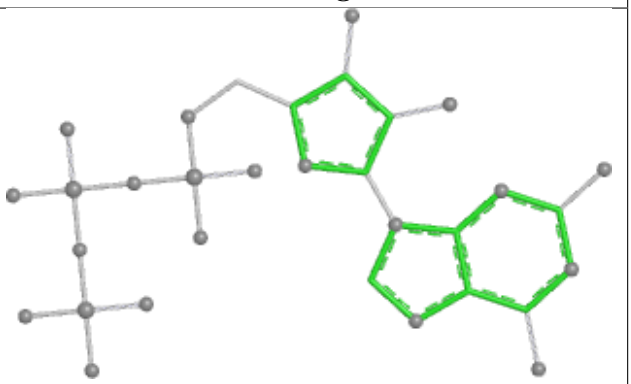
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Bond angles

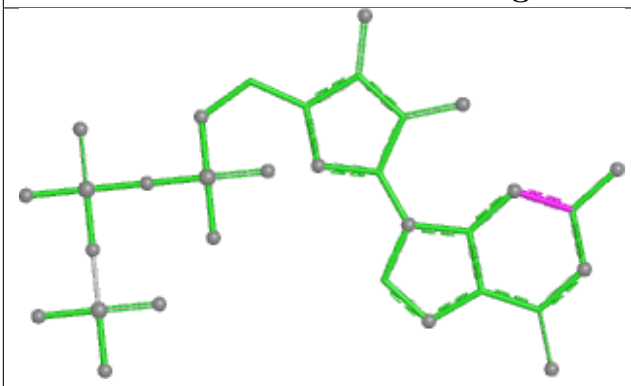


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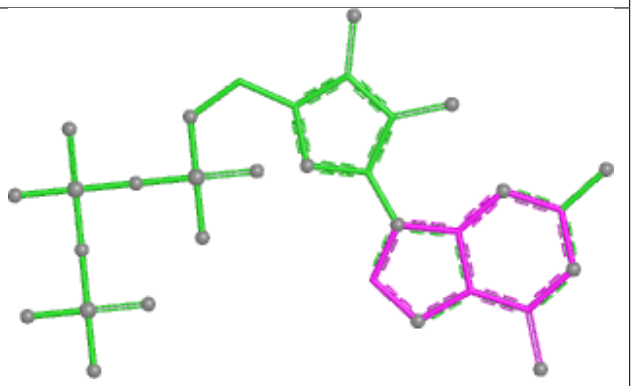


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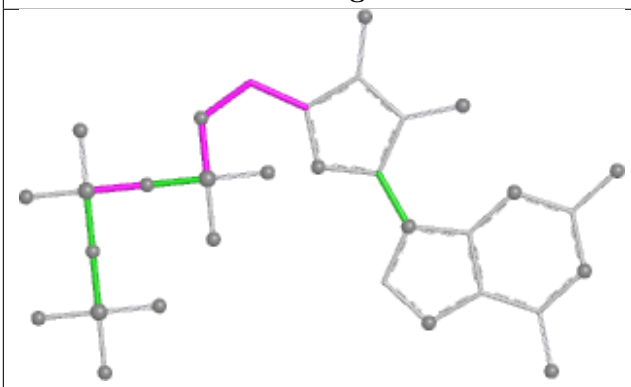
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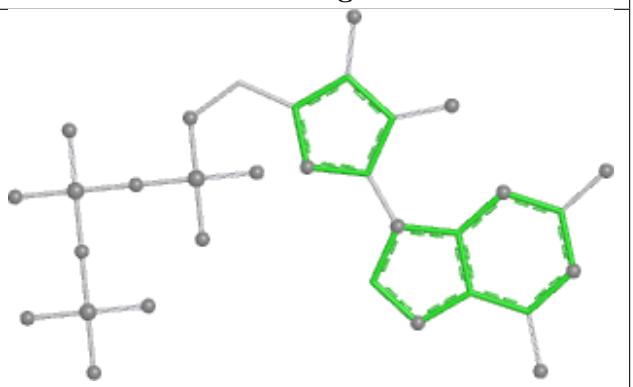
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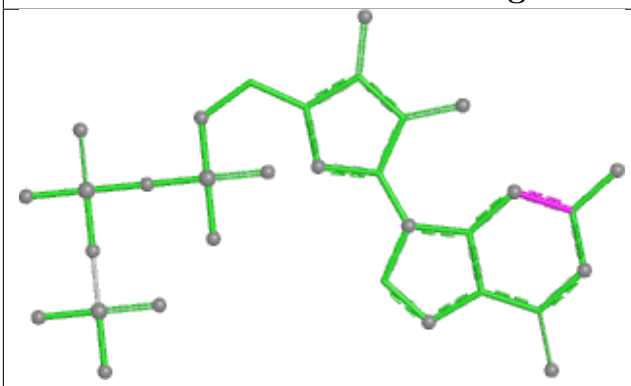


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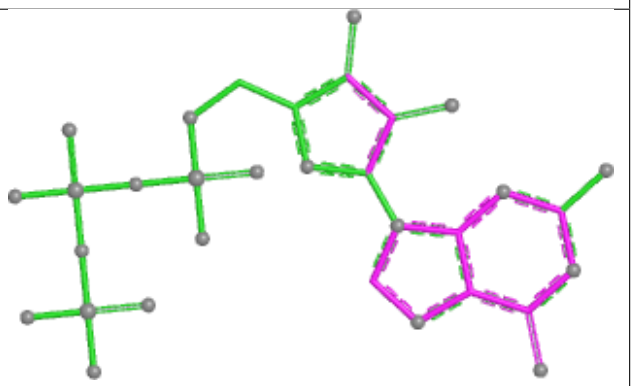


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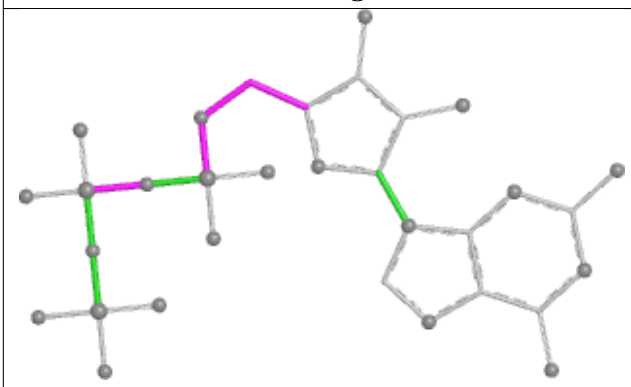
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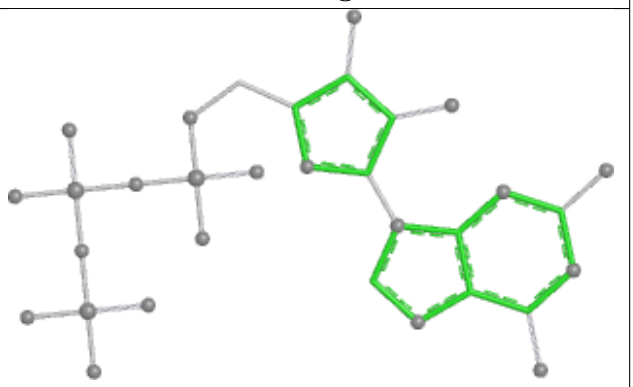
Bond lengths



Bond angles

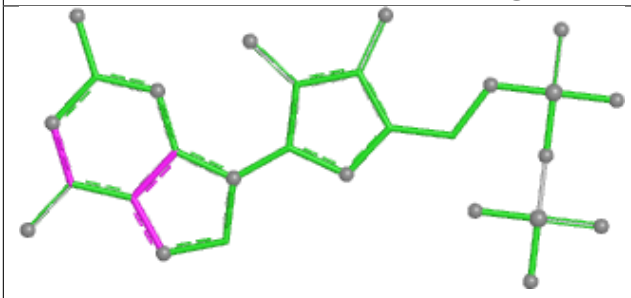


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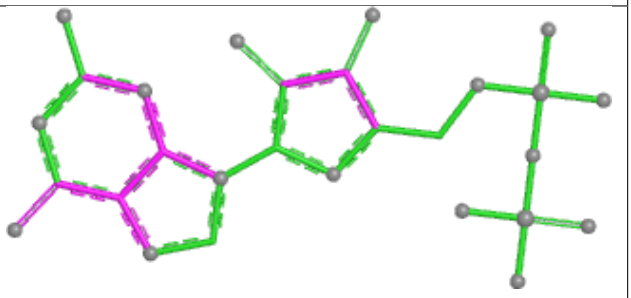


Rings

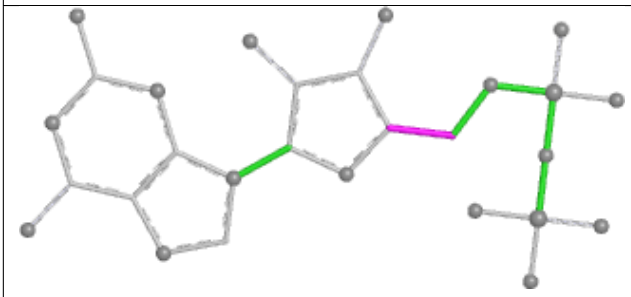
Ligand GDP MJ 501



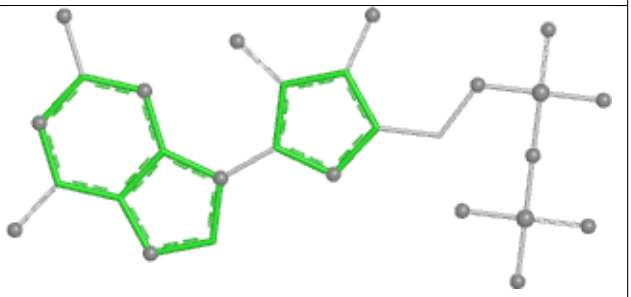
Bond lengths



Bond angles

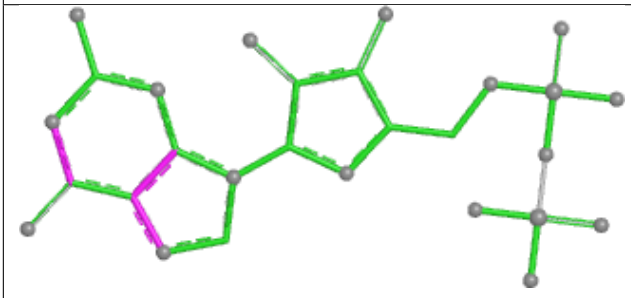


Torsions

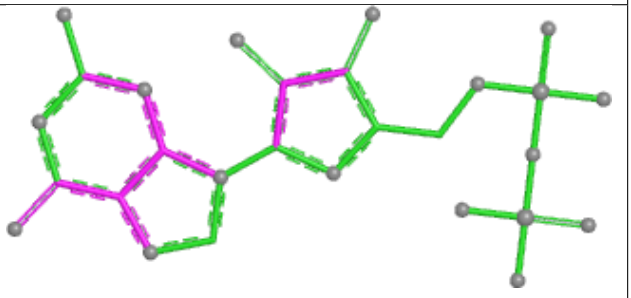


Rings

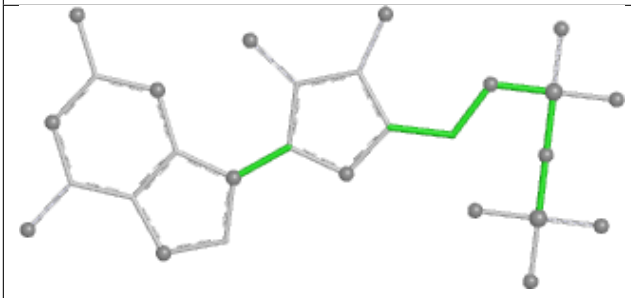
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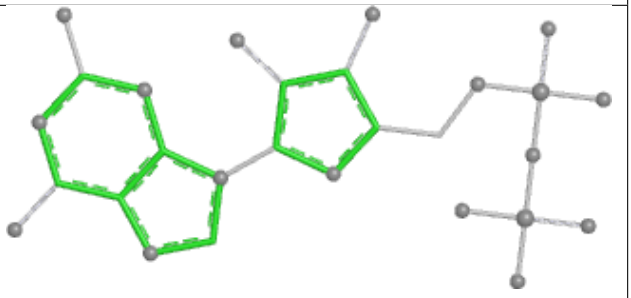
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Bond angles

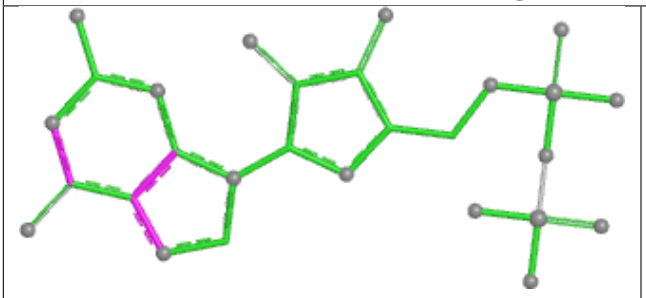


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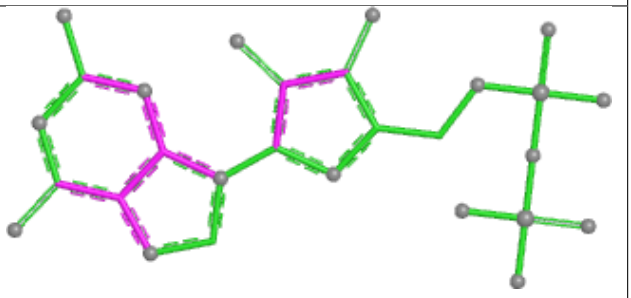


Rings

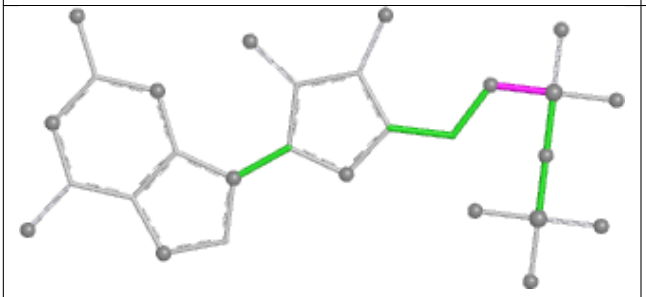
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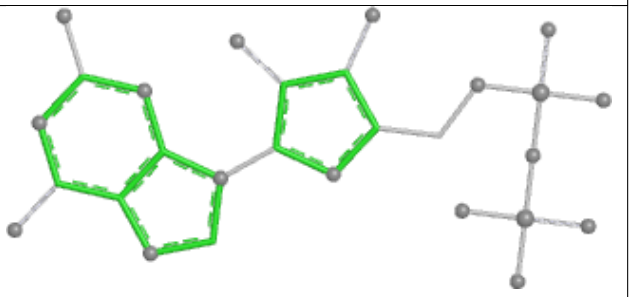
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Bond angles

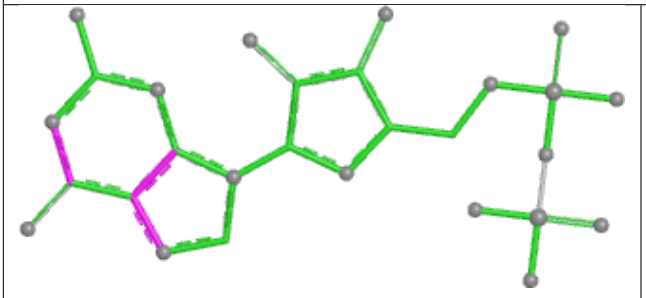


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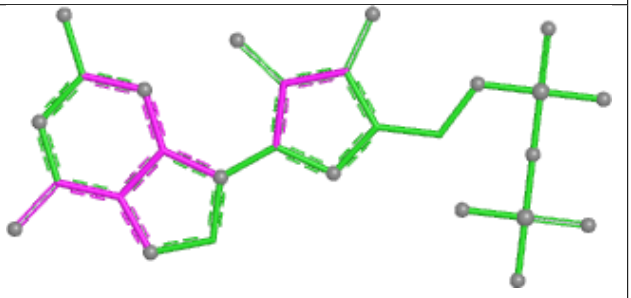


Rings

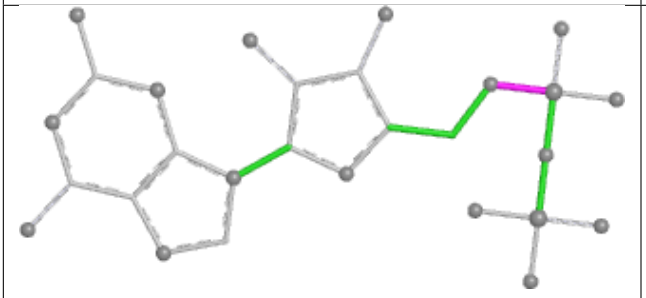
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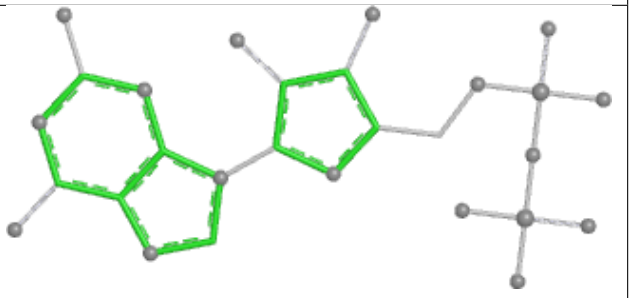
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Bond angles

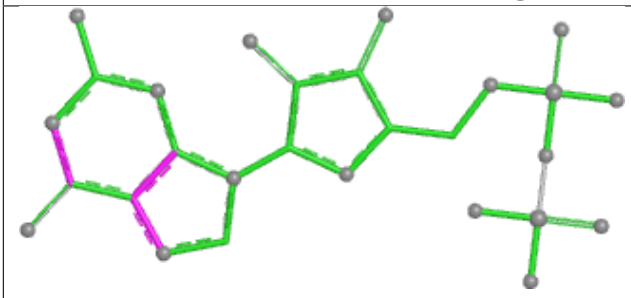


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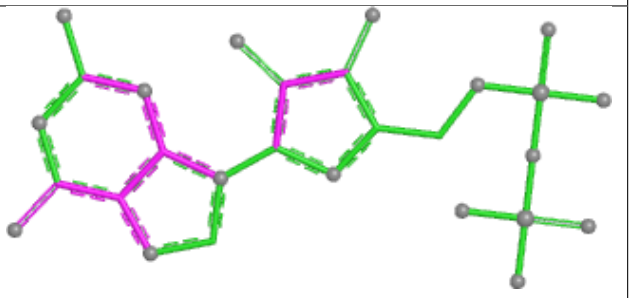


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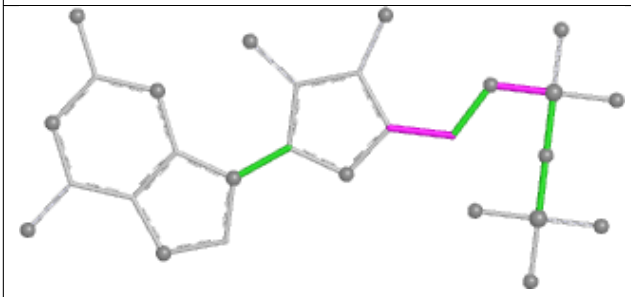
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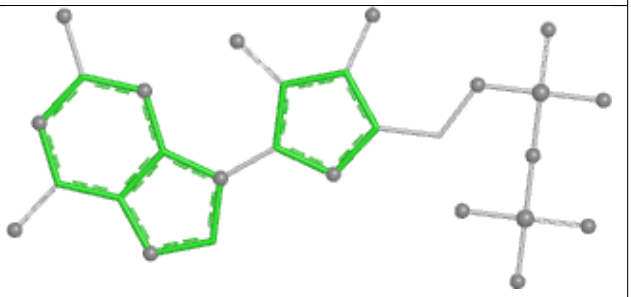
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Bond angles

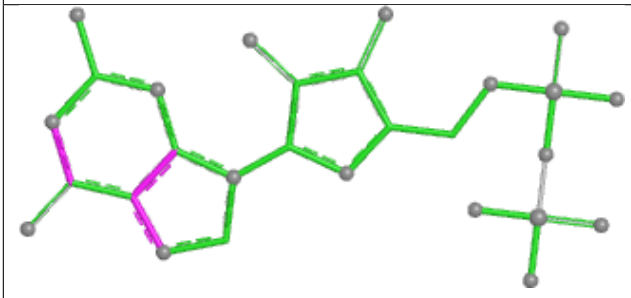


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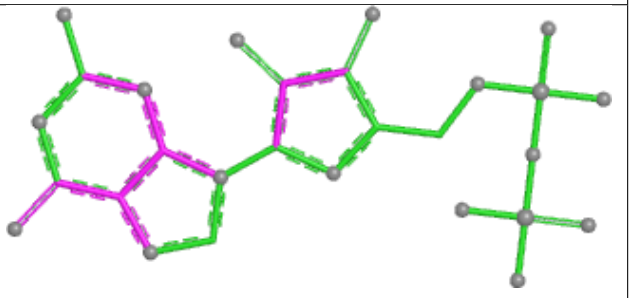


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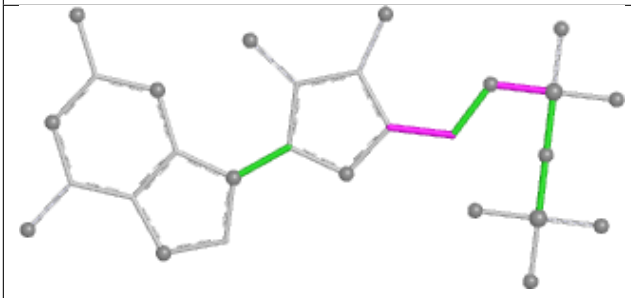
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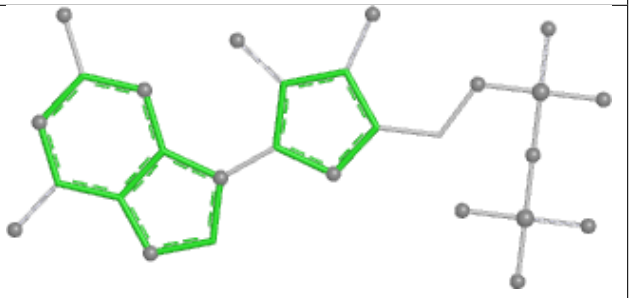
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Bond angles

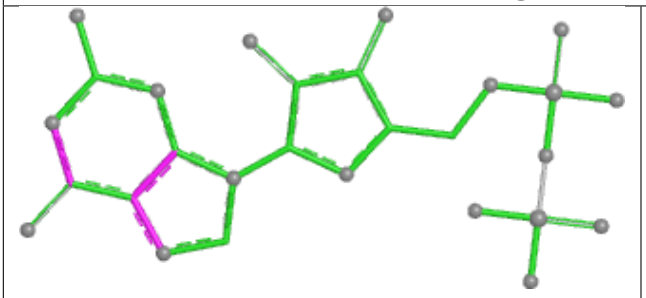


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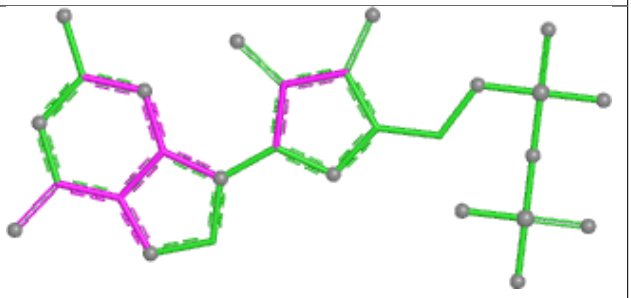


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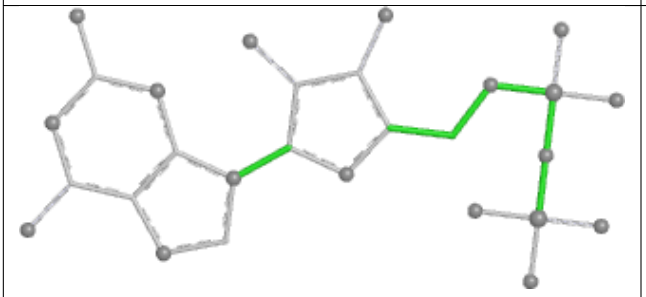
Ligand GDP BJ 501



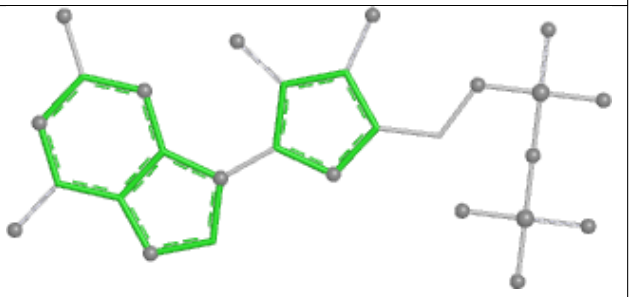
Bond lengths



Bond angles

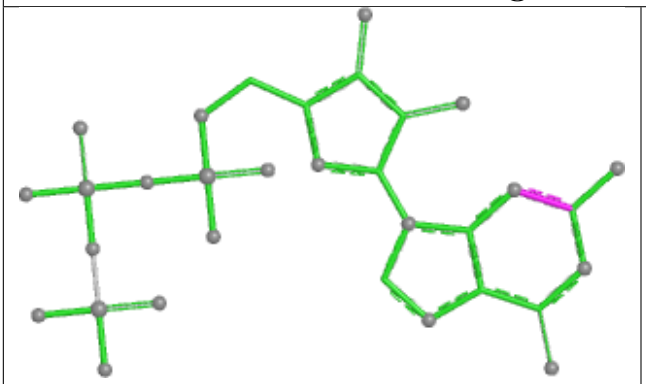


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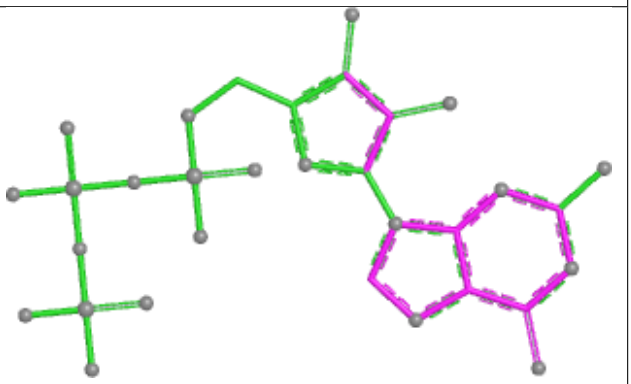


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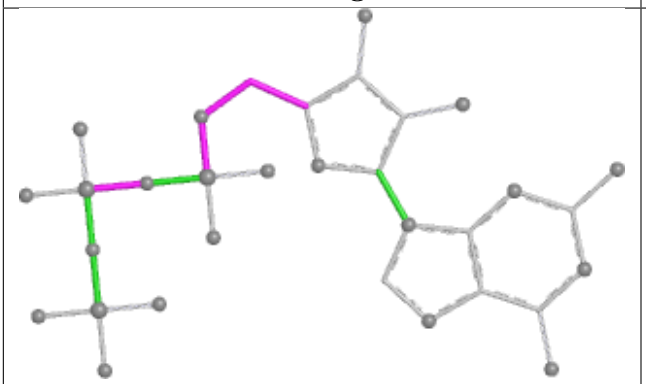
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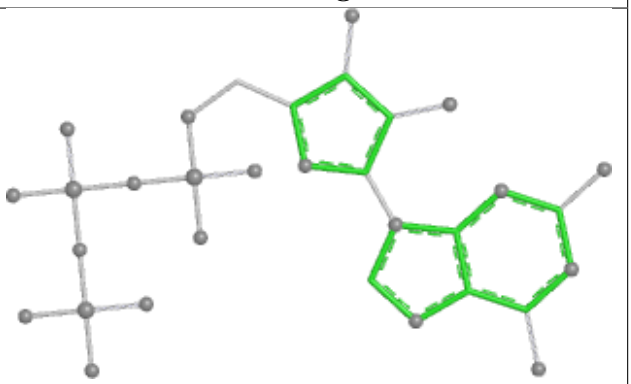
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Bond angles

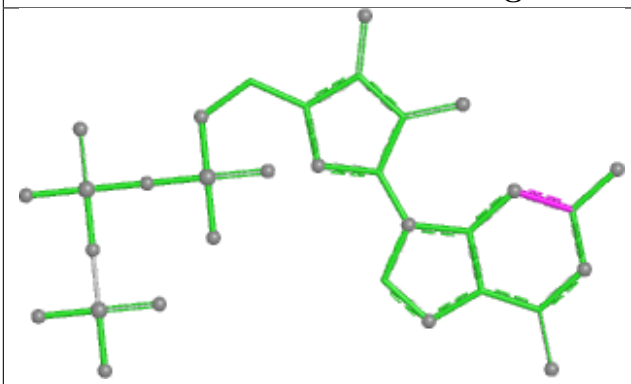


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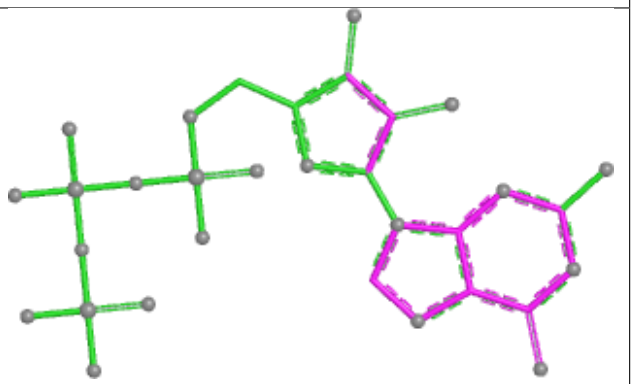


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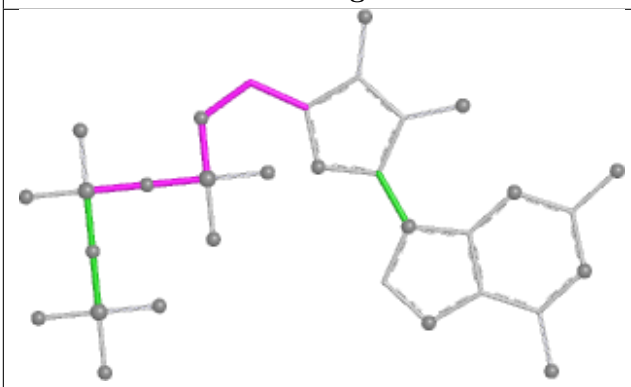
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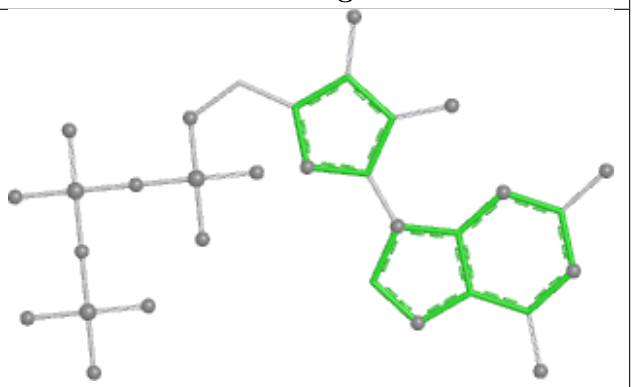
Bond lengths



Bond angles

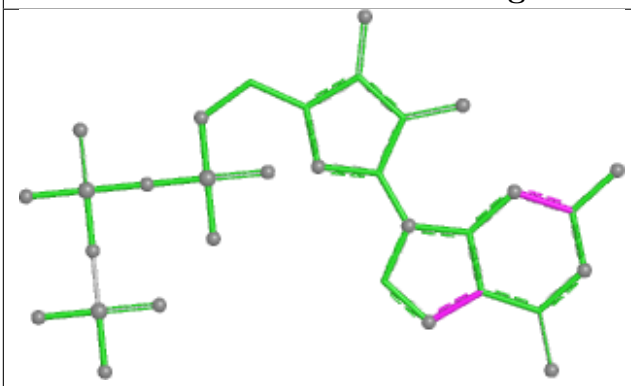


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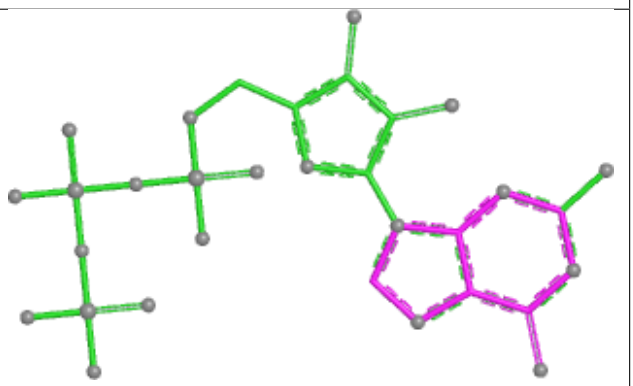


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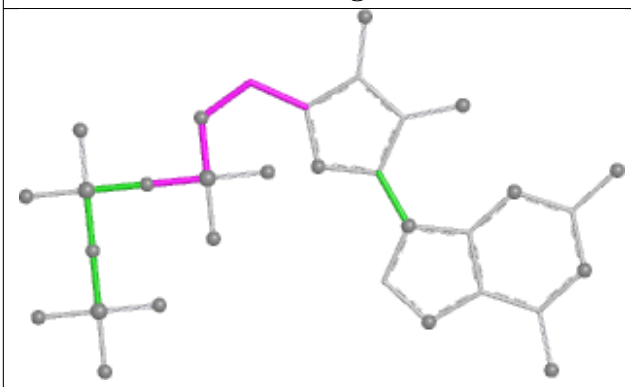
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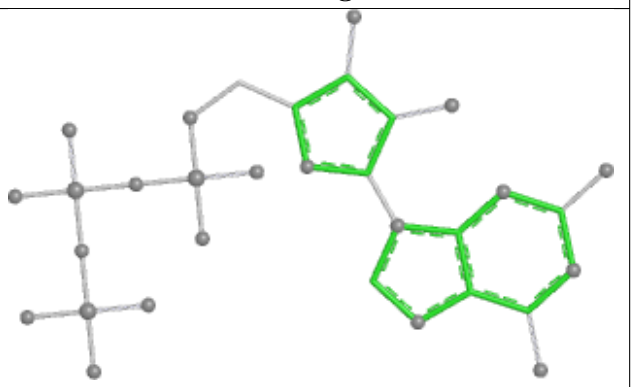
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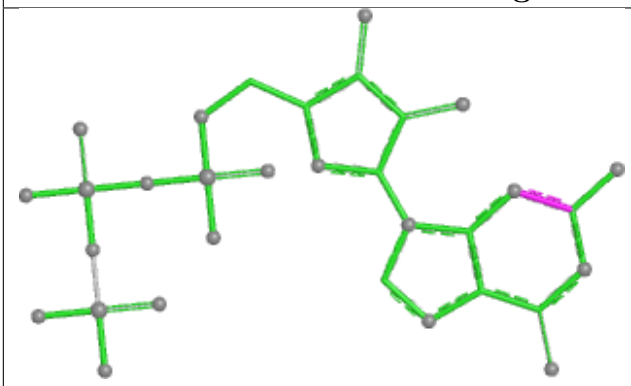


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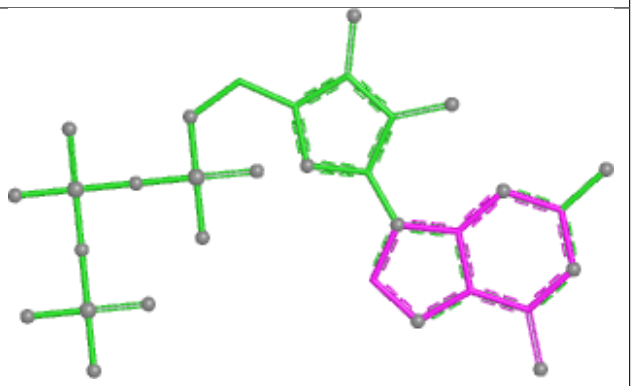


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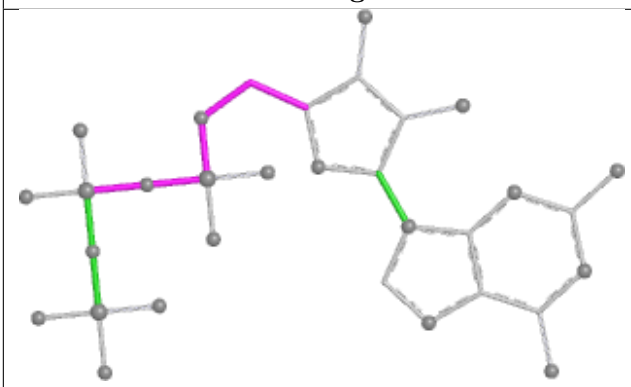
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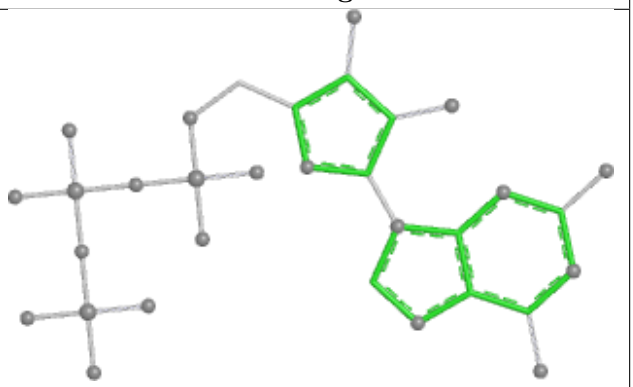
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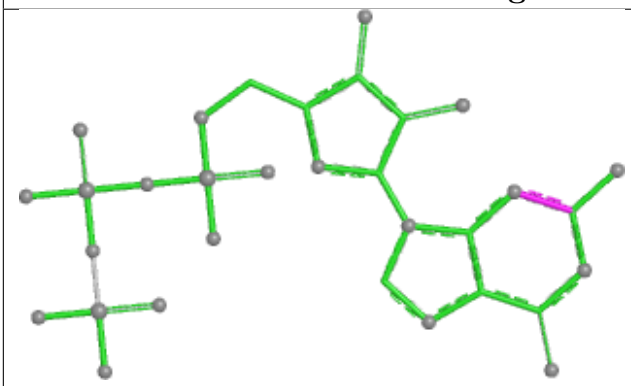


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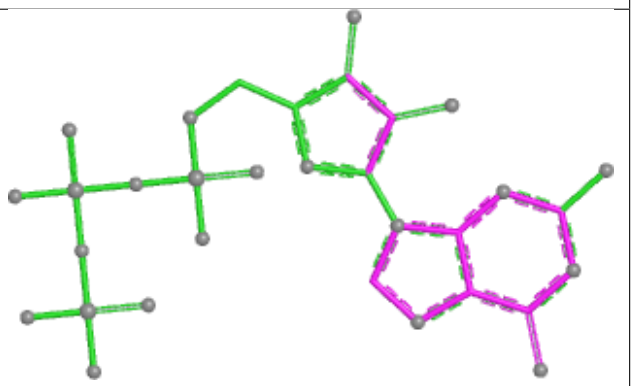


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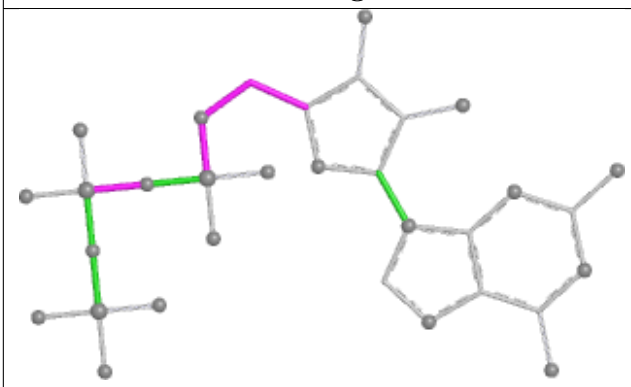
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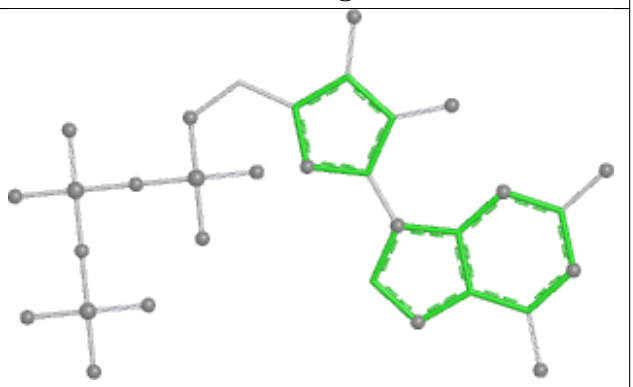
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Bond angles

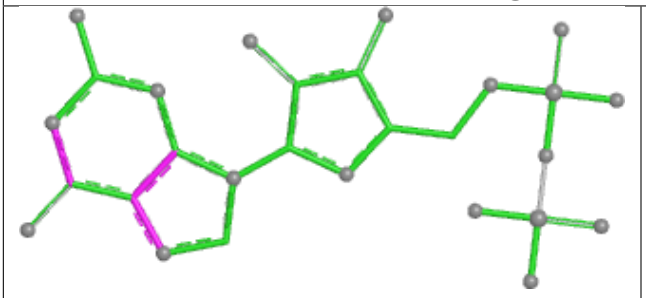


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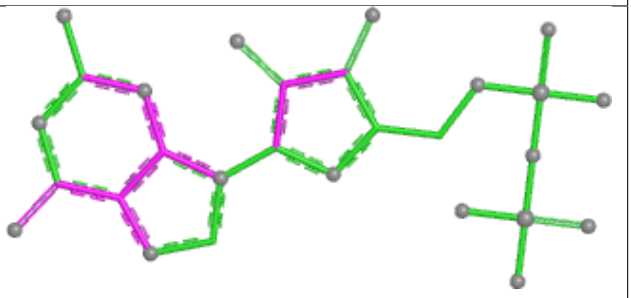


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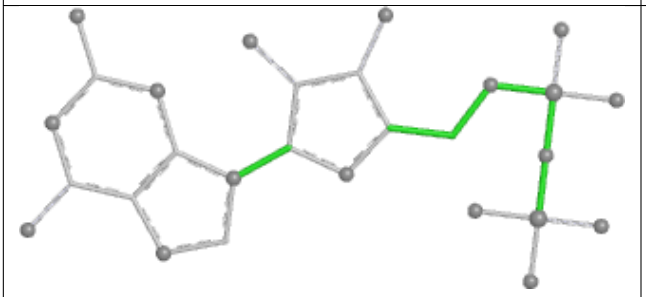
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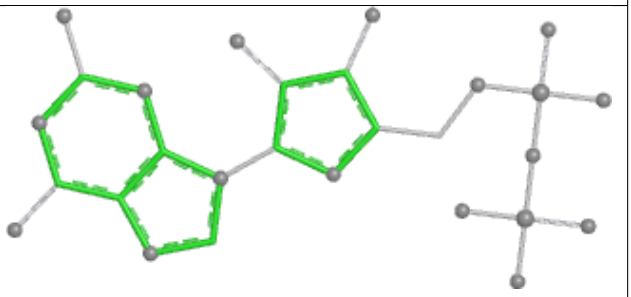
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Bond angles

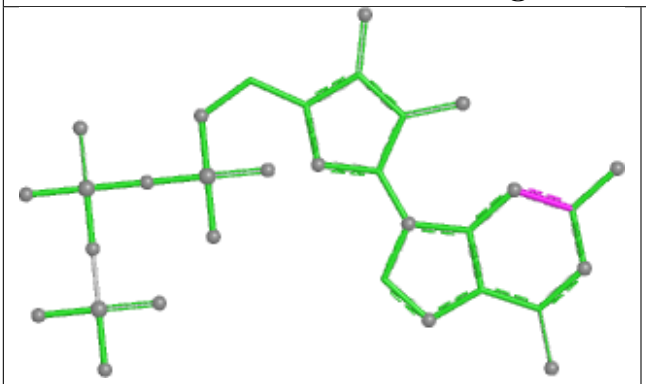


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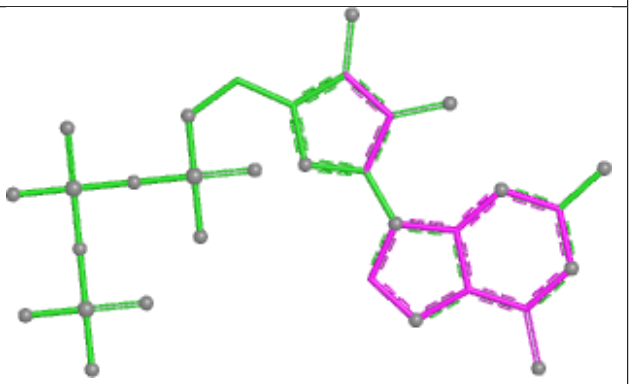


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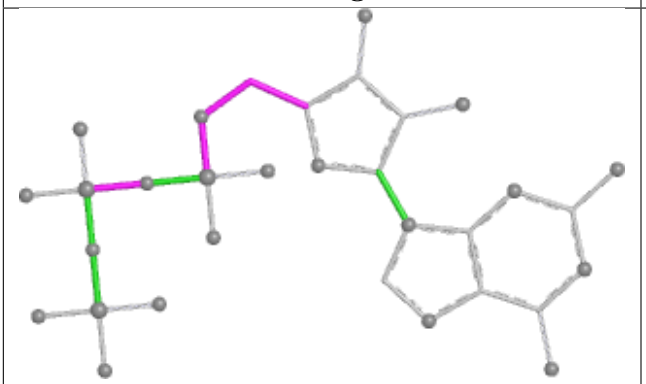
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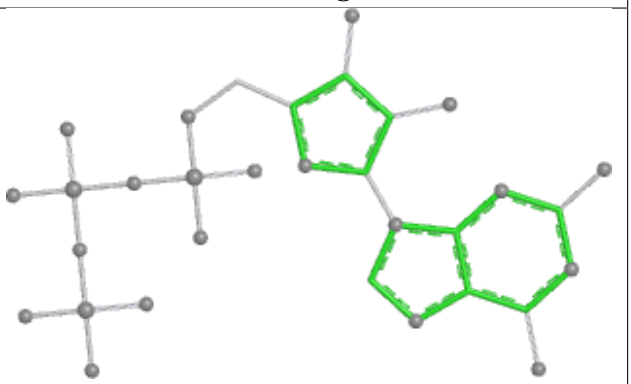
Bond lengths



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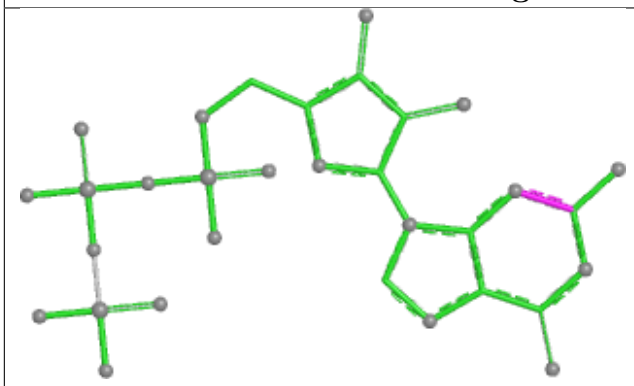


Torsions

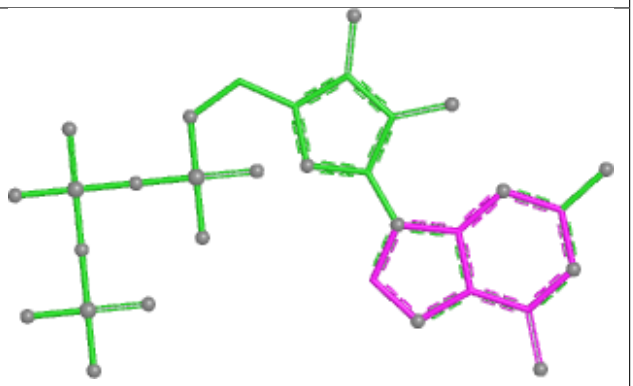


Rings

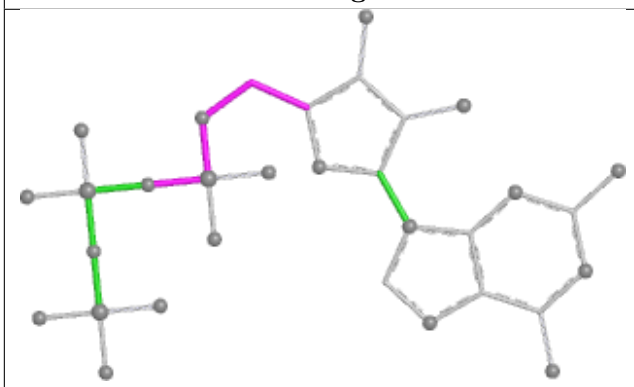
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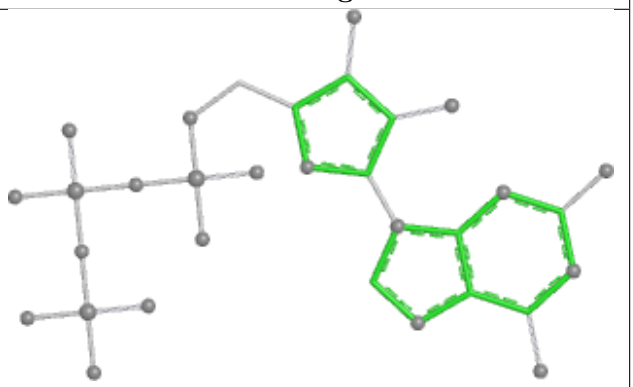
Bond lengths



Bond angles

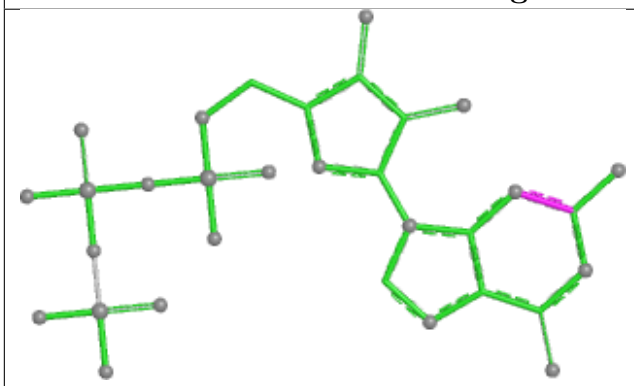


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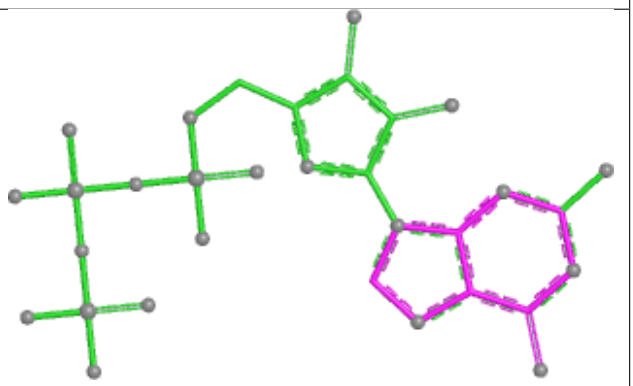


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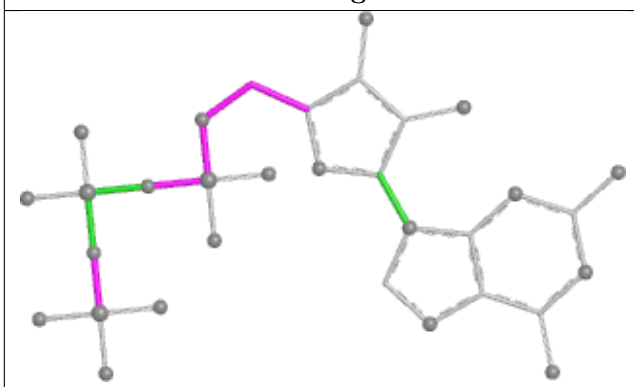
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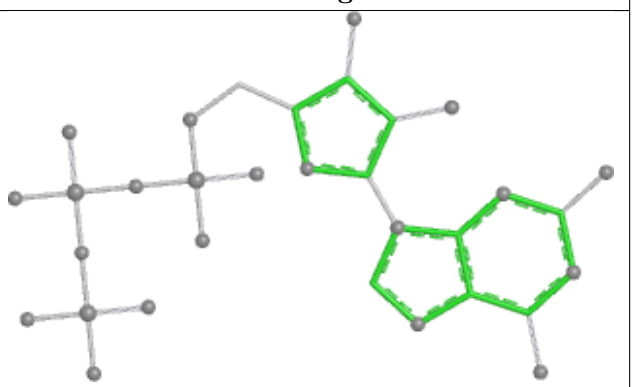
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Bond angles

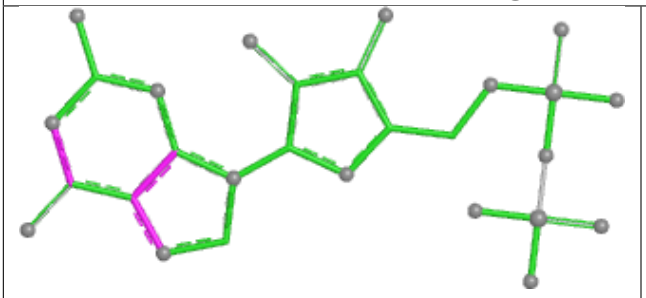


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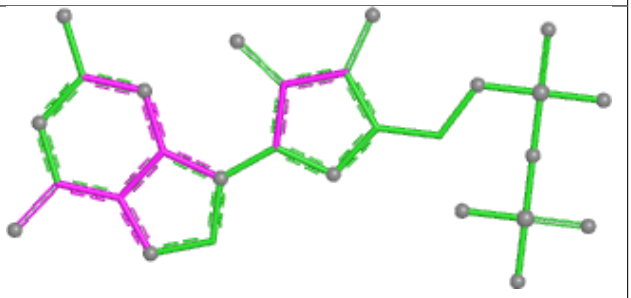


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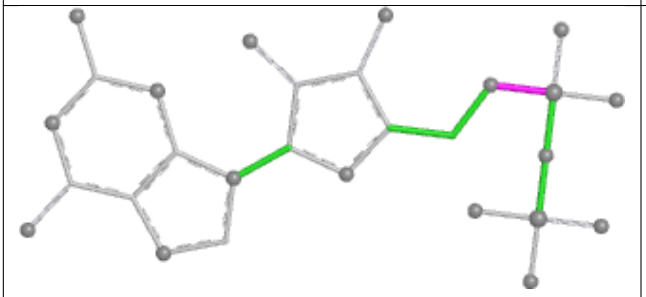
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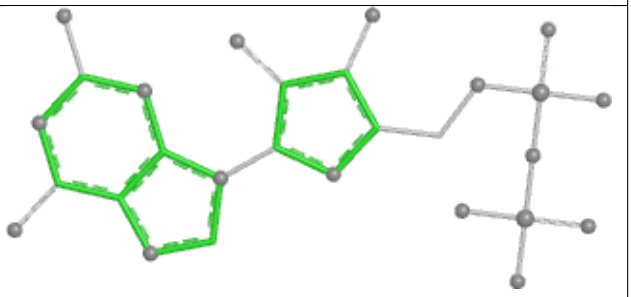
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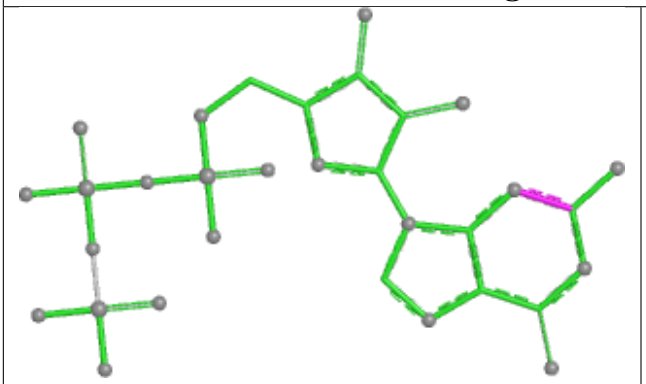


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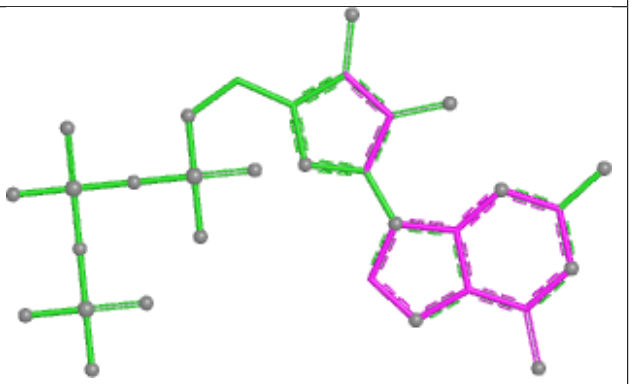


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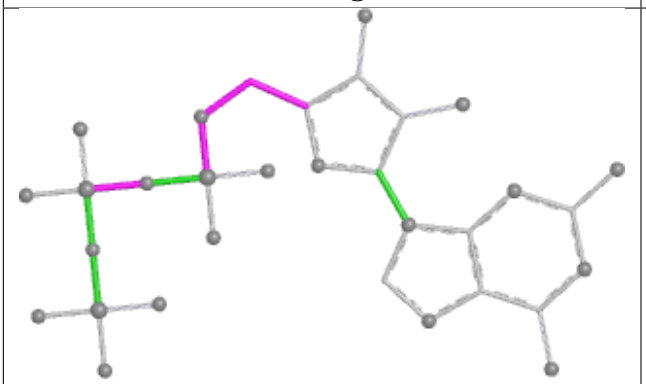
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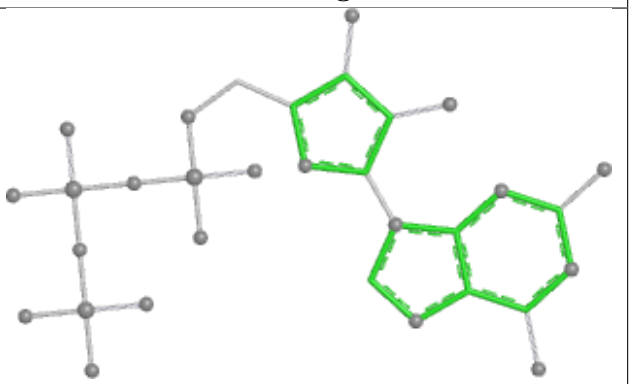
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Bond angles

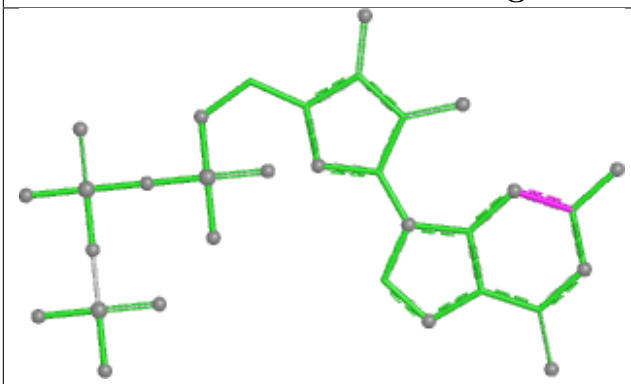


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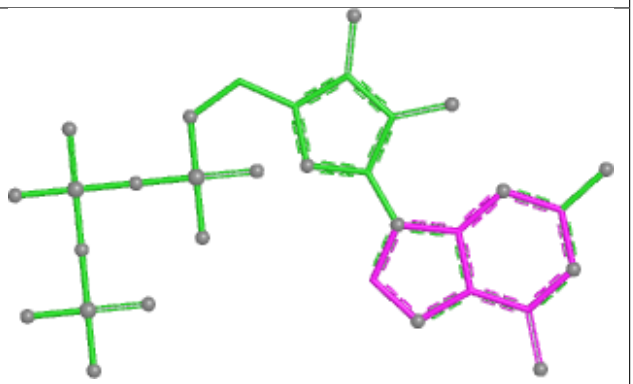


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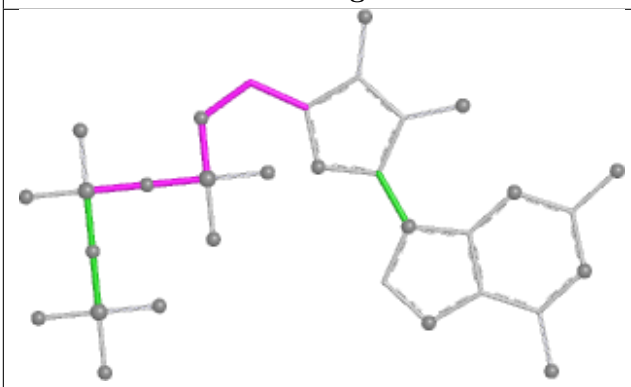
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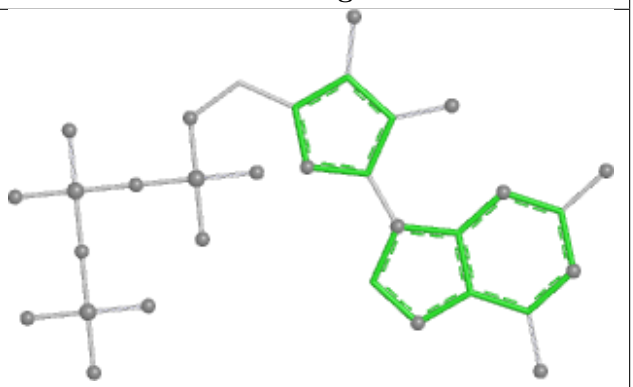
Bond lengths



Bond angles

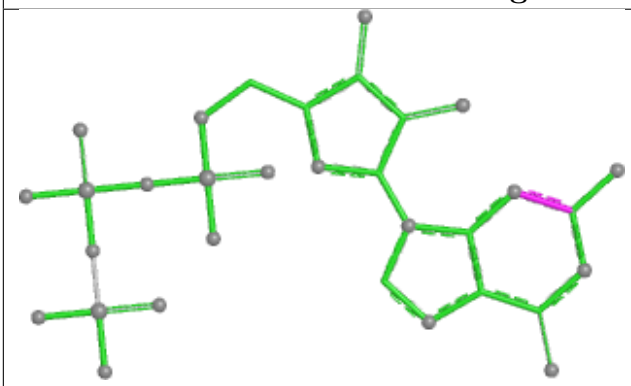


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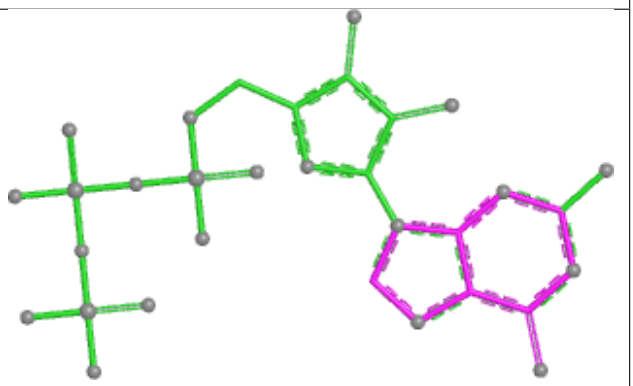


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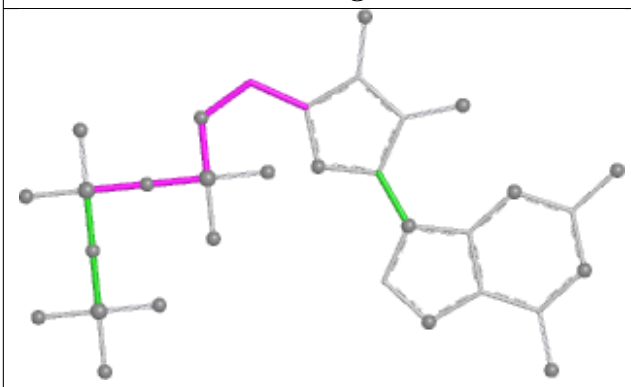
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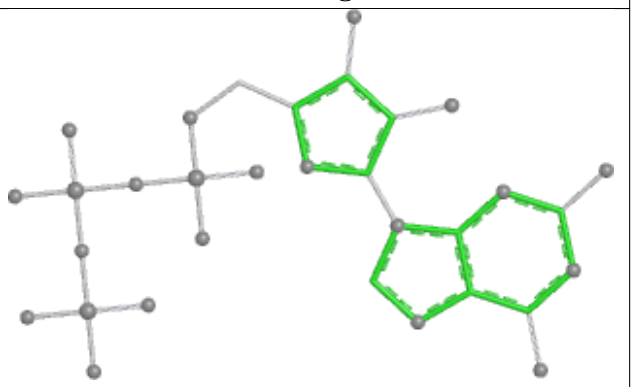
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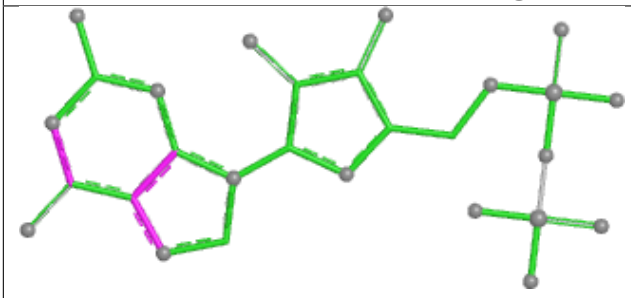


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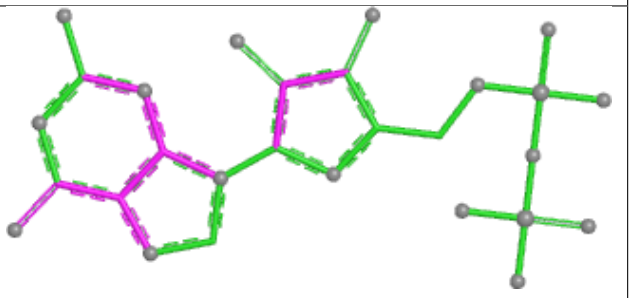


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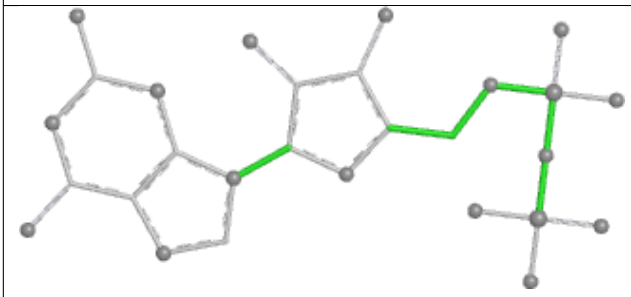
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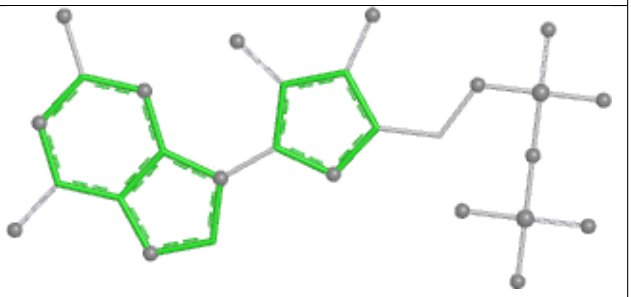
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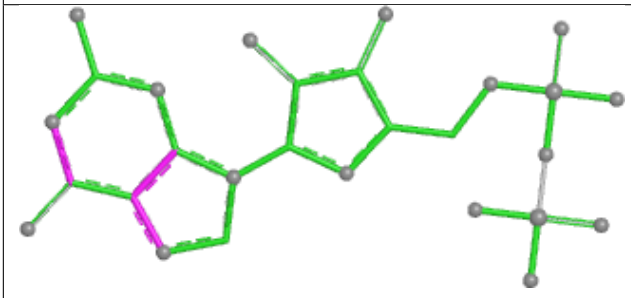


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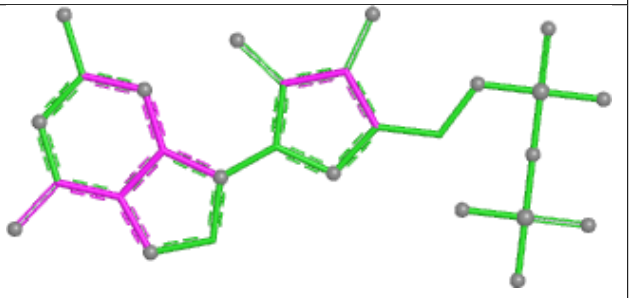


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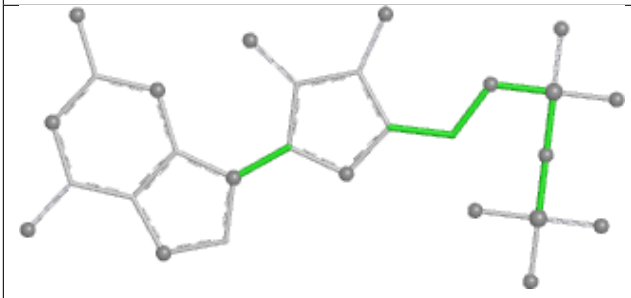
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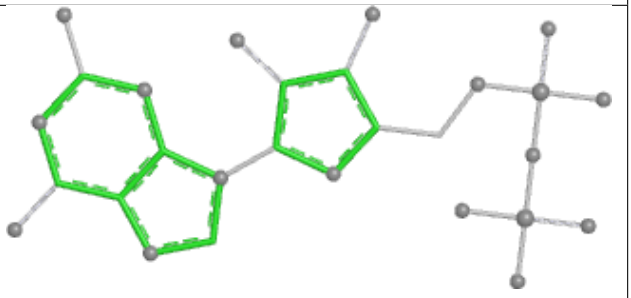
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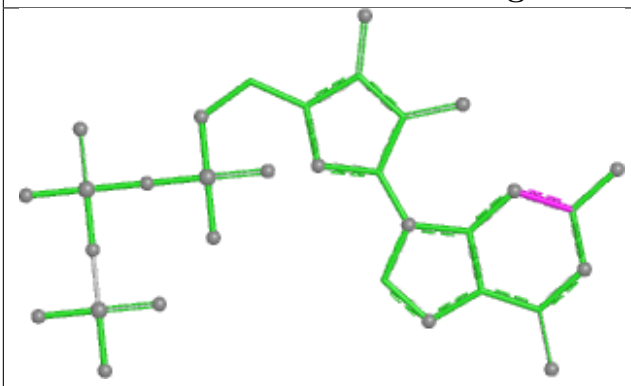


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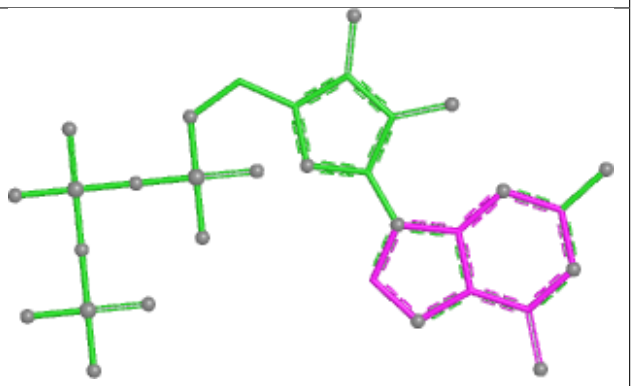


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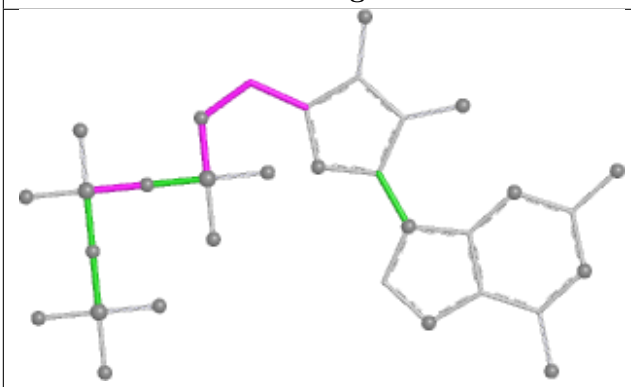
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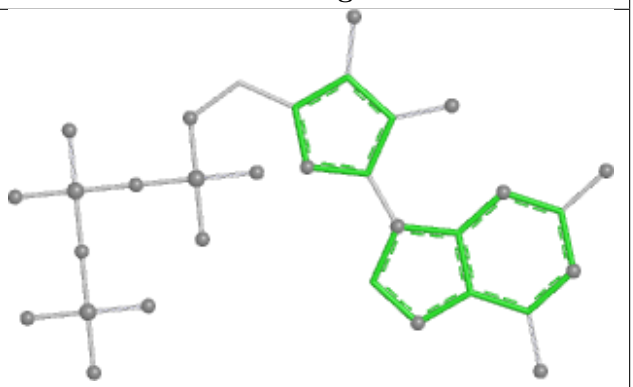
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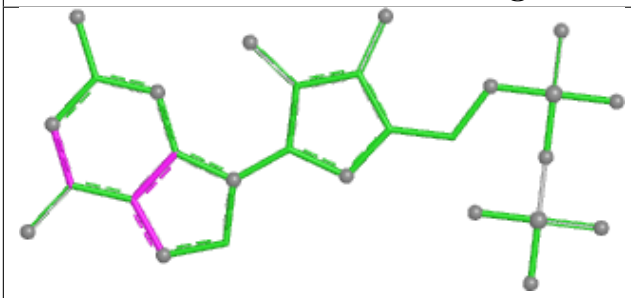


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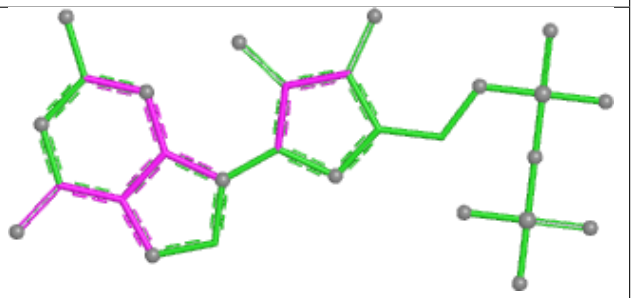


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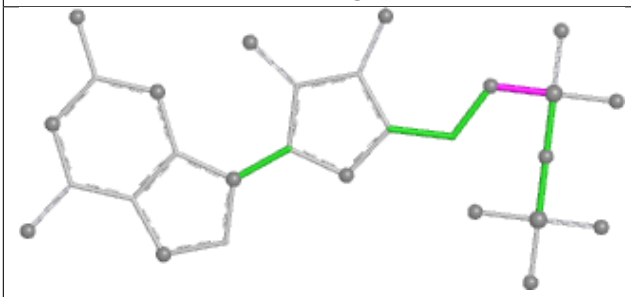
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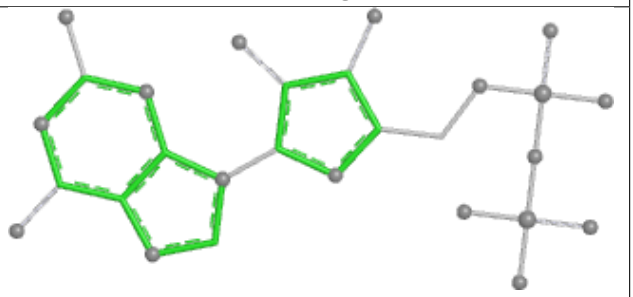
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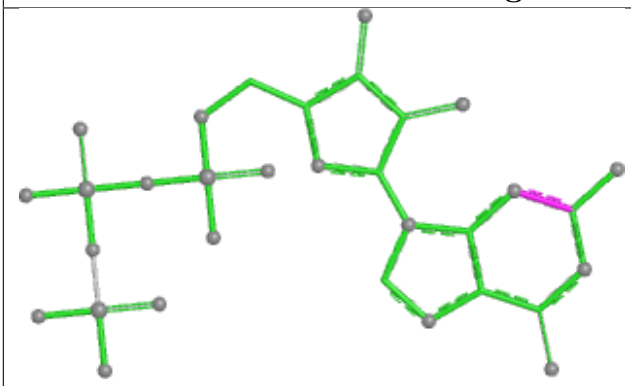


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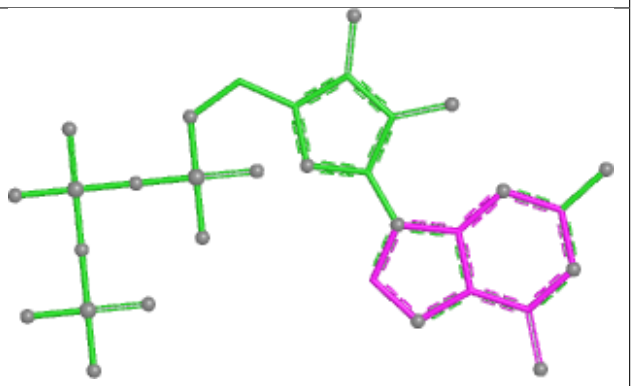


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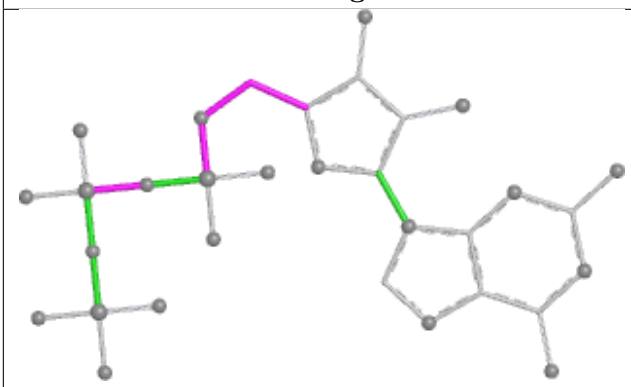
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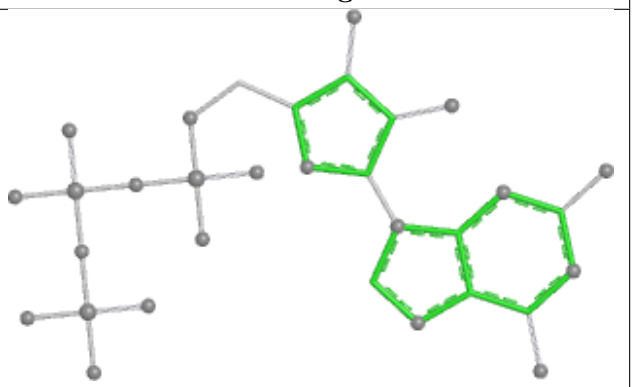
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Bond angles

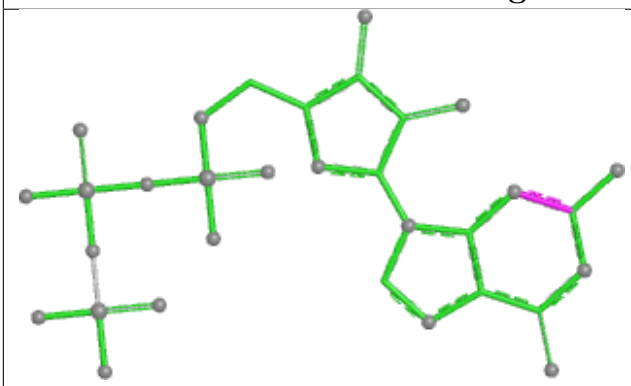


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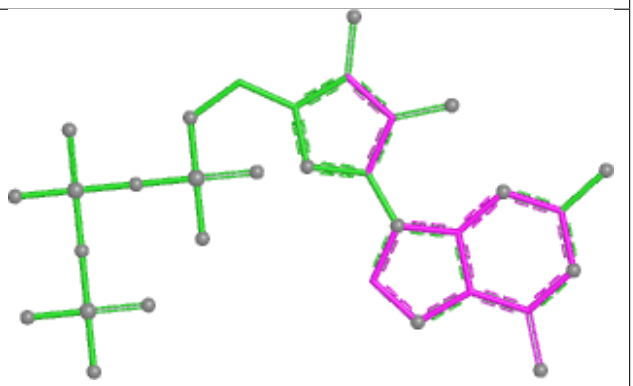


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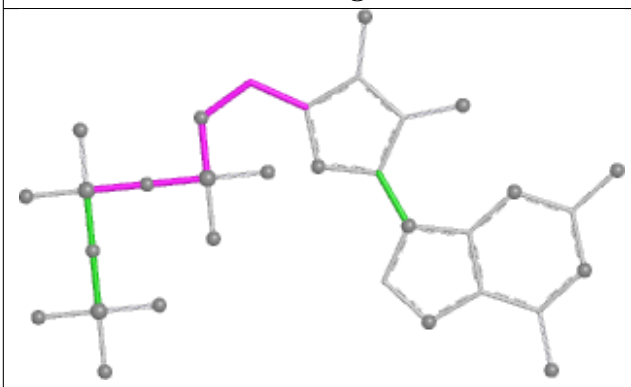
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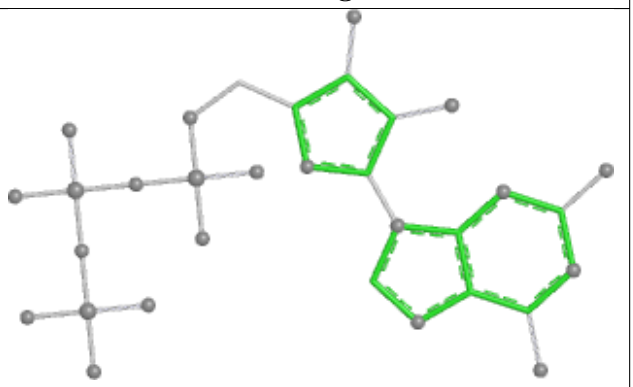
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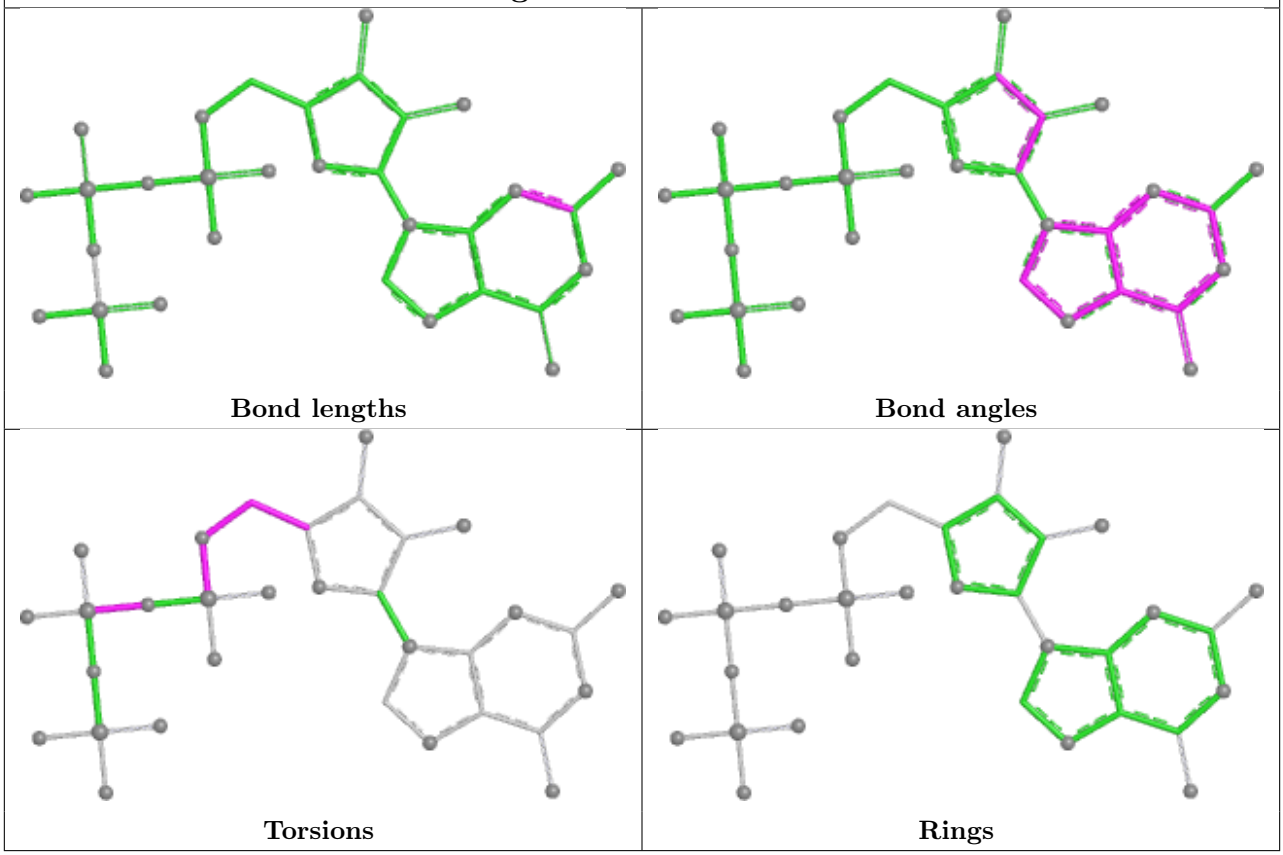


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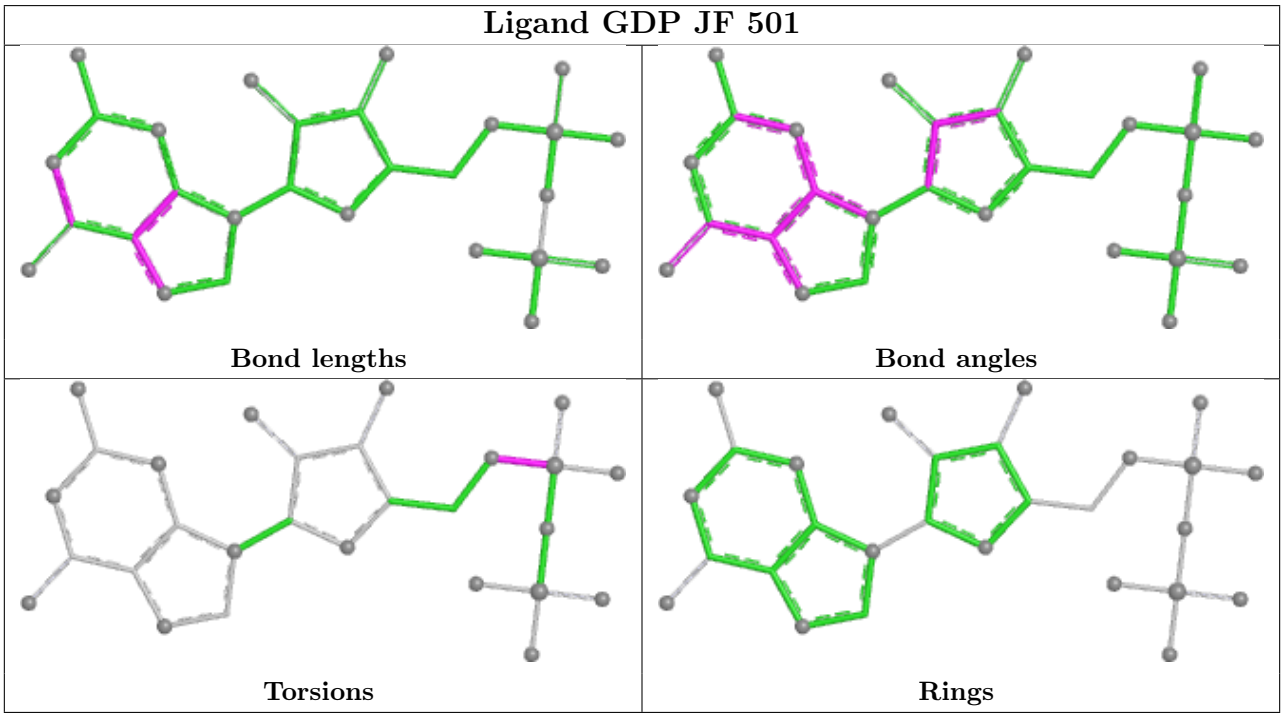


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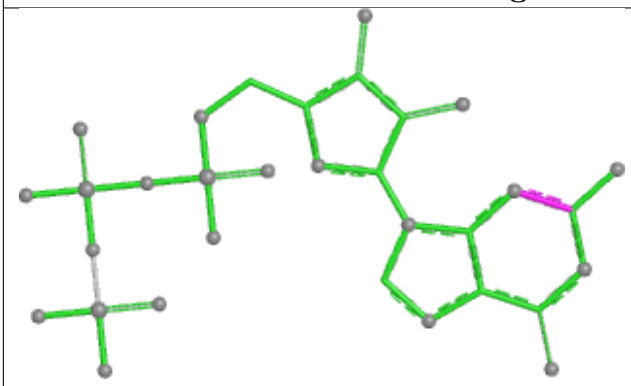
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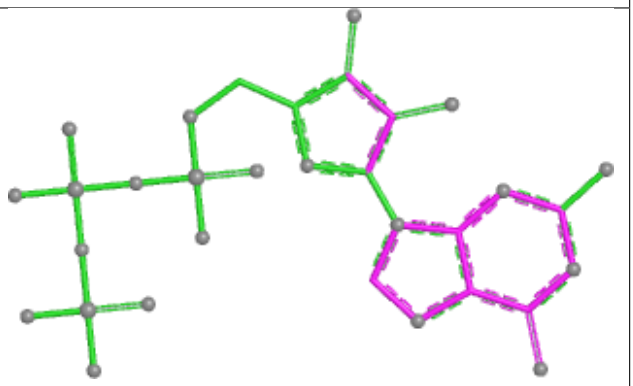
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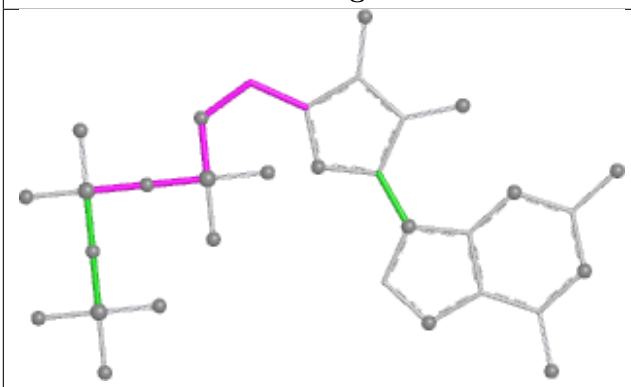
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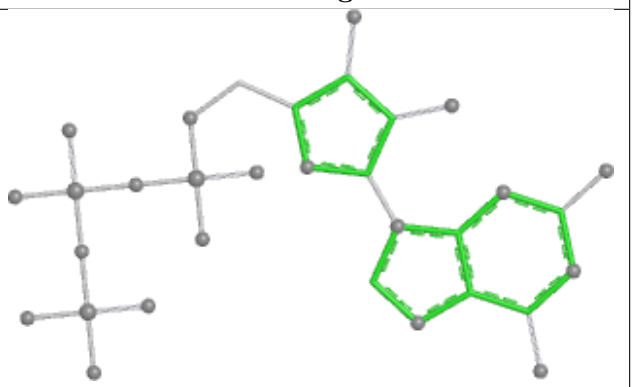
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Bond angles

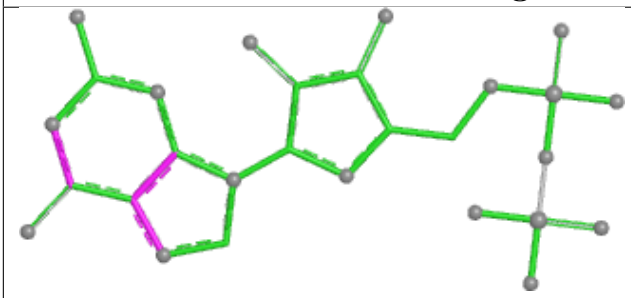


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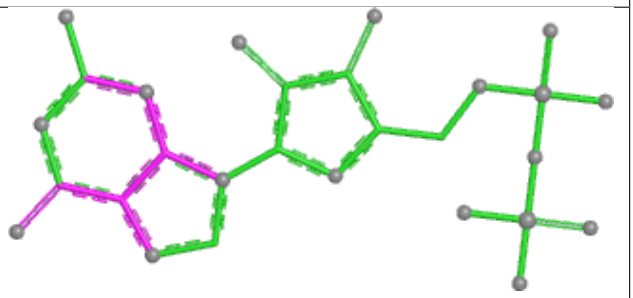


Rings

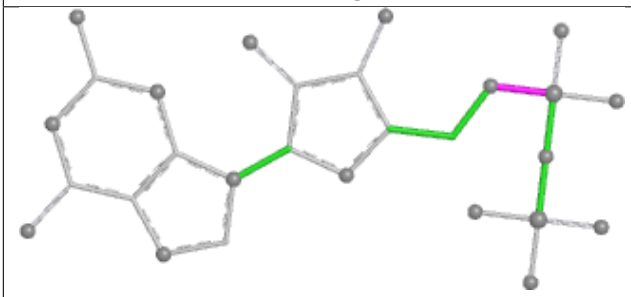
Ligand GDP JD 501



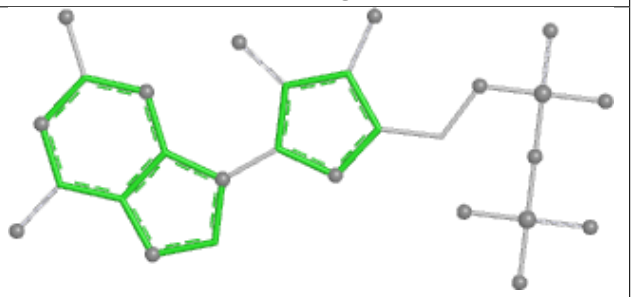
Bond lengths



Bond angles

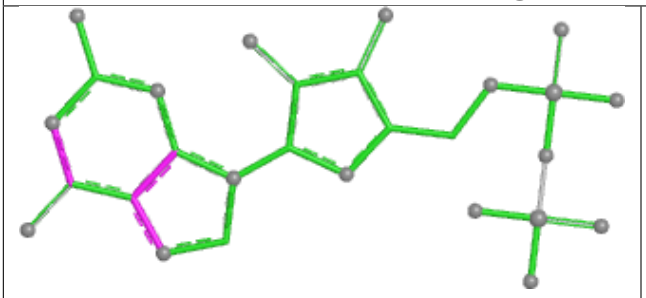


Torsions

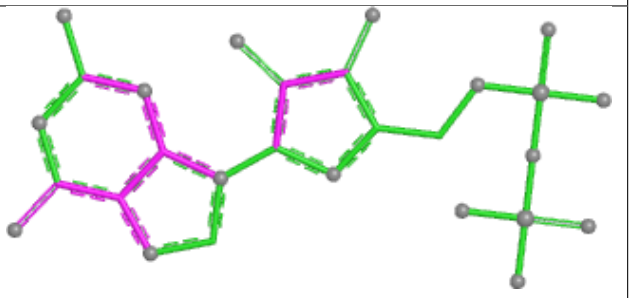


Rings

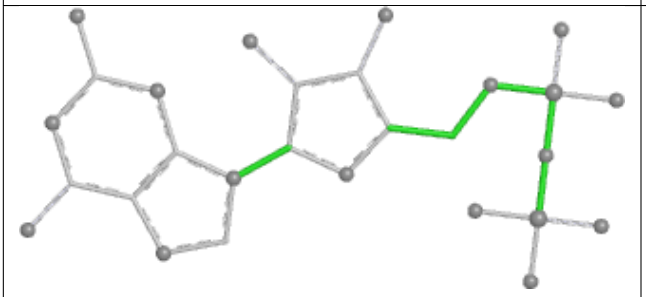
Ligand GDP PF 501



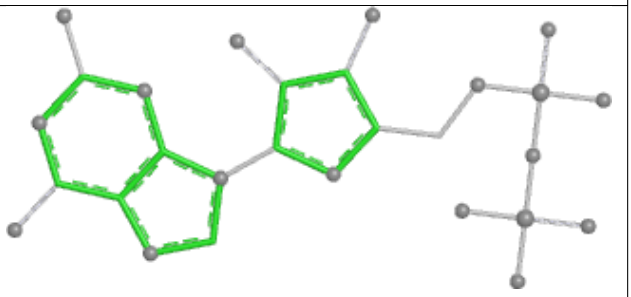
Bond lengths



Bond angles

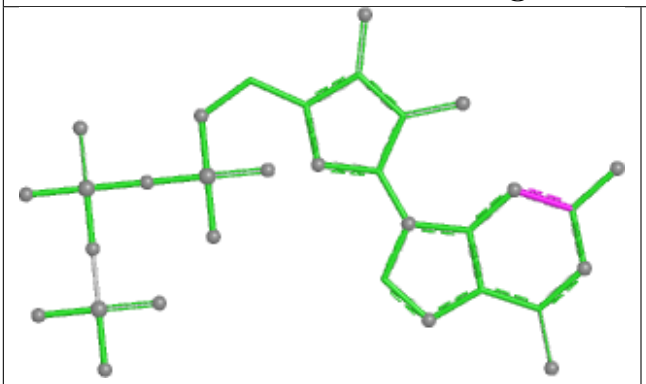


Torsions

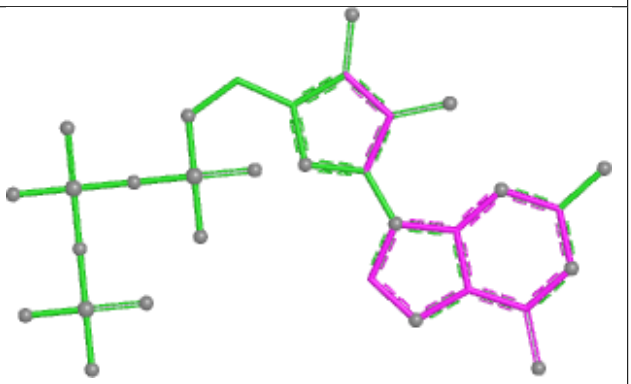


Rings

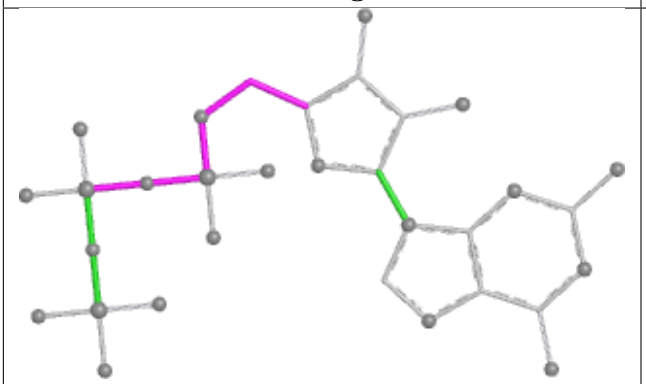
Ligand GTP BK 501



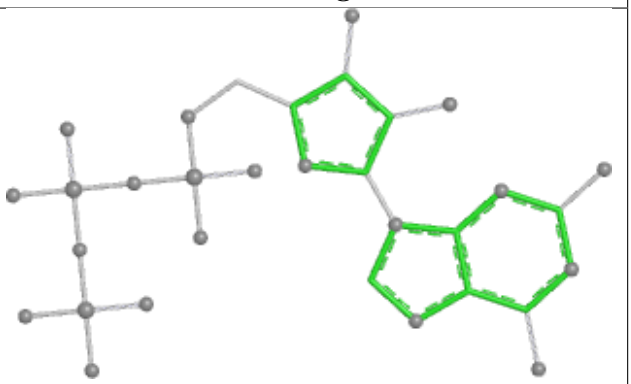
Bond lengths



Bond angles

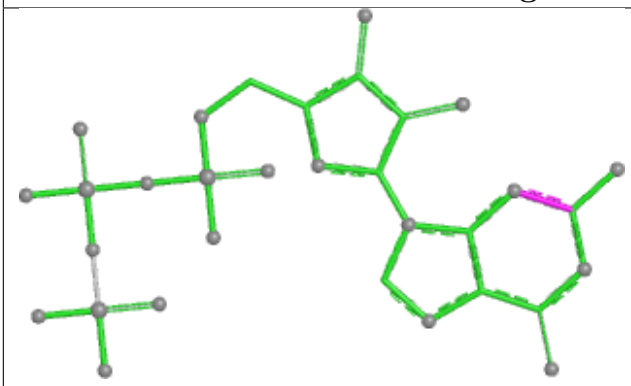


Torsions

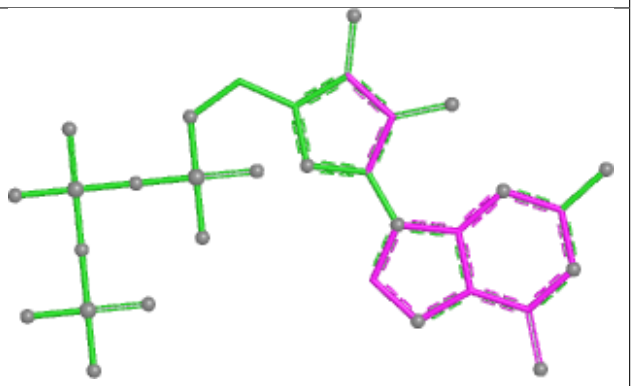


Rings

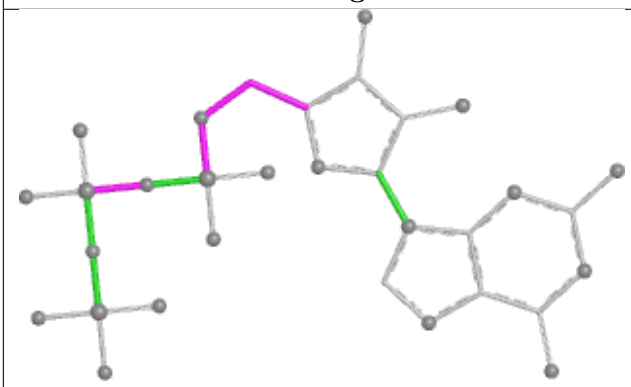
Ligand GTP JI 501



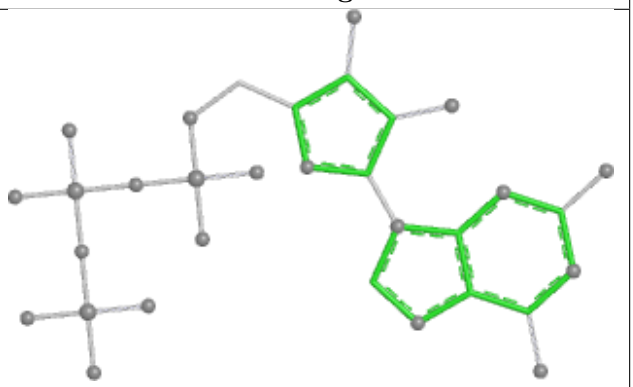
Bond lengths



Bond angles

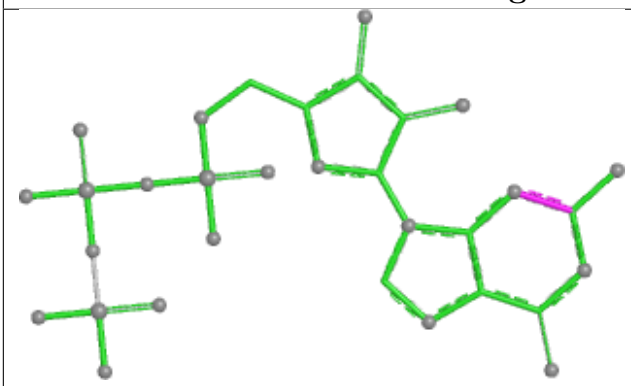


Torsions

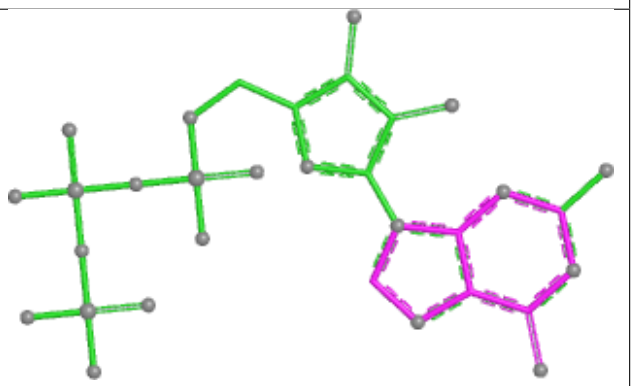


Rings

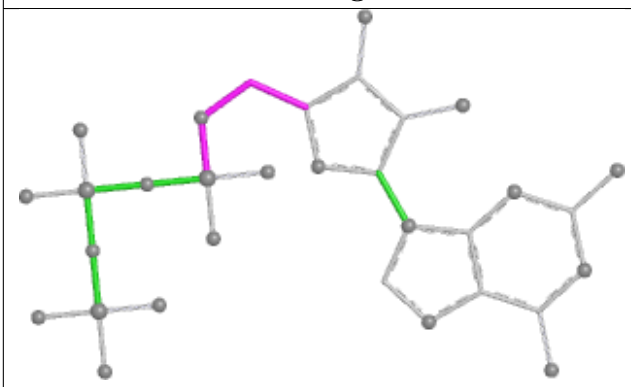
Ligand GTP OA 501



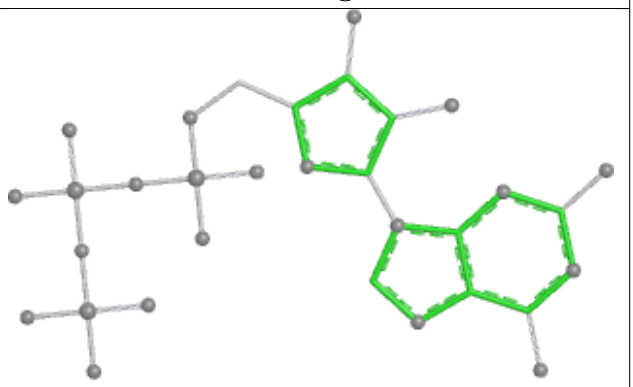
Bond lengths



Bond angles

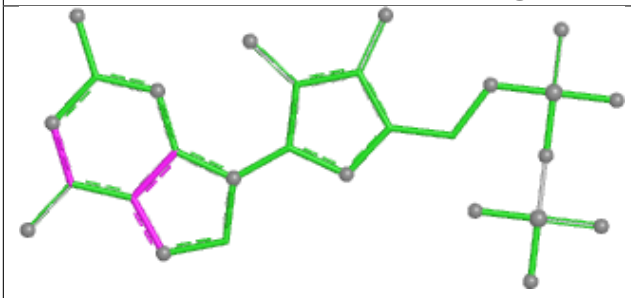


Torsions

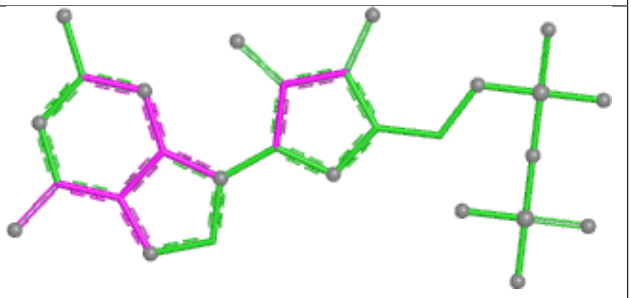


Rings

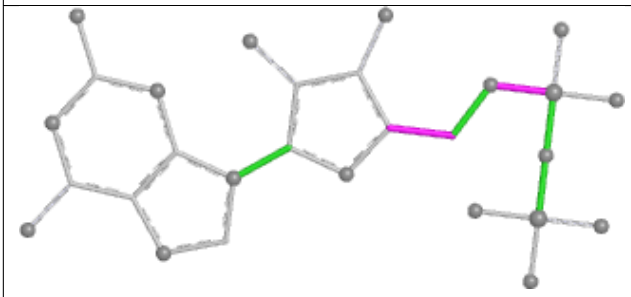
Ligand GDP TL 501



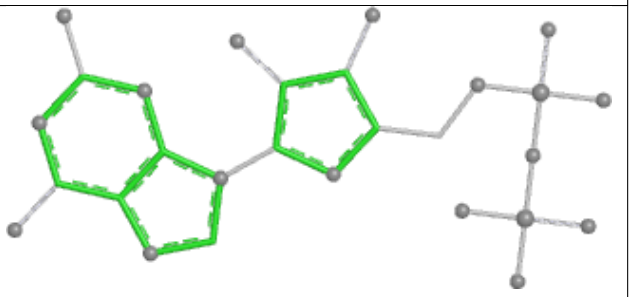
Bond lengths



Bond angles

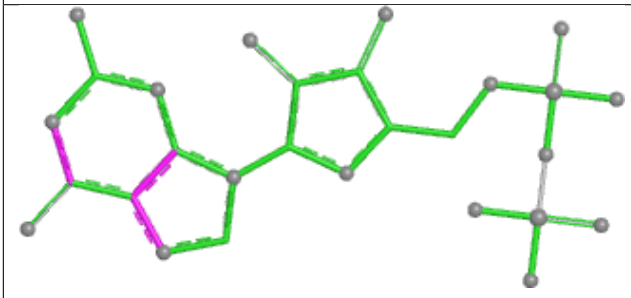


Torsions

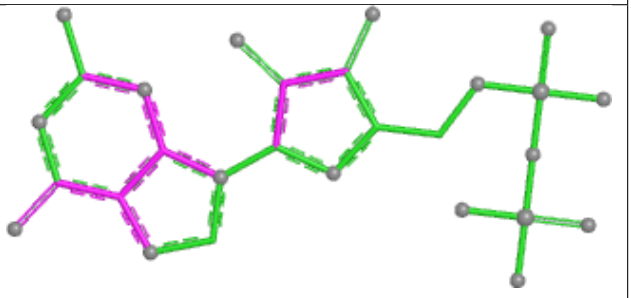


Rings

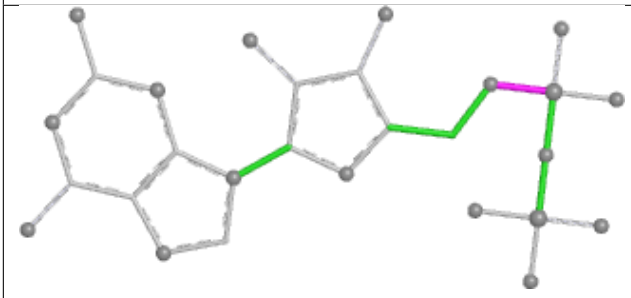
Ligand GDP WN 501



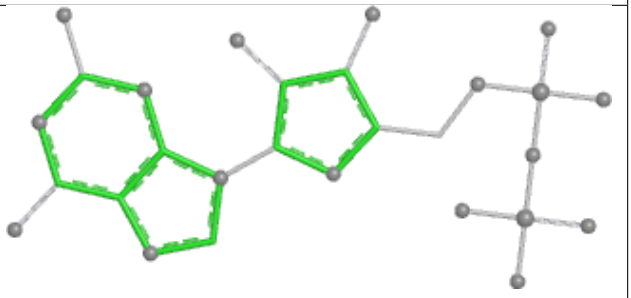
Bond lengths



Bond angles

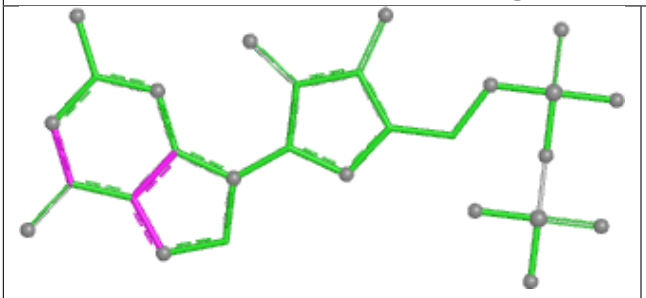


Torsions

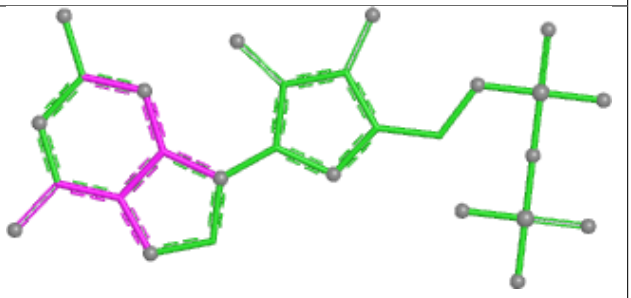


Rings

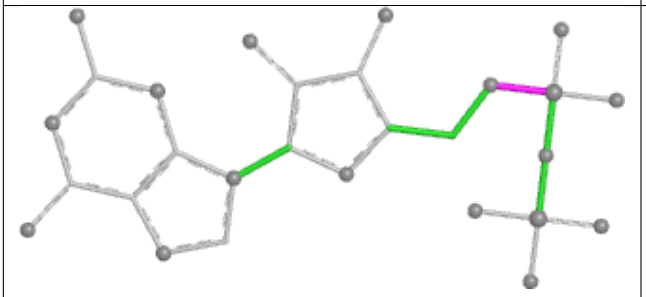
Ligand GDP EN 501



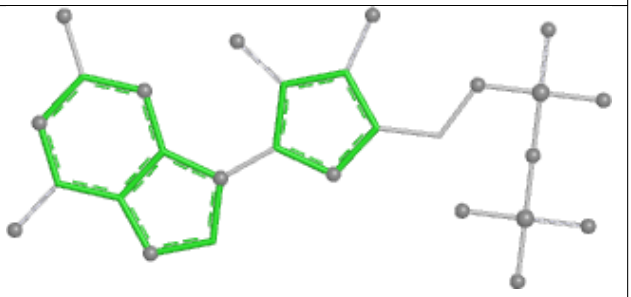
Bond lengths



Bond angles

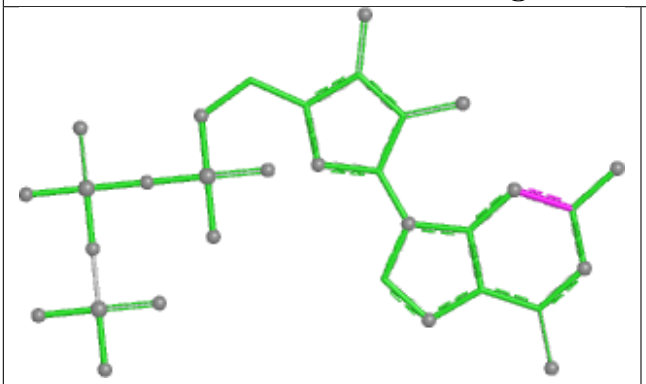


Torsions

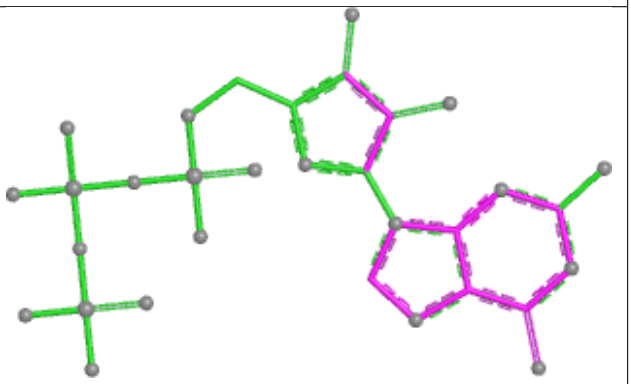


Rings

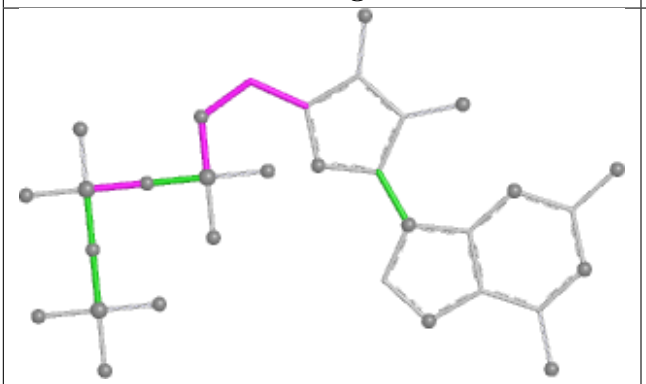
Ligand GTP GE 501



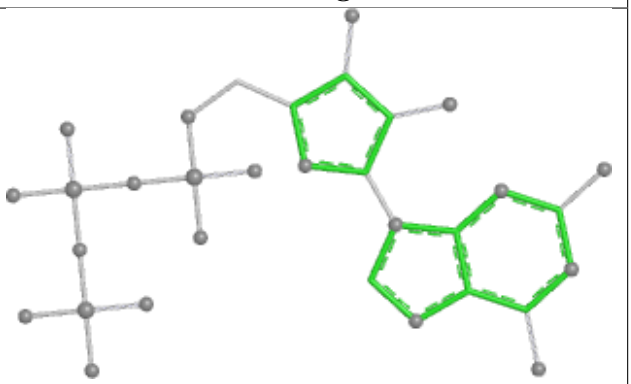
Bond lengths



Bond angles

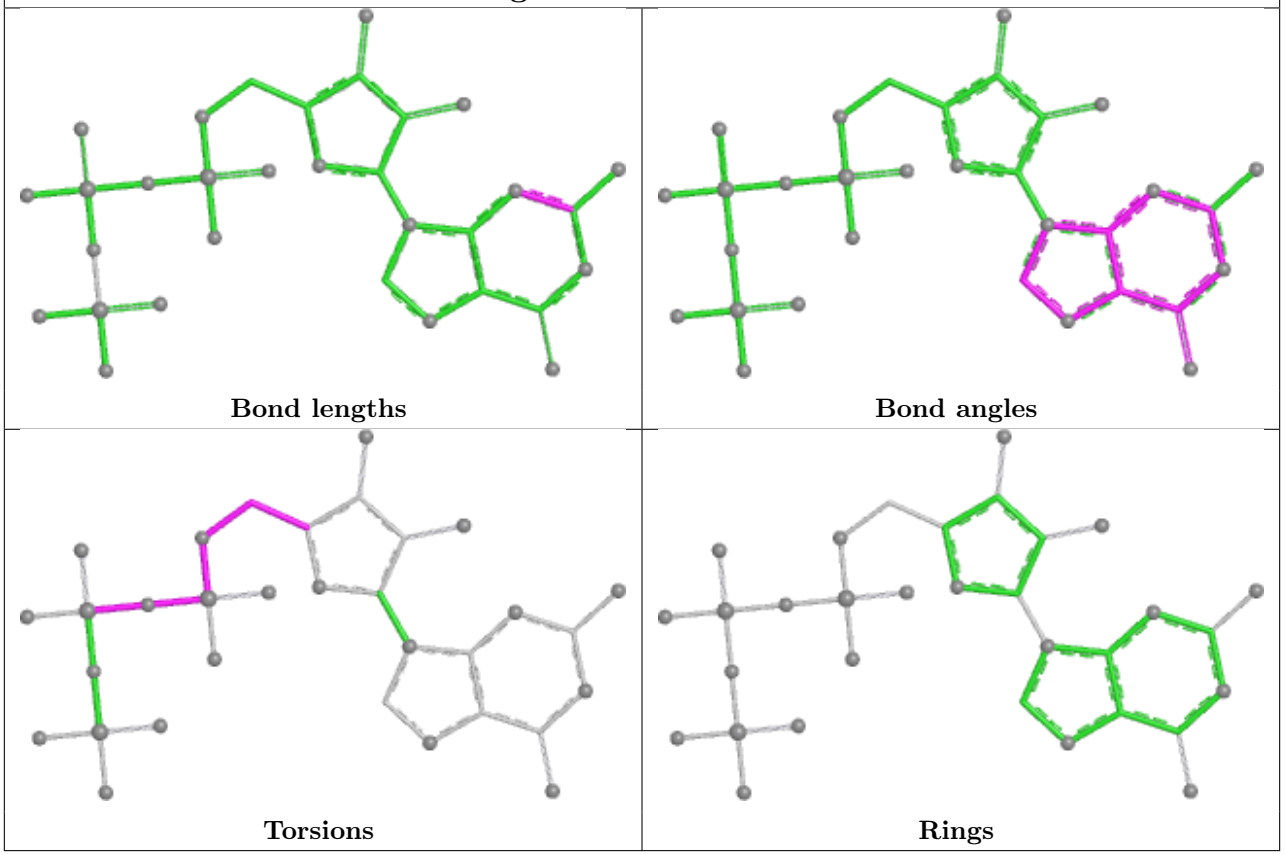


Torsions



Rings

Ligand GTP TG 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2A	1
1	1A	1
1	0A	1
28	2F	1
1	3A	1
12	0T	1
23	2O	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2A	110:PRO	C	111:SER	N	6.11
1	1A	110:PRO	C	111:SER	N	6.07
1	0A	110:PRO	C	111:SER	N	6.00
1	2F	68:THR	C	69:MET	N	5.77
1	3A	110:PRO	C	111:SER	N	5.47

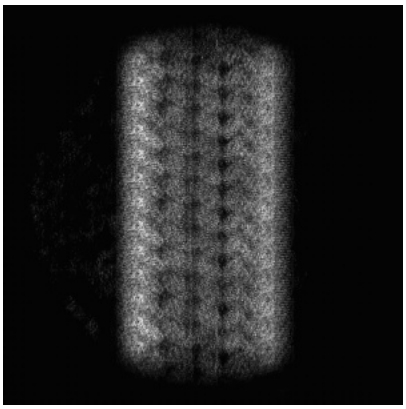
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29685. These allow visual inspection of the internal detail of the map and identification of artifacts.

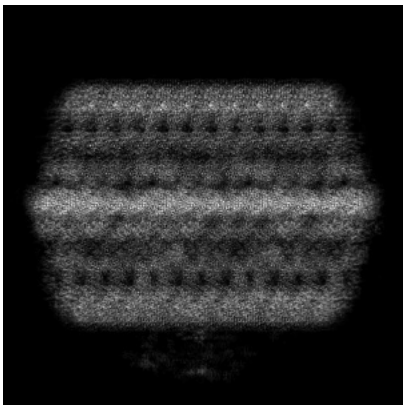
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

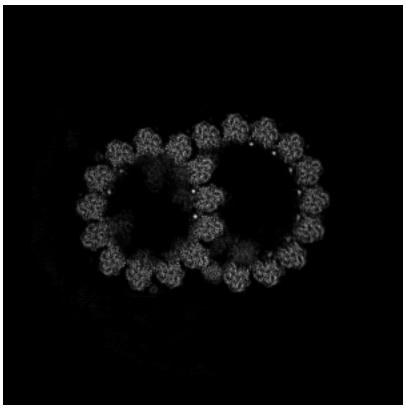
6.1.1 Primary map



X

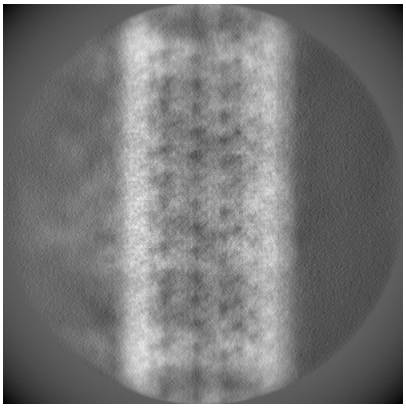


Y

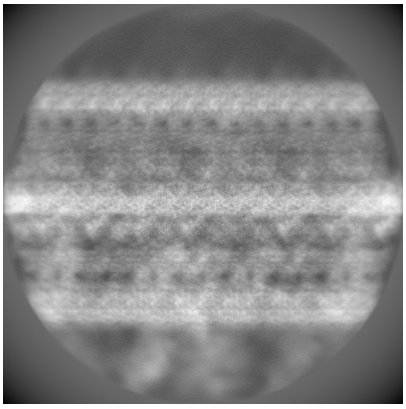


Z

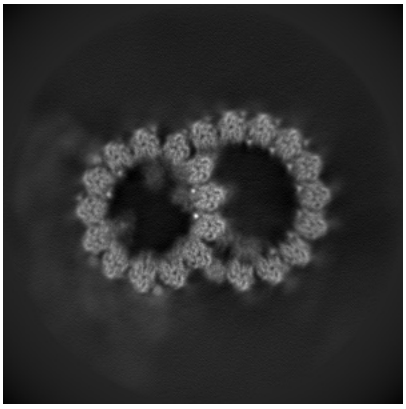
6.1.2 Raw map



X



Y

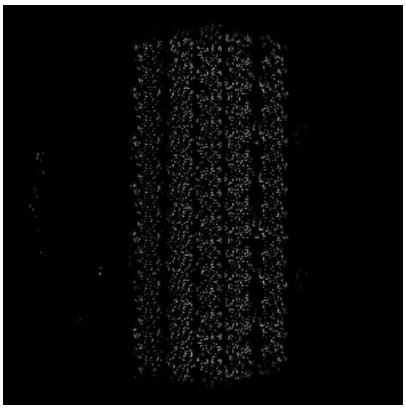


Z

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

6.2 Central slices (i)

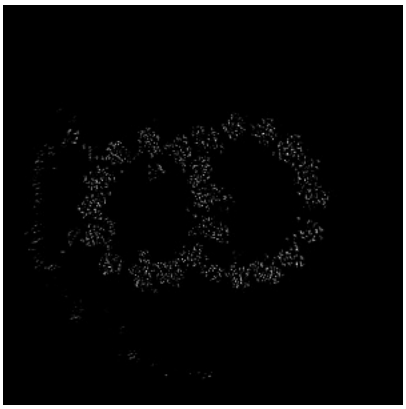
6.2.1 Primary map



X Index: 256

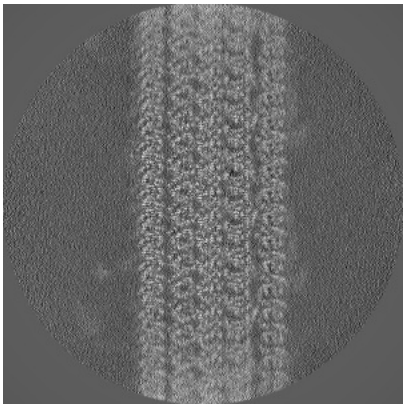


Y Index: 256

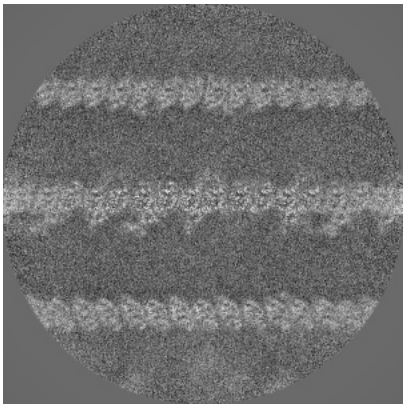


Z Index: 256

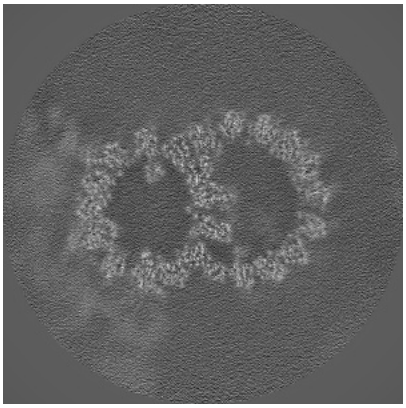
6.2.2 Raw map



X Index: 256



Y Index: 256

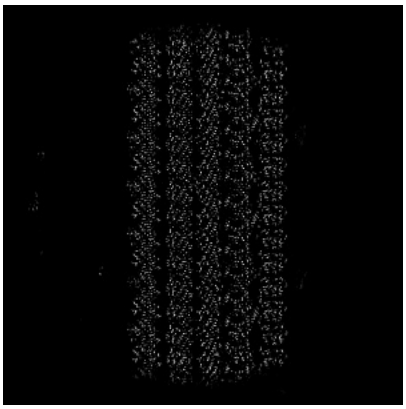


Z Index: 256

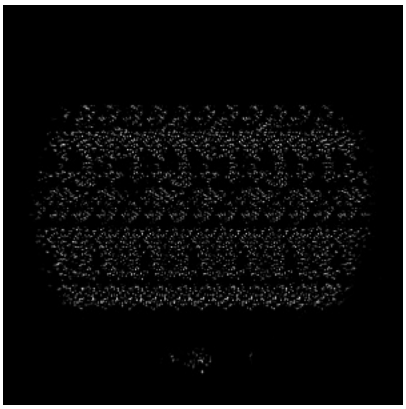
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

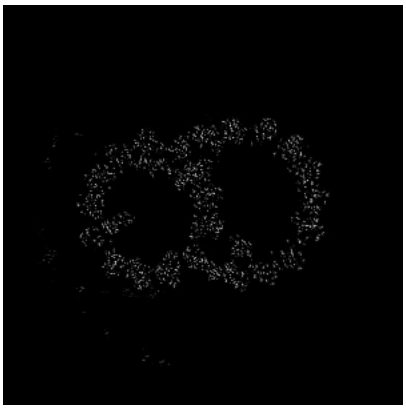
6.3.1 Primary map



X Index: 258

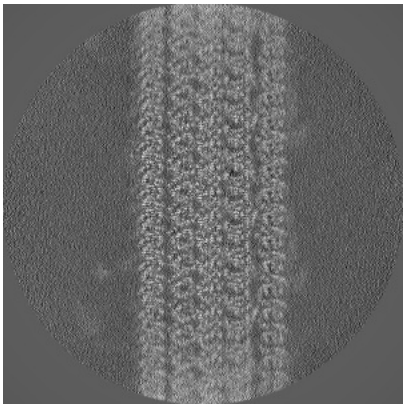


Y Index: 176

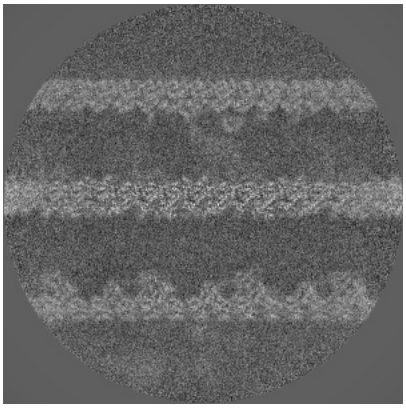


Z Index: 200

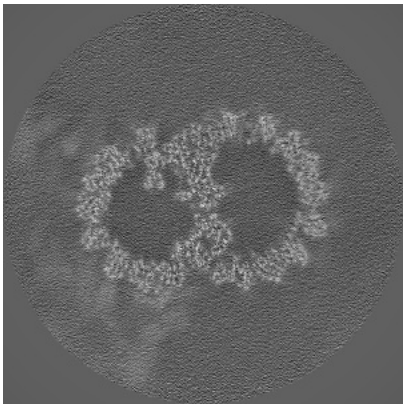
6.3.2 Raw map



X Index: 256



Y Index: 223

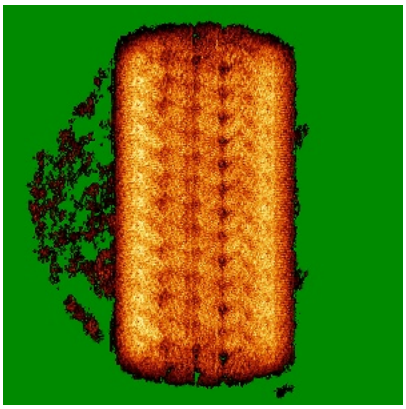


Z Index: 229

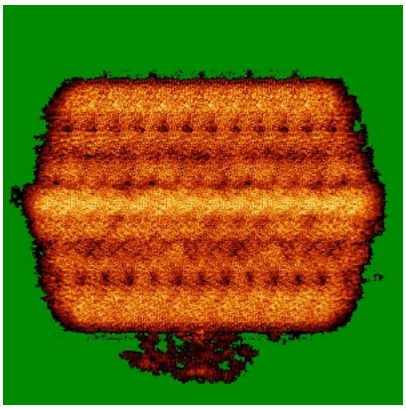
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

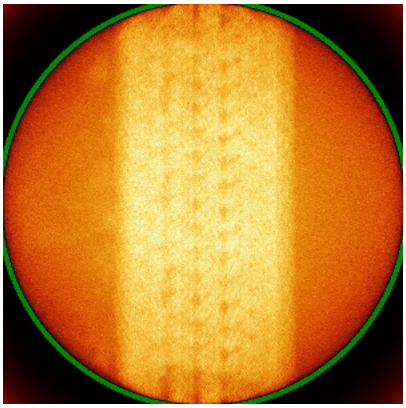


Y

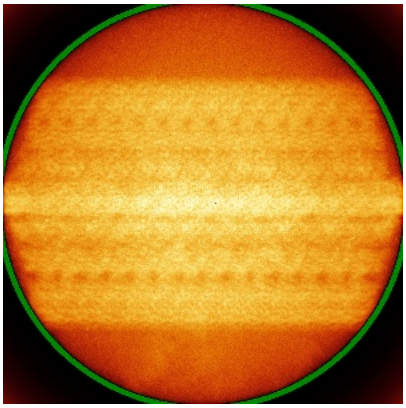


Z

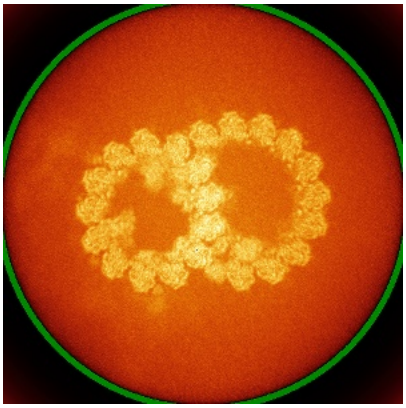
6.4.2 Raw map



X



Y

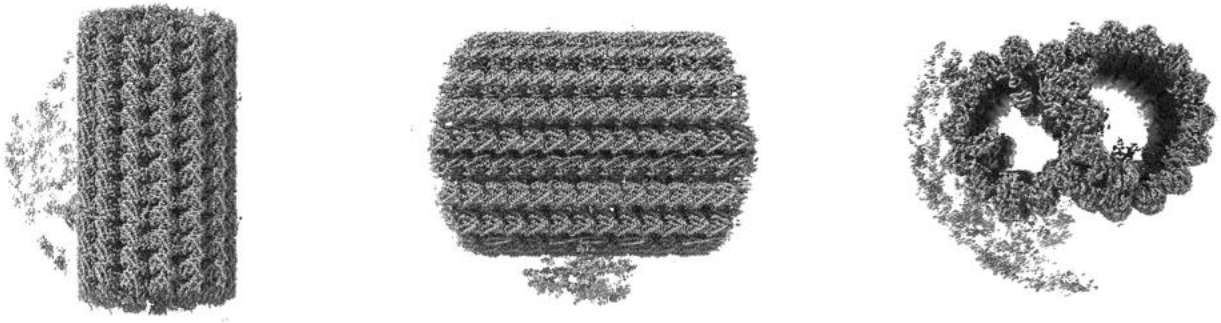


Z

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

6.5 Orthogonal surface views (i)

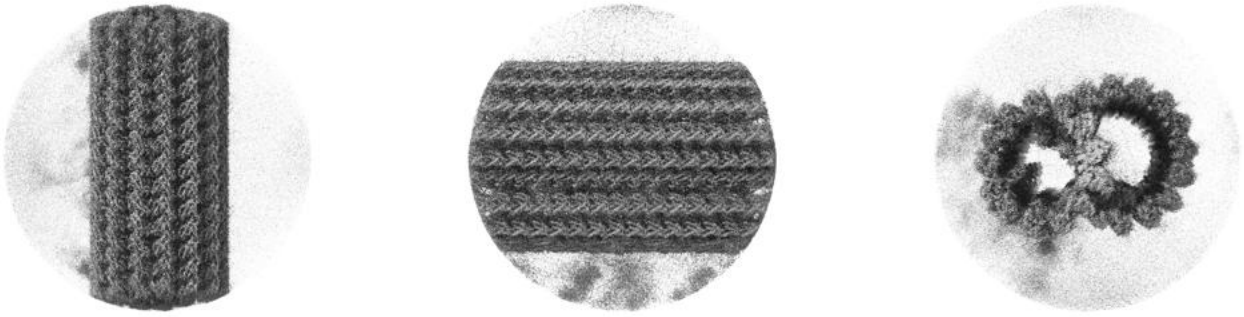
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

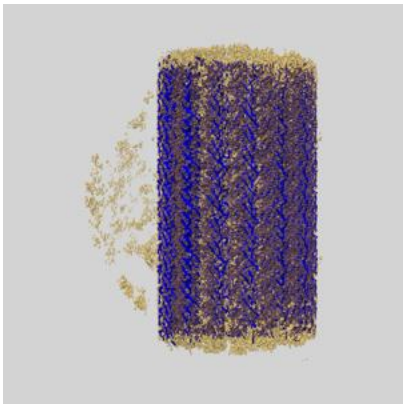
6.6 Mask visualisation

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

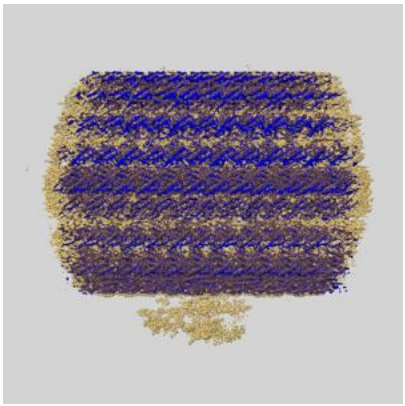
A mask typically either:

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

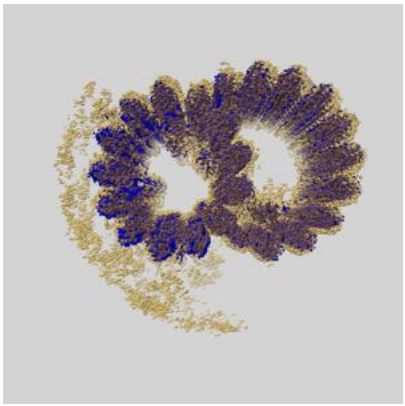
6.6.1 emd_29685_msk_1.map



X



Y

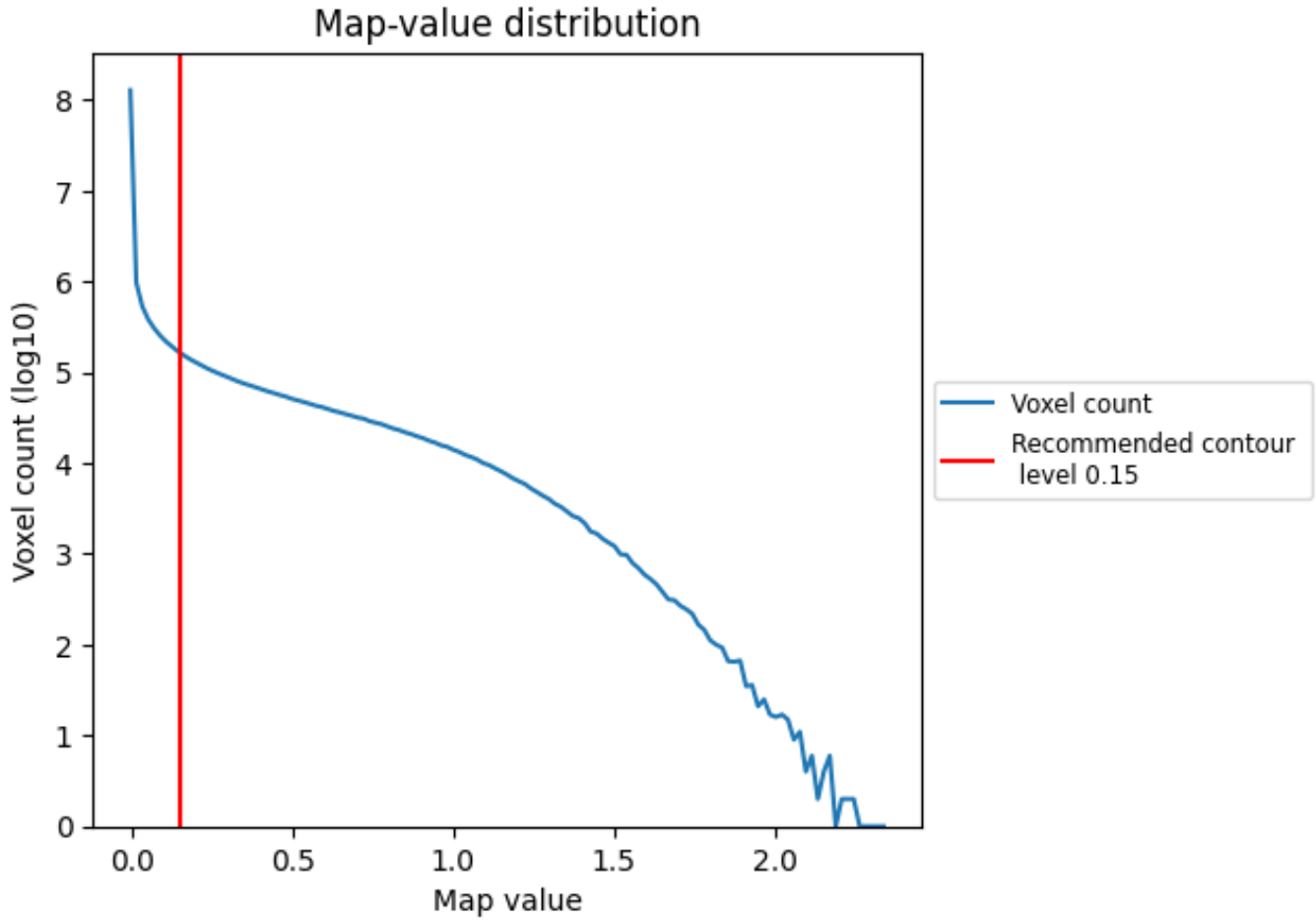


Z

7 Map analysis

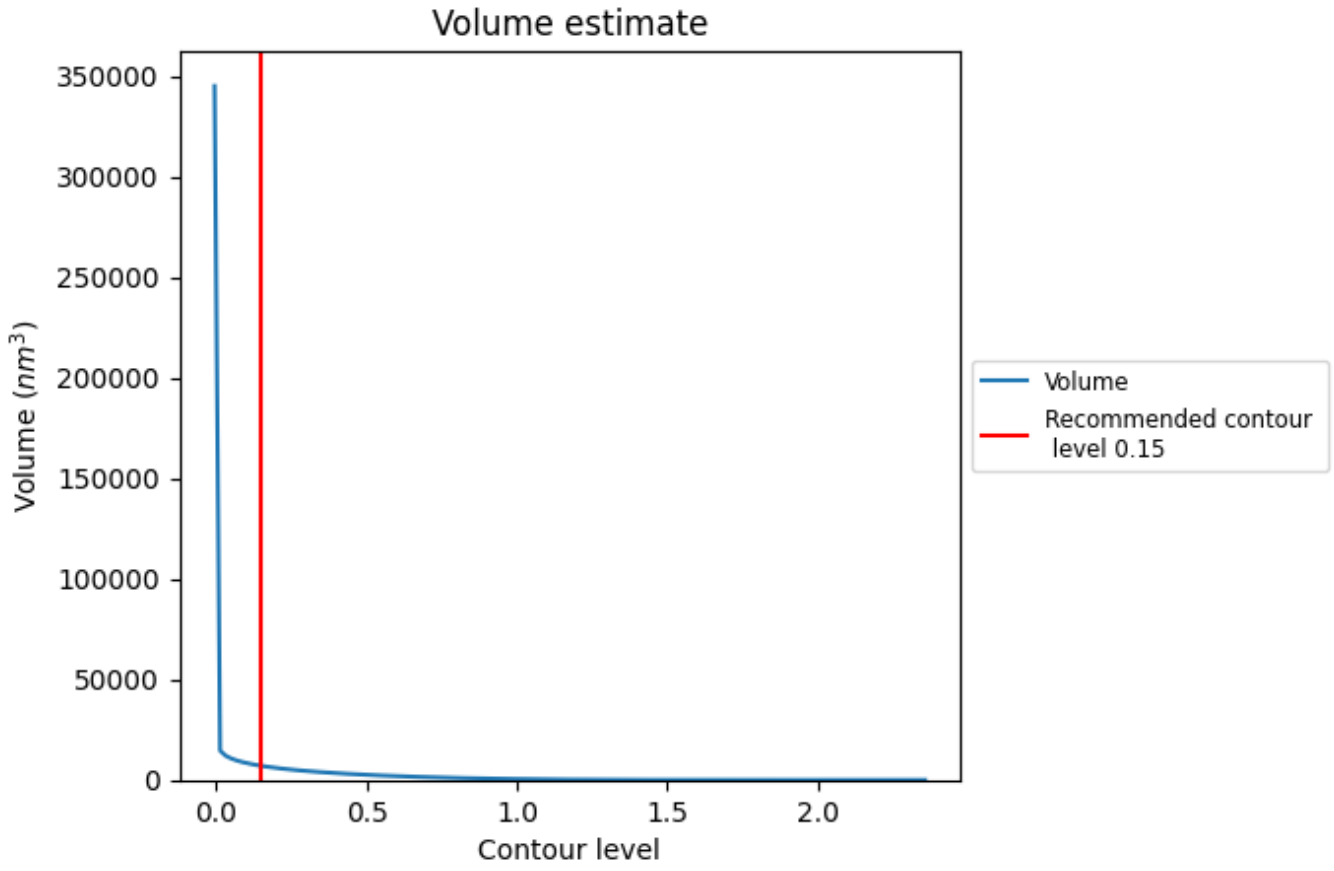
This section contains the results of statistical analysis of the map.

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.

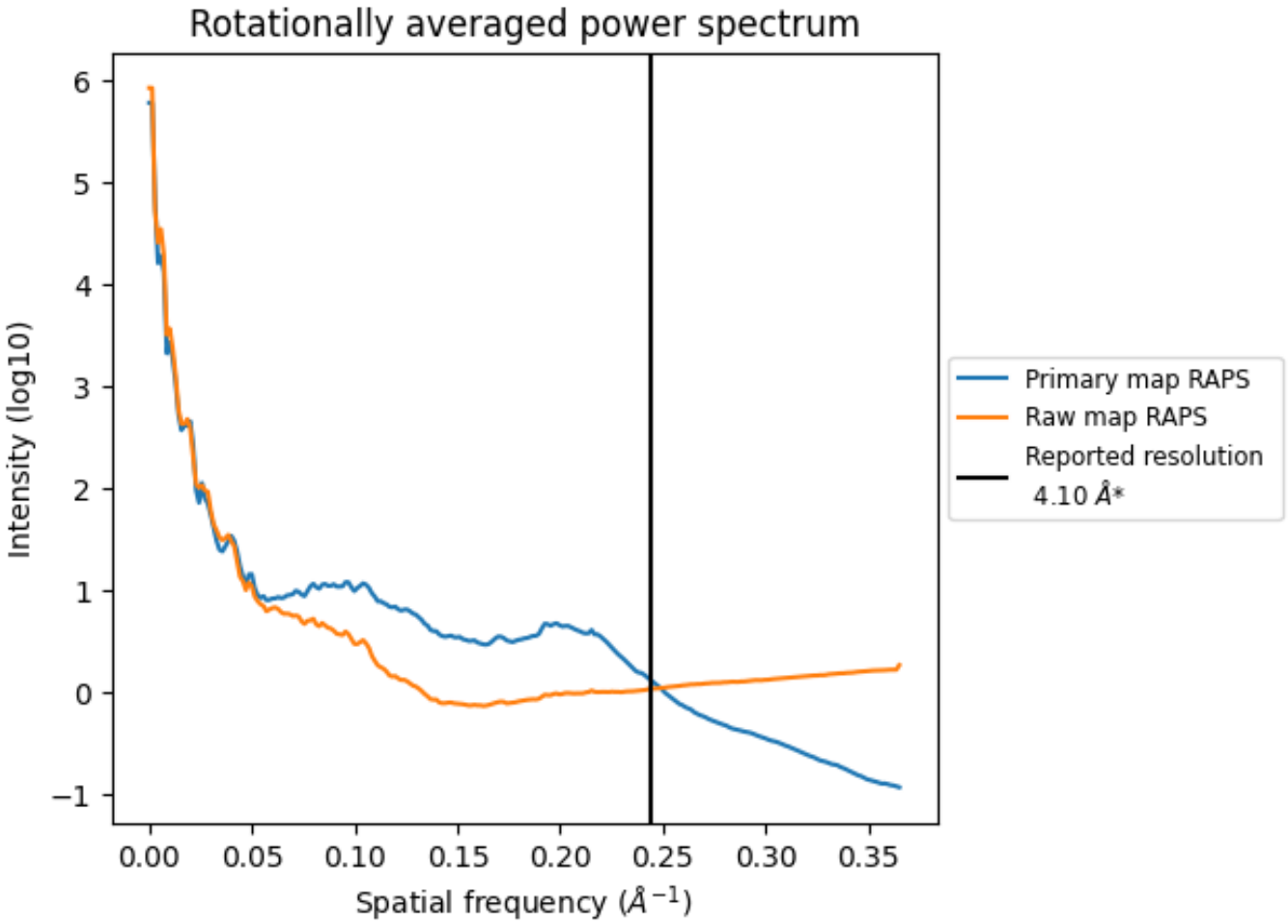
7.2 Volume estimate



The volume at the recommended contour level is 7038 nm^3; this corresponds to an approximate mass of 6357 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)

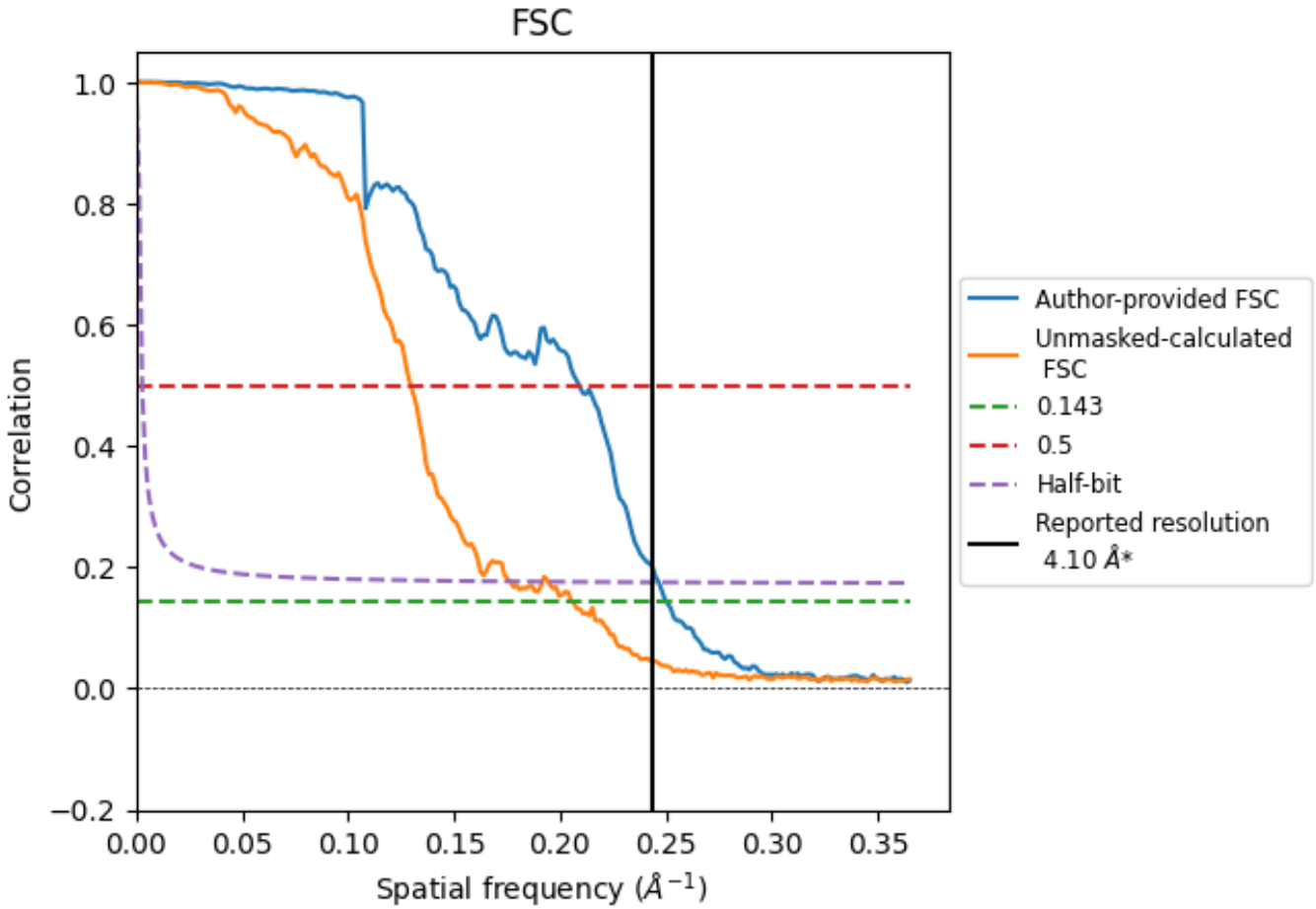


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8.2 Resolution estimates (i)

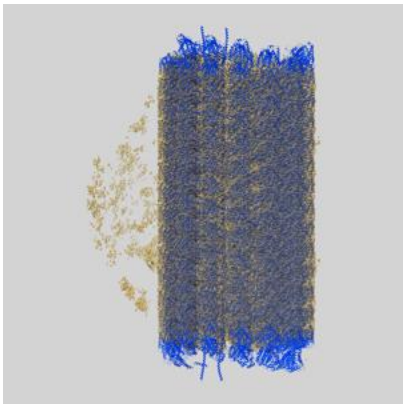
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.00	4.78	4.05
Unmasked-calculated*	4.86	7.72	5.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.86 differs from the reported value 4.1 by more than 10 %

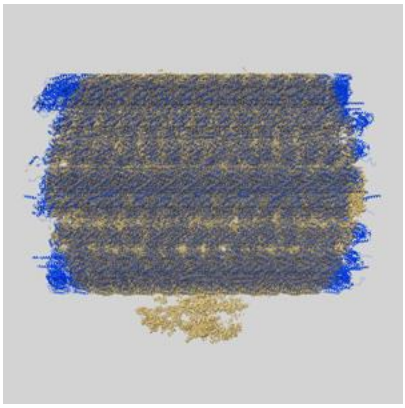
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29685 and PDB model 8G2Z. Per-residue inclusion information can be found in section 3 on page 72.

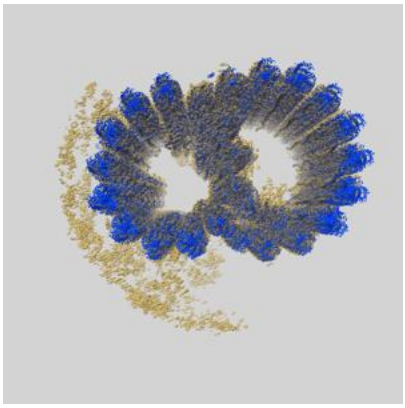
9.1 Map-model overlay



X



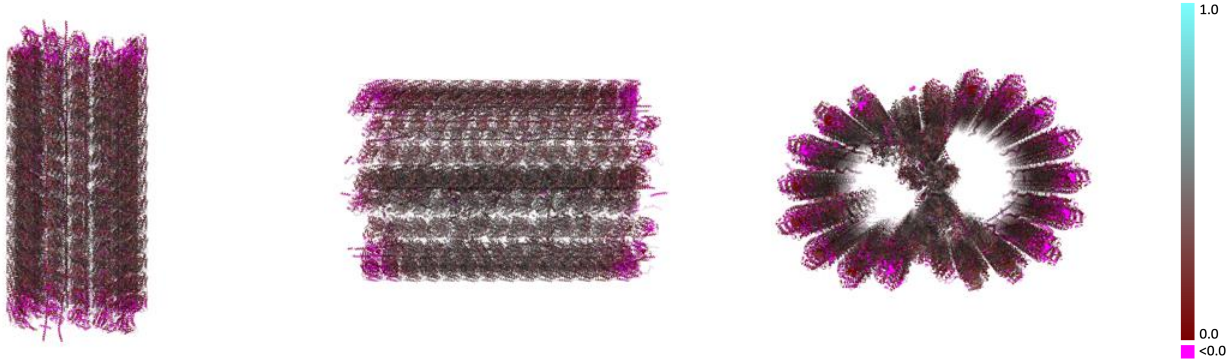
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

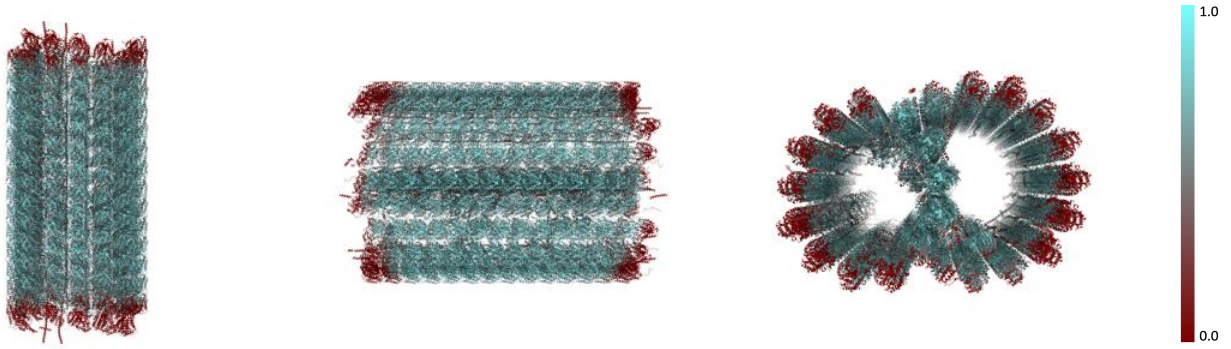
9.2 Q-score mapped to coordinate model (i)



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.

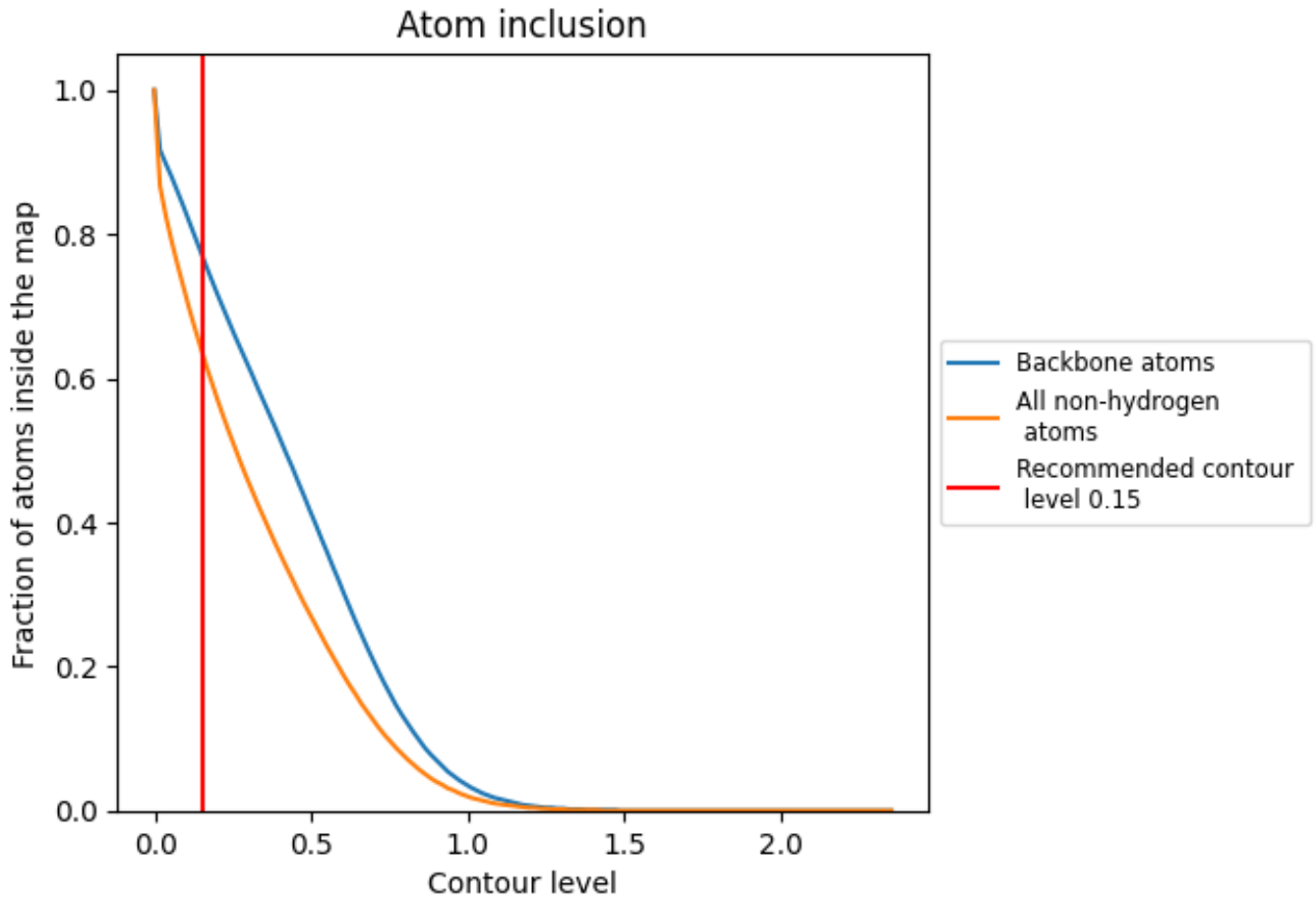
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 64% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6350	0.2870
0A	0.6270	0.2850
0B	0.7020	0.3390
0C	0.6590	0.2830
0D	0.4860	0.1340
0E	0.4270	0.1140
0F	0.6730	0.2870
0G	0.5630	0.2310
0H	0.3130	0.0690
0N	0.6690	0.2830
0Q	0.6950	0.3030
0S	0.3450	0.1700
0T	0.3810	0.2120
0U	0.6490	0.2860
0V	0.3220	0.1440
0X	0.6190	0.2700
1A	0.6250	0.3300
1B	0.6590	0.3000
1C	0.6690	0.2570
1D	0.5820	0.2640
1E	0.4750	0.2120
1F	0.6510	0.3180
1G	0.5670	0.2220
1H	0.3960	0.1160
1I	0.6710	0.3240
1J	0.5980	0.2620
1K	0.5000	0.1890
1L	0.5870	0.2700
1M	0.7080	0.3460
1N	0.7050	0.3380
1O	0.3310	0.0650
1P	0.4110	0.0930
1Q	0.7350	0.3550
1R	0.6960	0.3450
1S	0.7010	0.3410



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Chain	Atom inclusion	Q-score
1T	0.7190	0.3760
1U	0.7190	0.3500
1V	0.5620	0.2500
1W	0.6570	0.3050
1X	0.6790	0.3550
2A	0.6660	0.3430
2B	0.6340	0.2800
2C	0.5680	0.2020
2D	0.5680	0.2430
2E	0.5390	0.2350
2F	0.6600	0.2910
2G	0.6680	0.3100
2H	0.6050	0.3290
2I	0.5660	0.2640
2K	0.4450	0.1560
2L	0.3740	0.1590
2M	0.7450	0.3700
2N	0.5800	0.2080
2O	0.3850	0.0520
2P	0.4280	0.1250
2Q	0.7370	0.3520
2R	0.7090	0.3620
2S	0.6930	0.3390
2T	0.7380	0.3700
2U	0.7200	0.3410
2V	0.5600	0.2450
2W	0.4220	0.1170
2X	0.6870	0.3440
3A	0.6540	0.3140
3B	0.5800	0.2380
3C	0.6340	0.2710
3D	0.3550	0.2420
3E	0.2920	0.0800
3H	0.5950	0.3190
3I	0.7040	0.3220
3L	0.2740	0.0410
3O	0.3560	0.0500
3Q	0.7310	0.3560
3R	0.6980	0.3480
3S	0.6950	0.3200
3T	0.7160	0.3540
3U	0.6100	0.2660

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Chain	Atom inclusion	Q-score
3V	0.5220	0.2240
3X	0.6450	0.3150
4C	0.6120	0.2600
4F	0.6090	0.2780
4H	0.6190	0.3360
4Q	0.7280	0.3560
4R	0.6910	0.3500
4S	0.6600	0.3150
4X	0.6460	0.2980
5A	0.5170	0.2410
5B	0.6500	0.3190
5C	0.6580	0.3260
5D	0.5100	0.2510
5E	0.3130	0.1210
5F	0.4260	0.2120
5G	0.4780	0.2440
5H	0.3940	0.1430
5I	0.2700	0.1310
5J	0.3190	0.2170
5K	0.1850	0.0640
5Q	0.7190	0.3490
5R	0.7080	0.3460
5S	0.6700	0.3220
6F	0.6980	0.3660
6G	0.5490	0.1970
6H	0.6170	0.2460
6Q	0.6620	0.2980
6R	0.5210	0.2160
7R	0.5490	0.2300
8L	0.6500	0.1740
8N	0.5800	0.1110
8P	0.6570	0.1800
8R	0.6270	0.1770
AA	0.7390	0.3500
AB	0.4970	0.2450
AC	0.7700	0.4050
AD	0.7710	0.3870
AE	0.7780	0.4230
AF	0.7690	0.4050
AG	0.7670	0.4100
AH	0.7600	0.4020
AI	0.7750	0.4080

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Chain	Atom inclusion	Q-score
AJ	0.7620	0.4030
AK	0.7740	0.4080
AL	0.7730	0.4080
AM	0.7420	0.3490
AN	0.7690	0.3820
BA	0.5690	0.2260
BB	0.0830	0.0170
BC	0.7410	0.3410
BD	0.7260	0.3190
BE	0.7490	0.3730
BF	0.7460	0.3660
BG	0.7480	0.3710
BH	0.7350	0.3510
BI	0.7730	0.3870
BJ	0.7530	0.3790
BK	0.7520	0.3700
BL	0.7480	0.3700
BM	0.6930	0.2930
BN	0.7450	0.3380
CA	0.2480	0.0830
CB	0.6510	0.2380
CC	0.7040	0.3080
CD	0.7440	0.3450
CE	0.7300	0.3520
CF	0.7290	0.3270
CG	0.7280	0.3460
CH	0.7380	0.3550
CI	0.7480	0.3670
CJ	0.7500	0.3500
CK	0.7330	0.3470
CL	0.6950	0.2970
CM	0.5950	0.2200
CN	0.0150	0.0060
DA	0.0240	0.0130
DB	0.4770	0.1790
DC	0.6960	0.2740
DD	0.7530	0.3340
DE	0.7370	0.3480
DF	0.7590	0.3500
DG	0.7330	0.3320
DH	0.7510	0.3510
DI	0.7410	0.3490

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Chain	Atom inclusion	Q-score
DJ	0.7570	0.3480
DK	0.7510	0.3330
DL	0.7010	0.2760
DM	0.5790	0.2040
DN	0.0330	-0.0070
EA	0.0000	0.0450
EB	0.2380	0.0770
EC	0.6040	0.2260
ED	0.7040	0.3040
EE	0.7220	0.3390
EF	0.7180	0.3380
EG	0.7080	0.3380
EH	0.6980	0.3200
EI	0.7260	0.3510
EJ	0.7220	0.3410
EK	0.7290	0.3400
EL	0.6770	0.2890
EM	0.5610	0.2120
EN	0.0430	-0.0070
FA	0.6100	0.2230
FB	0.1590	0.0540
FC	0.7580	0.3550
FD	0.7300	0.3150
FE	0.7570	0.3710
FF	0.7560	0.3660
FG	0.7440	0.3560
FH	0.7380	0.3490
FI	0.7630	0.3700
FJ	0.7580	0.3650
FK	0.6930	0.2910
FL	0.7440	0.3340
FM	0.0000	0.0090
FN	0.1680	0.0210
GA	0.5900	0.2170
GB	0.0800	-0.0020
GC	0.7510	0.3590
GD	0.7480	0.3270
GE	0.7620	0.3770
GF	0.7510	0.3730
GG	0.7370	0.3660
GH	0.7570	0.3700
GI	0.7580	0.3810

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Chain	Atom inclusion	Q-score
GJ	0.7680	0.3820
GK	0.7440	0.3410
GL	0.7460	0.3600
GM	0.0000	0.0040
GN	0.4400	0.1860
HA	0.6100	0.2520
HB	0.1250	0.0330
HC	0.7540	0.3780
HD	0.7530	0.3540
HE	0.7610	0.3900
HF	0.7560	0.3810
HG	0.7380	0.3680
HH	0.7580	0.3820
HI	0.7640	0.3980
HJ	0.7560	0.3790
HK	0.7610	0.3700
HL	0.7480	0.3750
HM	0.0860	0.0010
HN	0.6170	0.2650
IA	0.6800	0.2860
IB	0.2470	0.1070
IC	0.7540	0.3780
ID	0.7450	0.3560
IE	0.7570	0.3930
IF	0.7650	0.3960
IG	0.7380	0.3720
IH	0.7590	0.3840
II	0.7650	0.3930
IJ	0.7540	0.3800
IK	0.7660	0.3810
IL	0.7520	0.3800
IM	0.5180	0.2510
IN	0.7370	0.3360
JA	0.7550	0.3670
JB	0.7380	0.3350
JC	0.7620	0.3940
JD	0.7610	0.3880
JE	0.7690	0.3980
JF	0.7760	0.4110
JG	0.7630	0.3880
JH	0.7610	0.3940
JI	0.7720	0.4020

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Chain	Atom inclusion	Q-score
JJ	0.7630	0.3950
JK	0.7530	0.3760
JL	0.7640	0.3990
JM	0.2250	0.1040
JN	0.7110	0.3350
KA	0.7570	0.3580
KB	0.6910	0.2970
KC	0.7680	0.4020
KD	0.7670	0.3940
KE	0.7760	0.4030
KF	0.7870	0.4100
KG	0.7770	0.4040
KH	0.7740	0.4060
KI	0.7710	0.3910
KJ	0.7760	0.3980
KK	0.7900	0.4020
KL	0.7830	0.4120
KM	0.6410	0.3100
KN	0.7710	0.3780
LA	0.7530	0.3740
LB	0.7300	0.3370
LC	0.7680	0.4130
LD	0.7750	0.3990
LE	0.7630	0.4010
LF	0.7590	0.4020
LG	0.7620	0.4080
LH	0.7760	0.4050
LI	0.7560	0.3930
LJ	0.7720	0.4100
LK	0.7640	0.4050
LL	0.7660	0.4050
LM	0.7290	0.3450
LN	0.7800	0.3960
MA	0.7670	0.3810
MB	0.7330	0.3340
MC	0.7680	0.4070
MD	0.7720	0.4050
ME	0.7650	0.4070
MF	0.7810	0.4120
MG	0.7530	0.3940
MH	0.7710	0.4090
MI	0.7550	0.3960

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Chain	Atom inclusion	Q-score
MJ	0.7840	0.4140
MK	0.7670	0.4000
ML	0.7620	0.4080
MM	0.7470	0.3510
MN	0.7900	0.3960
NA	0.6530	0.2780
NB	0.5050	0.1950
NC	0.7260	0.3500
ND	0.7040	0.3210
NE	0.7230	0.3630
NF	0.7280	0.3680
NG	0.7200	0.3510
NH	0.7050	0.3430
NI	0.7180	0.3520
NJ	0.7210	0.3470
NK	0.7210	0.3500
NL	0.7120	0.3510
NM	0.4200	0.2120
NN	0.6890	0.3130
OA	0.6240	0.2260
OB	0.2530	0.0810
OC	0.7140	0.3160
OD	0.7100	0.2830
OE	0.7340	0.3470
OF	0.7420	0.3430
OG	0.7300	0.3310
OH	0.7250	0.3340
OI	0.7250	0.3360
OJ	0.7240	0.3270
OK	0.7310	0.3360
OL	0.7370	0.3410
OM	0.4040	0.1940
ON	0.6890	0.2870
PA	0.4570	0.1270
PB	0.0730	0.0150
PC	0.6880	0.2650
PD	0.6350	0.2110
PE	0.7190	0.3070
PF	0.7030	0.2940
PG	0.6980	0.2950
PH	0.7030	0.2940
PI	0.7150	0.3160

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Chain	Atom inclusion	Q-score
PJ	0.6900	0.2960
PK	0.7260	0.3090
PL	0.7210	0.3080
PM	0.2980	0.1290
PN	0.6560	0.2510
QA	0.2050	0.0200
QB	0.5990	0.1940
QC	0.6820	0.2340
QD	0.7050	0.2810
QE	0.7300	0.2930
QF	0.7140	0.2910
QG	0.7000	0.2760
QH	0.7150	0.3030
QI	0.7250	0.3000
QJ	0.7160	0.3010
QK	0.7040	0.2820
QL	0.6440	0.2260
QM	0.2160	0.0710
QN	0.0000	0.0310
RA	0.0870	0.0150
RB	0.5350	0.1860
RC	0.6590	0.2270
RD	0.6940	0.2710
RE	0.7010	0.2870
RF	0.6990	0.2800
RG	0.6830	0.2670
RH	0.7000	0.2800
RI	0.7060	0.2980
RJ	0.6970	0.2860
RK	0.6910	0.2710
RL	0.6290	0.2190
RM	0.2500	0.0860
RN	0.0000	0.0250
SA	0.0180	0.0210
SB	0.4380	0.1350
SC	0.6670	0.2360
SD	0.7140	0.2840
SE	0.7160	0.2920
SF	0.7160	0.2890
SG	0.7120	0.2790
SH	0.7140	0.2950
SI	0.7180	0.3020

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Chain	Atom inclusion	Q-score
SJ	0.7170	0.3000
SK	0.7190	0.2910
SL	0.6630	0.2300
SM	0.3750	0.1260
SN	0.0000	0.0100
TA	0.0010	0.0270
TB	0.3000	0.0530
TC	0.6160	0.2070
TD	0.6780	0.2620
TE	0.6860	0.2580
TF	0.6920	0.2750
TG	0.6800	0.2610
TH	0.6700	0.2540
TI	0.6810	0.2690
TJ	0.6900	0.2710
TK	0.6830	0.2740
TL	0.6420	0.2200
TM	0.4850	0.1300
TN	0.0480	0.0030
UA	0.0170	0.0260
UB	0.3530	0.1120
UC	0.6310	0.2310
UD	0.6630	0.2510
UE	0.7050	0.2890
UF	0.6710	0.2670
UG	0.6830	0.2680
UH	0.6490	0.2400
UI	0.6810	0.2710
UJ	0.6640	0.2560
UK	0.6700	0.2720
UL	0.6420	0.2410
UM	0.5990	0.2090
UN	0.1950	0.0210
VA	0.6960	0.2830
VB	0.4690	0.1930
VC	0.7380	0.3310
VD	0.7350	0.3130
VE	0.7390	0.3230
VF	0.7300	0.3250
VG	0.7330	0.3190
VH	0.7070	0.2980
VI	0.7430	0.3270

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Chain	Atom inclusion	Q-score
VJ	0.7280	0.3210
VK	0.6950	0.2880
VL	0.7130	0.2990
VM	0.0210	0.0100
VN	0.4530	0.1240
WA	0.7190	0.3010
WB	0.5110	0.2200
WC	0.7390	0.3350
WD	0.7250	0.3210
WE	0.7280	0.3310
WF	0.7300	0.3360
WG	0.7220	0.3170
WH	0.7010	0.3050
WI	0.7480	0.3460
WJ	0.7320	0.3300
WK	0.7150	0.3010
WL	0.7130	0.3140
WM	0.2330	0.0860
WN	0.6270	0.2310