wwPDB EM Validation Summary Report (i)

Feb 1, 2025 – 07:40 PM EST

PDB ID	:	9CPB
EMDB ID	:	EMD-45801
Title	:	Atomic model of bovine Fallopian tube cilia doublet microtubule (48-nm periodicity)
Authors	:	Zeng, J.; Sun, C.; Zhang, R.
Deposited on	:	2024-07-18
Resolution	:	3.52 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 (1)) were used in the production of this report:

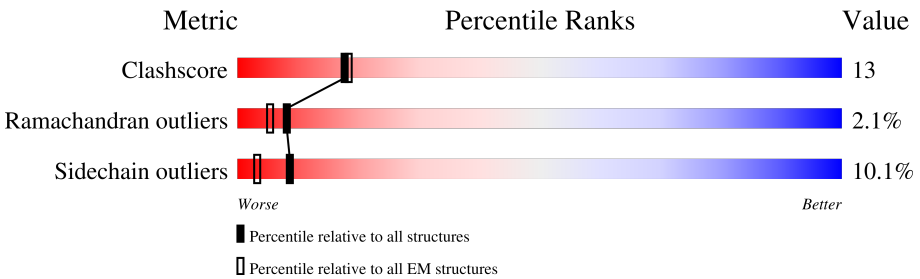
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.52 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1A	1044	39%, 46%, •, 53%
2	1D	687	14%, 15%, • •, 80%
2	1E	687	16%, 22%, • •, 73%
2	1F	687	10%, 11%, •, 88%
3	1H	547	•, 15%, 85%
3	1I	547	29%, 65%, •, 31%
4	1K	196	39%, 74%, 7%, 19%
4	1L	196	10%, 15%, •, 84%

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Mol	Chain	Length	Quality of chain
5	1N	196	8% 51% 7% 42%
5	1O	196	7% 55% 41%
5	1P	196	8% 57% 40%
6	1R	101	35% 86% 10%
7	1T	321	17% 77% 21%
7	1U	321	16% 74% 5% 21%
8	1W	193	17% 42% 24% 30%
8	1X	193	17% 92% 5%
8	1Y	193	15% 91% 5% 5%
8	1Z	193	15% 92% 5%
8	2A	193	18% 83% 10% 5%
8	2B	193	17% 92% 5%
9	2D	877	37% 45% 6% 49%
9	2E	877	11% 11% 88%
10	2F	170	9% 43% 54%
10	2G	170	15% 44% 54%
10	2H	170	16% 41% 5% 54%
11	2J	549	17% 28% 70%
11	2K	549	32% 49% 46%
11	2L	549	35% 46% 50%
11	2M	549	19% 32% 66%
12	2O	623	13% 95%
12	2P	623	17% 95%
12	2Q	623	15% 95%
13	2S	514	28% 51% 45%

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Mol	Chain	Length	Quality of chain
13	2T	514	19% 31% 7% 61%
14	2V	284	11% 11% 88%
14	2W	284	48% 71% 24%
14	2X	284	43% 68% 5% 26%
14	2Y	284	31% 53% 5% 42%
15	3A	232	38% 69% 9% 21%
16	3C	309	28% 55% 12% 32%
16	3D	309	6% 21% 77%
17	3F	212	49% 49% 50%
18	3H	1410	5% 7% 93%
19	3J	640	20% 57% 10% 33%
19	3K	640	27% 52% 17% 31%
19	3L	640	29% 54% 16% 29%
20	3N	733	20% 30% 8% 61%
20	3O	733	35% 61% 18% 21%
20	3P	733	45% 64% 15% 21%
20	3Q	733	31% 34% 5% 60%
21	3S	259	7% 22% 5% 73%
21	3T	259	32% 76% 15% 9%
21	3U	259	33% 77% 12% 9%
21	3V	259	33% 67% 12% 21%
22	3X	274	44% 39% 8% 53%
22	3Y	274	22% 35% 12% 48%
22	3Z	274	28% 37% 11% 51%
22	4A	274	36% 30% 9% 61%

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Mol	Chain	Length	Quality of chain
22	4B	274	27% 31% 8% 62%
22	4C	274	31% 23% 8% 69%
23	4D	135	30% 64% 21% 14%
24	4F	495	11% 18% 10% • 69%
24	4G	495	43% 55% 12% 32%
25	4I	377	65% 84% 15% •
25	4J	377	48% 76% 23% ••
26	4K	621	14% 16% 5% 79%
26	4L	621	19% 27% 9% 63%
26	4M	621	13% 12% 5% 83%
27	4O	257	18% 68% 17% 15%
27	4P	257	19% 72% 13% 15%
27	4Q	257	16% 66% 19% 15%
27	4R	257	20% 40% 32% 13% • 15%
27	4S	257	19% 75% 10% 15%
27	4T	257	60% 67% 16% •• 15%
28	4V	136	18% 18% 10% 73%
28	4W	136	17% 46% 10% • 42%
29	4Y	120	42% 59% 19% •• 20%
30	5A	377	31% 73% 19% • 7%
30	5B	377	• •• 96%
31	5D	169	91% 74% 19% 7%
31	5E	169	75% 69% 20% •• 7%
31	5F	169	92% 88% 7% 6%
31	5G	169	85% 73% 19% • 7%

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Mol	Chain	Length	Quality of chain
31	5H	169	92% 80% 12% • 7%
31	5I	169	91% 87% 6% 7%
31	5J	169	92% 73% 20% 7%
32	5L	418	• 22% 6% 72%
32	5M	418	15% 72% 22% 6%
32	5N	418	12% 77% 17% • 6%
32	5O	418	11% 33% 25% 10% • 30%
33	5Q	430	7% 20% 6% 75%
33	5R	430	9% 76% 16% • 7%
33	5S	430	9% 61% 21% 9% • 7%
33	5T	430	5% 32% 27% 10% • 29%
33	5V	430	64% 45% 23% • 28%
33	5W	430	85% 69% 25% • 5%
33	5X	430	83% 71% 22% • 5%
33	5Y	430	23% 19% 5% 75%
34	6A	490	38% 20% 25% 9% • 44%
34	6B	490	53% 52% 22% 5% 20%
34	6C	490	50% 38% 28% 12% • 20%
34	6D	490	17% 11% 9% • • 75%
34	6E	490	12% 5% 5% • 88%
34	6F	490	72% 56% 16% • 27%
34	6G	490	82% 68% 17% 15%
34	6H	490	74% 58% 16% • 25%
34	6I	490	13% 12% • 87%
34	6J	490	13% 10% • 87%

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Mol	Chain	Length	Quality of chain
34	6K	490	75% 62% 14% 24%
34	6L	490	83% 66% 18% 15%
34	6M	490	72% 57% 16% 26%
34	6N	490	11% 8% 89%
35	6P	447	20% 36% 60%
35	6Q	447	28% 77% 14% 8%
35	6R	447	32% 70% 17% 8%
35	6S	447	21% 38% 15% 43%
35	6T	447	53% 41% 11% 47%
35	6U	447	92% 72% 21% 6%
35	6V	447	96% 67% 27%
35	6W	447	47% 33% 12% 52%
36	6Y	683	15% 25% 72%
36	6Z	683	12% 26% 72%
37	7C	254	28% 26% 19% 53%
37	7D	254	13% 24% 6% 69%
37	7E	254	22% 22% 11% 67%
37	7F	254	14% 17% 7% 74%
38	7H	274	24% 18% 11% 69%
38	7I	274	8% 8% 5% 88%
39	7K	147	31% 64% 9% 27%
39	7L	147	18% 25% 5% 69%
40	7N	484	13% 10% 87%
41	AB	445	18% 68% 30%
41	AD	445	12% 74% 23%

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Mol	Chain	Length	Quality of chain
41	AF	445	11% 75% 22%
41	AH	445	6% 48% 36% 13%
41	AJ	445	11% 80% 18%
41	AL	445	7% 56% 31% 9%
41	BB	445	20% 76% 19%
41	BD	445	10% 42% 40% 12%
41	BF	445	16% 74% 22%
41	BH	445	15% 73% 22%
41	BJ	445	22% 72% 23%
41	BL	445	14% 72% 23%
41	CB	445	24% 69% 26%
41	CD	445	13% 41% 37% 15%
41	CF	445	11% 39% 39% 17%
41	CH	445	14% 65% 29%
41	CJ	445	11% 40% 38% 16%
41	CL	445	13% 62% 32%
41	DB	445	41% 62% 32%
41	DD	445	22% 66% 29%
41	DF	445	18% 63% 30%
41	DH	445	16% 28% 46% 18%
41	DJ	445	12% 29% 41% 24%
41	DL	445	15% 56% 35%
41	ED	445	9% 31% 45% 17%
41	EF	445	9% 63% 32%
41	EH	445	15% 65% 30%

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Mol	Chain	Length	Quality of chain
41	EJ	445	11% 65% 28%
41	EL	445	12% 61% 30%
41	FD	445	7% 36% 38% 18%
41	FF	445	14% 63% 29%
41	FH	445	23% 57% 38%
41	FJ	445	17% 58% 37%
41	FL	445	12% 32% 43% 17%
41	GD	445	8% 46% 36% 12%
41	GF	445	16% 69% 26%
41	GH	445	16% 70% 26%
41	GJ	445	6% 41% 40% 13%
41	GL	445	17% 74% 21%
41	HB	445	19% 70% 22%
41	HD	445	7% 38% 44% 12%
41	HF	445	12% 63% 32%
41	HH	445	10% 64% 31%
41	HJ	445	5% 39% 39% 16%
41	HL	445	9% 69% 25%
41	ID	445	15% 68% 28%
41	IF	445	15% 67% 29%
41	IH	445	12% 72% 23%
41	IJ	445	14% 73% 23%
41	IL	445	16% 67% 28%
41	IN	445	11% 42% 36% 14%
41	JD	445	10% 69% 25%

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Mol	Chain	Length	Quality of chain
41	JF	445	9% 75% 20%
41	JH	445	17% 70% 25%
41	JJ	445	10% 69% 26%
41	JL	445	7% 50% 35% 9%
41	KD	445	9% 73% 22%
41	KF	445	8% 76% 20%
41	KH	445	8% 73% 23%
41	KJ	445	8% 75% 20%
41	KL	445	6% 73% 23%
41	KN	445	10% 75% 20%
41	LD	445	56% 31% 8%
41	LF	445	7% 81% 15%
41	LH	445	6% 79% 17%
41	LJ	445	6% 75% 21%
41	LL	445	7% 74% 21%
41	LN	445	13% 78% 18%
41	MD	445	5% 42% 37% 15%
41	MF	445	44% 38% 12%
41	MH	445	8% 76% 20%
41	MJ	445	11% 71% 24%
41	ML	445	9% 60% 36%
41	MN	445	26% 43% 34% 17%
41	NB	445	11% 50% 31% 12%
41	ND	445	8% 42% 40% 11%
41	NF	445	10% 49% 31% 13%

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Mol	Chain	Length	Quality of chain
41	NH	445	10% 47% 36% 11%
41	NJ	445	15% 71% 24%
41	NL	445	26% 62% 26% 11%
41	OB	445	10% 35% 40% 18%
41	OD	445	16% 65% 30% 5%
41	OF	445	17% 64% 29%
41	OH	445	11% 45% 37% 11%
41	OJ	445	14% 44% 38% 12%
41	OL	445	20% 66% 28% 5%
41	PB	445	16% 36% 41% 18%
41	PD	445	17% 42% 36% 16%
41	PF	445	20% 38% 43% 13%
41	PH	445	14% 22% 42% 25% 7%
41	PJ	445	13% 24% 43% 25%
41	PL	445	22% 34% 39% 19%
41	QB	445	32% 62% 33%
41	QD	445	27% 60% 35%
41	QF	445	29% 64% 31%
41	QH	445	23% 36% 40% 16%
41	QJ	445	22% 34% 40% 19%
41	QL	445	33% 33% 38% 20%
41	RB	445	39% 60% 35%
41	RD	445	18% 34% 41% 18%
41	RF	445	18% 25% 49% 19%
41	RH	445	24% 63% 33%

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Mol	Chain	Length	Quality of chain
41	RJ	445	18% 38% 38% 19%
41	RL	445	32% 66% 29%
41	SD	445	18% 62% 33%
41	SF	445	18% 42% 37% 15%
41	SH	445	24% 60% 33%
41	SJ	445	19% 68% 27%
41	SL	445	24% 38% 39% 16%
41	TD	445	18% 63% 31%
41	TF	445	16% 66% 29%
41	TH	445	20% 64% 29%
41	TJ	445	16% 61% 33%
41	TL	445	17% 62% 32%
41	UD	445	15% 64% 29%
41	UF	445	12% 69% 27%
41	UH	445	14% 64% 31%
41	UJ	445	11% 64% 31%
41	UL	445	14% 61% 33%
41	VD	445	13% 69% 26%
41	VF	445	10% 65% 29%
41	VH	445	11% 71% 25%
41	VJ	445	12% 71% 24%
41	VL	445	11% 67% 29%
41	WD	445	6% 76% 20%
41	WF	445	5% 47% 33% 14%
41	WH	445	6% 50% 35% 10%

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Mol	Chain	Length	Quality of chain
41	WJ	445	8% 68% 26%
41	WL	445	7% 71% 24%
41	WN	445	15% 73% 22%
42	AC	452	10% 80% 17%
42	AE	452	11% 77% 21%
42	AG	452	10% 75% 21%
42	AI	452	8% 50% 34% 12%
42	AK	452	6% 47% 37% 13%
42	BC	452	17% 69% 28%
42	BE	452	13% 74% 21%
42	BG	452	13% 71% 24%
42	BI	452	6% 44% 34% 16% 5%
42	BK	452	14% 77% 20%
42	CC	452	13% 37% 41% 16%
42	CE	452	16% 69% 27%
42	CG	452	9% 35% 46% 14%
42	CI	452	16% 72% 25%
42	CK	452	13% 71% 25%
42	CM	452	29% 65% 29%
42	DC	452	23% 63% 31% 5%
42	DE	452	18% 64% 31% 5%
42	DG	452	19% 67% 28% 5%
42	DI	452	18% 62% 31% 5%
42	DK	452	15% 34% 43% 16% 5%
42	DM	452	27% 65% 29% 5%

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Mol	Chain	Length	Quality of chain
42	EC	452	22% 62% 34%
42	EE	452	11% 40% 40% 15%
42	EG	452	9% 36% 41% 17%
42	EI	452	12% 64% 31%
42	EK	452	14% 31% 42% 21%
42	EM	452	17% 34% 39% 19% 5%
42	FC	452	23% 30% 45% 18% 5%
42	FE	452	13% 61% 32% 6%
42	FG	452	16% 59% 34% 6%
42	FI	452	19% 56% 38% 6%
42	FK	452	11% 33% 38% 19% 6%
42	FM	452	29% 53% 40% 5%
42	GC	452	31% 72% 25%
42	GE	452	16% 72% 22% 5%
42	GG	452	17% 73% 22%
42	GI	452	11% 69% 26% 5%
42	GK	452	17% 70% 24% 5%
42	GM	452	13% 37% 41% 18%
42	HC	452	15% 33% 42% 18% 6%
42	HE	452	12% 63% 31% 5%
42	HG	452	7% 41% 39% 13% 5%
42	HI	452	5% 40% 40% 14% 5%
42	HK	452	12% 60% 35% 5%
42	HM	452	7% 46% 32% 14% 5%
42	IC	452	30% 75% 20% 5%

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Mol	Chain	Length	Quality of chain
42	IE	452	8% 50% 32% 12%
42	IG	452	13% 73% 23%
42	II	452	12% 71% 25%
42	IK	452	17% 71% 26%
42	IM	452	13% 71% 24% 5%
42	JC	452	15% 71% 23%
42	JE	452	11% 70% 25% 5%
42	JG	452	9% 73% 21% 5%
42	JI	452	15% 72% 22% 5%
42	JK	452	7% 40% 38% 17%
42	JM	452	6% 51% 30% 12% 5%
42	KC	452	10% 82% 14%
42	KE	452	8% 80% 15% 5%
42	KG	452	5% 75% 19% 5%
42	KI	452	5% 75% 20% 5%
42	KK	452	6% 75% 19% 5%
42	KM	452	57% 30% 8%
42	LC	452	7% 78% 17%
42	LE	452	9% 78% 19%
42	LG	452	6% 79% 16%
42	LI	452	8% 77% 19%
42	LK	452	7% 79% 17%
42	LM	452	8% 77% 17% 5%
42	MC	452	8% 69% 27%
42	ME	452	9% 74% 21% 5%

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Mol	Chain	Length	Quality of chain
42	MG	452	5% 54% 33% 8% 5%
42	MI	452	9% 74% 21% 5%
42	MK	452	21% 62% 34%
42	MM	452	10% 62% 33% 5%
42	NA	452	11% 45% 33% 15% 5%
42	NC	452	8% 42% 36% 15% 5%
42	NE	452	13% 71% 23% 5%
42	NG	452	10% 49% 33% 11%
42	NI	452	11% 44% 35% 13%
42	NK	452	10% 43% 37% 14% 5%
42	OA	452	23% 66% 28% 5%
42	OC	452	14% 65% 28% 5%
42	OE	452	13% 63% 31%
42	OG	452	13% 48% 33% 13%
42	OI	452	12% 67% 27%
42	OK	452	14% 65% 29% 5%
42	PA	452	29% 29% 33% 16% 19%
42	PC	452	17% 37% 38% 19%
42	PE	452	12% 35% 40% 17% 5%
42	PG	452	12% 21% 46% 23% 6% 5%
42	PI	452	12% 23% 40% 26% 5% 6%
42	PK	452	17% 42% 36% 16% 5%
42	QC	452	27% 64% 29% 5%
42	QE	452	22% 63% 31% 5%
42	QG	452	27% 62% 31% 5%

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Mol	Chain	Length	Quality of chain
42	QI	452	17% 38% 38% 16% • 5%
42	QK	452	24% 40% 39% 15% • 5%
42	RC	452	30% 61% 34% • •
42	RE	452	19% 65% 29% 5%
42	RG	452	24% 60% 33% • 5%
42	RI	452	20% 59% 35% • 5%
42	RK	452	25% 61% 33% • 5%
42	SC	452	25% 61% 34% • 5%
42	SE	452	17% 42% 36% 15% • 5%
42	SG	452	20% 66% 28% • 5%
42	SI	452	14% 40% 35% 17% • 6%
42	SK	452	21% 63% 31% • •
42	SM	452	57% 61% 33% • 5%
42	TC	452	29% 63% 32% • 5%
42	TE	452	18% 62% 33% • •
42	TG	452	25% 62% 31% • 5%
42	TI	452	17% 41% 35% 17% • 5%
42	TK	452	13% 43% 35% 14% • •
42	TM	452	40% 50% 43% • 5%
42	UC	452	16% 44% 37% 12% • •
42	UE	452	15% 69% 26% • •
42	UG	452	12% 65% 27% • •
42	UI	452	16% 67% 27% • •
42	UK	452	14% 63% 31% • •
42	UM	452	19% 64% 30% • 5%

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Mol	Chain	Length	Quality of chain
42	VC	452	14% 75% 22%
42	VE	452	10% 72% 24%
42	VG	452	12% 72% 25%
42	VI	452	11% 71% 25%
42	VK	452	11% 51% 32% 13%
42	VM	452	12% 68% 26% 5%
42	WC	452	10% 78% 19%
42	WE	452	5% 56% 30% 9% 5%
42	WG	452	10% 74% 23%
42	WI	452	6% 53% 32% 10% 5%
42	WK	452	8% 72% 24%
42	WM	452	9% 70% 25% 5%

2 Entry composition (i)

There are 45 unique types of molecules in this entry. The entry contains 1132145 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 Armadillo repeat containing 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	1A	493	2437	1451	493	493	0	0

- Molecule 2 is a protein called Coiled-coil domain containing 114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1D	134	1109	675	215	216	3	0	0
2	1E	187	1569	955	314	294	6	0	0
2	1F	83	698	424	145	125	4	0	0

- Molecule 3 is a protein called Coiled-coil domain containing 173.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1H	83	685	426	121	136	2	0	0
3	1I	377	3234	2007	605	612	10	0	0

- Molecule 4 is a protein called Uncharacterized protein C1orf158 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1K	159	1348	877	241	229	1	0	0
4	1L	32	Total	C	N	O		0	0
			269	170	48	51			

- Molecule 5 is a protein called Protein Flattop.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1N	114	894	569	162	161	2	0	0
5	1O	116	910	580	165	163	2	0	0
5	1P	118	928	590	169	167	2	0	0

- Molecule 6 is a protein called CFAP141.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	1R	91	785	495	151	133	6	0	0

- Molecule 7 is a protein called Cilia and flagella associated protein 161.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	1T	255	2055	1302	369	373	11	0	0
7	1U	255	2055	1302	369	373	11	0	0

- Molecule 8 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	1W	136	1143	741	196	200	6	0	0
8	1X	184	1532	984	268	273	7	0	0
8	1Y	184	1532	984	268	273	7	0	0
8	1Z	184	1532	984	268	273	7	0	0
8	2A	184	1532	984	268	273	7	0	0
8	2B	184	1532	984	268	273	7	0	0

- Molecule 9 is a protein called EF-hand domain family member B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	2D	451	3649	2326	650	660	13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	2E	101	816	513	145	156	2	0	0

- Molecule 10 is a protein called CFAP276.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	2F	79	631	395	116	120	0	0
10	2G	79	631	395	116	120	0	0
10	2H	79	631	395	116	120	0	0

- Molecule 11 is a protein called Cilia and flagella associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	2J	162	1349	837	245	258	9	0	0
11	2K	296	2554	1543	517	485	9	0	0
11	2L	275	2330	1426	438	450	16	0	0
11	2M	186	1589	961	327	299	2	0	0

- Molecule 12 is a protein called Cilia and flagella associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	2O	609	4713	2985	822	874	32	0	0
12	2P	609	4713	2985	822	874	32	0	0
12	2Q	609	4713	2985	822	874	32	0	0

- Molecule 13 is a protein called Methyl-CpG binding domain protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	2S	281	2081	1267	402	403	9	0	0
13	2T	199	1694	1032	321	329	12	0	0

- Molecule 14 is a protein called Cilia and flagella associated protein 77.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	2V	34	287	183	56	46	2	0	0
14	2W	215	1756	1109	335	303	9	0	0
14	2X	210	1711	1080	326	296	9	0	0
14	2Y	165	1327	838	250	232	7	0	0

- Molecule 15 is a protein called CFAP95.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	3A	183	1487	932	258	288	9	0	0

- Molecule 16 is a protein called Cilia-and flagella-associated protein 96.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	3C	211	1693	1077	291	318	7	0	0
16	3D	71	531	339	94	95	3	0	0

- Molecule 17 is a protein called EF-hand calcium-binding domain-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	3F	105	520	310	105	105	0	0

- Molecule 18 is a protein called EF-hand calcium binding domain 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	3H	97	481	287	97	97	0	0

- Molecule 19 is a protein called EF-hand domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	3J	431	3563	2303	597	649	14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	3K	443	3652	2361	613	664	14	0	0
19	3L	452	3726	2406	627	678	15	0	0

- Molecule 20 is a protein called EFHC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	3N	286	2388	1534	406	438	10	0	0
20	3O	579	4781	3067	810	878	26	0	0
20	3P	581	4787	3070	808	884	25	0	0
20	3Q	290	2409	1545	404	445	15	0	0

- Molecule 21 is a protein called Enkurin, TRPC channel interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	3S	70	563	356	95	110	2	0	0
21	3T	235	1939	1242	336	354	7	0	0
21	3U	235	1939	1242	336	354	7	0	0
21	3V	205	1696	1087	295	307	7	0	0

- Molecule 22 is a protein called Protein FAM166B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	3X	129	1014	662	172	174	6	0	0
22	3Y	142	1116	732	189	189	6	0	0
22	3Z	135	1059	690	181	182	6	0	0
22	4A	107	840	548	142	144	6	0	0
22	4B	105	830	538	143	143	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	4C	85	667	433	111	118	5	0	0

- Molecule 23 is a protein called Cilia- and flagella-associated protein 144.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	4D	116	992	627	186	177	2	0	0

- Molecule 24 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	4F	151	1261	772	241	244	4	0	0
24	4G	335	2883	1786	528	553	16	0	0

- Molecule 25 is a protein called Nucleoside diphosphate kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	4I	372	2533	1589	451	481	12	0	0
25	4J	372	2947	1880	499	546	22	0	0

- Molecule 26 is a protein called Outer dynein arm-docking complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	4K	132	1102	683	204	212	3	0	0
26	4L	228	1911	1190	353	364	4	0	0
26	4M	104	876	549	164	162	1	0	0

- Molecule 27 is a protein called PACRG protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	4O	219	1767	1144	298	316	9	0	0
27	4P	219	1767	1144	298	316	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	4Q	219	1767	1144	298	316	9	0	0
27	4R	219	1767	1144	298	316	9	0	0
27	4S	219	1767	1144	298	316	9	0	0
27	4T	219	1767	1144	298	316	9	0	0

- Molecule 28 is a protein called Pierce1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	4V	37	304	191	52	58	3	0	0
28	4W	79	654	415	118	119	2	0	0

- Molecule 29 is a protein called Pierce2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	4Y	96	775	496	130	142	7	0	0

- Molecule 30 is a protein called RIB43A-like with coiled-coils protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	5A	350	2915	1775	574	553	13	0	0
			Total	C	N	O			
30	5B	16	133	81	24	28		0	0

- Molecule 31 is a protein called Sperm acrosome associated 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	5D	157	1260	787	225	237	11	0	0
31	5E	157	1254	784	222	237	11	0	0
31	5F	159	1277	799	228	239	11	0	0
31	5G	157	1260	787	225	237	11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	5H	157	1260	787	225	237	11	0	0
31	5I	157	1260	787	225	237	11	0	0
31	5J	157	1260	787	225	237	11	0	0

- Molecule 32 is a protein called Tektin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	5L	116	943	585	176	180	2	0	0
32	5M	392	3231	2011	588	623	9	0	0
32	5N	392	3231	2011	588	623	9	0	0
32	5O	291	2414	1505	434	468	7	0	0

- Molecule 33 is a protein called Tektin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	5Q	109	901	548	176	175	2	0	0
33	5R	399	3250	2002	602	632	14	0	0
33	5S	399	3250	2002	602	632	14	0	0
33	5T	306	2498	1546	453	486	13	0	0
33	5V	308	2513	1560	453	487	13	0	0
33	5W	408	3336	2055	618	649	14	0	0
33	5X	408	3336	2055	618	649	14	0	0
33	5Y	107	877	533	170	172	2	0	0

- Molecule 34 is a protein called Tektin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	6A	273	2240	1377	412	440	11	0	0
34	6B	392	3189	1962	583	629	15	0	0
34	6C	393	3200	1968	587	630	15	0	0
34	6D	123	992	612	180	197	3	0	0
34	6E	59	487	301	91	93	2	0	0
34	6F	358	2896	1786	526	569	15	0	0
34	6G	416	3386	2084	618	667	17	0	0
34	6H	368	2989	1840	545	589	15	0	0
34	6I	63	531	324	101	104	2	0	0
34	6J	65	553	347	100	105	1	0	0
34	6K	371	3022	1869	546	593	14	0	0
34	6L	418	3411	2107	621	667	16	0	0
34	6M	361	2923	1804	532	572	15	0	0
34	6N	54	445	275	83	85	2	0	0

- Molecule 35 is a protein called Tektin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	6P	180	1491	915	272	298	6	0	0
35	6Q	410	3364	2070	628	651	15	0	0
35	6R	410	3364	2070	628	651	15	0	0
35	6S	254	2057	1269	390	389	9	0	0
35	6T	236	1917	1184	365	359	9	0	0
35	6U	419	3413	2097	638	663	15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	6V	437	3571	2201	666	688	16	0	0
35	6W	215	1766	1088	324	347	7	0	0

- Molecule 36 is a protein called TTC25 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	6Y	192	1300	812	232	249	7	0	0
36	6Z	192	1300	812	232	249	7	0	0

- Molecule 37 is a protein called Ciliary microtubule associated protein 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	7C	119	898	571	159	163	5	0	0
37	7D	80	618	404	113	99	2	0	0
37	7E	85	625	398	111	113	3	0	0
37	7F	67	519	338	89	91	1	0	0

- Molecule 38 is a protein called Ciliary microtubule associated protein 1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	7H	85	637	409	108	114	6	0	0
38	7I	34	238	151	43	42	2	0	0

- Molecule 39 is a protein called Cilia and flagella associated protein 90.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	7K	107	878	543	174	160	1	0	0
39	7L	46	382	249	65	67	1	0	0

- Molecule 40 is a protein called Sperm associated antigen 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	7N	64	524	324	93	104	3	0	0

- Molecule 41 is a protein called Tubulin beta-4B chain.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	DD	426	3348	2105	574	643	26	0	0
41	DF	426	3348	2105	574	643	26	0	0
41	DH	426	3348	2105	574	643	26	0	0
41	DJ	426	3348	2105	574	643	26	0	0
41	DL	425	3340	2100	573	642	25	0	0
41	ED	426	3348	2105	574	643	26	0	0
41	EF	426	3348	2105	574	643	26	0	0
41	EH	428	3361	2112	576	647	26	0	0
41	EJ	426	3348	2105	574	643	26	0	0
41	EL	425	3340	2100	573	642	25	0	0
41	FD	427	3356	2109	575	646	26	0	0
41	FF	426	3348	2105	574	643	26	0	0
41	FH	426	3348	2105	574	643	26	0	0
41	FJ	426	3348	2105	574	643	26	0	0
41	FL	425	3340	2100	573	642	25	0	0
41	GD	427	3356	2109	575	646	26	0	0
41	GF	428	3361	2112	576	647	26	0	0
41	GH	428	3361	2112	576	647	26	0	0
41	GJ	428	3361	2112	576	647	26	0	0
41	GL	425	3340	2100	573	642	25	0	0
41	HB	426	3348	2105	574	643	26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	HD	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	HF	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	HH	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	HJ	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	HL	425	3340	2100	573	642	25	0	0
			Total	C	N	O	S		
41	ID	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	IF	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	IH	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	IJ	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	IL	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	IN	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	JD	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	JF	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	JH	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	JJ	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	JL	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	KD	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	KF	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	KH	429	3368	2116	577	649	26	0	0
			Total	C	N	O	S		
41	KJ	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	KL	429	3368	2116	577	649	26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	KN	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	LD	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	LF	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	LH	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	LJ	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	LL	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	LN	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	MD	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	MF	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	MH	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	MJ	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	ML	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	MN	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	NB	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	ND	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	NF	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	NH	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	NJ	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	NL	396	3118	1966	533	597	22	0	0
			Total	C	N	O	S		
41	OB	425	3339	2100	572	641	26	0	0
			Total	C	N	O	S		
41	OD	424	3327	2091	571	639	26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	OF	425	3339	2100	572	641	26	0	0
			Total	C	N	O	S		
41	OH	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	OJ	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	OL	424	3327	2091	571	639	26	0	0
			Total	C	N	O	S		
41	PB	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	PD	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	PF	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	PH	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	PJ	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	PL	425	3340	2100	573	642	25	0	0
			Total	C	N	O	S		
41	QB	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	QD	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	QF	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	QH	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	QJ	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	QL	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	RB	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	RD	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	RF	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	RH	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	RJ	428	3361	2112	576	647	26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	RL	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	SD	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	SF	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	SH	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	SJ	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	SL	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	TD	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	TF	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	TH	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	TJ	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	TL	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	UD	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	UF	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	UH	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	UJ	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	UL	426	3348	2105	574	643	26	0	0
			Total	C	N	O	S		
41	VD	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	VF	427	3356	2109	575	646	26	0	0
			Total	C	N	O	S		
41	VH	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	VJ	428	3361	2112	576	647	26	0	0
			Total	C	N	O	S		
41	VL	426	3348	2105	574	643	26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	WD	427	3356	2109	575	646	26	0	0
41	WF	426	3348	2105	574	643	26	0	0
41	WH	426	3348	2105	574	643	26	0	0
41	WJ	426	3348	2105	574	643	26	0	0
41	WL	426	3348	2105	574	643	26	0	0
41	WN	426	3348	2105	574	643	26	0	0

- Molecule 42 is a protein called Tubulin alpha-1D chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	AC	440	3437	2175	584	655	23	0	0
42	AE	440	3437	2175	584	655	23	0	0
42	AG	440	3437	2175	584	655	23	0	0
42	AI	440	3437	2175	584	655	23	0	0
42	AK	440	3437	2175	584	655	23	0	0
42	BC	440	3437	2175	584	655	23	0	0
42	BE	433	3396	2151	576	646	23	0	0
42	BG	440	3437	2175	584	655	23	0	0
42	BI	430	3374	2138	573	640	23	0	0
42	BK	439	3430	2170	583	654	23	0	0
42	CC	438	3424	2167	582	652	23	0	0
42	CE	438	3424	2167	582	652	23	0	0
42	CG	439	3430	2170	583	654	23	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	CI	439	3430	2170	583	654	23	0	0
			Total	C	N	O	S		
42	CK	439	3430	2170	583	654	23	0	0
			Total	C	N	O	S		
42	CM	439	3430	2170	583	654	23	0	0
			Total	C	N	O	S		
42	DC	429	3366	2134	572	637	23	0	0
			Total	C	N	O	S		
42	DE	430	3372	2137	573	639	23	0	0
			Total	C	N	O	S		
42	DG	431	3379	2142	574	640	23	0	0
			Total	C	N	O	S		
42	DI	429	3364	2133	572	636	23	0	0
			Total	C	N	O	S		
42	DK	430	3372	2137	573	639	23	0	0
			Total	C	N	O	S		
42	DM	430	3372	2137	573	639	23	0	0
			Total	C	N	O	S		
42	EC	439	3430	2170	583	654	23	0	0
			Total	C	N	O	S		
42	EE	441	3446	2180	585	658	23	0	0
			Total	C	N	O	S		
42	EG	434	3404	2157	578	646	23	0	0
			Total	C	N	O	S		
42	EI	436	3408	2158	580	648	22	0	0
			Total	C	N	O	S		
42	EK	440	3437	2175	584	655	23	0	0
			Total	C	N	O	S		
42	EM	428	3358	2130	571	634	23	0	0
			Total	C	N	O	S		
42	FC	431	3379	2142	574	640	23	0	0
			Total	C	N	O	S		
42	FE	425	3339	2118	568	631	22	0	0
			Total	C	N	O	S		
42	FG	426	3346	2123	569	632	22	0	0
			Total	C	N	O	S		
42	FI	427	3347	2121	570	633	23	0	0
			Total	C	N	O	S		
42	FK	424	3326	2109	566	629	22	0	0
			Total	C	N	O	S		
42	FM	429	3365	2132	572	638	23	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	GC	440	3437	2175	584	655	23	0	0
			Total	C	N	O	S		
42	GE	430	3371	2138	573	637	23	0	0
			Total	C	N	O	S		
42	GG	433	3393	2149	576	645	23	0	0
			Total	C	N	O	S		
42	GI	429	3365	2135	572	635	23	0	0
			Total	C	N	O	S		
42	GK	429	3364	2133	572	636	23	0	0
			Total	C	N	O	S		
42	GM	439	3430	2170	583	654	23	0	0
			Total	C	N	O	S		
42	HC	427	3350	2126	570	631	23	0	0
			Total	C	N	O	S		
42	HE	430	3374	2138	573	640	23	0	0
			Total	C	N	O	S		
42	HG	430	3371	2138	573	637	23	0	0
			Total	C	N	O	S		
42	HI	430	3371	2138	573	637	23	0	0
			Total	C	N	O	S		
42	HK	431	3379	2142	574	640	23	0	0
			Total	C	N	O	S		
42	HM	429	3365	2132	572	638	23	0	0
			Total	C	N	O	S		
42	IC	429	3365	2135	572	635	23	0	0
			Total	C	N	O	S		
42	IE	432	3388	2147	575	643	23	0	0
			Total	C	N	O	S		
42	IG	440	3437	2175	584	655	23	0	0
			Total	C	N	O	S		
42	II	432	3387	2146	575	643	23	0	0
			Total	C	N	O	S		
42	IK	440	3437	2175	584	655	23	0	0
			Total	C	N	O	S		
42	IM	431	3378	2140	574	641	23	0	0
			Total	C	N	O	S		
42	JC	432	3384	2143	575	643	23	0	0
			Total	C	N	O	S		
42	JE	430	3372	2137	573	639	23	0	0
			Total	C	N	O	S		
42	JG	428	3358	2130	571	634	23	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	JI	429	3366	2134	572	637	23	0	0
			Total	C	N	O	S		
42	JK	440	3437	2175	584	655	23	0	0
			Total	C	N	O	S		
42	JM	430	3372	2137	573	639	23	0	0
			Total	C	N	O	S		
42	KC	432	3384	2143	575	643	23	0	0
			Total	C	N	O	S		
42	KE	431	3380	2141	574	642	23	0	0
			Total	C	N	O	S		
42	KG	430	3370	2136	573	638	23	0	0
			Total	C	N	O	S		
42	KI	428	3358	2130	571	634	23	0	0
			Total	C	N	O	S		
42	KK	430	3372	2137	573	639	23	0	0
			Total	C	N	O	S		
42	KM	432	3376	2138	575	641	22	0	0
			Total	C	N	O	S		
42	LC	433	3393	2149	576	645	23	0	0
			Total	C	N	O	S		
42	LE	440	3437	2175	584	655	23	0	0
			Total	C	N	O	S		
42	LG	433	3393	2149	576	645	23	0	0
			Total	C	N	O	S		
42	LI	434	3397	2151	577	646	23	0	0
			Total	C	N	O	S		
42	LK	435	3401	2153	578	647	23	0	0
			Total	C	N	O	S		
42	LM	431	3378	2140	574	641	23	0	0
			Total	C	N	O	S		
42	MC	439	3430	2170	583	654	23	0	0
			Total	C	N	O	S		
42	ME	429	3366	2134	572	637	23	0	0
			Total	C	N	O	S		
42	MG	430	3372	2137	573	639	23	0	0
			Total	C	N	O	S		
42	MI	431	3379	2142	574	640	23	0	0
			Total	C	N	O	S		
42	MK	440	3437	2175	584	655	23	0	0
			Total	C	N	O	S		
42	MM	431	3376	2138	574	642	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	NA	430	3372	2136	573	641	22	0	0
			Total	C	N	O	S		
42	NC	429	3365	2135	572	635	23	0	0
			Total	C	N	O	S		
42	NE	430	3374	2140	573	638	23	0	0
			Total	C	N	O	S		
42	NG	432	3387	2146	575	643	23	0	0
			Total	C	N	O	S		
42	NI	432	3387	2146	575	643	23	0	0
			Total	C	N	O	S		
42	NK	430	3374	2138	573	640	23	0	0
			Total	C	N	O	S		
42	OA	428	3358	2129	571	636	22	0	0
			Total	C	N	O	S		
42	OC	429	3366	2134	572	637	23	0	0
			Total	C	N	O	S		
42	OE	433	3396	2151	576	646	23	0	0
			Total	C	N	O	S		
42	OG	433	3391	2148	576	644	23	0	0
			Total	C	N	O	S		
42	OI	432	3387	2146	575	643	23	0	0
			Total	C	N	O	S		
42	OK	431	3380	2141	574	642	23	0	0
			Total	C	N	O	S		
42	PA	368	2872	1820	487	545	20	0	0
			Total	C	N	O	S		
42	PC	432	3386	2144	575	644	23	0	0
			Total	C	N	O	S		
42	PE	431	3380	2143	574	640	23	0	0
			Total	C	N	O	S		
42	PG	430	3371	2138	573	637	23	0	0
			Total	C	N	O	S		
42	PI	427	3349	2123	570	634	22	0	0
			Total	C	N	O	S		
42	PK	430	3371	2138	573	637	23	0	0
			Total	C	N	O	S		
42	QC	430	3372	2137	573	639	23	0	0
			Total	C	N	O	S		
42	QE	430	3372	2137	573	639	23	0	0
			Total	C	N	O	S		
42	QG	431	3380	2141	574	642	23	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	QI	429	3366	2134	572	637	23	0	0
			Total	C	N	O	S		
42	QK	431	3380	2141	574	642	23	0	0
			Total	C	N	O	S		
42	RC	432	3387	2146	575	643	23	0	0
			Total	C	N	O	S		
42	RE	428	3358	2130	571	634	23	0	0
			Total	C	N	O	S		
42	RG	430	3372	2137	573	639	23	0	0
			Total	C	N	O	S		
42	RI	431	3379	2142	574	640	23	0	0
			Total	C	N	O	S		
42	RK	431	3379	2142	574	640	23	0	0
			Total	C	N	O	S		
42	SC	430	3372	2137	573	639	23	0	0
			Total	C	N	O	S		
42	SE	431	3381	2142	574	642	23	0	0
			Total	C	N	O	S		
42	SG	431	3379	2142	574	640	23	0	0
			Total	C	N	O	S		
42	SI	427	3358	2129	569	637	23	0	0
			Total	C	N	O	S		
42	SK	432	3387	2146	575	643	23	0	0
			Total	C	N	O	S		
42	SM	431	3378	2140	574	641	23	0	0
			Total	C	N	O	S		
42	TC	430	3371	2138	573	637	23	0	0
			Total	C	N	O	S		
42	TE	432	3388	2147	575	643	23	0	0
			Total	C	N	O	S		
42	TG	430	3371	2138	573	637	23	0	0
			Total	C	N	O	S		
42	TI	430	3371	2138	573	637	23	0	0
			Total	C	N	O	S		
42	TK	432	3387	2146	575	643	23	0	0
			Total	C	N	O	S		
42	TM	430	3372	2137	573	639	23	0	0
			Total	C	N	O	S		
42	UC	433	3393	2149	576	645	23	0	0
			Total	C	N	O	S		
42	UE	432	3388	2147	575	643	23	0	0

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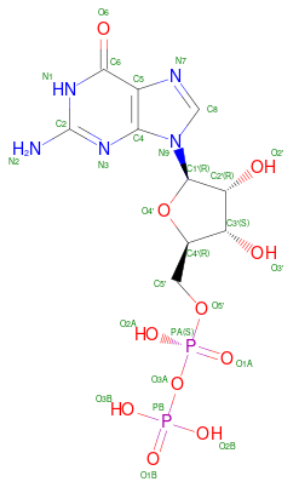
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	UG	433	3393	2149	576	645	23	0	0
			Total	C	N	O	S		
42	UI	433	3393	2149	576	645	23	0	0
			Total	C	N	O	S		
42	UK	433	3391	2148	576	644	23	0	0
			Total	C	N	O	S		
42	UM	431	3378	2140	574	641	23	0	0
			Total	C	N	O	S		
42	VC	440	3437	2175	584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

- Molecule 43 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).

GDP



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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
43	CF	1	28	10	5	11	2	0
43	CH	1	28	10	5	11	2	0
43	CJ	1	28	10	5	11	2	0
43	CL	1	28	10	5	11	2	0
43	DB	1	28	10	5	11	2	0
43	DD	1	28	10	5	11	2	0
43	DF	1	28	10	5	11	2	0
43	DH	1	28	10	5	11	2	0
43	DJ	1	28	10	5	11	2	0
43	DL	1	28	10	5	11	2	0
43	ED	1	28	10	5	11	2	0
43	EF	1	28	10	5	11	2	0
43	EH	1	28	10	5	11	2	0
43	EJ	1	28	10	5	11	2	0
43	EL	1	28	10	5	11	2	0
43	FD	1	28	10	5	11	2	0
43	FF	1	28	10	5	11	2	0
43	FH	1	28	10	5	11	2	0
43	FJ	1	28	10	5	11	2	0
43	FL	1	28	10	5	11	2	0
43	GD	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
43	GF	1	28	10	5	11	2	0
43	GH	1	28	10	5	11	2	0
43	GJ	1	28	10	5	11	2	0
43	GL	1	28	10	5	11	2	0
43	HB	1	28	10	5	11	2	0
43	HD	1	28	10	5	11	2	0
43	HF	1	28	10	5	11	2	0
43	HH	1	28	10	5	11	2	0
43	HJ	1	28	10	5	11	2	0
43	HL	1	28	10	5	11	2	0
43	ID	1	28	10	5	11	2	0
43	IF	1	28	10	5	11	2	0
43	IH	1	28	10	5	11	2	0
43	IJ	1	28	10	5	11	2	0
43	IL	1	28	10	5	11	2	0
43	IN	1	28	10	5	11	2	0
43	JD	1	28	10	5	11	2	0
43	JF	1	28	10	5	11	2	0
43	JH	1	28	10	5	11	2	0
43	JJ	1	28	10	5	11	2	0
43	JL	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
43	KD	1	28	10	5	11	2	0
43	KF	1	28	10	5	11	2	0
43	KG	1	28	10	5	11	2	0
43	KJ	1	28	10	5	11	2	0
43	KL	1	28	10	5	11	2	0
43	KN	1	28	10	5	11	2	0
43	LD	1	28	10	5	11	2	0
43	LF	1	28	10	5	11	2	0
43	LH	1	28	10	5	11	2	0
43	LJ	1	28	10	5	11	2	0
43	LL	1	28	10	5	11	2	0
43	LN	1	28	10	5	11	2	0
43	MD	1	28	10	5	11	2	0
43	MF	1	28	10	5	11	2	0
43	MH	1	28	10	5	11	2	0
43	MJ	1	28	10	5	11	2	0
43	ML	1	28	10	5	11	2	0
43	MN	1	28	10	5	11	2	0
43	NB	1	28	10	5	11	2	0
43	ND	1	28	10	5	11	2	0
43	NF	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
43	NH	1	28	10	5	11	2	0
43	NJ	1	28	10	5	11	2	0
43	NL	1	28	10	5	11	2	0
43	OB	1	28	10	5	11	2	0
43	OD	1	28	10	5	11	2	0
43	OF	1	28	10	5	11	2	0
43	OH	1	28	10	5	11	2	0
43	OJ	1	28	10	5	11	2	0
43	OL	1	28	10	5	11	2	0
43	PB	1	28	10	5	11	2	0
43	PD	1	28	10	5	11	2	0
43	PF	1	28	10	5	11	2	0
43	PH	1	28	10	5	11	2	0
43	PJ	1	28	10	5	11	2	0
43	PL	1	28	10	5	11	2	0
43	QB	1	28	10	5	11	2	0
43	QD	1	28	10	5	11	2	0
43	QF	1	28	10	5	11	2	0
43	QH	1	28	10	5	11	2	0
43	QJ	1	28	10	5	11	2	0
43	QL	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
43	RB	1	28	10	5	11	2	0
43	RD	1	28	10	5	11	2	0
43	RF	1	28	10	5	11	2	0
43	RH	1	28	10	5	11	2	0
43	RJ	1	28	10	5	11	2	0
43	RL	1	28	10	5	11	2	0
43	SD	1	28	10	5	11	2	0
43	SF	1	28	10	5	11	2	0
43	SH	1	28	10	5	11	2	0
43	SJ	1	28	10	5	11	2	0
43	SL	1	28	10	5	11	2	0
43	TD	1	28	10	5	11	2	0
43	TF	1	28	10	5	11	2	0
43	TH	1	28	10	5	11	2	0
43	TJ	1	28	10	5	11	2	0
43	TL	1	28	10	5	11	2	0
43	UD	1	28	10	5	11	2	0
43	UF	1	28	10	5	11	2	0
43	UH	1	28	10	5	11	2	0
43	UJ	1	28	10	5	11	2	0
43	UL	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
43	VD	1	28	10	5	11	2	0
43	VF	1	28	10	5	11	2	0
43	VH	1	28	10	5	11	2	0
43	VJ	1	28	10	5	11	2	0
43	VL	1	28	10	5	11	2	0
43	WD	1	28	10	5	11	2	0
43	WF	1	28	10	5	11	2	0
43	WH	1	28	10	5	11	2	0
43	WJ	1	28	10	5	11	2	0
43	WL	1	28	10	5	11	2	0
43	WN	1	28	10	5	11	2	0

- Molecule 44 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
44	AB	1	1	1	0
44	AE	1	1	1	0
44	AG	1	1	1	0
44	AI	1	1	1	0
44	AK	1	1	1	0
44	BC	1	1	1	0
44	BE	1	1	1	0
44	BG	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
44	BI	1	1	1	0
44	BK	1	1	1	0
44	CC	1	1	1	0
44	CE	1	1	1	0
44	CI	1	1	1	0
44	CK	1	1	1	0
44	CM	1	1	1	0
44	DM	1	1	1	0
44	EK	1	1	1	0
44	FC	1	1	1	0
44	FD	1	1	1	0
44	FG	1	1	1	0
44	FI	1	1	1	0
44	FK	1	1	1	0
44	FL	1	1	1	0
44	GC	1	1	1	0
44	GE	1	1	1	0
44	GG	1	1	1	0
44	GI	1	1	1	0
44	GK	1	1	1	0
44	GM	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
44	HC	1	1	1	0
44	HE	1	1	1	0
44	HG	1	1	1	0
44	HI	1	1	1	0
44	HK	1	1	1	0
44	HM	1	1	1	0
44	IC	1	1	1	0
44	IE	1	1	1	0
44	IG	1	1	1	0
44	IK	1	1	1	0
44	IL	1	1	1	0
44	JC	1	1	1	0
44	JE	1	1	1	0
44	JG	1	1	1	0
44	JI	1	1	1	0
44	JK	1	1	1	0
44	JM	1	1	1	0
44	KC	1	1	1	0
44	KE	1	1	1	0
44	KG	1	1	1	0
44	KI	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
44	KK	1	1	1	0
44	KM	1	1	1	0
44	LC	1	1	1	0
44	LD	1	1	1	0
44	LG	1	1	1	0
44	LI	1	1	1	0
44	LK	1	1	1	0
44	LM	1	1	1	0
44	MC	1	1	1	0
44	ME	1	1	1	0
44	MH	1	1	1	0
44	MK	1	1	1	0
44	MM	1	1	1	0
44	NA	1	1	1	0
44	NB	1	1	1	0
44	NE	1	1	1	0
44	NG	1	1	1	0
44	NI	1	1	1	0
44	NK	1	1	1	0
44	OA	1	1	1	0
44	OC	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
44	OE	1	1	1	0
44	OI	1	1	1	0
44	OK	1	1	1	0
44	PC	1	1	1	0
44	PE	1	1	1	0
44	PG	1	1	1	0
44	PI	1	1	1	0
44	SC	1	1	1	0
44	SD	1	1	1	0
44	SF	1	1	1	0
44	SH	1	1	1	0
44	SJ	1	1	1	0
44	TC	1	1	1	0
44	TD	1	1	1	0
44	TF	1	1	1	0
44	TI	1	1	1	0
44	TK	1	1	1	0
44	TL	1	1	1	0
44	UE	1	1	1	0
44	UG	1	1	1	0
44	UI	1	1	1	0

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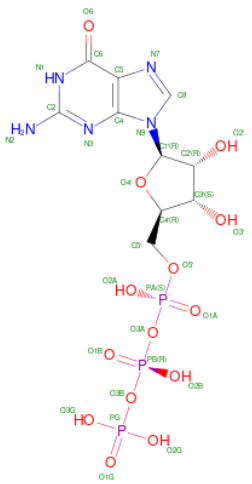
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
44	UK	1	1	1	0
44	UM	1	1	1	0
44	VC	1	1	1	0
44	VE	1	1	1	0
44	VG	1	1	1	0
44	VI	1	1	1	0
44	VJ	1	1	1	0
44	VM	1	1	1	0
44	WC	1	1	1	0
44	WD	1	1	1	0
44	WG	1	1	1	0
44	WI	1	1	1	0
44	WK	1	1	1	0
44	WM	1	1	1	0

- Molecule 45 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

GTP



Mol	Chain	Residues	Atoms					AltConf
45	AC	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	AF	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	AI	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	AK	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	BC	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	BG	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	BI	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	BK	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	CC	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	CE	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	CG	1	Total	C	N	O	P	0
			32	10	5	14	3	
45	CI	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	CK	1	32	10	5	14	3	0
45	CM	1	32	10	5	14	3	0
45	DC	1	32	10	5	14	3	0
45	DE	1	32	10	5	14	3	0
45	DG	1	32	10	5	14	3	0
45	DI	1	32	10	5	14	3	0
45	DK	1	32	10	5	14	3	0
45	DM	1	32	10	5	14	3	0
45	EC	1	32	10	5	14	3	0
45	EE	1	32	10	5	14	3	0
45	EG	1	32	10	5	14	3	0
45	EI	1	32	10	5	14	3	0
45	EK	1	32	10	5	14	3	0
45	EM	1	32	10	5	14	3	0
45	FC	1	32	10	5	14	3	0
45	FE	1	32	10	5	14	3	0
45	FF	1	32	10	5	14	3	0
45	FI	1	32	10	5	14	3	0
45	FK	1	32	10	5	14	3	0
45	FM	1	32	10	5	14	3	0
45	GC	1	32	10	5	14	3	0

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	JK	1	32	10	5	14	3	0
45	JM	1	32	10	5	14	3	0
45	KC	1	32	10	5	14	3	0
45	KE	1	32	10	5	14	3	0
45	KG	1	32	10	5	14	3	0
45	KI	1	32	10	5	14	3	0
45	KK	1	32	10	5	14	3	0
45	KM	1	32	10	5	14	3	0
45	LC	1	32	10	5	14	3	0
45	LE	1	32	10	5	14	3	0
45	LF	1	32	10	5	14	3	0
45	LI	1	32	10	5	14	3	0
45	LK	1	32	10	5	14	3	0
45	LM	1	32	10	5	14	3	0
45	MC	1	32	10	5	14	3	0
45	ME	1	32	10	5	14	3	0
45	MG	1	32	10	5	14	3	0
45	MI	1	32	10	5	14	3	0
45	MK	1	32	10	5	14	3	0
45	MM	1	32	10	5	14	3	0
45	NA	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	NC	1	32	10	5	14	3	0
45	NE	1	32	10	5	14	3	0
45	NG	1	32	10	5	14	3	0
45	NI	1	32	10	5	14	3	0
45	NK	1	32	10	5	14	3	0
45	OA	1	32	10	5	14	3	0
45	OC	1	32	10	5	14	3	0
45	OE	1	32	10	5	14	3	0
45	OG	1	32	10	5	14	3	0
45	OI	1	32	10	5	14	3	0
45	OK	1	32	10	5	14	3	0
45	PA	1	32	10	5	14	3	0
45	PC	1	32	10	5	14	3	0
45	PE	1	32	10	5	14	3	0
45	PG	1	32	10	5	14	3	0
45	PI	1	32	10	5	14	3	0
45	PK	1	32	10	5	14	3	0
45	QC	1	32	10	5	14	3	0
45	QE	1	32	10	5	14	3	0
45	QG	1	32	10	5	14	3	0
45	QI	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	QK	1	32	10	5	14	3	0
45	RC	1	32	10	5	14	3	0
45	RE	1	32	10	5	14	3	0
45	RG	1	32	10	5	14	3	0
45	RI	1	32	10	5	14	3	0
45	RK	1	32	10	5	14	3	0
45	SC	1	32	10	5	14	3	0
45	SE	1	32	10	5	14	3	0
45	SG	1	32	10	5	14	3	0
45	SI	1	32	10	5	14	3	0
45	SK	1	32	10	5	14	3	0
45	SM	1	32	10	5	14	3	0
45	TC	1	32	10	5	14	3	0
45	TE	1	32	10	5	14	3	0
45	TG	1	32	10	5	14	3	0
45	TI	1	32	10	5	14	3	0
45	TK	1	32	10	5	14	3	0
45	TM	1	32	10	5	14	3	0
45	UC	1	32	10	5	14	3	0
45	UE	1	32	10	5	14	3	0
45	UG	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	UI	1	32	10	5	14	3	0
45	UK	1	32	10	5	14	3	0
45	UM	1	32	10	5	14	3	0
45	VC	1	32	10	5	14	3	0
45	VE	1	32	10	5	14	3	0
45	VG	1	32	10	5	14	3	0
45	VI	1	32	10	5	14	3	0
45	VK	1	32	10	5	14	3	0
45	VM	1	32	10	5	14	3	0
45	WC	1	32	10	5	14	3	0
45	WE	1	32	10	5	14	3	0
45	WG	1	32	10	5	14	3	0
45	WI	1	32	10	5	14	3	0
45	WK	1	32	10	5	14	3	0
45	WM	1	32	10	5	14	3	0

3 Residue-property plots (i)

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

- Molecule 1: Armadillo repeat containing 4

Chain 1A:

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

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

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

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

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

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

SER GLN LEU THR LYS ARG LEU GLU PRO SER LEU ASN TRP ARG THR SER VAL SER SER LYS ASP ARG ASN THR LEU ARG ASP THR GLN VAL GLU LYS HIS GLY GLY LYS LEU GLU LYS SER ARG SER SER VAL SER PRO GLY ARG ALA GLN LEU ILE ARG LYS SER VAL GLU LYS ILE GLU

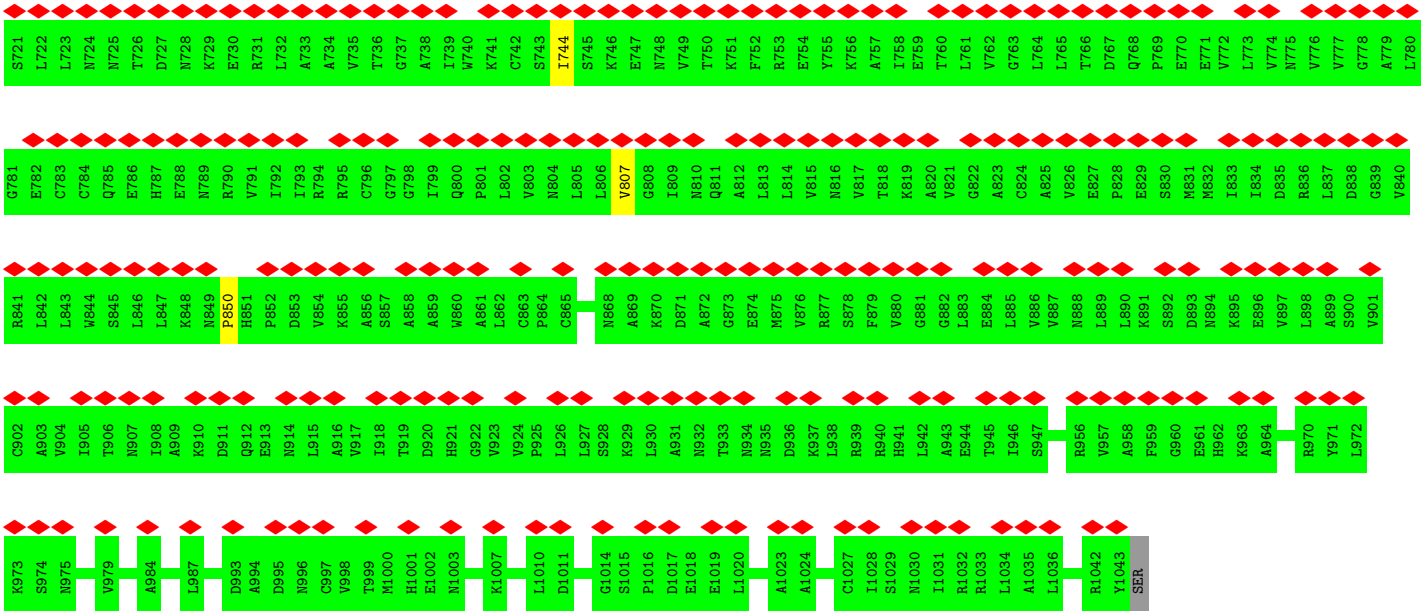
GLU ILE ILE SER ASP SER SER SER GLU SER GLU GLU ASP GLU GLU GLN PRO ASP HIS ARG GLN GLU ALA ASN ALA ASP LEU PRO SER GLU TYR TRP GLN ILE GLN LYS LEU VAL LYS TYR LEU LYS GLY GLY ASN GLN THR ALA THR VAL ILE ALA LEU CYS SER MET LYS ASP PHE ASN

LEU ALA GLN GLU THR CYS GLN LEU ALA ILE ARG ASP VAL GLY GLY LEU GLU VAL LEU ILE ASN LEU LEU GLU THR ASP GLU VAL LYS CYS LYS ILE GLY LYS SER LEU LYS ILE LEU LYS GLU ILE SER HIS ASN PRO GLN ILE ARG ARG ASN ILE VAL ASP L534 G535 G536 L537 P538 V539 M540

V541 N542 I543 L544 D545 S546 P547 H548 K549 S550 L551 K552 C553 L554 A555 A556 E557 T558 I559 A560 N561 V562 A563 K564 F565 R566 R567 A568 R569 R570 V571 V572 R573 R574 H575 G576 G577 I578 T579 K580 L581 V582 A583 L584 L585 D586 CYS GLY LYS HIS SER GLY GLU PRO ALA GLN SER SER LEU TYR

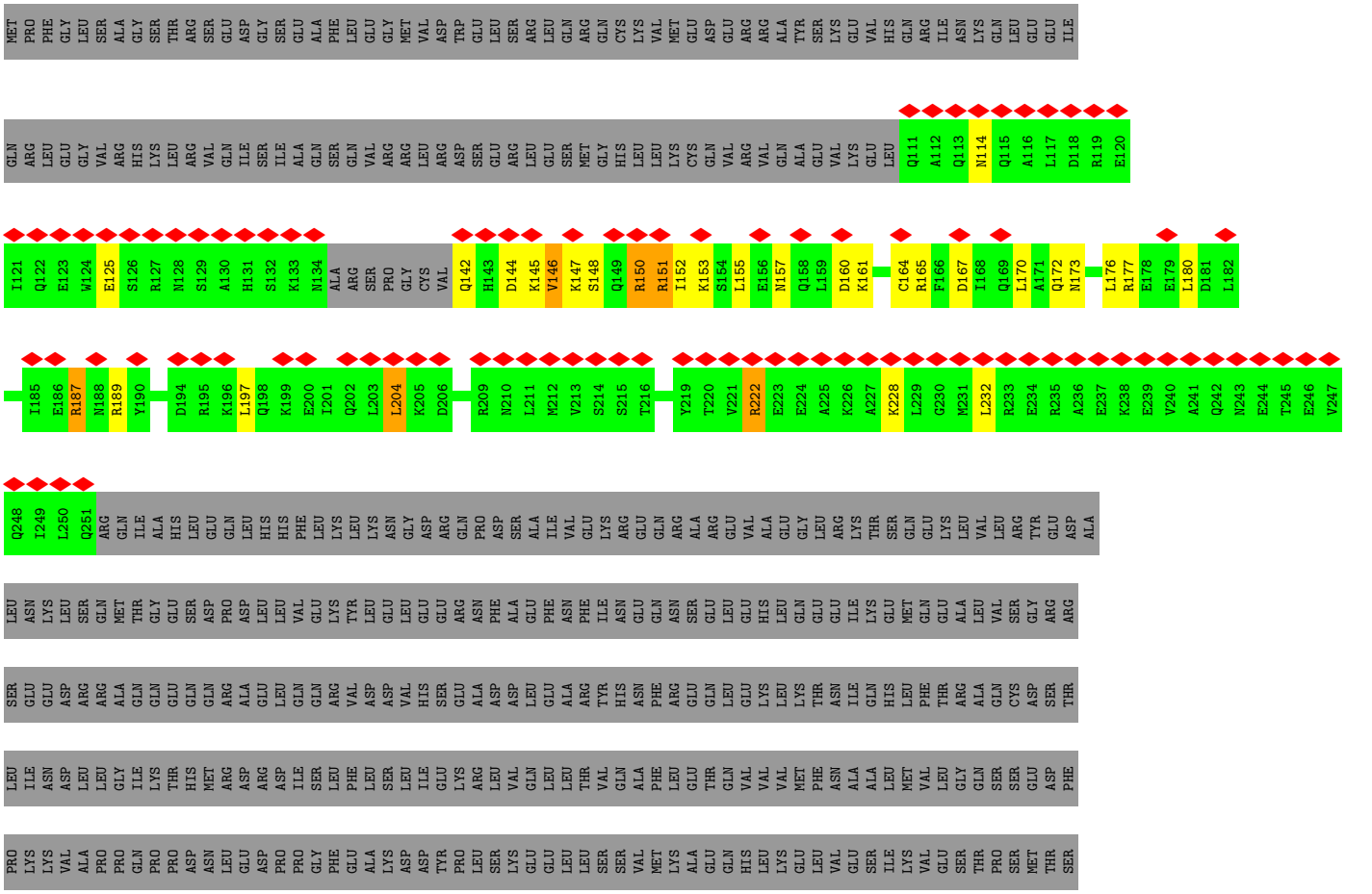
GLU THR ARG D604 V605 E606 V607 A608 R609 G610 G611 A612 L613 A614 L615 W616 S617 C618 S619 K620 S621 Y622 A623 N624 K625 E626 A627 I628 R629 K630 A631 G632 G633 I634 P635 L636 L637 A638 R639 L640 L641 K642 T643 S644 H645 E646 N647 M648 L649 I650 P651 V652 V653 G654 T655 L656 Q657 E658 C659 A660

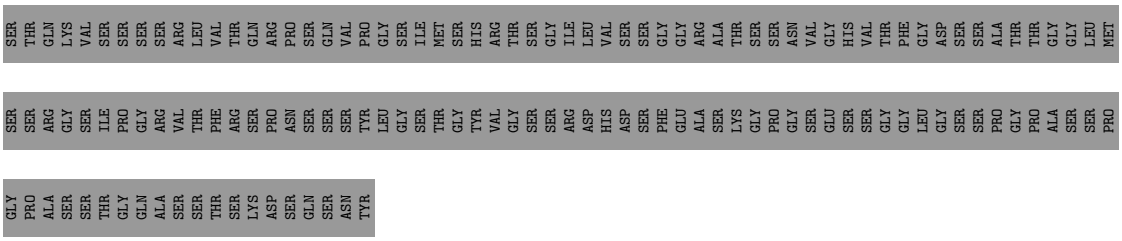
S661 E662 E663 N664 Y665 R666 A667 A668 I669 K670 A671 E672 R673 I674 I675 E676 N677 L678 V679 K680 N681 L682 N683 S684 E685 N686 E687 Q688 L689 Q690 E691 H692 C693 A694 M695 A696 I697 Y698 Q699 C700 A701 E702 D703 E704 E705 T706 R707 D708 L709 V710 R711 L712 H713 G714 G715 L716 K717 P718 L719 A720



- Molecule 2: Coiled-coil domain containing 114

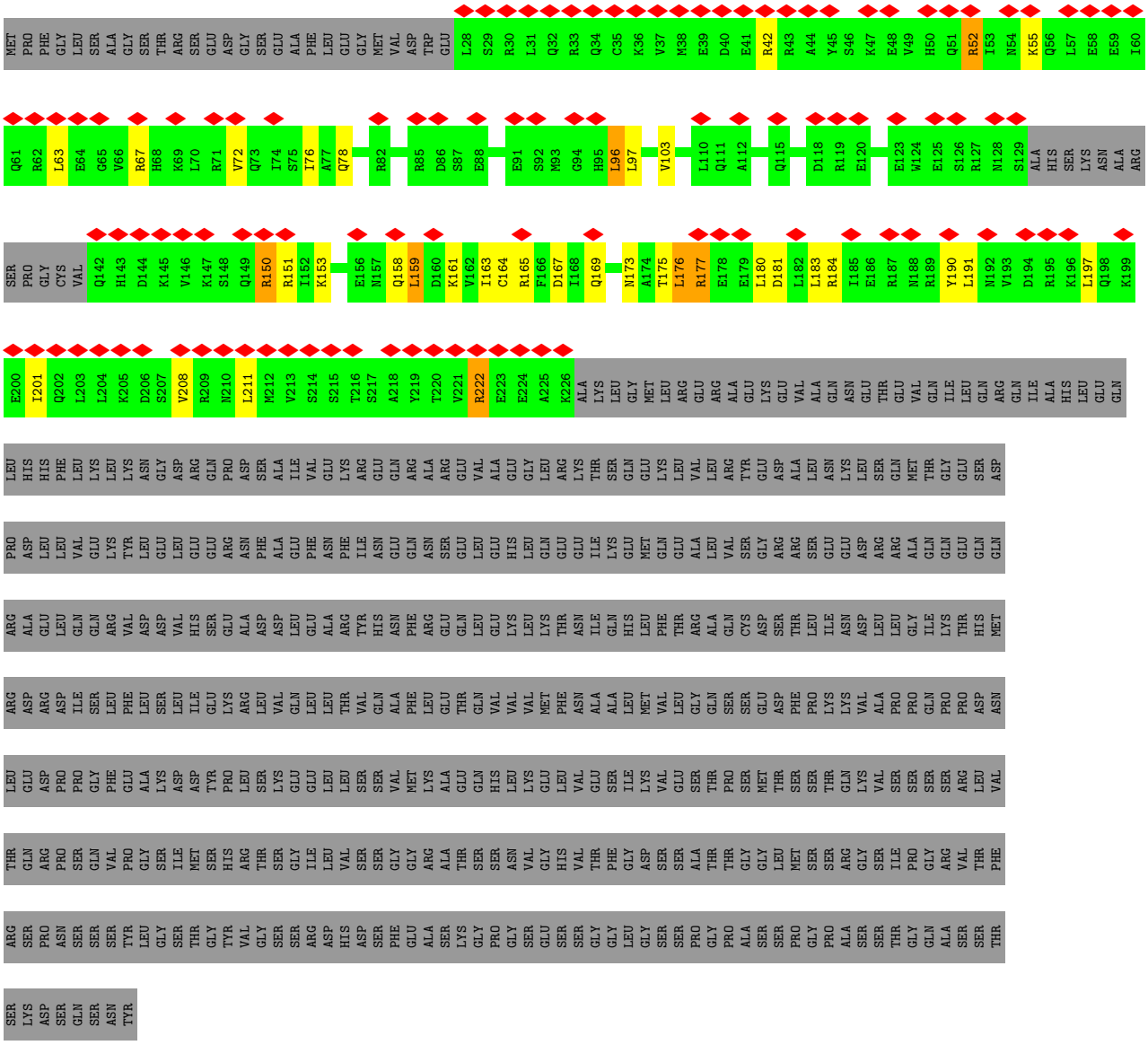
Chain 1D:





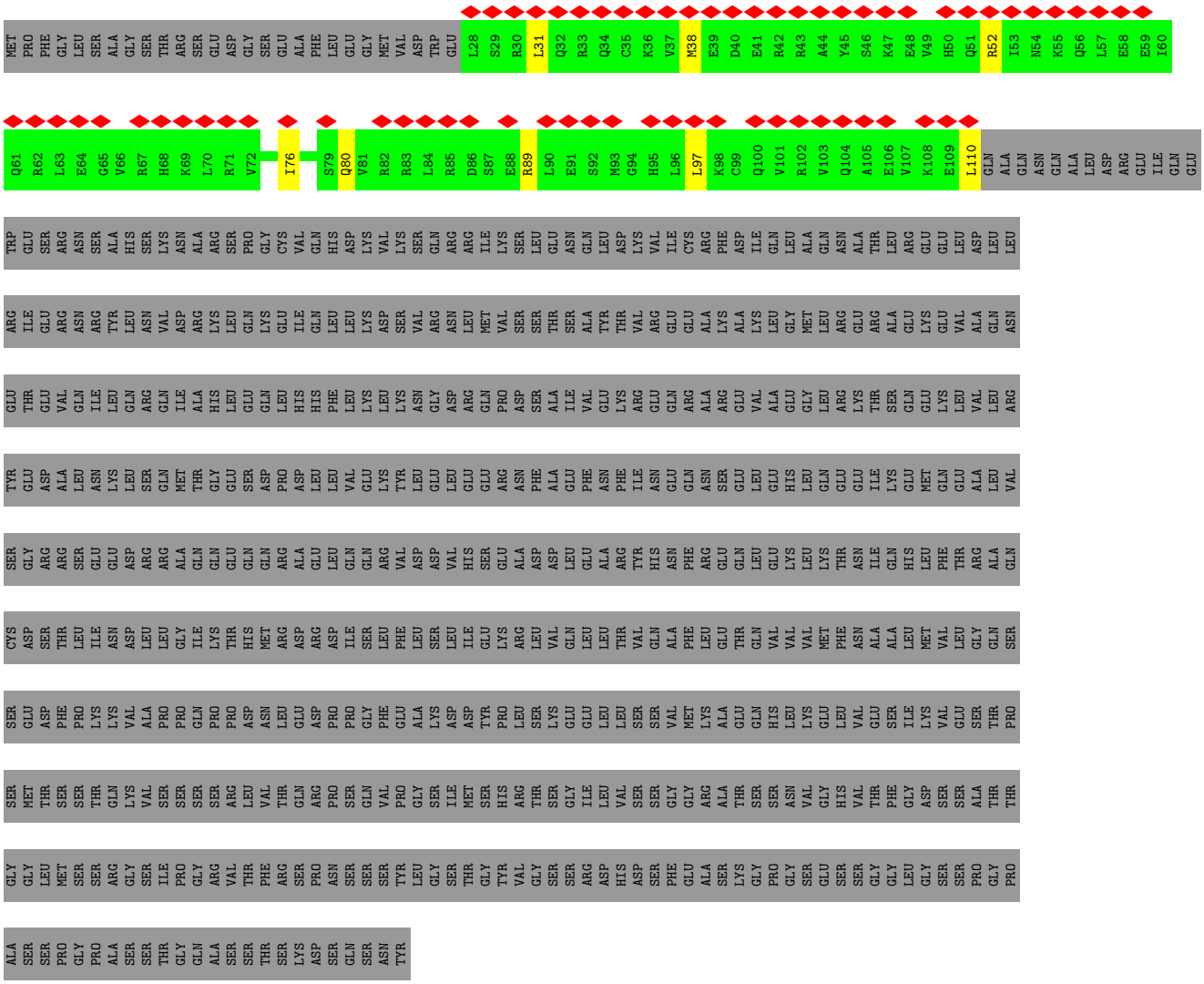
• Molecule 2: Coiled-coil domain containing 114

Chain 1E:



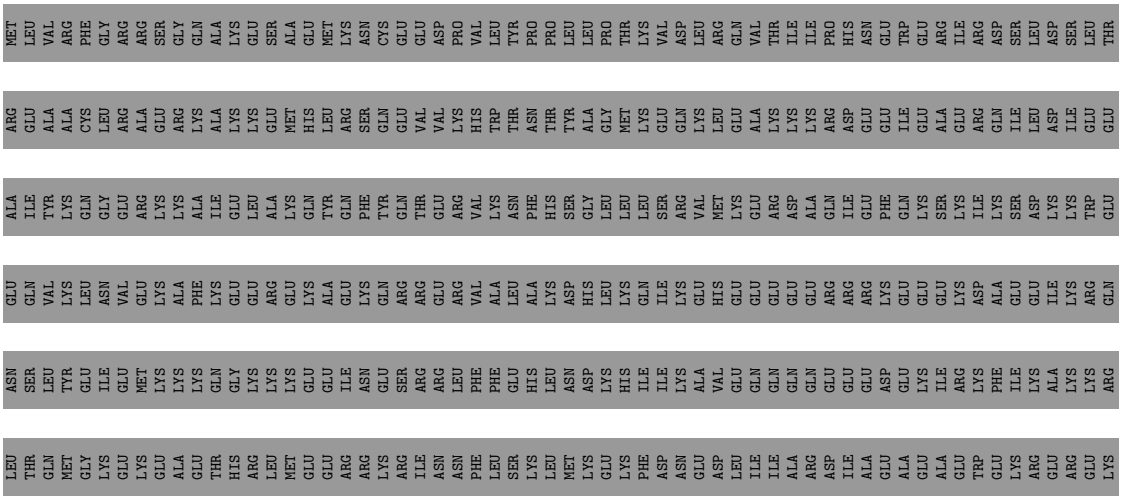
• Molecule 2: Coiled-coil domain containing 114

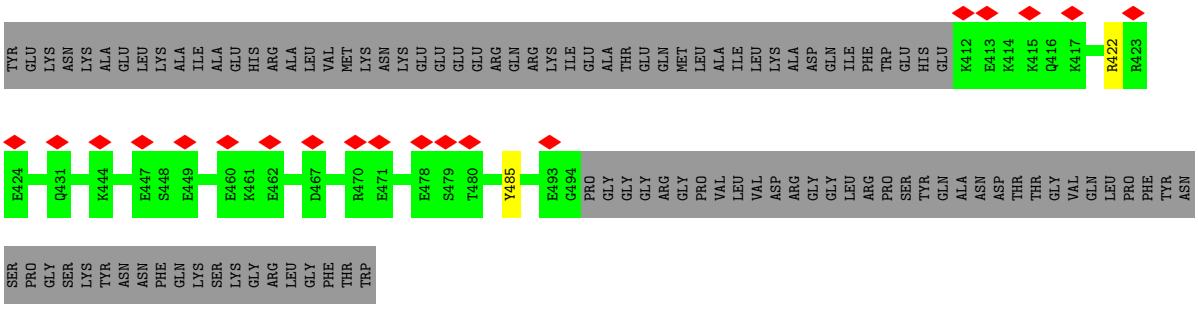
Chain 1F:



- Molecule 3: Coiled-coil domain containing 173

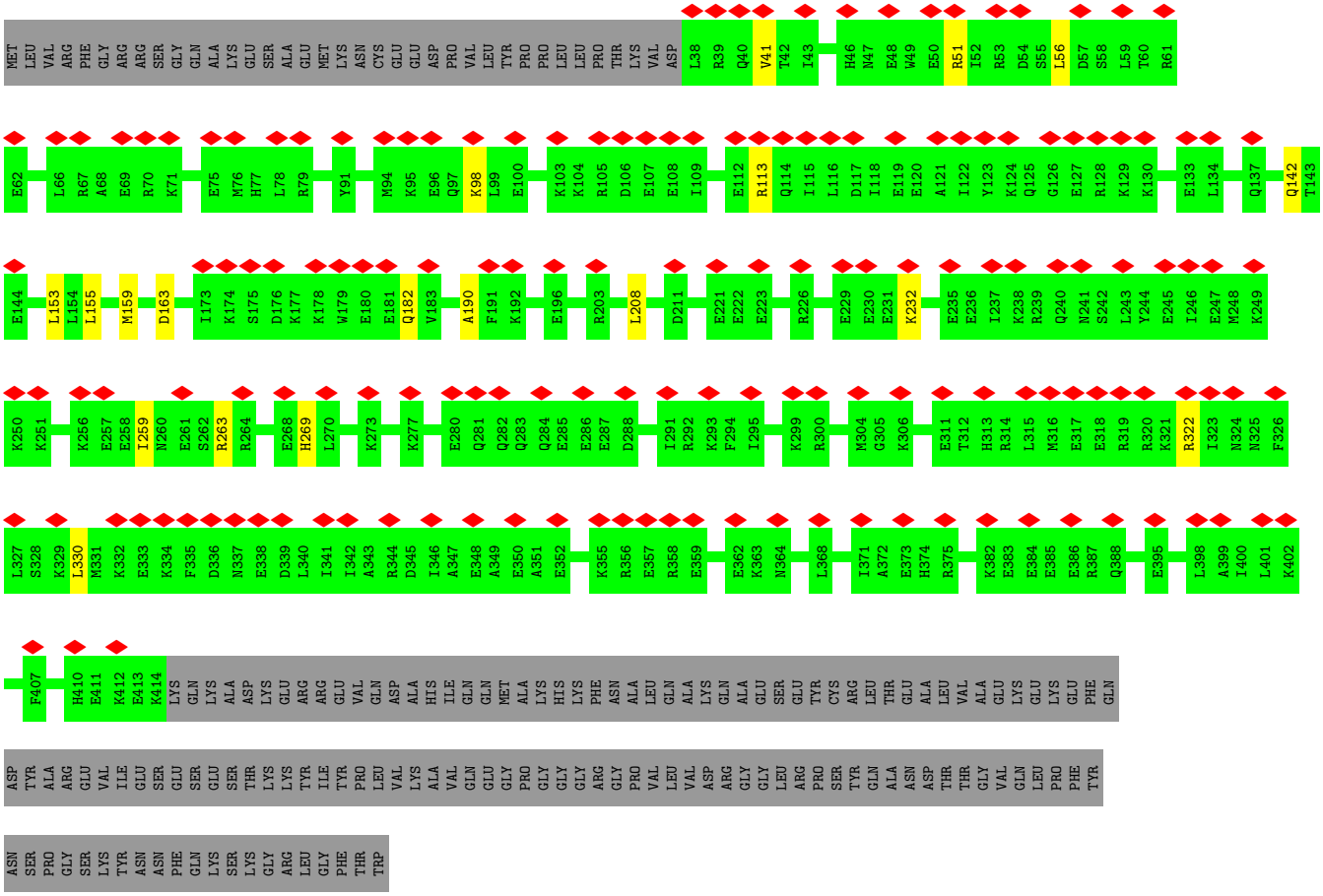
Chain 1H:





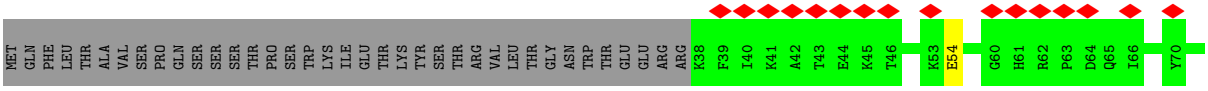
- Molecule 3: Coiled-coil domain containing 173

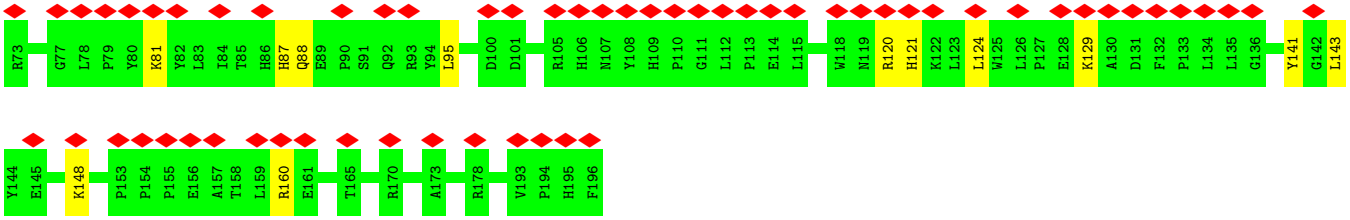
Chain 1I:



- Molecule 4: Uncharacterized protein C1orf158 homolog

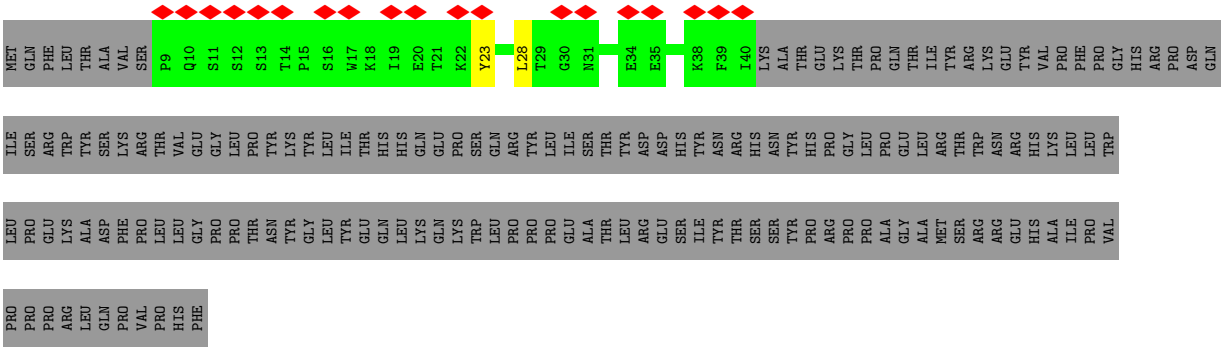
Chain 1K:





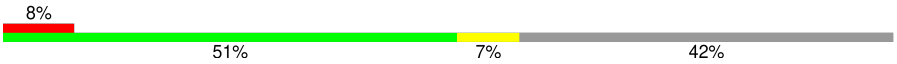
- Molecule 4: Uncharacterized protein C1orf158 homolog

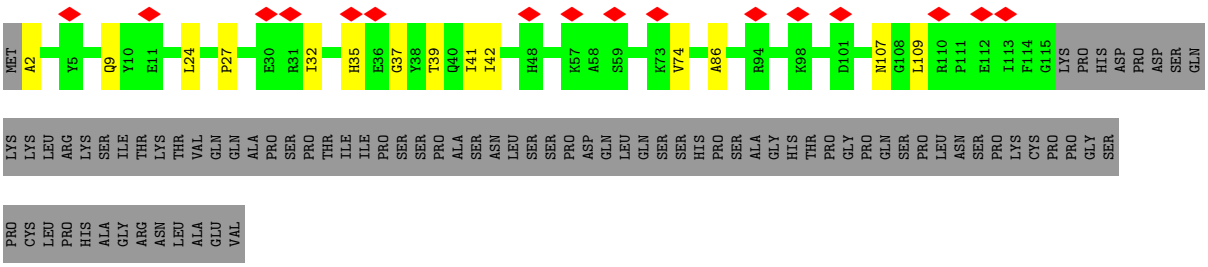
Chain 1L:



- Molecule 5: Protein Flattop

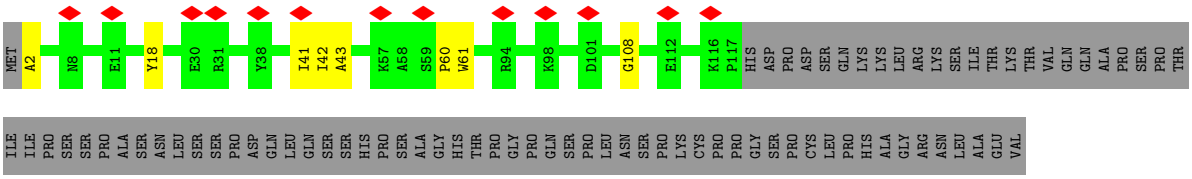
Chain 1N:





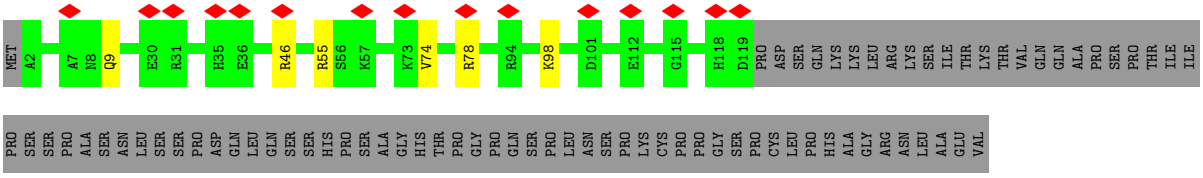
- Molecule 5: Protein Flattop

Chain 1O:



- Molecule 5: Protein Flattop

Chain 1P:

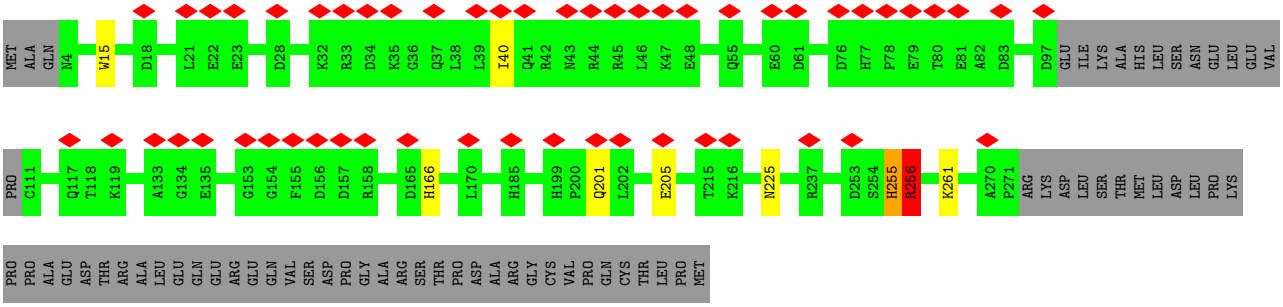


- Molecule 6: CFAP141

Chain 1R:

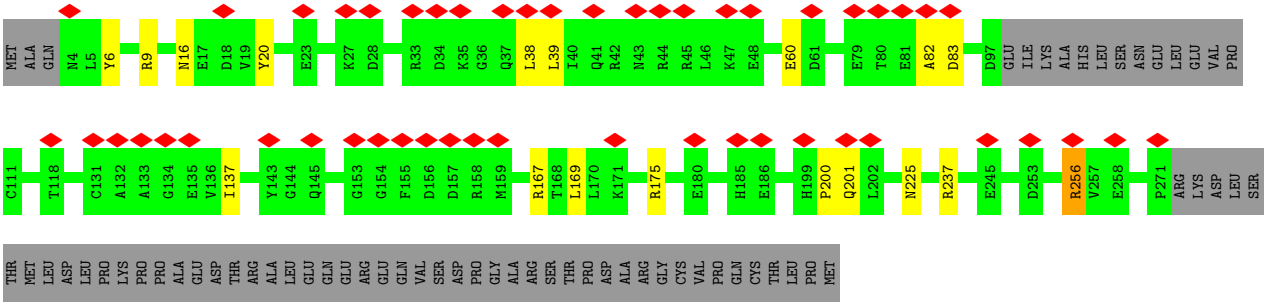
- Molecule 7: Cilia and flagella associated protein 161

Chain 1T:



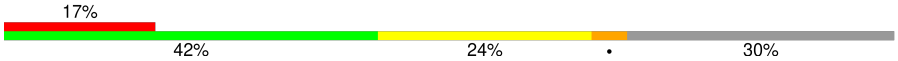
- Molecule 7: Cilia and flagella associated protein 161

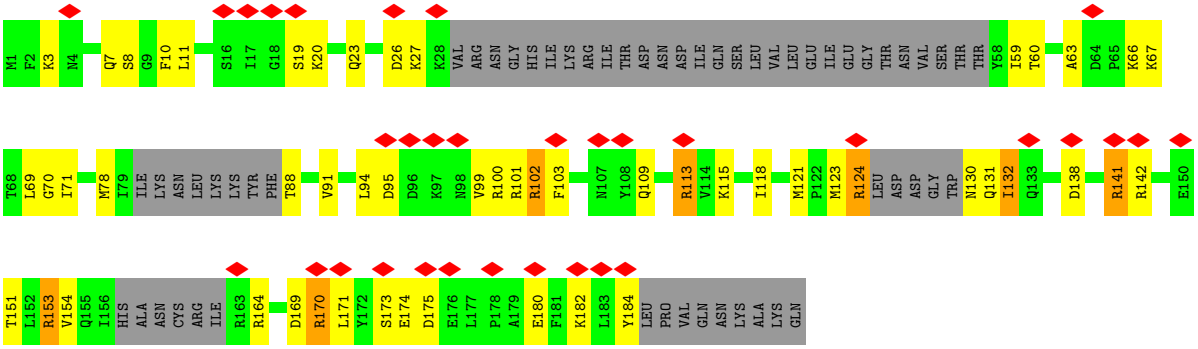
Chain 1U:



- Molecule 8: Cilia- and flagella-associated protein 20

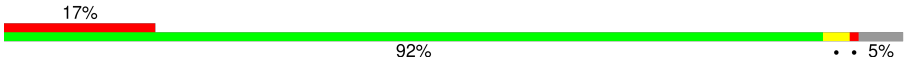
Chain 1W:

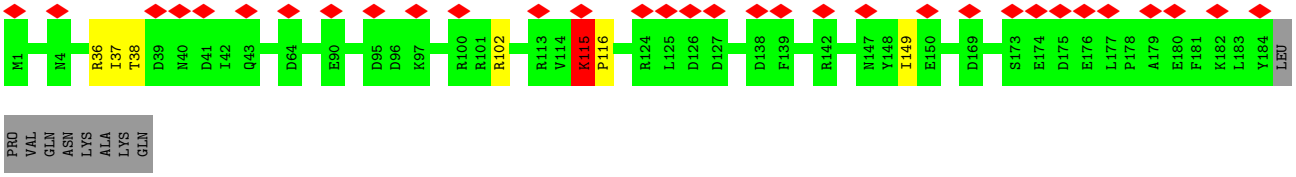




• Molecule 8: Cilia- and flagella-associated protein 20

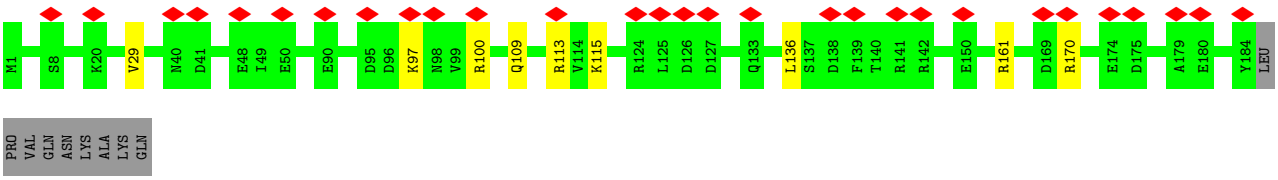
Chain 1X:





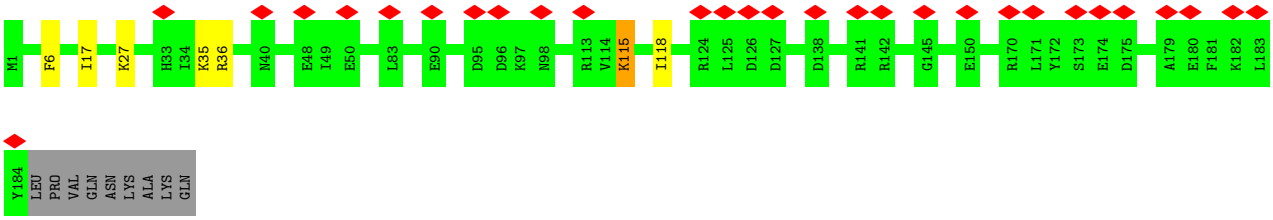
• Molecule 8: Cilia- and flagella-associated protein 20

Chain 1Y:



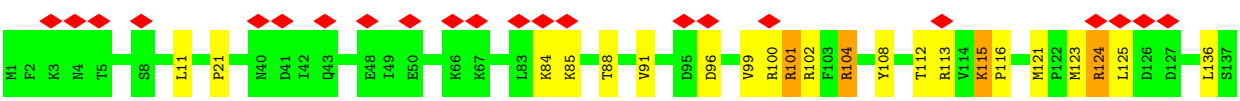
• Molecule 8: Cilia- and flagella-associated protein 20

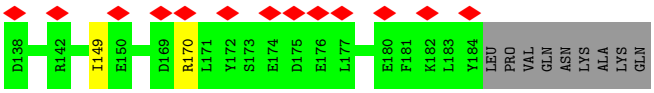
Chain 1Z:



• Molecule 8: Cilia- and flagella-associated protein 20

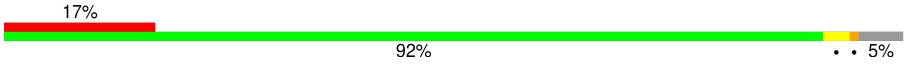
Chain 2A:

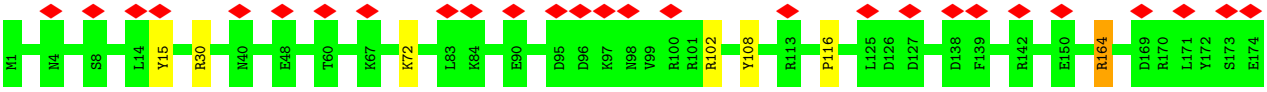


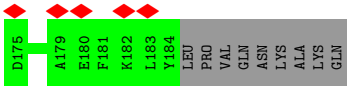


- Molecule 8: Cilia- and flagella-associated protein 20

Chain 2B:

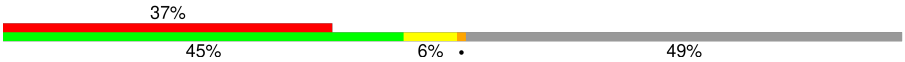


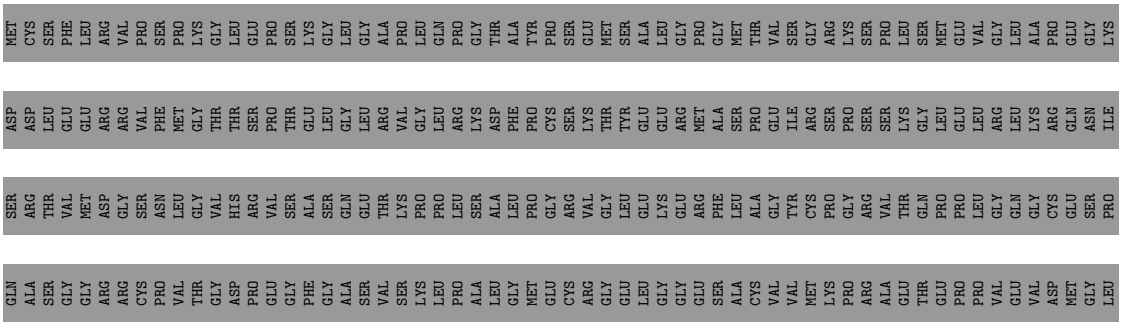


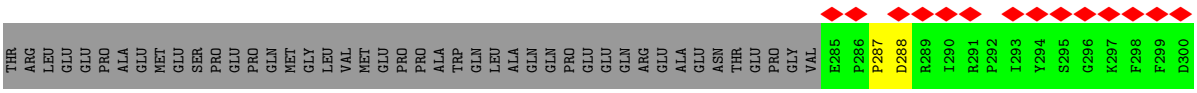


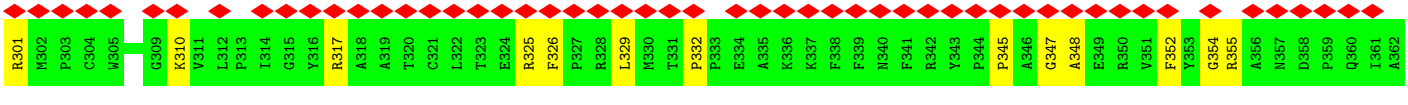
- Molecule 9: EF-hand domain family member B

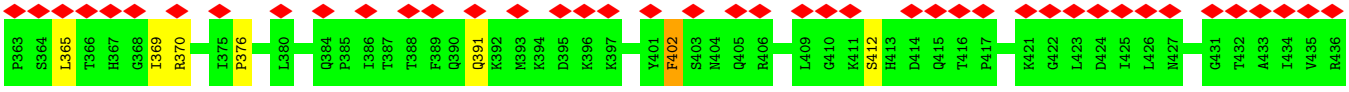
Chain 2D:

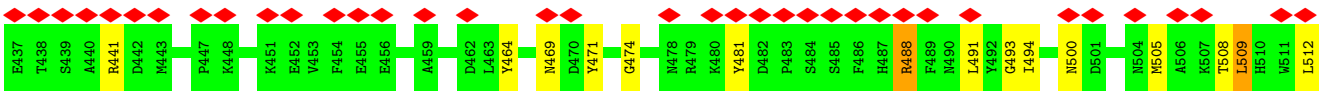


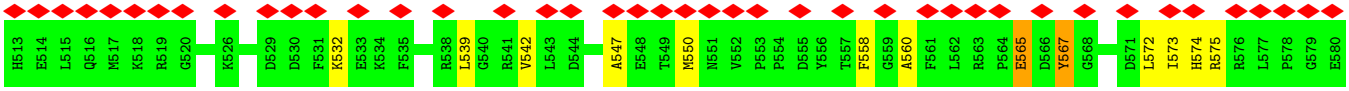


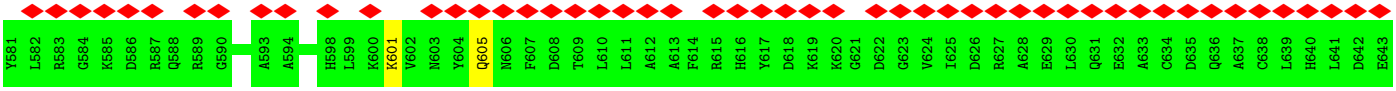


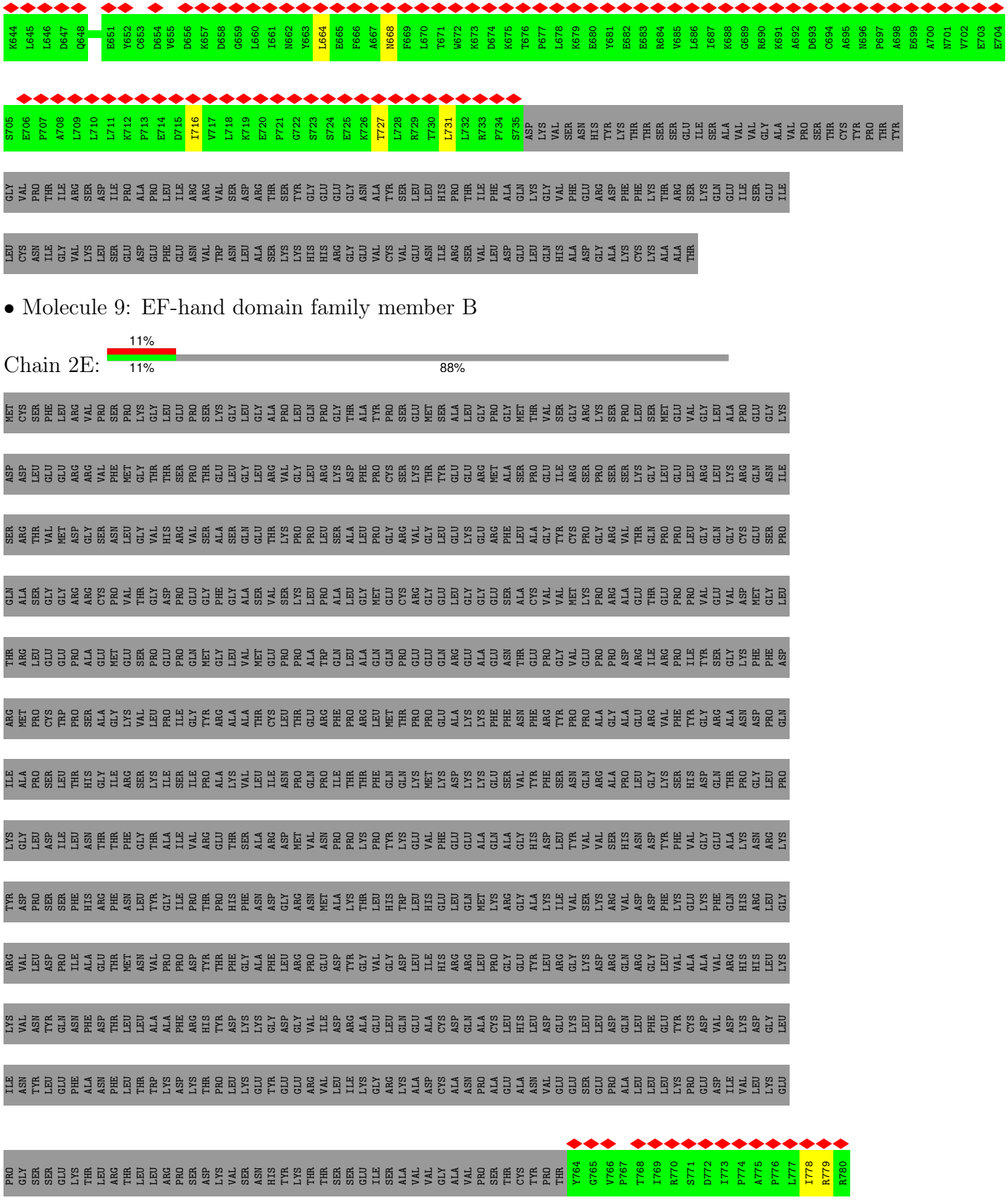






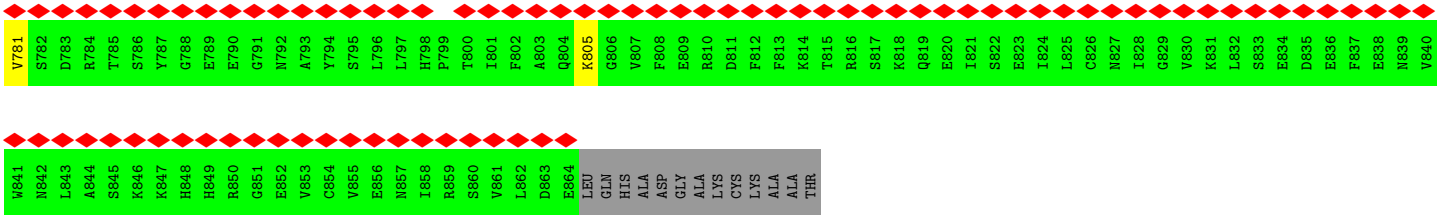






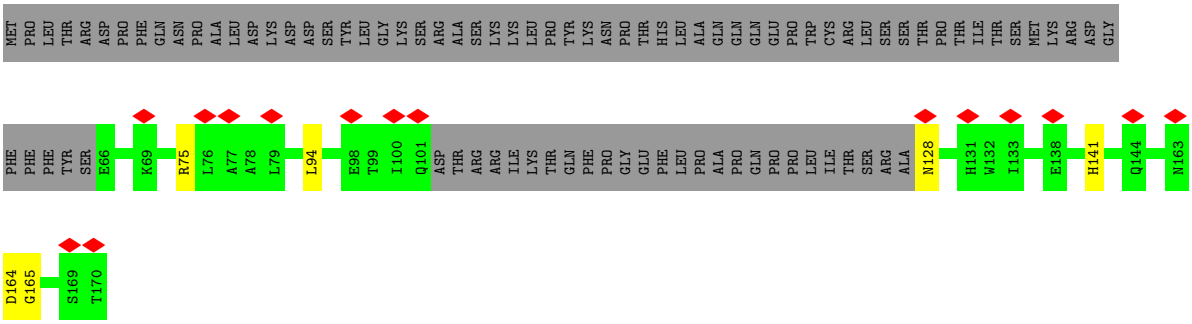
• Molecule 9: EF-hand domain family member B

Chain 2E: 11% 11% 88%



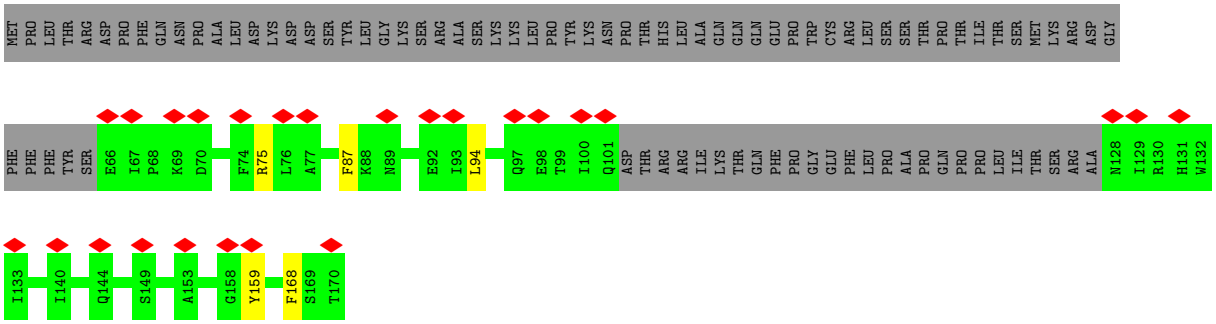
• Molecule 10: CFAP276

Chain 2F:



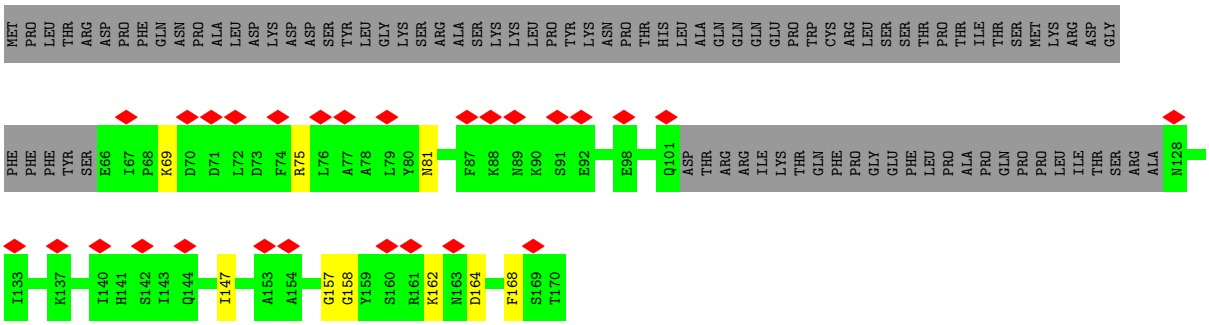
• Molecule 10: CFAP276

Chain 2G:



• Molecule 10: CFAP276

Chain 2H:



• Molecule 11: Cilia and flagella associated protein 45

Chain 2J: 17% 28% • 70%

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

ILE ARG LYS THR LEU THR ALA LEU GLY LEU ASP HIS LYS PRO E75 Q78 M84 T92 K93 D94 P95 S96 G97 Q98 S99 L100 I101 M102 E105 E106 F107 E108 R109 W112 H115 V116 L117 T118 K119 E120 E121 L122 E123 A124 R125 E126 Q127 A128 F129 K130 K131 E132 K133 E134

A135 I136 V137 D138 T139 V140 T141 T142 R143 K144 K145 I146 M147 K148 Q149 K150 E151 M152 V153 W154 R155 N156 N157 R158 K159 L160 S161 D162 L163 E164 E165 K168 E169 R170 A171 Q172 N173 L174 L175 Q176 R177 A178 N179 Q180 L181 R182 M183 E184 Q185 E186 K190 D191 M192 K193 I204 R205

E211 E218 L219 D220 A221 E222 E223 K224 R225 L226 D227 Q228 M229 M230 E231 V232 E233 K236 SER VAL GLN ARG GLN GLU GLU LEU ASP ARG LYS ARG ARG GLU GLU ARG ILE ARG GLY ARG ARG HIS ILE VAL GLU GLN MET GLU LYS ASN GLN GLU GLU ARG SER LEU LEU ALA GLU GLN

ARG GLU GLN GLU LYS GLU GLN MET LEU GLU TYR MET GLU LYS LEU GLN GLU GLU ASP LEU ARG ASP LEU GLU GLN ARG HIS GLN GLN LYS LEU LYS MET GLN ALA GLU ILE LYS ARG ILE ASN ASP GLU ASN GLN ARG GLN LYS ALA GLU LEU ARG ALA ALA GLN GLU LYS LEU ALA ASP GLN

MET VAL MET GLU PHE THR LYS LYS LYS MET ALA ARG GLU ALA GLU PHE GLU ALA GLU GLN GLU ARG ILE ARG ARG GLU LYS GLU LYS GLU ILE ALA ARG LEU ARG ALA MET GLN GLU LYS ALA GLN ASP TYR GLN ALA GLU GLN ASP ALA LEU ARG ALA ALA LYS ARG ASN GLN GLU VAL ALA

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

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

ARG LYS LYS LEU GLU GLU LEU ARG ALA THR GLY LEU PRO GLU LYS TYR CYS ILE GLU ALA GLU ARG LYS ALA ASN ILE PRO VAL ASN THR SER VAL ASN

- Molecule 11: Cilia and flagella associated protein 45

Chain 2K: 32% 49% • • 46%

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

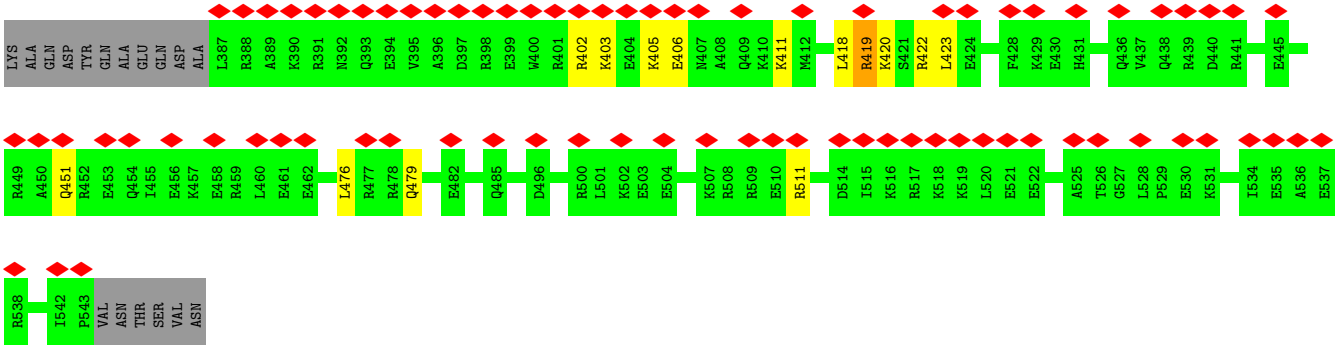
ILE ARG LYS THR LEU THR ALA LEU GLY LEU ASP HIS LYS PRO GLU THR ILE GLN LEU ILE THR ARG ASP MET VAL ARG GLU LEU ILE ILE PRO THR LYS ASP PRO SER GLY GLN SER LEU ILE MET SER PRO GLU GLU PHE GLU ARG ILE LYS TRP ALA SER HIS VAL LEU THR LYS GLU

GLU LEU GLU ALA ARG GLU GLN ALA PHE LYS LYS GLU LYS GLU ALA THR VAL ASP THR VAL THR THR ARG ARG LYS LYS ILE MET LYS GLN LYS GLU MET VAL TRP ARG ASN ASN ARG LYS LEU SER ASP LEU GLU GLU VAL ALA LYS GLU ARG ALA GLN ASN LEU LEU GLN ARG ALA ASN GLN

LEU ARG MET GLU GLN GLU GLU LEU LYS ASP MET LYS LYS ILE ILE LEU ASN ALA LYS CYS HIS ALA ILE ARG ASP ALA GLN ILE ILE LEU GLU LYS GLN LEU ILE GLN LYS GLU LEU ASP ALA GLU GLU LYS ARG LEU ASP GLN MET MET GLU V232 E233 R234 Q235 K236 R240 Q241 E242

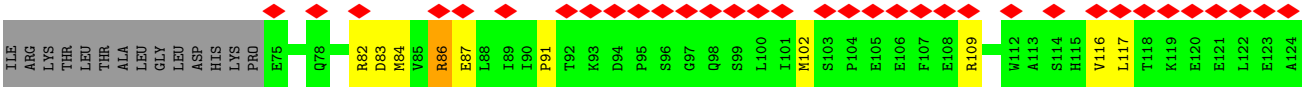
E243 L244 D245 R246 K247 R248 R249 I253 R254 R257 H258 Q262 M263 E264 Q267 L273 A274 E275 E278 Q279 E280 K281 E282 Q283 M284 L285 E286 Y287 M288 E289 K290 L291 Q292 E293 E294 D295 L296 R297 D298 L299 E300 Q301 R302 H303 Q304 Q305 K306 L307 K308 M309 Q310 A311 E312 I313

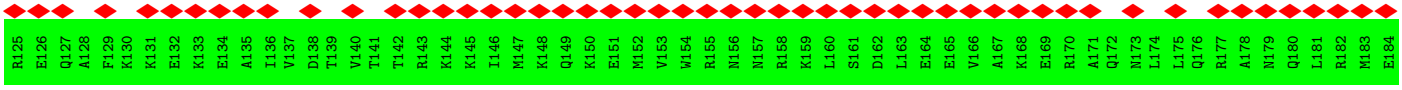
K314 R315 I316 N317 D318 E319 N320 Q321 R322 Q323 K324 A325 E326 L327 I328 A329 Q330 E331 K332 L333 A334 D335 Q336 M337 V338 M339 E340 F341 T342 K343 K344 K345 M346 A347 R348 E349 A350 E351 F352 E353 A354 E355 Q356 E357 R358 I359 R360 R361 E364 K365 E366 R369 L370 ARG ALA MET GLN GLU

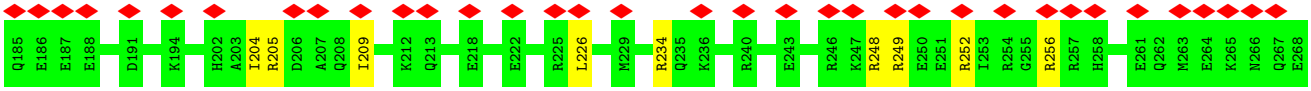


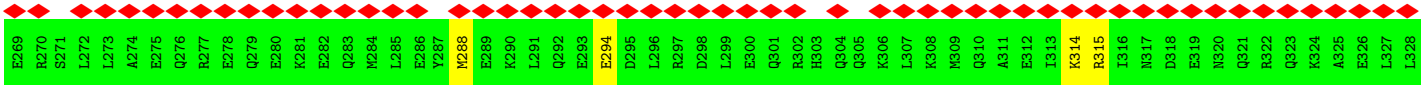
• Molecule 11: Cilia and flagella associated protein 45

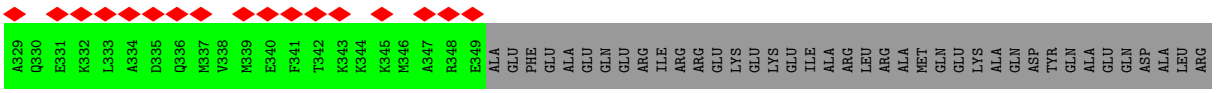
Chain 2L:

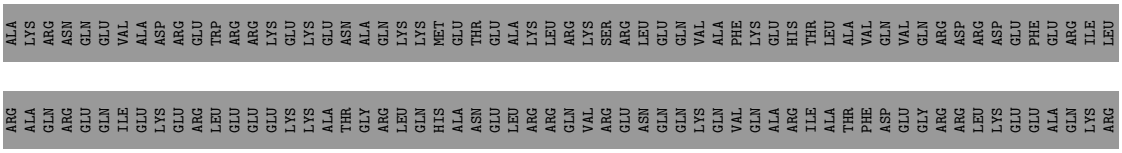






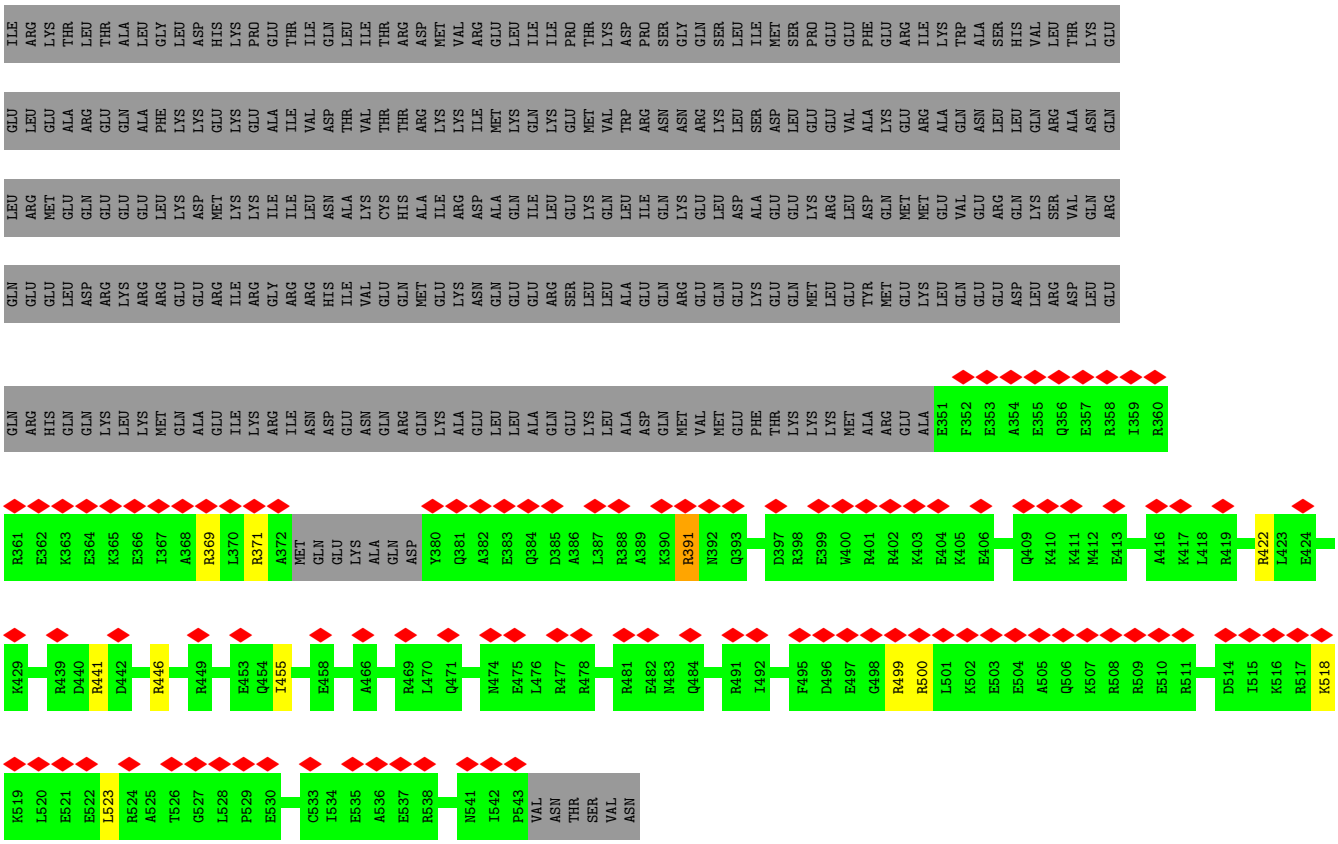






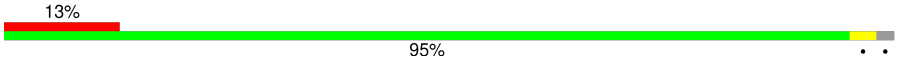
• Molecule 11: Cilia and flagella associated protein 45

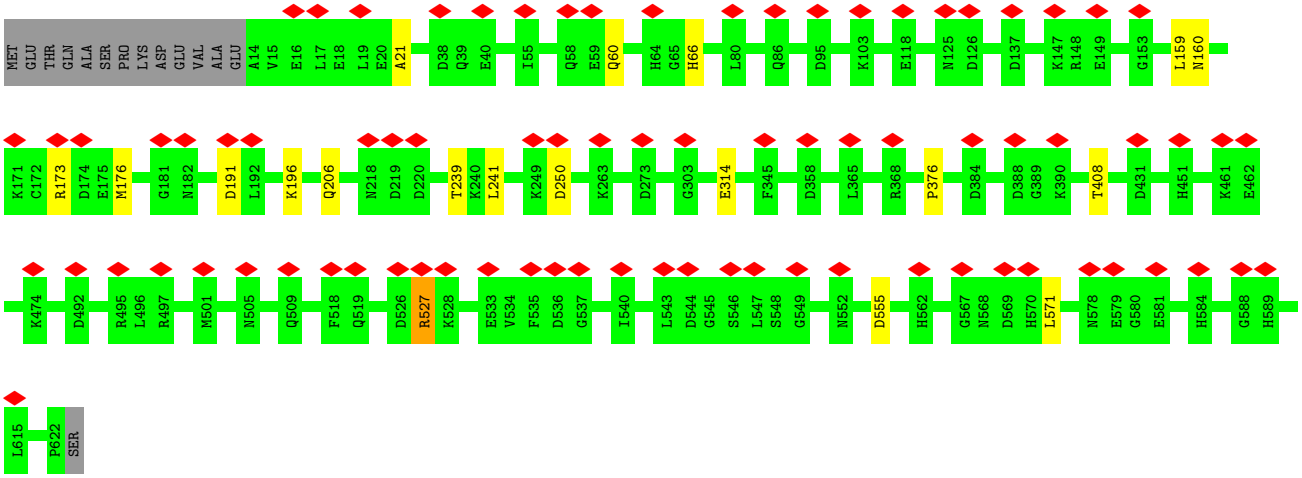
Chain 2M:



• Molecule 12: Cilia and flagella associated protein 52

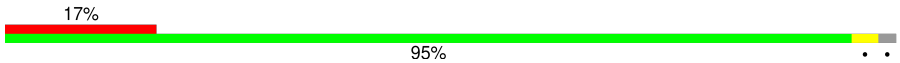
Chain 2O:

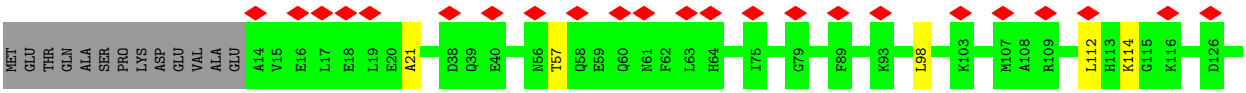


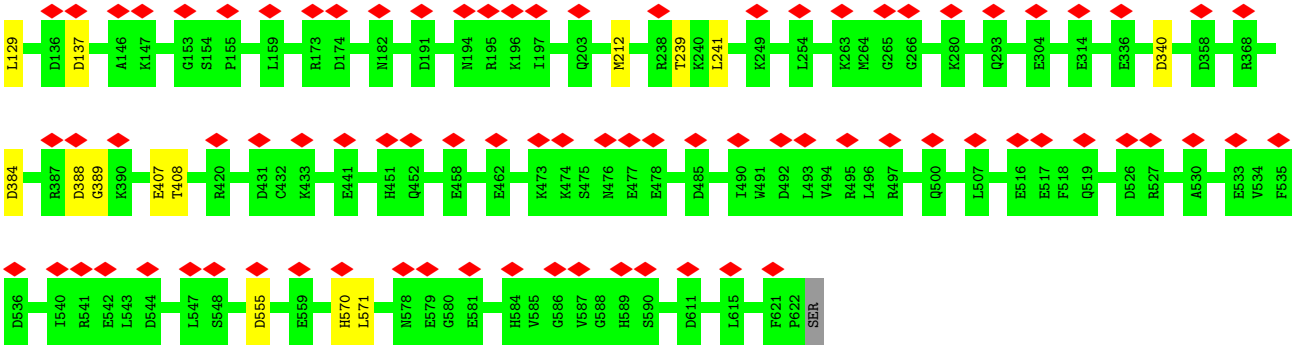


• Molecule 12: Cilia and flagella associated protein 52

Chain 2P:

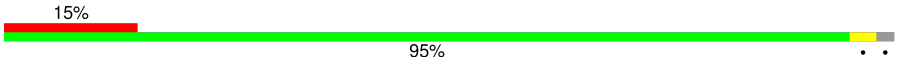


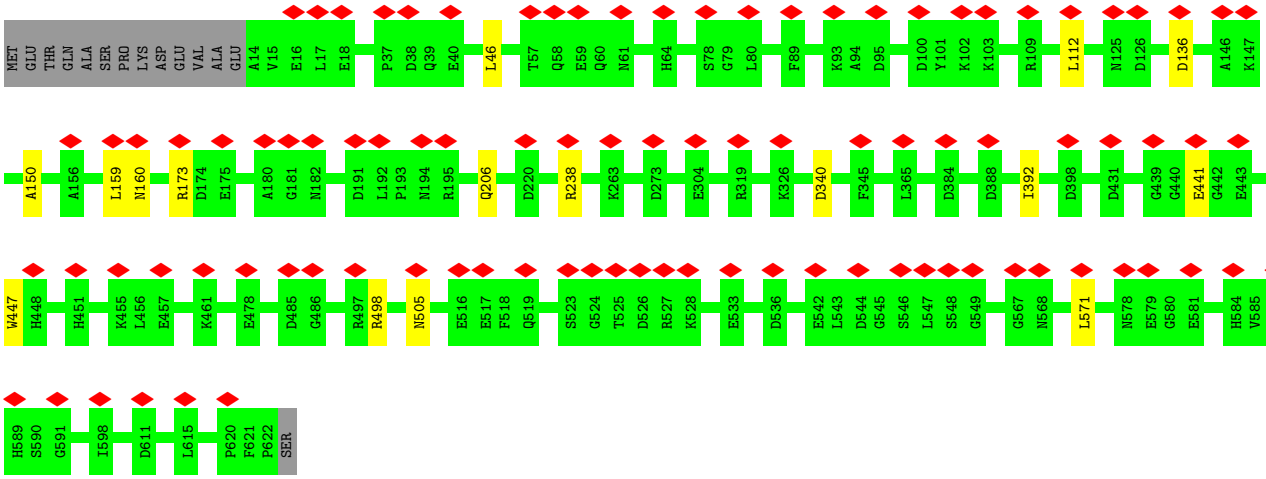




• Molecule 12: Cilia and flagella associated protein 52

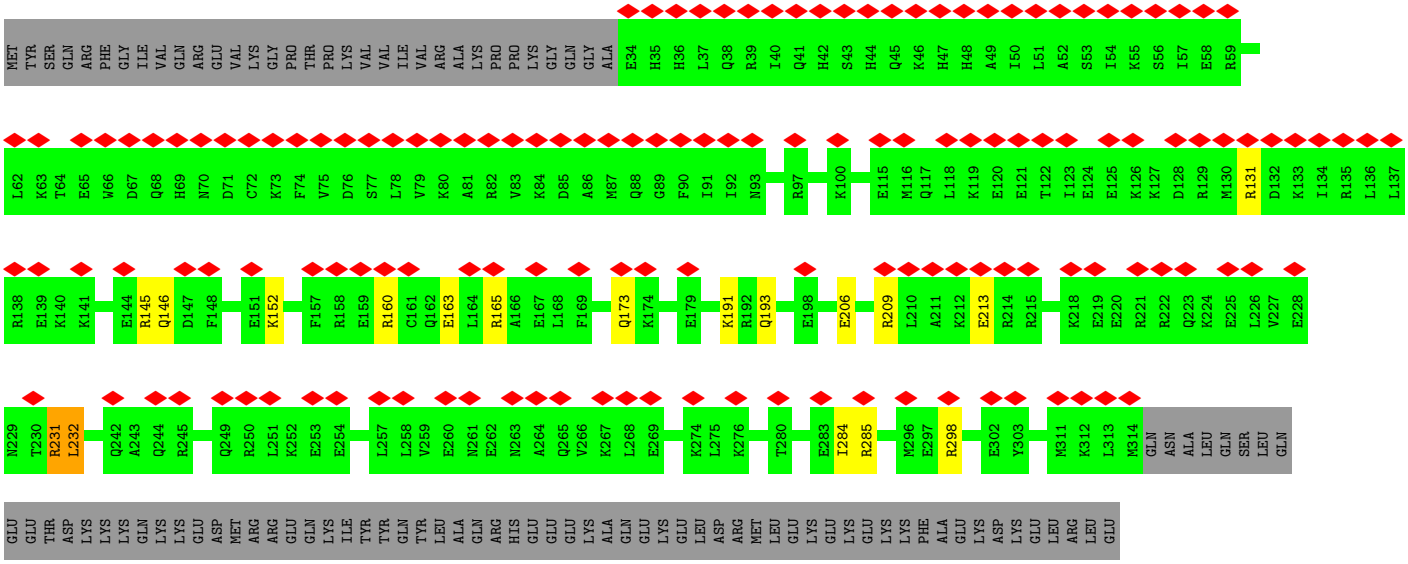
Chain 2Q:

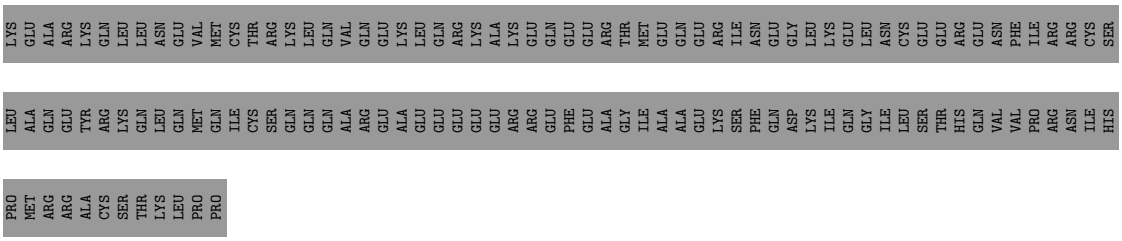




• Molecule 13: Methyl-CpG binding domain protein 1

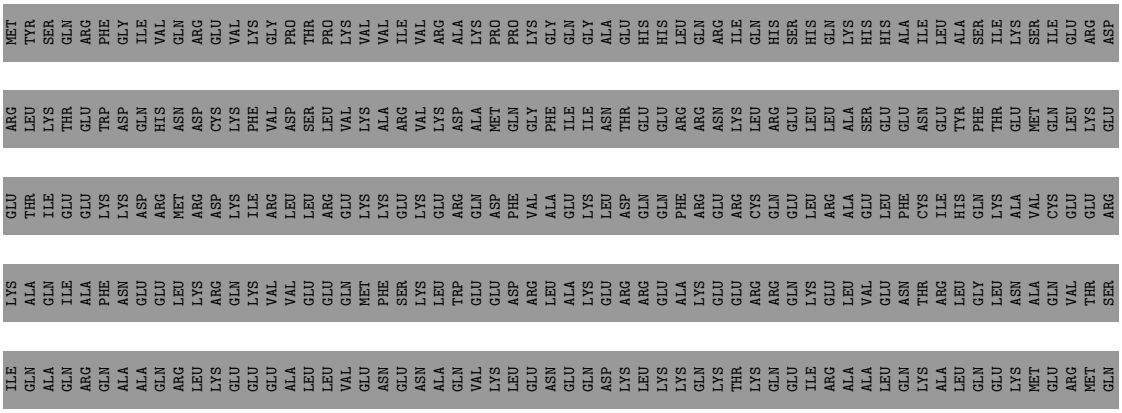
Chain 2S:

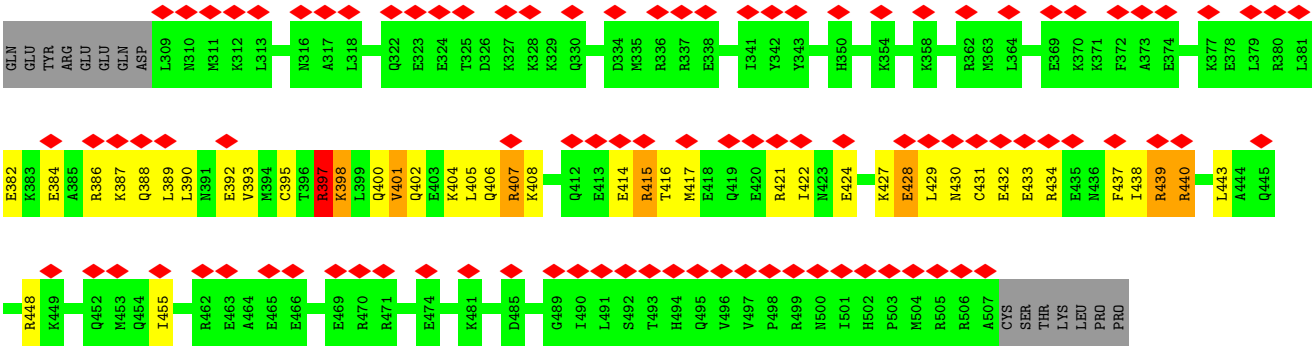




- Molecule 13: Methyl-CpG binding domain protein 1

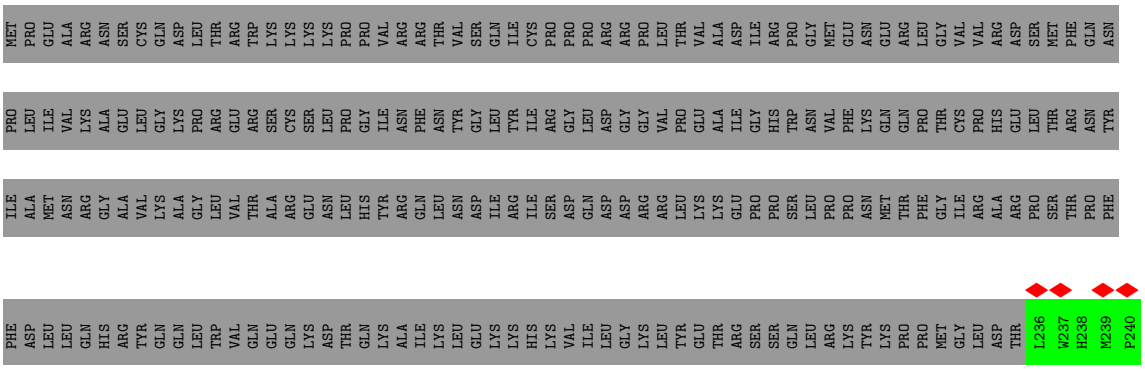
Chain 2T:

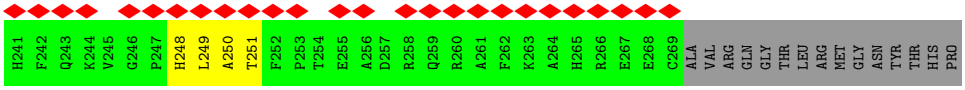




- Molecule 14: Cilia and flagella associated protein 77

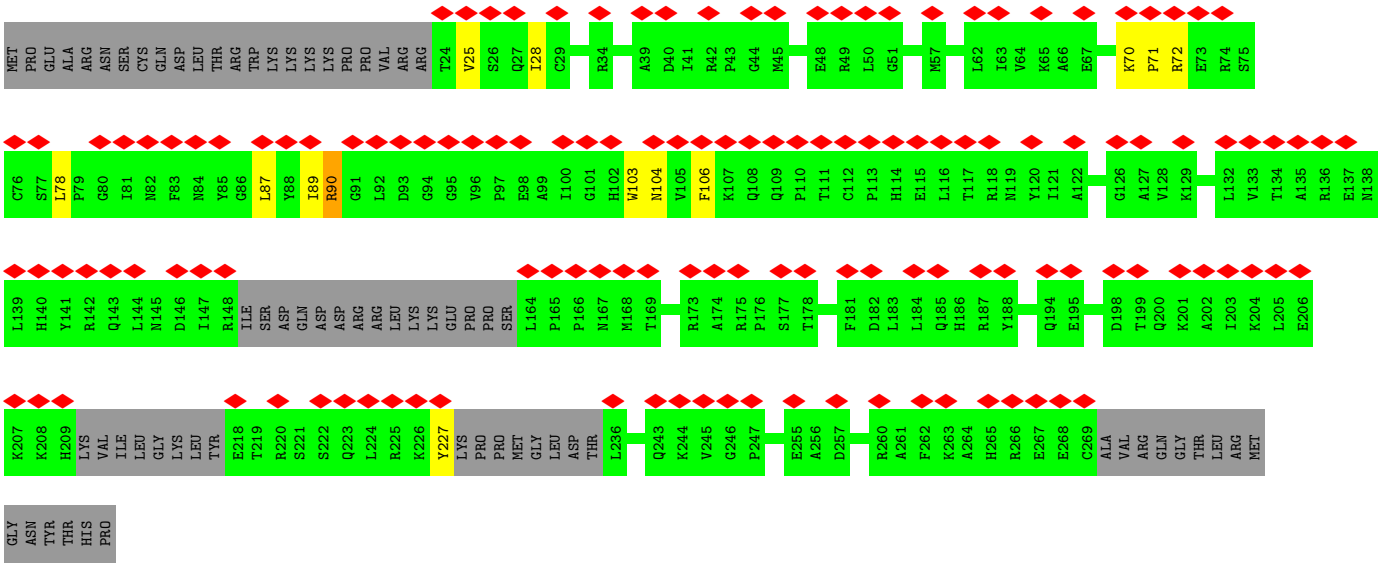
Chain 2V:





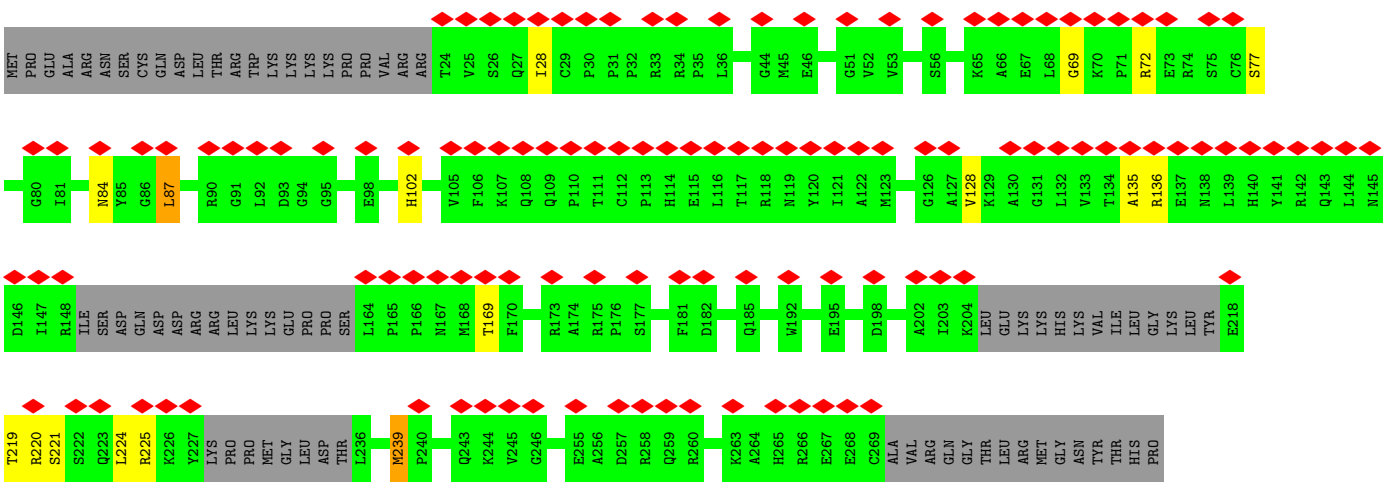
• Molecule 14: Cilia and flagella associated protein 77

Chain 2W:



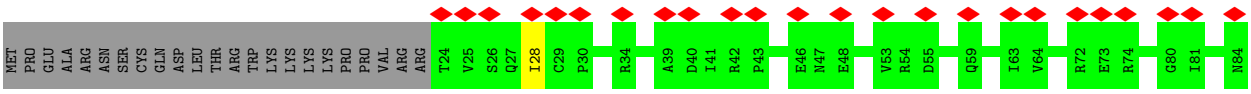
• Molecule 14: Cilia and flagella associated protein 77

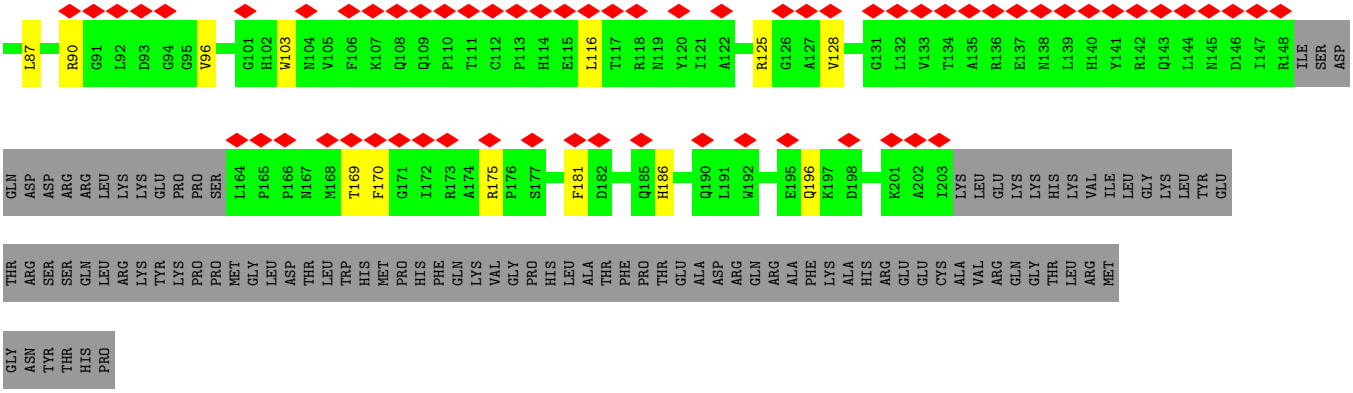
Chain 2X:



• Molecule 14: Cilia and flagella associated protein 77

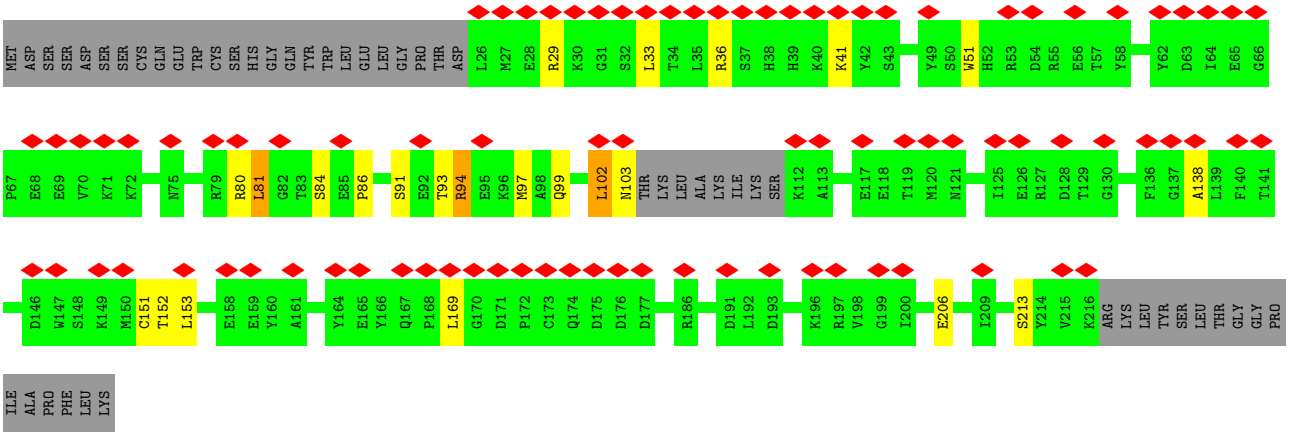
Chain 2Y:





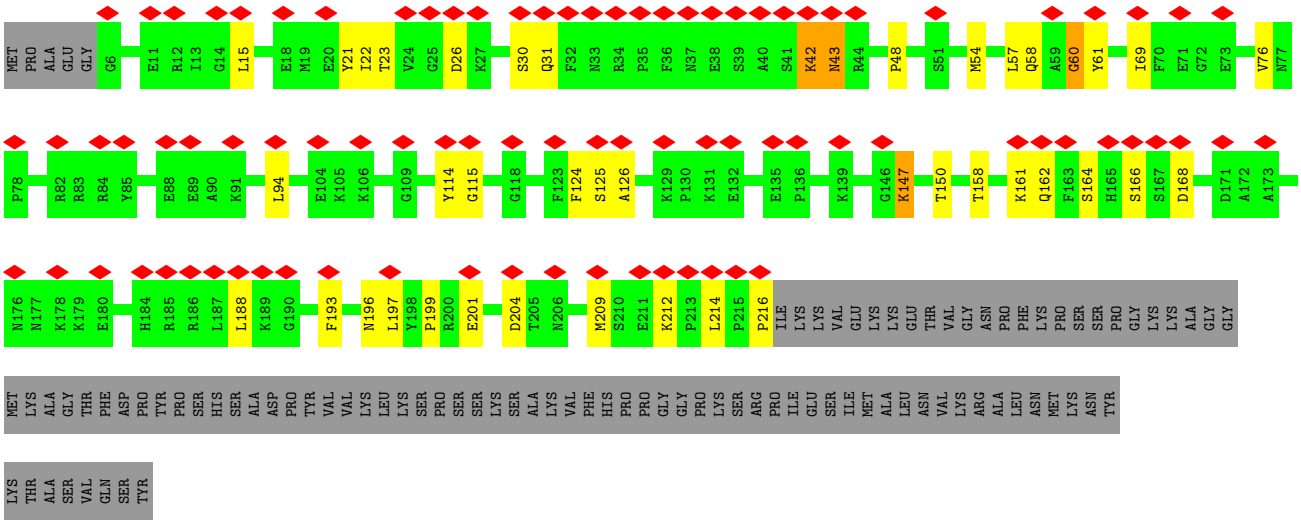
- Molecule 15: CFAP95

Chain 3A:



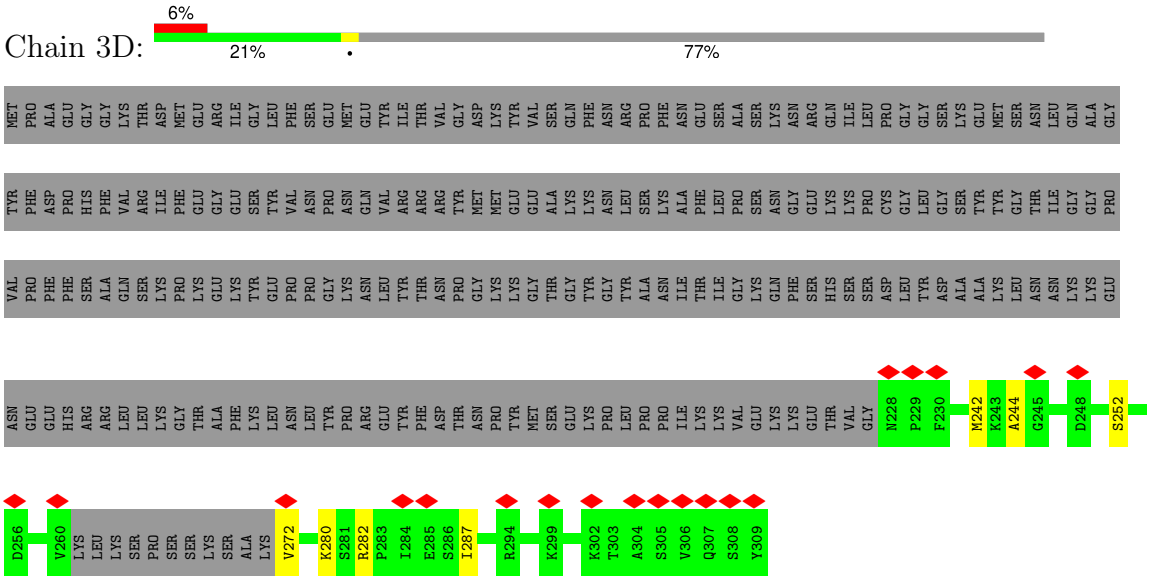
- Molecule 16: Cilia-and flagella-associated protein 96

Chain 3C:



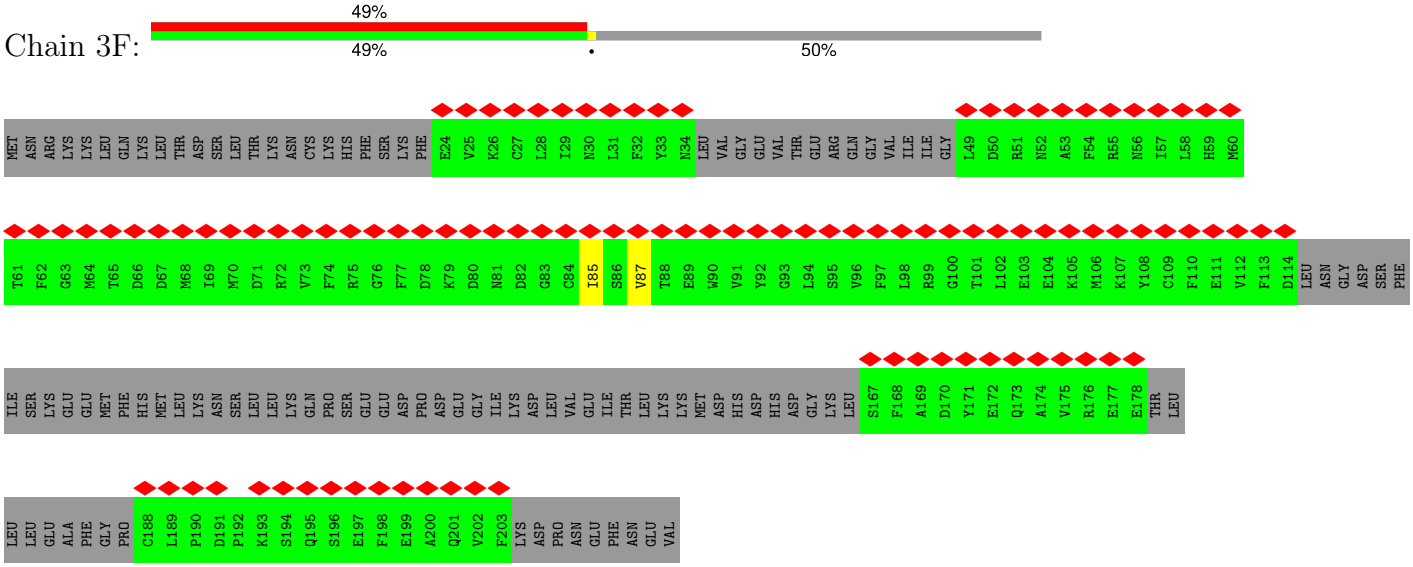
- Molecule 16: Cilia-and flagella-associated protein 96

Chain 3D:



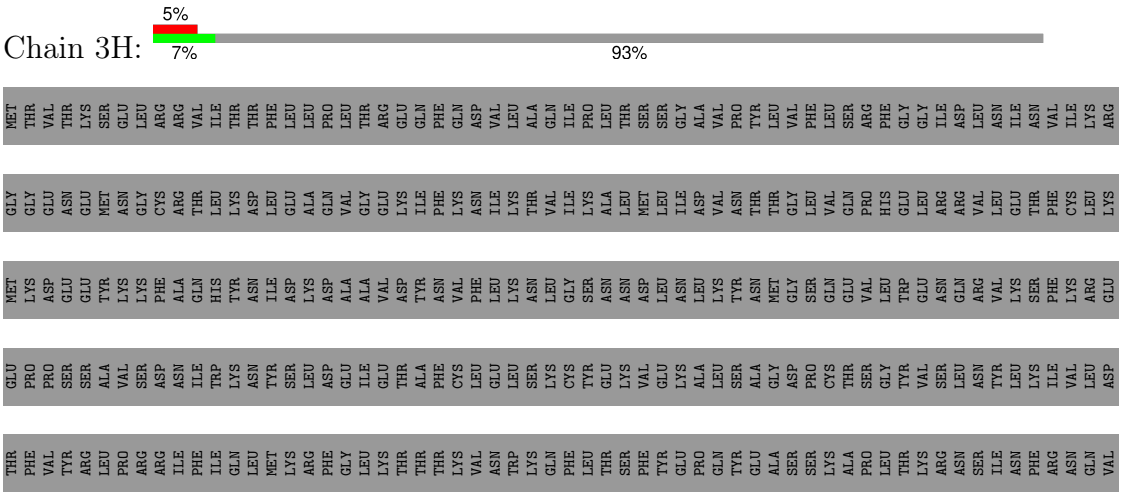
- Molecule 17: EF-hand calcium-binding domain-containing protein 1

Chain 3F:



- Molecule 18: EF-hand calcium binding domain 6

Chain 3H:



HIS LYS GLU ASN VAL ILE THR LYS LEU PHE ARG HIS GLU ASP HIS ASP SER SER LEU LYS LYS ALA LEU LEU LEU ILE LYS SER LYS PRO ASP GLY GLN ILE THR GLY GLN GLU LEU GLN ARG ILE LEU ASN CYS MET VAL VAL LYS ILE SER ASP SER GLU PHE ARG GLU LEU MET ARG
ILE LEU ASP PRO GLY CYS THR GLY CYS VAL ASN VAL SER ARG PHE ILE GLU LEU ILE GLU GLU SER PRO LYS LEU HIS LYS ILE PRO ALA TYR LYS ASP THR LYS MET PRO LEU PHE LEU ALA TRP ASP SER VAL GLU GLU ILE ILE HIS ASP SER ILE ALA LYS ASN LEU MET PHE
CYS ASN MET LEU ARG SER TYR ASP LEU GLY ASP THR GLY LEU ASN ASN PHE LYS LYS ILE MET ARG VAL PHE CYS PRO PHE LEU THR THR GLU HIS LEU VAL LYS LEU CYS SER LYS PHE GLN ASP ILE ALA SER GLY ARG ILE LEU TYR LYS LYS LEU LEU ALA CYS LEU
GLY ILE ASN ARG PRO PRO THR VAL SER PRO VAL SER MET PRO LYS GLY GLN LEU LEU GLN LYS GLU GLU GLN PRO LEU PRO ASP HIS SER GLU ARG ALA THR PRO ALA GLU SER GLN GLY ALA VAL THR ARG ASN MET THR LYS ASP GLU VAL ILE GLU LYS LEU LYS
SER CYS ILE GLN GLN GLN ASP PRO ALA PHE ARG LYS ARG PHE LEU ASP PHE THR LYS GLU PRO ASN ASN GLY GLY LYS ILE HIS THR HIS HIS ASP PHE LYS LYS VAL THR GLY MET PRO MET ASP ASP ASP GLN TYR ALA LEU LEU THR THR LYS LEU GLY TYR LYS LYS GLU GLY MET
SER TYR LEU ASP PHE ALA ALA GLY PHE GLU ASP PRO LYS MET ASN GLU PRO VAL THR PRO PRO GLN THR PRO VAL LEU PRO LYS GLY ASP VAL SER SER PHE PHE VAL THR ALA GLU GLU GLU CYS LEU ARG GLN TYR ALA LEU ARG GLN PHE PRO ARG ARG LEU LYS GLU PHE PHE ARG ASP PRO TYR ALA ALA
PHE PHE LYS MET ASP THR ASP ARG ASP GLY ILE LEU THR MET HIS ASP LEU HIS ARG LEU LEU LEU GLN HIS LEU LEU PHE ASN LEU LYS ASP GLU GLU PHE GLU GLY GLY LEU LEU ARG LEU SER ILE LEU LYS ARG
SER PHE SER ALA ASP ASP ASP ALA PRO GLN ARG LEU LEU PRO ARG PRO LYS GLN LYS VAL ALA ASP SER GLU LEU ALA CYS GLU GLN ALA HIS GLN TYR LEU VAL SER ASP LEU SER LYS ASN PHE ILE GLU THR ASP SER GLU GLY ASN GLY ILE LEU ARG
ARG ARG ASP MET LYS ASN ALA LEU TYR GLY PHE ASP ILE PRO LEU THR PRO ARG GLU PHE GLU LYS LEU TRP MET ARG TYR ASP SER GLU GLY ARG GLY HIS ILE THR TYR GLN GLU PHE GLU GLY PHE LEU ASN SER ALA ASP ILE HIS ARG PRO TYR ALA GLU TYR
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ILE ASN PHE ALA ALA LEU SER PRO GLU GLU VAL LEU LYS ASN ILE GLN GLY VAL ILE ALA ALA SER SER LEU ALA LEU SER THR ALA PHE SER ALA LEU ASP LYS GLU VAL LYS ALA SER ASP PHE GLY GLN VAL LEU LYS ASP PHE CYS TYR LYS LEU THR ASP ASN
GLN TYR HIS TYR PHE LEU ARG LYS LEU ARG LEU HIS LEU THR PRO TYR ILE ASN TRP LYS TYR PHE LEU GLN ASN PHE SER SER TYR VAL GLU GLU THR ALA VAL GLU TRP ALA GLU LYS MET PRO ARG GLY PRO ARG PRO LEU SER PRO LYS GLU MET ALA ASN GLN GLU LEU LEU ALA
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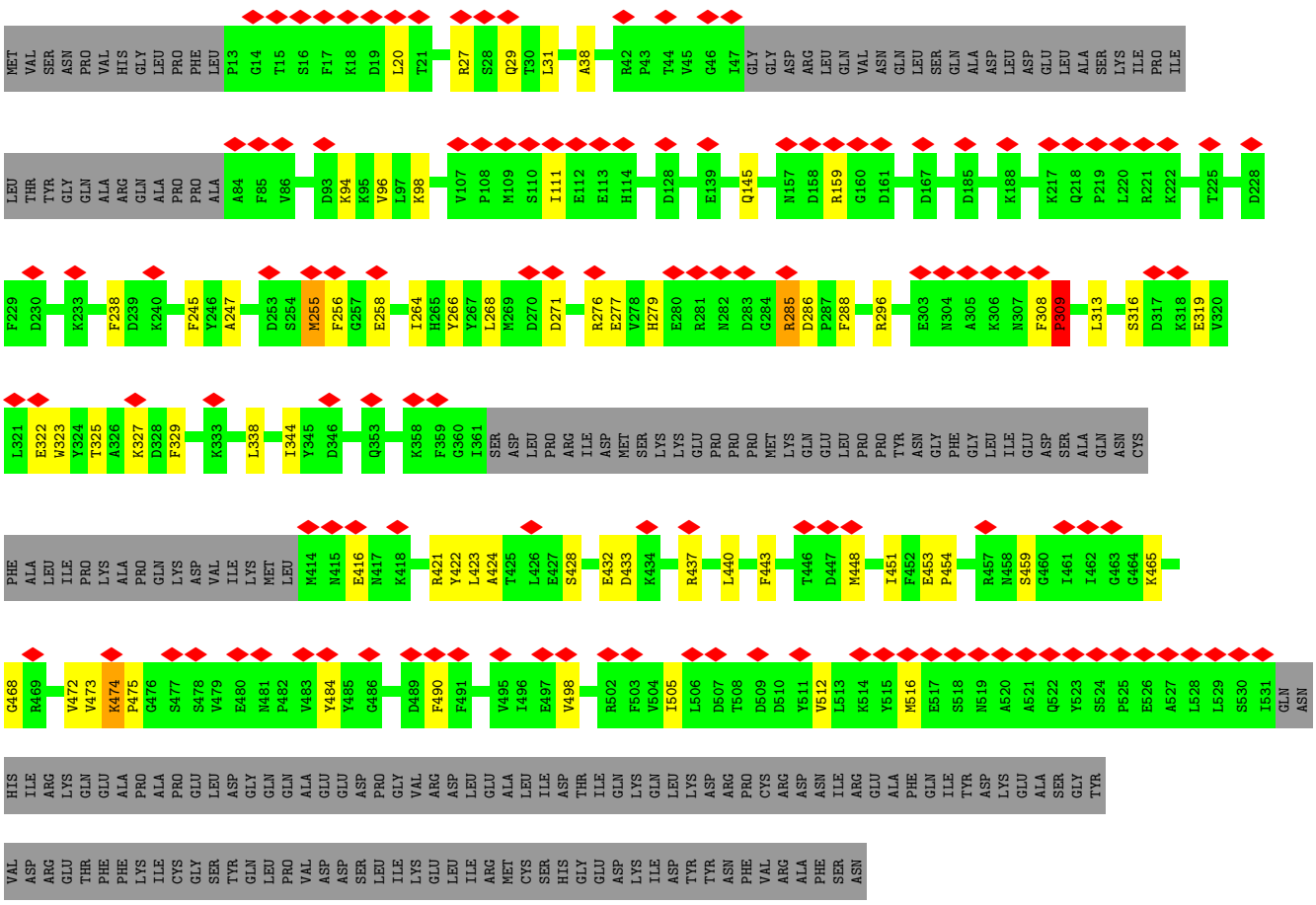
VAL GLU LYS PHE ASN LEU SER ARG ASP GLU CYS GLN GLN LEU LEU ILE LYS TYR ASP LEU LYS ASN ASN GLY LYS PHE ALA TYR CYS SER PHE ILE GLN SER CYS VAL LEU LEU LEU LYS ALA LYS GLU THR SER LEU MET GLN ARG MET K1400 I1401 Q1402 N1403 A1404 N1405 K1406 M1407
K1408 E1409 A1410 G1411 A1412 E1413 T1414 C1415 S1416 F1417 L1421 Q1425 P1426 K1427 I1428 V1429 H1430 C1431 M1435 R1436 F1439 K1440 D1443 E1444 G1445 G1446 T1447 G1448 L1449 L1450 S1451 D1454 F1455 R1456 K1457 V1458 L1459 Y1462 S1463 I1464 N1465 L1466 S1467 E1468 E1469 E1470 F1471 F1472 H1473 I1474 L1475 E1476 Y1477
Y1478 T1481 L1482 S1483 S1484 K1485 Y1488 N1489 D1490 F1491 L1492 R1493 A1494 F1495 L1496 GLN

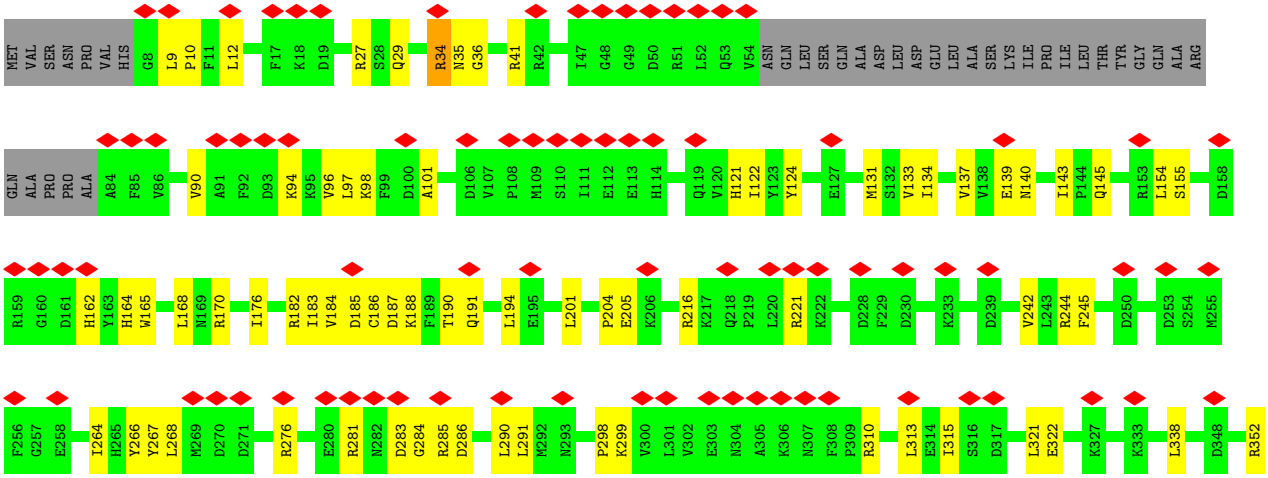
- Molecule 19: EF-hand domain containing 1

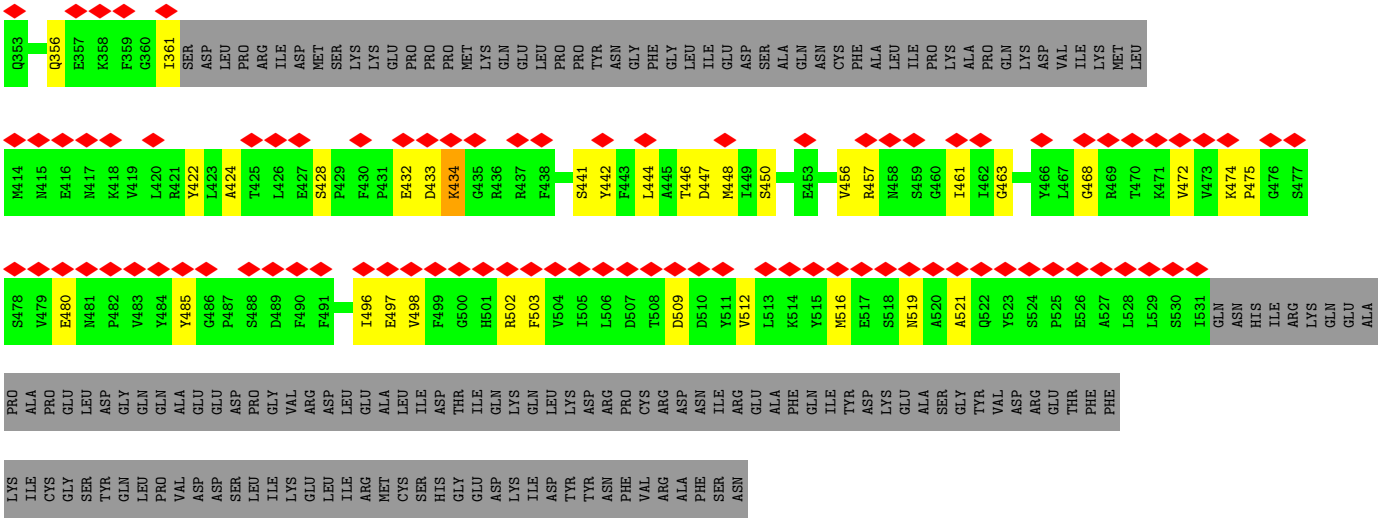
Chain 3J:



- Molecule 19: EF-hand domain containing 1

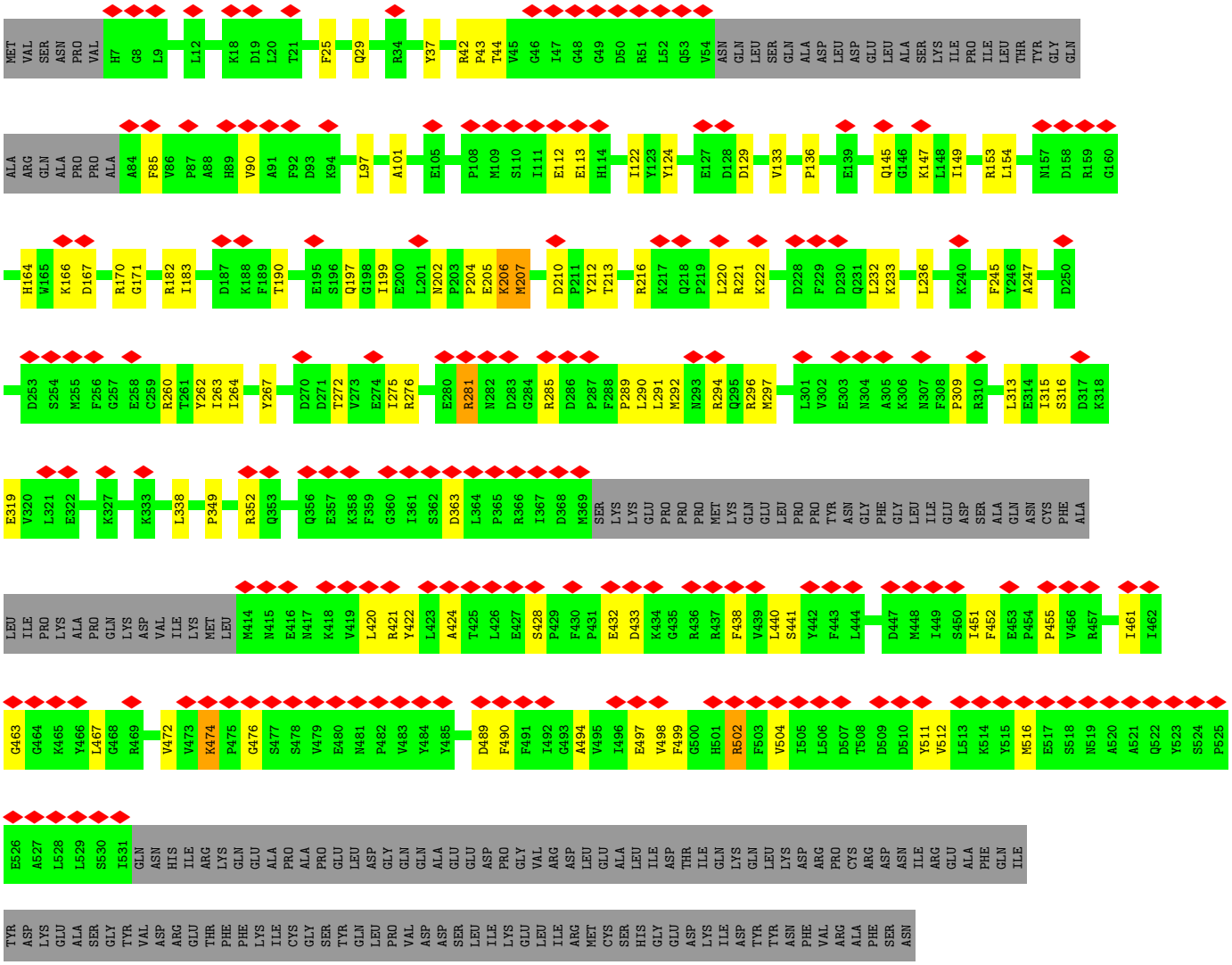
Chain 3K:





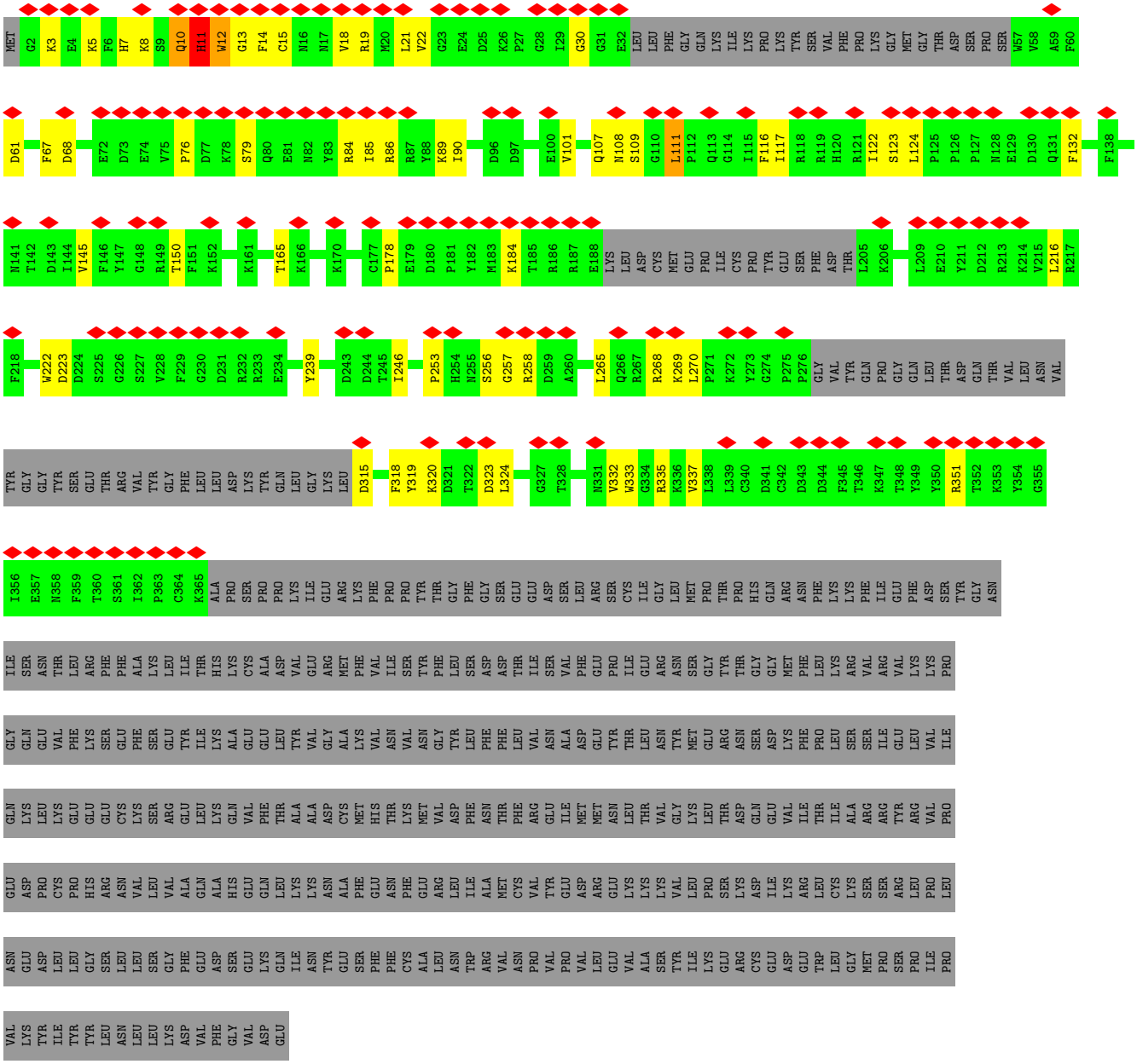
- Molecule 19: EF-hand domain containing 1

Chain 3L:



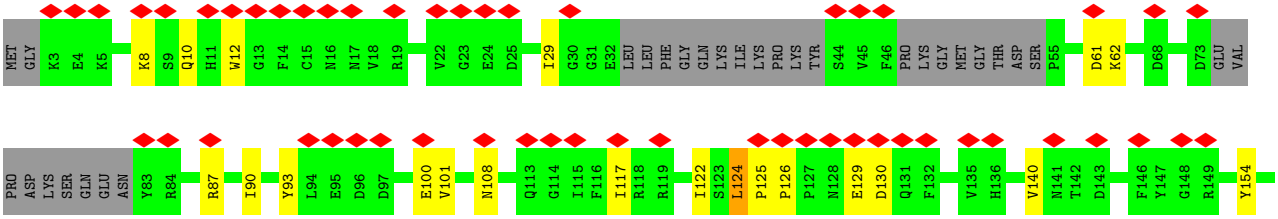
- Molecule 20: EFHC2

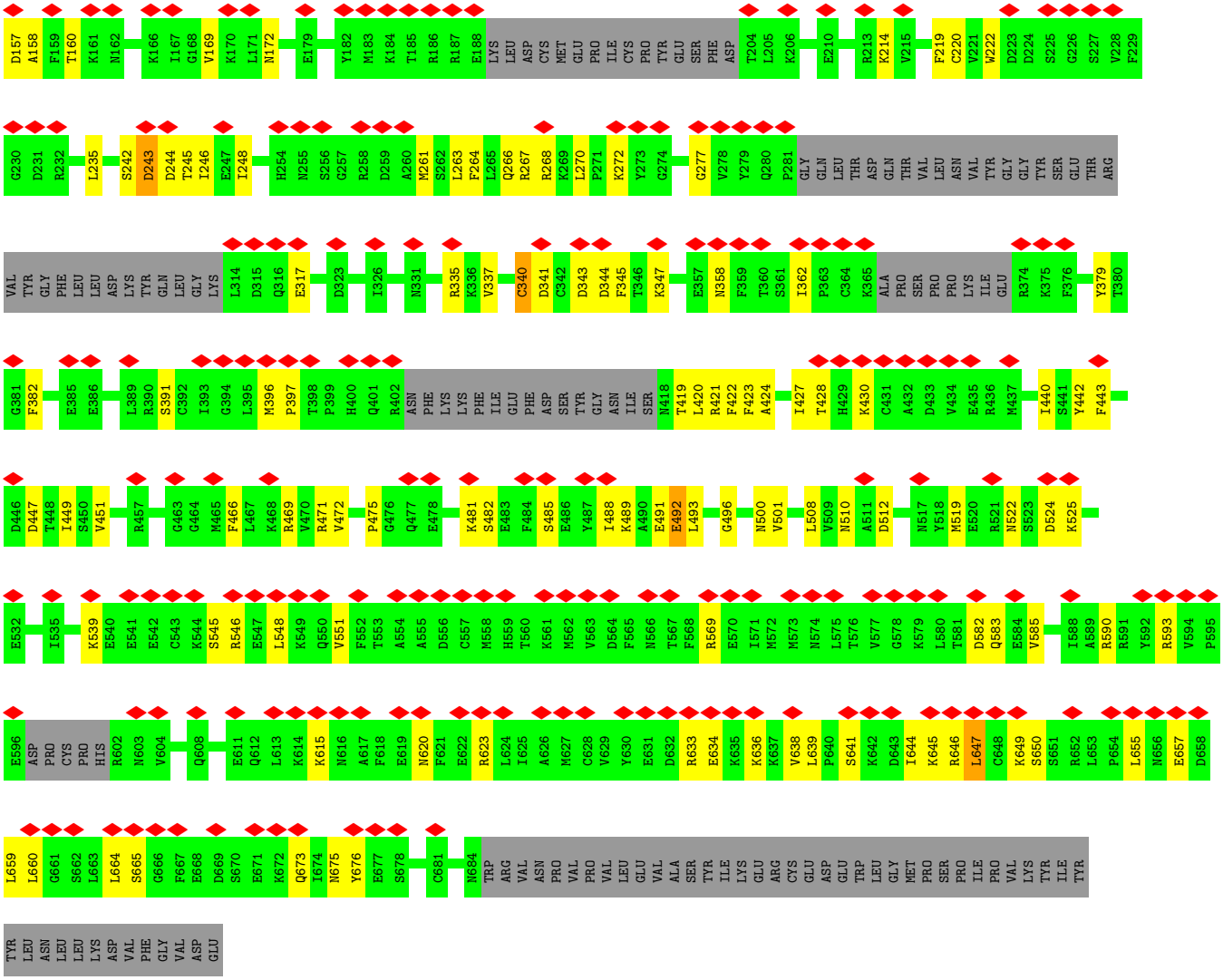
Chain 3N:



- Molecule 20: EFHC2

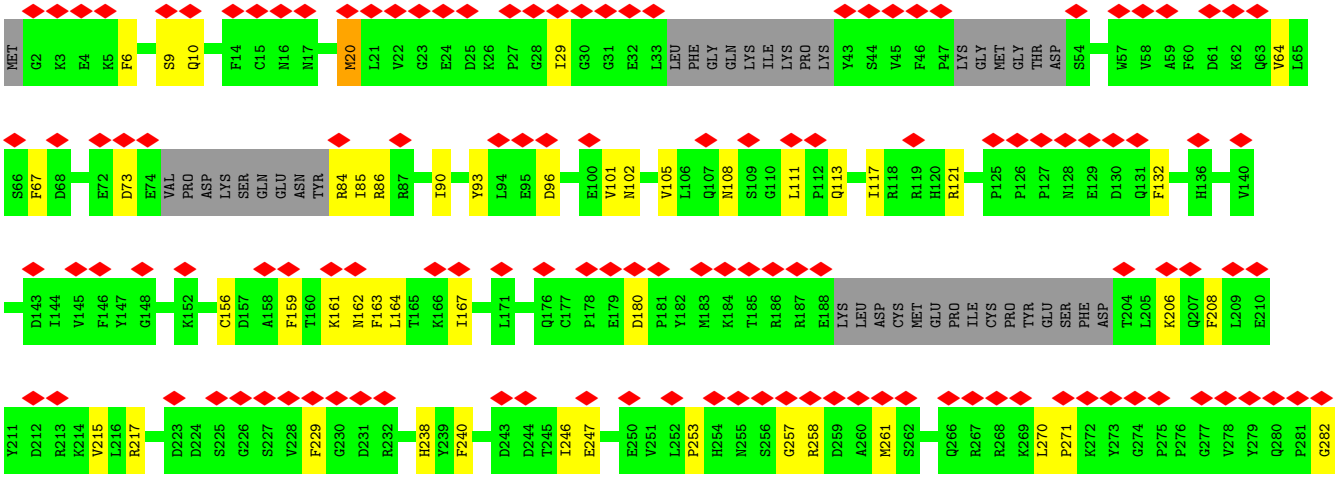
Chain 3O:

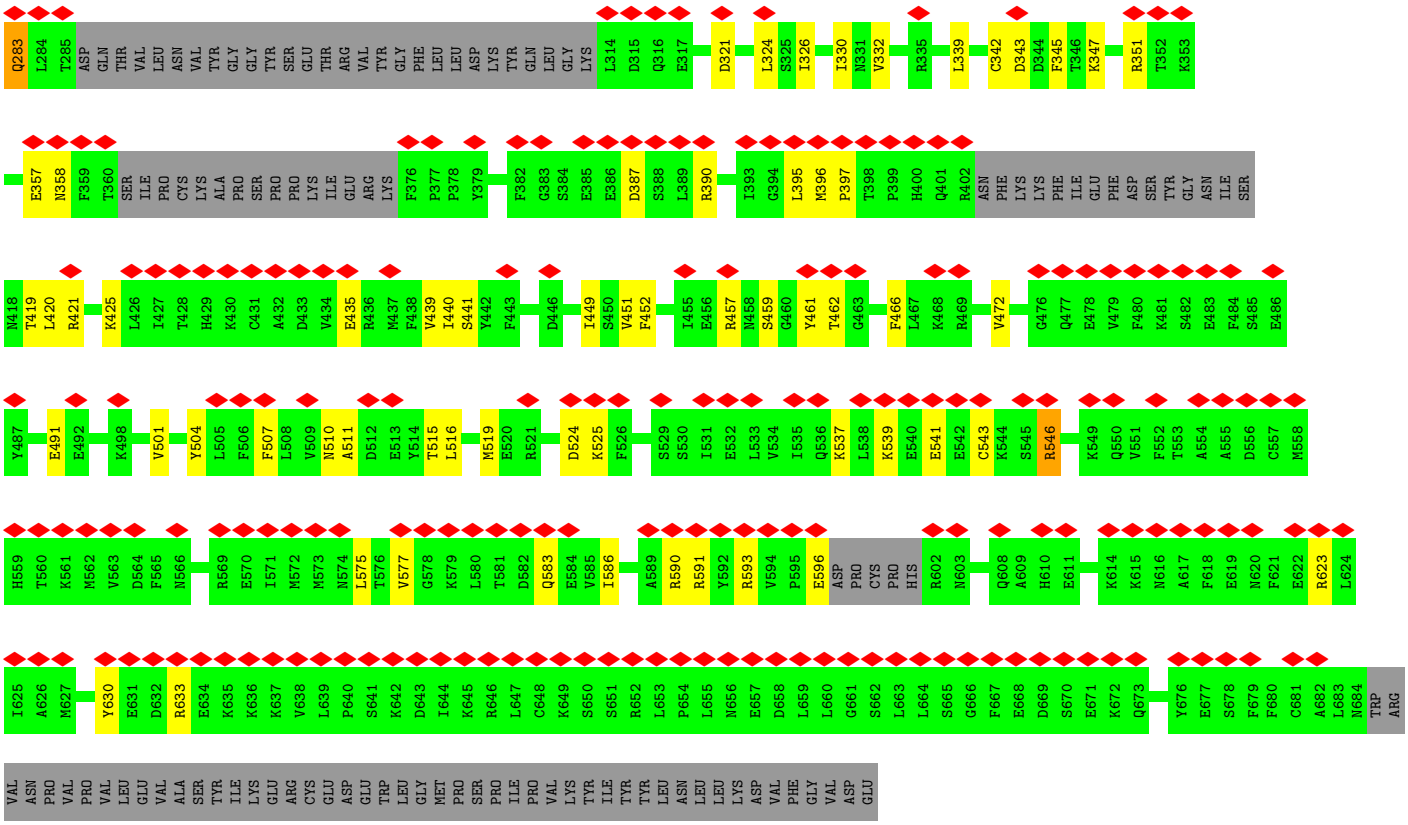




- Molecule 20: EFHC2

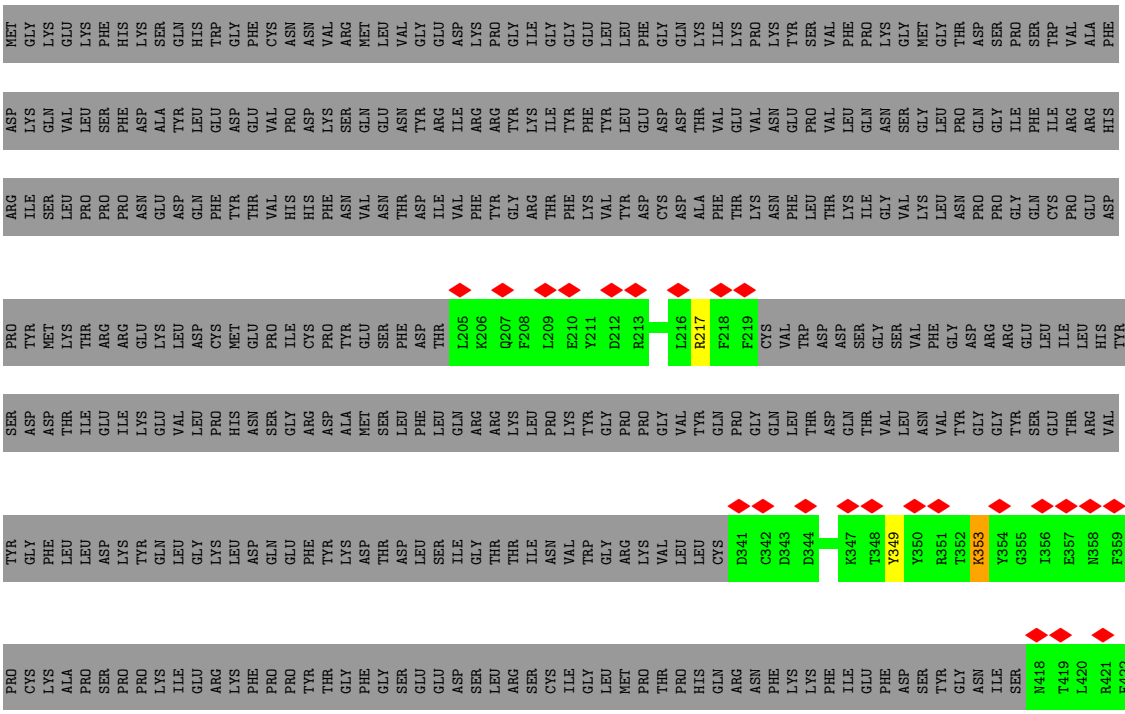
Chain 3P:





- Molecule 20: EFHC2

Chain 3Q:



F423 A424 K425 L426 I427 T428 H429 K430 C431 A432 D433 V434 E435 R436 M437 F438 S441 Y442 F443 L444 S445 D446 D447 T448 I449 F452 E453 P454 I455 N458 S459 G460 Y461 T462 G463 G464 M465 F466 L467 K468 R469 V470 R471 V472 K473 K474 PRO GLY GLN GLU VAL PHE LYS SER GLU PHE S485

E486 Y487 I488 K489 A490 E491 E492 L493 Y494 V495 G496 A497 K498 V499 N500 V501 N502 G503 Y504 L505 F506 F507 L508 V509 N510 A511 D512 E513 L516 N517 Y518 M519 E520 R521 N522 S523 D524 K525 F526 P527 L528 S529 S530 I531 E532 L533 V534 I535 Q536 K537 L538 K539 E540 E541 E542 C543 K544 S545 R546

E547 L548 K549 Q550 V551 F552 T553 A554 A555 D556 C557 M558 H559 T560 K561 M562 V563 D564 F565 N566 T567 F568 R569 E570 I571 M572 M573 N574 L575 T576 K579 L580 T581 D582 Q583 E584 V585 I586 T587 I588 A589 R590 R591 Y592 R593 V594 P595 E596 ASP PRO CYS PRO HIS R602 N603 V604 L605 V606 A607

Q608 A609 H610 E611 Q612 L613 K614 K615 N616 A617 F618 E619 N620 F621 E622 R623 L624 I625 A626 M627 C628 V629 Y630 E631 D632 R633 E634 K635 K636 K637 V638 L639 P640 S641 K642 D643 I644 K645 R646 L647 C648 K649 S650 S651 R652 L653 P654 L655 N656 E657 D658 L659 L660 G661 S662 L663 L664 S665 G666 F667

E668 D669 S670 E671 K672 Q673 I674 N675 Y676 E677 S678 F679 F680 C681 A682 L683 N684 W685 ARG VAL ASN PRO VAL PRO VAL LEU GLU VAL ALA SER TYR ILE LYS GLU ARG CYS GLU ASP GLU TRP LEU GLY MET PRO SER PRO ILE PRO VAL LYS TYR ILE TYR TYR LEU ASN LEU LEU LYS ASP

VAL PHE GLY VAL ASP GLU

- Molecule 21: Enkurin, TRPC channel interacting protein

Chain 3S:

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

SER PRO LYS ASP PHE LEU LYS LYS HIS SER LYS GLU LYS ILE LEU PRO PRO LYS LYS LYS PHE GLU TRP ASN GLU ARG ARG LYS PRO PRO VAL PRO LEU ARG THR ASP HIS PRO VAL MET GLY ILE GLN SER GLU LYS N107 F108 I109 N110 T111 N112 A113 A114 M118 K122 I127

D130 K131 R132 K136 H137 D138 T141 K151 Y154 E159 Y160 I161 C162 K163 E166 E167 K170 A171 Q172 E173 E174 Y175 D176 ASN TYR ILE GLN GLU ASN LEU ARG LYS ALA ALA MET LYS ARG LEU SER ASP GLU GLU ARG GLU ALA VAL LEU GLU GLN GLY LEU LYS LYS

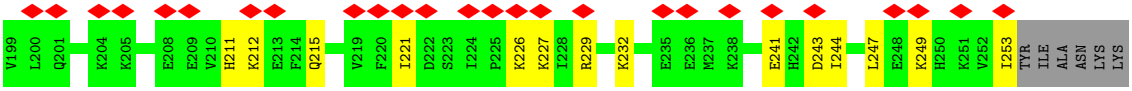
ASN TRP GLU GLU VAL HIS LYS GLU PHE GLN SER LEU SER VAL PHE ILE ASP SER ILE PRO LYS LYS ILE ARG LYS GLN LYS LEU GLU GLU GLU MET LYS GLN LEU GLU HIS ASP ILE GLY VAL LEU GLU LYS HIS LYS VAL ILE TYR ILE ALA ASN LYS LYS

- Molecule 21: Enkurin, TRPC channel interacting protein

Chain 3T:

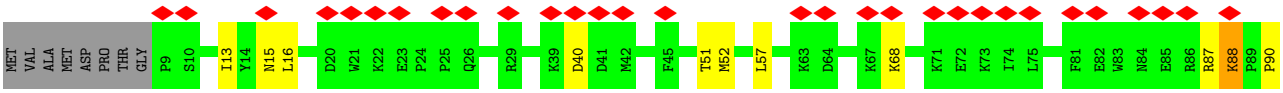
MET VAL ALA MET ASP PRO THR GLY P9 S10 S19 D20 W21 K22 E23 R29 Y30 V31 S32 I33 F34 K35 K39 D40 D41 T51 M52 P60 S61 P62 K63 D64 F65 L66 K71 E72 K73 I74 L75 K78 K79 K80 F81 E82 W83 N84 E85 R86 R87 P92 L93 R94

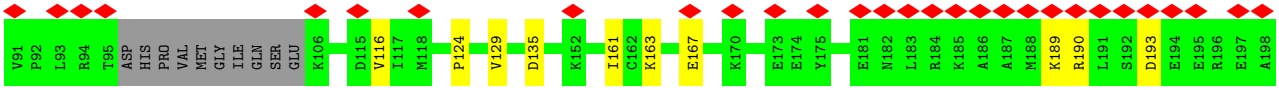
T95 ASP HIS PRO VAL MET GLY ILE GLN SER GLU K106 T111 D115 V116 I117 M118 K123 P124 I127 Y128 V129 D130 D135 D138 K152 N165 K170 N177 Y178 I179 Q180 E181 N182 L183 R184 K185 A186 A187 M188 K189 R190 L191 S192 D193 E194 E195 R196 E197 A198

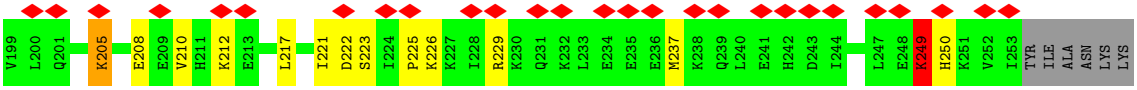


• Molecule 21: Enkurin, TRPC channel interacting protein

Chain 3U:

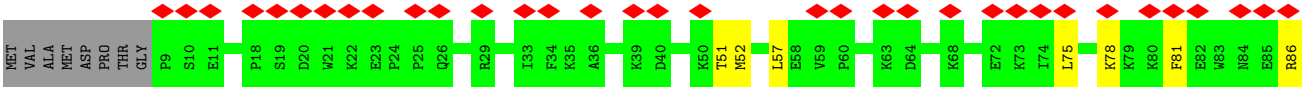


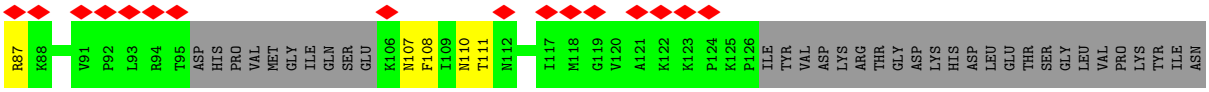


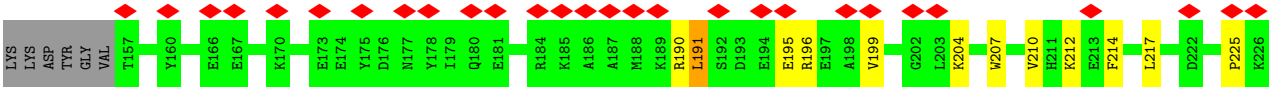


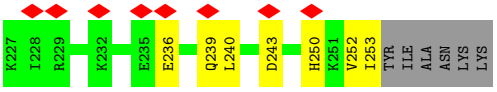
• Molecule 21: Enkurin, TRPC channel interacting protein

Chain 3V:



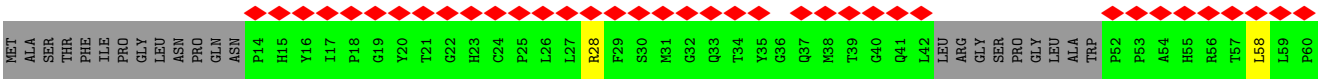


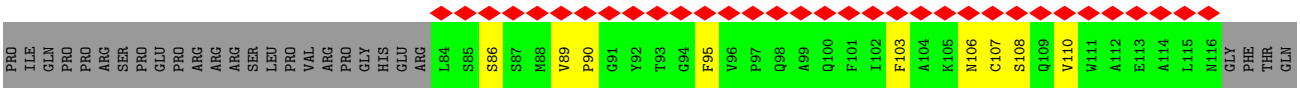


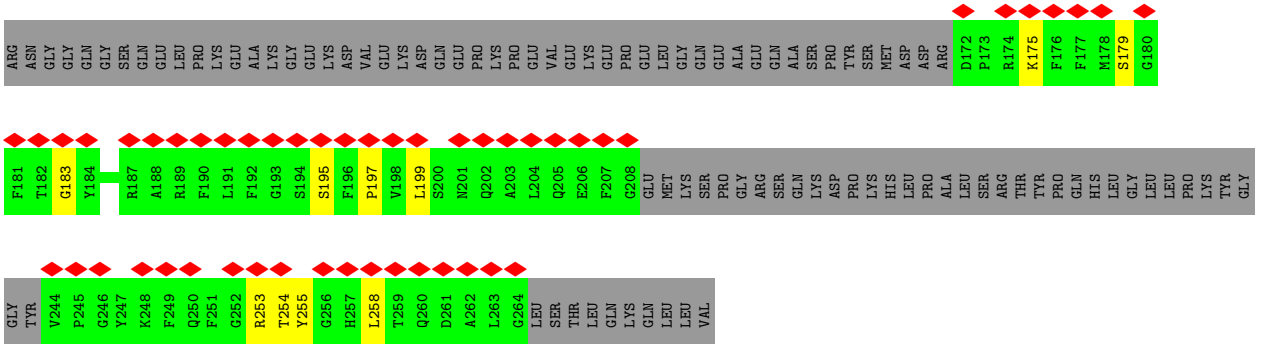


• Molecule 22: Protein FAM166B

Chain 3X:

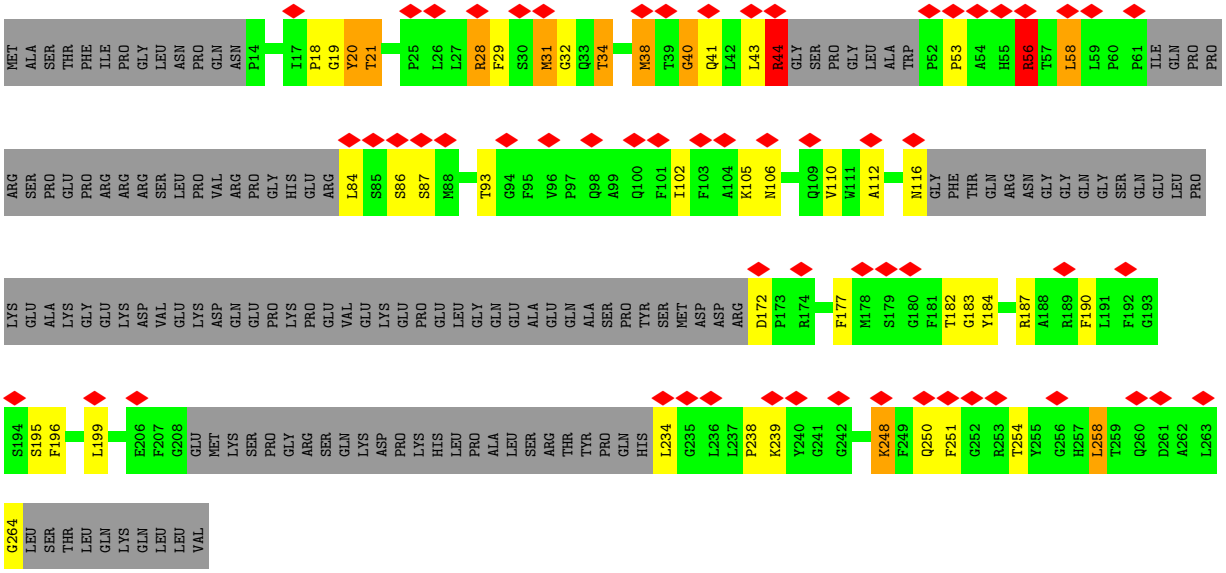






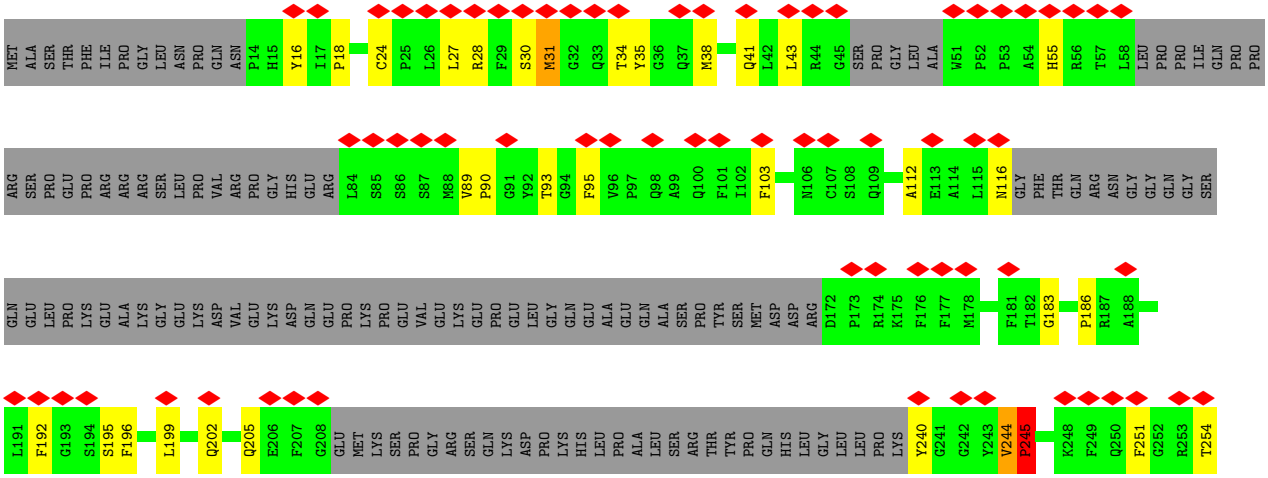
- Molecule 22: Protein FAM166B

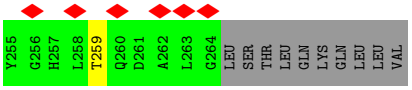
Chain 3Y:



- Molecule 22: Protein FAM166B

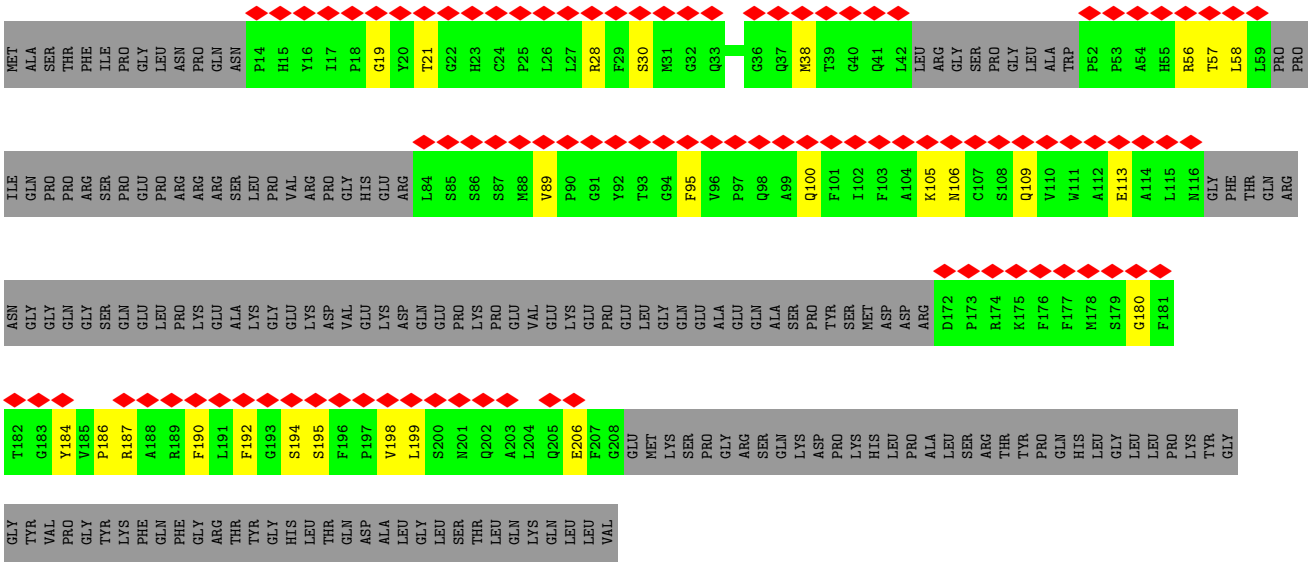
Chain 3Z:





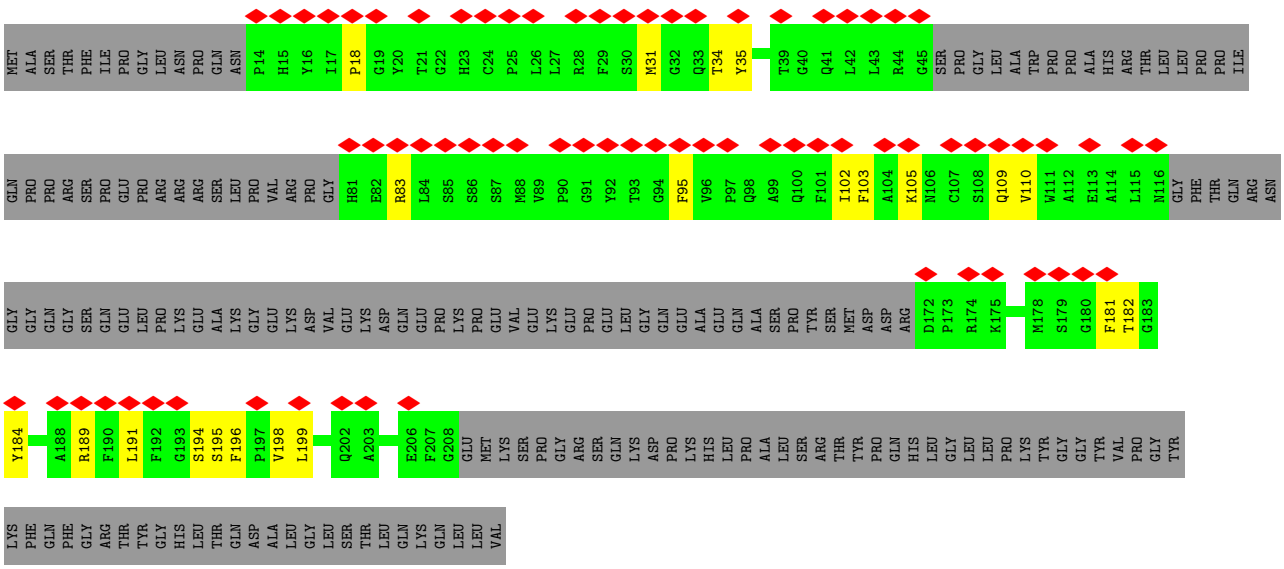
• Molecule 22: Protein FAM166B

Chain 4A:



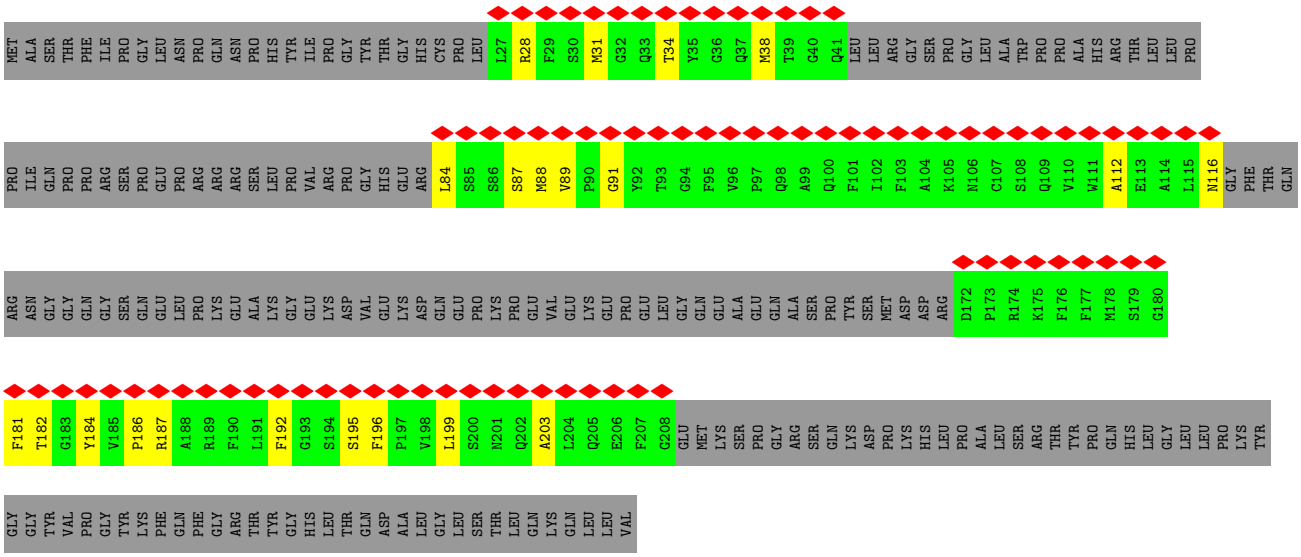
• Molecule 22: Protein FAM166B

Chain 4B:



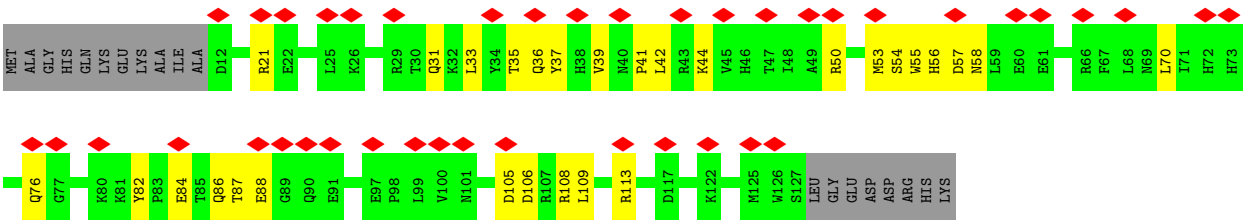
• Molecule 22: Protein FAM166B

Chain 4C:



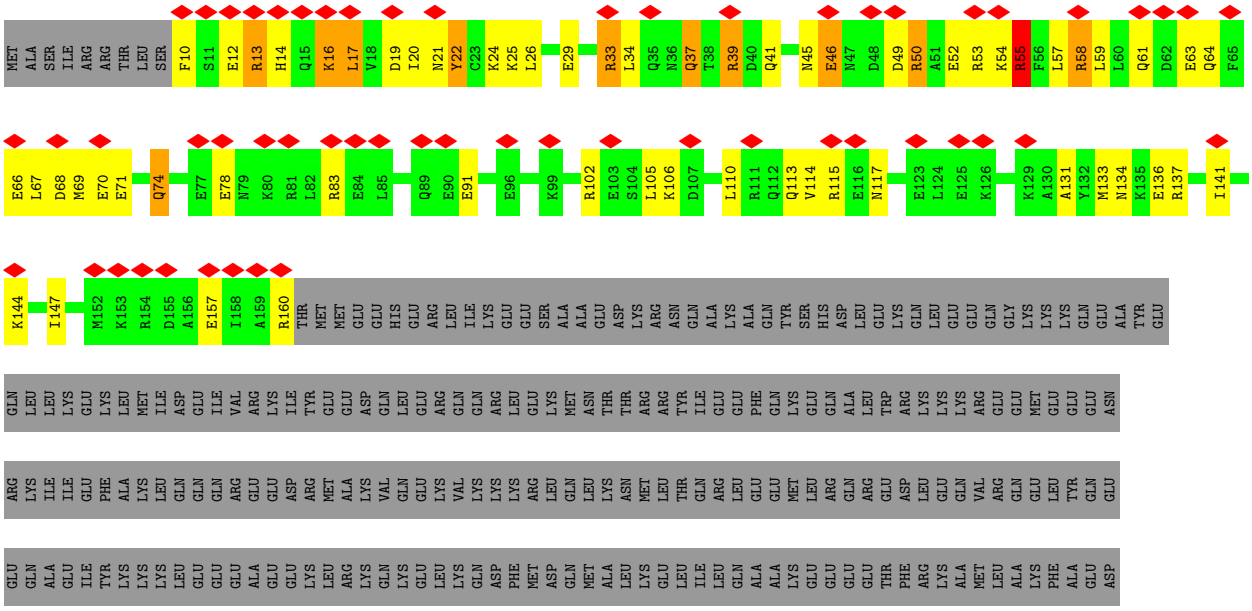
- Molecule 23: Cilia- and flagella-associated protein 144

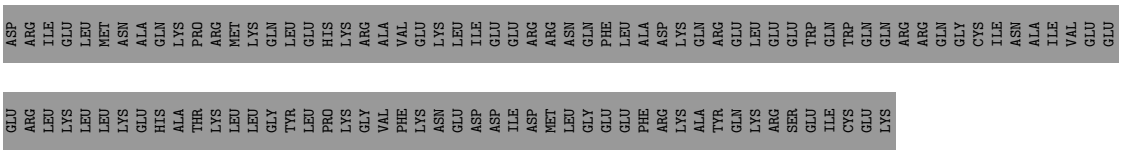
Chain 4D:



- Molecule 24: Meiosis-specific nuclear structural protein 1

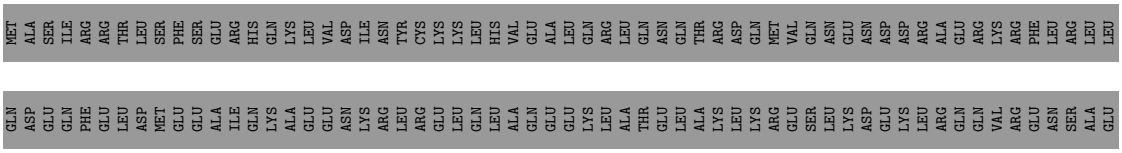
Chain 4F:

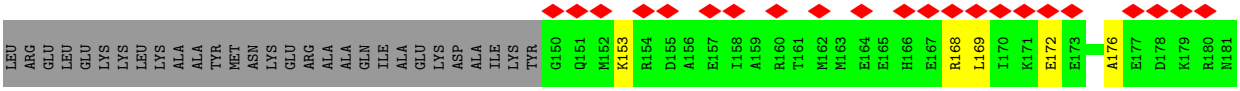


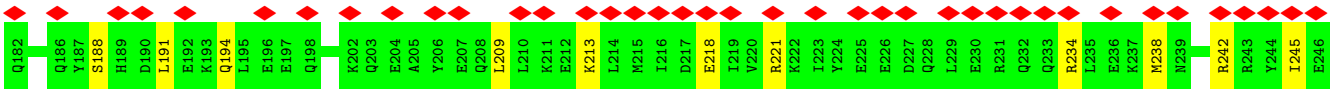


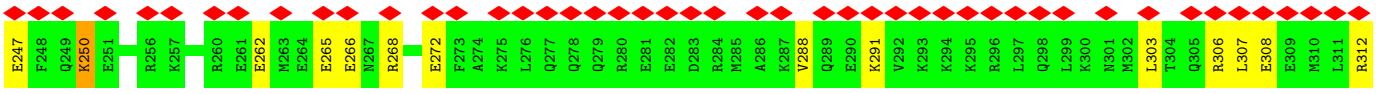
- Molecule 24: Meiosis-specific nuclear structural protein 1

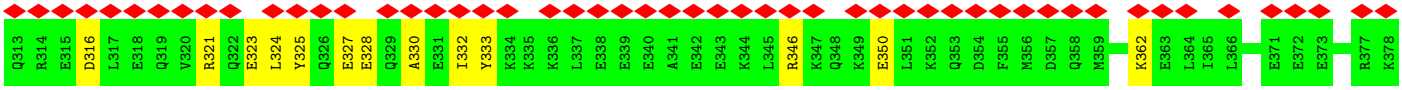
Chain 4G:

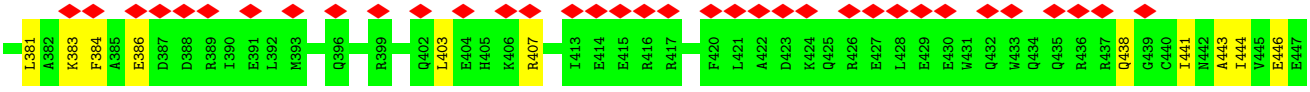


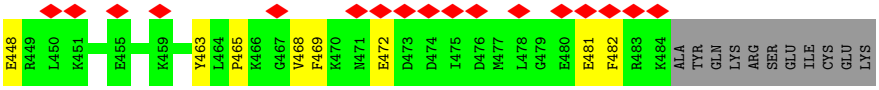






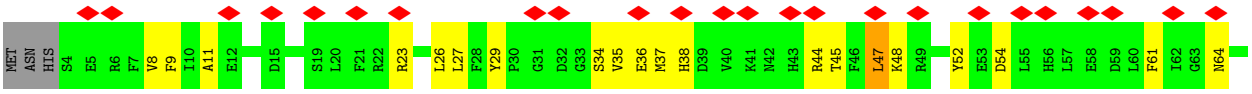


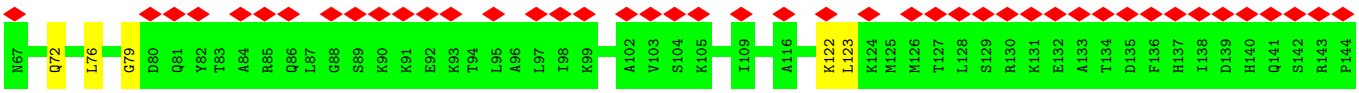


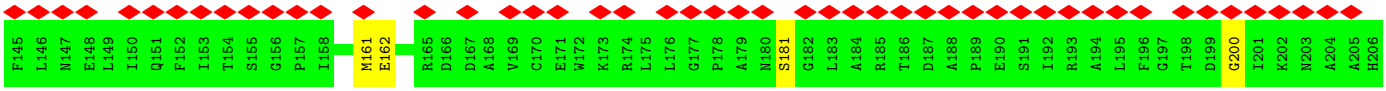


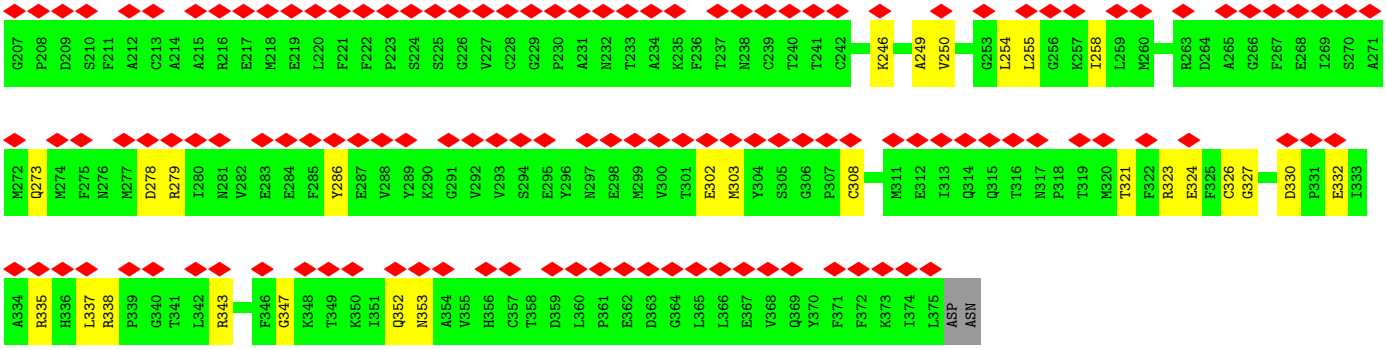
- Molecule 25: Nucleoside diphosphate kinase 7

Chain 4I:



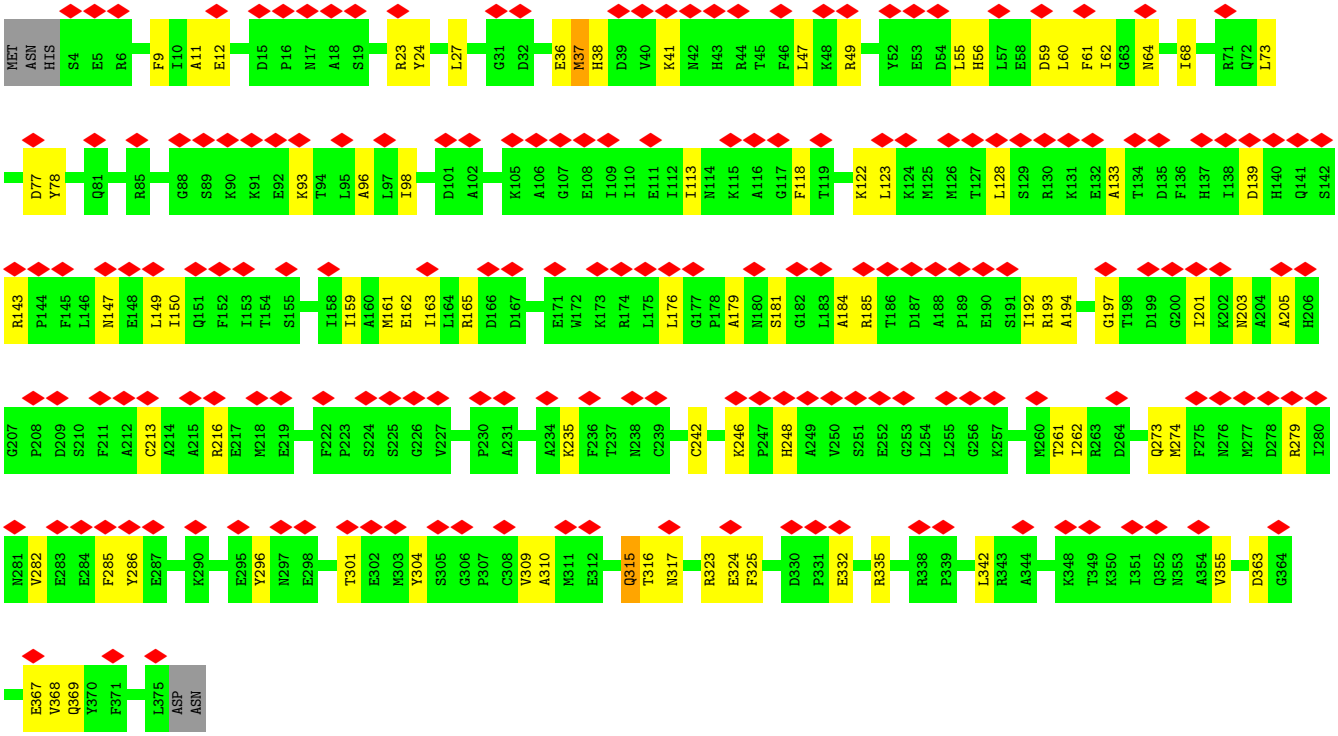






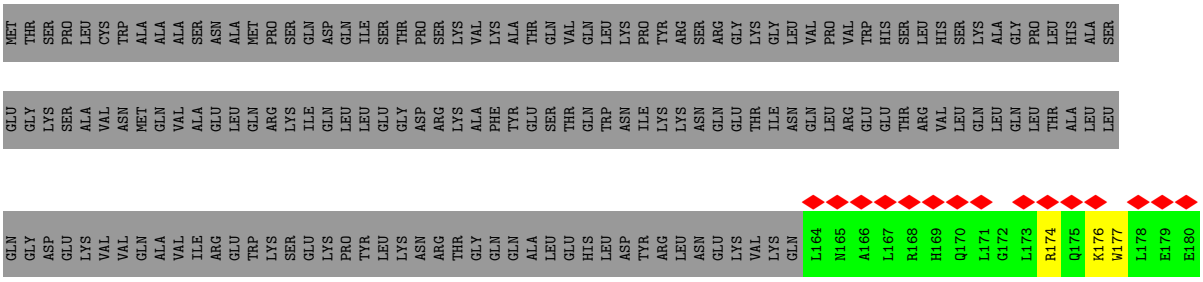
• Molecule 25: Nucleoside diphosphate kinase 7

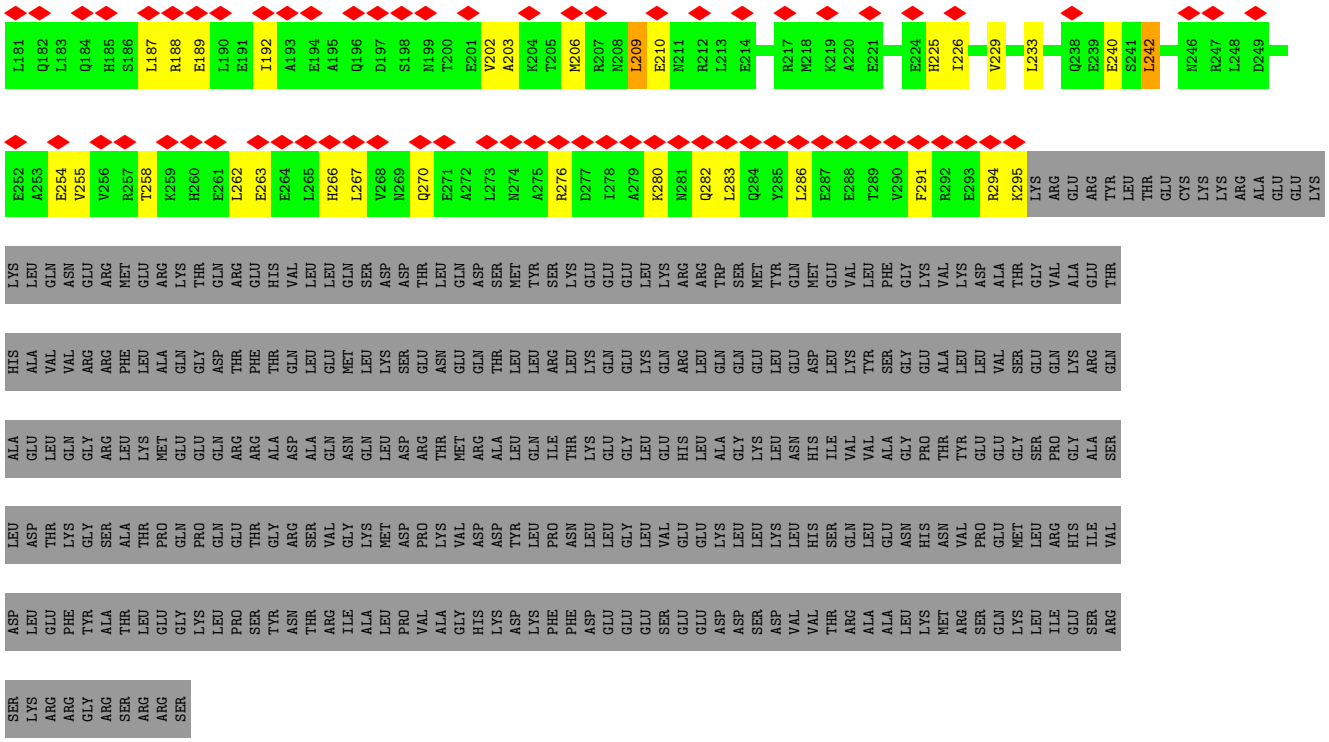
Chain 4J:



• Molecule 26: Outer dynein arm-docking complex subunit 3

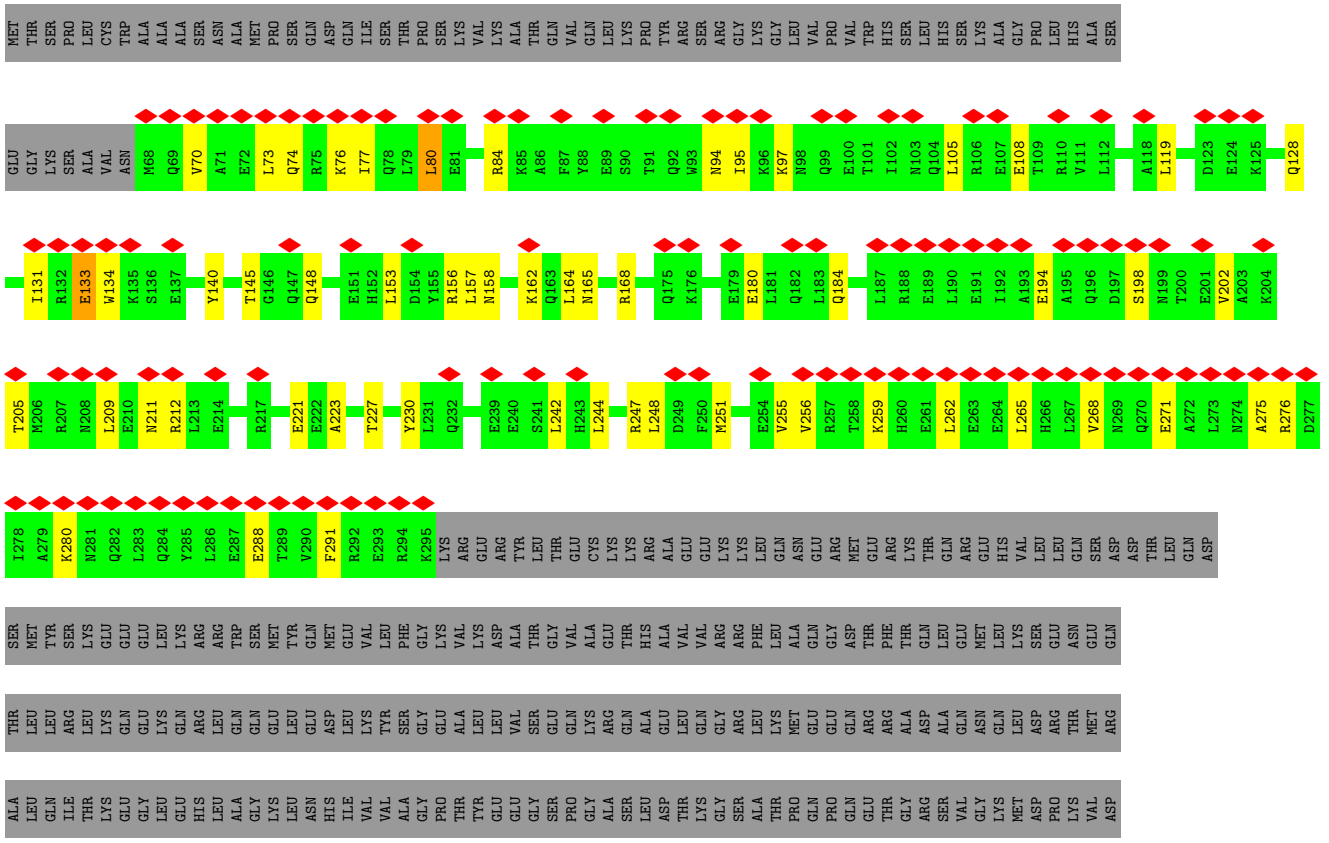
Chain 4K:

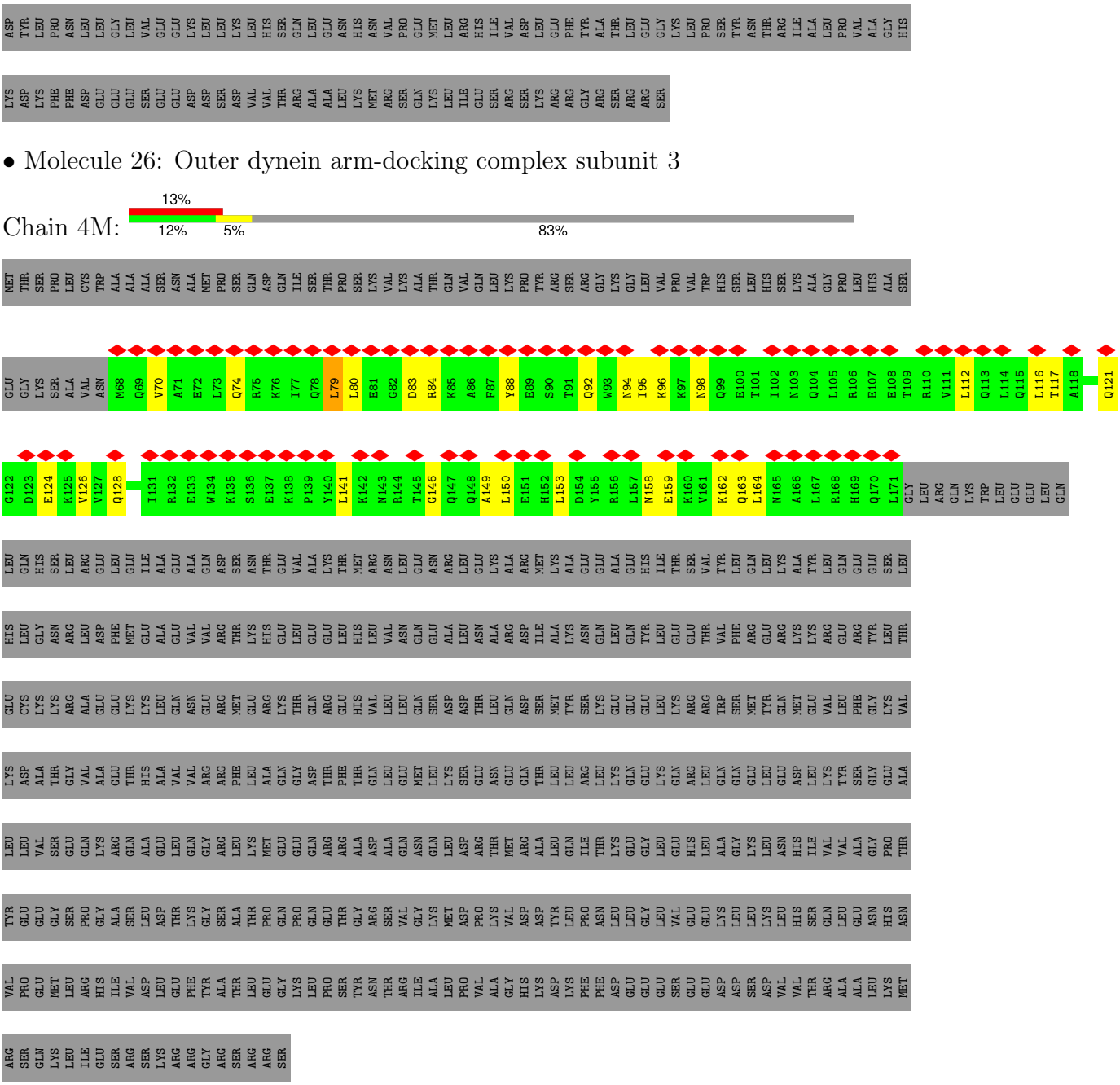




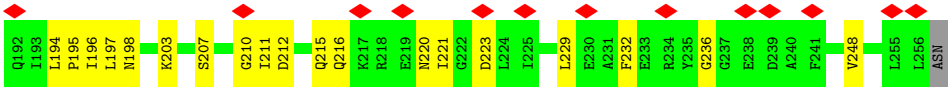
• Molecule 26: Outer dynein arm-docking complex subunit 3

Chain 4L:



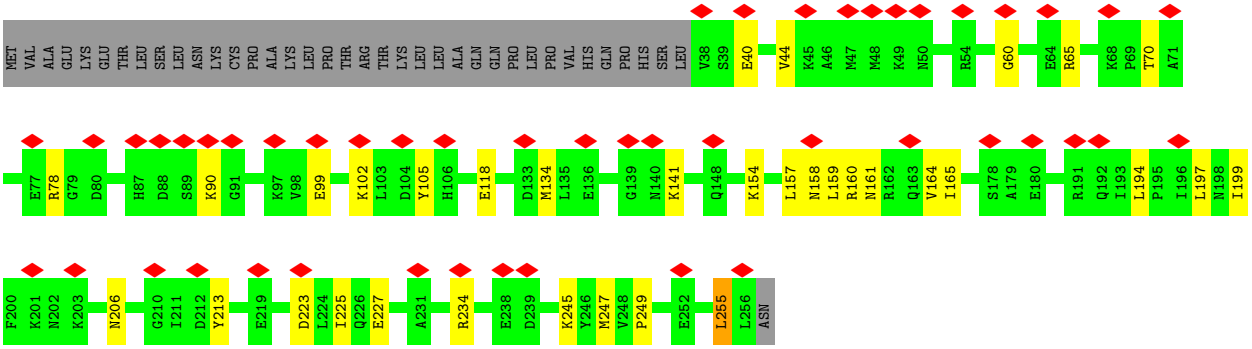

• Molecule 26: Outer dynein arm-docking complex subunit 3
Chain 4M:
13%
12%
5%
83%

• Molecule 27: PACRG protein
Chain 4O:
18%
68%
17%
15%



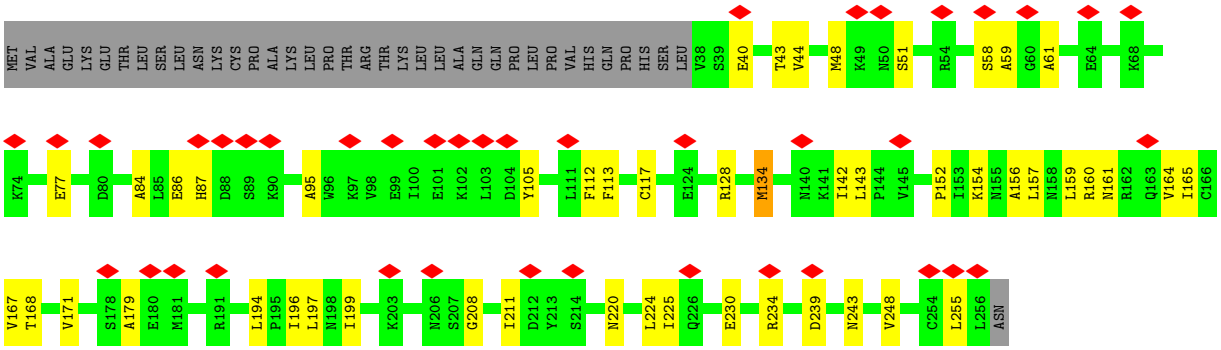
- Molecule 27: PACRG protein

Chain 4P:



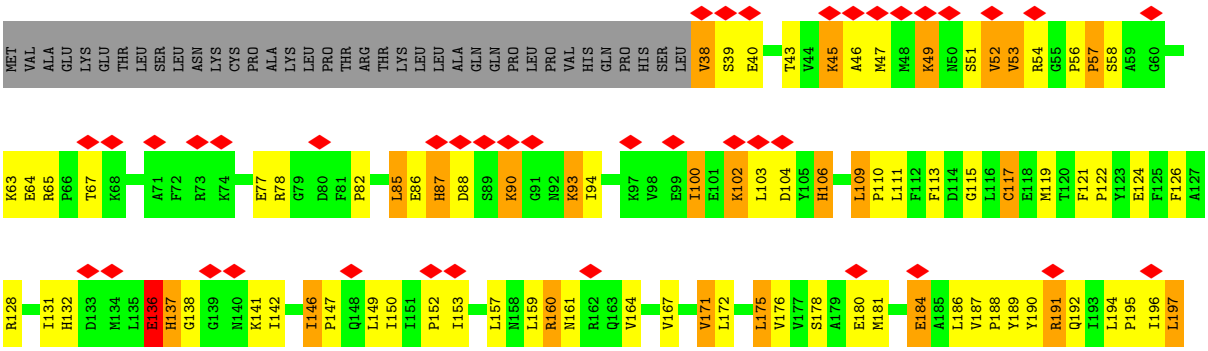
- Molecule 27: PACRG protein

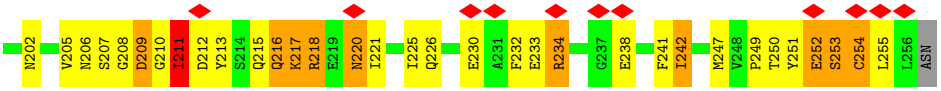
Chain 4Q:



- Molecule 27: PACRG protein

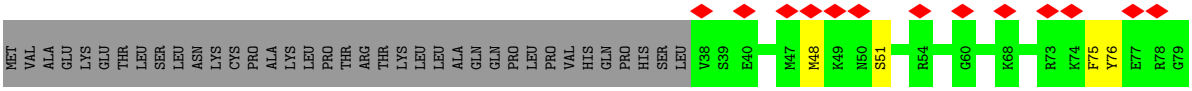
Chain 4R:

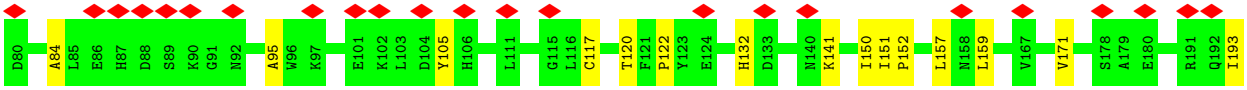


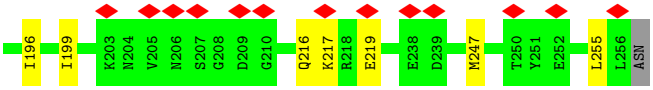


- Molecule 27: PACRG protein

Chain 4S:

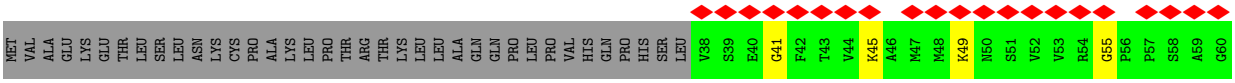


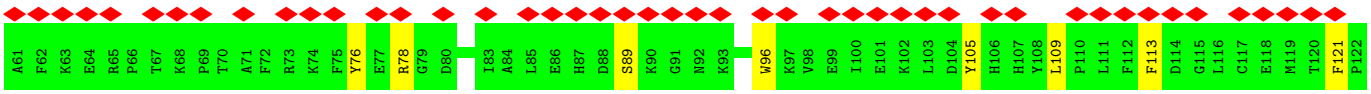


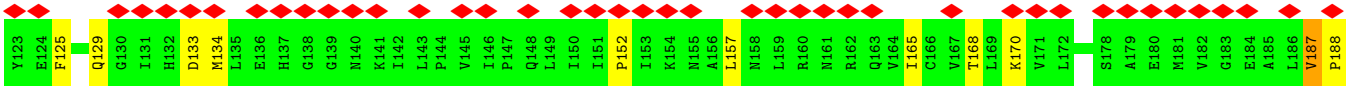


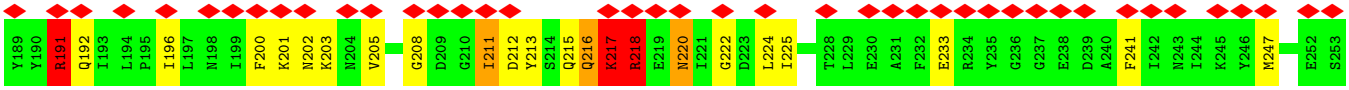
- Molecule 27: PACRG protein

Chain 4T:



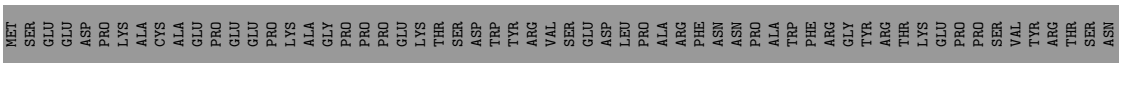


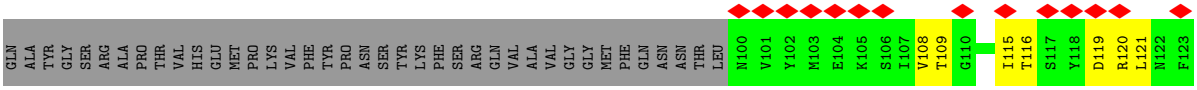


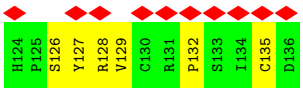


- Molecule 28: Pierce1

Chain 4V:

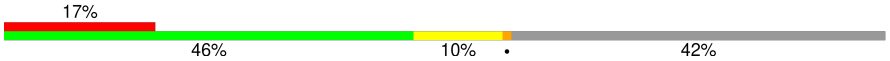


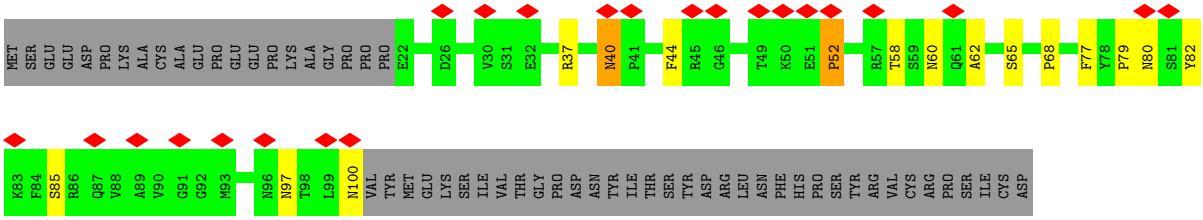




- Molecule 28: Pierce1

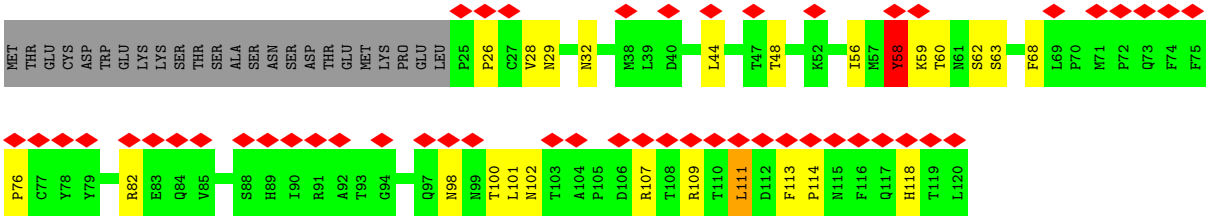
Chain 4W:





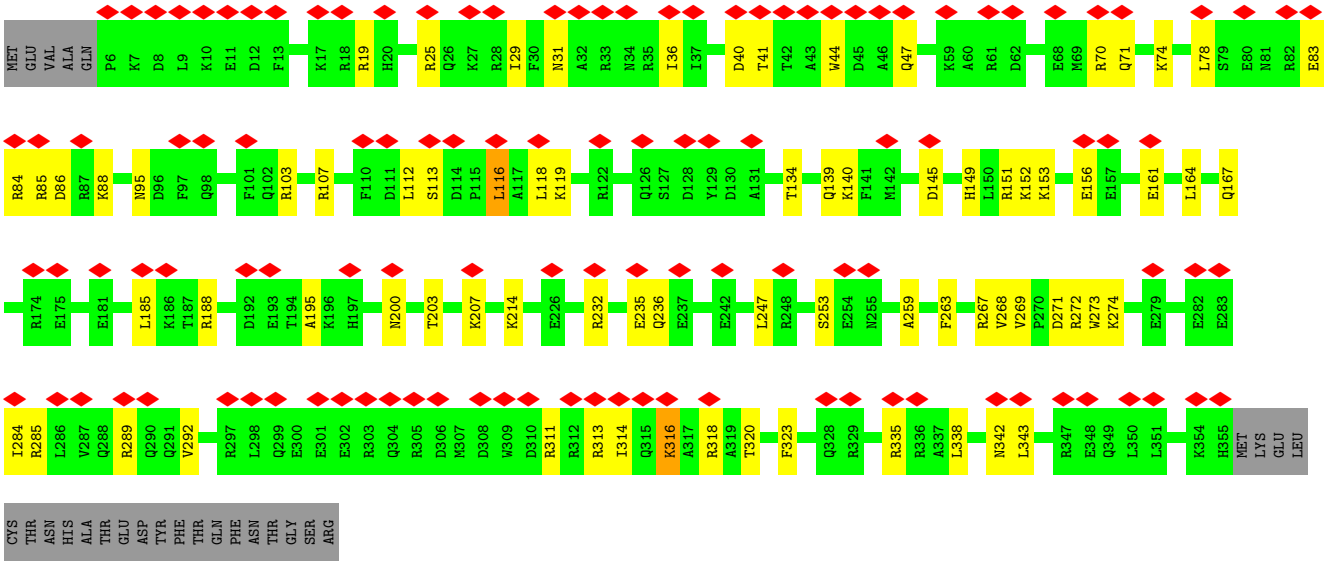
- Molecule 29: Pierce2

Chain 4Y:



- Molecule 30: RIB43A-like with coiled-coils protein 2

Chain 5A:



- Molecule 30: RIB43A-like with coiled-coils protein 2

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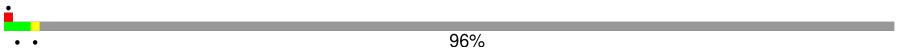
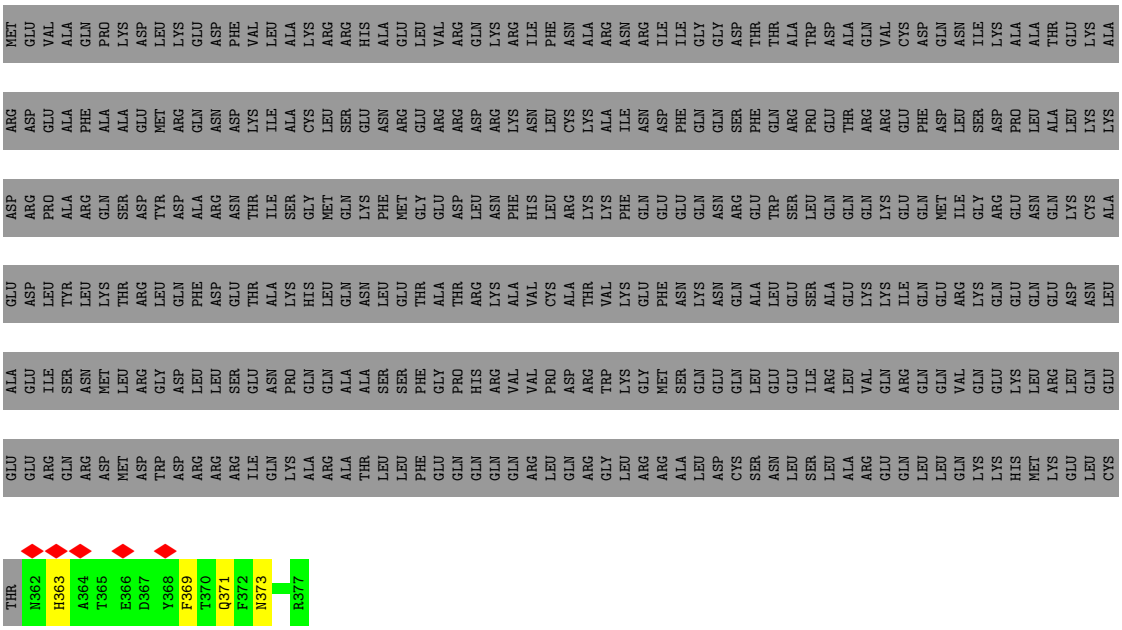
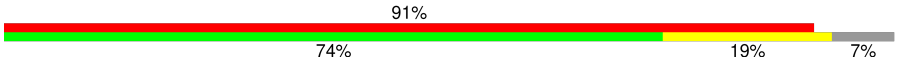
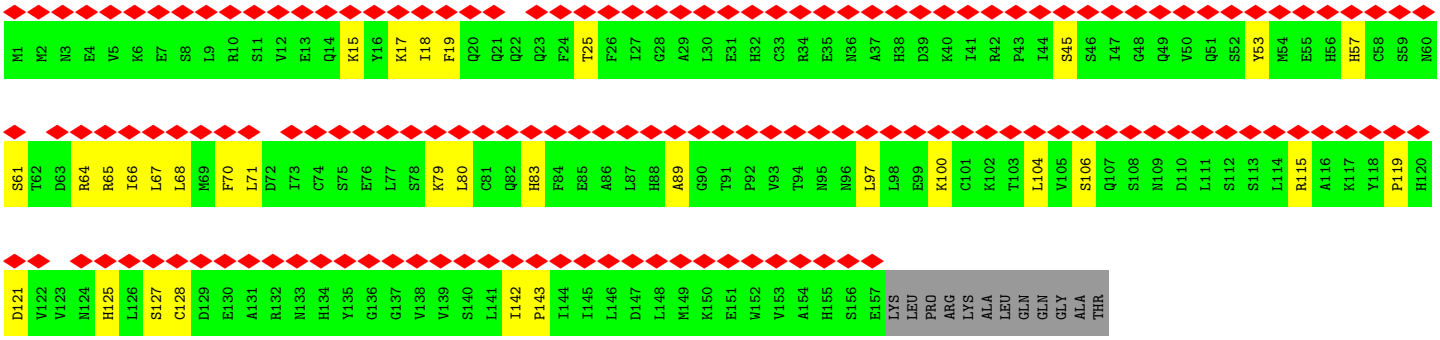




• Molecule 31: Sperm acrosome associated 9

Chain 5D:





• Molecule 31: Sperm acrosome associated 9

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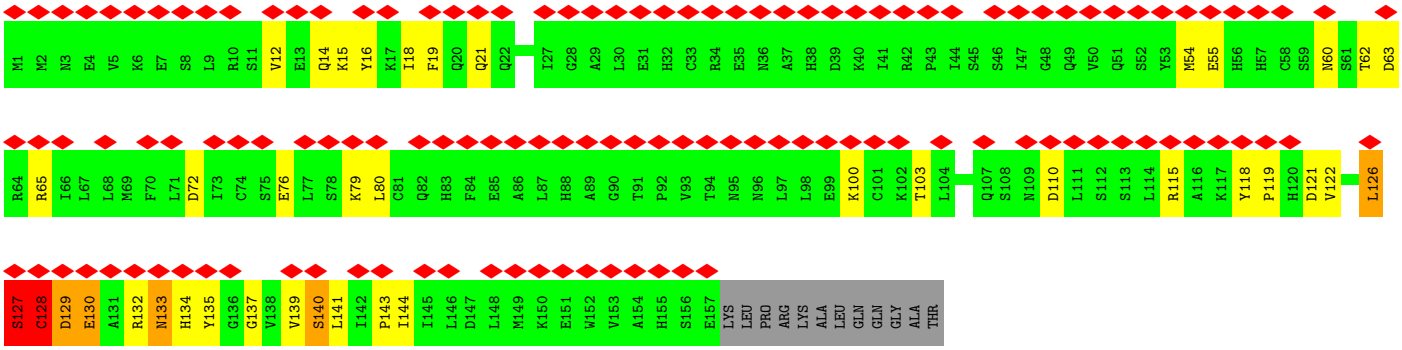

• Molecule 31: Sperm acrosome associated 9

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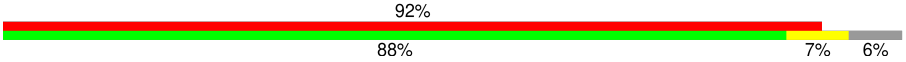
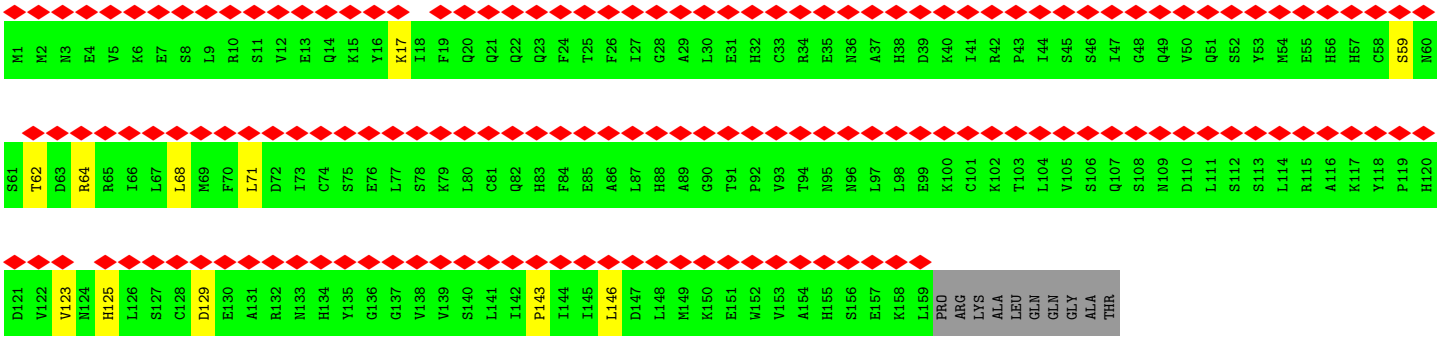
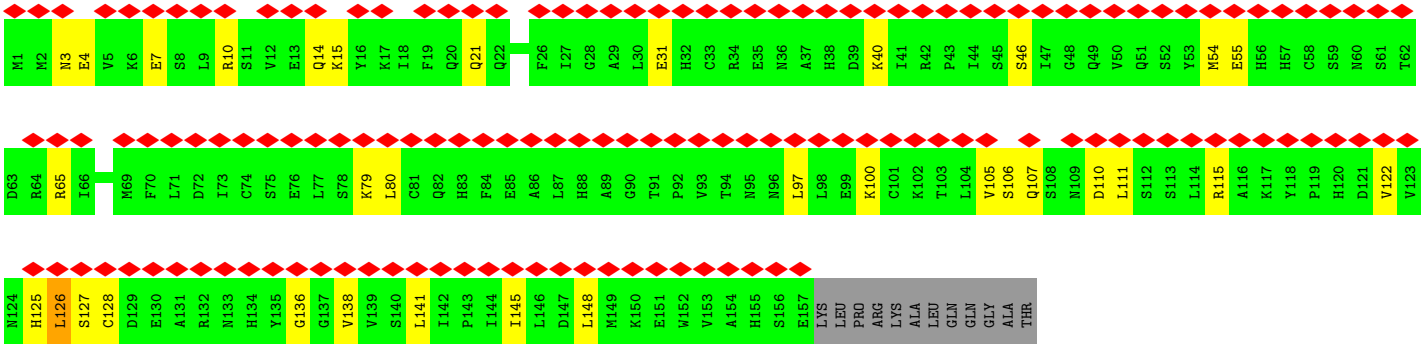




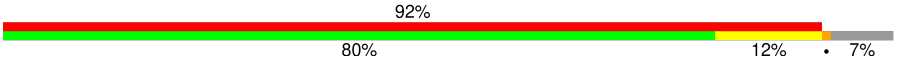
- Molecule 31: Sperm acrosome associated 9

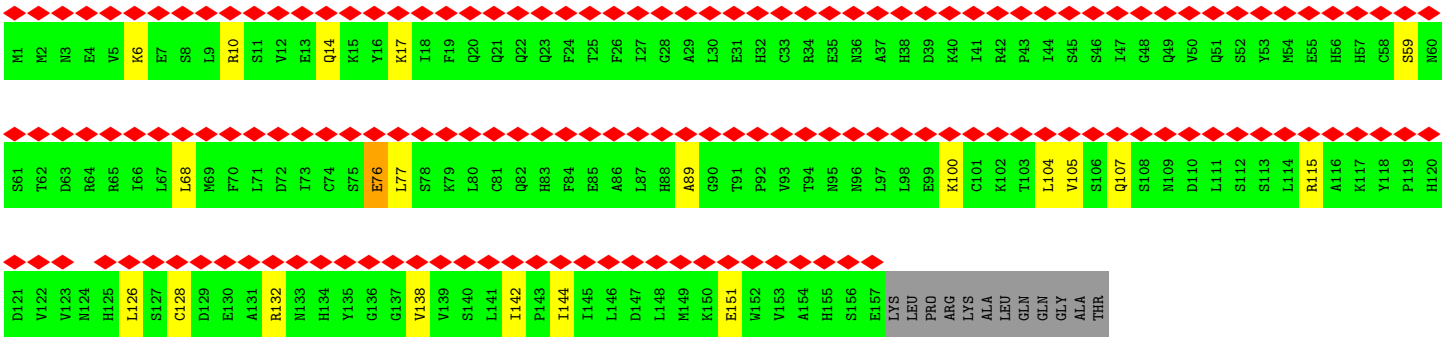
Chain 5G:



- Molecule 31: Sperm acrosome associated 9

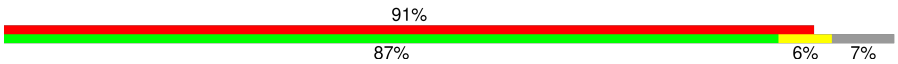
Chain 5H:

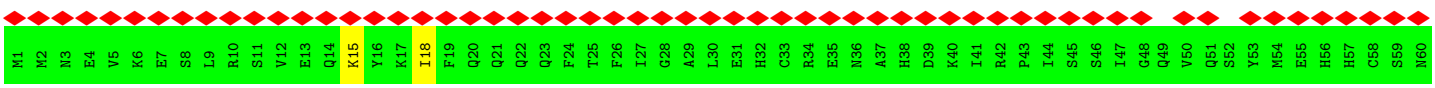


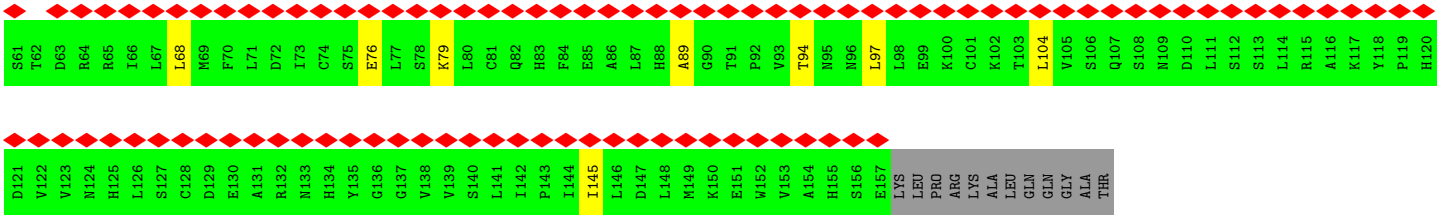


- Molecule 31: Sperm acrosome associated 9

Chain 5I:

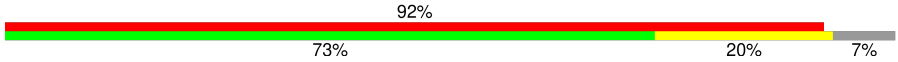


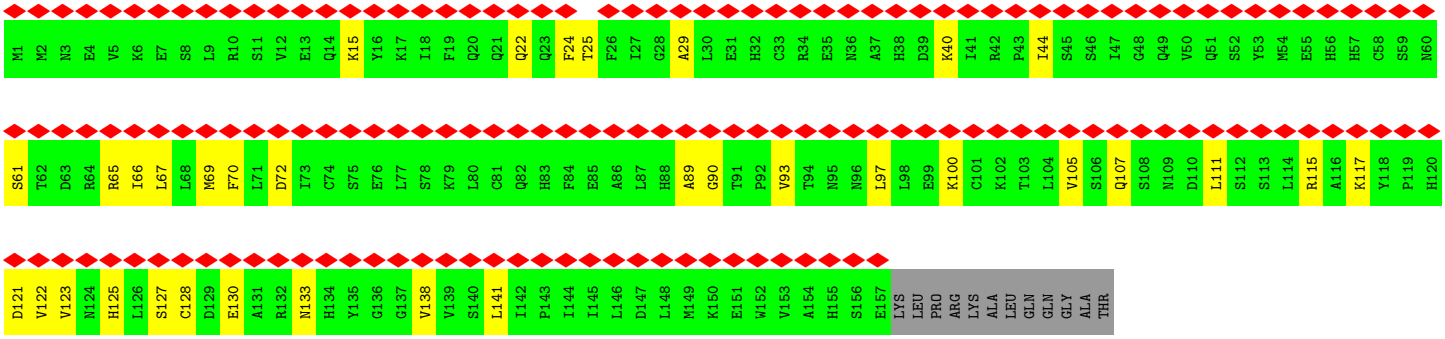




• Molecule 31: Sperm acrosome associated 9

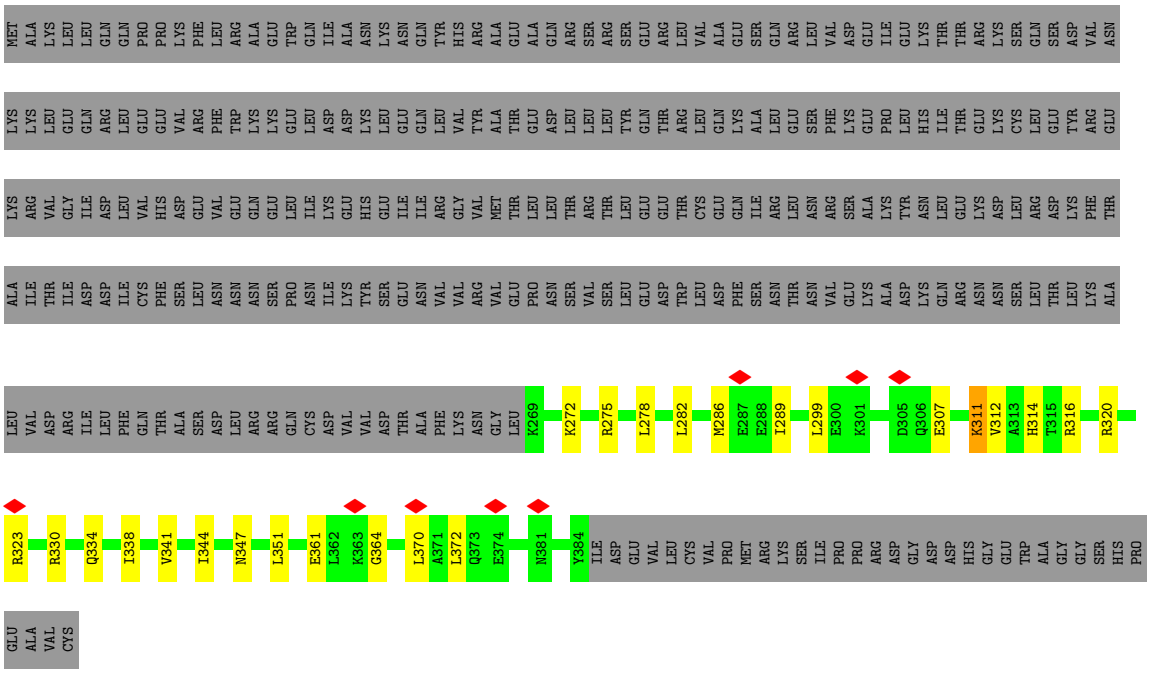
Chain 5J:





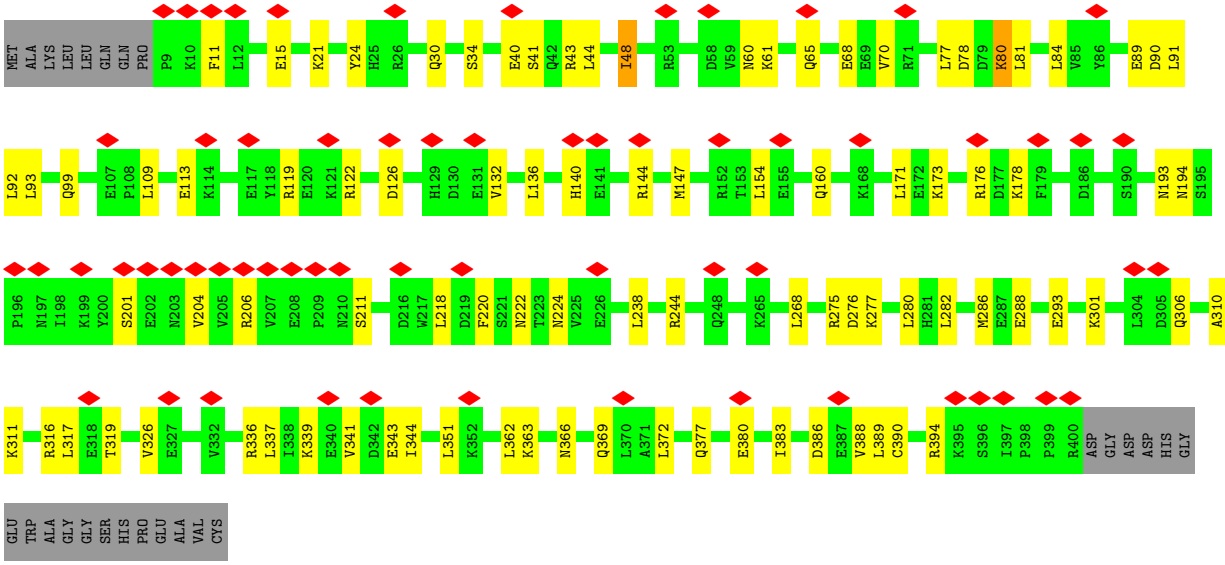
• Molecule 32: Tektin-1

Chain 5L:



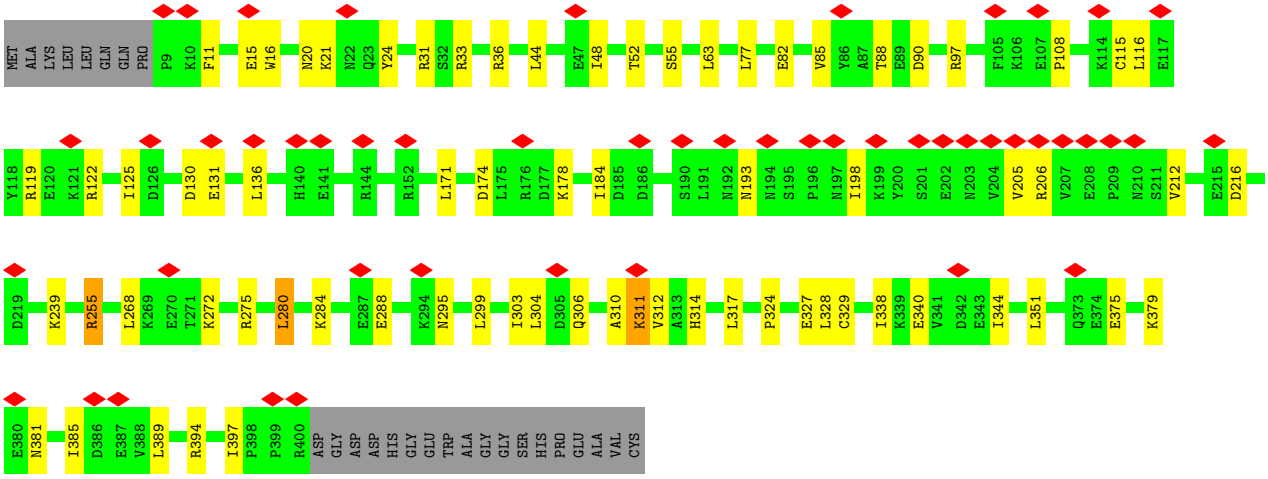
• Molecule 32: Tektin-1

Chain 5M:



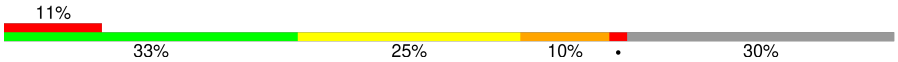
- Molecule 32: Tektin-1

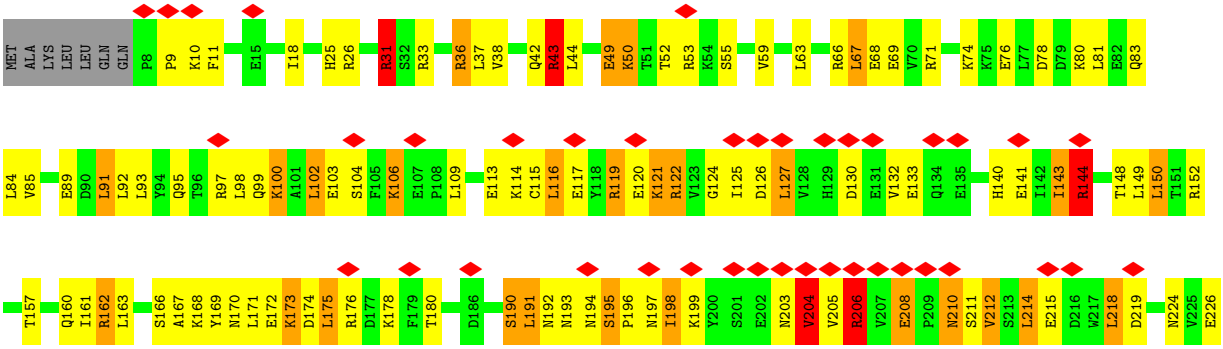
Chain 5N:

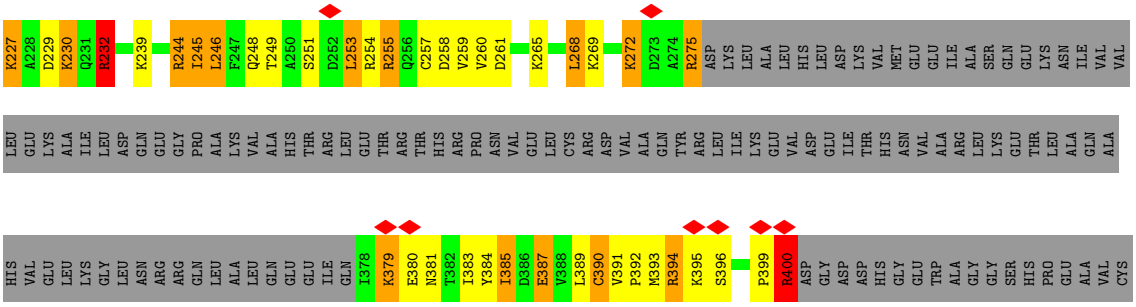


- Molecule 32: Tektin-1

Chain 5O:

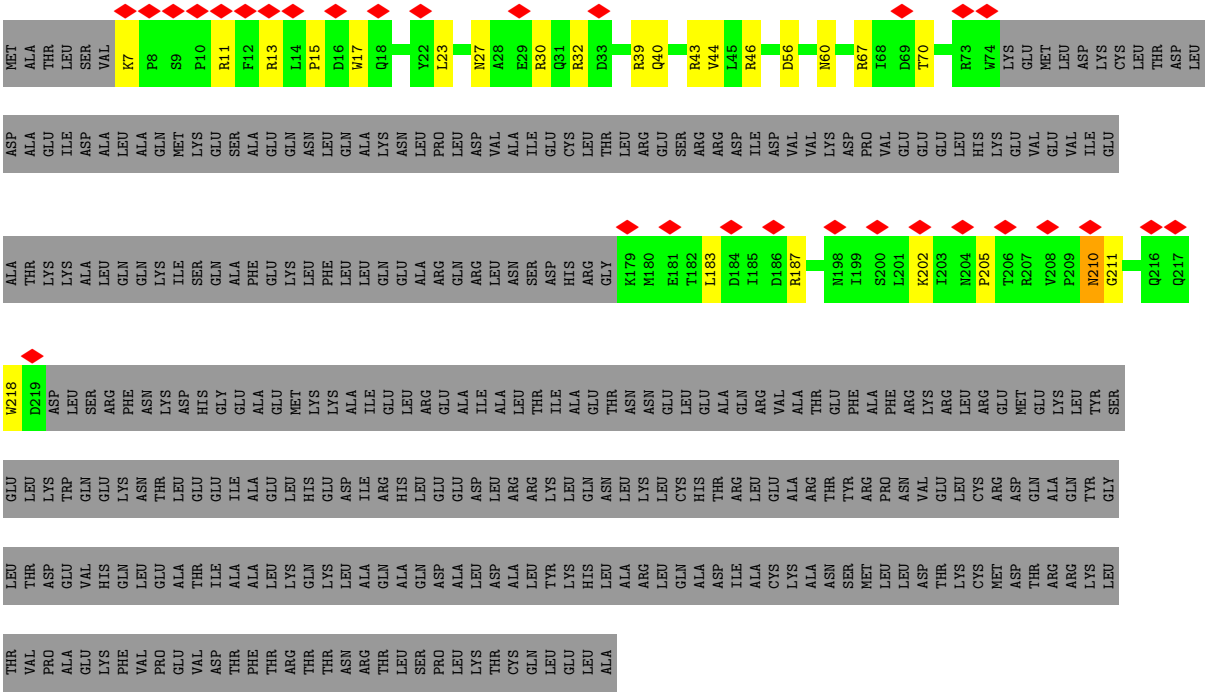






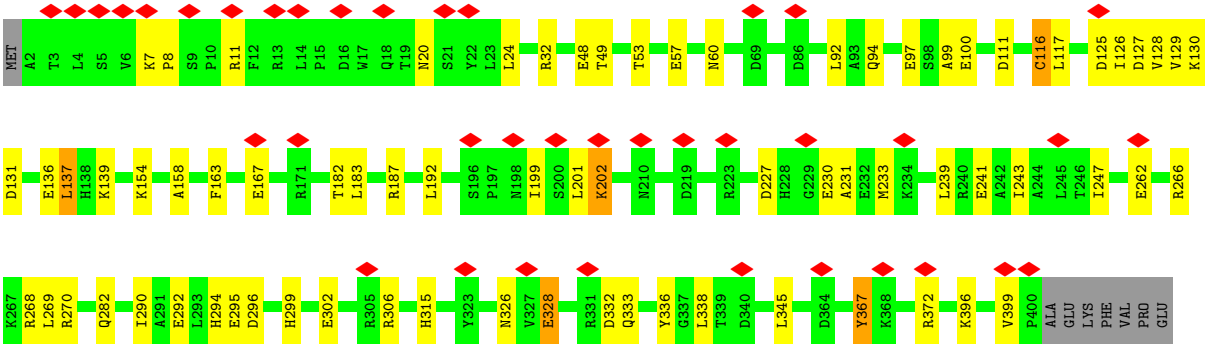
- Molecule 33: Tektin-2

Chain 5Q:



- Molecule 33: Tektin-2

Chain 5R:



VAL ASP THR PHE THR ARG THR THR ASN ARG THR LEU SER PRO LEU LYS THR CYS GLN LEU GLU LEU ALA

- Molecule 33: Tektin-2

Chain 5S:

MET A2 T3 L4 S5 V6 K7 P8 S9 P10 R11 F12 R13 L14 P15 D16 W17 Q18 T19 N20 S21 Y22 L23 L24 S25 R30 Q31 R32 D33 A34 S35 I38 R39 Q40 E41 A42 R43 V44 L45 R46 N51 I54 R61 T62 R63 L64 R67 I68 D69 S72 R73 W74 K75

E76 M77 L78 D79 K80 D86 I89 D90 A91 L92 Q104 A105 K106 R124 D125 I126 K130 K139 Q152 Q153 K154 A158 F159 E160 K161 L162 L165 A168 R169 Q170 R171 L172 D175 H176 R177 G178 K179 M180 I185 D186 R187 G188 C189 L190 S191 L192 N193 L194

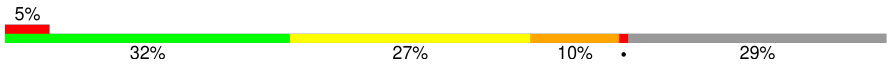
T195 S196 P197 N198 T199 S200 L201 K202 I203 N204 R207 V208 P209 N210 G211 S212 T213 S214 L215 Q216 L221 S222 R223 K226 D227 E232 M233 K234 K235 A236 I237 I243 E253 L254 R258 T261 E262 R266 K267 R268 E271 E278 Q282 L293 H294 R305

R306 K307 K312 H315 T316 R317 L318 E319 R324 P325 E328 L329 C330 R331 E341 L345 T348 Q360 L363 D364 Y367 K368 R372 S383 L386 K389 D392 L397 T398 V399 P400 ALA GLU LYS PHE VAL PRO GLU VAL ASP THR PHE THR ARG

THR THR ASN ARG THR LEU SER PRO LEU LYS THR CYS GLN LEU GLU LEU ALA

- Molecule 33: Tektin-2

Chain 5T:



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

ARG THR ARG LEU ALA GLU R67 I68 D69 T70 R73 W74 K75 D79 L82 T83 D86 A87 E88 I89 D90 A91 L92 M95 K96 E97 L103 Q104 A105 K106 M107 L108 P109 L110 D111 V112 A113 I114 L117 T118 L119 R120 E121 S122 R123 R124 D125 I126 D127 V128 V129 K130 D131

P132 V133 E134 E135 E136 L137 H138 K139 E140 V141 E142 V143 I144 E145 K148 K149 Q152 Q153 K154 I155 E160 K161 L162 F163 L164 L165 Q166 E167 A168 R169 Q170 R171 L172 N173 S174 D175 H176 R177 M180 E181 T182 L183 D184 ILE ASP ARG GLY CYS LEU SER LEU ASN LEU THR SER PRO

ASN ILE SER LEU LYS ILE ASN PRO THR ARG VAL PRO ASN GLY SER T213 S214 L215 Q216 Q217 D220 R223 E232 M233 K234 K235 A236 I237 E238 L239 R240 E241 L245 T246 I247 A248 E249 Q257 R258 T261 F265 R266 K267 R268 L269 R270 E271 K274 L275 Y276 S277 E278

L279 K280 W281 Q282 E283 K284 I290 A291 E292 E295 R298 H299 L300 E301 E302 D303 L304 R305 R306 K307 L308 L311 K312 L313 C314 H315 T316 R317 L318 E319 A320 R321 T322 Y323 R324 P325 N326 V327 E328 L329 C330 R331 L338 T339 D340 Q344 L345 I349 A350 A351 L352 K353 Q354

K355 L356 A357 Q358 A359 Q360 D361 A362 L363 D364 A365 L366 Y367 K368 R372 I377 A378 C379 S383 D387 T388 K389 C390 M391 D392 T393 R394 R395 K396 L397 T398 V399 P400 ALA GLU LYS PHE VAL PRO GLU VAL ASP THR PHE THR ARG THR THR ASN ARG THR LEU SER PRO LEU LYS

THR CYS GLN LEU GLU LEU ALA

- Molecule 33: Tektin-2

Chain 5V:

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

ARG THR ARG LEU ALA GLU ARG ILE ASP THR VAL SER R73 W74 K75 E76 M77 L78 D79 K80 C81 L82 T83 D84 L85 D86 A87 E88 I89 D90 A91 L92 A93 Q94 M95 K96 E97 S98 A99 E100 Q101 N102 L103 Q104 A105 K106 N107 L108 P109 L110 D111 V112 A113 I114 E115 C116 L117 T118 L119 R120

E121 S122 R123 R124 D125 I126 D127 V128 V129 K130 D131 P132 V133 E134 E135 E136 L137 H138 K139 E140 V141 E142 V143 I144 E145 A146 T147 K148 K149 A150 L151 Q152 Q153 K154 I155 S156 Q157 A158 F159 E160 K161 L162 F163 L164 L165 Q166 E167 A168 R169 Q170 R171 L172 N173 S174 D175 H176 R177 G178 K179 M180

GLU THR LEU ASP ILE ASP ARG GLY CYS LEU SER LEU ASN LEU THR SER PRO ASN ILE SER LEU LYS ILE ASN PRO THR ARG VAL PRO ASN GLY SER THR SER LEU GLN Q217 W218 D219 D220 L221 S222 R223 F224 N225 K226 D227 H228 G229 E230 A231 E232 M233 K234 K235 A236 I237 E238 L239 R240

E241 A242 I243 A244 L245 T246 I247 A248 E249 T250 N251 N252 E253 L254 E255 A256 Q257 R258 V259 A260 T261 E262 F263 A264 F265 R266 K267 R268 L269 R270 E271 M272 E273 K274 L275 Y276 S277 E278 L279 K280 W281 Q282 E283 K284 N285 T286 L287 E288 E289 I290 A291 E292 L293 H294 E295 D296 I297 R298 H299 L300

E301 E302 D303 L304 R305 R306 K307 L308 Q309 N310 L311 K312 L313 C314 H315 T316 R317 L318 E319 A320 R321 T322 Y323 R324 P325 N326 V327 E328 L329 C330 R331 D332 Q333 A334 Q335 Y336 G337 L338 T339 D340 E341 V342 H343 Q344 L345 E346 A347 T348 I349 A350 K353 Q354 K355 L356 A357 Q358 A359 Q360 D361

A362 L363 D364 A365 L366 Y367 K368 H369 L370 A371 R372 L373 Q374 A375 D376 I377 A378 C379 K380 A381 N382 S383 M384 L385 L386 D387 T388 K389 C390 M391 D392 T393 R394 R395 K396 L397 T398 V399 P400 A401 E402 K403 F404 V405 P406 E407 V408 D409 T410 F411 T412 R413 T414 T415 N416 ARG THR LEU SER PRO

LEU LYS THR CYS GLN LEU GLU LEU ALA

- Molecule 33: Tektin-2

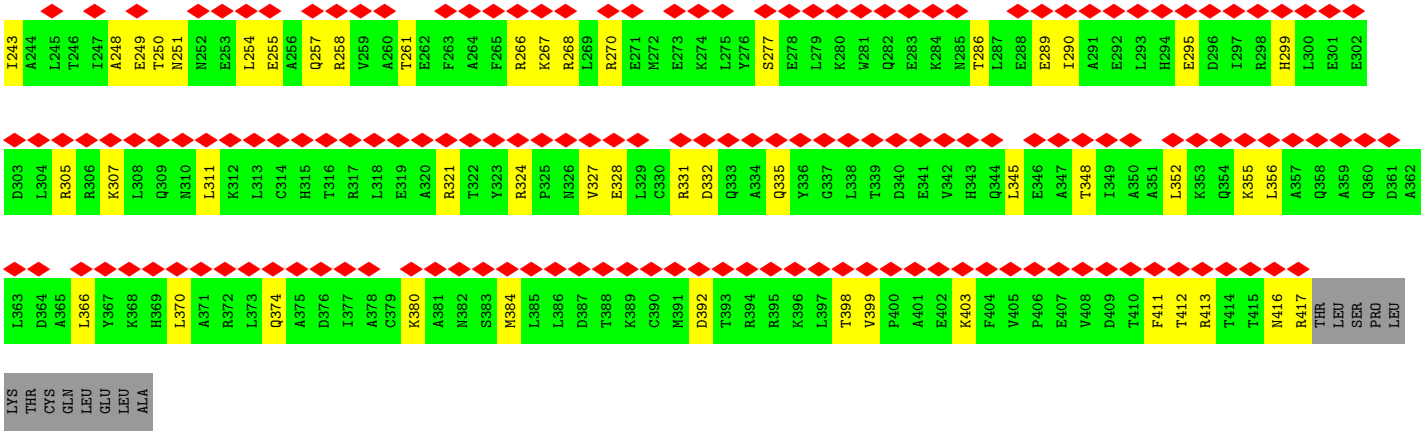
Chain 5W:

MET ALA THR LEU SER VAL LYS PRO SER P10 R11 F12 R13 L14 P15 D16 W17 Q18 T19 N20 S21 Y22 L23 L24 S25 T26 N27 A28 E29 R30 Q31 R32 D33 A34 S35 H36 Q37 I38 R39 Q40 E41 A42 R43 V44 L45 R46 N47 E48 T49 N50 N51 Q52 T53 I54 W55 D56 E57 H58 D59 N60

R61 T62 R63 L64 A65 E66 R67 I68 D69 R73 W74 K75 E76 M77 L78 D79 K80 C81 L82 T83 D84 L85 D86 A87 E88 I89 D90 A91 L92 A93 Q94 M95 K96 E97 S98 A99 E100 Q101 N102 L103 Q104 A105 K106 N107 L108 P109 L110 D111 V112 A113 I114 E115 C116 L117 T118 L119 R120 E121 S122

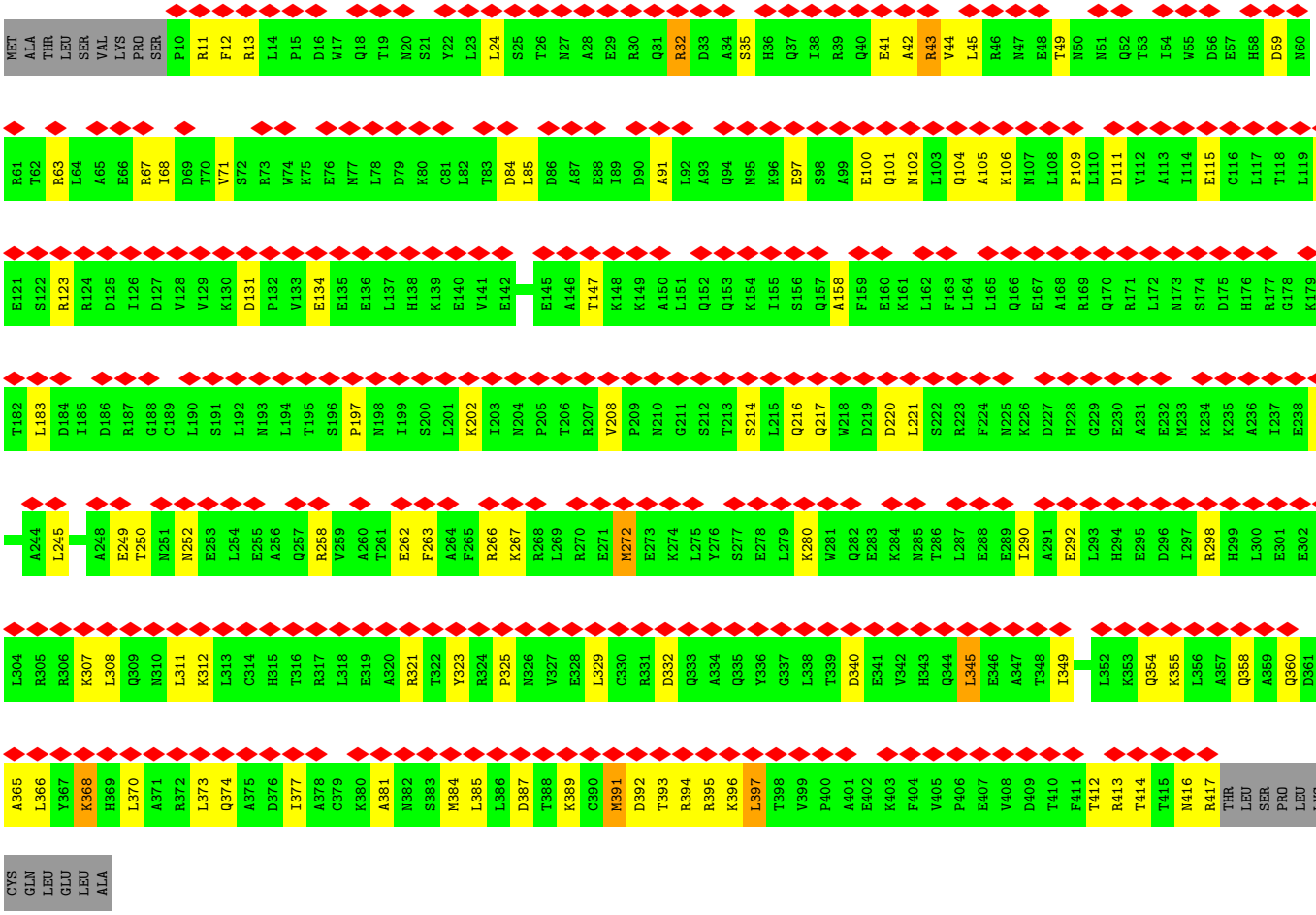
R123 R124 D125 I126 D127 V128 V129 K130 D131 P132 V133 E134 E135 E136 L137 H138 K139 E140 V141 E142 V143 I144 E145 A146 T147 K148 K149 A150 L151 Q152 Q153 K154 I155 S156 Q157 A158 F159 E160 K161 L162 F163 L164 L165 Q166 E167 A168 R169 Q170 R171 L172 N173 S174 D175 H176 R177 G178 K179 M180 E181 T182

L183 D184 I185 D186 R187 G188 C189 L190 S191 L192 N193 L194 T195 S196 P197 N198 I199 S200 L201 K202 I203 N204 P205 T206 R207 V208 P209 N210 G211 S212 T213 S214 L215 Q216 Q217 W218 D219 D220 L221 S222 R223 F224 N225 K226 D227 H228 G229 E230 A231 E232 M233 K234 K235 A236 I237 E238 L239 R240 E241 A242



- Molecule 33: Tektin-2

Chain 5X:



- Molecule 33: Tektin-2

Chain 5Y:

MET ALA THR LEU SER VAL LYS PRO SER P10 R11 F12 R13 L14 P15 D16 W17 Q18 T19 N20 S21 Y22 L23 L24 S25 T26 N27 A28 E29 R30 Q31 R32 D33 A34 S35 H36 Q37 I38 R39 Q40 E41 A42 R43 V44 L45 R46 N47 E48 T49 N50 N51 Q52 T53 I54 W55 D56 E57 H58 D59 N60

R61 T62 R63 E66 R67 I68 D69 T70 V71 S72 R73 W74 LYS GLU MET LEU ASP LYS CYS LEU THR ASP LEU ASP ALA GLU ILE ASP ALA LEU ALA GLN MET LYS GLU SER ALA GLU GLN ASN LEU GLN ALA LYS ASN LEU PRO LEU ASP VAL ALA ILE GLU CYS LEU THR LEU ARG GLU

SER ARG ARG ASP ILE ASP VAL VAL LYS ASP PRO VAL GLU GLU GLU LEU HIS LYS GLU VAL GLU VAL ILE GLU ALA THR LYS LYS ALA LEU GLN GLN LYS ILE SER GLN ALA PHE GLU LYS LEU PHE LEU LEU GLN GLU ALA ARG GLN ARG LEU ASN SER ASP HIS ARG G178 K179 M180 E181

T182 L183 D184 I185 D186 R187 G188 C189 L190 S191 L192 N193 L194 T195 S196 P197 N198 I199 S200 L201 K202 I203 N204 P205 T206 R207 V208 P209 N210 G211 S212 T213 S214 L215 Q216 Q217 W218 D219 ASP LEU SER ARG PHE ASN LYS ASP HIS GLY GLU ALA GLU MET LYS LYS ALA ILE GLU LEU ARG GLU

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

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

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

LEU LYS THR CYS GLN LEU GLU LEU ALA

- Molecule 34: Tektin-3

Chain 6A: 38% 20% 25% 9% 44%

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

ASN TRP PRO THR LEU ASP PRO TYR CYS THR ARG SER GLN ARG VAL SER GLU SER THR MET LEU PRO PHE VAL SER ASN ARG THR THR LEU PHE THR R93 Y94 T95 P96 D97 D98 W99 Y100 R101 S102 N103 L104 T105 N106 F107 Q108 E109 S110 N111 T112 S113 R114 H115 N116 S117 E118 R119 L120

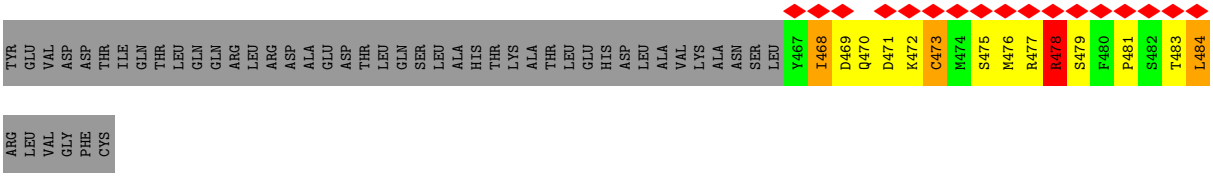
R121 V122 D123 T124 S125 R126 L127 I128 Q129 D130 K131 Y132 Q133 Q134 T135 R136 K137 T138 Q139 A140 D141 S142 T143 Q144 N145 L146 G147 E148 R149 V150 N151 D152 I153 G154 F155 W156 K157 S158 E159 I160 I161 H162 E163 L164 D165 A166 M167 I168 G169 E170 T171 N172 E173 L174 T175 D176 I177 K178 K179 R180

L181 E182 R183 A184 L185 M186 E187 T188 E189 A190 P191 L192 Q193 V194 A195 R196 E197 C198 L199 F200 H201 R202 E203 K204 R205 MET GLY ILE ASP L210 V211 H212 D213 E214 V215 E216 K217 E218 L219 L220 T221 E222 V223 D224 T225 I226 L227 C228 C229 Q230 E231 R232 M233 K234 L235 Y236 L237 D238 K239 A240

I241 A242 Q243 L244 A245 R248 A249 A250 Q251 H252 E253 L254 E255 K256 D257 L258 S259 D260 K261 Q262 S263 A264 Y265 R266 I267 D268 D269 K270 C271 H272 H273 L274 R275 N276 T277 S278 D279 G280 V281 S282 Y283 F284 H285 G286 V287 E288 R289 V290 D291 A292 T293 V294 S295 V296 P297 E298 S299 W300 A301

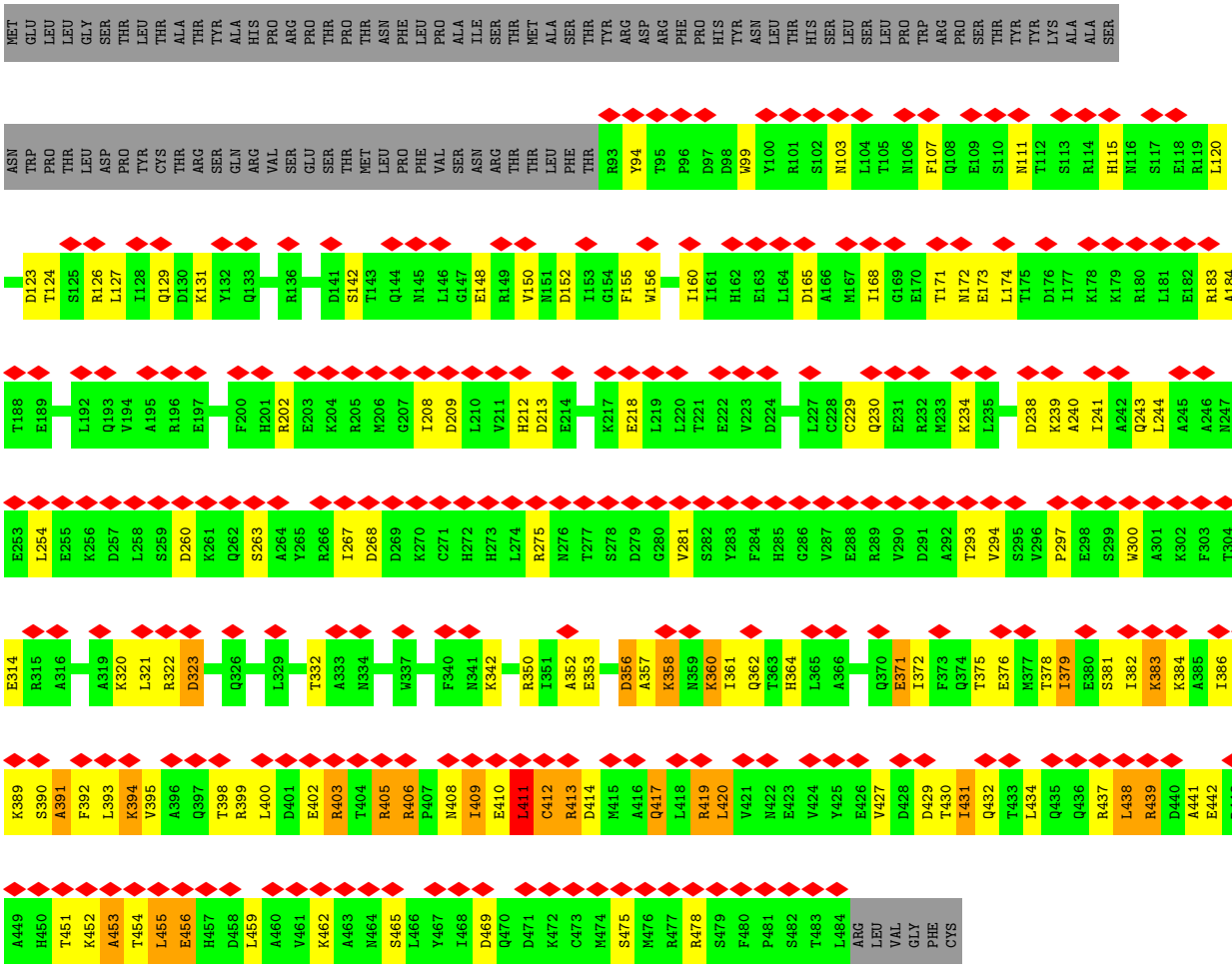
K302 F303 T304 D305 D306 N307 I308 L309 R310 S311 Q312 S313 E314 R315 A316 A319 K320 L321 R322 D323 D324 I325 Q326 N327 V328 L329 V330 V331 T332 A333 M336 W337 N338 Q339 F340 N341 K342 V343 N344 L345 T348 N349 R350 I351 ALA GLU THR ALA ASP ALA LYS ASN LYS ILE GLN THR HIS

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



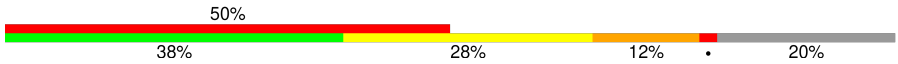
- Molecule 34: Tektin-3

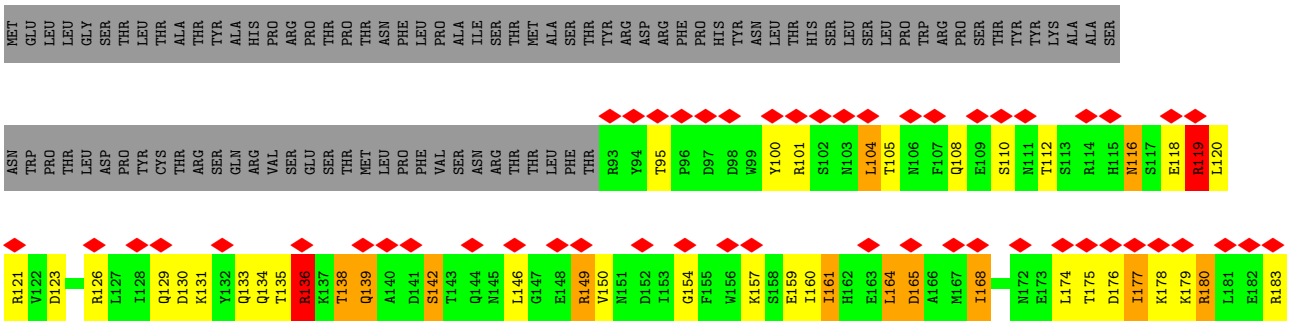
Chain 6B:

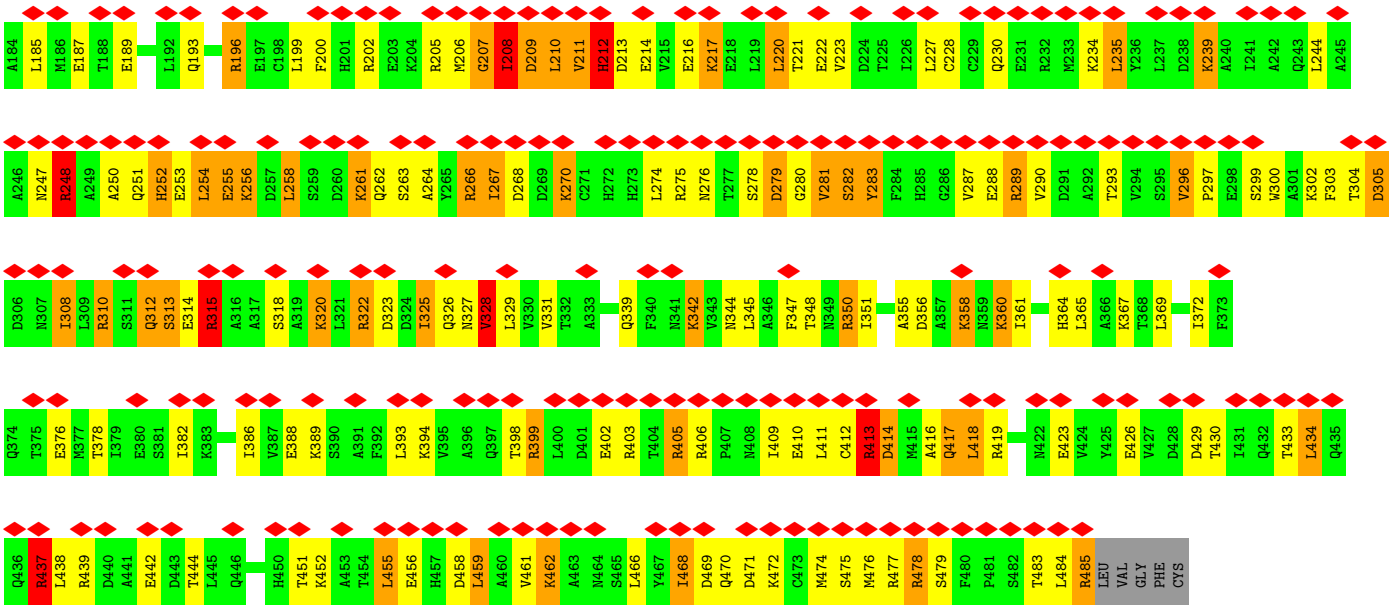


- Molecule 34: Tektin-3

Chain 6C:

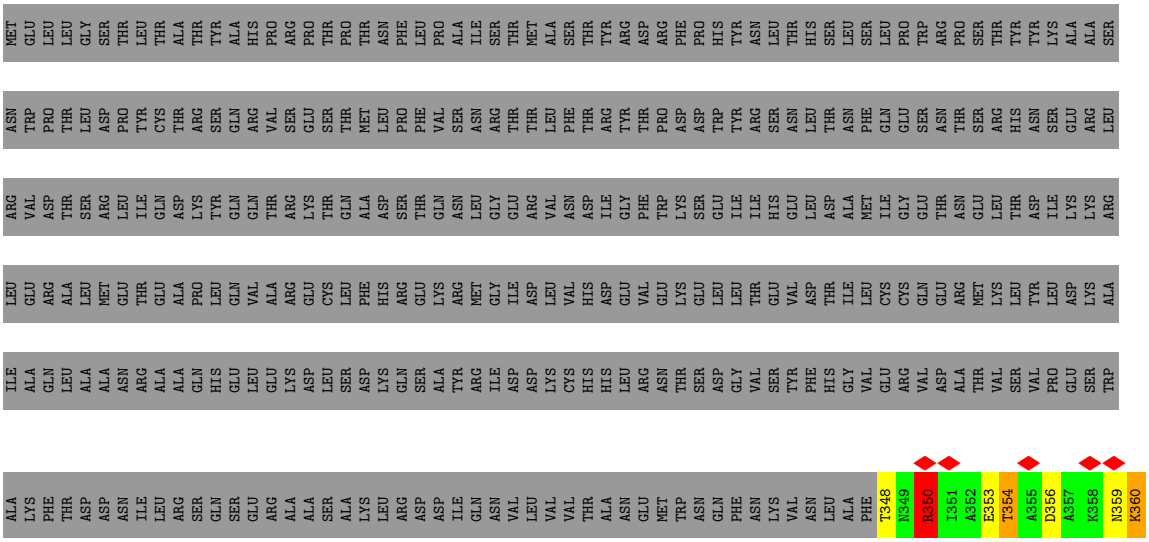






- Molecule 34: Tektin-3

Chain 6D:



- Molecule 34: Tektin-3

Chain 6E:

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

ASN TRP PRO THR LEU ASP PRO PRO TYR CYS THR ARG SER GLN ARG VAL SER GLU SER THR MET LEU PRO PHE VAL SER ASN LEU ARG THR THR LEU PHE THR ARG TYR THR PRO ASP ASP TRP TYR ARG SER ASN LEU THR ASN PHE GLN GLU SER ASN THR SER ARG HIS ASN SER GLU ARG LEU

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

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

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

ALA LYS PHE THR ASP ASN ILE LEU ARG SER GLN SER GLU ARG ALA ALA SER ALA LYS LEU ARG ASP ASP ILE GLN ASN VAL LEU VAL VAL THR ALA ASN GLU MET TRP ASN GLN PHE ASN LYS VAL ASN LEU ALA PHE THR ASN ARG ILE ALA GLU THR ALA ASP ALA LYS ASN LYS

ILE GLN THR HIS LEU ALA LYS THR LEU GLN GLU ILE PHE GLN THR GLU MET THR ILE E380 S381 I382 K383 K384 A385 I386 V387 E388 K389 S390 A391 F392 L393 K394 V395 A396 Q397 T398 R399 L400 D401 E402 R403 T404 R405 R406 P407 N408 I409 E410 L411 C412 R413 D414 M415 A416 Q417 L418 R419 L420

V421 N422 E423 V424 Y425 E426 V427 D428 D429 T430 I431 Q432 T433 L434 Q435 Q436 R437 L438 ARG ASP ALA GLU ASP THR LEU GLN SER LEU ALA HIS THR LYS ALA THR LEU GLU HIS ASP LEU ALA VAL LYS ALA ASN SER LEU TYR ILE ASP GLN ASP LYS CYS MET SER MET ARG ARG SER PHE

PRO SER THR LEU ARG LEU VAL GLY PHE CYS

- Molecule 34: Tektin-3

Chain 6F:

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

ASN TRP PRO THR LEU ASP PRO PRO TYR CYS THR ARG SER GLN ARG VAL SER GLU SER THR MET LEU PRO PHE VAL SER ASN LEU ARG THR THR LEU PHE THR ARG TYR THR PRO ASP ASP TRP TYR ARG SER ASN LEU THR ASN PHE GLN GLU SER ASN THR SER ARG HIS ASN SER GLU ARG LEU

ARG VAL ASP T124 S125 R126 L127 I128 Q129 D130 K131 Y132 Q133 Q134 T135 R136 K137 T138 Q139 A140 D141 S142 T143 Q144 N145 L146 G147 E148 R149 V150 N151 D152 I153 G154 F155 W156 K157 S158 E159 I160 I161 H162 E163 L164 D165 A166 M167 I168 G169 E170 T171 N172 E173 L174 T175 D176 I177 K178 K179 R180

L181 E182 R183 A184 L185 M186 E187 T188 E189 A190 P191 L192 Q193 V194 A195 R196 E197 C198 L199 F200 H201 R202 E203 K204 R205 M206 G207 I208 D209 L210 V211 H212 D213 E214 V215 E216 K217 E218 L219 L220 T221 E222 V223 D224 T225 I226 L227 C228 C229 Q230 E231 R232 M233 K234 L235 Y236 L237 D238 K239 A240

I241 A242 Q243 L244 A245 A246 N247 R248 A249 A250 Q251 H252 E253 L254 E255 K256 D257 L258 S259 D260 K261 Q262 S263 A264 Y265 R266 I267 D268 D269 K270 C271 H272 H273 L274 R275 N276 T277 S278 D279 G280 V281 S282 Y283 F284 H285 G286 V287 E288 R289 V290 D291 A292 T293 V294 S295 V296 P297 E298 S299 W300

A301 K302 F303 T304 D305 D306 N307 I308 L309 R310 S311 Q312 S313 E314 R315 A316 A317 S318 A319 K320 L321 R322 D323 D324 I325 Q326 N327 V328 L329 V330 V331 T332 A333 N334 E335 M336 W337 N338 Q339 F340 N341 K342 V343 N344 L345 A346 F347 T348 N349 R350 I351 A352 E353 T354 A355 D356 A357 K358 N359 K360

I361 Q362 T363 H364 L365 A366 K367 T368 L369 Q370 E371 I372 F373 Q374 T375 E376 M377 T378 I379 E380 S381 I382 K383 K384 A385 I386 V387 E388 K389 S390 A391 F392 L393 K394 V395 A396 Q397 T398 R399 L400 D401 E402 R403 T404 R405 R406 P407 N408 I409 E410 L411 C412 R413 D414 M415 A416 Q417 L418 R419 L420

V421 N422 E423 V424 Y425 E426 V427 D428 D429 T430 I431 Q432 T433 L434 Q435 Q436 R437 L438 R439 D440 A441 E442 D443 T444 L445 Q446 S447 L448 A449 H450 T451 K452 A453 T454 L455 E456 H457 D458 L459 A460 V461 K462 A463 N464 S465 L466 Y467 I468 D469 Q470 D471 K472 C473 M474 S475 M476 R477 R478 S479 F480

P481 SER THR LEU ARG LEU VAL GLY PHE CYS

- Molecule 34: Tektin-3

Chain 6G: 82% 68% 17% 15%

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

ASN TRP PRO THR LEU D66 P67 Y68 C69 T70 R71 S72 Q73 R74 V75 S76 E77 S78 T79 M80 L81 P82 F83 V84 S85 N86 R87 T88 T89 L90 F91 T92 R93 Y94 T95 P96 D97 D98 W99 Y100 R101 S102 N103 L104 T105 N106 F107 Q108 E109 S110 N111 T112 S113 R114 H115 N116 S117 E118 R119 L120

R121 V122 D123 T124 S125 R126 L127 I128 Q129 D130 K131 Y132 Q133 Q134 T135 R136 K137 T138 Q139 A140 D141 S142 T143 Q144 N145 L146 G147 E148 R149 V150 N151 D152 I153 G154 F155 W156 K157 S158 E159 I160 I161 H162 E163 L164 D165 A166 M167 I168 G169 E170 T171 N172 E173 L174 T175 D176 I177 K178 K179 R180

L181 E182 R183 A184 L185 M186 E187 T188 E189 A190 P191 L192 Q193 V194 A195 R196 E197 C198 L199 F200 H201 R202 E203 K204 R205 M206 G207 I208 D209 L210 V211 H212 D213 E214 V215 E216 K217 E218 L219 L220 T221 E222 V223 D224 T225 I226 L227 C228 C229 Q230 E231 R232 M233 K234 L235 Y236 L237 D238 K239 A240

I241 A242 Q243 L244 A245 A246 N247 R248 A249 A250 Q251 H252 E253 L254 E255 K256 D257 L258 S259 D260 K261 Q262 S263 A264 Y265 R266 I267 D268 D269 K270 C271 H272 H273 L274 R275 N276 T277 S278 D279 G280 V281 S282 Y283 F284 H285 G286 V287 E288 R289 V290 D291 A292 T293 V294 S295 V296 P297 E298 S299 W300

A301 K302 F303 T304 D305 D306 N307 I308 L309 R310 S311 Q312 S313 E314 R315 A316 A317 S318 A319 K320 L321 R322 D323 D324 I325 Q326 N327 V328 L329 V330 V331 T332 A333 N334 E335 M336 W337 N338 Q339 F340 N341 K342 V343 N344 L345 A346 F347 T348 N349 R350 I351 A352 E353 T354 A355 D356 N359 K360 I361

Q362 T363 H364 L365 A366 K367 T368 L369 Q370 E371 I372 F373 Q374 T375 E376 M377 T378 I379 E380 S381 I382 K383 K384 A385 I386 V387 E388 K389 S390 A391 F392 L393 K394 V395 A396 Q397 T398 R399 L400 D401 E402 R403 T404 R405 R406 P407 N408 I409 E410 L411 C412 R413 D414 M415 A416 Q417 L418 R419 L420 V421

N422 E423 V424 Y425 E426 V427 D428 D429 T430 I431 Q432 T433 L434 Q435 Q436 R437 L438 R439 D440 A441 E442 D443 T444 L445 Q446 S447 L448 A449 H450 T451 K452 A453 T454 L455 E456 H457 D458 L459 A460 V461 K462 A463 N464 S465 L466 Y467 I468 D469 Q470 D471 K472 C473 M474 S475 M476 R477 R478 S479 F480 P481

SER THR LEU ARG LEU VAL GLY PHE CYS

- Molecule 34: Tektin-3

Chain 6H: 74% 58% 16% • 25%

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

ASN TRP PRO THR LEU ASP P67 Y68 C69 T70 R71 S72 Q73 R74 V75 S76 E77 S78 T79 M80 L81 P82 F83 V84 S85 N86 R87 T88 T89 L90 F91 T92 R93 Y94 T95 P96 D97 D98 W99 Y100 R101 S102 N103 L104 T105 N106 F107 Q108 E109 S110 N111 T112 S113 R114 H115 N116 S117 E118 R119 L120

R121 V122 D123 T124 S125 R126 L127 I128 Q129 D130 K131 Y132 Q133 Q134 T135 R136 K137 T138 Q139 A140 D141 S142 T143 Q144 N145 L146 G147 E148 R149 V150 N151 D152 I153 G154 F155 W156 K157 S158 E159 I160 I161 H162 E163 L164 D165 A166 M167 I168 G169 E170 T171 N172 E173 L174 T175 D176 I177 K178 K179 R180

L181 E182 R183 A184 L185 M186 E187 T188 E189 A190 P191 L192 Q193 V194 A195 R196 E197 C198 L199 F200 H201 R202 E203 K204 R205 M206 G207 I208 D209 L210 V211 H212 D213 E214 V215 E216 K217 E218 L219 L220 T221 E222 V223 D224 T225 I226 L227 C228 C229 Q230 E231 R232 M233 K234 L235 Y236 L237 D238 K239 A240

I241 A242 Q243 L244 A245 A246 N247 R248 A249 A250 Q251 H252 E253 L254 E255 K256 D257 L258 S259 D260 K261 Q262 S263 A264 Y265 R266 I267 D268 D269 K270 C271 H272 H273 L274 R275 N276 T277 S278 D279 G280 V281 S282 Y283 F284 H285 G286 V287 E288 R289 V290 D291 A292 T293 V294 S295 V296 P297 E298 S299 W300

A301 K302 F303 T304 D305 D306 N307 I308 L309 R310 S311 Q312 S313 E314 R315 A316 A317 S318 A319 K320 L321 R322 D323 D324 I325 Q326 N327 V328 L329 V330 V331 T332 A333 N334 E335 M336 W337 N338 Q339 F340 N341 K342 V343 N344 L345 A346 F347 T348 N349 R350 I351 A352 E353 T354 A355 D356 A357 K358 N359 K360

I361 Q362 T363 H364 L365 A366 K367 T368 L369 Q370 E371 I372 F373 Q374 T375 E376 M377 T378 I379 E380 S381 I382 K383 K384 A385 ILE VAL GLU LYS SER ALA PHE LEU LYS VAL ALA GLN THR ARG LEU ASP GLU ARG THR ARG ARG PRO ASN ILE GLU LEU CYS ARG ASP MET ALA GLN LEU ARG LEU

VAL ASN GLU VAL TYR GLU VAL ASP ASP THR ILE GLN T433 L434 Q435 Q436 R437 L438 R439 D440 A441 E442 D443 T444 L445 Q446 S447 L448 A449 H450 T451 K452 A453 T454 L455 E456 H457 D458 L459 A460 V461 K462 A463 N464 S465 L466 Y467 I468 D469 Q470 D471 K472 C473 M474 S475 M476 R477 R478 S479 F480

P481 SER THR LEU ARG LEU VAL GLY PHE CYS

- Molecule 34: Tektin-3

Chain 6I: 13% 12% 87%

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

ASN TRP PRO THR LEU ASP P67 Y68 C69 T70 R71 S72 Q73 R74 V75 S76 E77 S78 T79 M80 L81 P82 F83 V84 S85 N86 R87 T88 T89 L90 F91 T92 R93 Y94 T95 P96 D97 D98 W99 Y100 R101 S102 N103 L104 T105 N106 F107 Q108 E109 S110 N111 T112 S113 R114 H115 N116 S117 E118 R119 L120

R121 V122 D123 T124 S125 R126 L127 I128 Q129 ASP LYS TYR GLN GLN GLN THR ARG LYS THR GLN ALA ASP SER THR GLN ASN LEU GLY GLU ARG VAL ASN ASP ILE GLY PHE TRP LYS SER GLU ILE ILE HIS GLU LEU ASP ALA MET ILE GLY GLU THR ASN GLU LEU THR ASP ILE LYS LYS ARG

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

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

ALA LYS PHE THR ASP ASP ASN ILE LEU ARG SER GLN SER GLU ARG ALA ALA SER ALA LYS LEU ARG ASP ASP ILE GLN ASN VAL LEU VAL VAL THR ALA ASN GLU MET TRP ASN GLN PHE ASN LYS VAL ASN LEU ALA PHE THR ASN ARG ILE ALA GLU THR ASP ALA LYS ASN LYS

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

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

PRO SER THR LEU ARG LEU VAL GLY PHE CYS

- Molecule 34: Tektin-3

Chain 6J:

MET GLU LEU LEU GLY SER THR LEU THR ALA THR TYR ALA HIS PRO ARG PRO THR PRO THR ASN PHE LEU PRO ALA ILE SER THR MET ALA SER THR TYR ARG ASP ARG PHE PRO HIS TYR ASN LEU THR H44 S45 L46 S47 L48 P49 W50 R51 P52 S53 T54 Y55 Y56 K57 A58 A59 S60

N61 W62 P63 T64 L65 D66 P67 Y68 G69 T70 ARG SER GLN ARG VAL SER GLU SER THR MET LEU PRO PHE VAL SER ASN ARG THR THR LEU F91 T92 R93 Y94 T95 P96 D97 D98 W99 Y100 R101 S102 N103 L104 T105 N106 F107 Q108 E109 S110 N111 T112 S113 R114 H115 N116 S117 E118 R119 L120

R121 V122 D123 T124 S125 R126 L127 I128 GLN ASP LYS TYR GLN GLN THR ARG LYS THR GLN ALA ASP SER THR GLN ASN LEU GLY GLU ARG VAL ASN ASP ILE GLY PHE TRP LYS SER GLU ILE ILE HIS GLU LEU ASP ALA MET ILE GLY GLU THR ASN GLU LEU THR ASP ILE LYS LYS ARG

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

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

ALA LYS PHE THR ASP ASP ASN ILE LEU ARG SER GLN SER GLU ARG ALA ALA SER ALA LYS LEU ARG ASP ASP ILE GLN ASN VAL LEU VAL VAL THR ALA ASN GLU MET TRP ASN GLN PHE ASN LYS VAL ASN LEU ALA PHE THR ASN ARG ILE ALA GLU THR ALA ASP ALA LYS ASN LYS

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

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

PRO SER THR LEU ARG LEU VAL GLY PHE CYS

- Molecule 34: Tektin-3

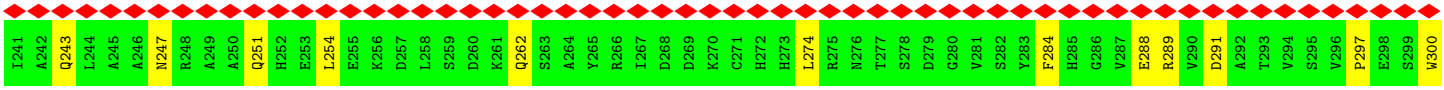
Chain 6K:

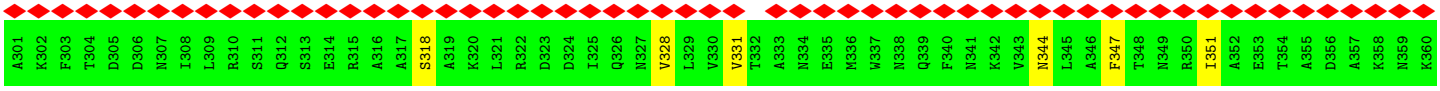
MET GLU LEU LEU GLY SER THR LEU THR ALA THR TYR ALA HIS PRO ARG PRO THR PRO THR ASN PHE LEU PRO ALA ILE SER THR MET ALA SER THR TYR ARG ASP ARG PHE PRO HIS TYR ASN LEU T43 H44 S45 L46 S47 L48 P49 W50 R51 P52 S53 T54 Y55 Y56 K57 A58 A59 S60

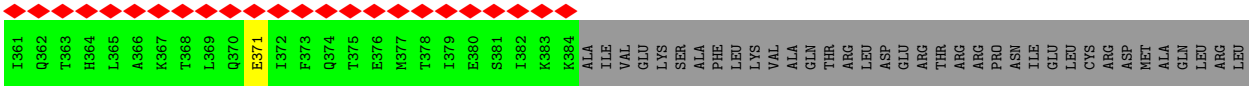
N61 W62 P63 T64 L65 D66 P67 Y68 C69 T70 ARG SER GLN ARG VAL SER GLU SER THR MET LEU PRO PHE VAL SER ASN ARG THR THR LEU F91 T92 R93 Y94 T95 P96 D97 D98 W99 Y100 R101 S102 N103 L104 T105 N106 F107 Q108 E109 S110 N111 T112 S113 R114 H115 N116 S117 E118 R119 L120

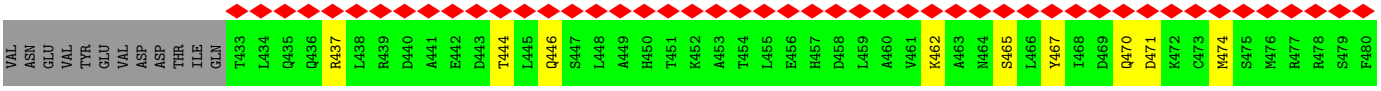
R121 V122 D123 T124 S125 R126 L127 I128 Q129 D130 K131 Y132 Q133 Q134 T135 R136 K137 T138 Q139 A140 D141 S142 T143 Q144 N145 L146 G147 E148 R149 V150 N151 D152 I153 G154 F155 W156 K157 S158 E159 I160 I161 H162 E163 L164 D165 A166 M167 I168 G169 E170 T171 N172 E173 L174 T175 D176 I177 K178 K179 R180

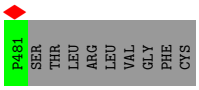
L181 E182 R183 A184 L185 M186 E187 T188 E189 A190 P191 L192 Q193 V194 A195 R196 E197 C198 L199 F200 H201 R202 E203 K204 R205 M206 G207 I208 D209 L210 V211 H212 D213 E214 V215 E216 K217 E218 L219 L220 T221 E222 V223 D224 T225 I226 L227 C228 C229 Q230 E231 R232 M233 K234 L235 Y236 L237 D238 K239 A240





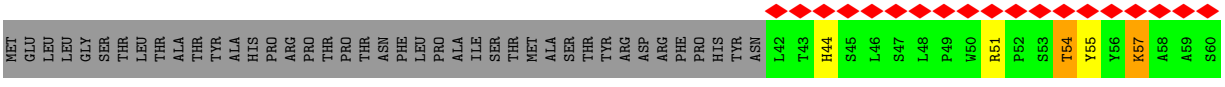


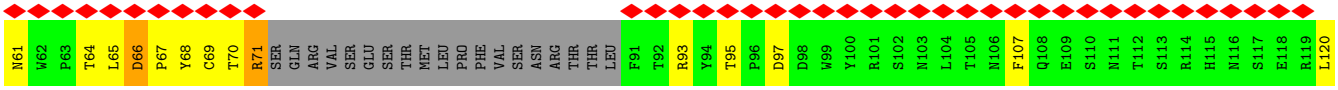


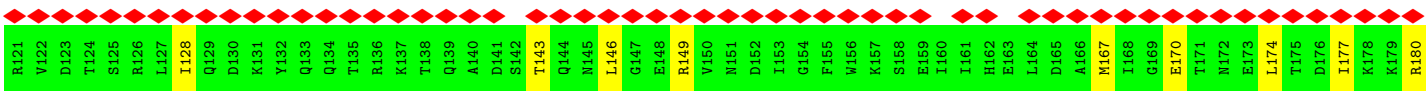


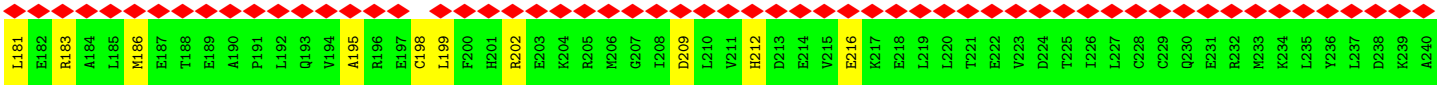
- Molecule 34: Tektin-3

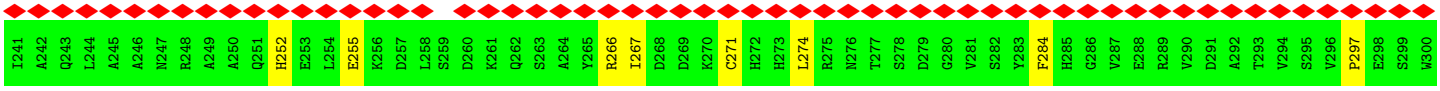
Chain 6L:

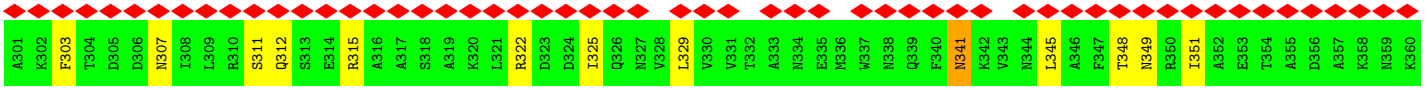


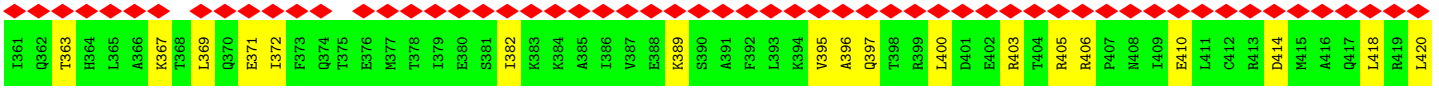


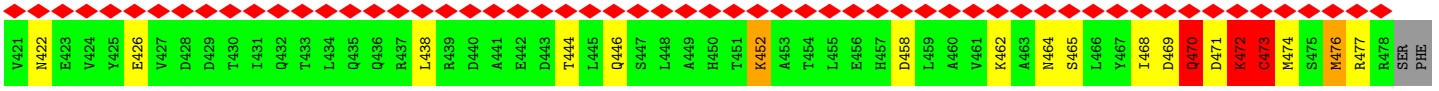












PRO SER THR LEU ARG LEU VAL GLY PHE CYS

- Molecule 34: Tektin-3

Chain 6M:

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

ASN TRP PRO THR LEU ASP PRO TYR CYS THR ARG SER GLN ARG VAL SER GLU SER THR MET LEU PRO PHE VAL SER ASN ARG THR THR LEU PHE THR ARG TYR THR PRO ASP ASP TRP TYR ARG SER ASN LEU THR ASN PHE GLN GLU SER ASN THR SER ARG HIS ASN SER GLU ARG LEU

ARG VAL ASP THR SER R126 L127 I128 Q129 D130 K131 Y132 Q133 Q134 T135 R136 K137 T138 Q139 A140 D141 S142 T143 Q144 N145 L146 G147 E148 R149 V150 N151 D152 I153 G154 F155 W156 K157 S158 E159 I160 I161 H162 E163 L164 D165 A166 M167 I168 G169 E170 T171 N172 E173 L174 T175 D176 I177 K178 K179 R180

L181 E182 R183 A184 L185 M186 E187 T188 E189 A190 P191 L192 Q193 V194 A195 R196 E197 C198 L199 F200 H201 R202 E203 K204 R205 M206 G207 I208 D209 L210 V211 H212 D213 E214 V215 E216 K217 E218 L219 L220 T221 E222 V223 D224 T225 I226 L227 C228 C229 Q230 E231 R232 M233 K234 L235 Y236 L237 D238 K239 A240

I241 A242 Q243 L244 A245 A246 N247 R248 A249 A250 Q251 H252 E253 L254 E255 K256 D257 L258 S259 D260 K261 Q262 S263 A264 Y265 R266 I267 D268 D269 K270 C271 H272 H273 L274 R275 N276 T277 S278 D279 G280 V281 S282 Y283 F284 H285 G286 V287 E288 R289 V290 D291 A292 T293 V294 S295 V296 P297 E298 S299 W300

A301 K302 F303 T304 D305 D306 N307 I308 L309 R310 S311 Q312 S313 E314 R315 A316 A317 S318 A319 K320 L321 R322 D323 D324 I325 Q326 N327 V328 L329 V330 V331 T332 A333 N334 E335 M336 W337 N338 Q339 F340 N341 K342 V343 N344 L345 A346 F347 T348 N349 R350 I351 A352 E353 T354 A355 D356 A357 K358 N359 K360

I361 Q362 T363 H364 L365 A366 K367 T368 L369 Q370 E371 I372 F373 Q374 T375 E376 M377 T378 I379 E380 S381 I382 K383 K384 A385 I386 V387 E388 K389 S390 A391 F392 L393 K394 V395 A396 Q397 T398 R399 L400 D401 E402 R403 T404 R405 R406 P407 N408 I409 E410 L411 C412 R413 D414 M415 A416 Q417 L418 R419 L420

V421 N422 E423 V424 Y425 E426 V427 D428 D429 T430 I431 Q432 T433 L434 Q435 Q436 R437 L438 R439 D440 A441 E442 D443 T444 L445 Q446 S447 L448 A449 H450 T451 K452 A453 T454 L455 E456 H457 D458 L459 A460 V461 K462 A463 N464 S465 L466 Y467 I468 D469 Q470 D471 K472 C473 M474 S475 M476 R477 R478 S479 F480

P481 S482 T483 L484 R485 L486 VAL GLY PHE CYS

- Molecule 34: Tektin-3

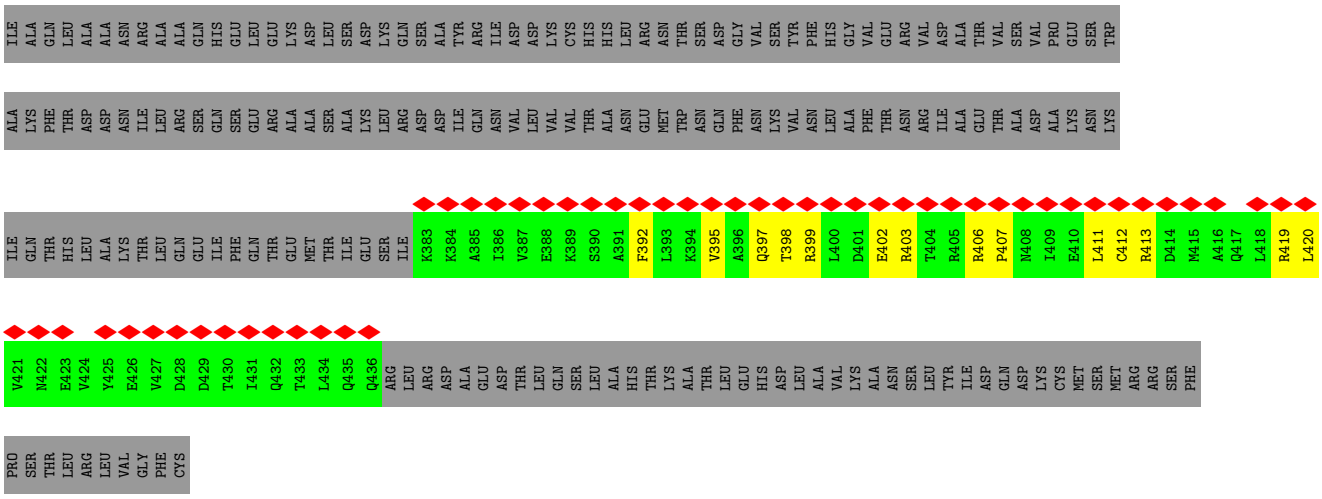
Chain 6N:

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

ASN TRP PRO THR LEU ASP PRO TYR CYS THR ARG SER GLN ARG VAL SER GLU SER THR MET LEU PRO PHE VAL SER ASN ARG THR THR LEU PHE THR ARG TYR THR PRO ASP ASP TRP TYR ARG SER ASN LEU THR ASN PHE GLN GLU SER ASN THR SER ARG HIS ASN SER GLU ARG LEU

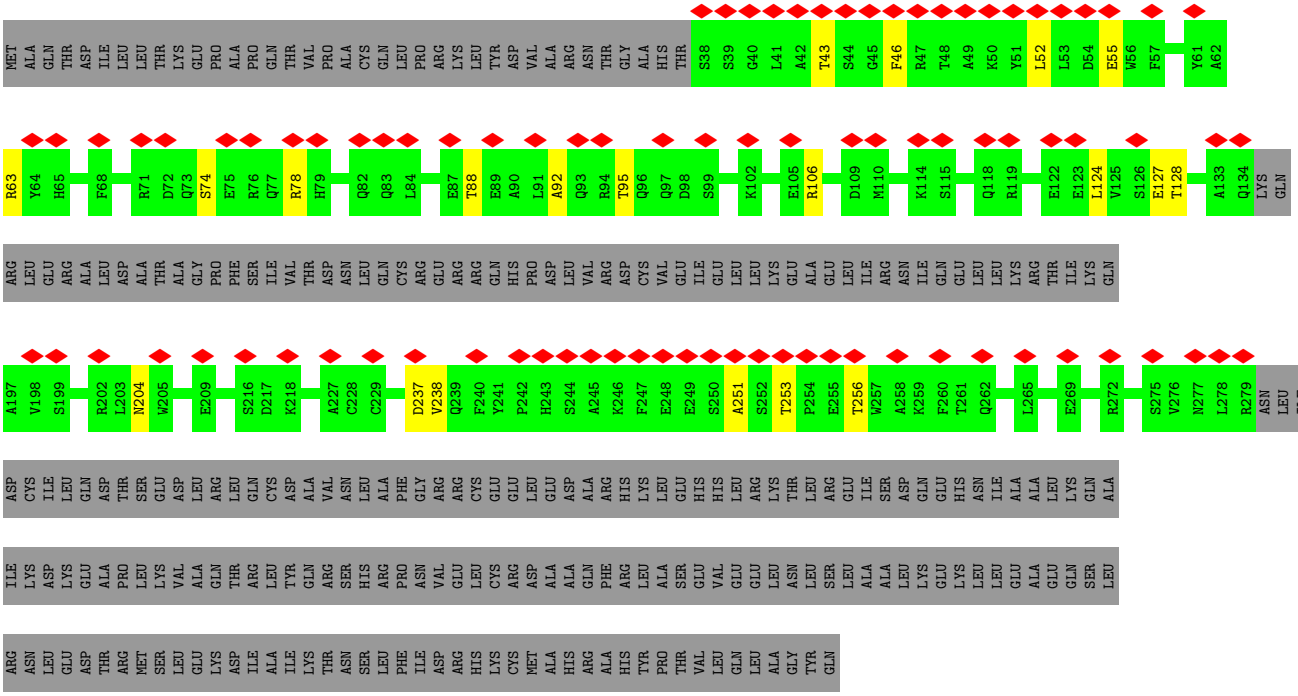
ARG VAL ASP THR SER ARG LEU ILE GLN ASP LYS TYR GLN GLN THR ARG LYS THR GLN ASN ASN LEU GLY GLU ARG VAL ASN ASP ILE GLY PHE TRP LYS SER GLU ILE ILE HIS GLU LEU ASP ALA MET ILE GLY GLU THR ASN GLU LEU THR ASP ILE LYS LYS ARG

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



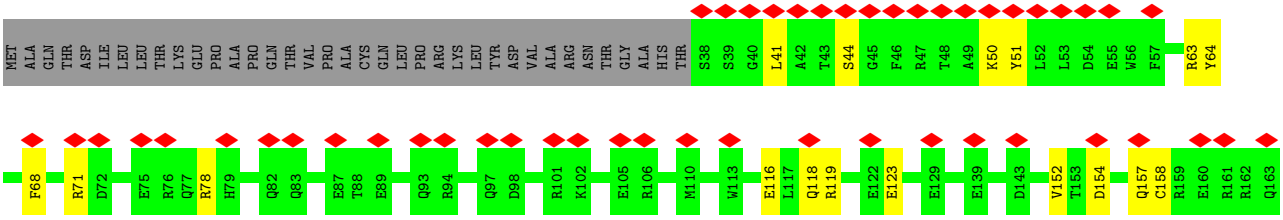
- Molecule 35: Tektin-4

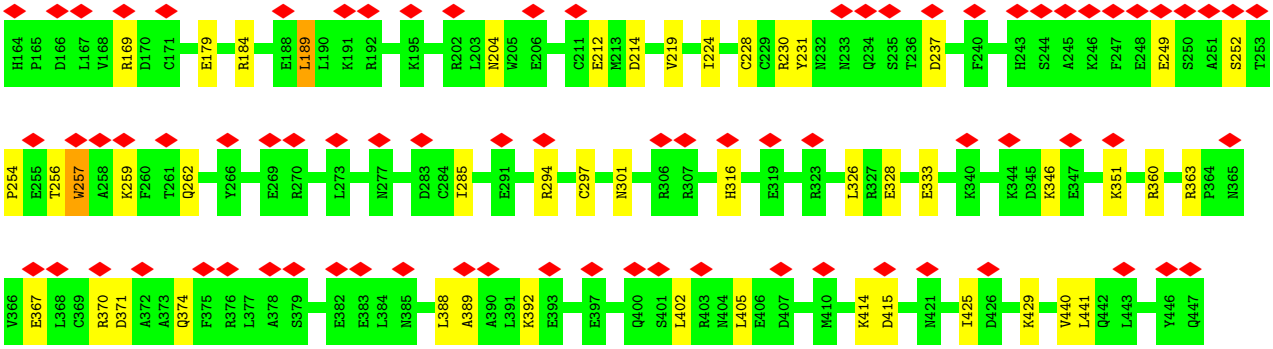
Chain 6P:



- Molecule 35: Tektin-4

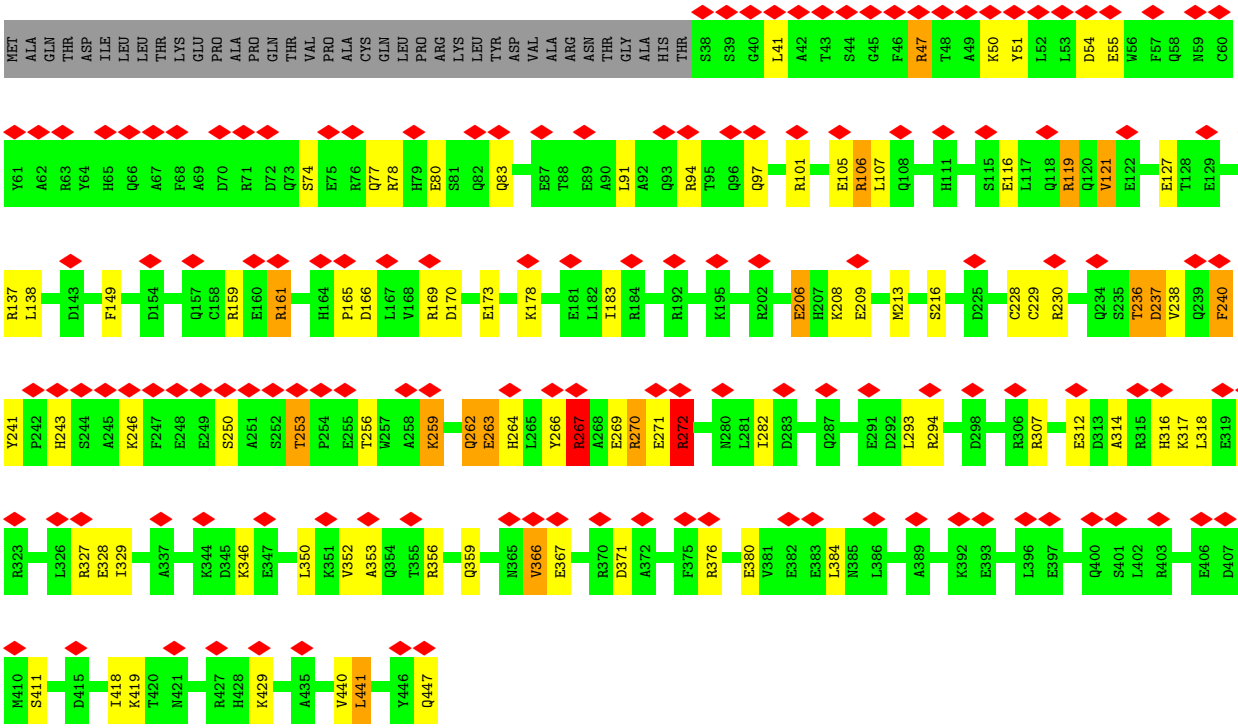
Chain 6Q:





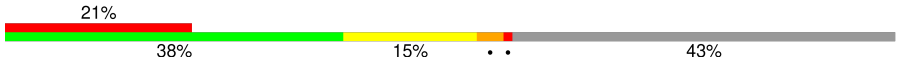
- Molecule 35: Tektin-4

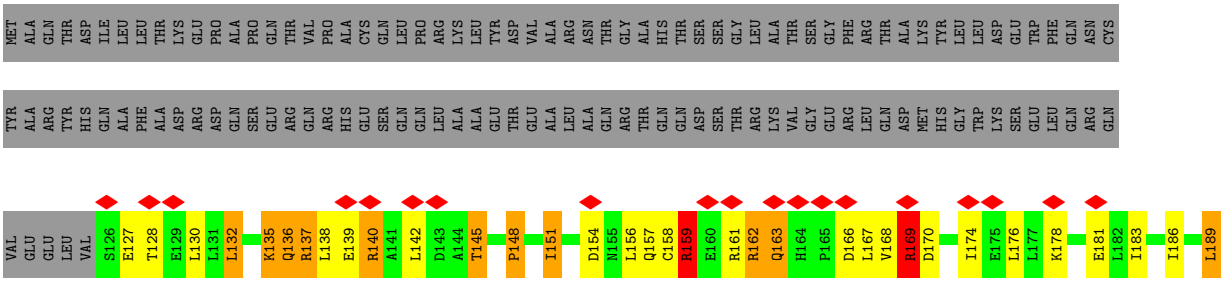
Chain 6R:

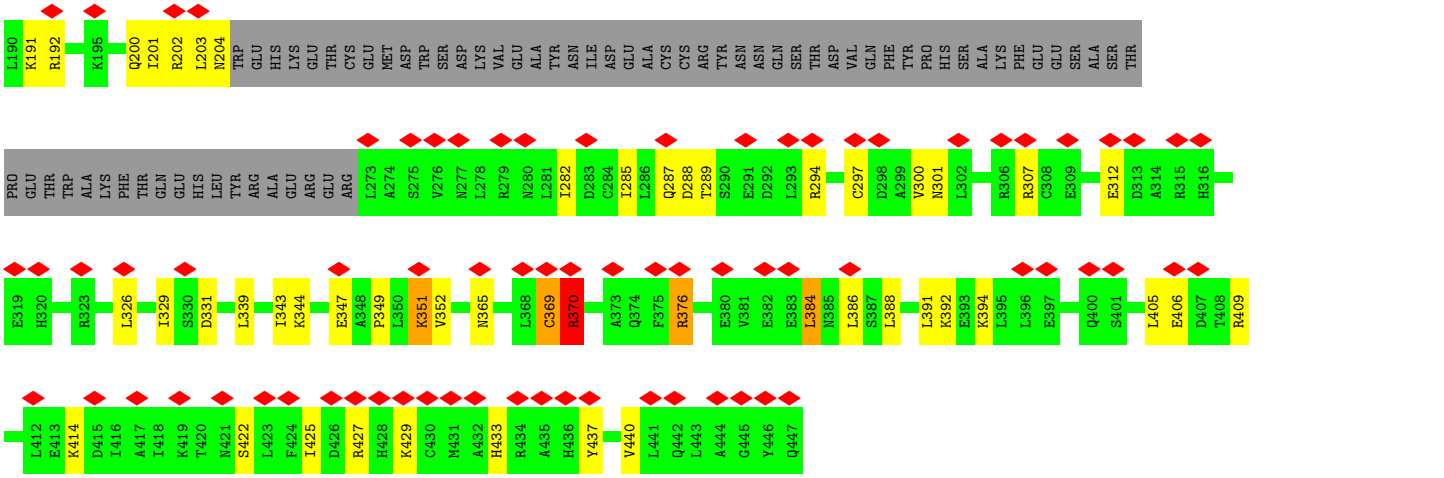


- Molecule 35: Tektin-4

Chain 6S:

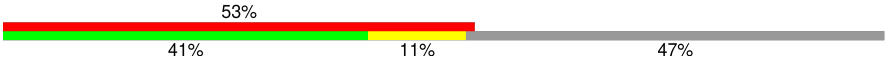


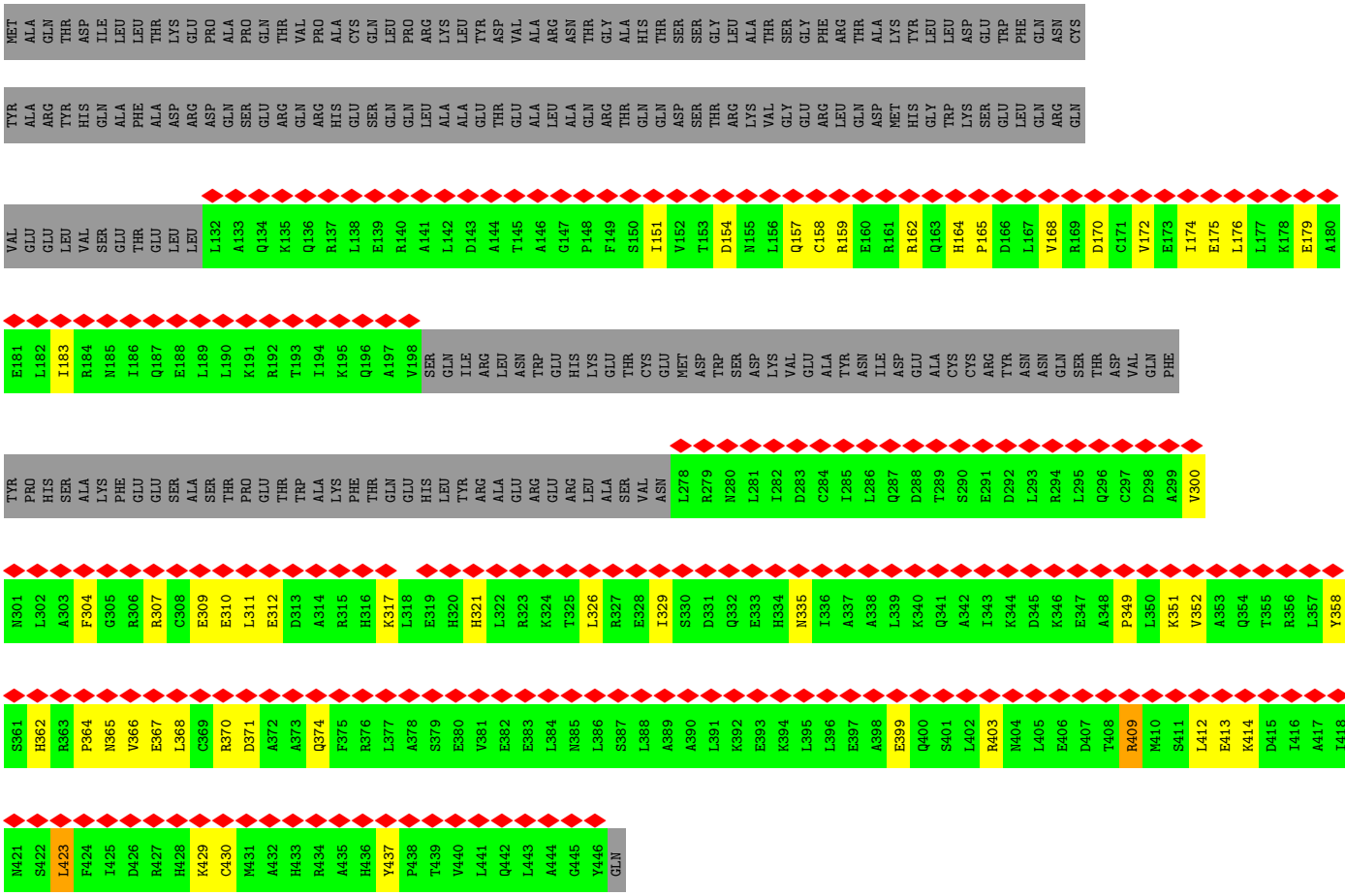




- Molecule 35: Tektin-4

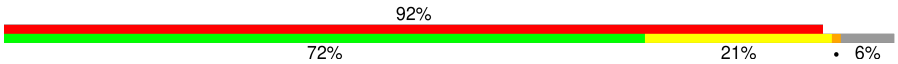
Chain 6T:





- Molecule 35: Tektin-4

Chain 6U:



MET ALA GLN THR ASP ILE LEU LEU THR LYS GLU PRO ALA PRO GLN THR VAL PRO ALA CYS GLN LEU PRO ARG LYS LEU TYR D28 V29 A30 R31 N32 T33 G34 A35 H36 T37 S38 S39 G40 L41 A42 T43 S44 G45 F46 R47 T48 A49 K50 Y51 L52 L53 D54 E55 W56 F57 Q58 N59 C60

Y61 A62 R63 Y64 H65 Q66 A67 F68 A69 D70 R71 D72 Q73 S74 E75 R76 Q77 R78 H79 E80 S81 Q82 Q83 L84 A85 A86 E87 T88 E89 A90 L91 A92 Q93 R94 T95 Q96 Q97 D98 S99 T100 R101 K102 V103 G104 E105 R106 L107 Q108 D109 M110 H111 G112 W113 K114 S115 E116 L117 Q118 R119 Q120

V121 E122 E123 L124 V125 S126 E127 T128 E129 L130 L131 L132 A133 Q134 K135 Q136 R137 L138 E139 R140 A141 L142 D143 A144 T145 A146 G147 P148 F149 S150 I151 V152 T153 D154 N155 L156 Q157 C158 R159 E160 R161 R162 Q163 H164 P165 D166 L167 V168 R169 D170 C171 V172 E173 I174 E175 L176 L177 K178 E179 A180

E181 L182 I183 R184 N185 I186 Q187 E188 L189 L190 K191 R192 T193 I194 K195 Q196 A197 V198 S199 Q200 I201 R202 L203 N204 W205 E206 H207 K208 E209 T210 C211 E212 M213 D214 W215 S216 D217 K218 V219 E220 A221 Y222 N223 I224 D225 E226 A227 C228 C229 R230 Y231 N232 N233 Q234 S235 T236 D237 V238 Q239 F240

Y241 P242 H243 S244 A245 K246 F247 E248 E249 S250 A251 S252 T253 P254 E255 T256 W257 A258 K259 F260 T261 Q262 E263 H264 L265 Y266 R267 A268 E269 R270 E271 R272 L273 A274 S275 V276 N277 L278 R279 N280 L281 I282 D283 C284 I285 L286 Q287 D288 T289 S290 E291 D292 L293 R294 L295 Q296 C297 D298 A299 V300

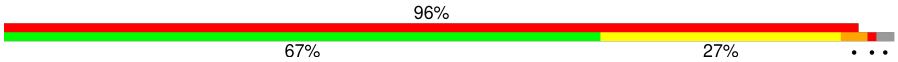
N301 L302 A303 F304 G305 R306 R307 C308 E309 E310 L311 E312 D313 A314 R315 H316 K317 L318 E319 H320 H321 L322 R323 K324 T325 L326 R327 E328 I329 S330 D331 Q332 E333 H334 N335 I336 A337 A338 L339 K340 Q341 A342 I343 K344 D345 K346 E347 A348 P349 L350 K351 V352 A353 Q354 T355 R356 L357 Y358 Q359 R360

S361 H362 R363 P364 N365 V366 E367 L368 C369 R370 D371 A372 A373 Q374 F375 R376 L377 A378 S379 E380 V381 E382 E383 L384 N385 L386 S387 L388 A389 A390 L391 K392 E393 K394 L395 L396 E397 A398 E399 Q400 S401 L402 R403 N404 L405 E406 D407 T408 R409 M410 S411 L412 E413 K414 D415 I416 A417 I418 K419 T420

N421 S422 L423 F424 I425 D426 R427 H428 K429 C430 M431 A432 H433 R434 A435 H436 Y437 P438 T439 V440 L441 Q442 L443 A444 G445 Y446 GLN

- Molecule 35: Tektin-4

Chain 6V:



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Y61 A62 R63 Y64 H65 Q66 A67 F68 A69 D70 R71 D72 Q73 S74 E75 R76 Q77 R78 H79 E80 S81 Q82 Q83 L84 A85 A86 E87 T88 E89 A90 L91 A92 Q93 R94 T95 Q96 Q97 D98 S99 T100 R101 K102 V103 G104 E105 R106 L107 Q108 D109 M110 H111 G112 W113 K114 S115 E116 L117 Q118 R119 Q120

V121 E122 E123 L124 V125 S126 E127 T128 E129 L130 L131 L132 A133 Q134 K135 Q136 R137 L138 E139 R140 A141 L142 D143 A144 T145 A146 G147 P148 F149 S150 I151 V152 T153 D154 N155 L156 Q157 C158 R159 E160 R161 R162 Q163 H164 P165 D166 L167 V168 R169 D170 C171 V172 E173 I174 E175 L176 L177 K178 E179 A180

E181 L182 I183 R184 N185 I186 Q187 E188 L189 L190 K191 R192 T193 I194 K195 Q196 A197 V198 S199 Q200 I201 R202 L203 N204 W205 E206 H207 K208 E209 T210 C211 E212 M213 D214 W215 S216 D217 K218 V219 E220 A221 Y222 N223 I224 D225 E226 A227 C228 C229 R230 Y231 N232 N233 Q234 S235 T236 D237 V238 Q239 F240

Y241 P242 H243 S244 A245 K246 F247 E248 E249 S250 A251 S252 T253 P254 E255 T256 W257 A258 K259 F260 T261 Q262 E263 H264 L265 Y266 R267 A268 E269 R270 E271 R272 L273 A274 S275 V276 N277 L278 R279 N280 L281 I282 D283 C284 I285 L286 Q287 D288 T289 S290 E291 D292 L293 R294 L295 Q296 C297 D298 A299 V300

N301 L302 A303 F304 G305 R306 R307 C308 E309 E310 L311 E312 D313 A314 R315 H316 K317 L318 E319 H320 H321 L322 R323 K324 T325 L326 R327 E328 I329 S330 D331 Q332 E333 H334 N335 I336 A337 A338 L339 K340 Q341 A342 I343 K344 D345 K346 E347 A348 P349 L350 K351 V352 A353 Q354 T355 R356 L357 Y358 Q359 R360

S361 H362 R363 P364 N365 V366 E367 L368 C369 R370 D371 A372 A373 Q374 F375 R376 L377 A378 S379 E380 V381 E382 E383 L384 N385 L386 S387 L388 A389 A390 L391 K392 E393 K394 L395 L396 E397 A398 E399 Q400 S401 L402 R403 N404 L405 E406 D407 T408 R409 M410 S411 L412 E413 K414 D415 I416 A417 I418 K419 T420

N421 S422 L423 F424 I425 D426 R427 H428 K429 C430 M431 A432 H433 R434 A435 H436 Y437 P438 T439 V440 L441 Q442 L443 A444 G445 Y446 GLN

- Molecule 35: Tektin-4

Chain 6W: 47% 33% 12% 52%

MET ALA GLN THR D5 I6 L7 L8 T9 K10 GLU PRO ALA P14 Q15 T16 V17 P18 A19 C20 Q21 L22 P23 R24 K25 L26 Y27 D28 V29 A30 R31 N32 T33 G34 A35 H36 T37 S38 S39 G40 L41 A42 T43 S44 G45 F46 R47 T48 A49 K50 Y51 L52 L53 D54 E55 W56 F57 Q58 N59 C60

Y61 A62 R63 Y64 H65 Q66 A67 F68 A69 D70 R71 D72 Q73 S74 E75 R76 Q77 R78 H79 E80 S81 Q82 Q83 L84 A85 A86 E87 T88 E89 A90 L91 A92 Q93 R94 T95 Q96 Q97 D98 S99 T100 R101 K102 V103 G104 E105 R106 L107 Q108 D109 M110 H111 G112 W113 K114 S115 E116 L117 Q118 R119 Q120

V121 E122 E123 L124 V125 S126 E127 T128 E129 L130 L131 L132 A133 Q134 K135 GLN ARG LEU GLU ARG ALA LEU ASP ALA THR ALA GLY PRO PHE SER ILE VAL THR ASP ASN LEU GLN CYS ARG GLU ARG ARG GLN HIS PRO ASP LEU VAL ARG ASP CYS VAL GLU ILE GLU LEU LEU LYS GLU ALA

GLU LEU ILE ARG ASN ILE GLN GLU LEU LEU LYS ARG THR ILE K195 Q196 A197 V198 S199 Q200 I201 R202 L203 N204 W205 E206 H207 K208 E209 T210 C211 E212 M213 D214 W215 S216 D217 K218 V219 E220 A221 Y222 N223 I224 D225 E226 A227 C228 C229 R230 Y231 N232 N233 Q234 S235 T236 D237 V238 Q239 F240

Y241 P242 H243 S244 A245 K246 F247 E248 E249 S250 A251 S252 T253 P254 E255 T256 W257 A258 K259 F260 T261 Q262 E263 H264 L265 Y266 R267 A268 E269 R270 E271 R272 L273 A274 S275 V276 N277 L278 R279 N280 L281 ILE ASP CYS ILE LEU GLN ASP THR SER GLU ASP LEU ARG LEU GLN CYS ASP ALA VAL

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

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

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

- Molecule 36: TTC25 protein

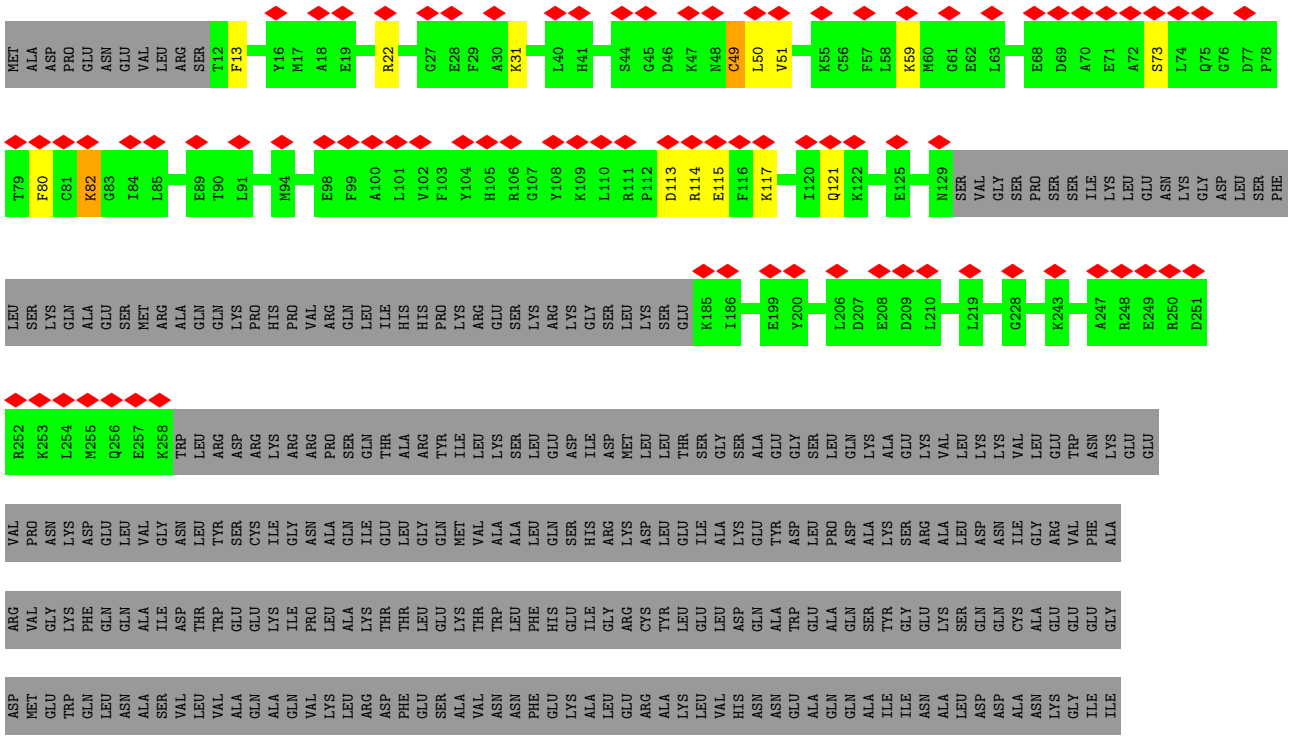
Chain 6Y: 15% 25% 72%

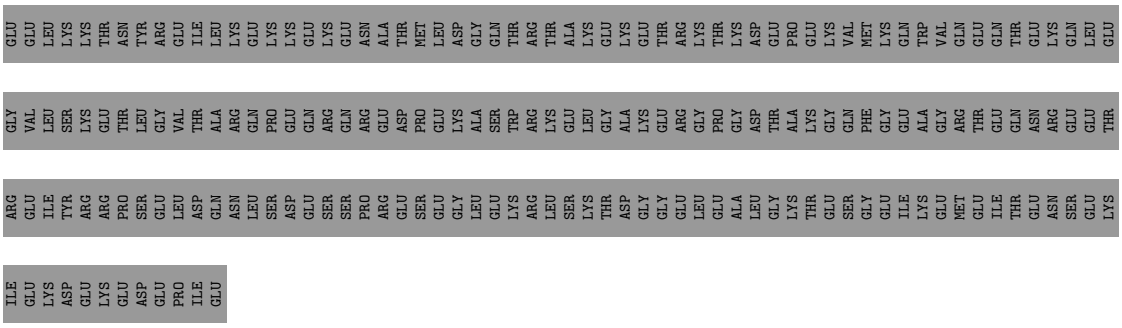
MET ALA ASP PRO GLU ASN GLU VAL LEU ARG SER T12 F13 P14 A18 E19 G20 E21 R22 L23 Y24 L25 C26 G27 E28 F29 A30 K31 A32 A33 H34 L40 H41 L42 Q43 S44 G45 D46 K47 L50 V51 A52 R53 S54 K55 C56 F57 L58 K59 M60 G61 E62 L63 E64 K65 S66 L67

E68 D69 A70 E71 A72 S73 L74 Q75 G76 D77 P78 T79 F80 C81 K82 G83 I84 L85 Q86 K87 A88 E89 T90 L91 Y92 T93 M94 G95 D96 F97 E98 F99 A100 L101 V102 F103 Y104 H105 R106 G107 Y108 K109 L110 R111 P112 D113 R114 E115 F116 K117 V118 G119 I120 Q121 K122 A123 Q124 E125 A126 I127

- Molecule 36: TTC25 protein

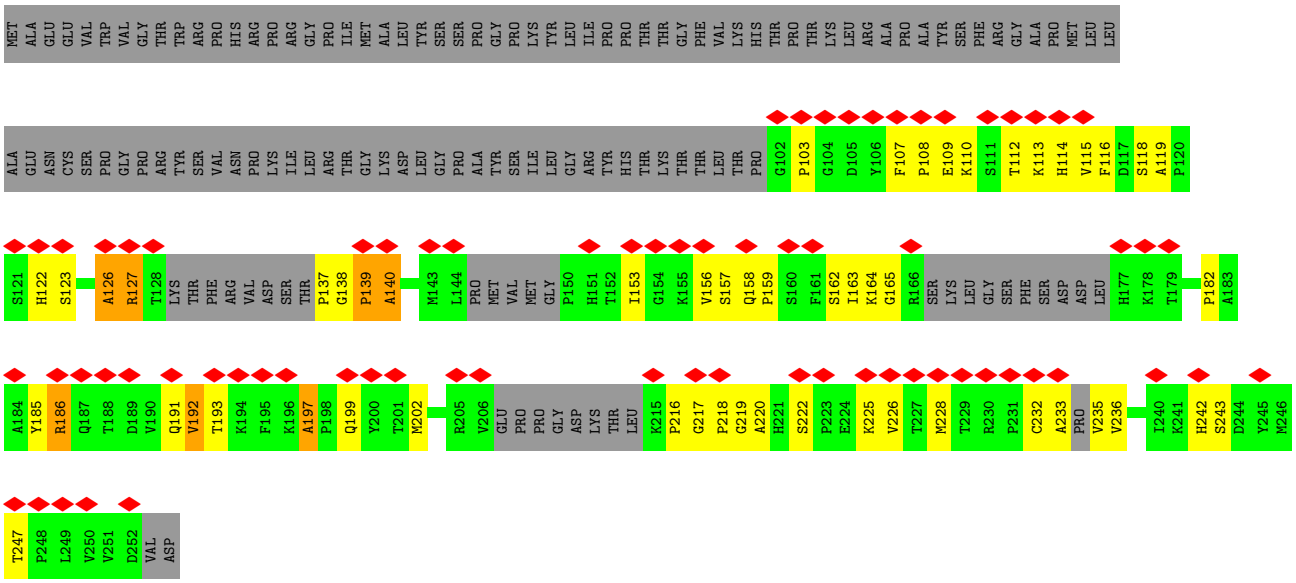
Chain 6Z:





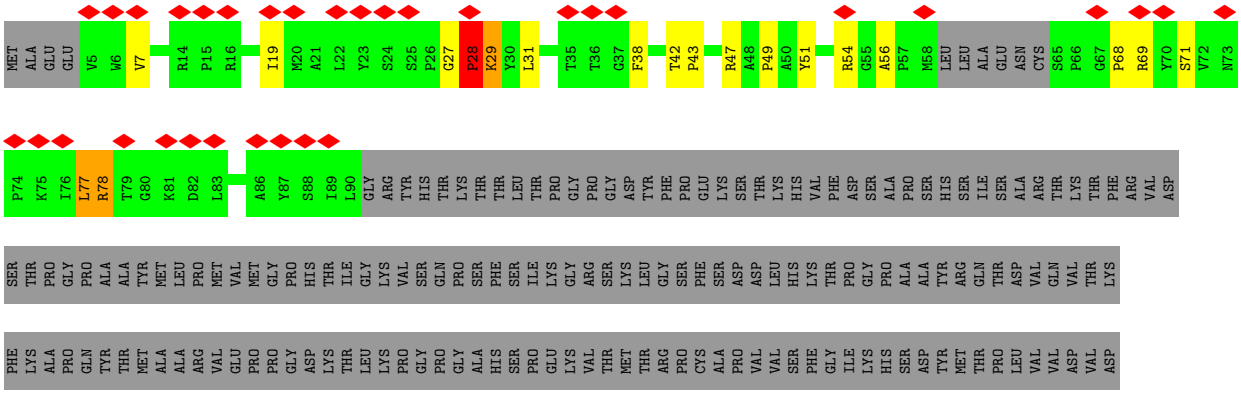
- Molecule 37: Ciliary microtubule associated protein 1A

Chain 7C:



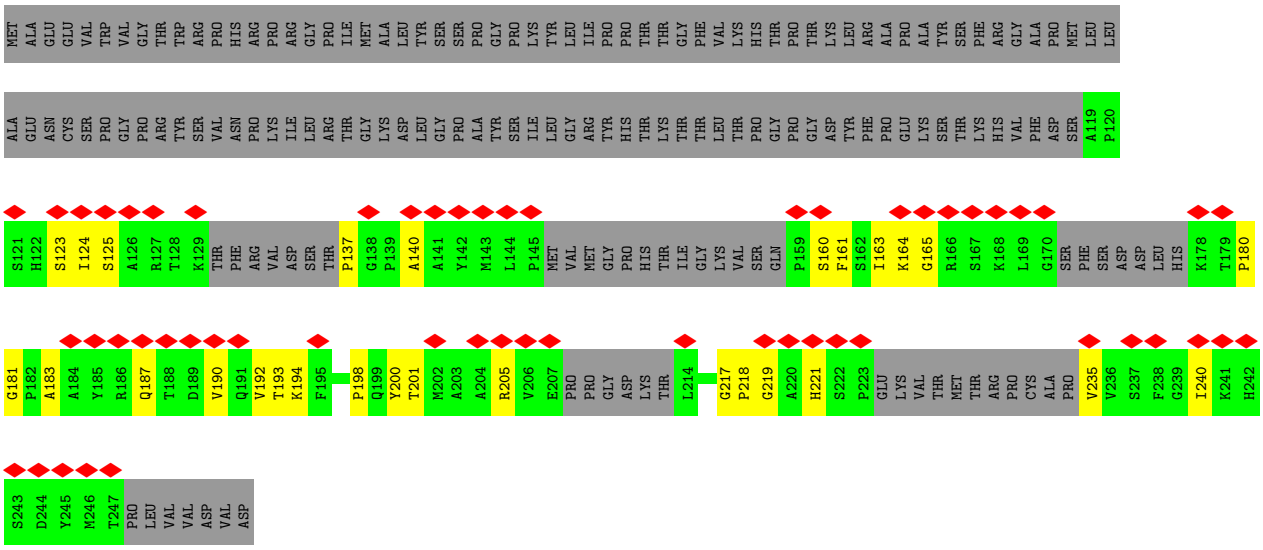
- Molecule 37: Ciliary microtubule associated protein 1A

Chain 7D:



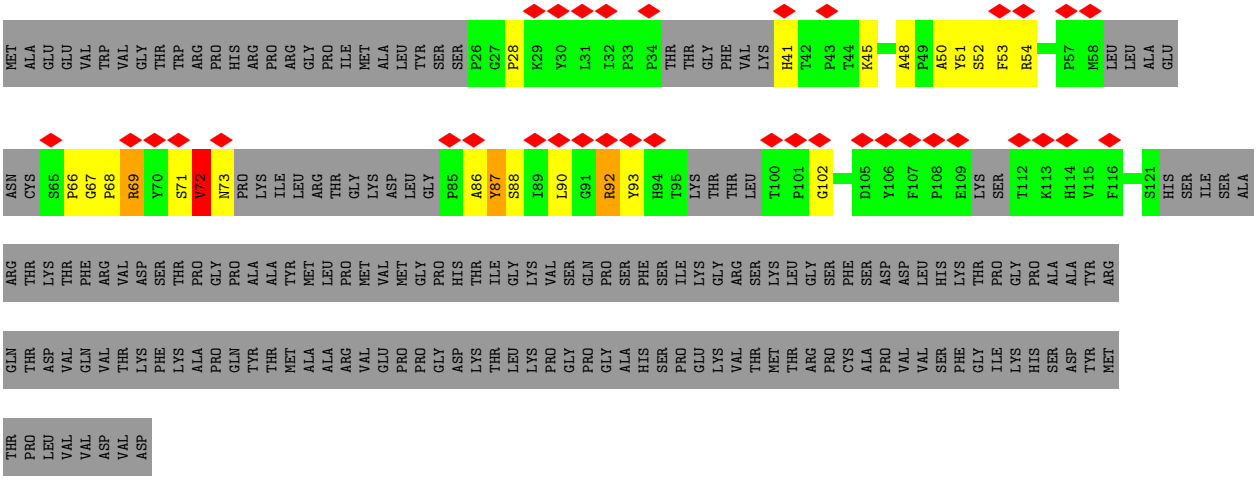
- Molecule 37: Ciliary microtubule associated protein 1A

Chain 7E:



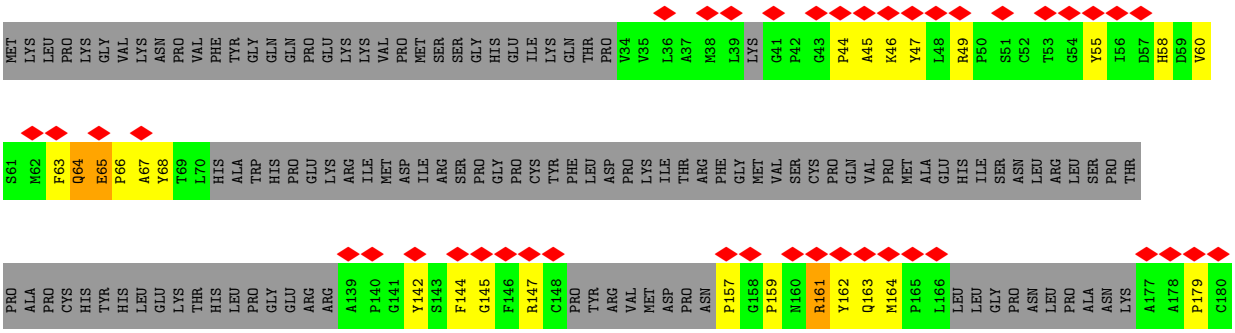
- Molecule 37: Ciliary microtubule associated protein 1A

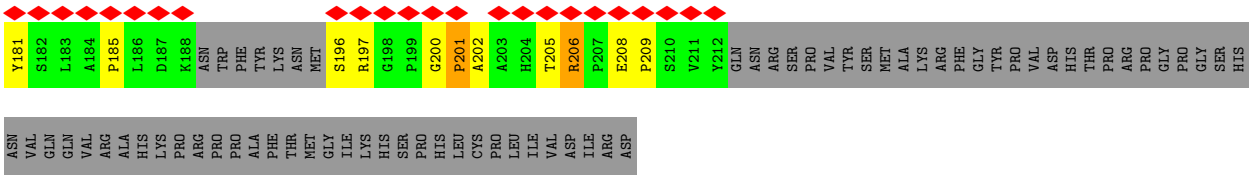
Chain 7F:



- Molecule 38: Ciliary microtubule associated protein 1C

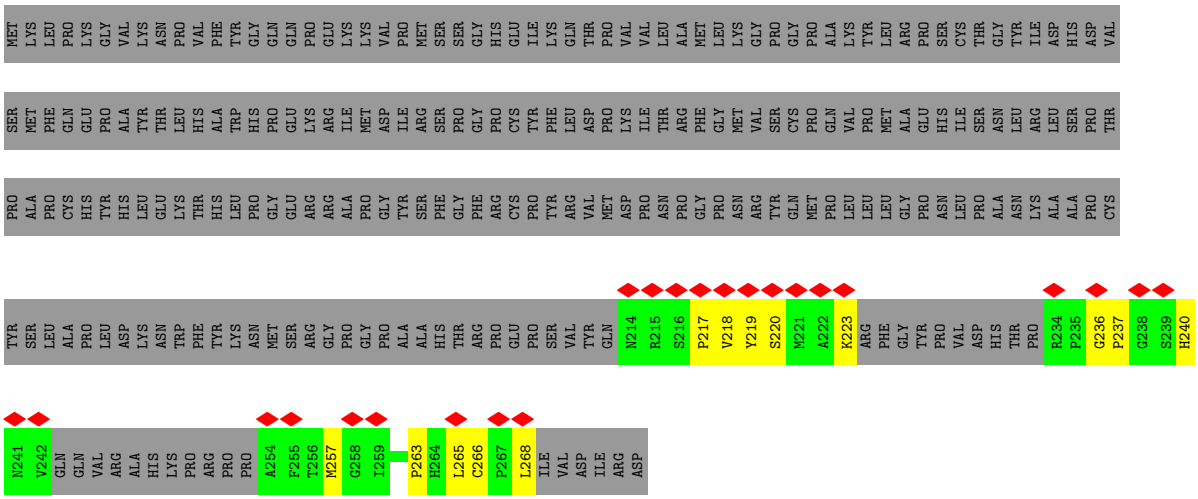
Chain 7H:





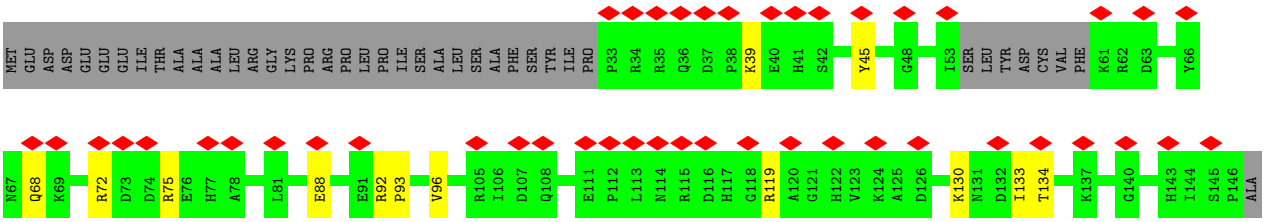
- Molecule 38: Ciliary microtubule associated protein 1C

Chain 7I:



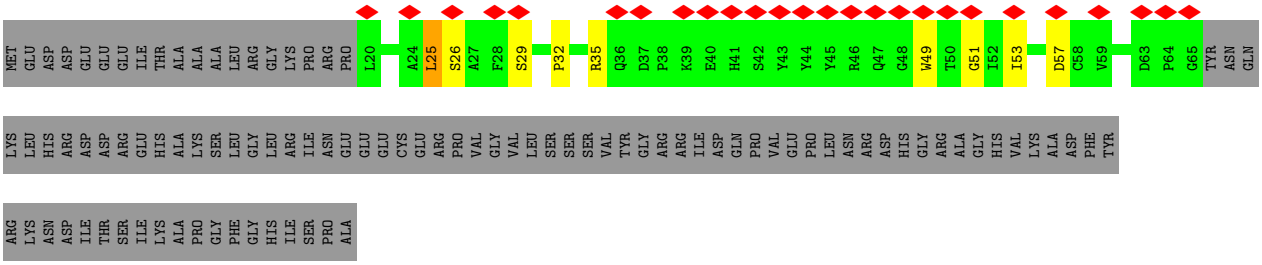
- Molecule 39: Cilia and flagella associated protein 90

Chain 7K:



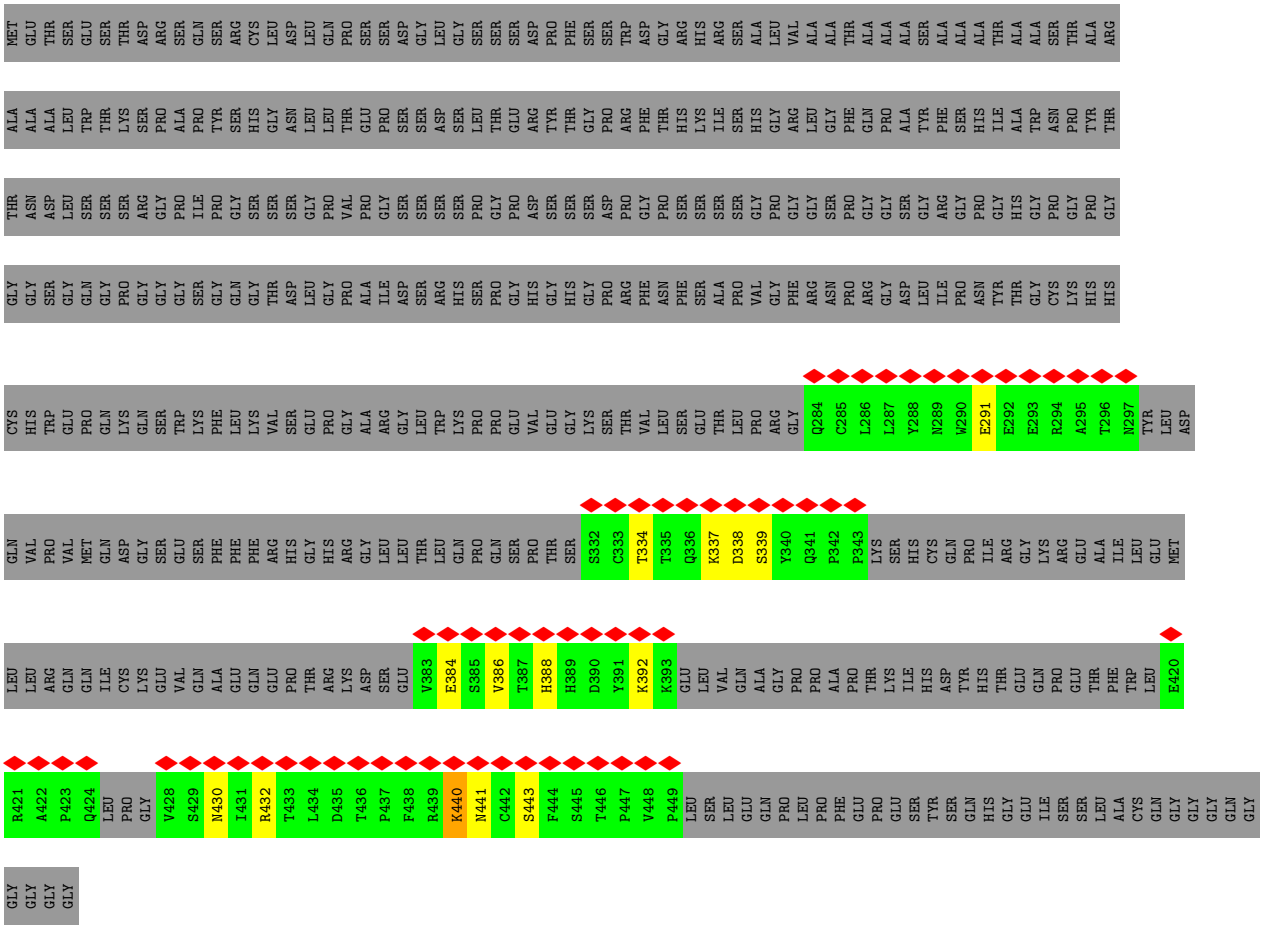
- Molecule 39: Cilia and flagella associated protein 90

Chain 7L:



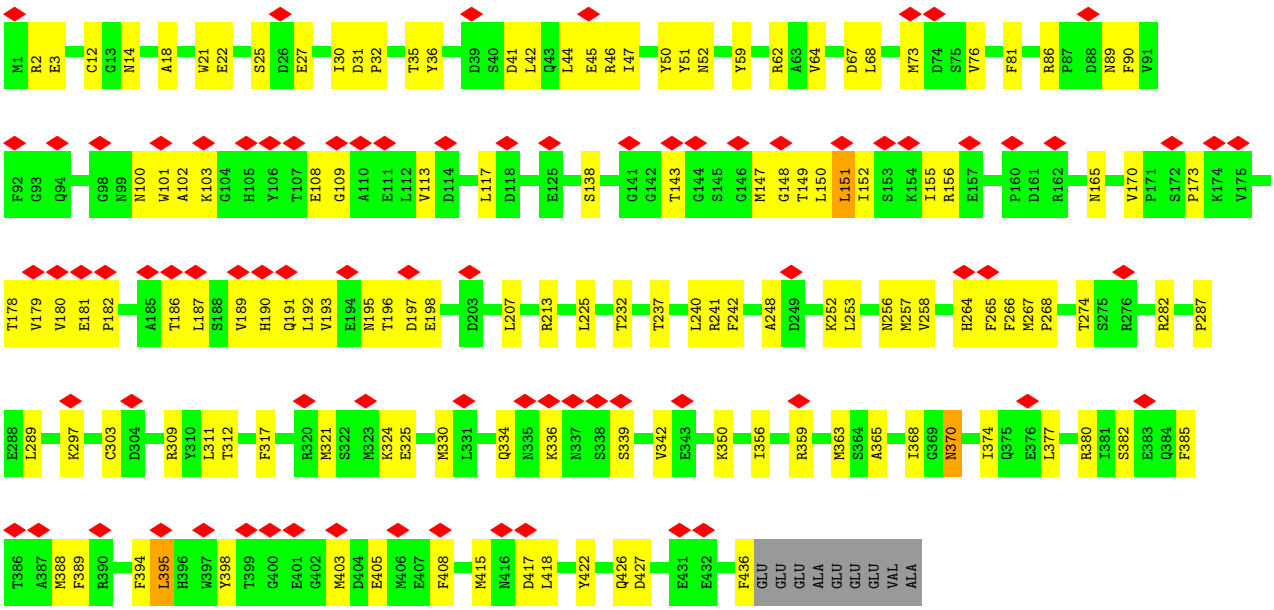
- Molecule 40: Sperm associated antigen 8

Chain 7N:



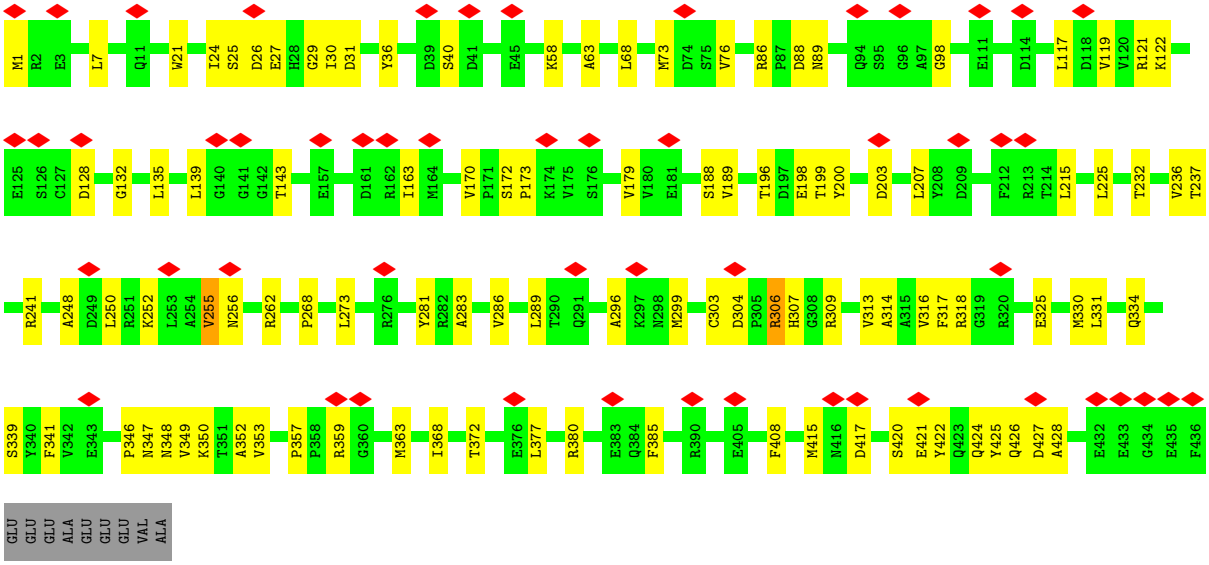
- Molecule 41: Tubulin beta-4B chain

Chain AB:



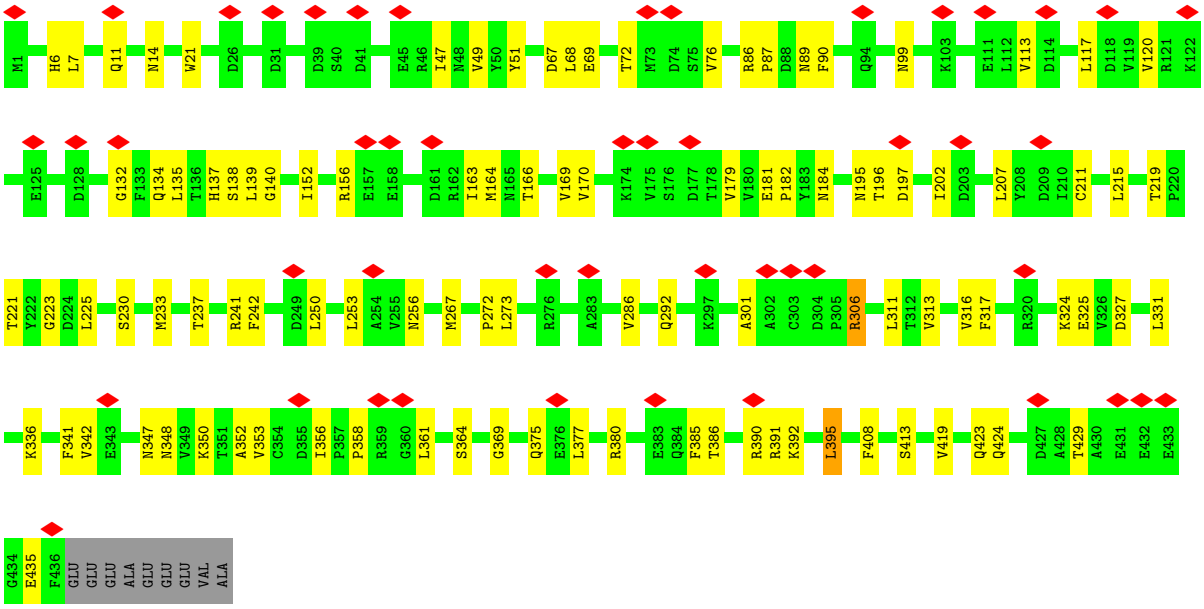
- Molecule 41: Tubulin beta-4B chain

Chain AD:



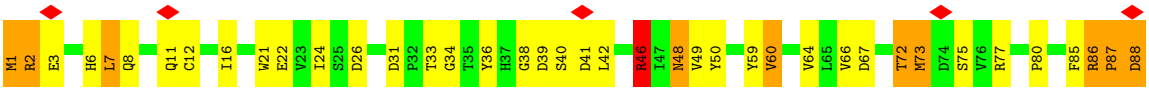
- Molecule 41: Tubulin beta-4B chain

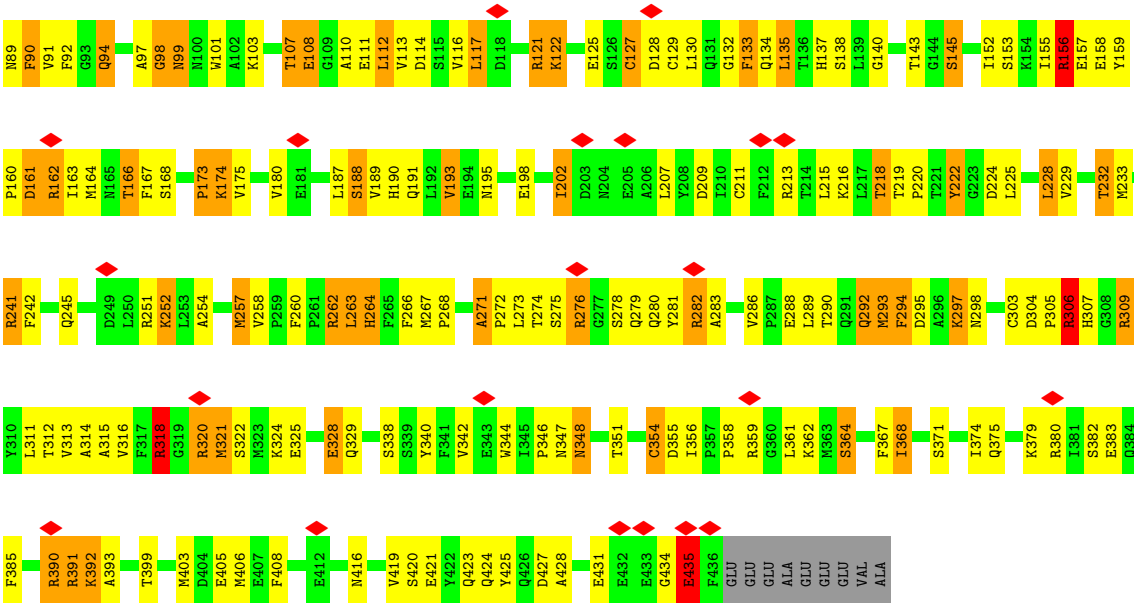
Chain AF:



- Molecule 41: Tubulin beta-4B chain

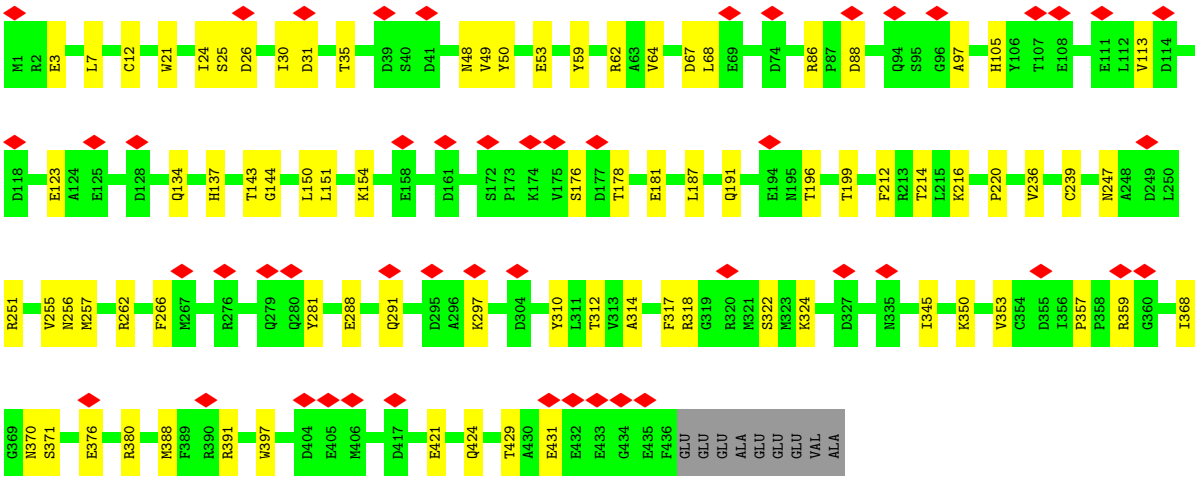
Chain AH:





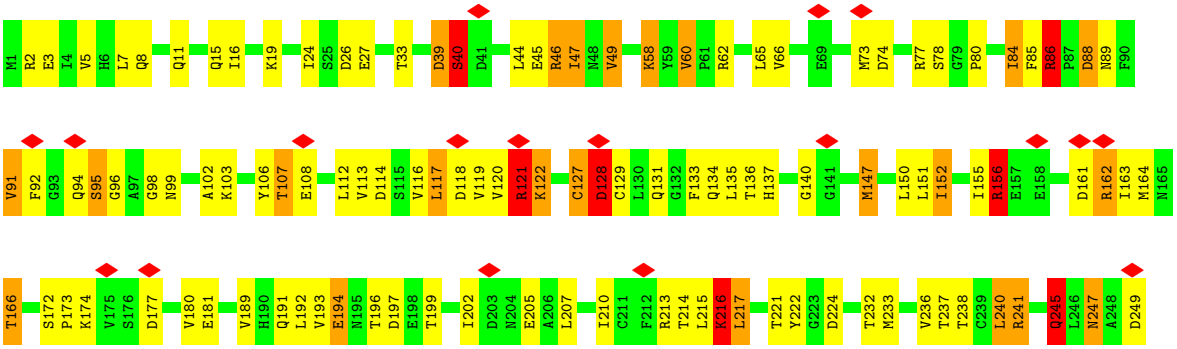
• Molecule 41: Tubulin beta-4B chain

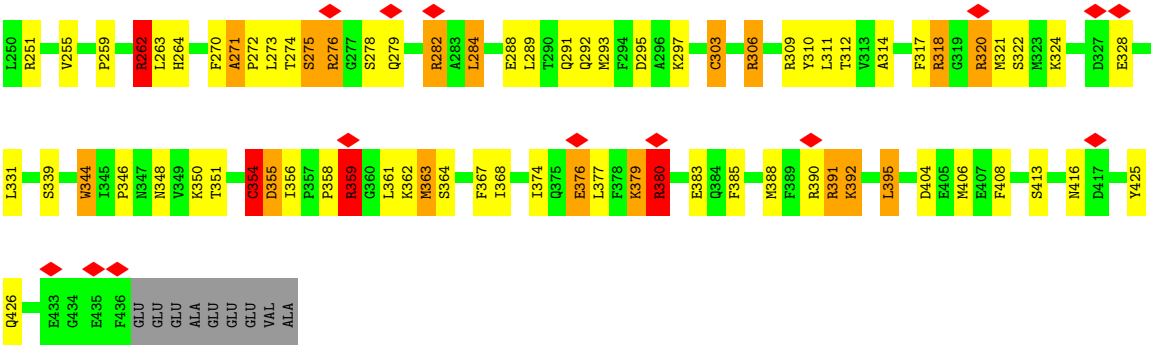
Chain AJ:



• Molecule 41: Tubulin beta-4B chain

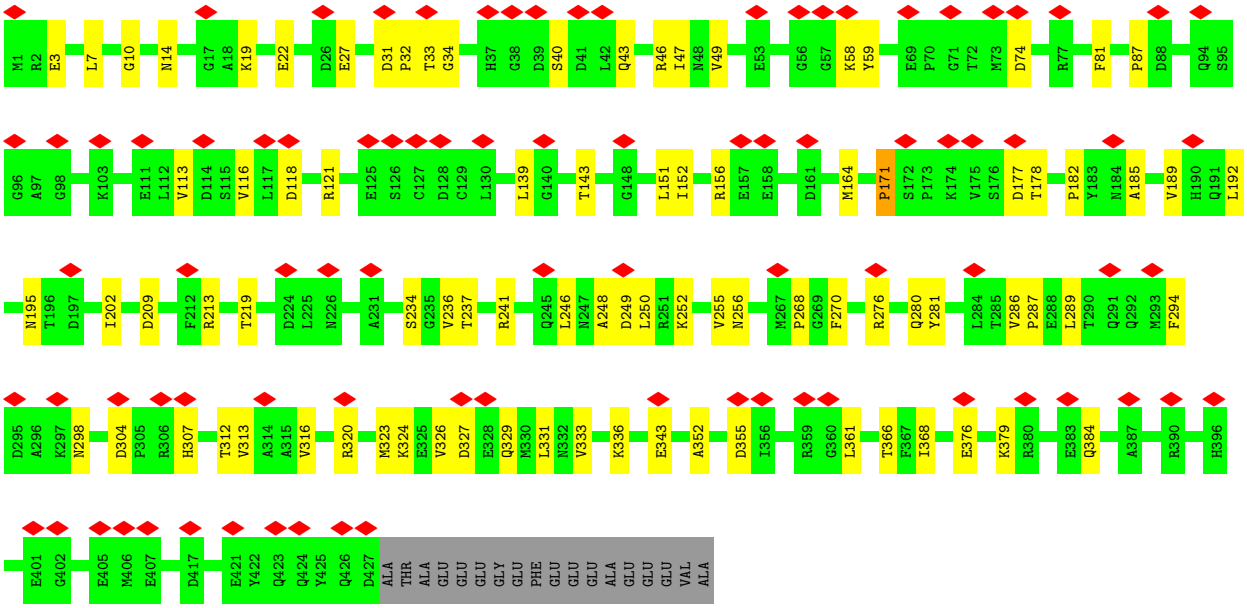
Chain AL:





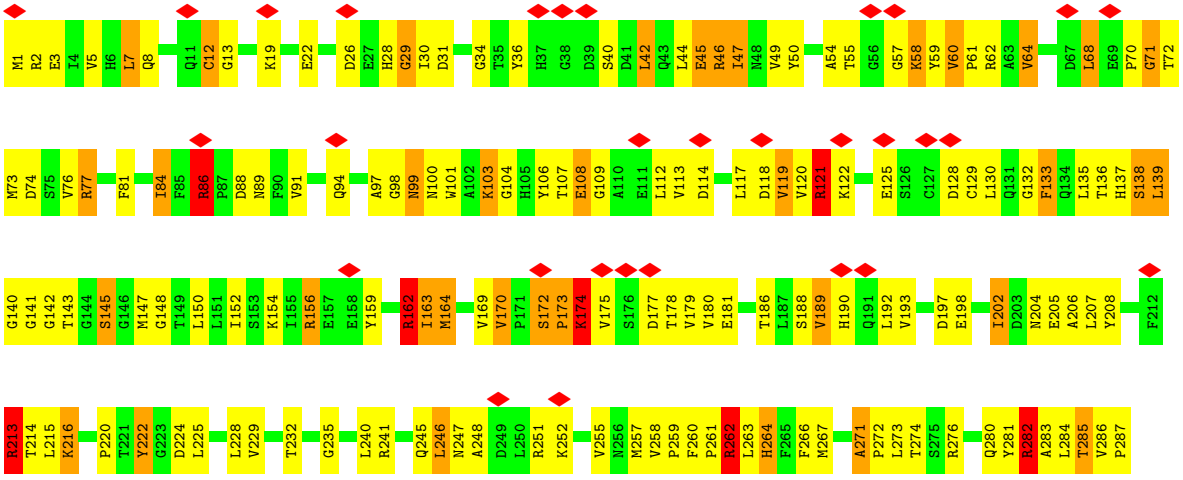
- Molecule 41: Tubulin beta-4B chain

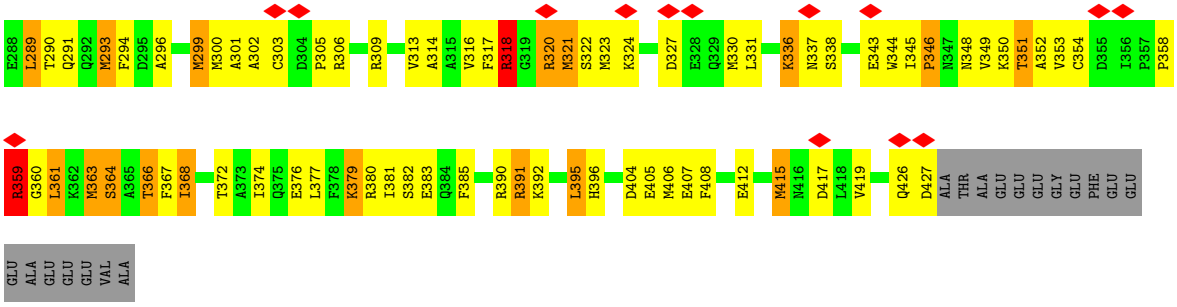
Chain BB:



- Molecule 41: Tubulin beta-4B chain

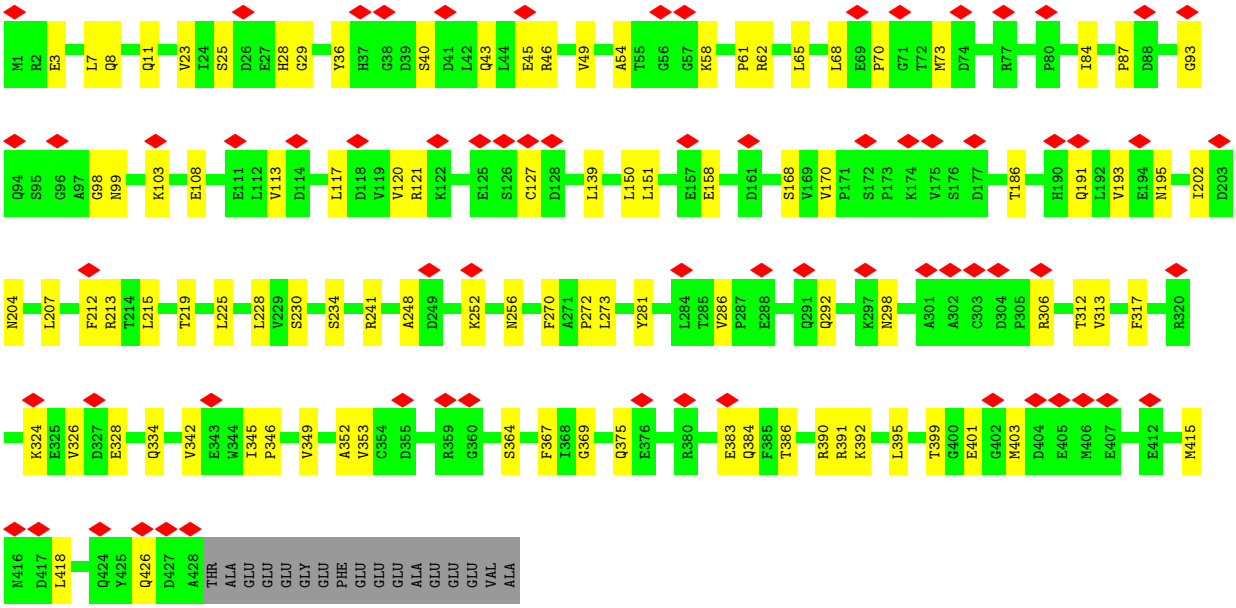
Chain BD:





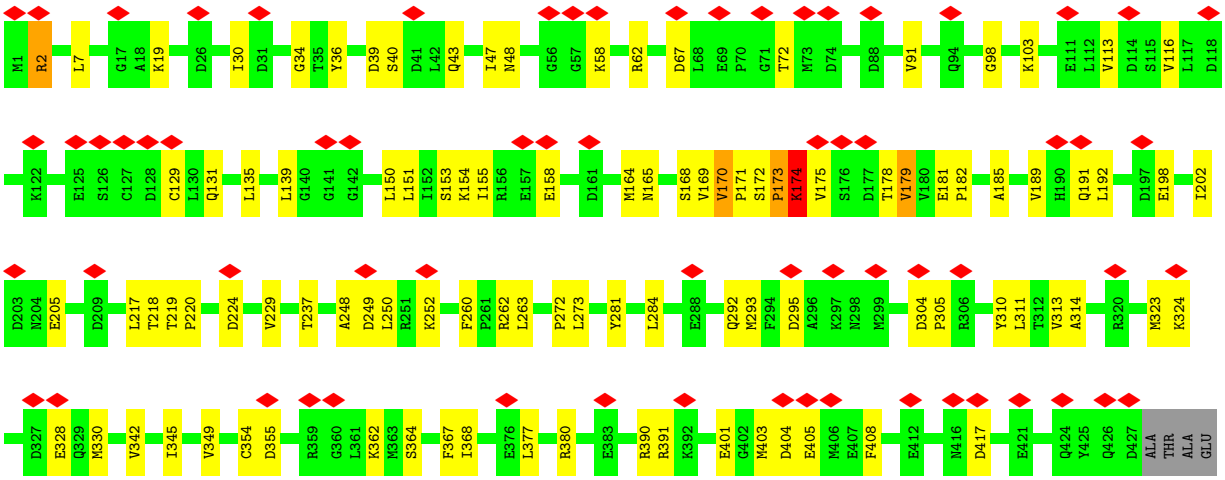
- Molecule 41: Tubulin beta-4B chain

Chain BF:



- Molecule 41: Tubulin beta-4B chain

Chain BH:



GLU GLU GLY GLU PHE GLU GLU GLU ALA GLU GLU GLU VAL ALA

- Molecule 41: Tubulin beta-4B chain

Chain BJ:

M1 L7 Q8 A9 G10 Q11 C12 G13 N14 K19 E22 D26 E27 D31 T35 Y36 H37 G38 D39 S40 D41 L42 Q43 E53 G56 G57 K58 L65 V66 D67 L68 E69 D74 S75 V76 R77 G82 F85 R86 P87 D88 W101 A102 K103 A110 E111

D114 S115 V116 L117 D118 R121 K122 E125 S126 C127 D128 Q131 S138 L139 G140 G141 G142 T143 G144 S145 G146 M147 G148 T149 L150 L151 R156 E157 E158 Y159 P160 D161 M164 N165 V169 V170 P171 S172 P173 K174 V175 S176 D177 T178 V179 V180 E181 N184 H190 Q191

N195 T196 D197 E198 T199 Y200 C201 I202 D203 N204 E205 A206 L207 C211 F212 R213 T214 L215 K216 L217 T218 T219 L225 L228 T237 R241 F242 L246 W247 A248 D249 L250 R251 K252 N256 M257 R262 L263 H264 P268 G269 F270 A271 P272 L273 R276 Y281 R282

E288 L289 T290 Q291 Q292 M293 F294 D295 A296 K297 N298 A301 A302 C303 D304 P305 R306 R309 Y310 A314 R318 G319 R320 K324 D327 E328 Q329 M330 L331 N332 V333 Q334 N335 K336 N337 S338 S339 Y340 F341 V342 E343 P346 M347 A352 D355 I356 P357 P358 R359 G360

S364 I368 E376 K379 R380 E383 Q384 F385 T386 R390 R391 K392 L395 H396 W397 G402 M403 D404 E405 M406 E407 E410 S413 N414 M415 N416 D417 S420 E421 Y422 Q423 Q424 D427 ALA THR ALA GLU GLU GLY GLU PHE GLU GLU GLU ALA GLU GLU

GLU VAL ALA

- Molecule 41: Tubulin beta-4B chain

Chain BL:

MET R2 E3 I4 V5 H6 L7 Q8 A9 G10 Q11 N14 D26 D31 P32 T33 G34 T35 Y36 S40 D41 L42 Q43 L44 G56 G57 K58 P61 R62 A63 V64 D67 L68 M73 D74 P80 I84 F85 R86 P87 D88 N89 F90 V91 Q94 S95 G96 K103

T107 E111 L112 V113 D114 S115 V116 L117 D118 E125 S126 C127 D128 Q131 G132 F133 Q134 H137 S138 L139 G140 G141 M147 E158 D161 M164 N165 T166 F167 V170 P171 S172 P173 K174 V175 S176 D177 T178 V179 V180 E181 P182 S188 V189 H190 Q191 L192 V193 E194

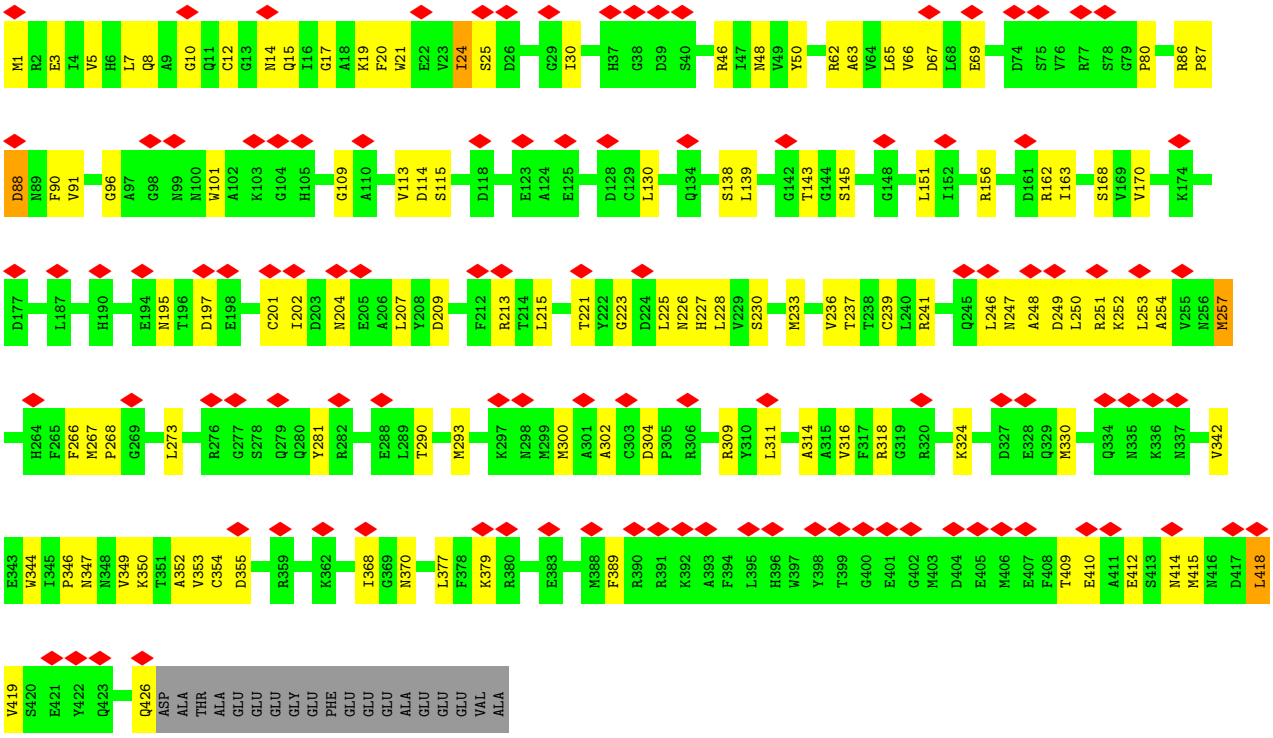
N195 D203 N204 E205 A206 L207 C211 F212 R213 T214 L215 T221 Y222 G223 D224 L225 L228 V229 S230 M233 V236 T237 F242 D249 K252 R262 L273 Y281 L284 E288 Q292 D295 A296 K297 N298 D304 P305 R306 R309 Y310 V316

F317 R318 G319 R320 M321 S322 M323 K324 E325 V326 D327 E328 Q329 M330 F341 V342 E343 P346 M347 N348 V349 A352 D355 I356 R359 G360 S364 I368 S371 T372 Q375 E376 L377 F378 K379 R380 Q384 F385 T386 R390 R391 F394 G400 E401 G402 M403 D404

E405 M406 E412 S413 N414 M415 N416 D417 Q424 Y425 Q426 ASP ALA THR ALA GLU GLU GLY GLU PHE GLU GLU GLU ALA GLU GLU GLU VAL ALA

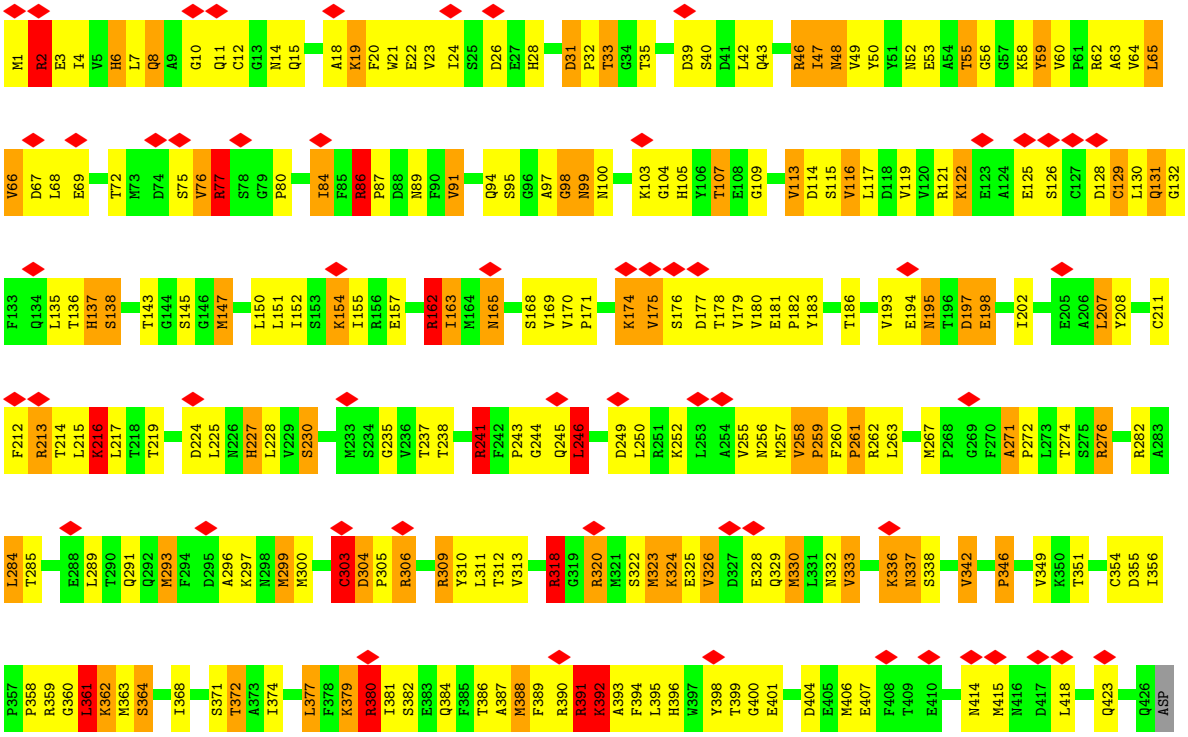
- Molecule 41: Tubulin beta-4B chain

Chain CB: 24% 69% 26%



- Molecule 41: Tubulin beta-4B chain

Chain CD: 13% 41% 37% 15%



ALA THR ALA GLU GLU GLU GLY GLU PHE GLU GLU GLU ALA GLU GLU GLU VAL ALA

- Molecule 41: Tubulin beta-4B chain

Chain CF:

M1 R2 E3 I4 V5 H6 L7 Q8 C12 A18 K19 F20 W21 E22 V23 I24 S25 D26 E27 H28 G29 I30 D31 G34 T35 D39 S40 D41 L42 Q43 L44 E45 R46 I47 N48 V49 Y50 Y51 N52 E53 G57 K58 Y59 V60 P61 R62 A63 V64 L65 V66 D67 L68 E69 P70 G71

T72 M73 D74 S75 V76 R77 S78 G79 P80 F81 G82 Q83 I84 F85 R86 P87 D88 N89 F90 V91 Q94 S95 G96 N99 N100 W101 A102 K103 G104 H105 Y106 T107 E108 E111 L112 V113 D114 S115 V116 L117 D118 V119 V120 R121 K122 S126 C127 D128 C129 L130 Q131 G132 L135 T136 H137

S138 L139 T143 L150 K154 I155 R156 E157 D161 R162 I163 M164 N165 T166 F167 S168 V169 V170 P171 S172 P173 K174 V175 S176 D177 T178 V179 V180 E181 P182 Y183 L187 S188 V189 H190 Q191 L192 D197 E198 T199 Y200 C201 I202 D203 N204 L207 Y208 D209 R213 T214 L215 K216

P220 T221 Y222 G223 D224 L225 N226 H227 L228 V229 S230 A231 T232 M233 T237 T238 C239 L240 R241 F242 P243 G244 N247 A248 D249 L250 R251 K252 L253 A254 Y255 N256 M257 V258 P259 F260 P261 R262 L263 H264 F265 F266 M267 P268 G269 F270 A271 P272 I273 T274 S275 R276 G277 S278 Q279 Q280 Y281

R282 A283 L284 T285 V286 P287 E288 L289 Q292 M299 M300 A301 A302 C303 D304 P305 R306 H307 G308 R309 Y310 L311 T312 V316 F317 R318 G319 R320 M321 S322 M323 K324 E325 V326 D327 E328 Q329 M330 L331 Q334 N335 K336 N337 Y340 F341 V342 I345 P346 N347 T351 C354 D355

I356 P357 P358 R359 K362 M363 S364 I368 G369 N370 S371 T372 A373 I374 Q375 E376 L377 F378 K379 R380 I381 F385 T386 A387 M388 F389 R390 R391 K392 A393 F394 L395 H396 W397 Y398 E401 G402 M403 D404 E405 M406 E410 A411 E412 S413 N414 M415 N416 D417 L418 V419 S420 E421 Y422 Q423

Q424 Y425 Q426 D427 A428 THR ALA GLU GLU GLU GLY GLU PHE GLU GLU GLU ALA GLU GLU GLU VAL ALA

- Molecule 41: Tubulin beta-4B chain

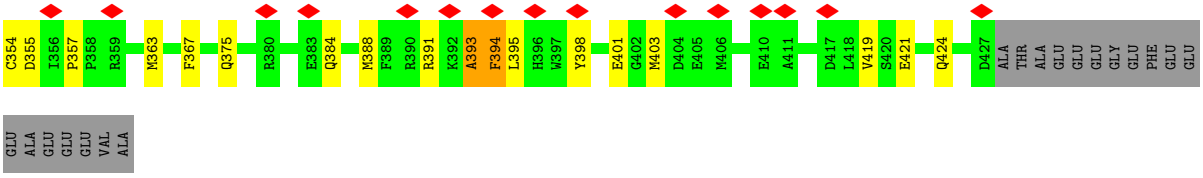
Chain CH:

M1 R2 G10 Q11 C12 G13 N14 G17 A18 K19 F20 W21 E22 V23 I24 E27 I30 D39 S40 L44 E45 R46 Y51 A54 T55 G56 Y59 V60 P61 V64 L65 V66 D67 L68 E69 P70 G71 D74 S75 V76 R77 F81 R86 P87 D88 N89 F90

A97 G98 N99 N100 W101 A102 K103 G104 H105 Y106 T107 E108 G109 V113 D114 S115 V116 L117 D118 V119 V120 R121 K122 E125 S126 C127 L130 Q131 G132 F133 S138 L139 T143 G144 S145 G146 M147 G148 T149 L150 L151 I152 S153 K154 I155 R156 R162 N165 T166 F167 S172

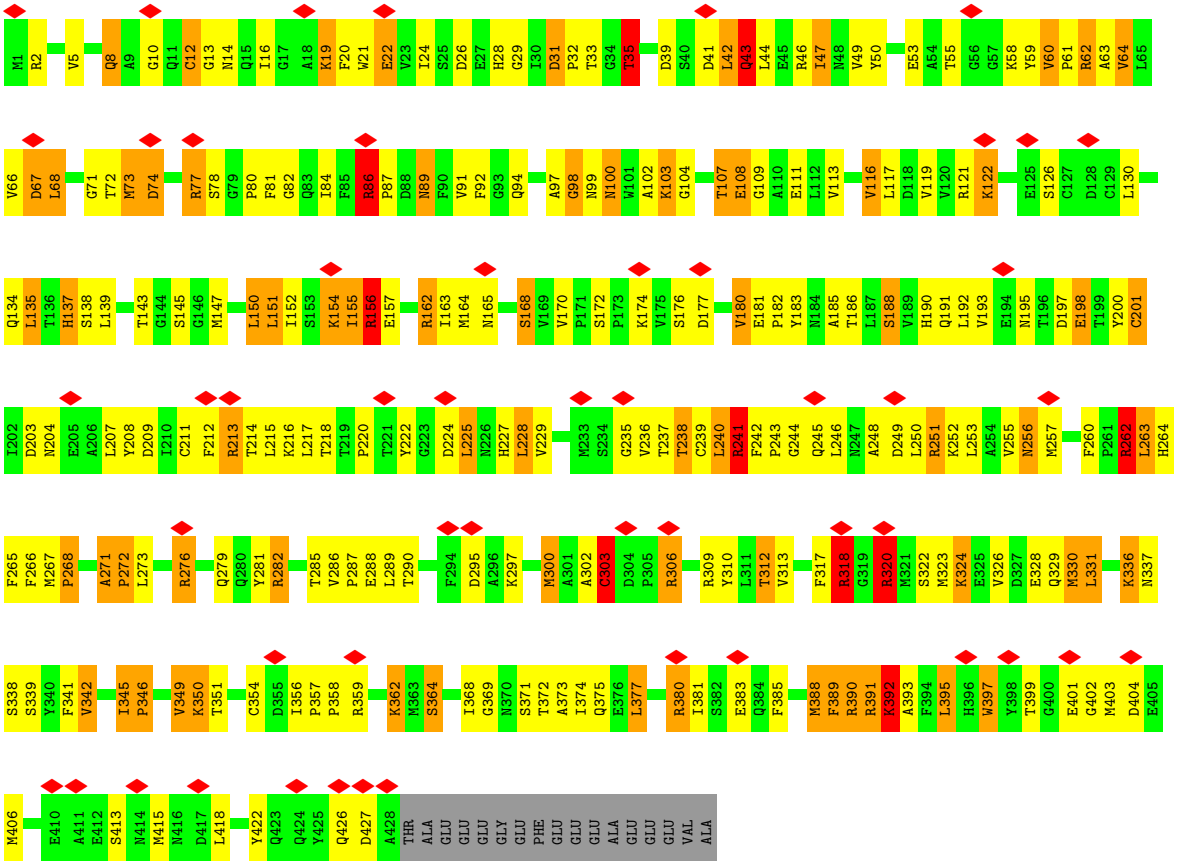
P173 K174 V175 S176 D177 T178 E181 P182 Y183 N184 S188 V189 H190 Q191 L192 V193 E194 N195 T196 D197 E198 I202 E205 A206 L207 Y208 D209 I210 C211 F212 R213 T214 L215 G223 D224 L225 N226 H227 L228 V229 S230 A231 T232 M233 V236 T237 T238 C239 L240 R241 Q245 L246 N247

A248 D249 L250 R251 K252 N256 F260 L263 M267 P268 G269 R282 E288 L289 T290 Q291 Q292 M293 F294 D295 A302 R306 R309 Y310 L311 T312 V313 F317 R318 G319 R320 E325 M330 V333 K336 V342 E343 W344 I345 P346 N347 M348 V349 V353



• Molecule 41: Tubulin beta-4B chain

Chain CJ:



• Molecule 41: Tubulin beta-4B chain

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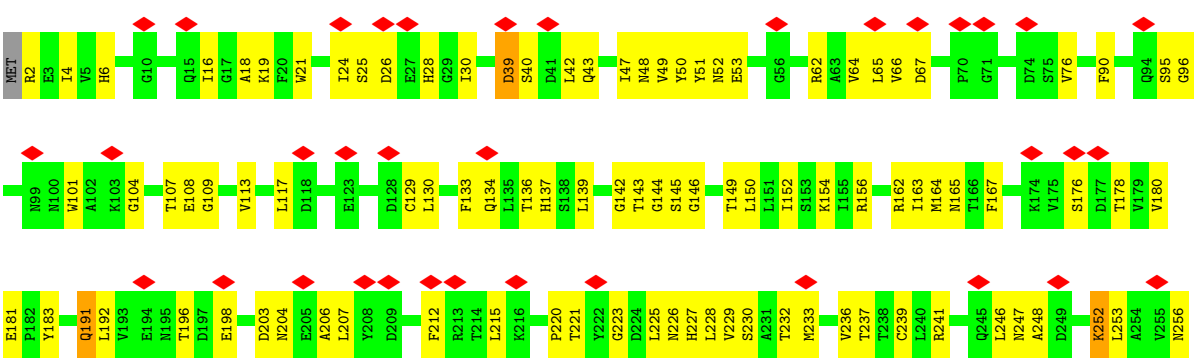
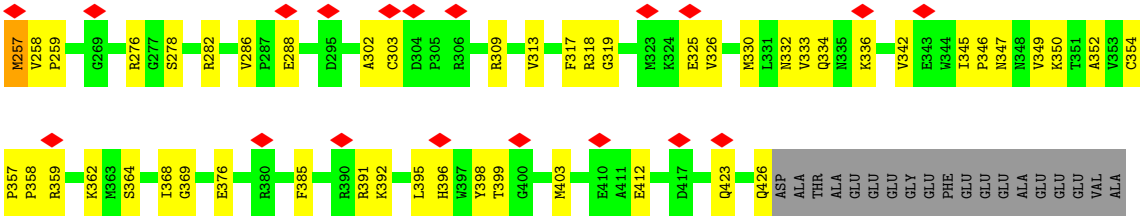
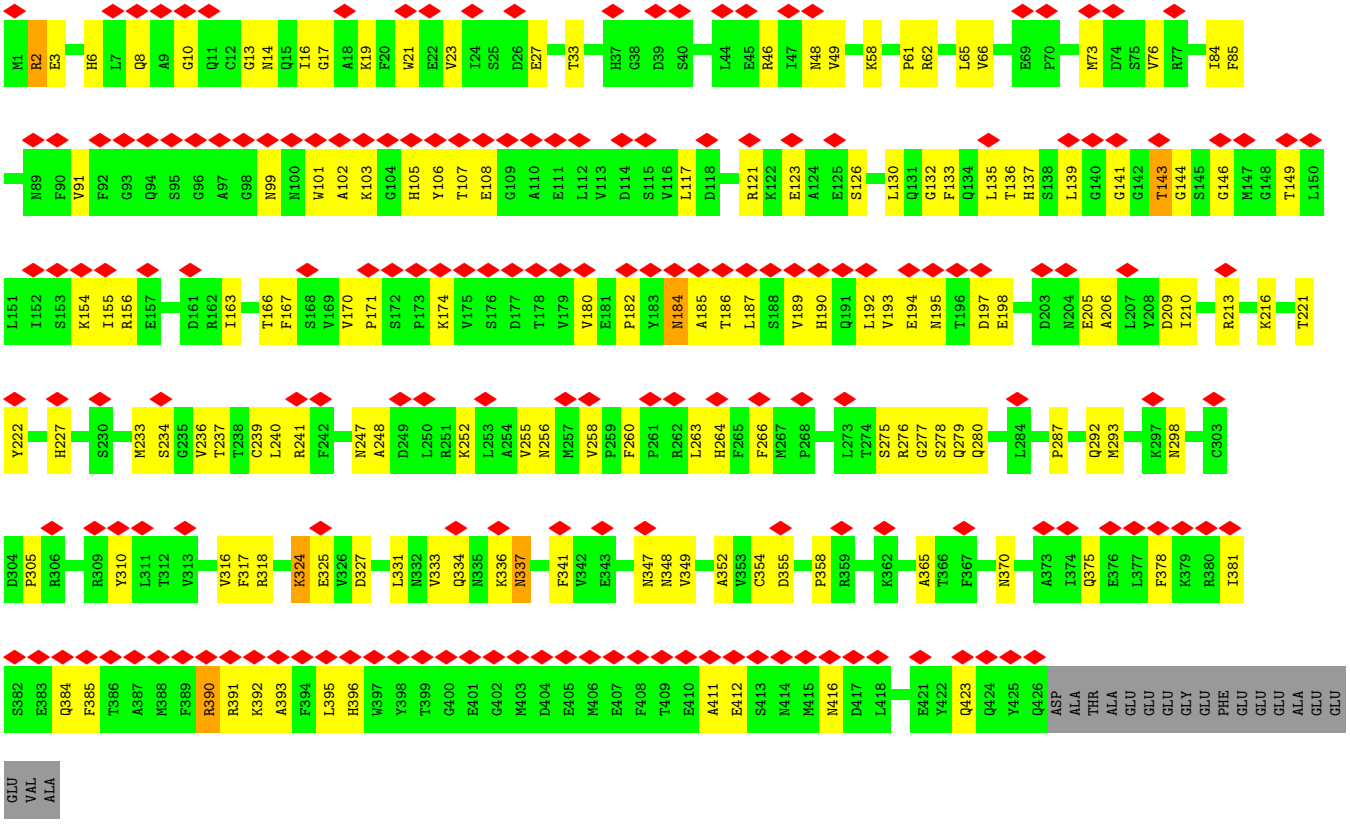




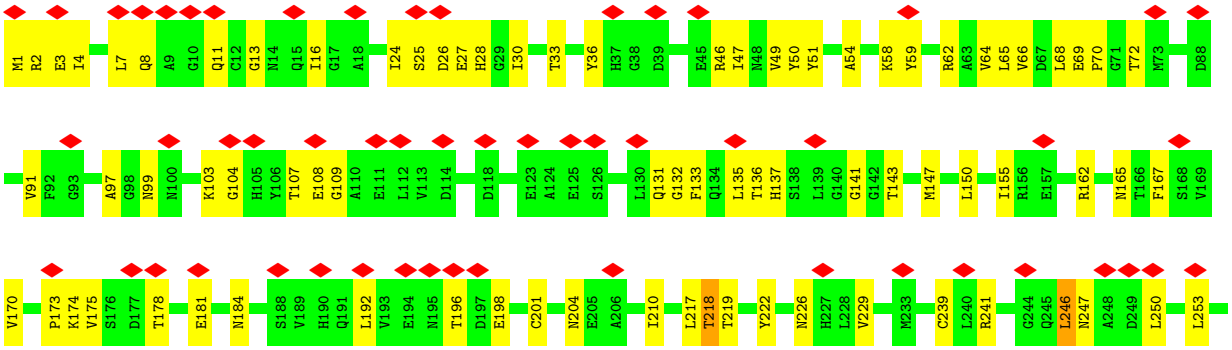
• Molecule 41: Tubulin beta-4B chain

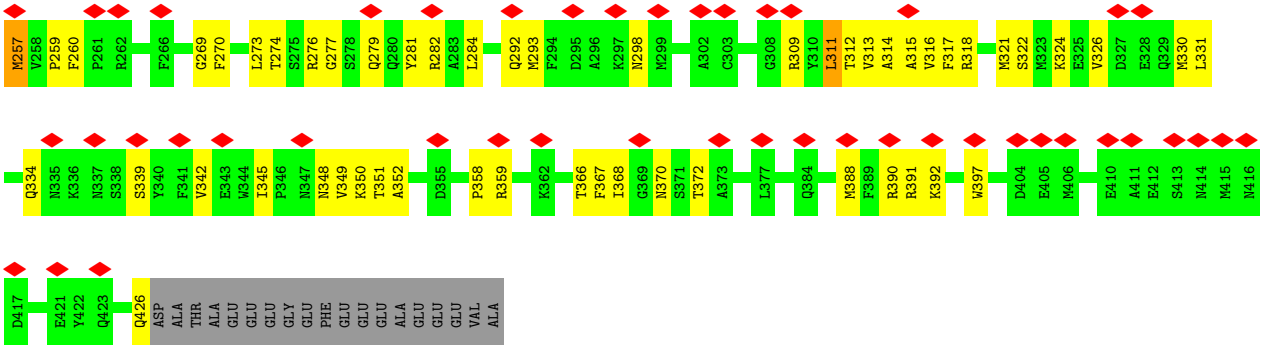
Chain DB:



• Molecule 41: Tubulin beta-4B chain

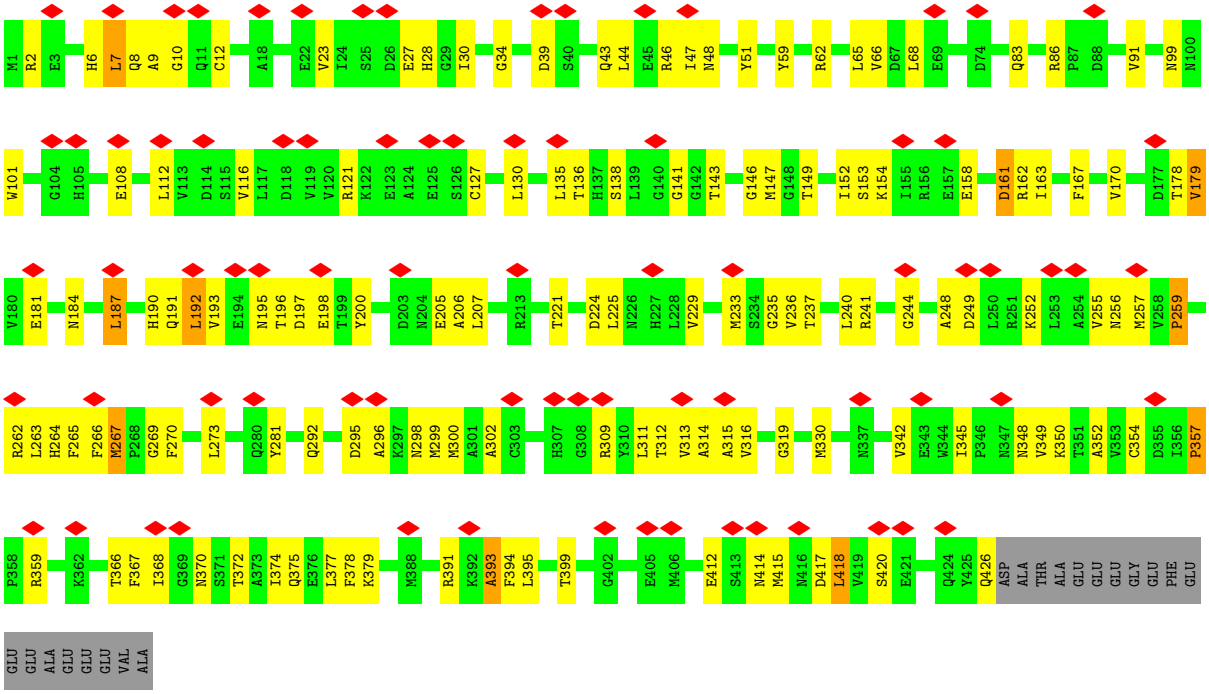
Chain DD:





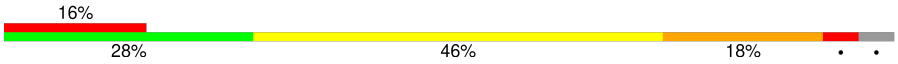
- Molecule 41: Tubulin beta-4B chain

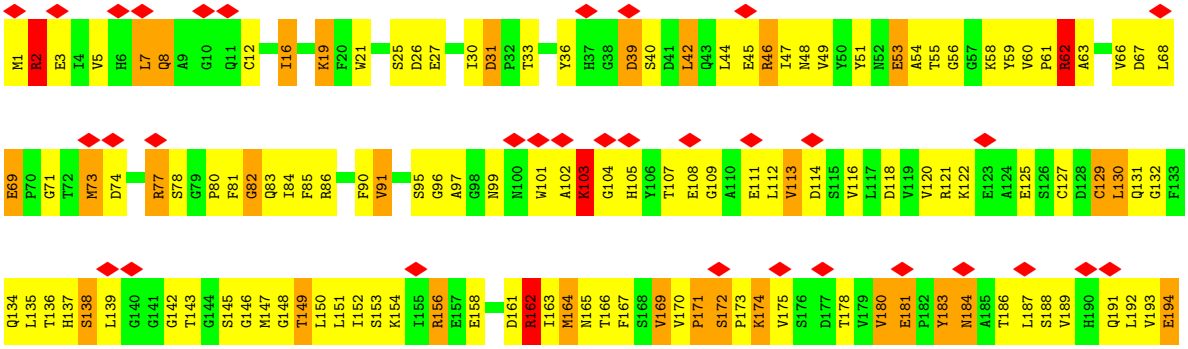
Chain DF:

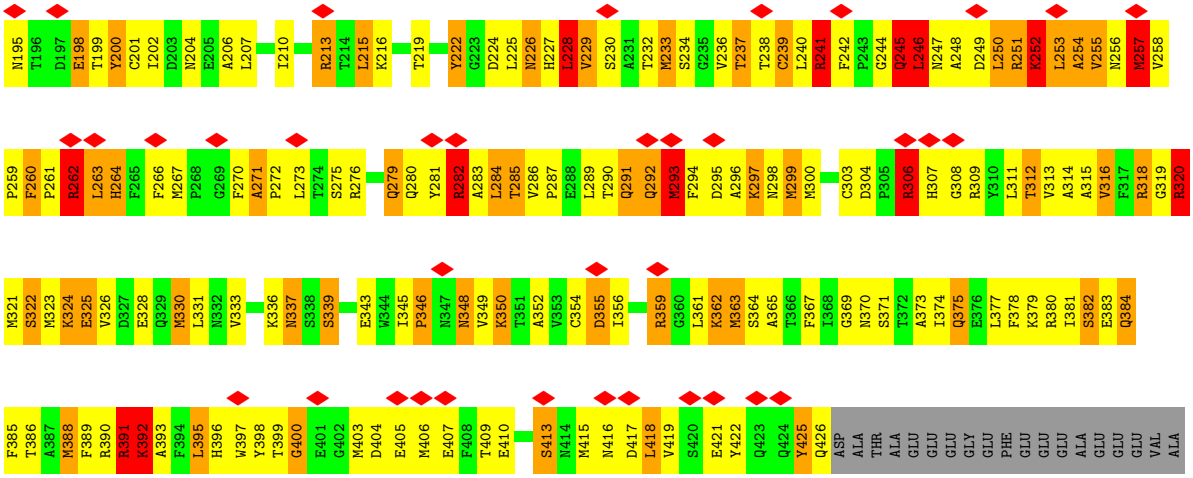


- Molecule 41: Tubulin beta-4B chain

Chain DH:

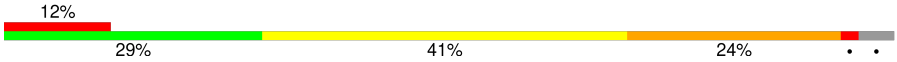


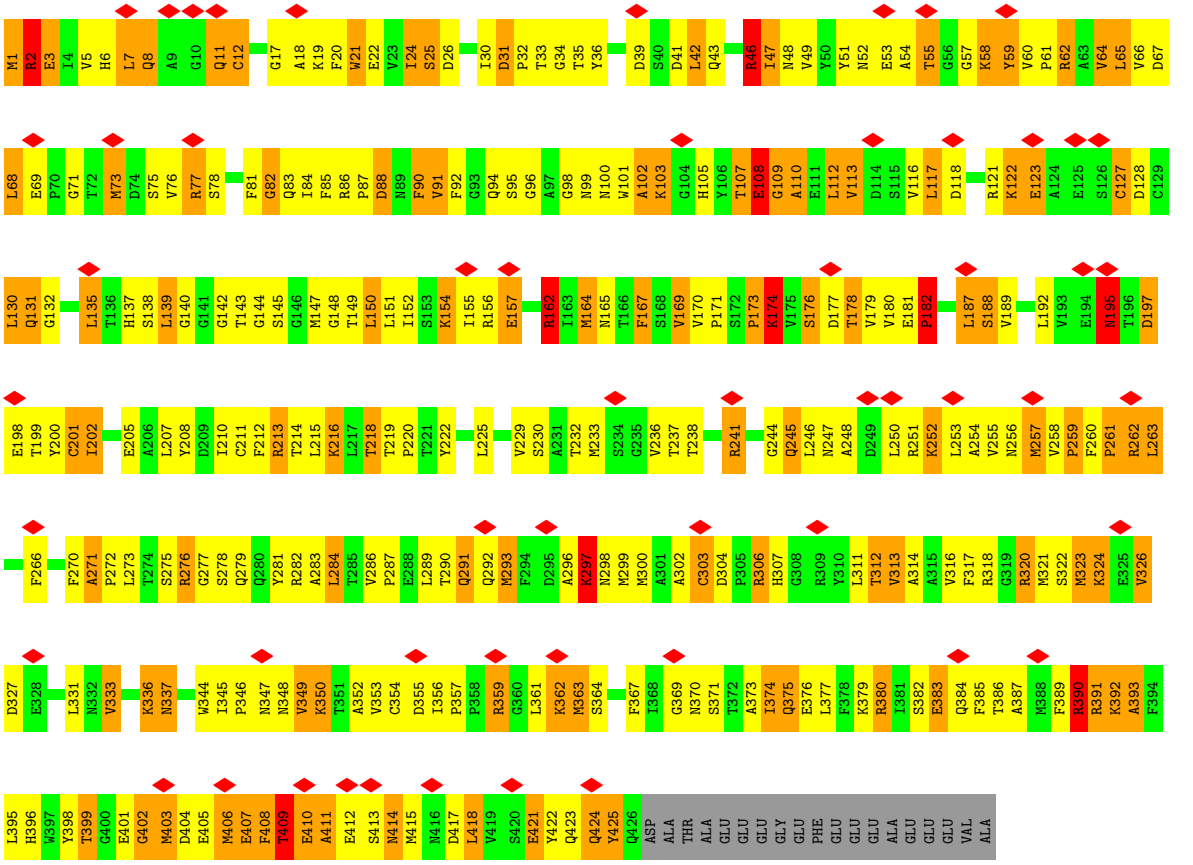




- Molecule 41: Tubulin beta-4B chain

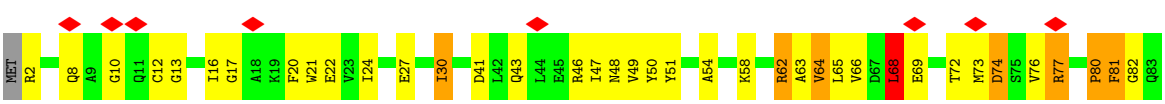
Chain DJ:

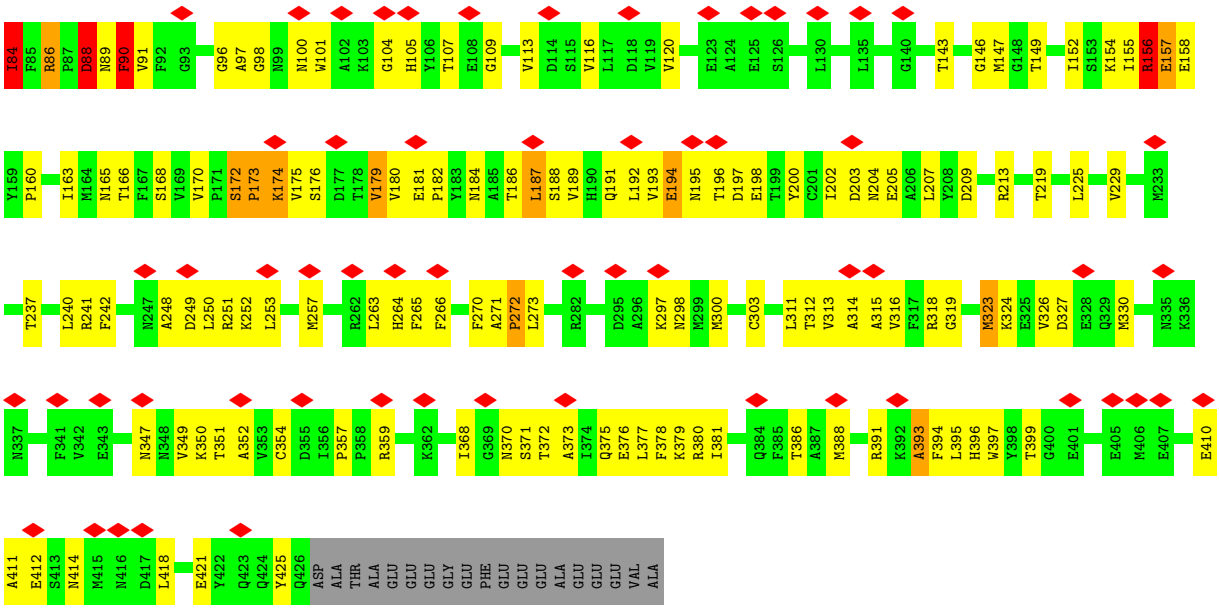




- Molecule 41: Tubulin beta-4B chain

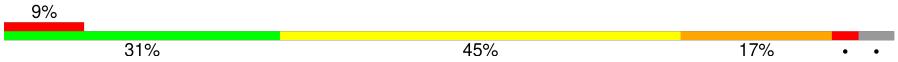
Chain DL:

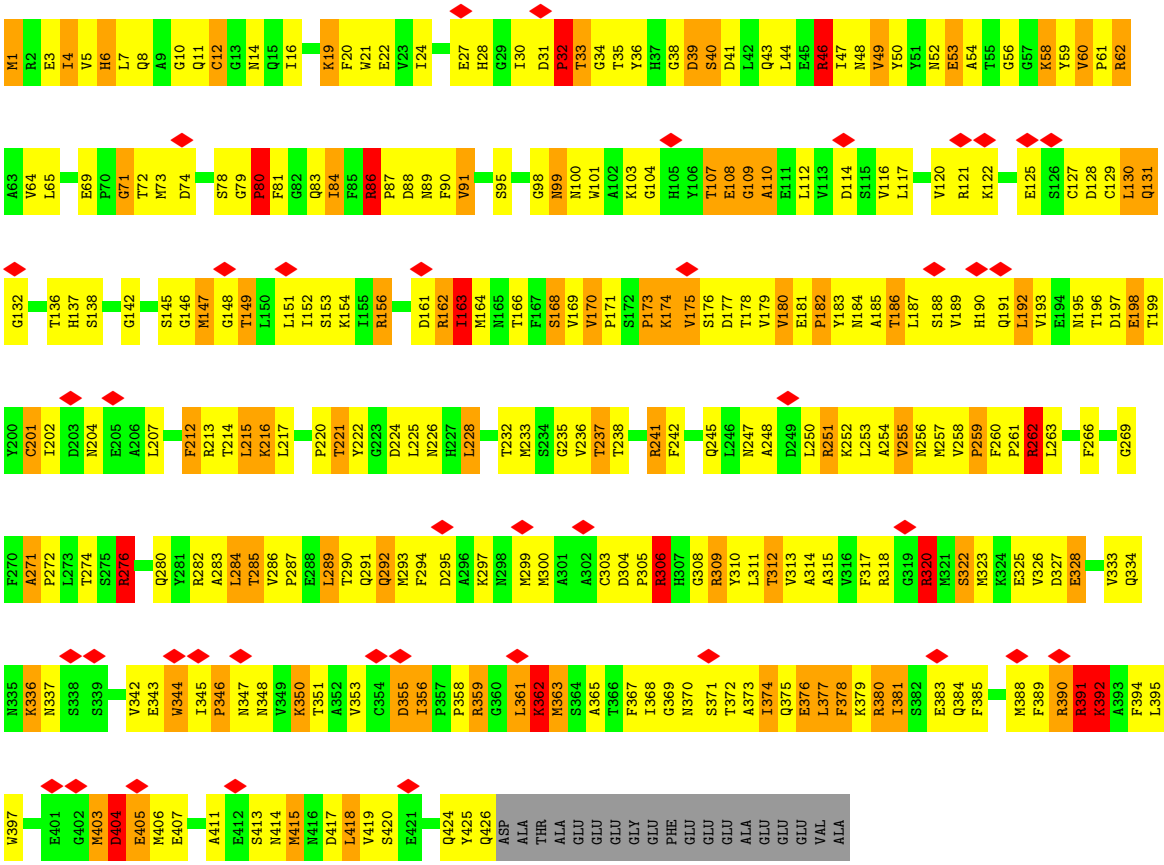




• Molecule 41: Tubulin beta-4B chain

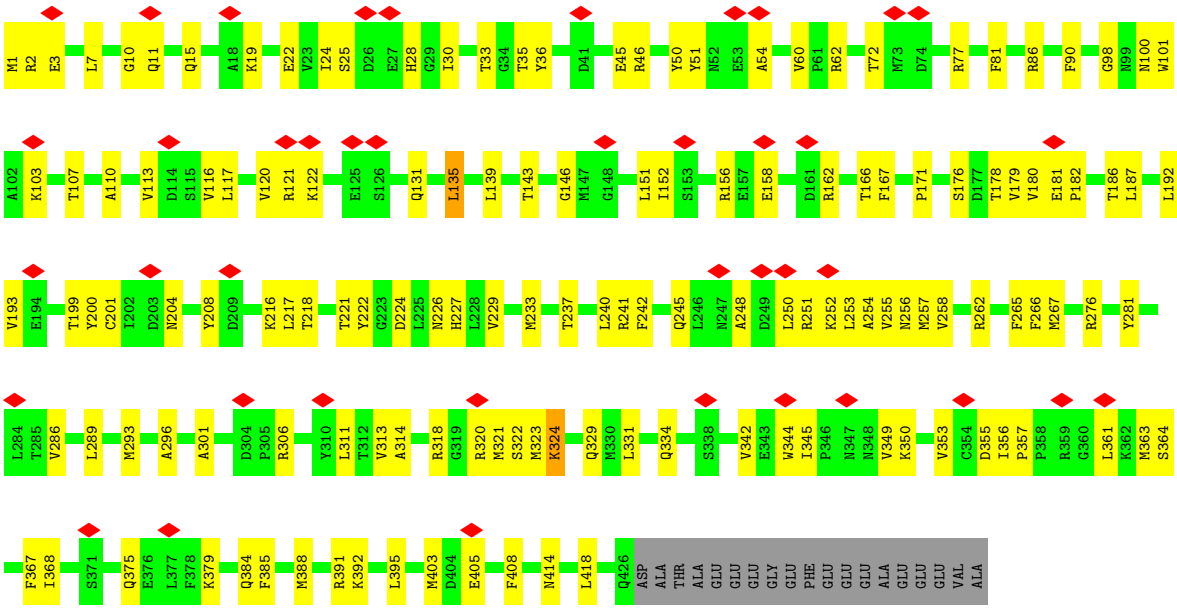
Chain ED:





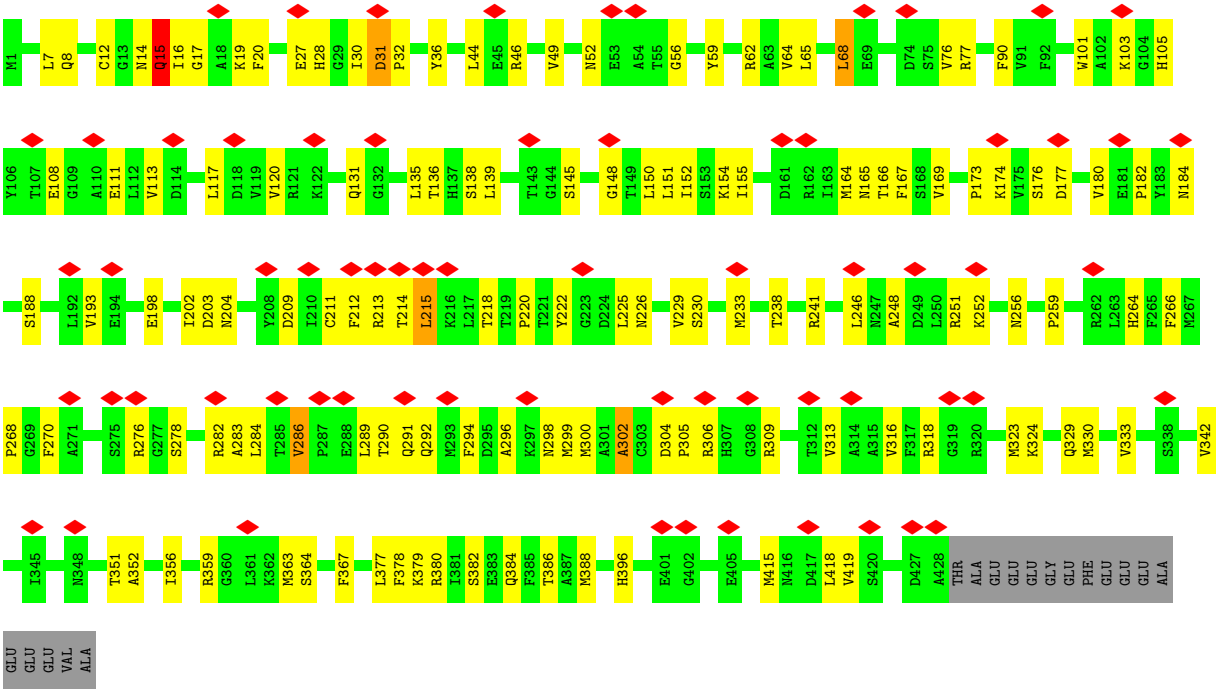
• Molecule 41: Tubulin beta-4B chain

Chain EF:



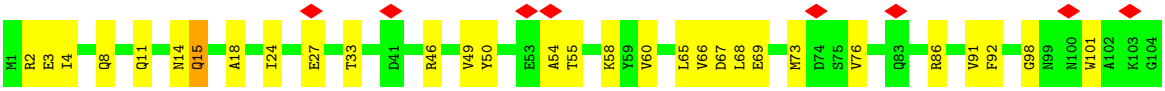
- Molecule 41: Tubulin beta-4B chain

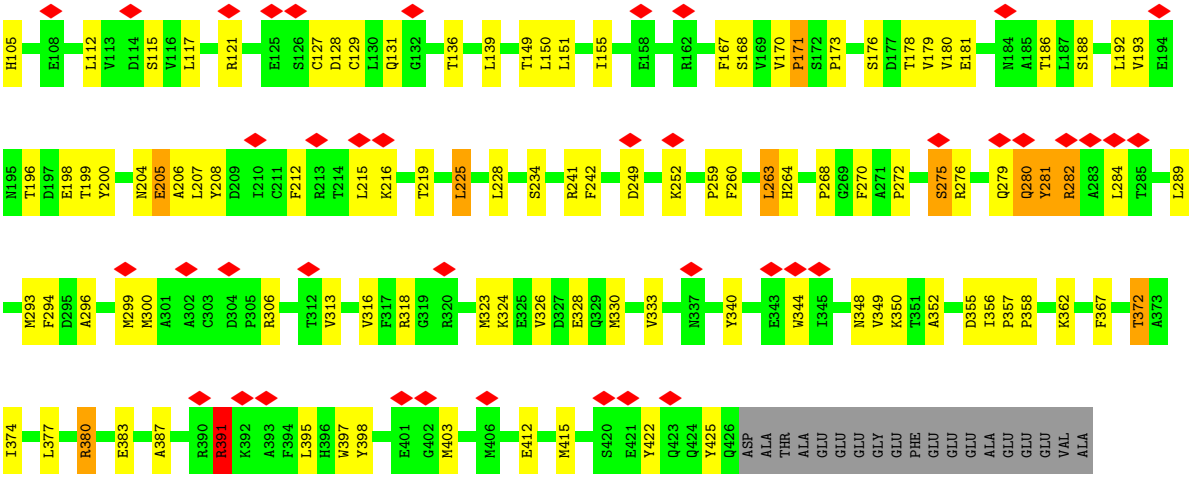
Chain EH:



- Molecule 41: Tubulin beta-4B chain

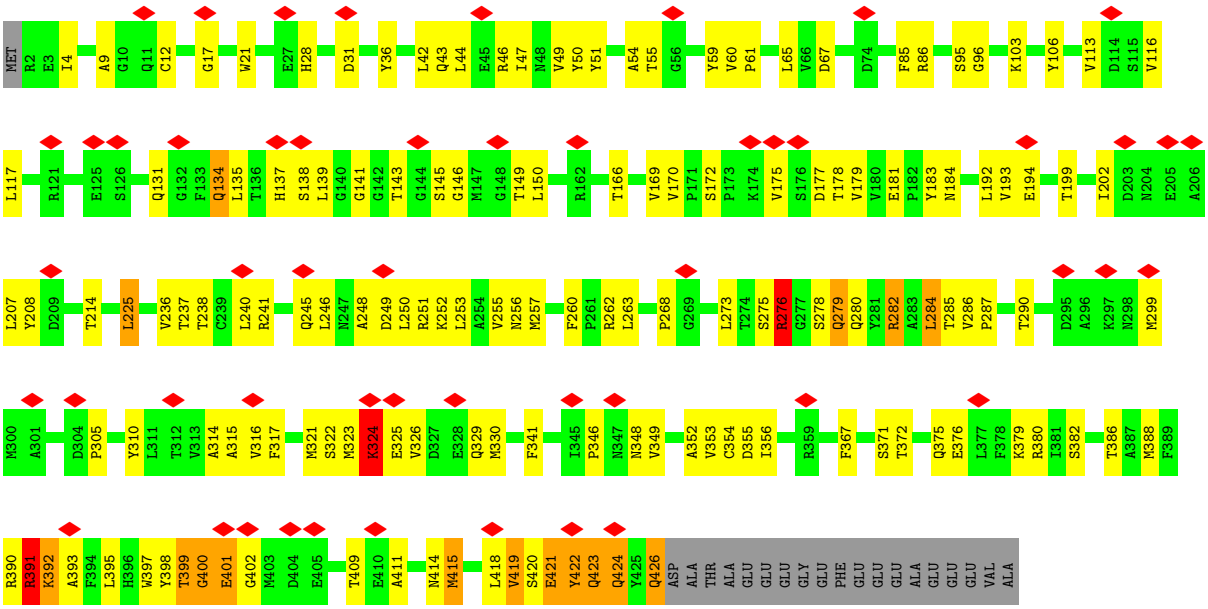
Chain EJ:





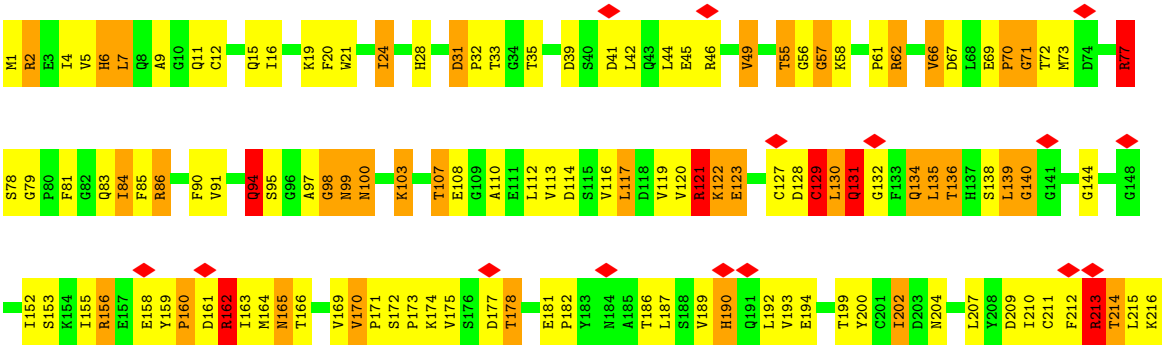
• Molecule 41: Tubulin beta-4B chain

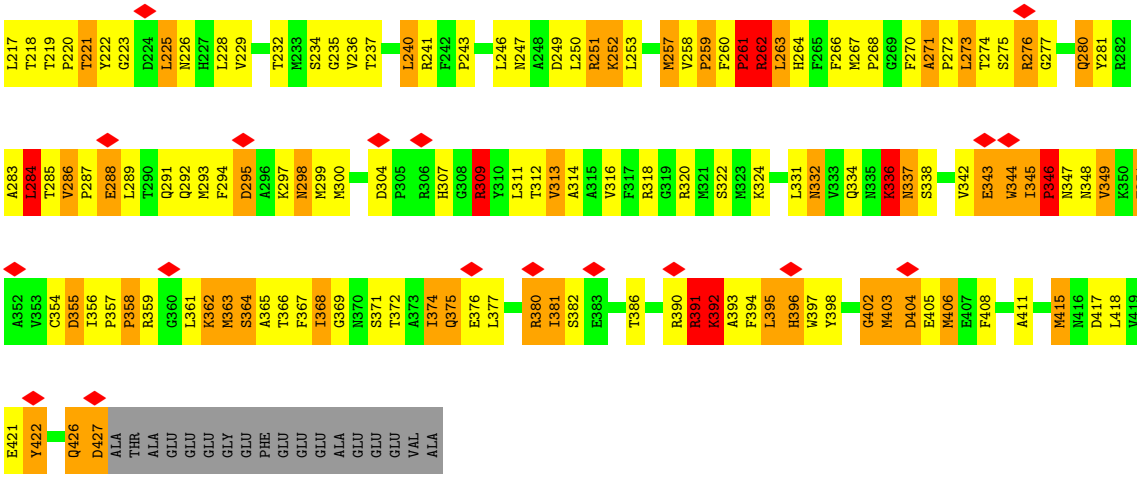
Chain EL:



• Molecule 41: Tubulin beta-4B chain

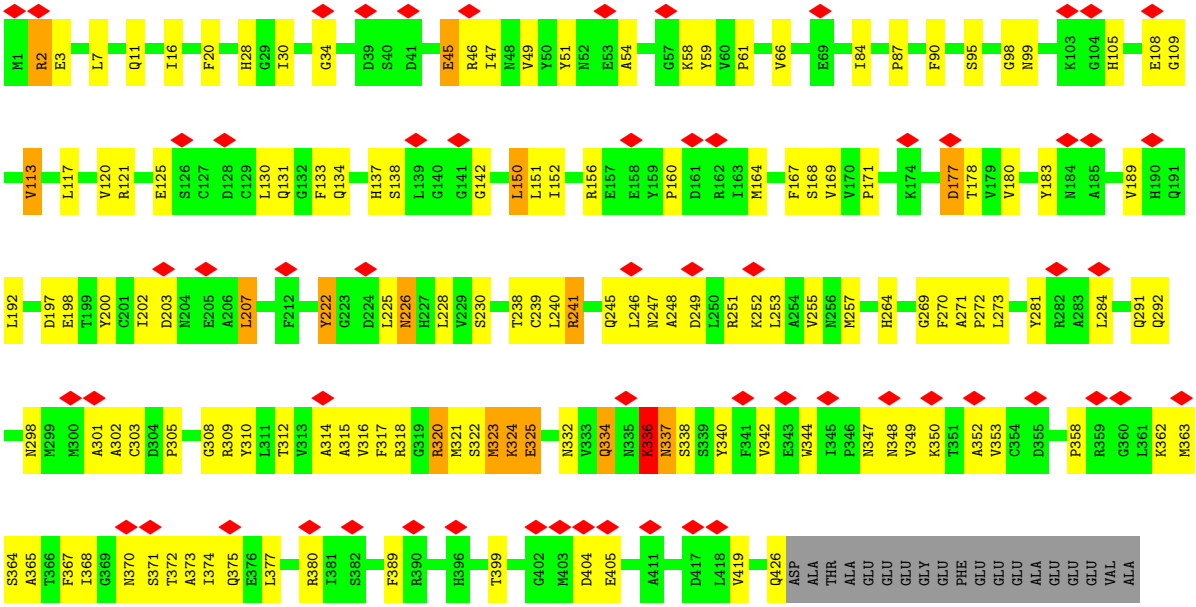
Chain FD:





• Molecule 41: Tubulin beta-4B chain

Chain FF:



• Molecule 41: Tubulin beta-4B chain

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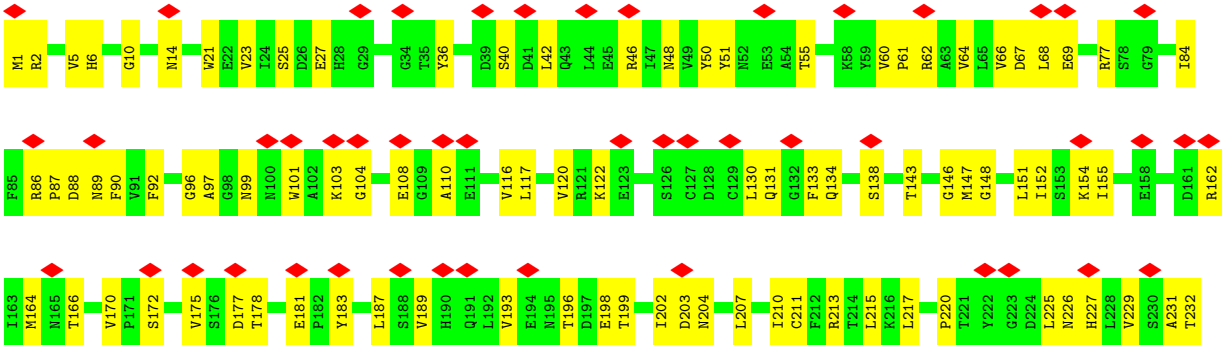

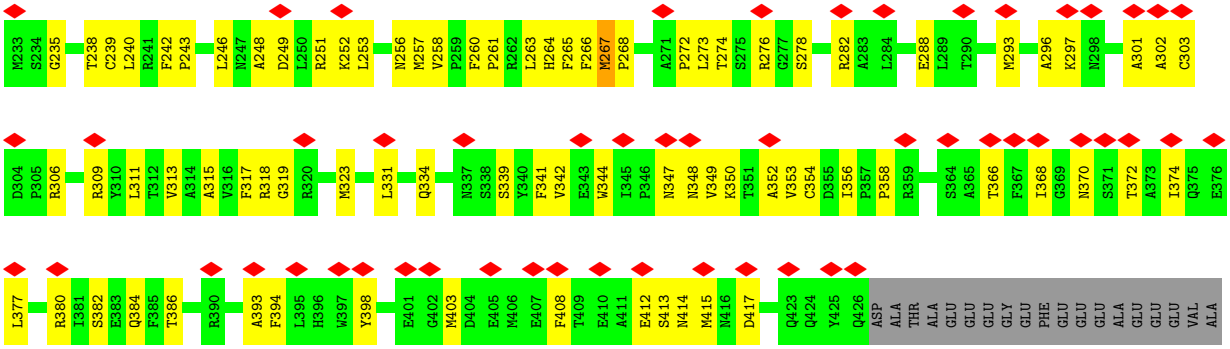

- Molecule 41: Tubulin beta-4B chain

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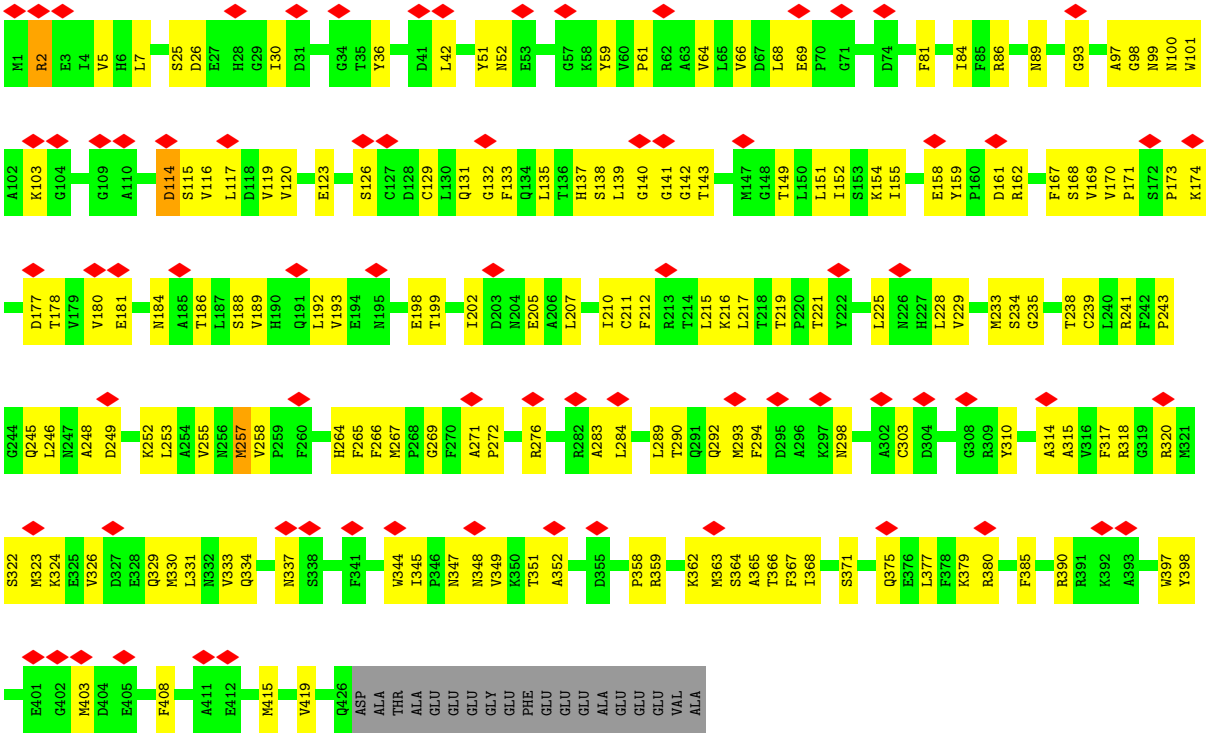
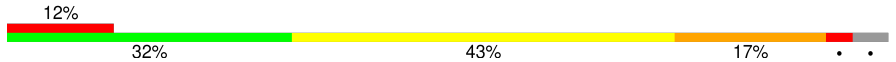
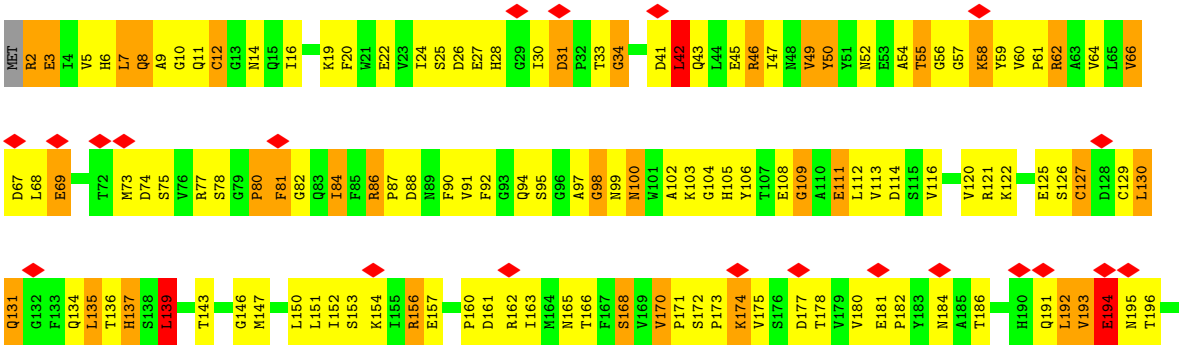
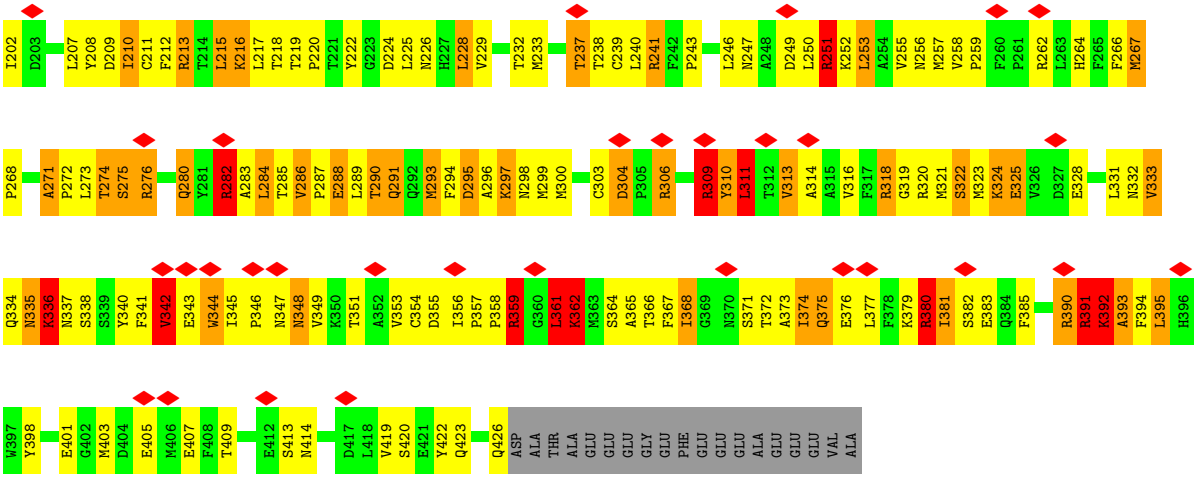


- Molecule 41: Tubulin beta-4B chain

Chain FL:

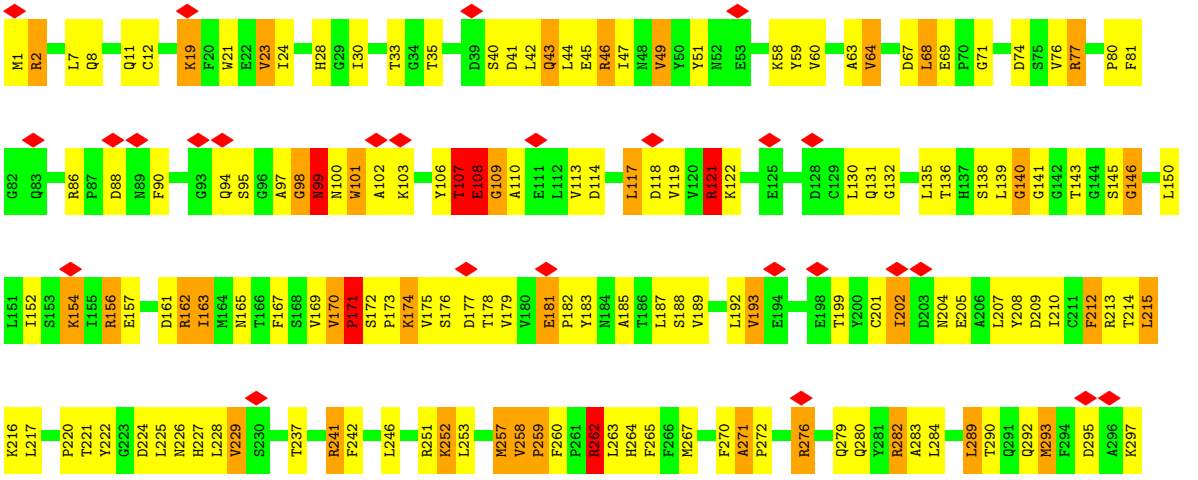






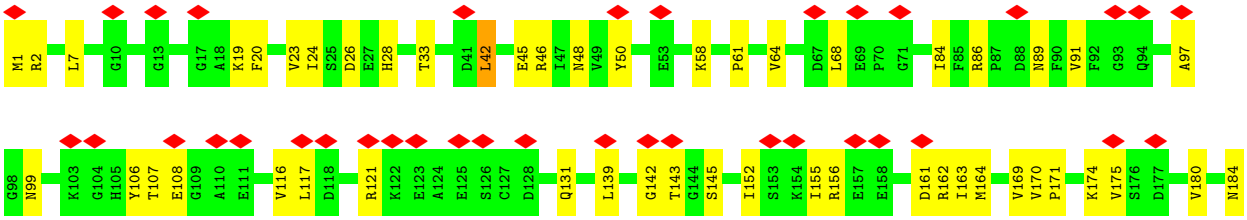
- Molecule 41: Tubulin beta-4B chain

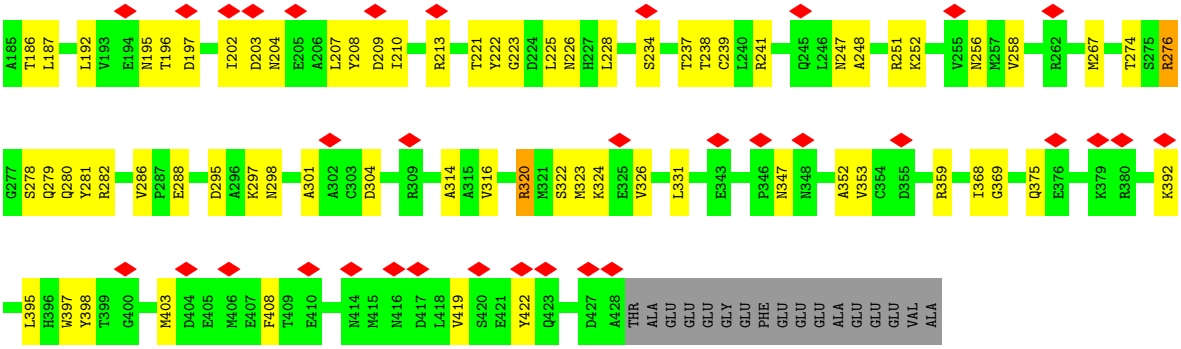
Chain GD:



- Molecule 41: Tubulin beta-4B chain

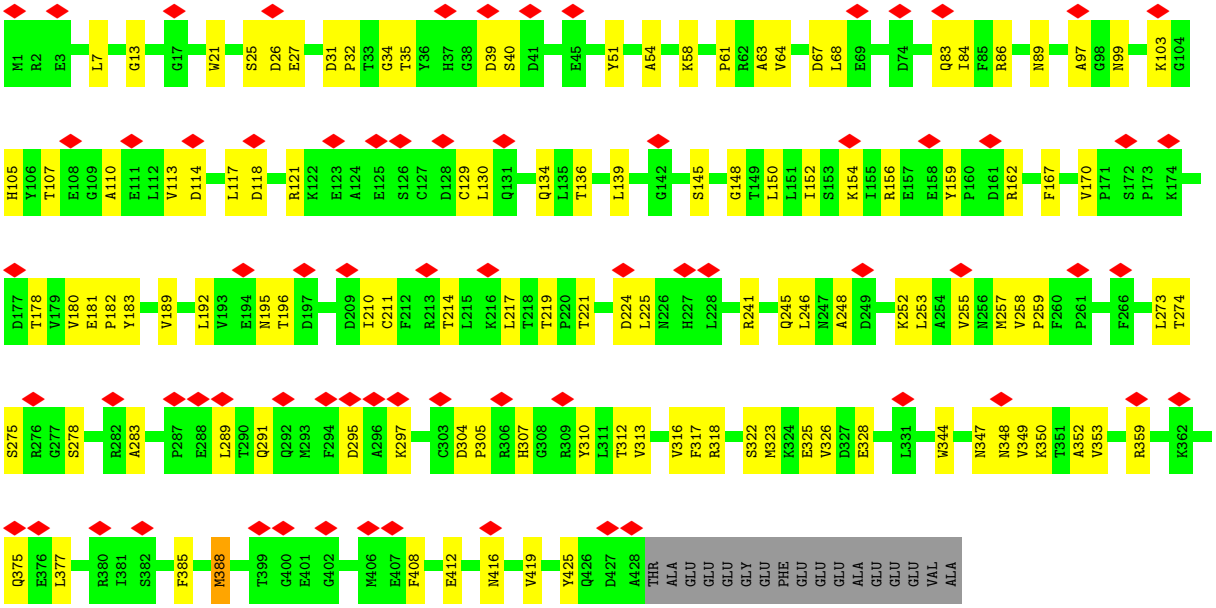
Chain GF:





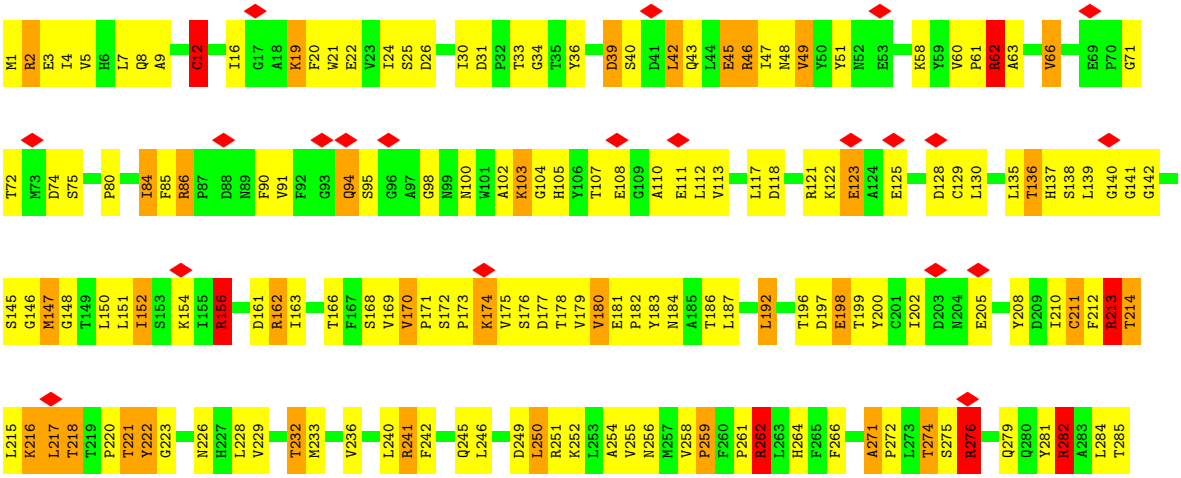
• Molecule 41: Tubulin beta-4B chain

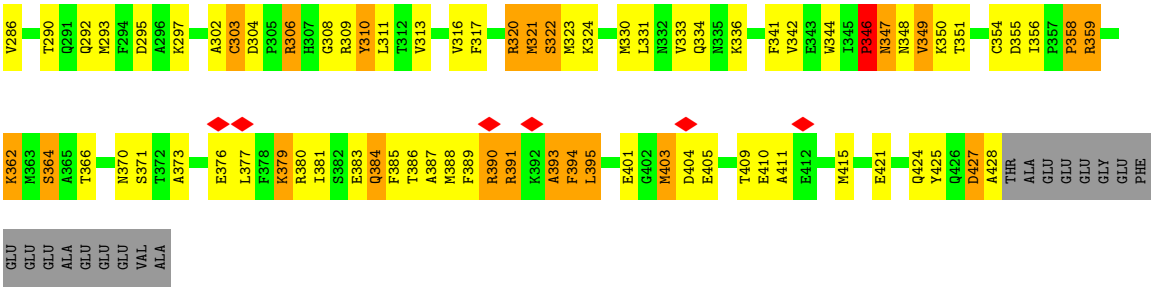
Chain GH:



• Molecule 41: Tubulin beta-4B chain

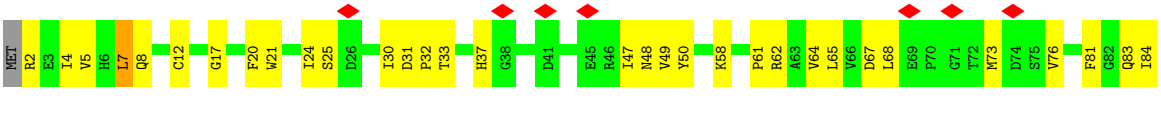
Chain GJ:

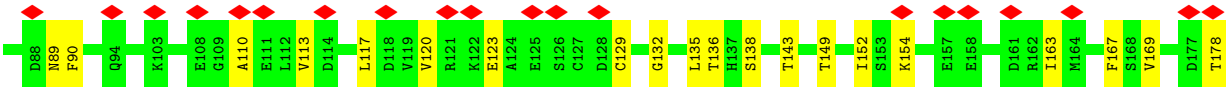


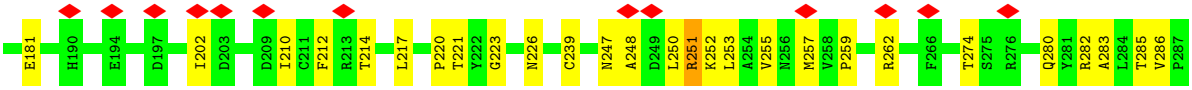


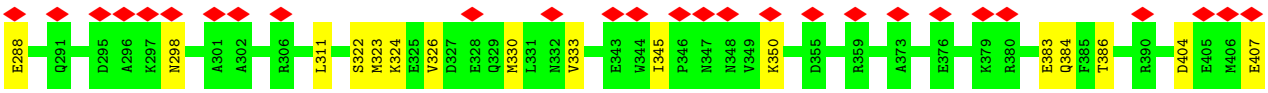
- Molecule 41: Tubulin beta-4B chain

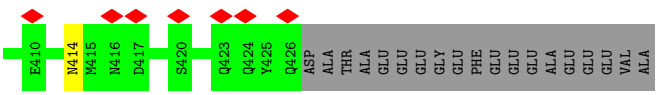
Chain GL:





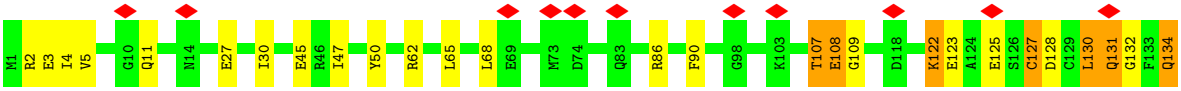


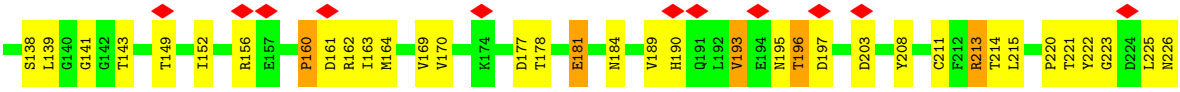


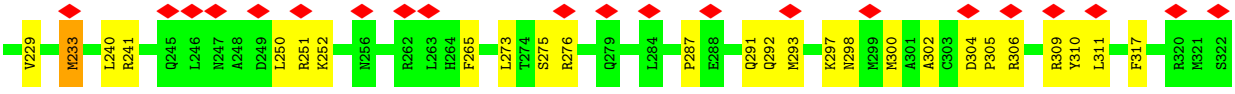


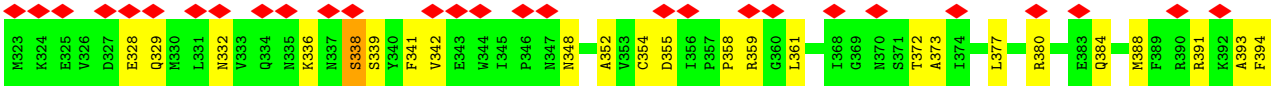
- Molecule 41: Tubulin beta-4B chain

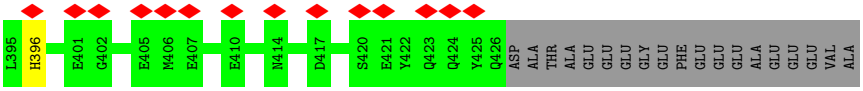
Chain HB:





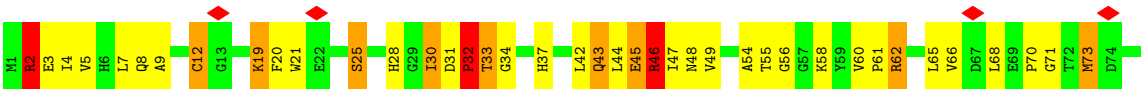


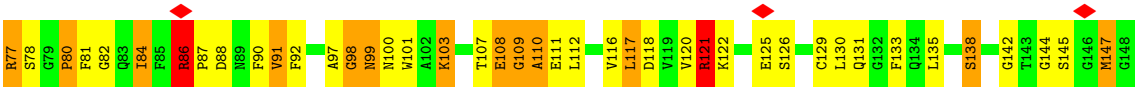


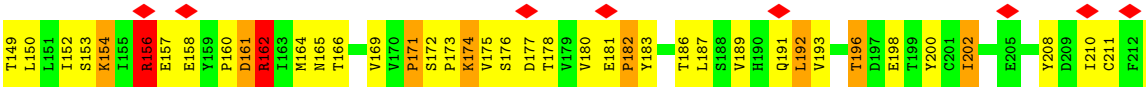


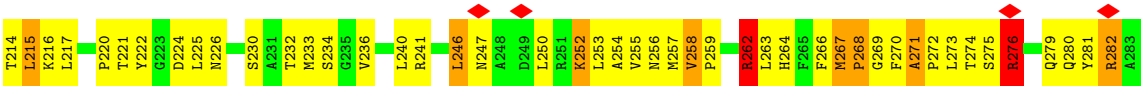
- Molecule 41: Tubulin beta-4B chain

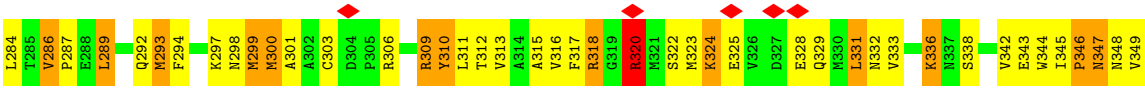
Chain HD:

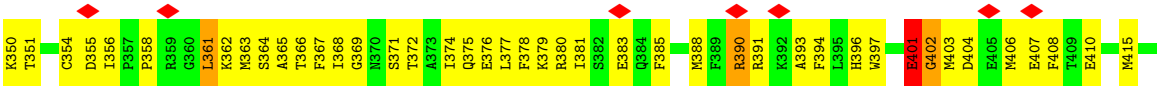






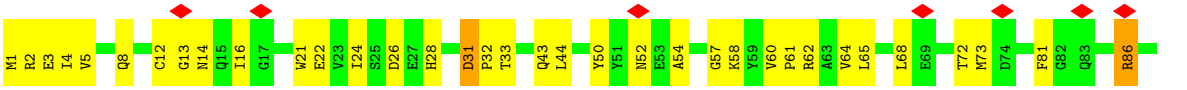


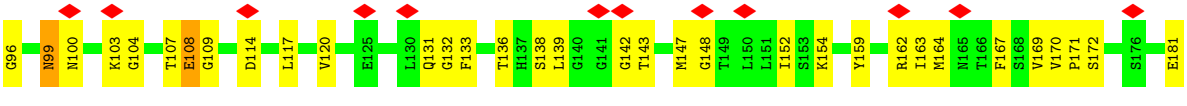


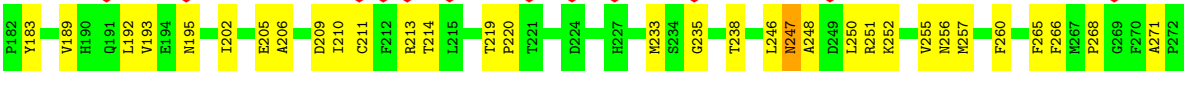


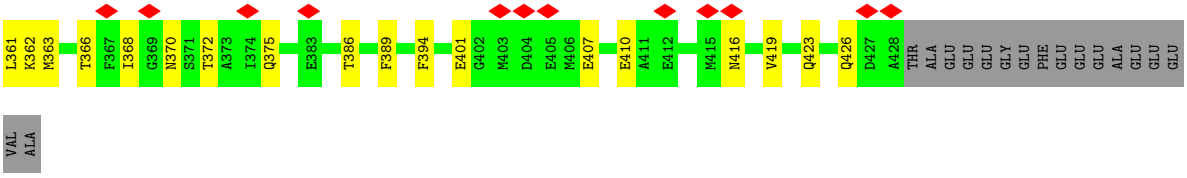
- Molecule 41: Tubulin beta-4B chain

Chain HF:



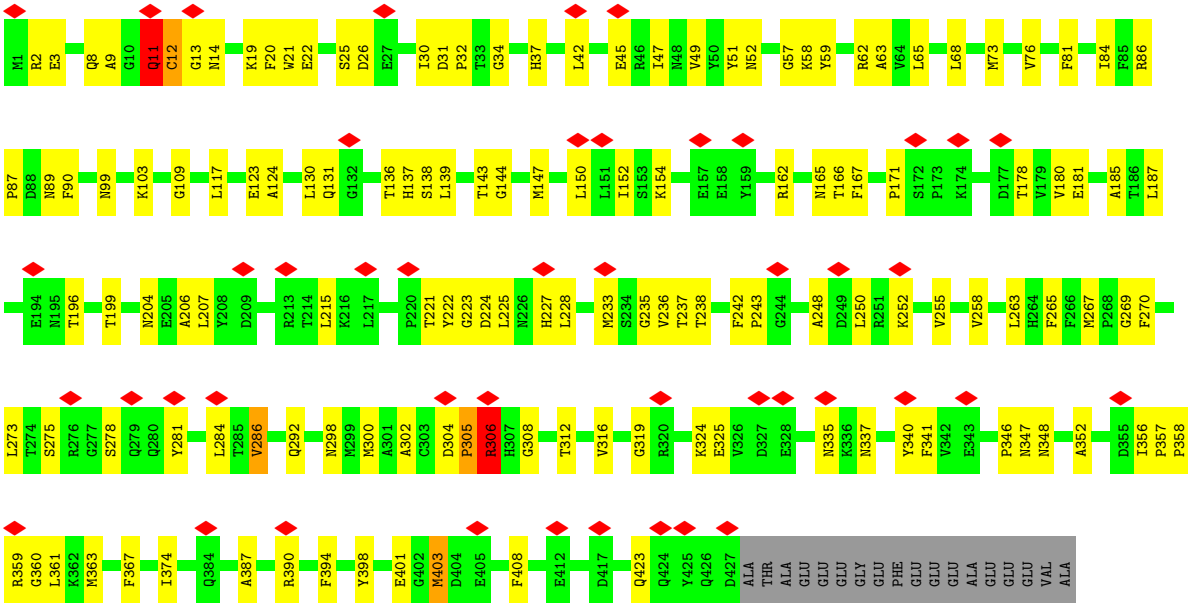






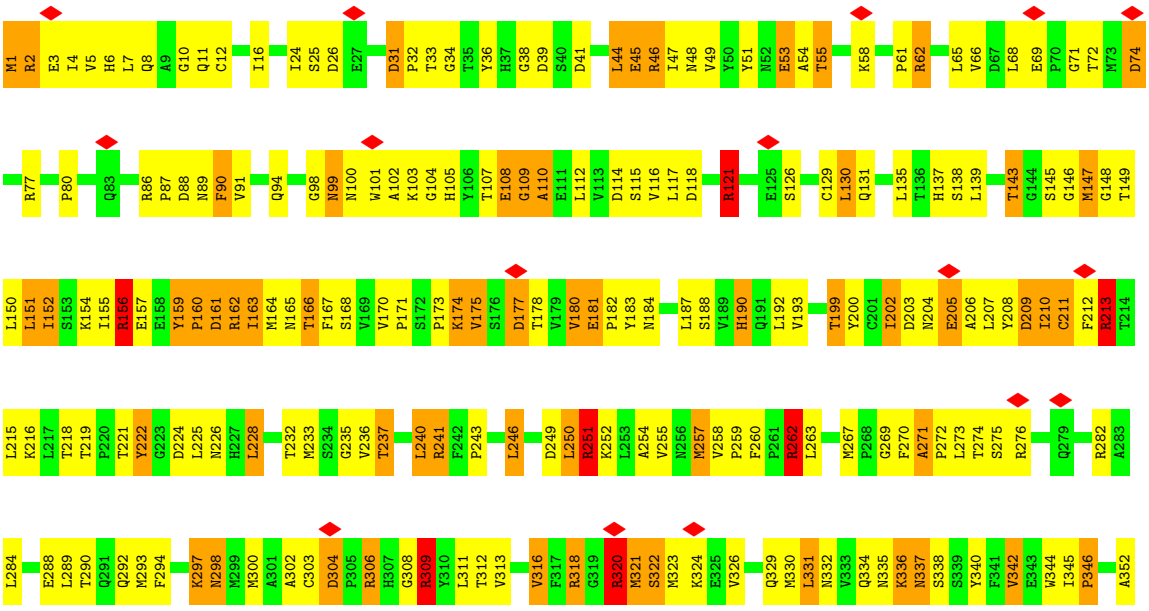
• Molecule 41: Tubulin beta-4B chain

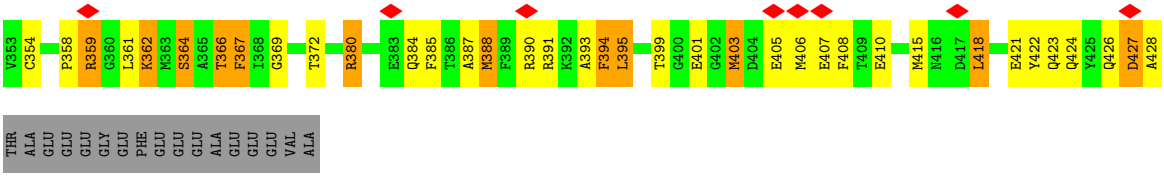
Chain HH:



• Molecule 41: Tubulin beta-4B chain

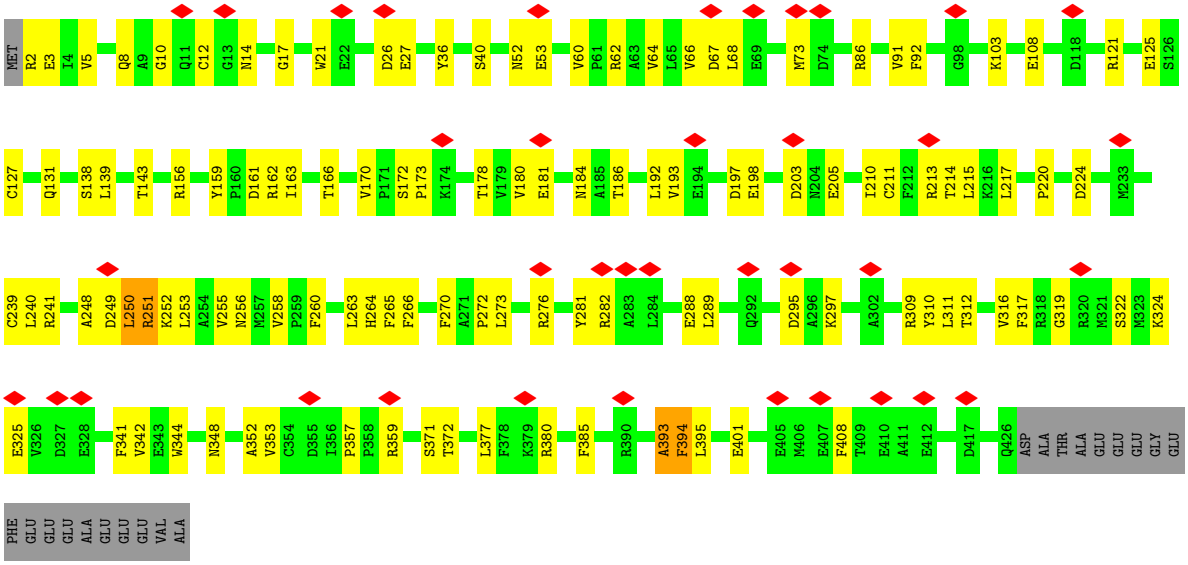
Chain HJ:





• Molecule 41: Tubulin beta-4B chain

Chain HL:



• Molecule 41: Tubulin beta-4B chain

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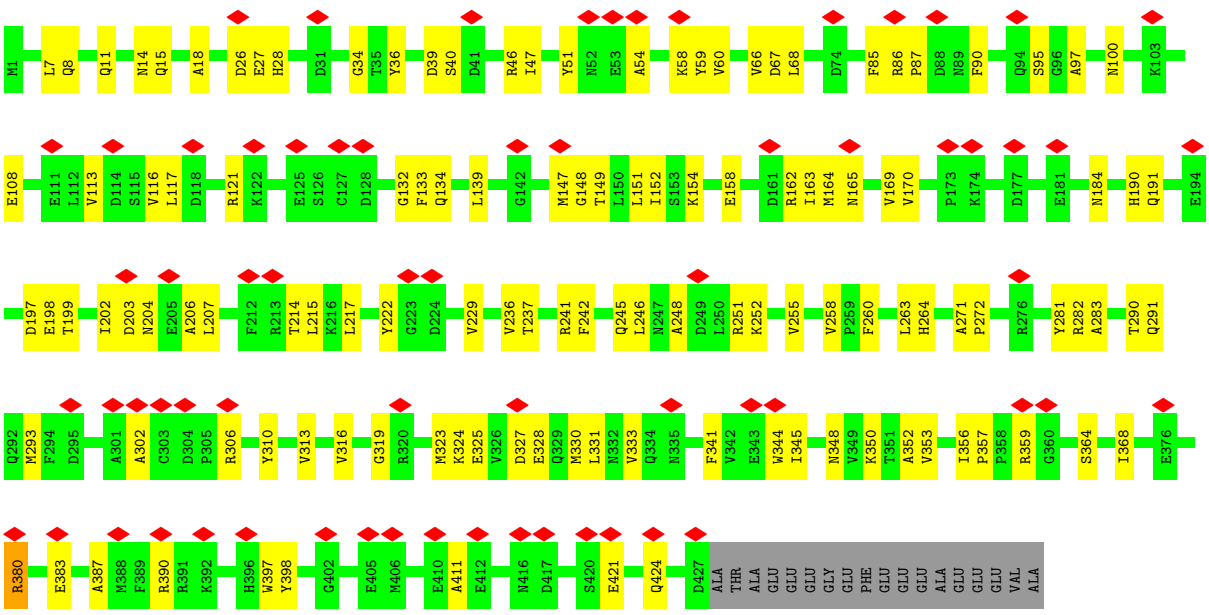
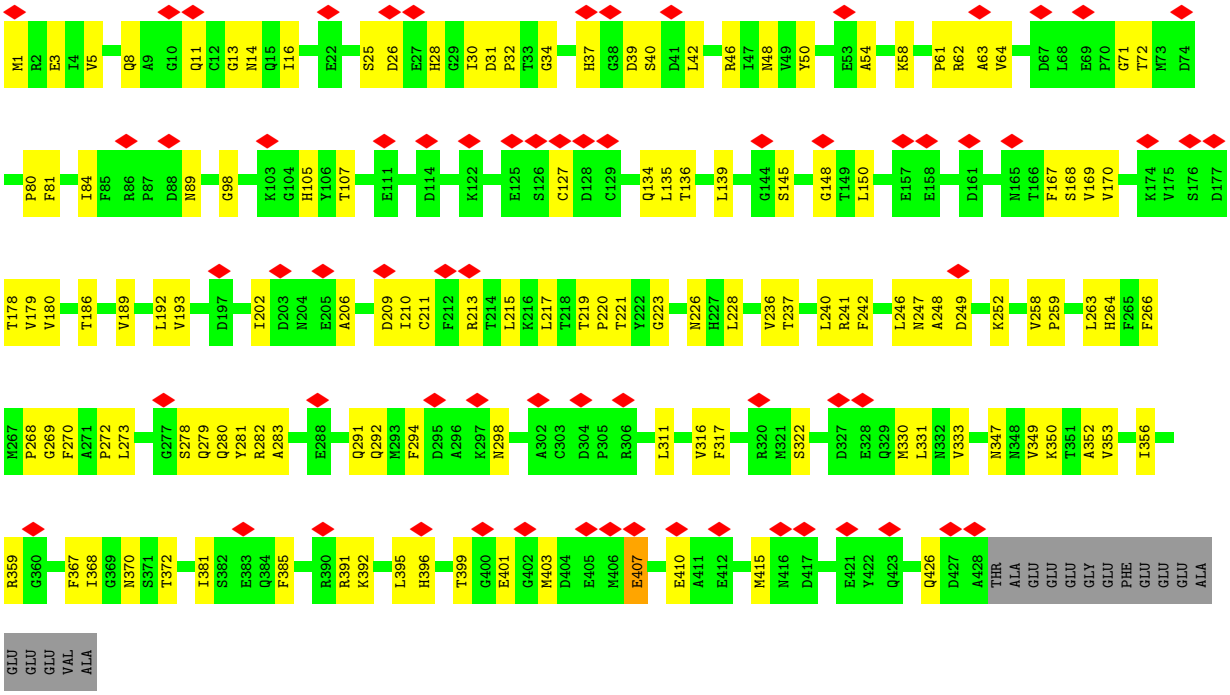


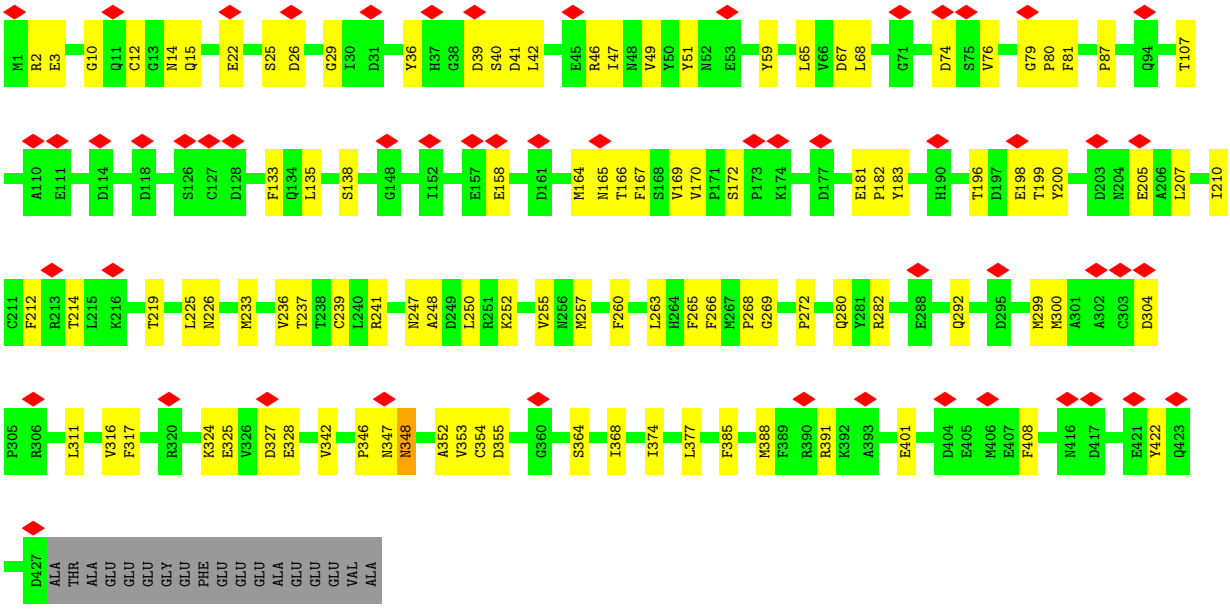
• Molecule 41: Tubulin beta-4B chain

Chain IF: 15% 67% 29%



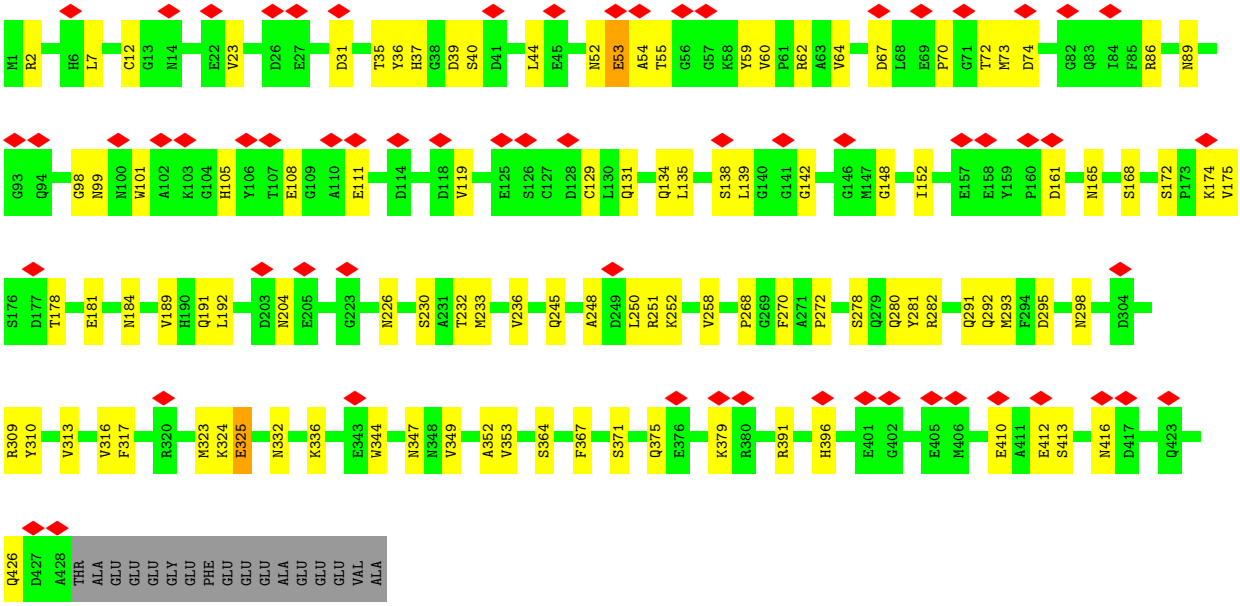
- Molecule 41: Tubulin beta-4B chain

Chain IH: 12% 72% 23%



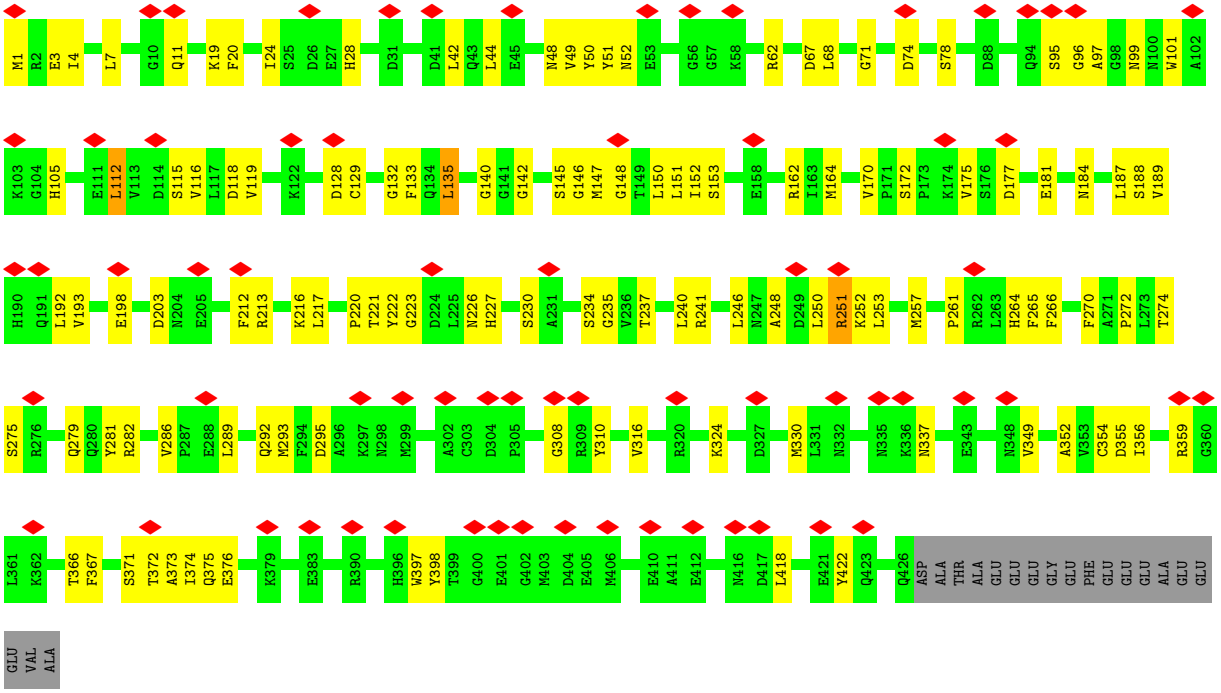
- Molecule 41: Tubulin beta-4B chain

Chain IJ: 14% 73% 23%



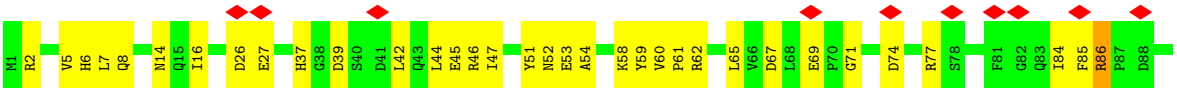
- Molecule 41: Tubulin beta-4B chain

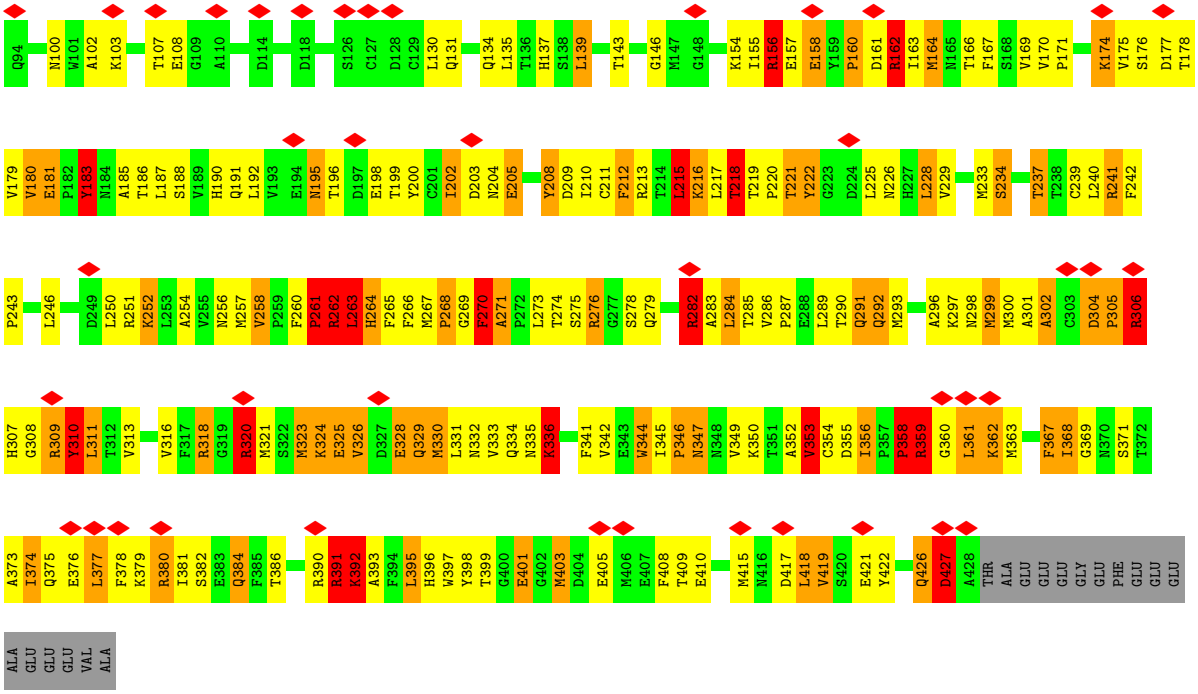
Chain IL:



- Molecule 41: Tubulin beta-4B chain

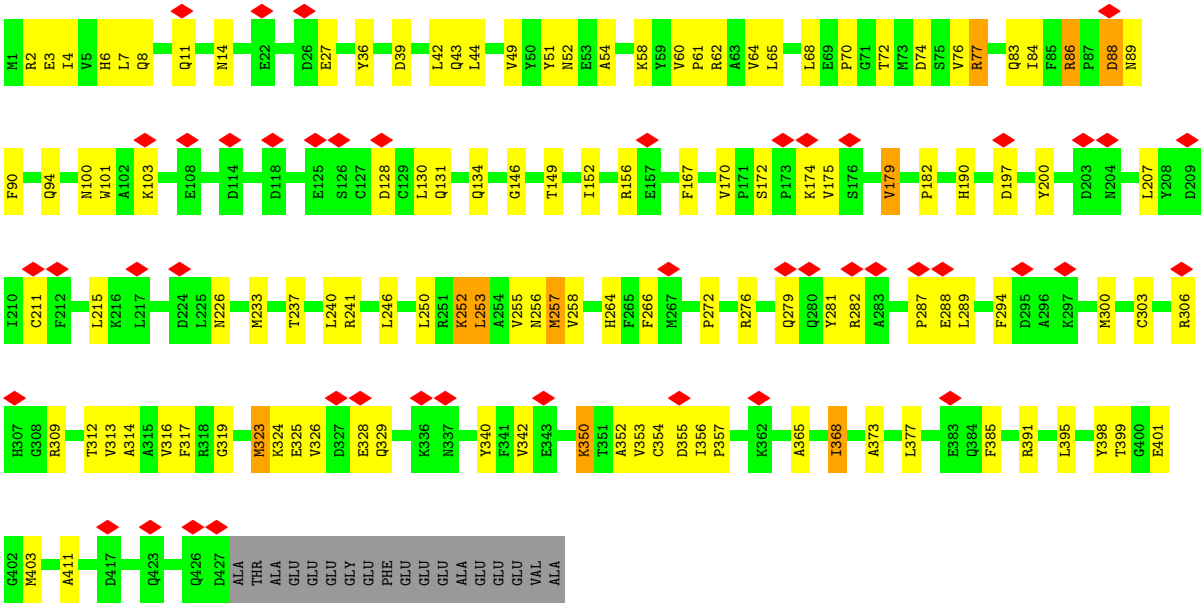
Chain IN:





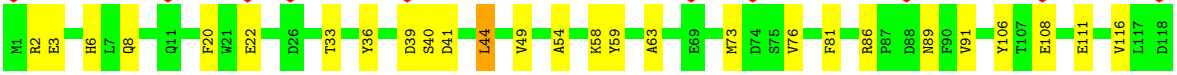
• Molecule 41: Tubulin beta-4B chain

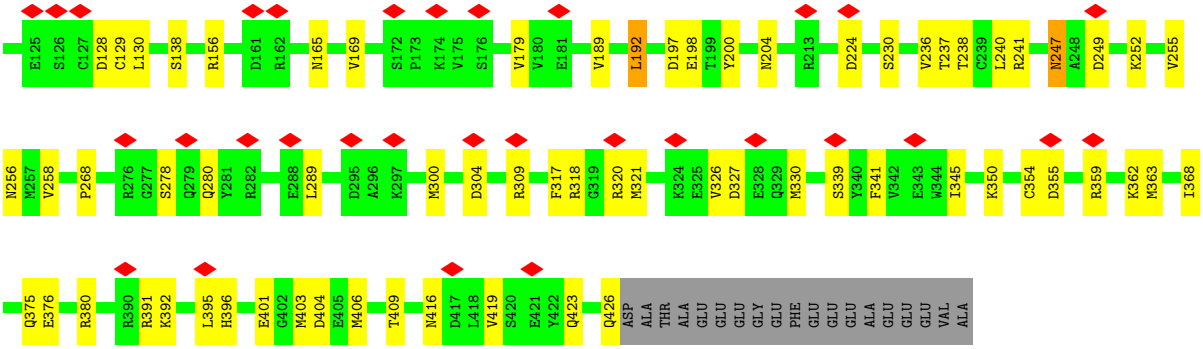
Chain JD:



• Molecule 41: Tubulin beta-4B chain

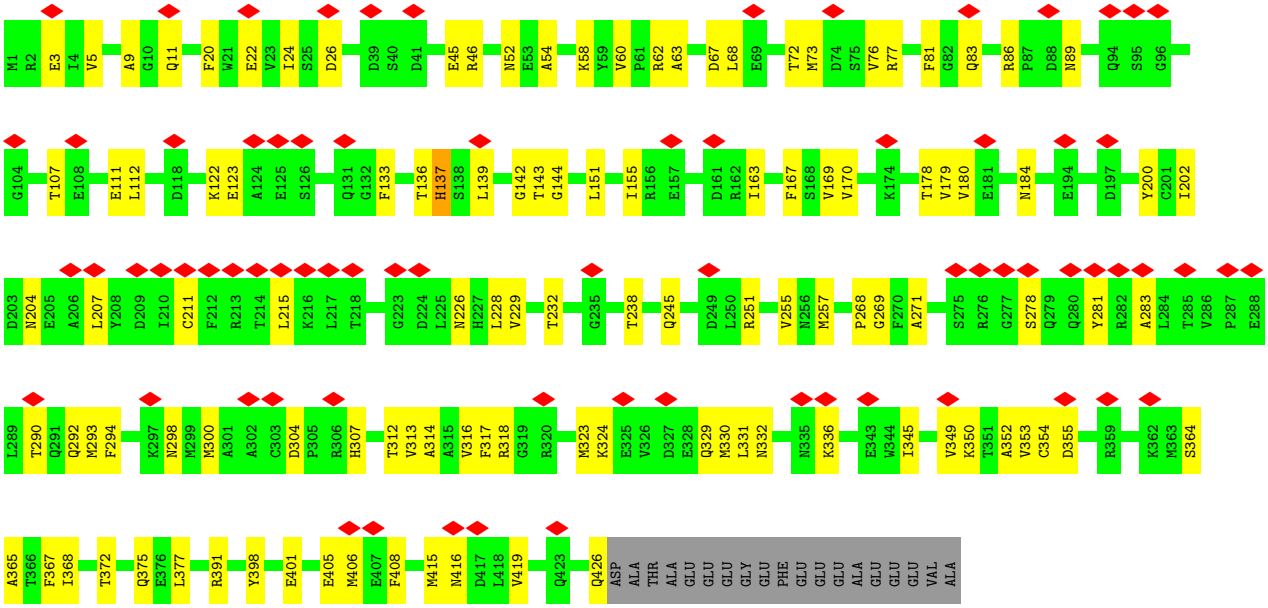
Chain JF:





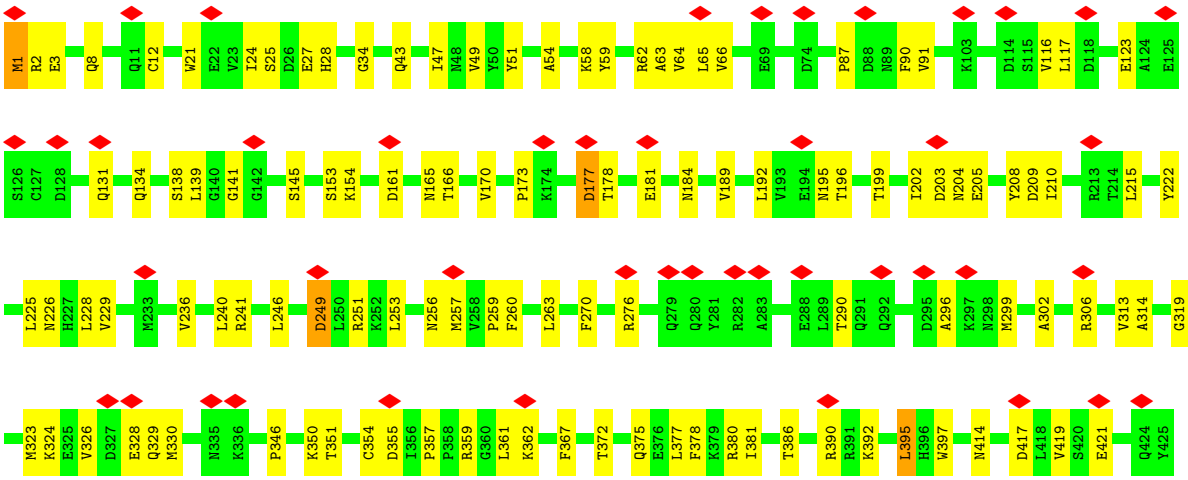
- Molecule 41: Tubulin beta-4B chain

Chain JH:



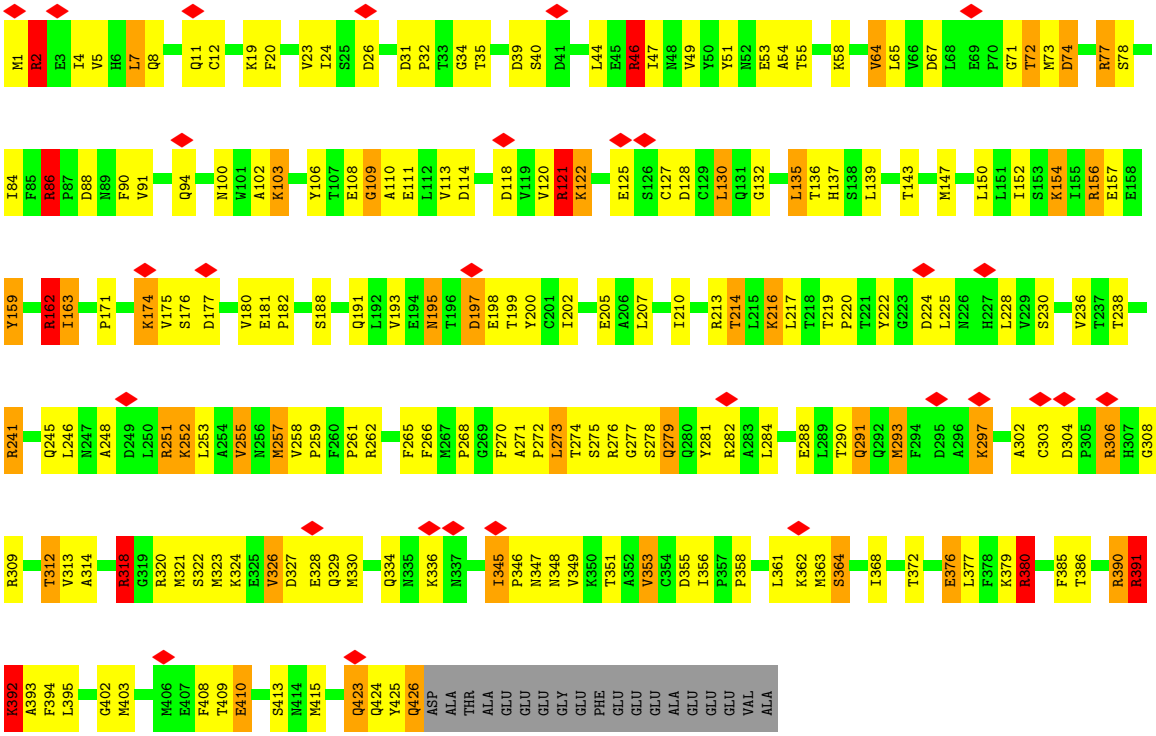
- Molecule 41: Tubulin beta-4B chain

Chain JJ:



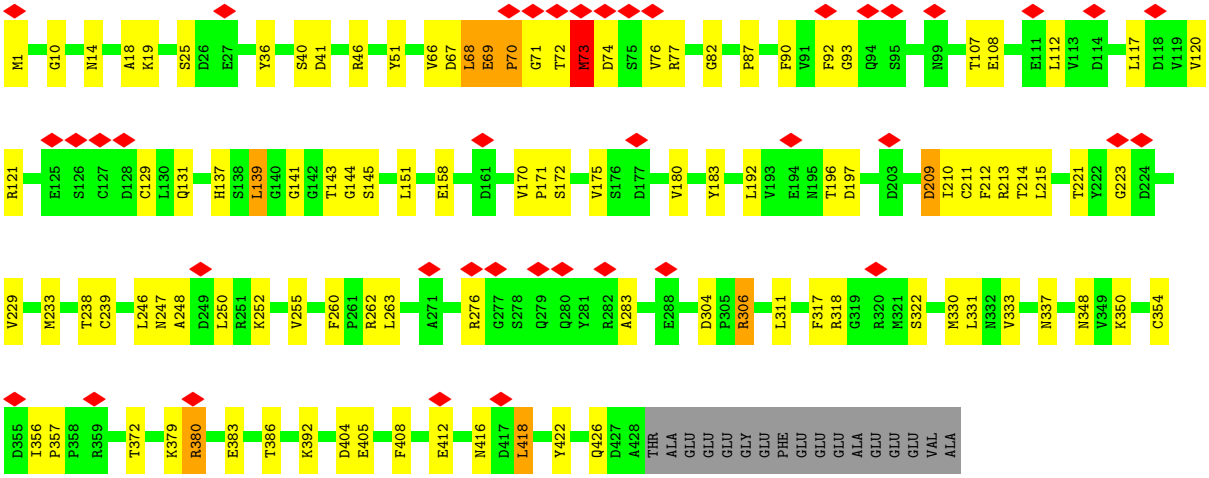
- Molecule 41: Tubulin beta-4B chain

Chain JL:



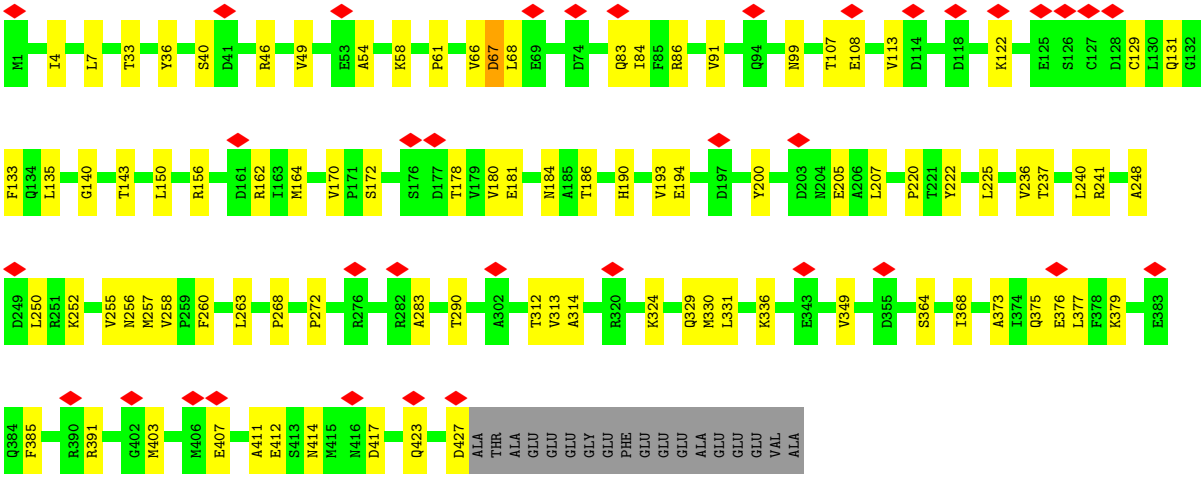
- Molecule 41: Tubulin beta-4B chain

Chain KD:



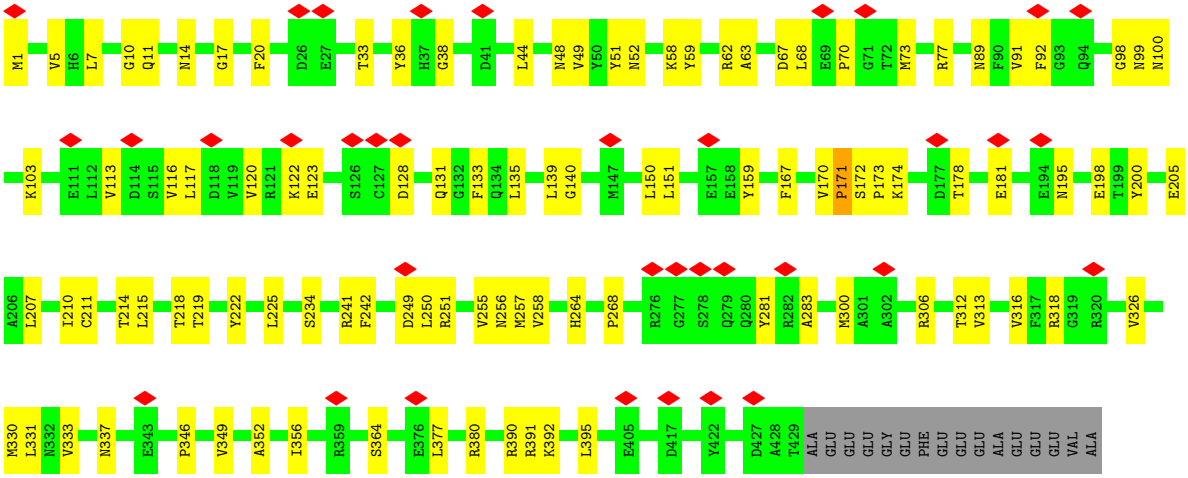
- Molecule 41: Tubulin beta-4B chain

Chain KF:



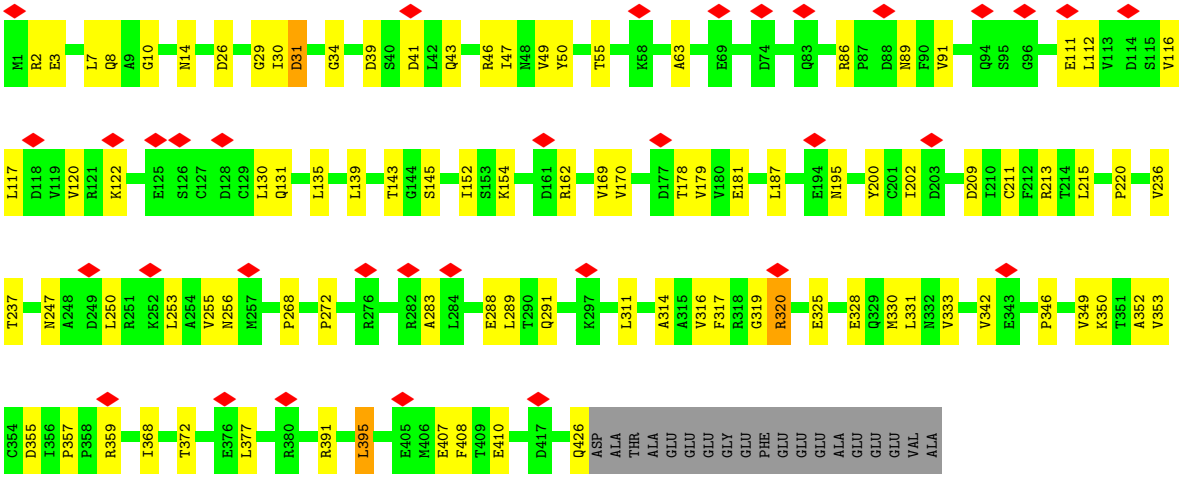
- Molecule 41: Tubulin beta-4B chain

Chain KH:



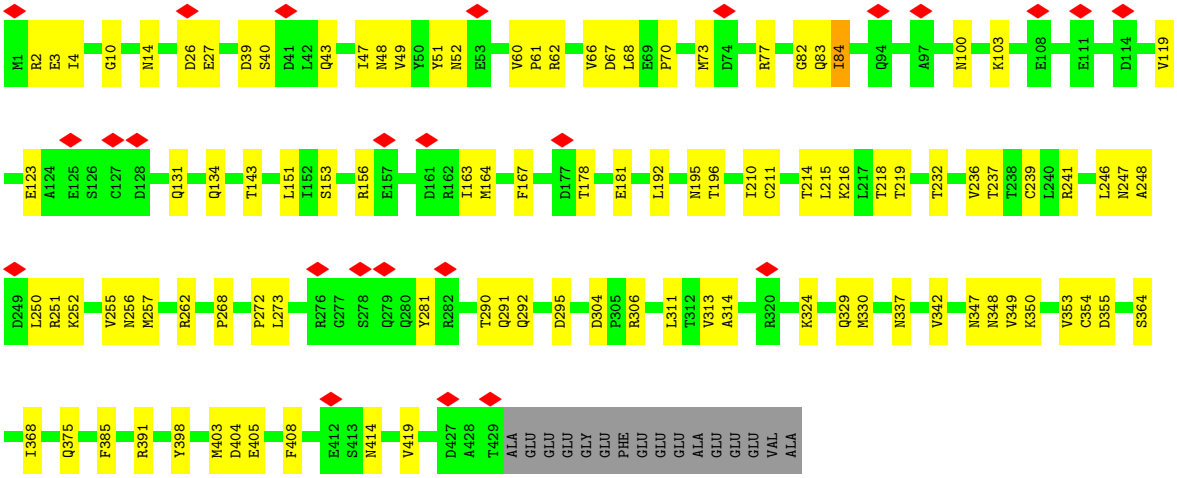
- Molecule 41: Tubulin beta-4B chain

Chain KJ:



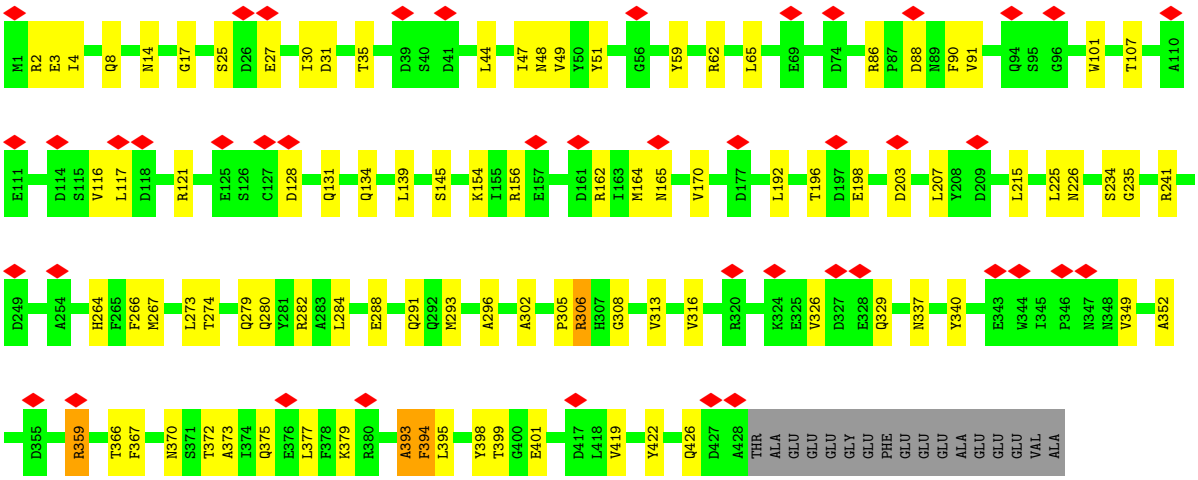
• Molecule 41: Tubulin beta-4B chain

Chain KL:



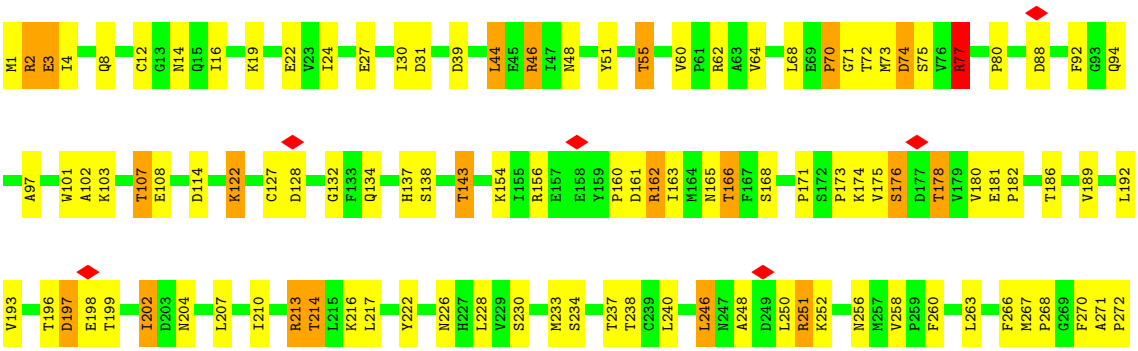
• Molecule 41: Tubulin beta-4B chain

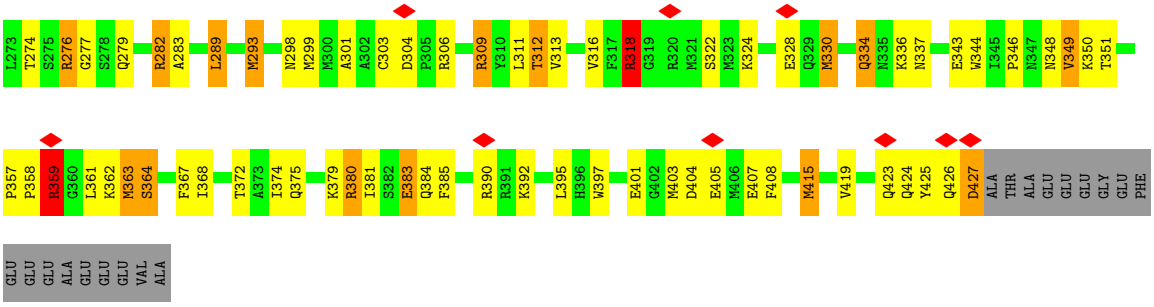
Chain KN:



• Molecule 41: Tubulin beta-4B chain

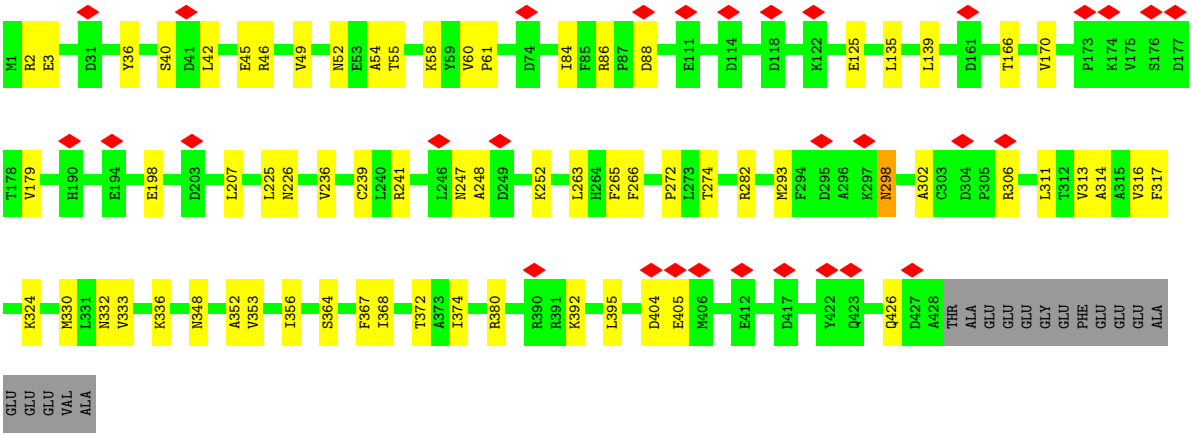
Chain LD:





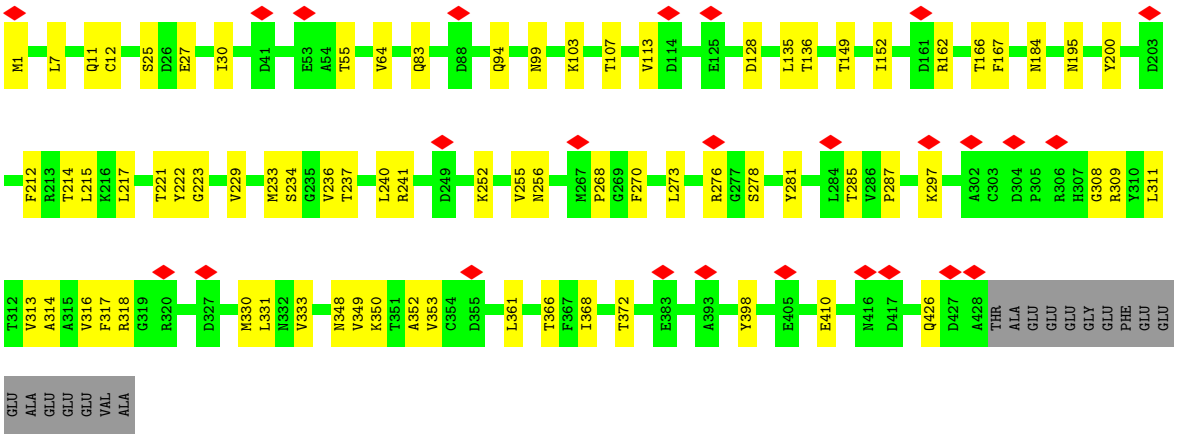
• Molecule 41: Tubulin beta-4B chain

Chain LF:



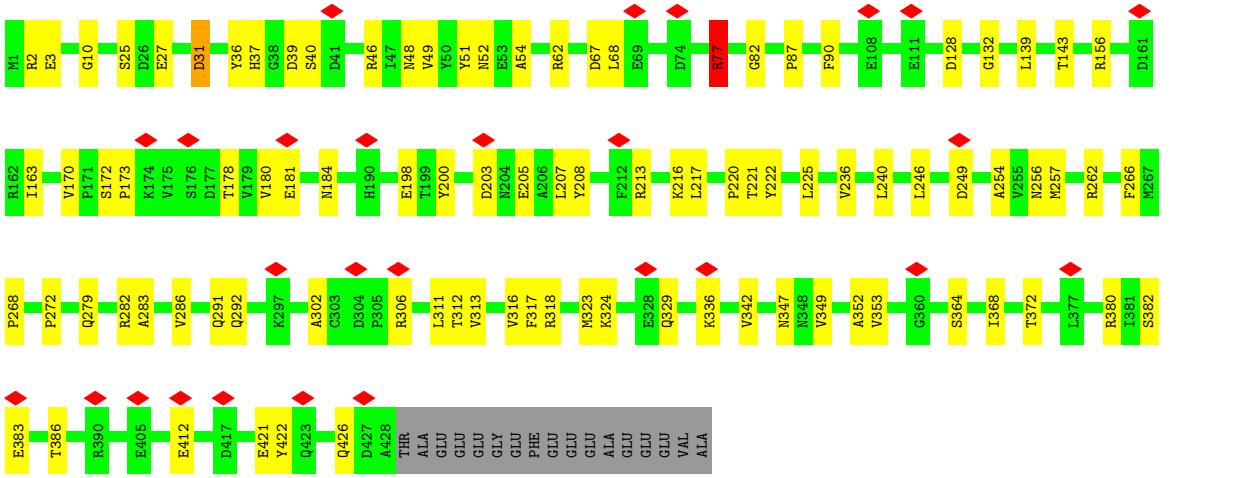
• Molecule 41: Tubulin beta-4B chain

Chain LH:



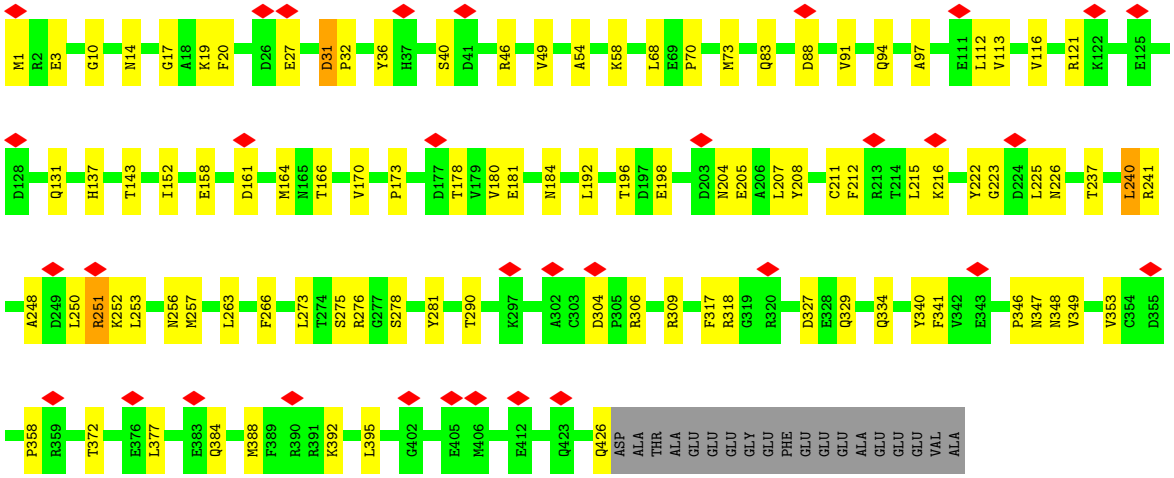
• Molecule 41: Tubulin beta-4B chain

Chain LJ:



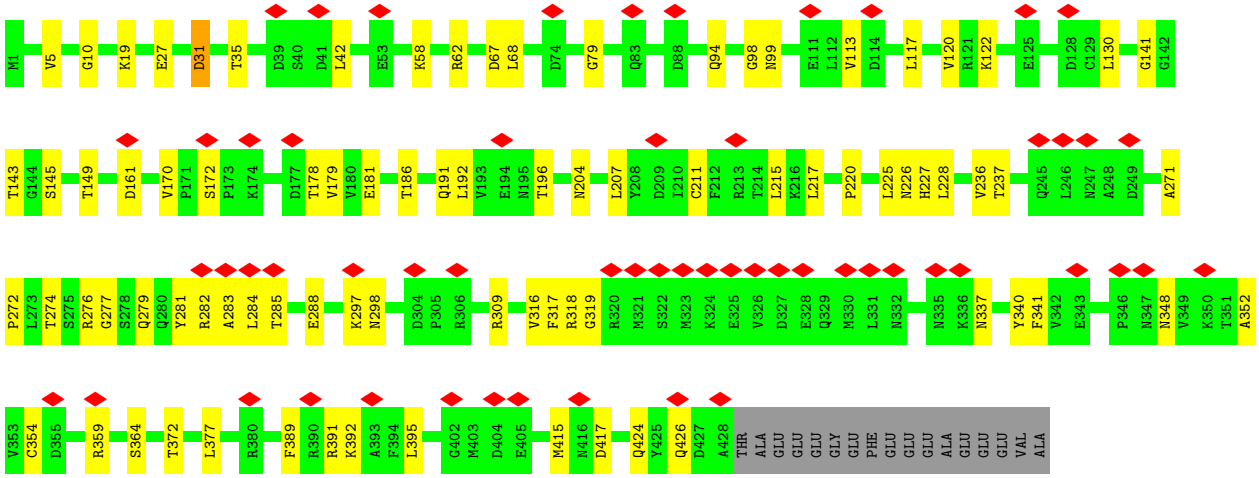
- Molecule 41: Tubulin beta-4B chain

Chain LL:



- Molecule 41: Tubulin beta-4B chain

Chain LN:



- Molecule 41: Tubulin beta-4B chain

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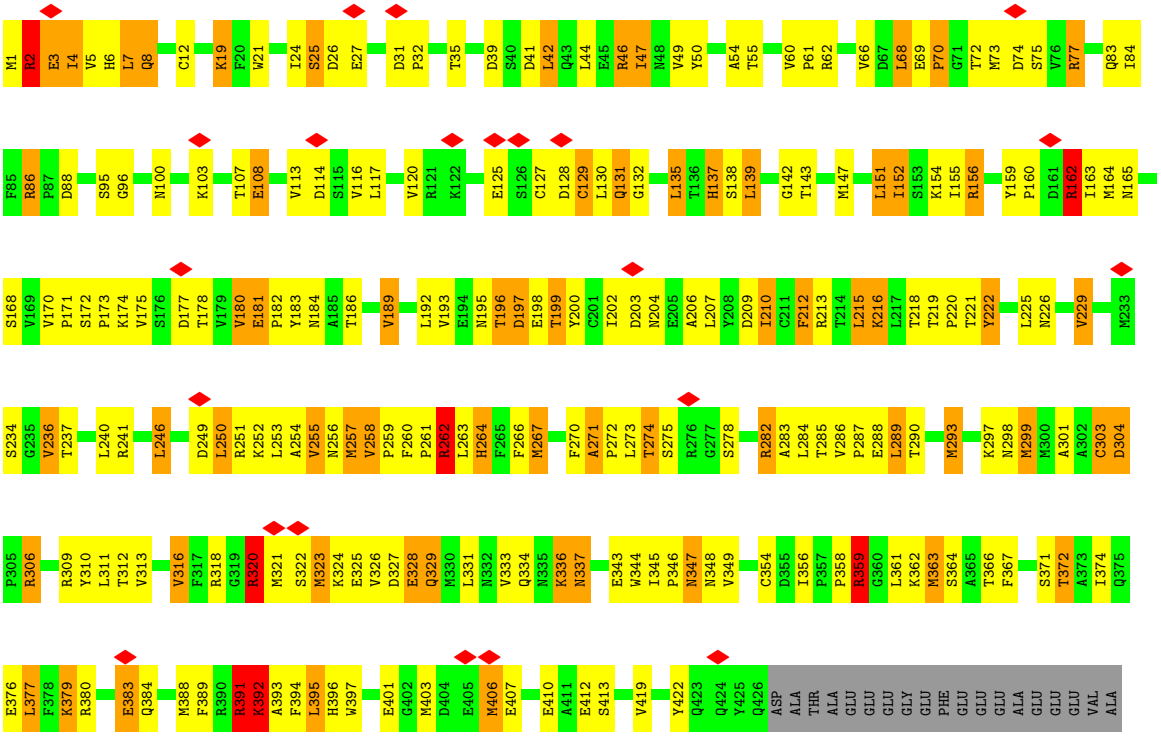
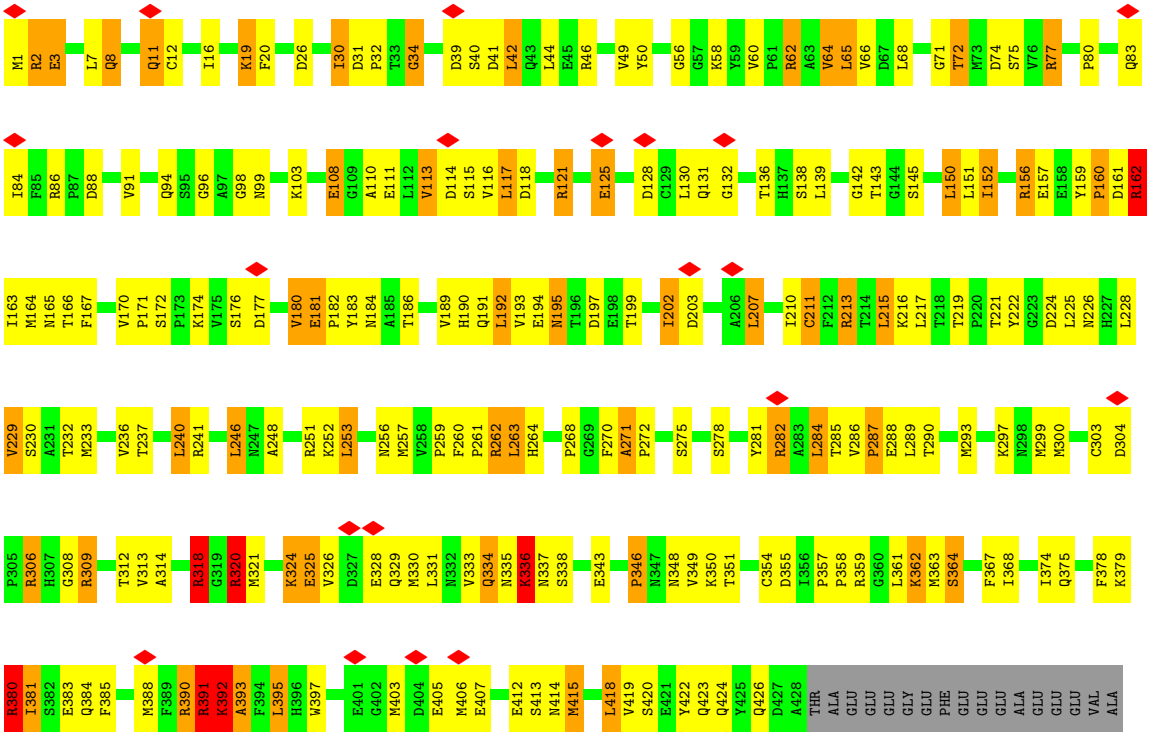


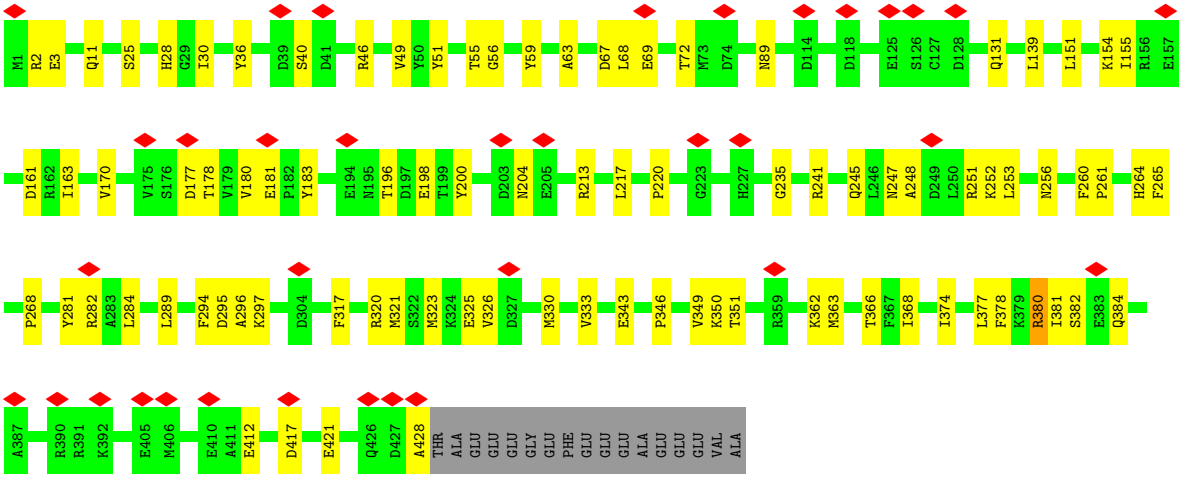
- Molecule 41: Tubulin beta-4B chain

Chain MF:



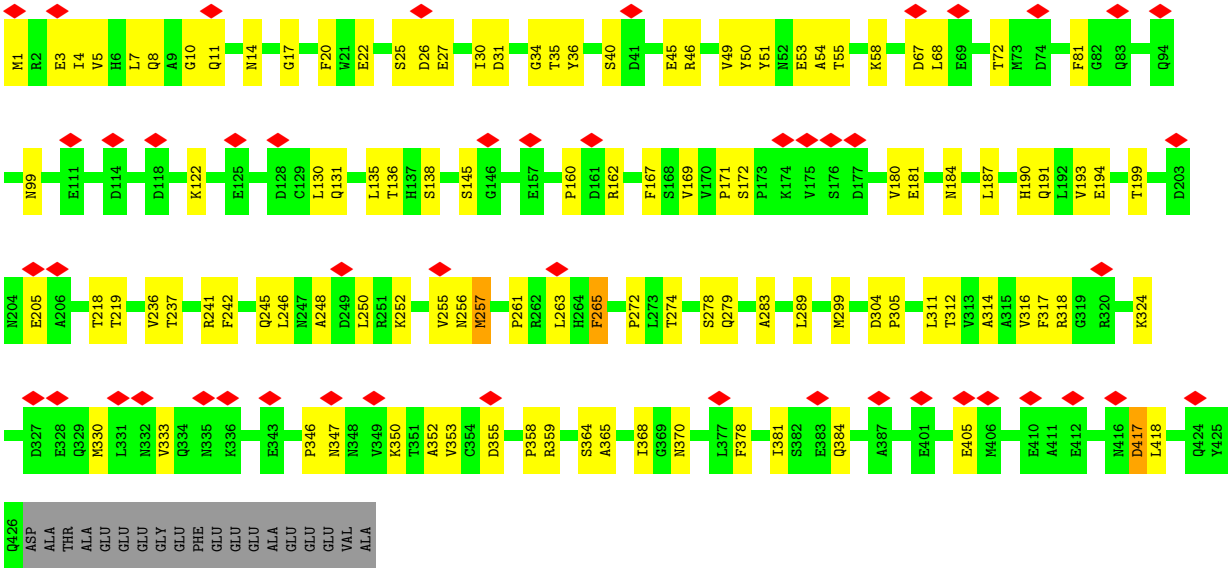
- Molecule 41: Tubulin beta-4B chain

Chain MH:



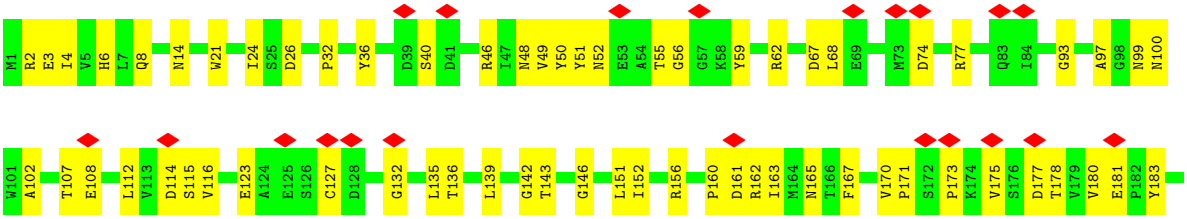
- Molecule 41: Tubulin beta-4B chain

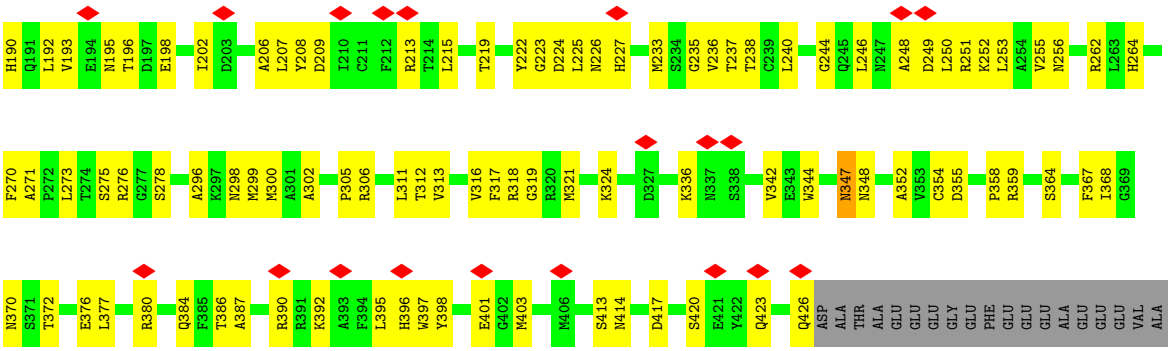
Chain MJ:



- Molecule 41: Tubulin beta-4B chain

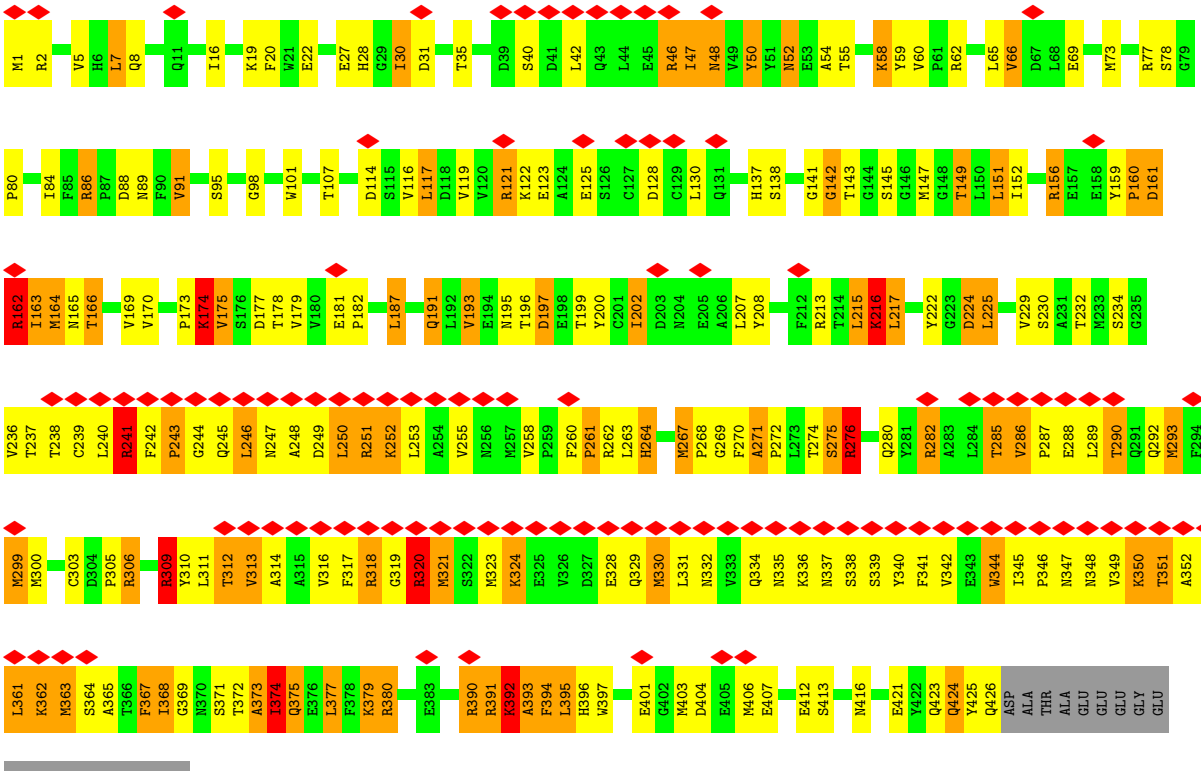
Chain ML:





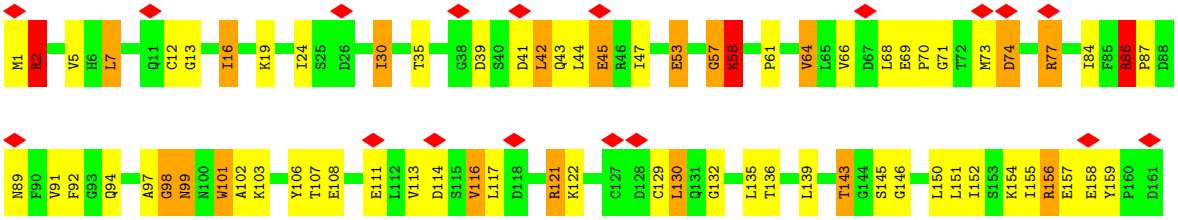
• Molecule 41: Tubulin beta-4B chain

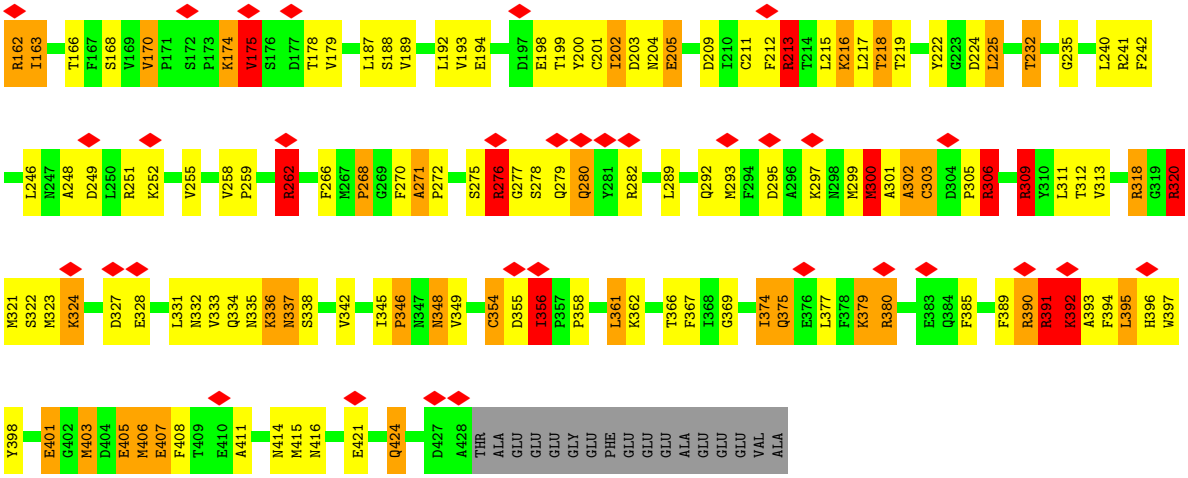
Chain MN:



• Molecule 41: Tubulin beta-4B chain

Chain NB:





- Molecule 41: Tubulin beta-4B chain

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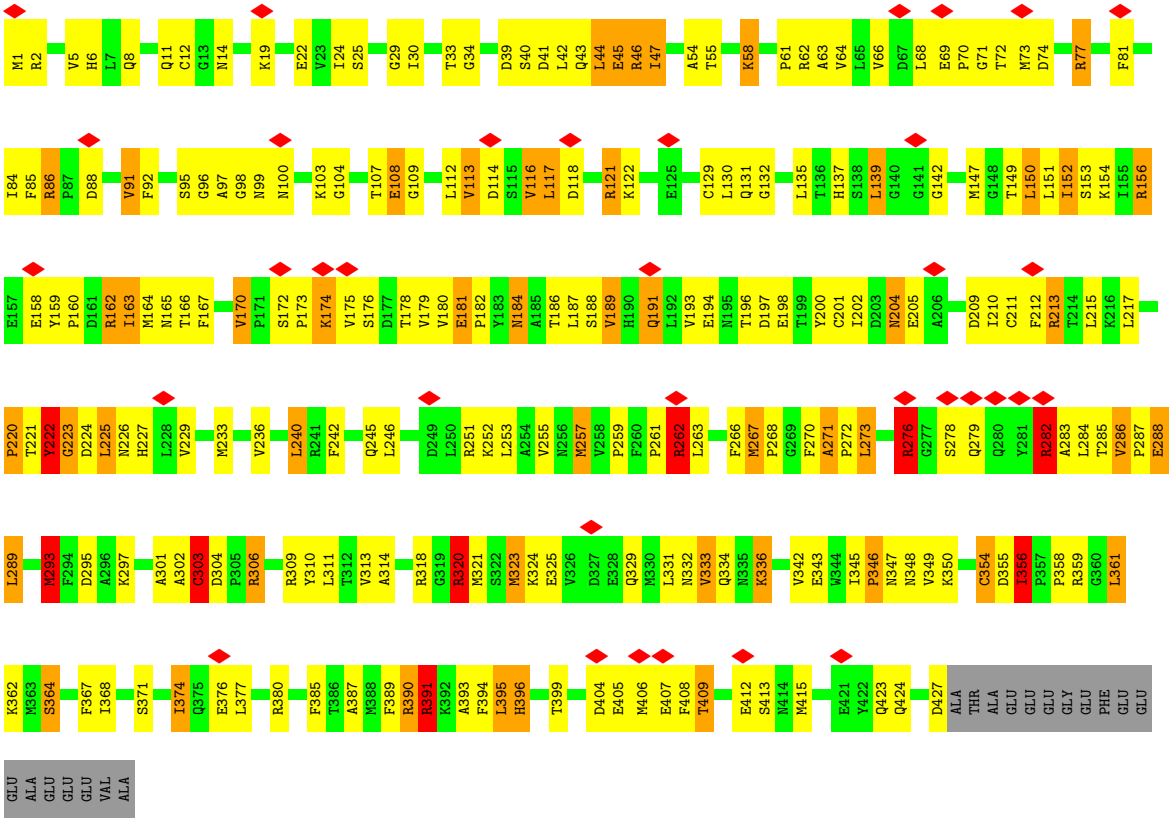
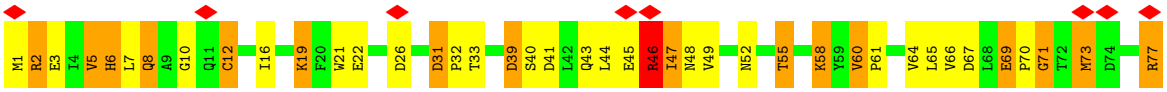
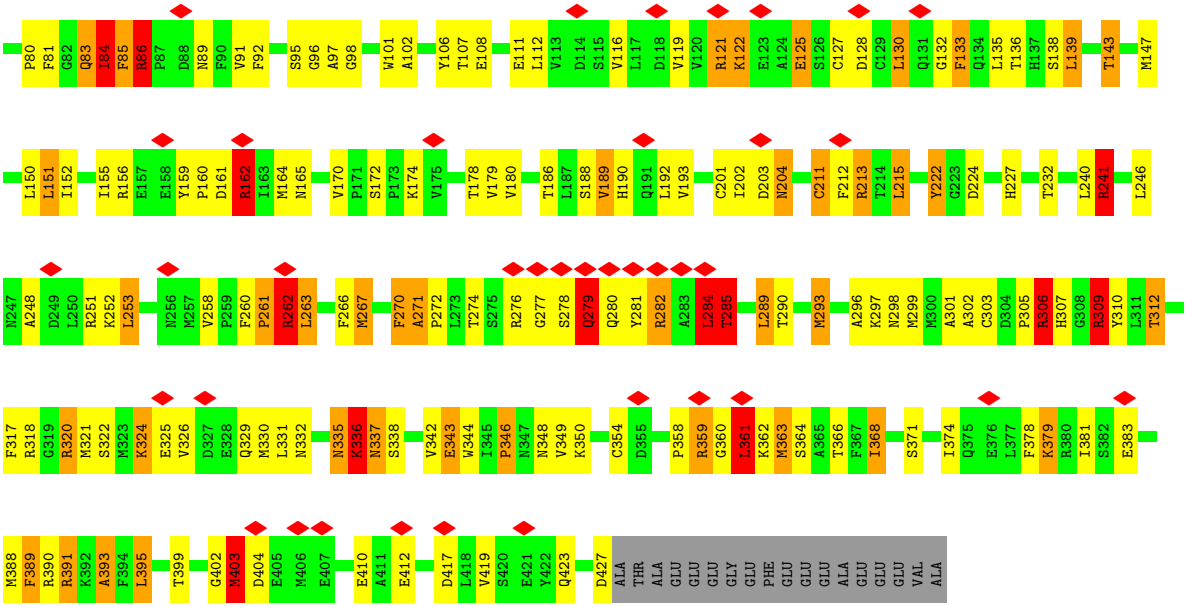


- Molecule 41: Tubulin beta-4B chain

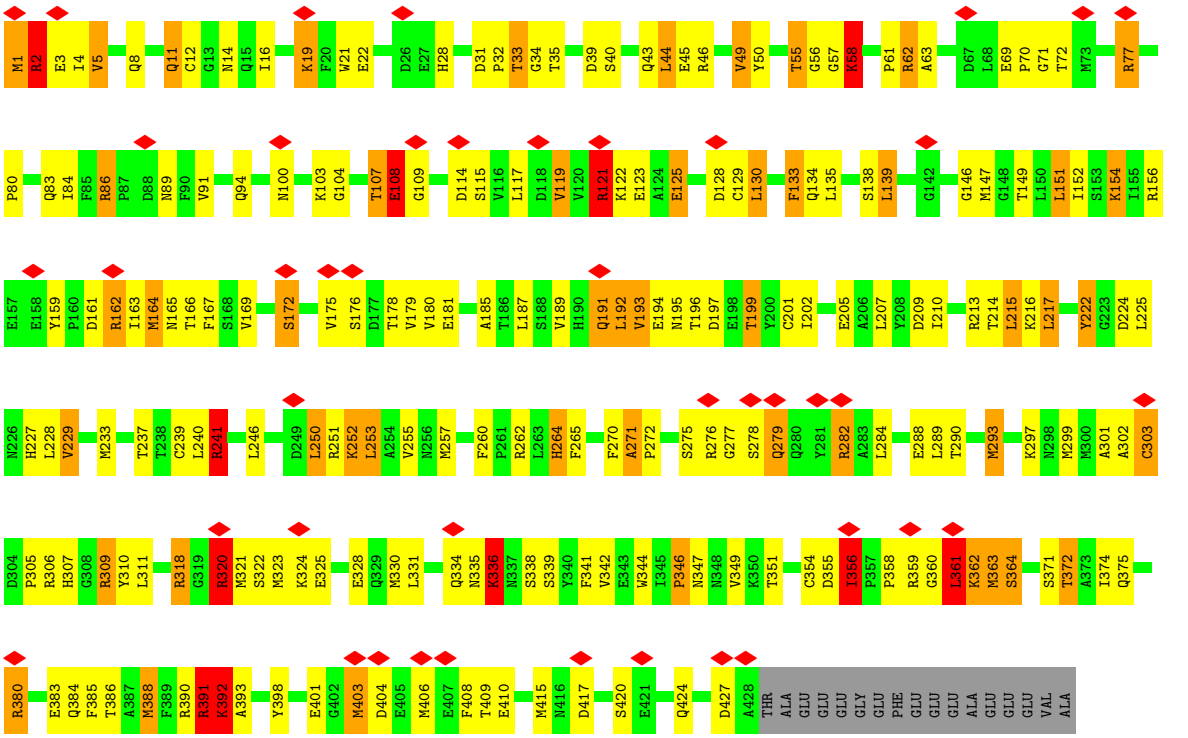
Chain NF:





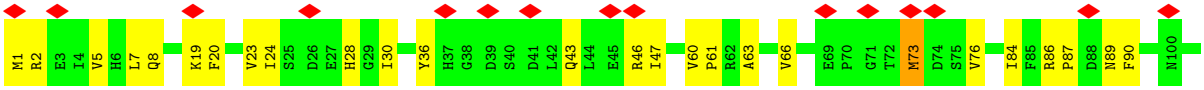
- Molecule 41: Tubulin beta-4B chain

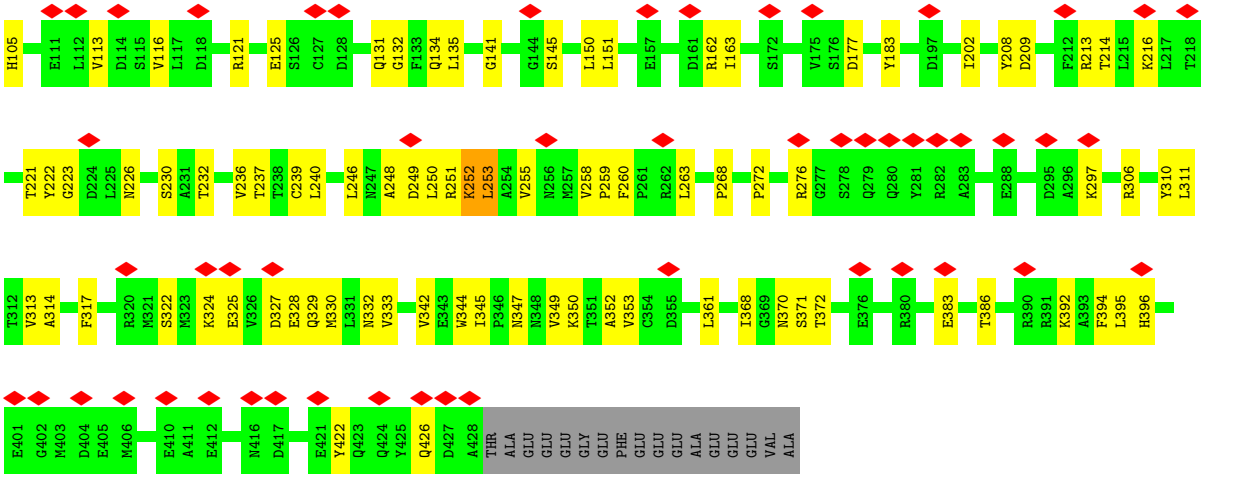
Chain NH:



- Molecule 41: Tubulin beta-4B chain

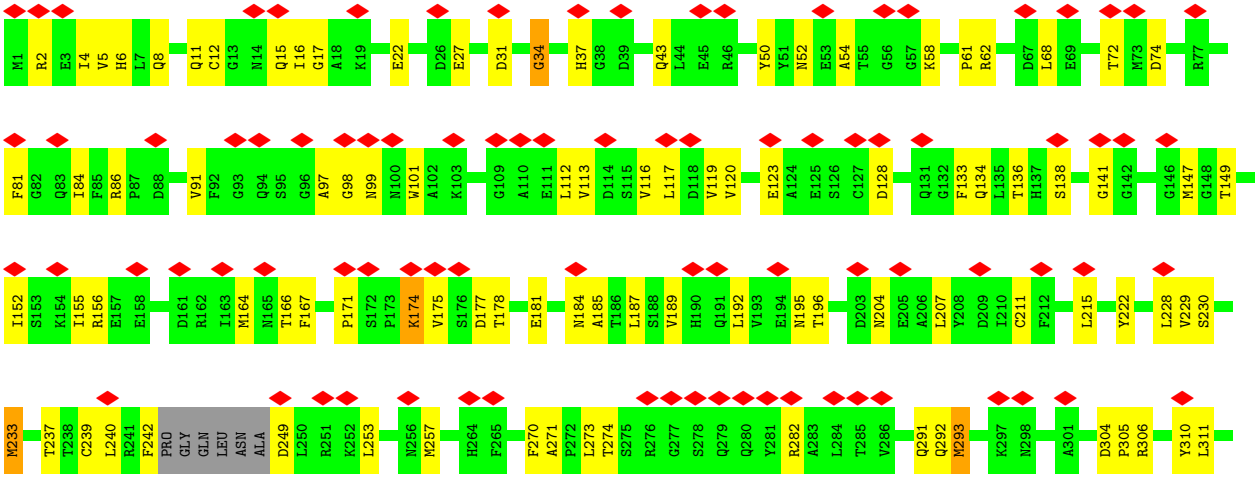
Chain NJ:





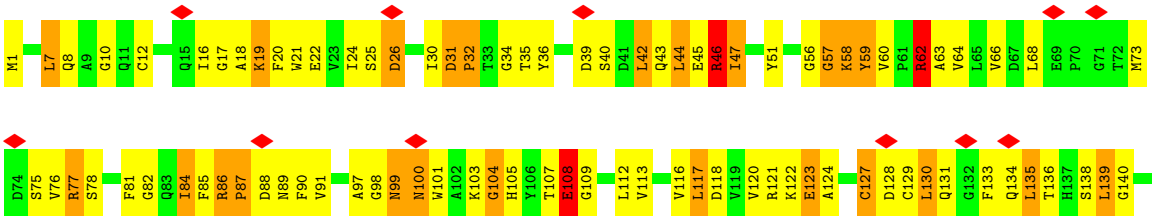
- Molecule 41: Tubulin beta-4B chain

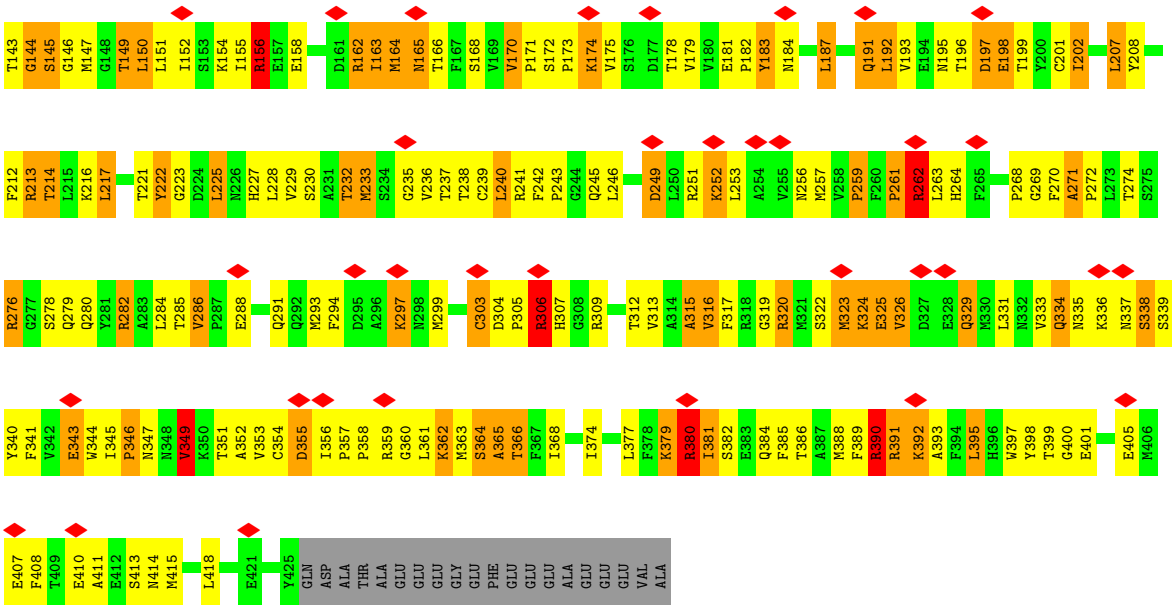
Chain NL:



- Molecule 41: Tubulin beta-4B chain

Chain OB:





- Molecule 41: Tubulin beta-4B chain

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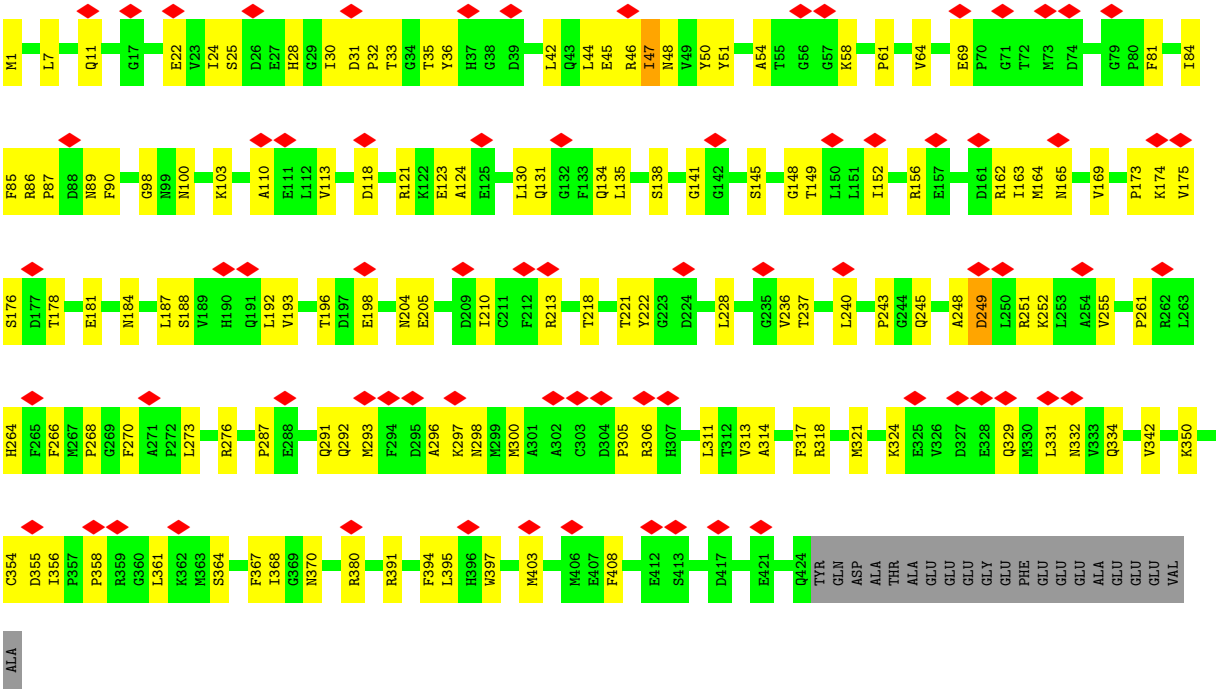

- Molecule 41: Tubulin beta-4B chain

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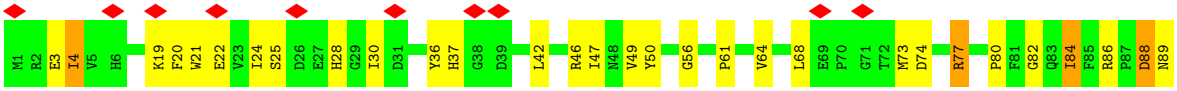
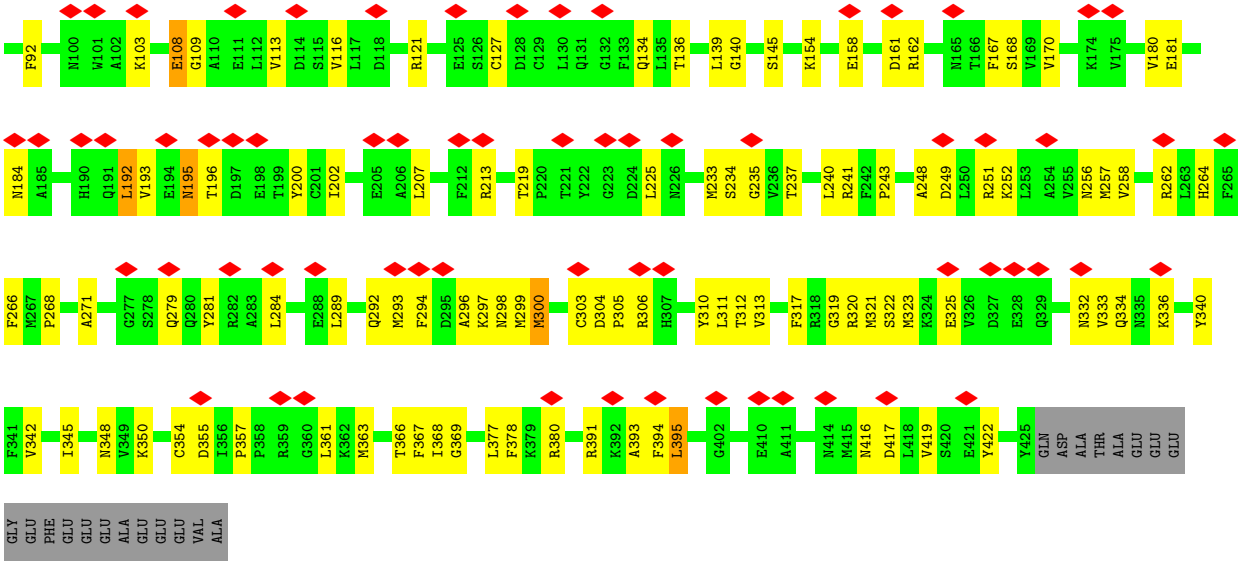
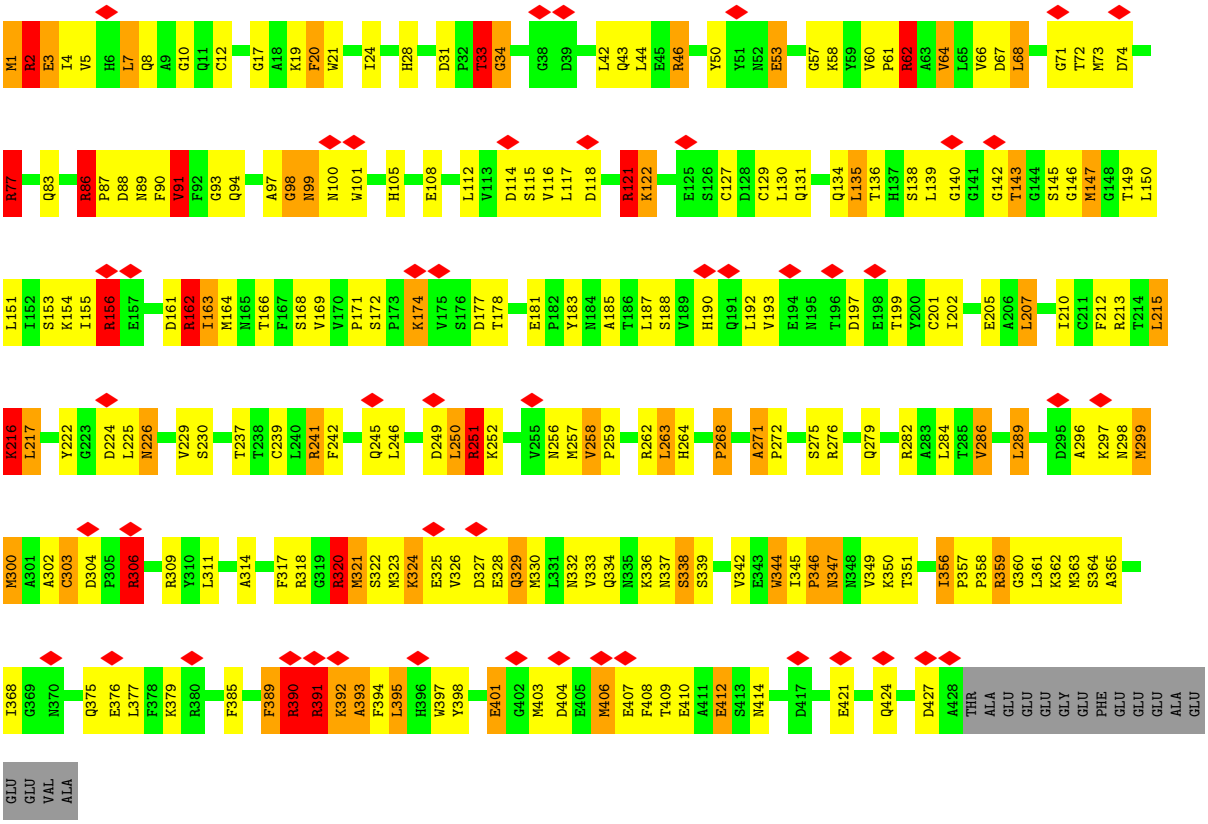




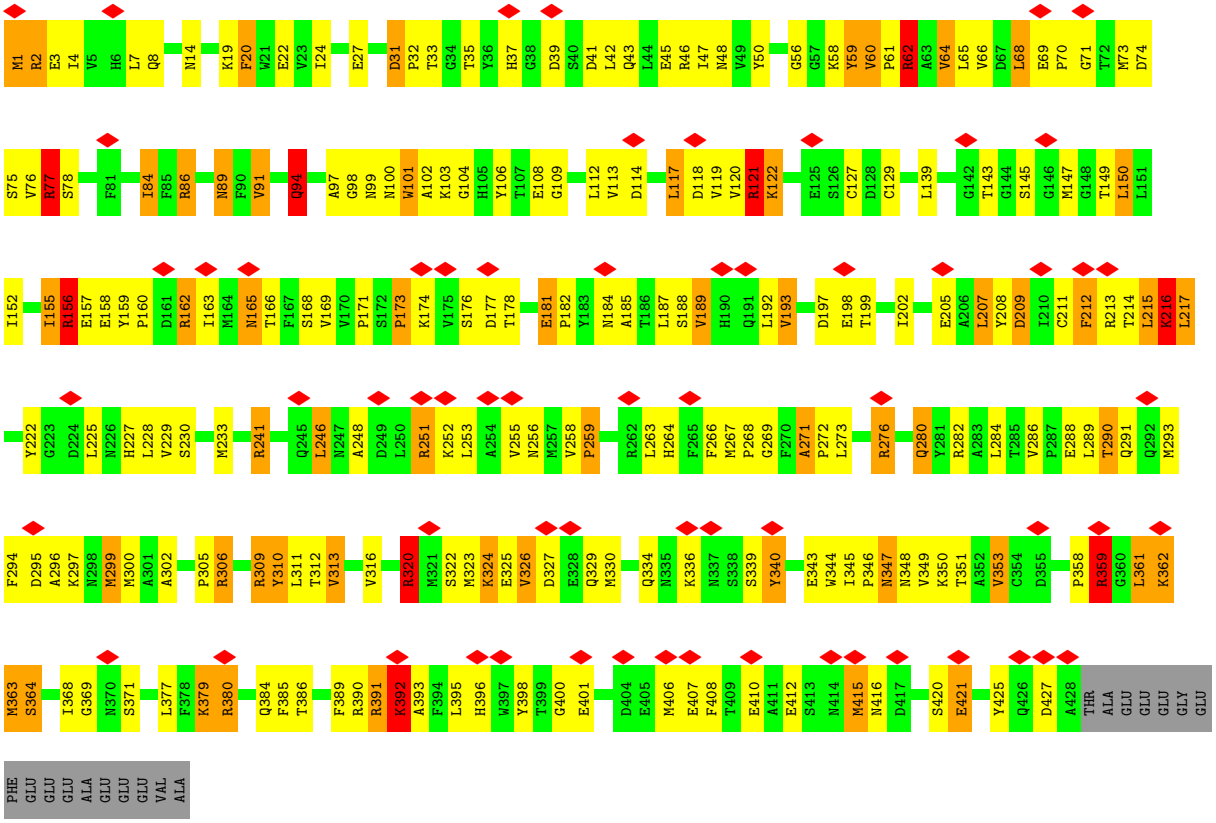
- Molecule 41: Tubulin beta-4B chain

Chain OH:



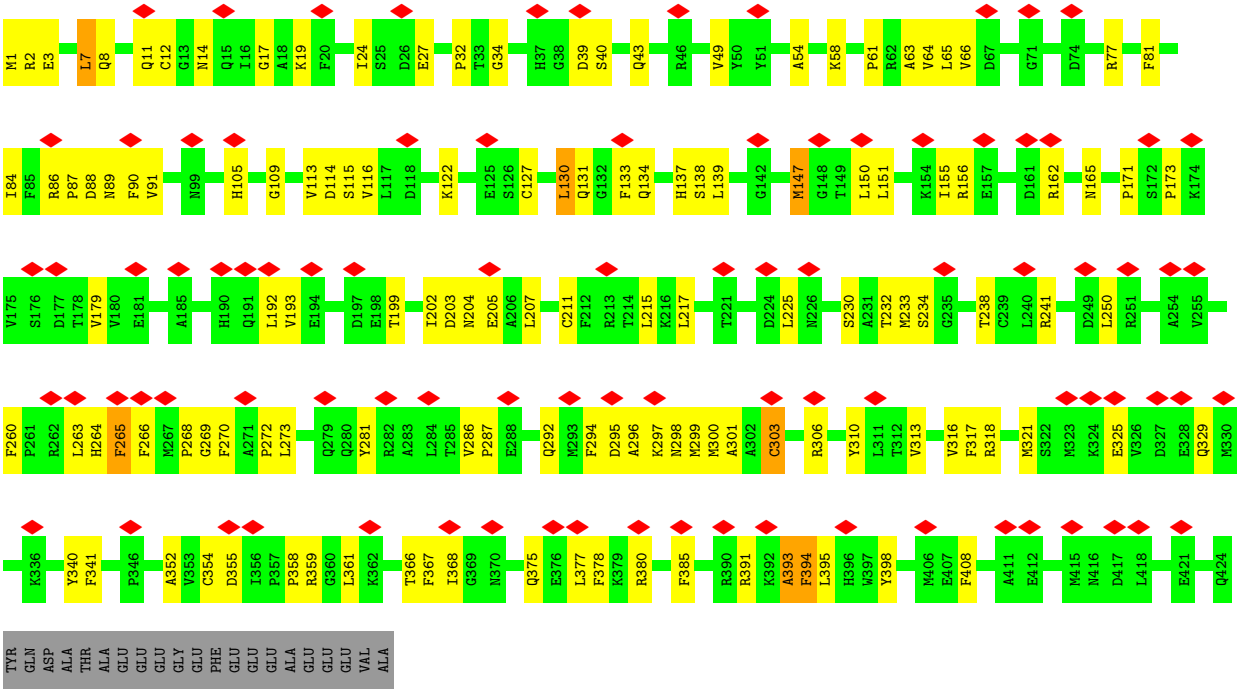
- Molecule 41: Tubulin beta-4B chain

Chain OJ:



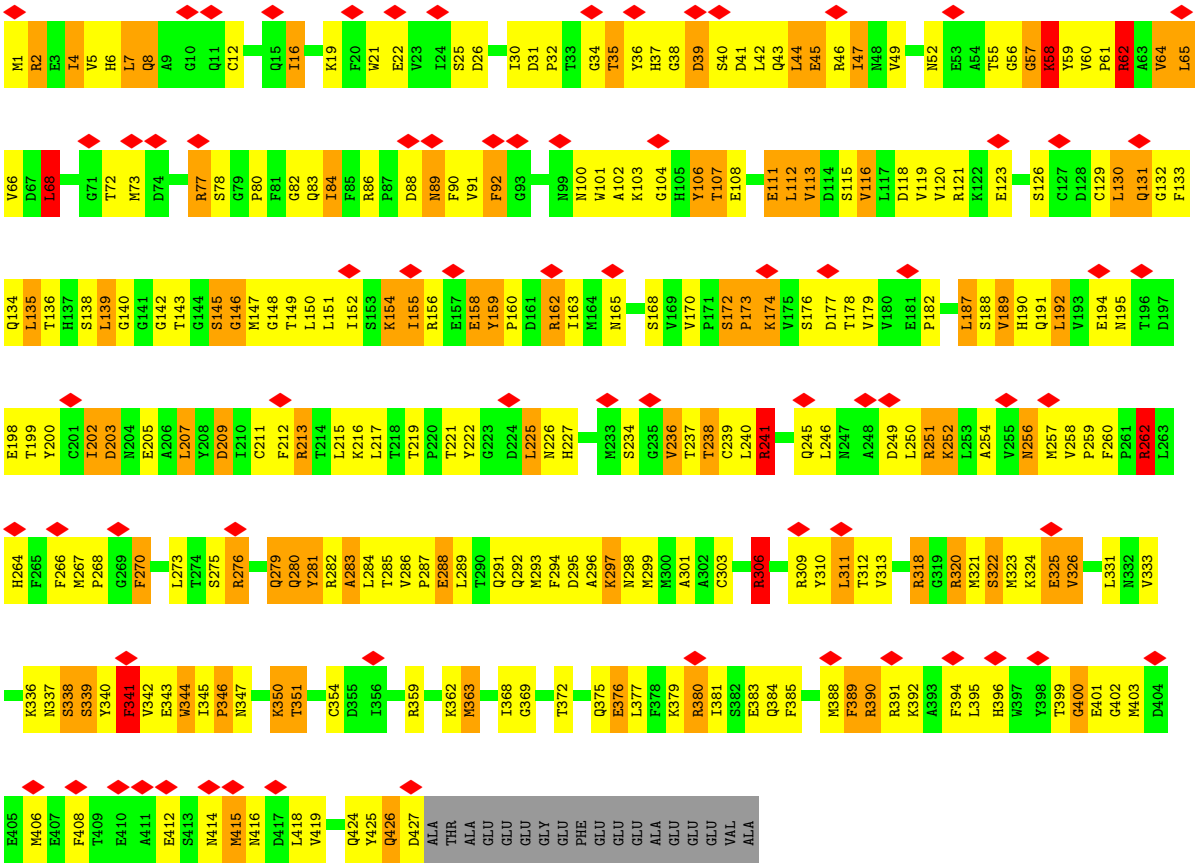
- Molecule 41: Tubulin beta-4B chain

Chain OL:



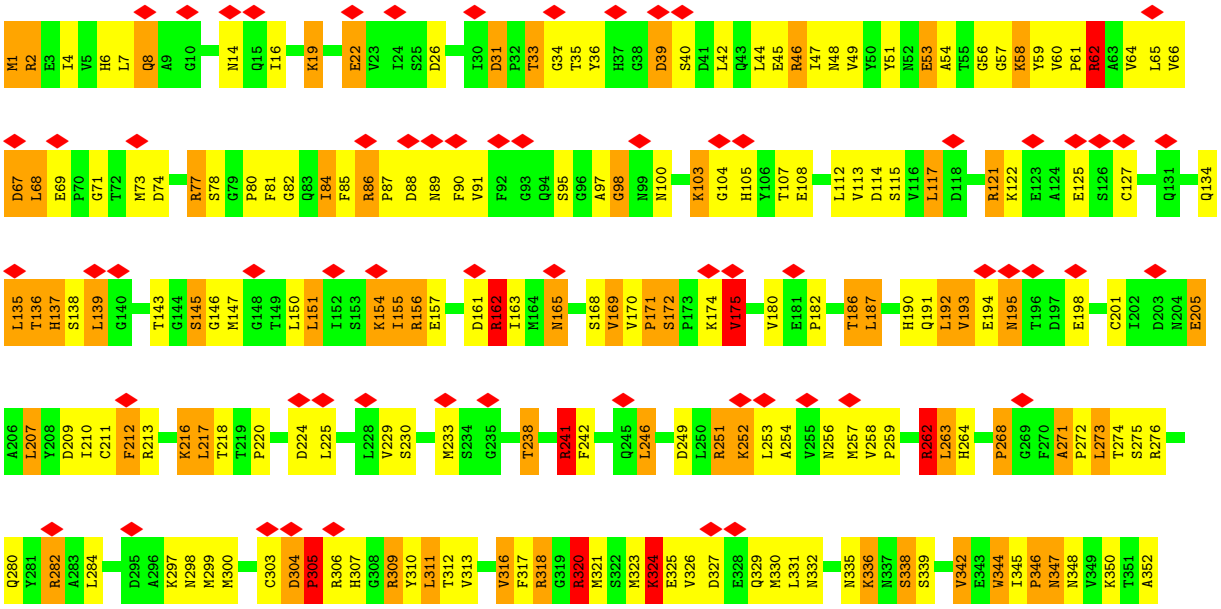
- Molecule 41: Tubulin beta-4B chain

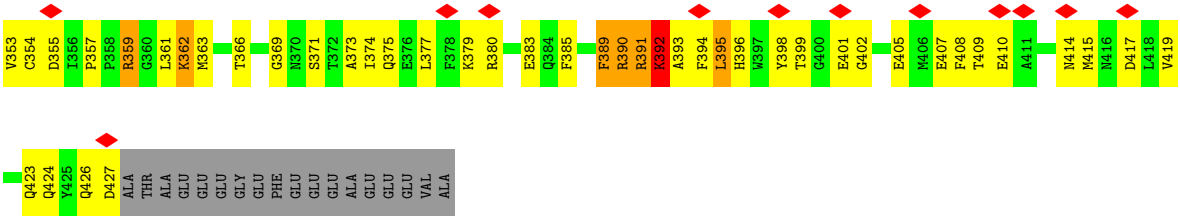
Chain PB:



- Molecule 41: Tubulin beta-4B chain

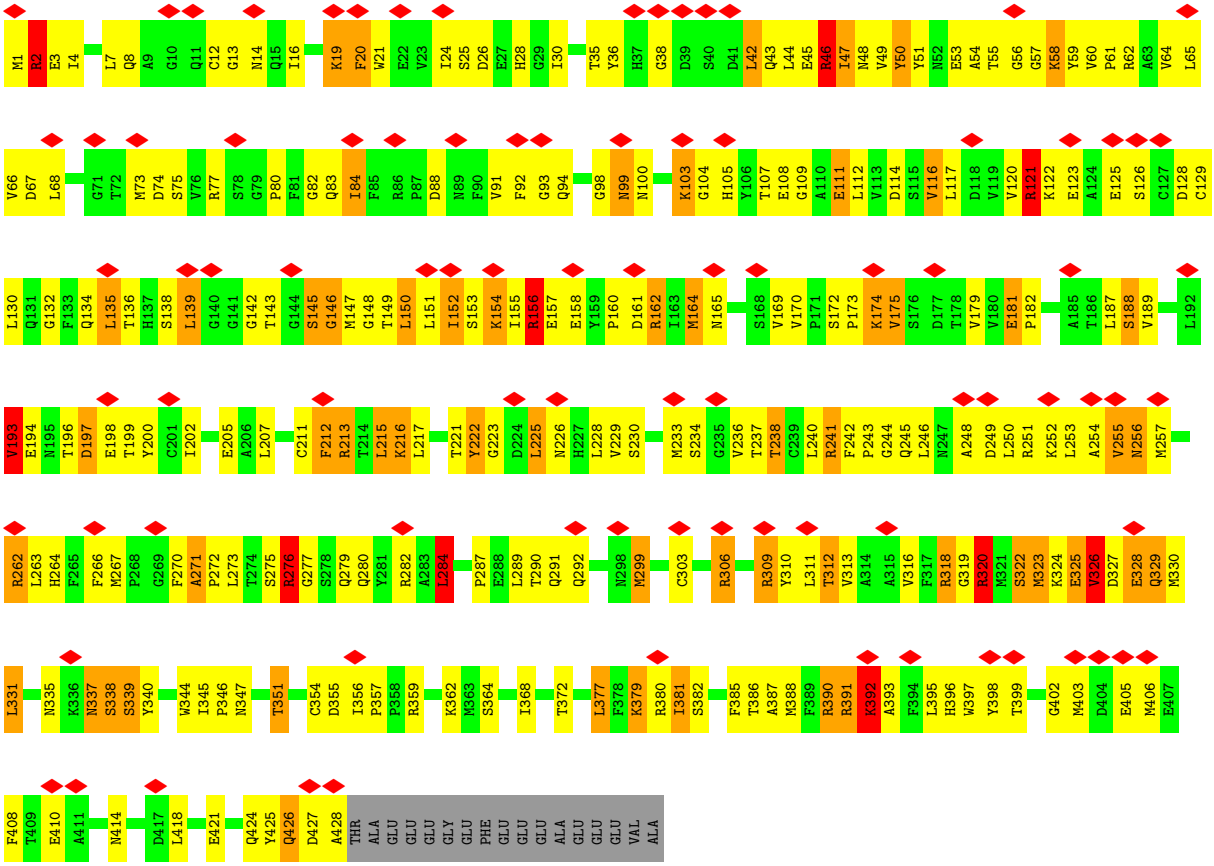
Chain PD:





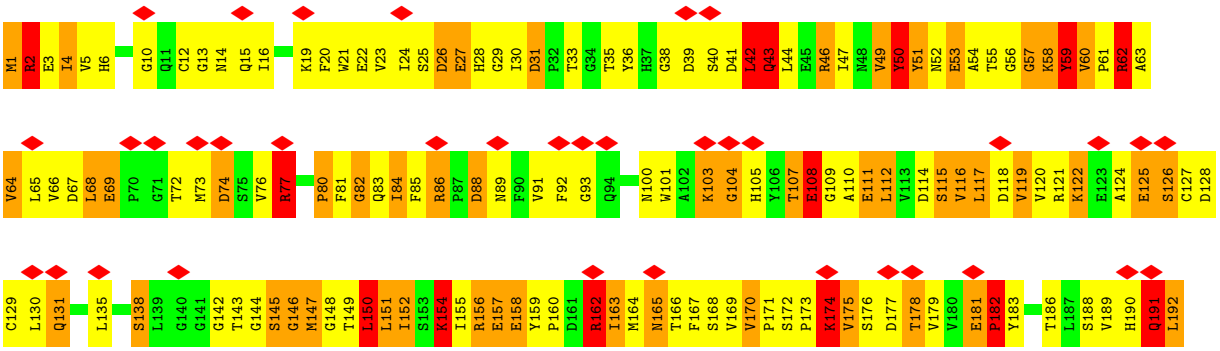
• Molecule 41: Tubulin beta-4B chain

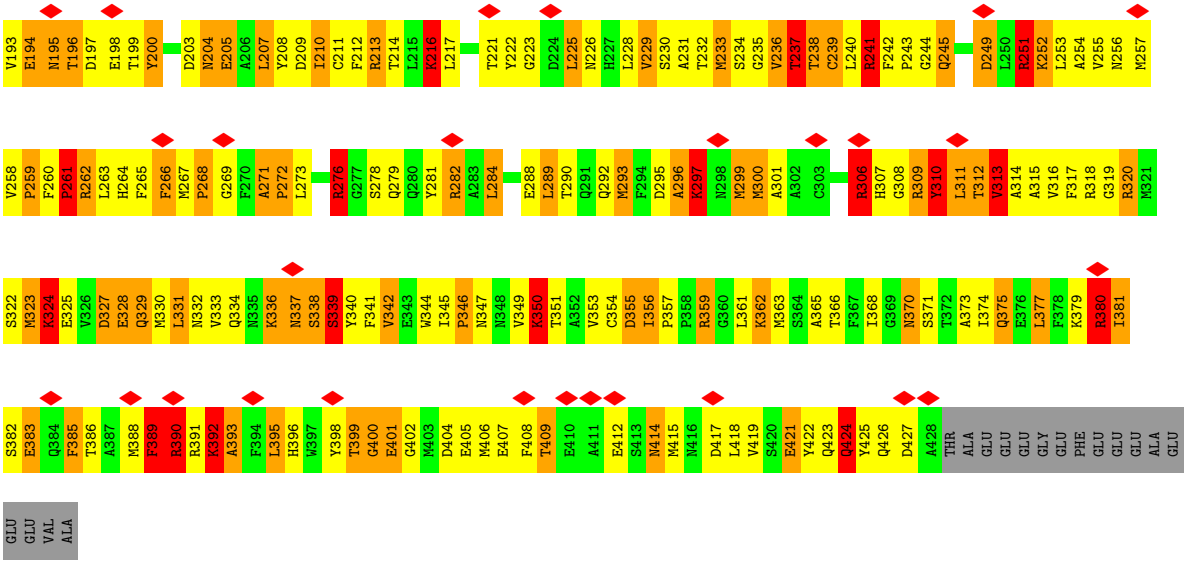
Chain PF:



• Molecule 41: Tubulin beta-4B chain

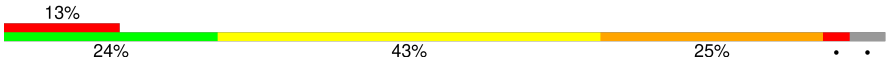
Chain PH:

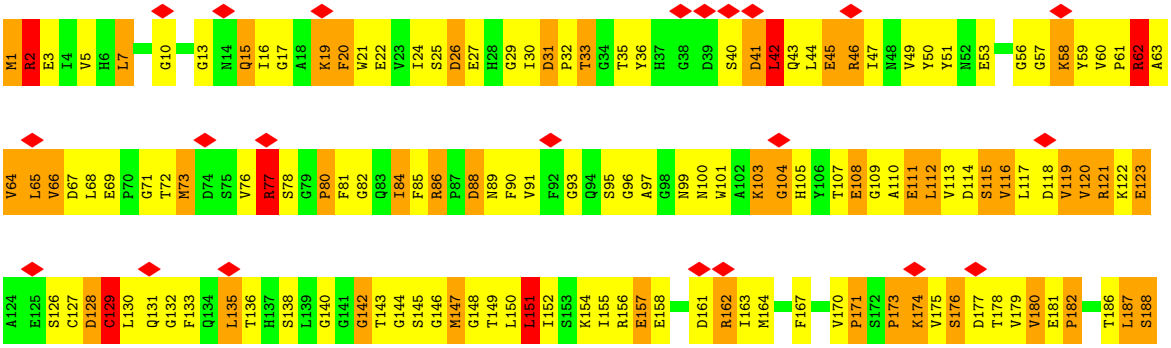




- Molecule 41: Tubulin beta-4B chain

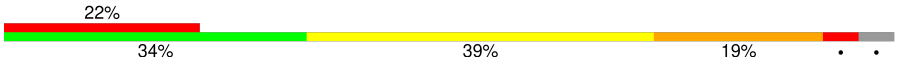
Chain PJ:

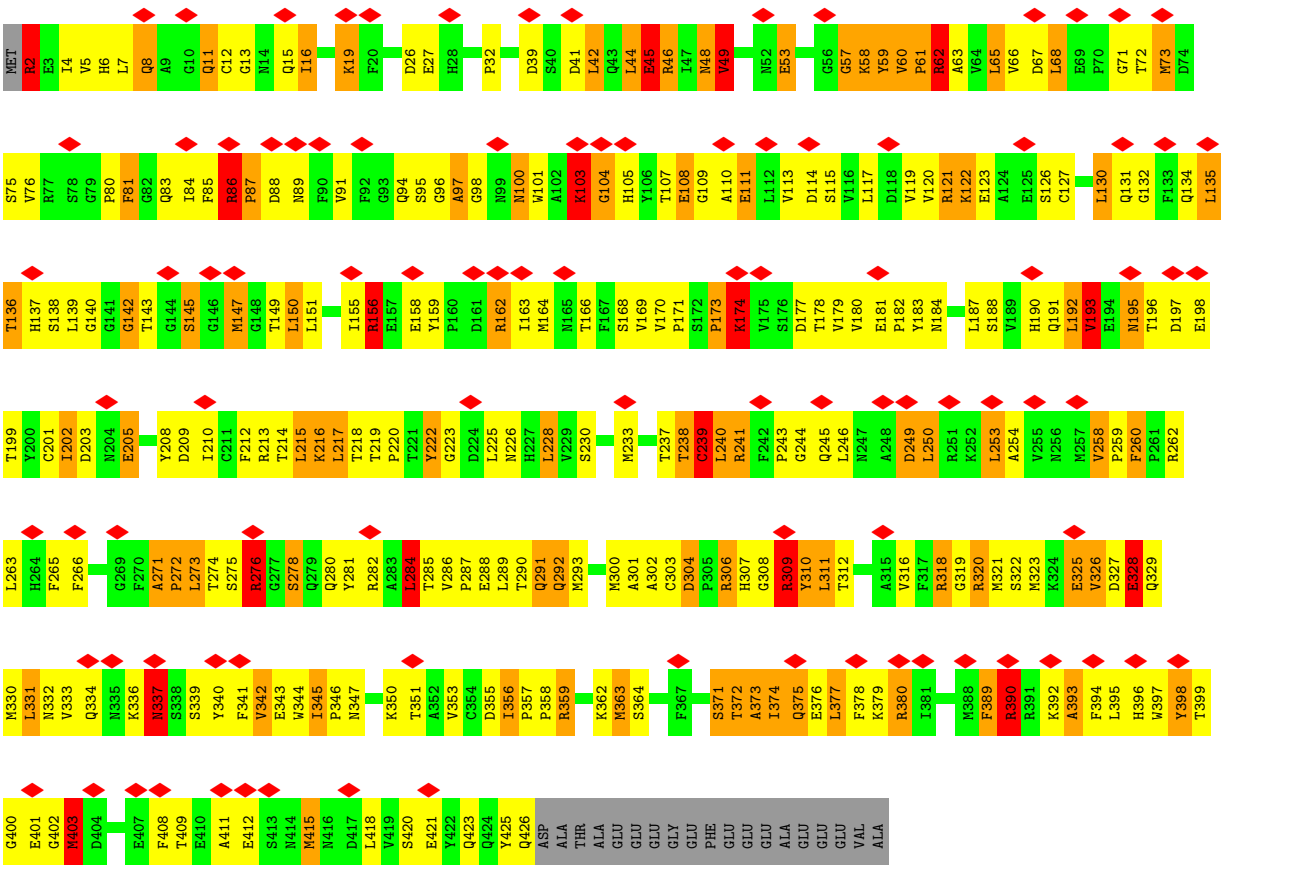




- Molecule 41: Tubulin beta-4B chain

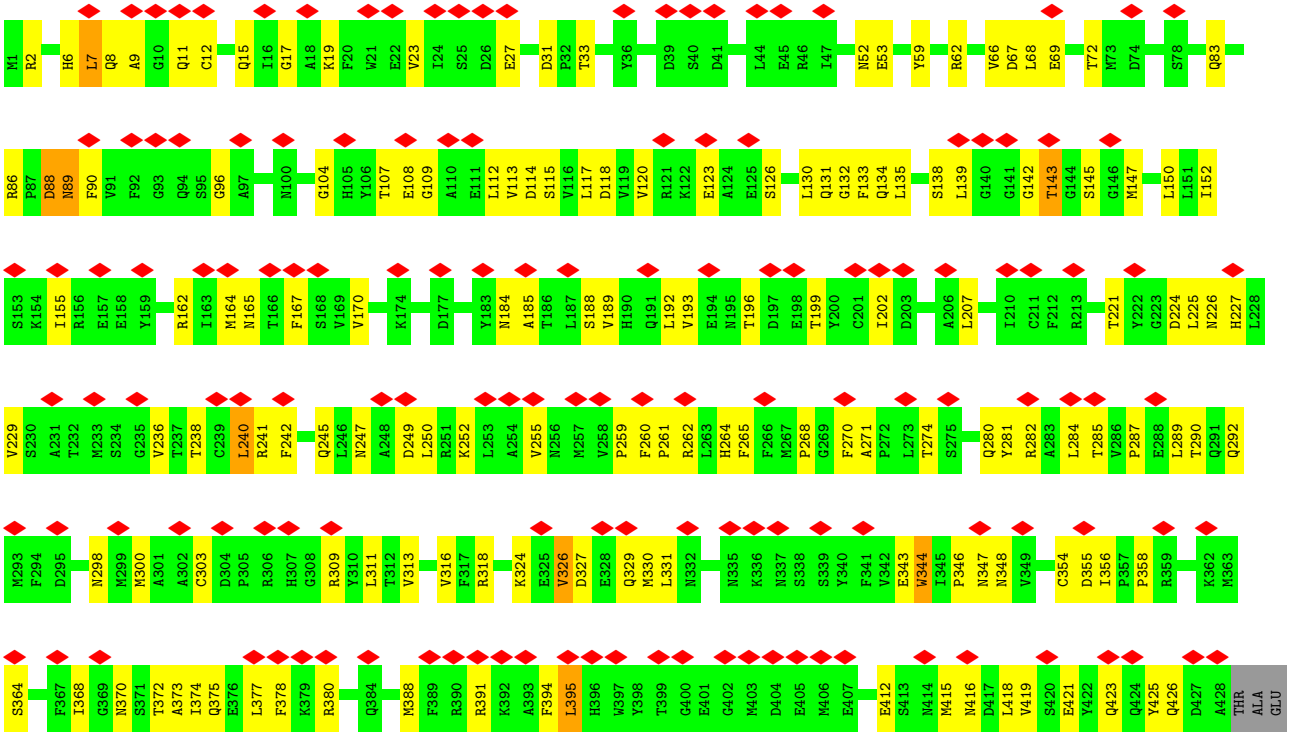
Chain PL:





- Molecule 41: Tubulin beta-4B chain

Chain QB:



GLU GLU GLY GLU PHE GLU GLU GLU ALA GLU GLU GLU GLU VAL ALA

• Molecule 41: Tubulin beta-4B chain

Chain QD: 27% 60% 35%

M1 R2 E3 L7 Q8 A9 G10 Q11 C12 G13 N14 Q15 I16 G17 A18 K19 E22 V23 I24 S25 D26 I30 T35 Y36 D39 S40 D41 L42 Q43 L44 E45 R46 L47 N48 V49 Y50 P61 R62 V66 D67 L68 E69 P70 G71 D74 S78 I84 F85 R86 P87

D88 N89 F90 V91 F92 G93 G96 N99 G104 H105 Y106 T107 E108 G109 A110 E111 L112 V113 D114 S115 V116 L117 D118 V119 V120 R121 S126 C127 L130 Q131 L135 T136 H137 S138 L139 G140 T143 G144 L150 L151 I152 S153 K154 I155 R156 E157 M164 N165 T166 F167 S168

V169 V170 P171 S172 P173 K174 V175 S176 D177 T178 V179 V180 E181 N184 A185 T186 L187 S188 Q191 L192 V193 E194 N195 T196 D197 E198 T199 Y200 D203 N204 E205 A206 L207 F212 R213 T214 L215 K216 Y222 G223 D224 L225 N226 H227 L228 V229 S230 A231 T232 M233 S234 C239 L240 R241

F242 L246 N247 A248 D249 L250 R251 K252 L253 A254 V255 N256 M257 F260 P261 R262 L263 H264 F265 F266 M267 P268 G269 F270 A271 P272 L273 T274 S275 R276 G277 S278 Q279 Q280 Y281 R282 E288 L289 T290 Q291 Q292 M293 F294 D295 N298 M299 M300 A301 A302 C303 D304 P305 R306 H307 G308 R309

Y310 L311 A314 R318 S322 M323 K324 E325 V326 D327 E328 L331 N332 V333 Q334 N335 K336 N337 Y340 F341 W344 N347 N348 V349 K350 V353 C354 D355 I356 P357 P358 R359 G360 L361 S364 A365 T366 F367 I368 G369 N370 I374 Q375 E376 L377 F378 K379 R380 I381 S382

E383 Q384 F385 T386 A387 H388 F389 R390 R391 K392 A393 W397 Y398 E401 M406 E407 F408 T409 E410 A411 E412 S413 N414 M415 N416 D417 L418 V419 S420 Q423 Q424 Y425 Q426 D427 ALA THR ALA GLU GLU GLU GLY GLU PHE GLU GLU GLU ALA GLU GLU GLU VAL ALA

• Molecule 41: Tubulin beta-4B chain

Chain QF: 29% 64% 31%

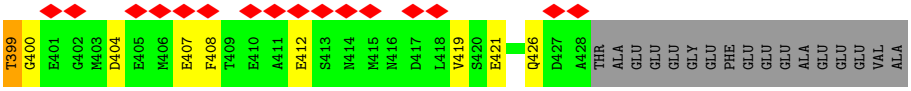
M1 R2 E3 H6 L7 G10 Q11 N14 Q15 I16 G17 A18 S25 D26 G29 I30 D31 G34 D39 S40 D41 L44 E45 R46 I47 A63 V64 L65 V66 D67 L68 E69 P70 G71 D74 R77 R86 P87 D88 N89 F90 V91 N100 K103 G104 H105

Y106 T107 E108 G109 L112 V113 D114 S115 D118 V119 V120 R121 K122 E125 S126 C127 L130 Q134 L135 T136 L139 G146 M147 G148 T149 L150 L151 I155 R156 E157 D161 N165 T166 F167 S168 V169 V170 P173 K174 V175 S176 D177 T178 V179 V180 E181 P182 A185

T186 L187 S188 V189 H190 Q191 L192 V193 E194 N195 T196 D197 E198 T199 Y200 C201 I202 D203 N204 E205 A206 L207 Y208 D209 I210 C211 F212 R213 Y222 G223 D224 L225 N226 H227 A231 T232 M233 V236 T237 L240 R241 F242 Q245 L246 N247 A248 D249 L250 R251 K252 L253 A254 V255 N256 M257

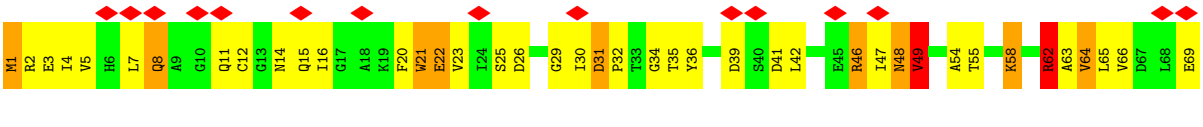
V258 P259 R262 L263 H264 F265 F266 M267 P268 G269 F270 A271 P272 L273 R276 Q280 Y281 R282 A283 L284 T285 E288 Q292 M293 F294 D295 A296 K297 N298 M299 M300 A301 A302 C303 D304 P305 R306 R309 T312 V313 A314 A315 R318 M323 K324 E325 V326 D327 E328 Q329 M330

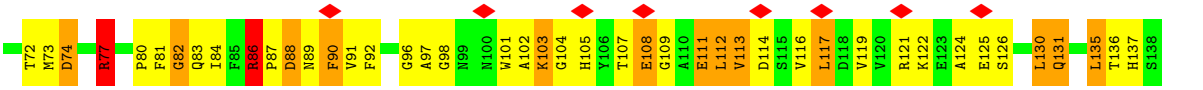
L331 N332 V333 Q334 N335 K336 N337 S338 S339 Y340 F341 V342 E343 W344 I345 P346 N347 N348 V349 K350 T351 A352 V353 C354 D355 I356 P357 S364 A365 T366 F367 I368 G369 N370 S371 T372 A373 I374 Q375 E376 L377 F378 K379 E383 Q384 F385 M388 F389 R390 R391 K392 A393 F394 L395 H396 W397 Y398

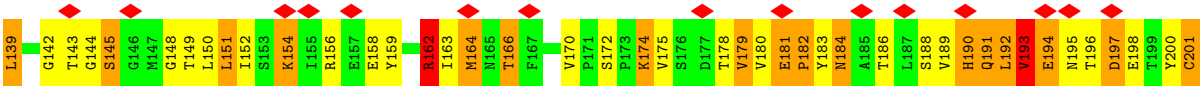


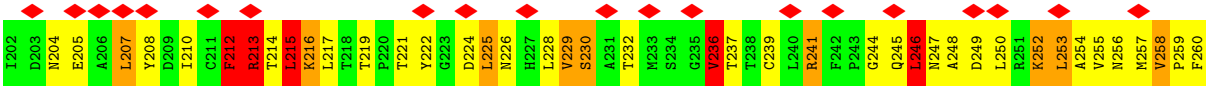
- Molecule 41: Tubulin beta-4B chain

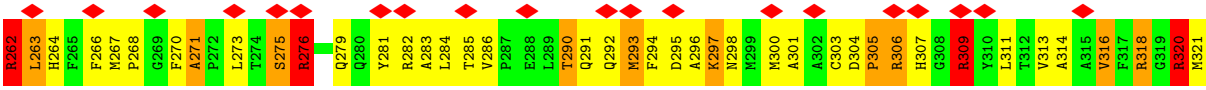
Chain QH:

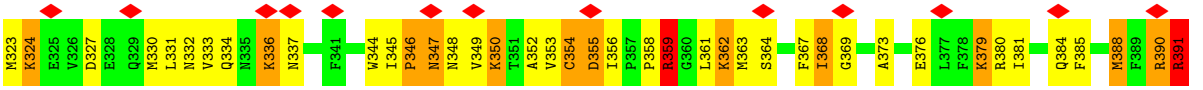


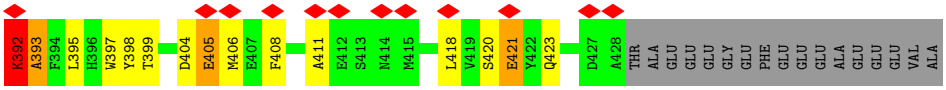






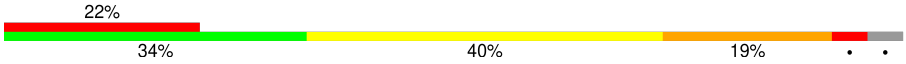


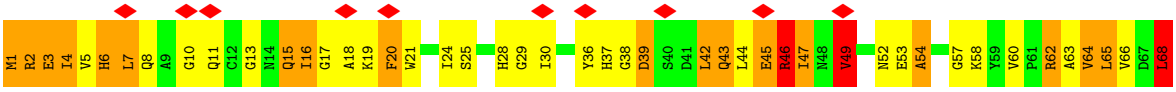


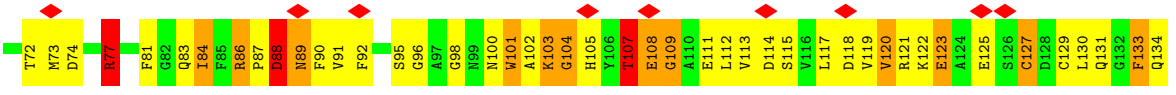


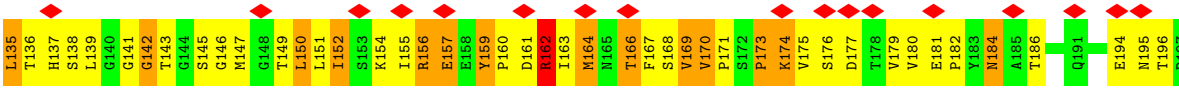
- Molecule 41: Tubulin beta-4B chain

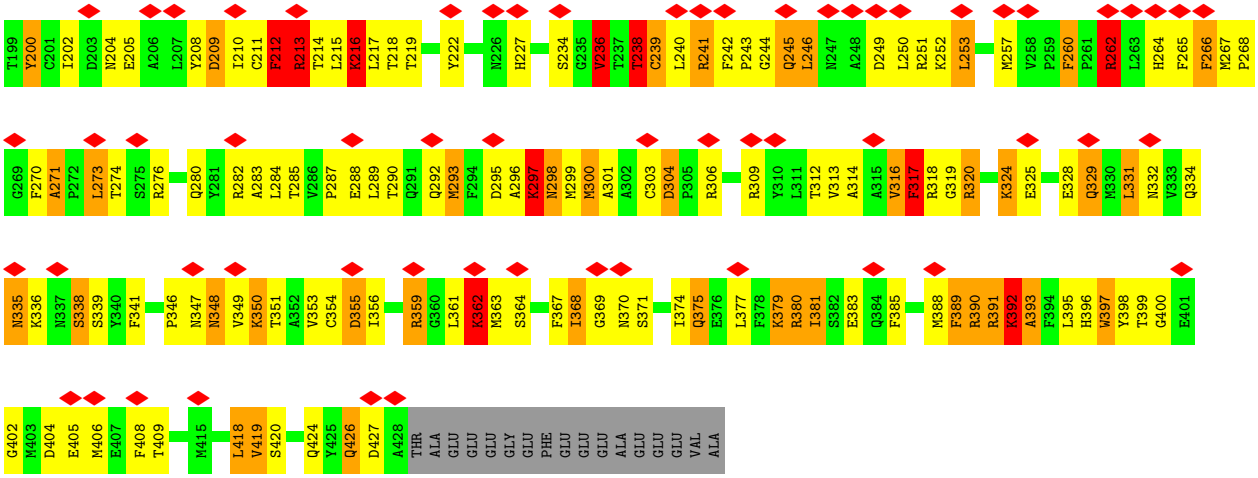
Chain QJ:





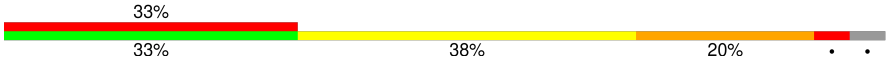


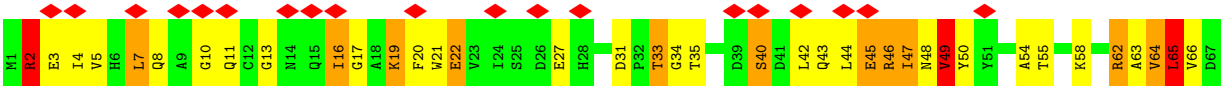


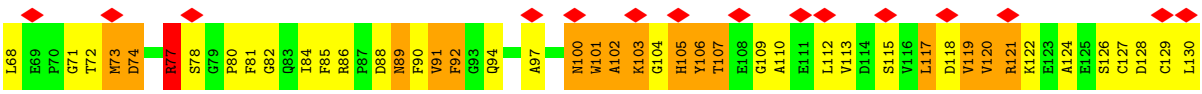


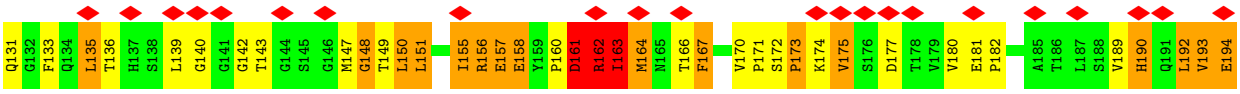
- Molecule 41: Tubulin beta-4B chain

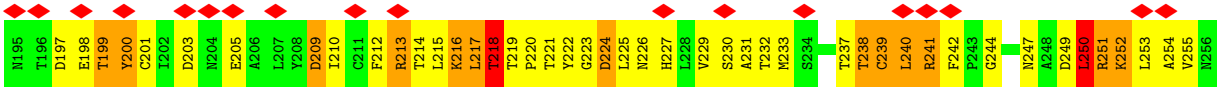
Chain QL:

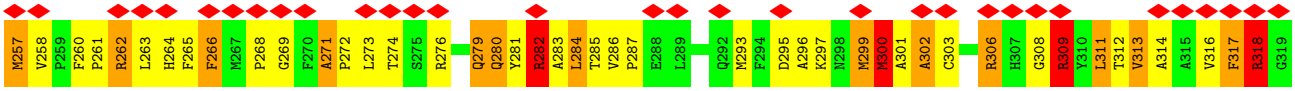


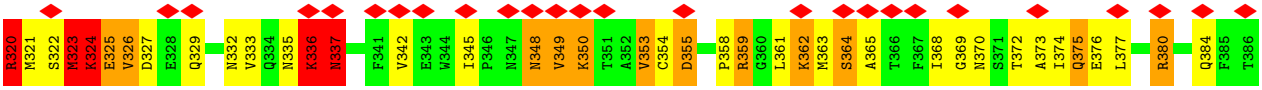


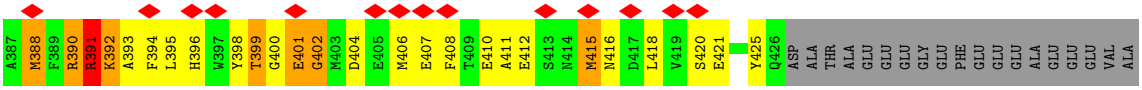






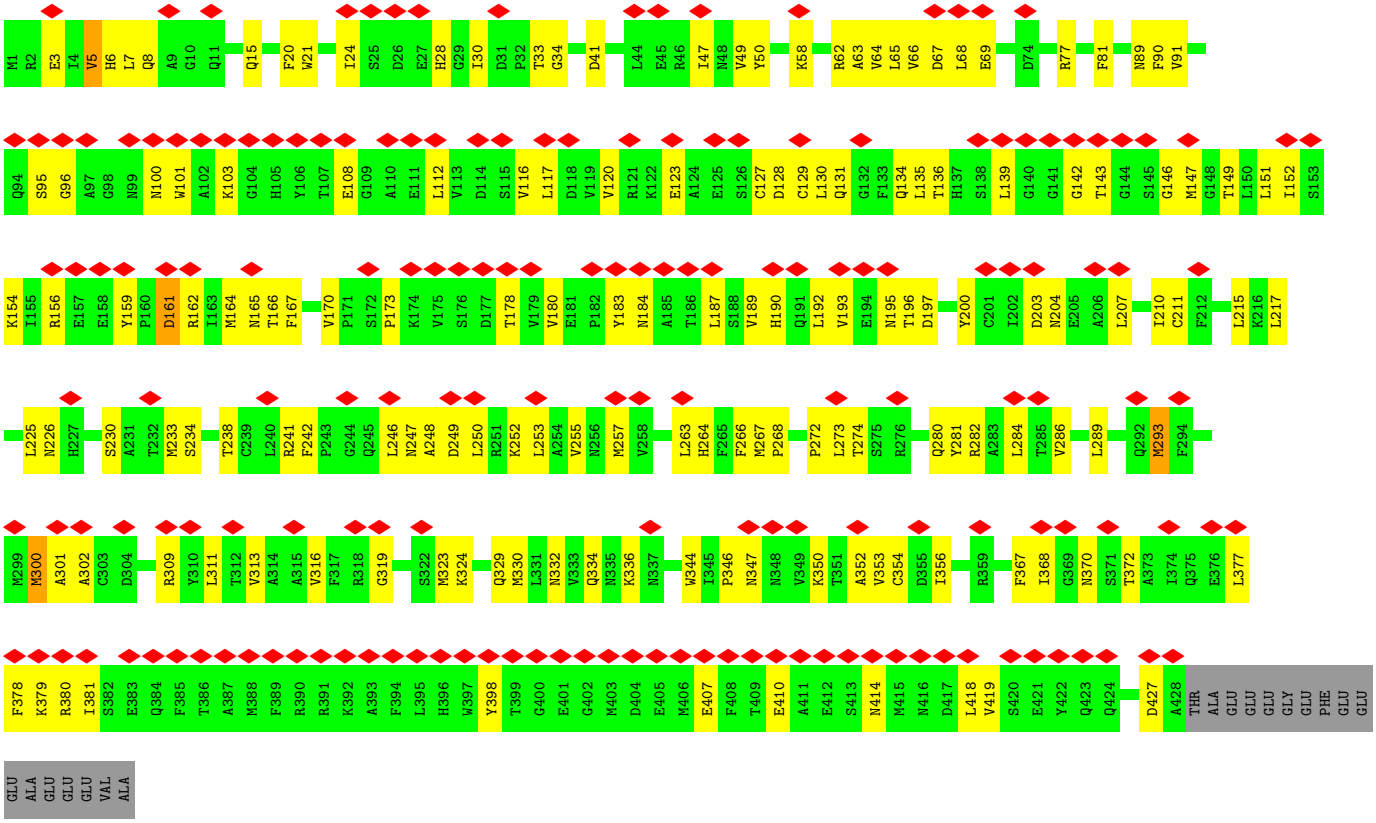






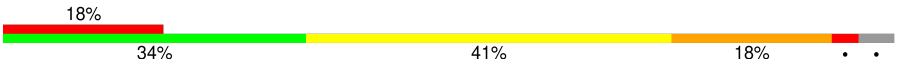
- Molecule 41: Tubulin beta-4B chain

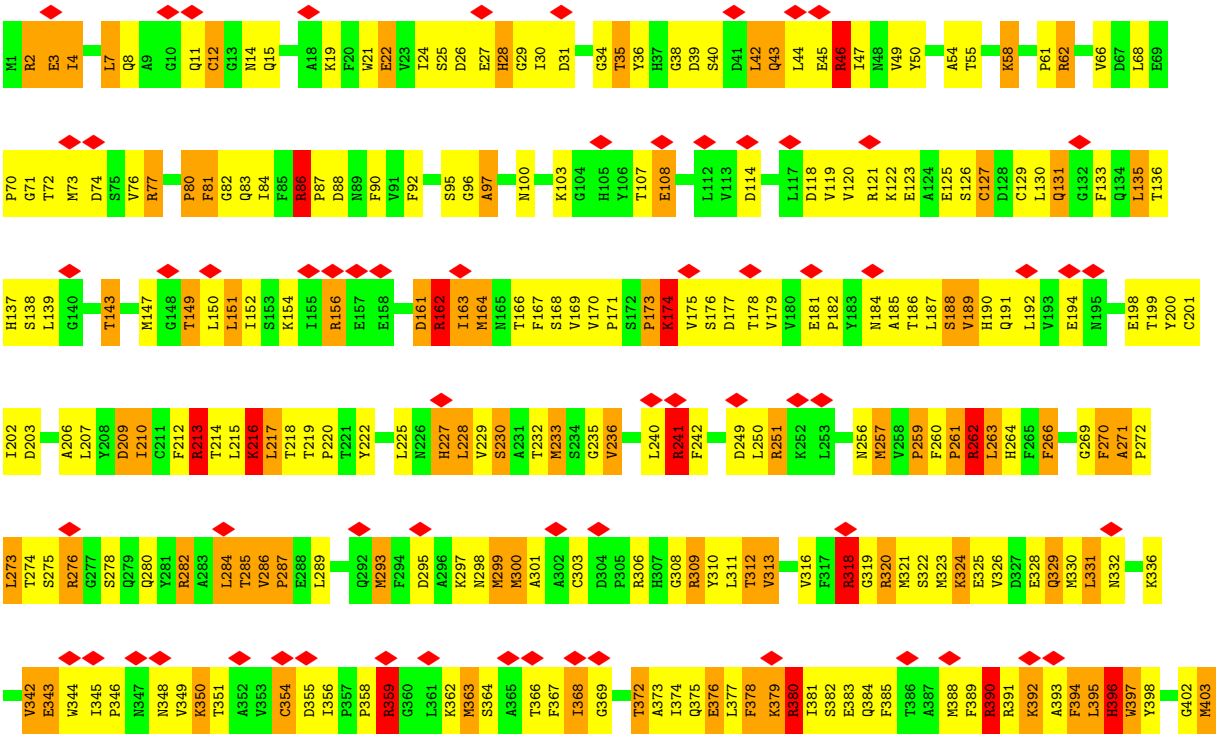
Chain RB:

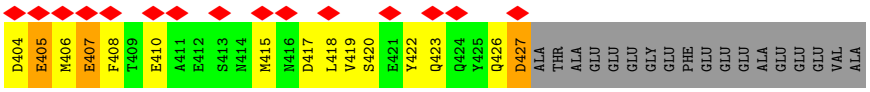


- Molecule 41: Tubulin beta-4B chain

Chain RD:

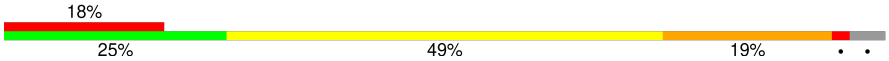


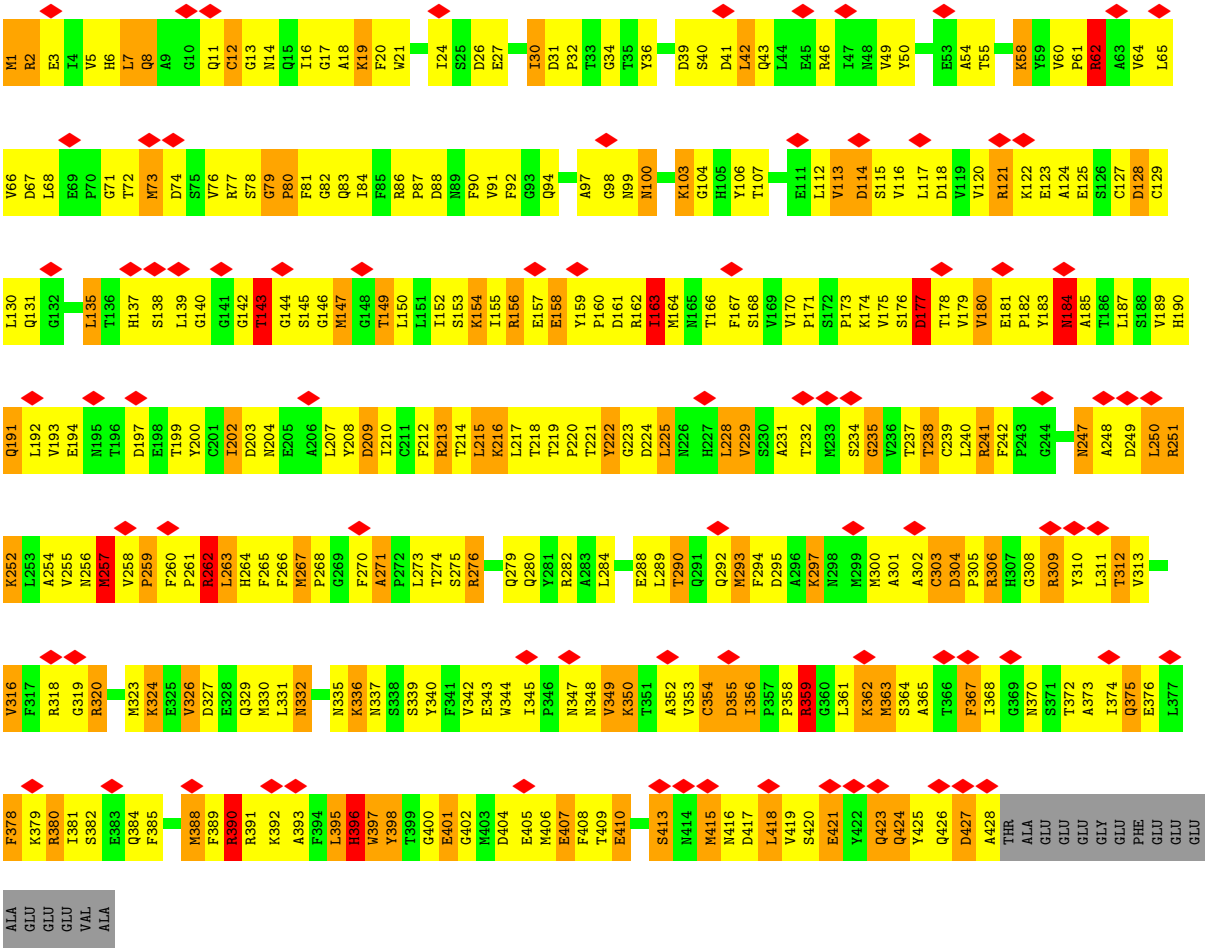




- Molecule 41: Tubulin beta-4B chain

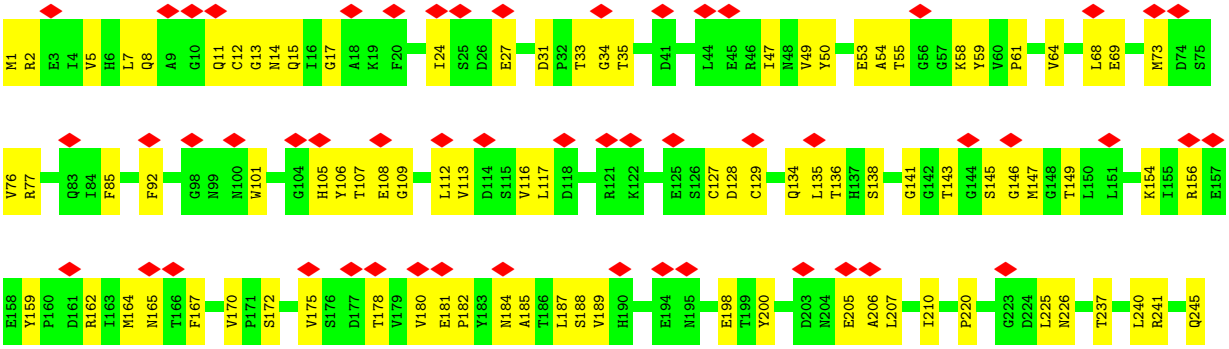
Chain RF:

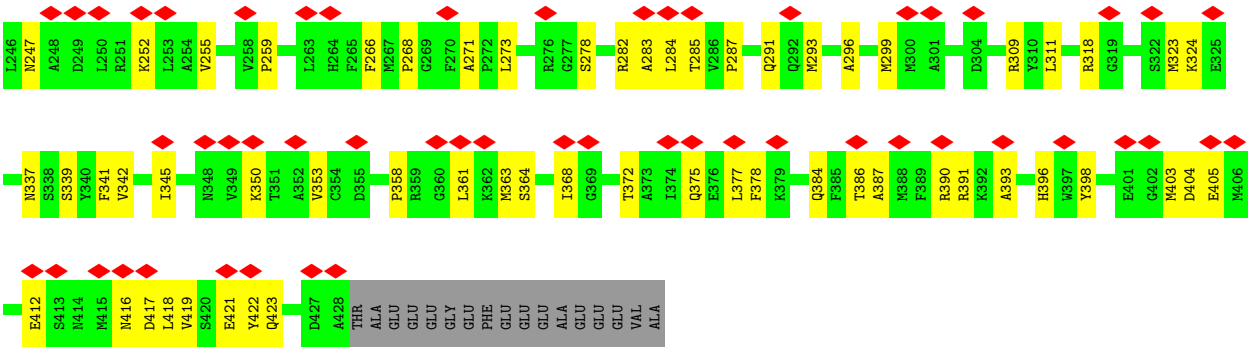




- Molecule 41: Tubulin beta-4B chain

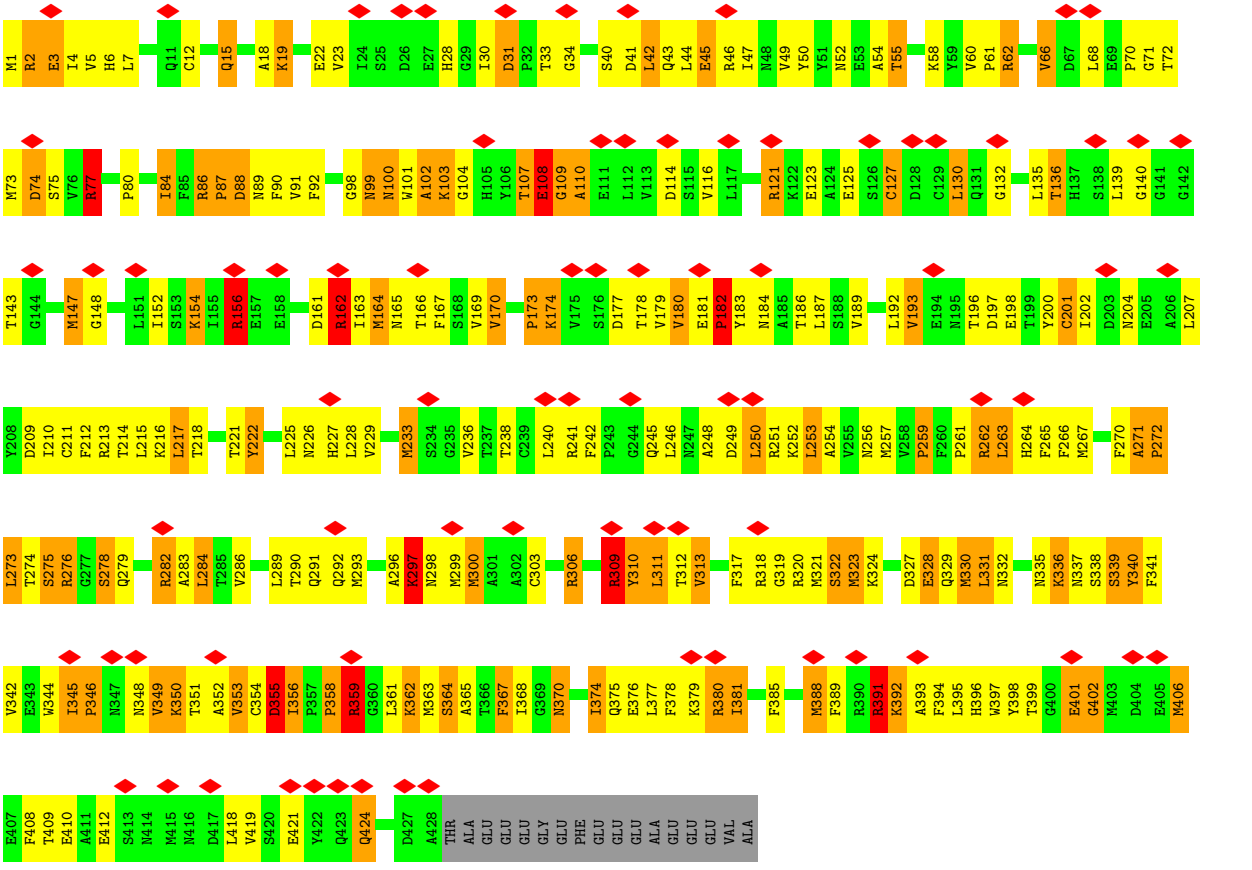
Chain RH:





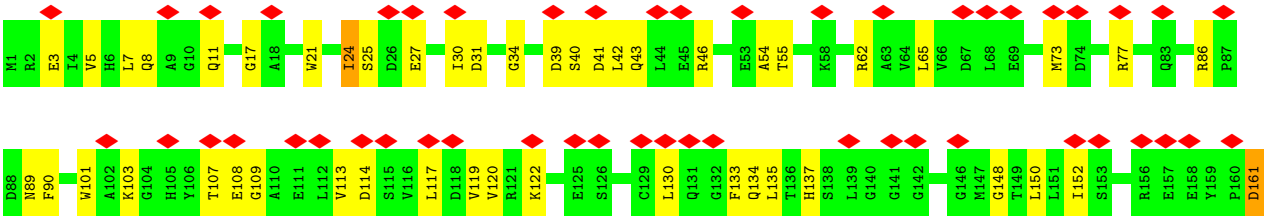
- Molecule 41: Tubulin beta-4B chain

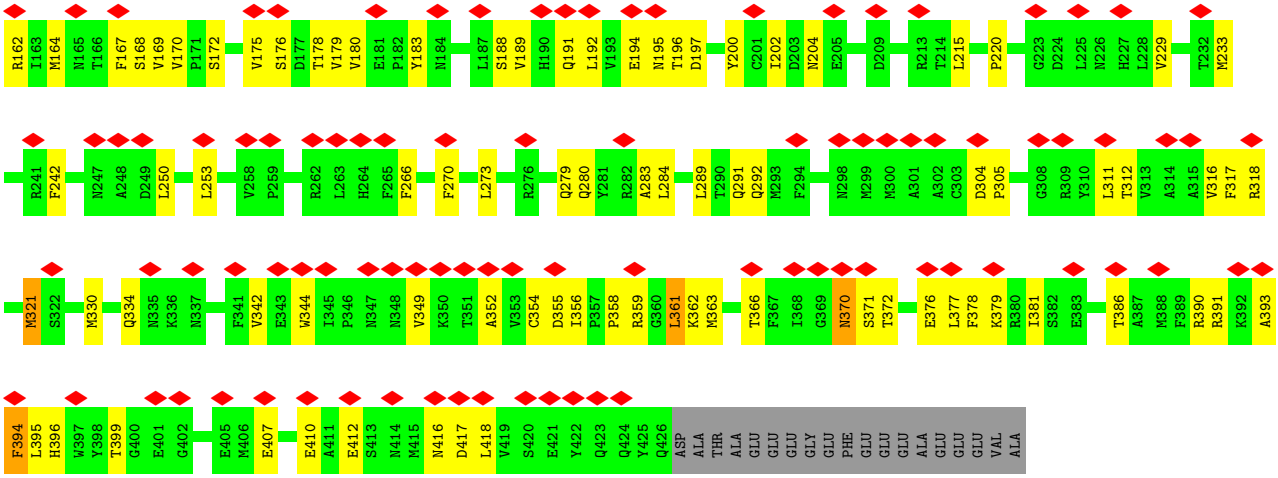
Chain RJ:



- Molecule 41: Tubulin beta-4B chain

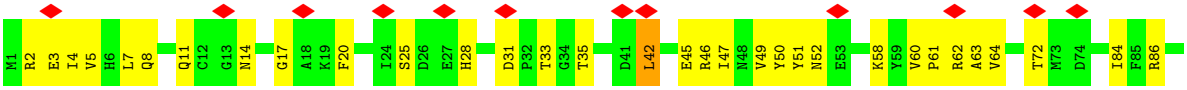
Chain RL:

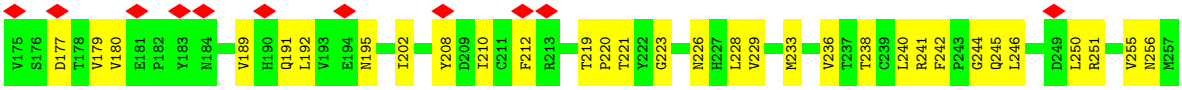


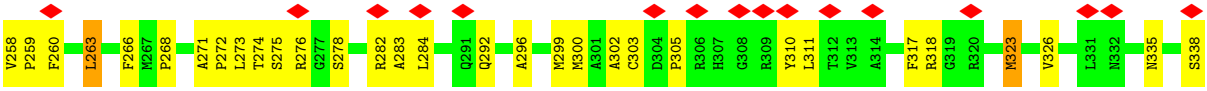


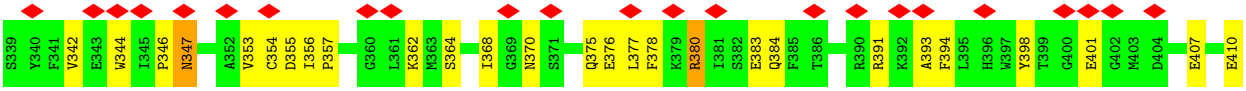
- Molecule 41: Tubulin beta-4B chain

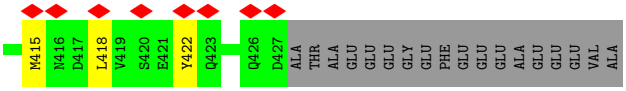
Chain SD:





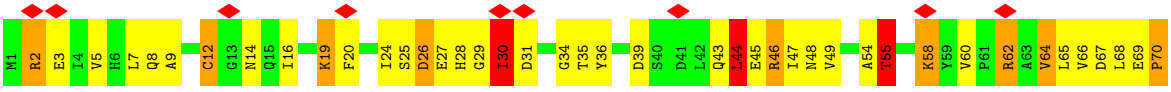


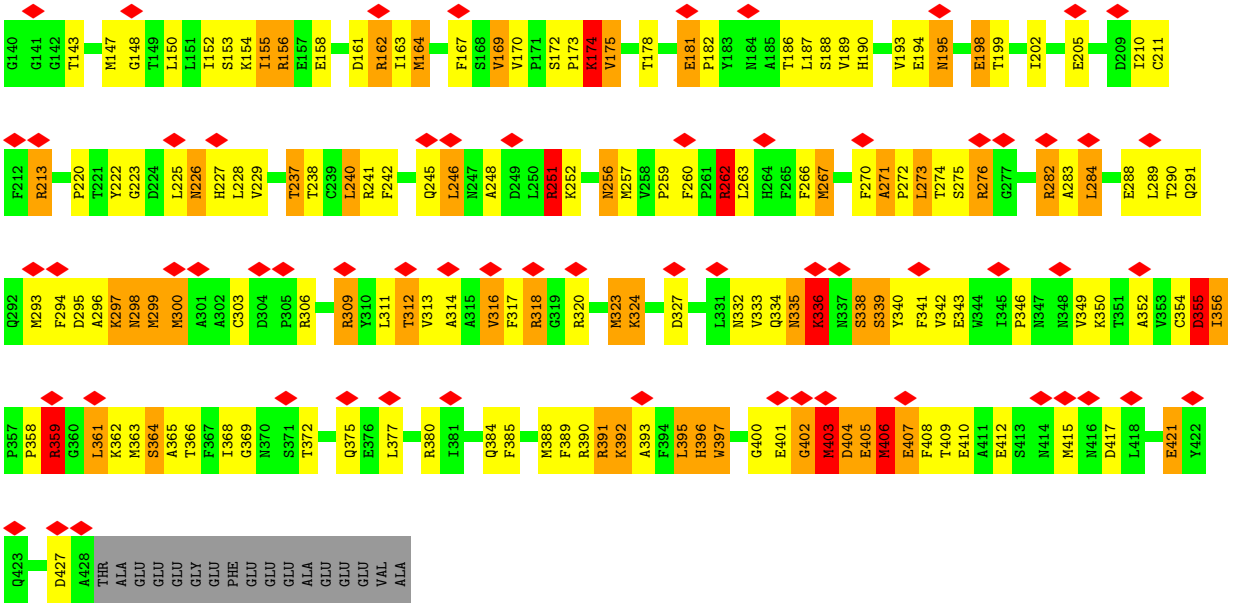




- Molecule 41: Tubulin beta-4B chain

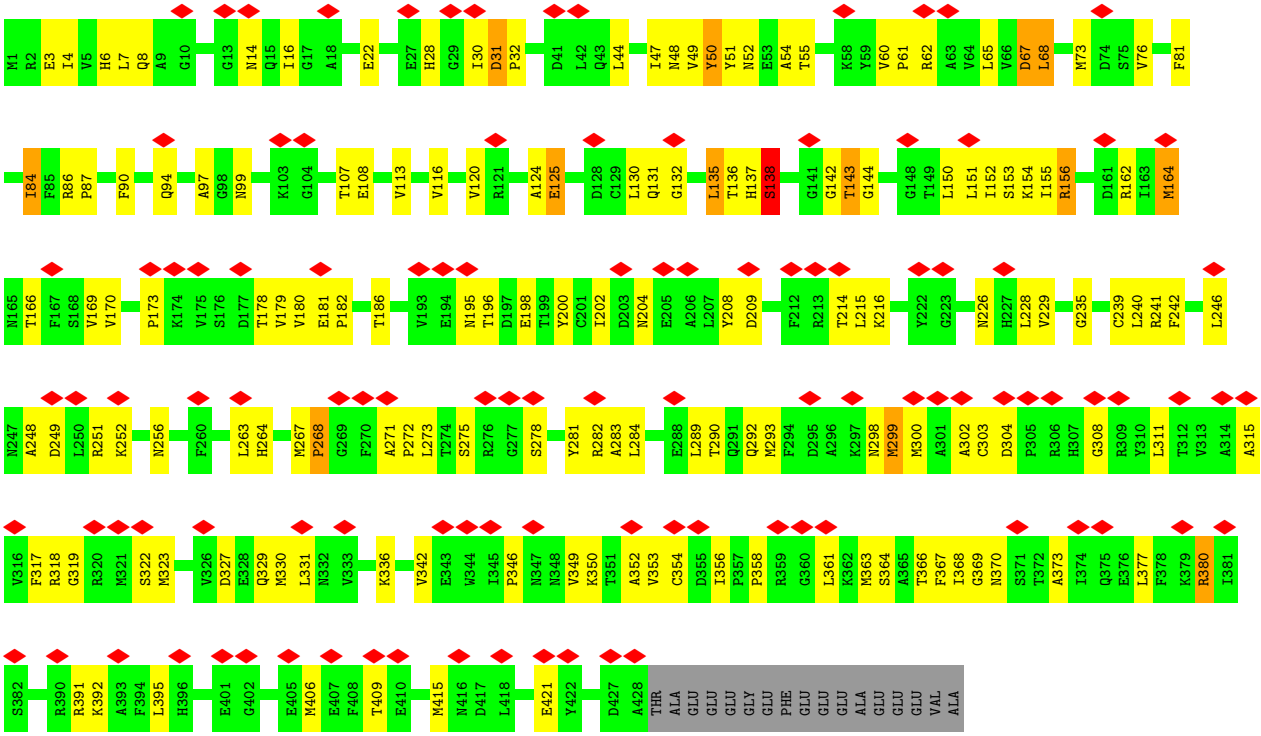
Chain SF:





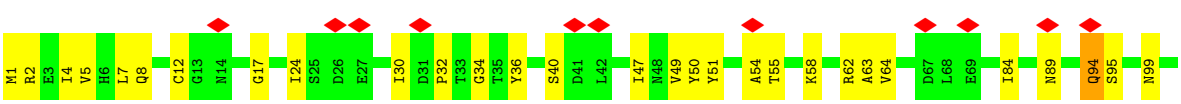
- Molecule 41: Tubulin beta-4B chain

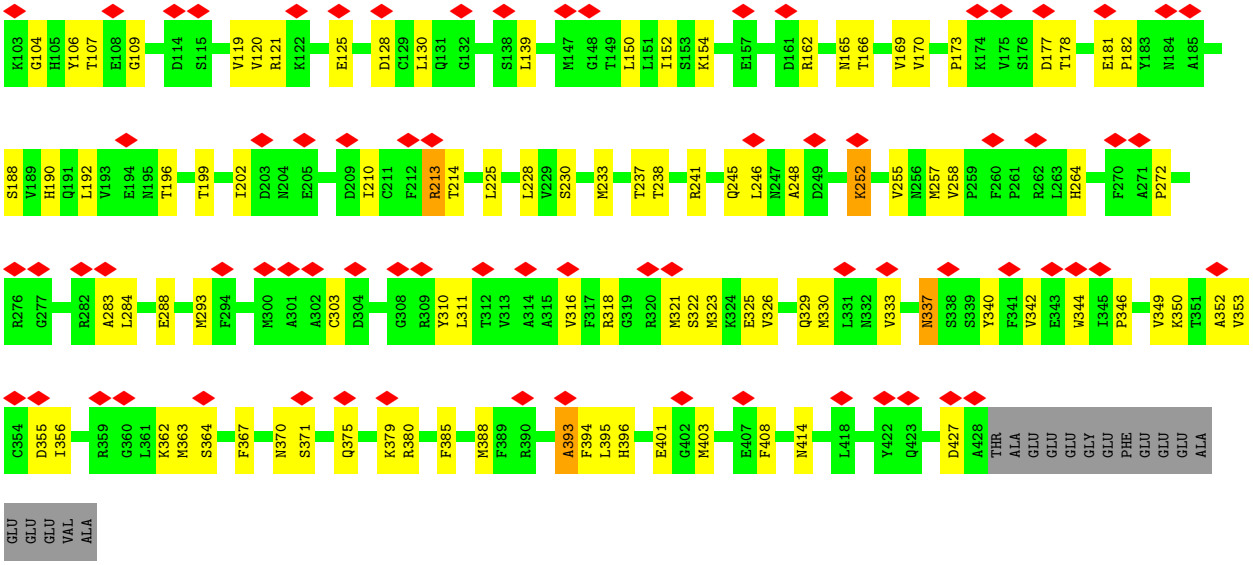
Chain SH:



- Molecule 41: Tubulin beta-4B chain

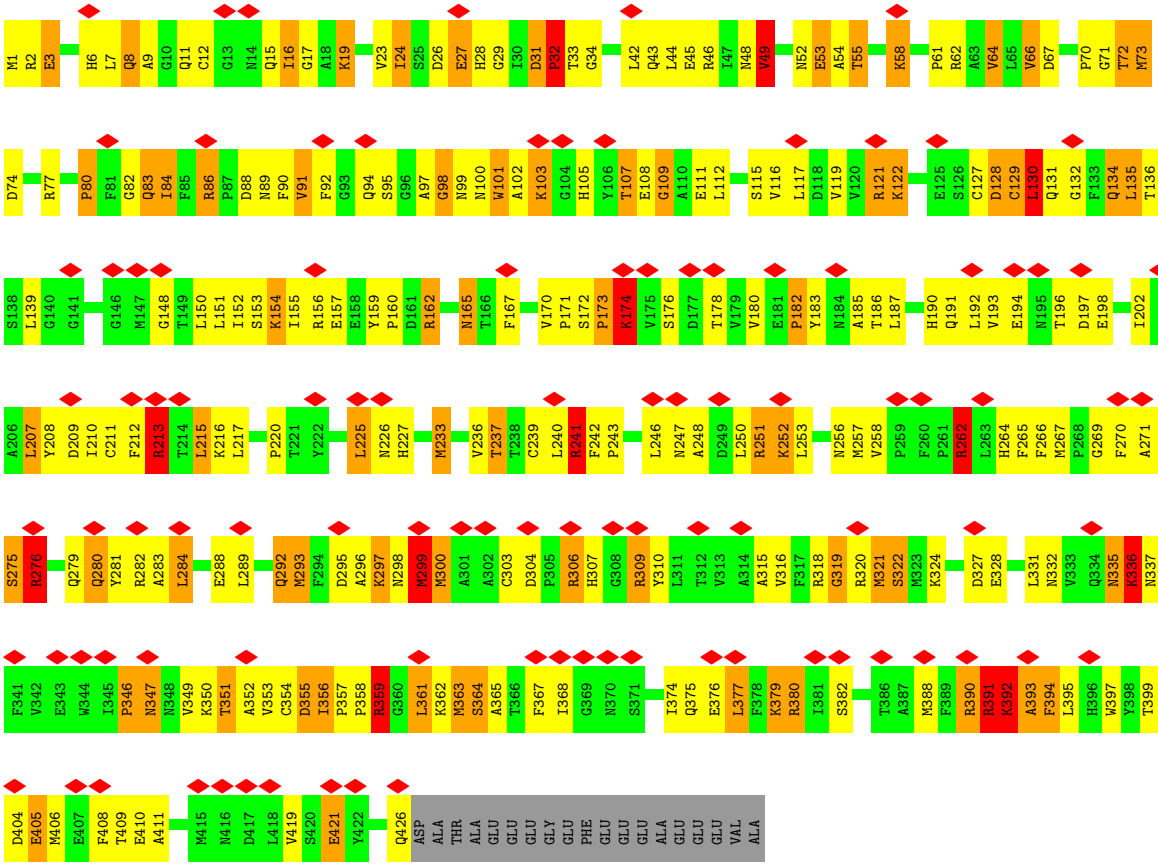
Chain SJ:





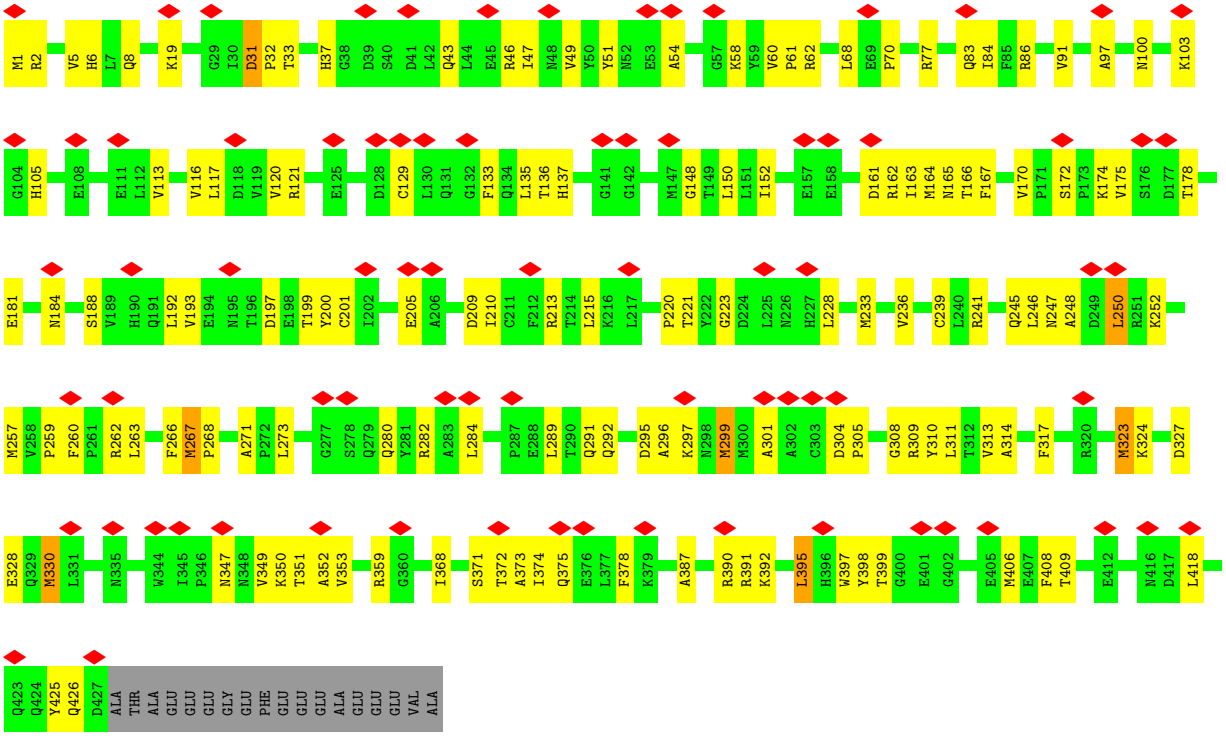
- Molecule 41: Tubulin beta-4B chain

Chain SL:



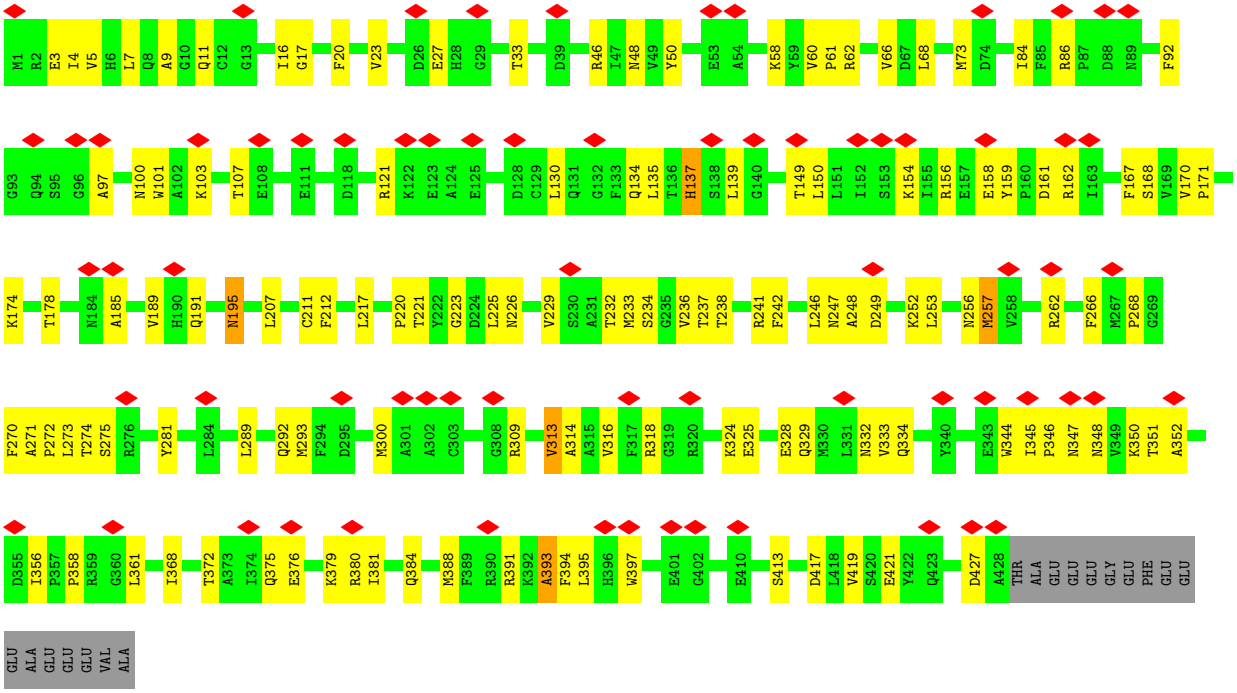
- Molecule 41: Tubulin beta-4B chain

Chain TD:



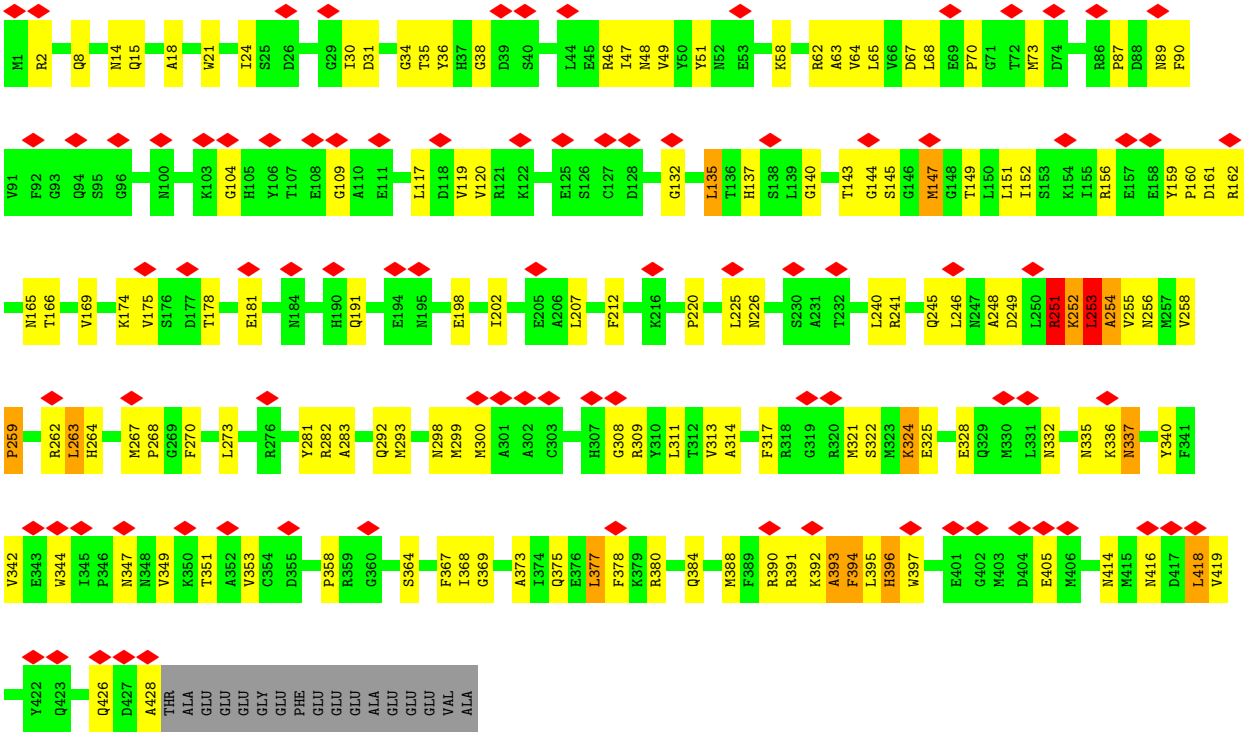
- Molecule 41: Tubulin beta-4B chain

Chain TF:



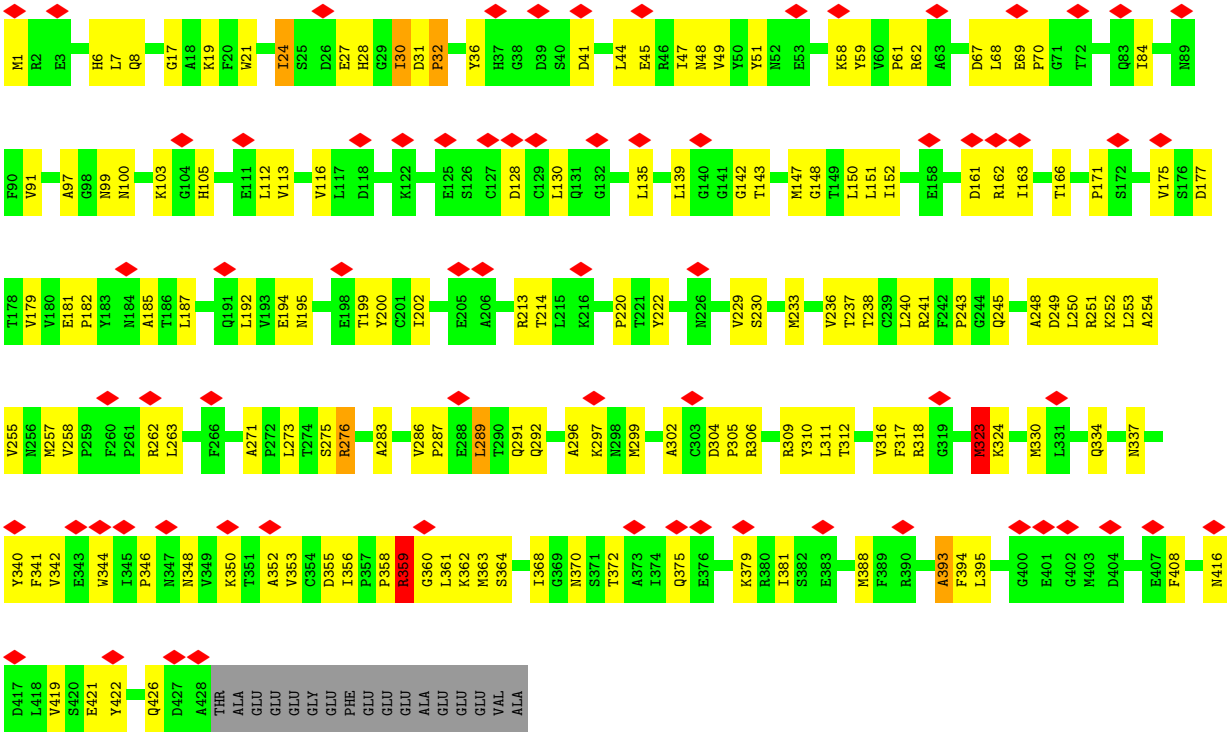
- Molecule 41: Tubulin beta-4B chain

Chain TH:



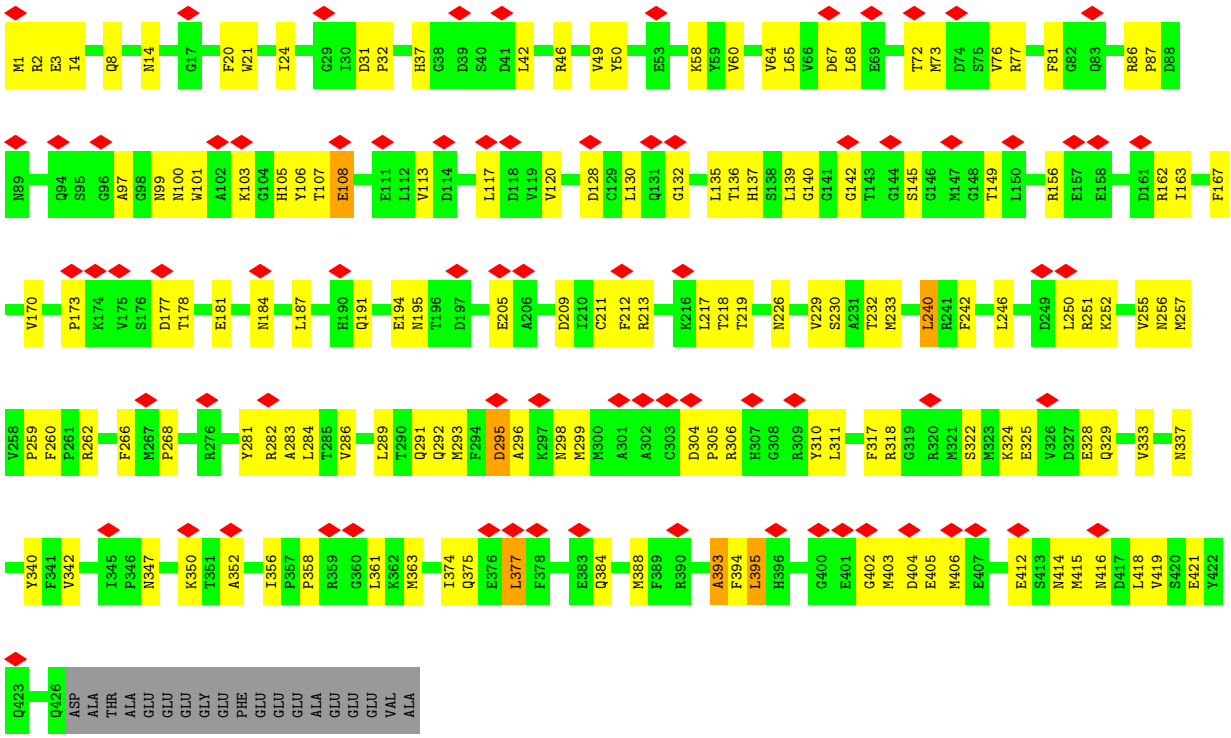
- Molecule 41: Tubulin beta-4B chain

Chain TJ:



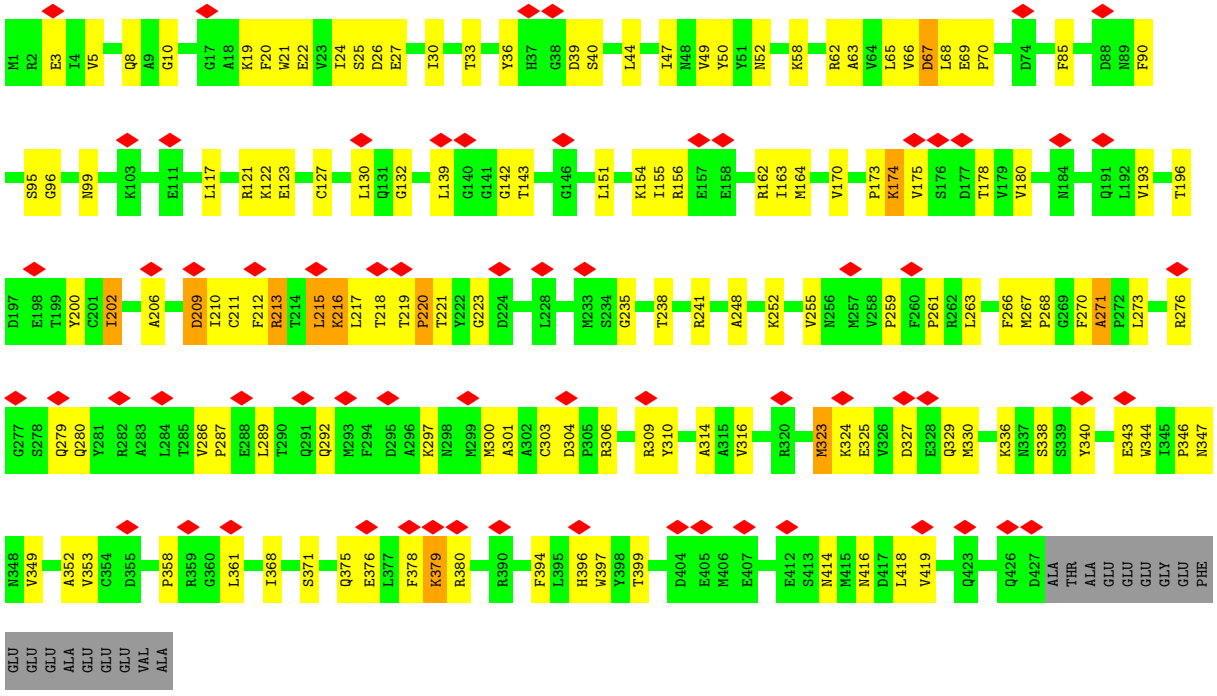
- Molecule 41: Tubulin beta-4B chain

Chain TL:



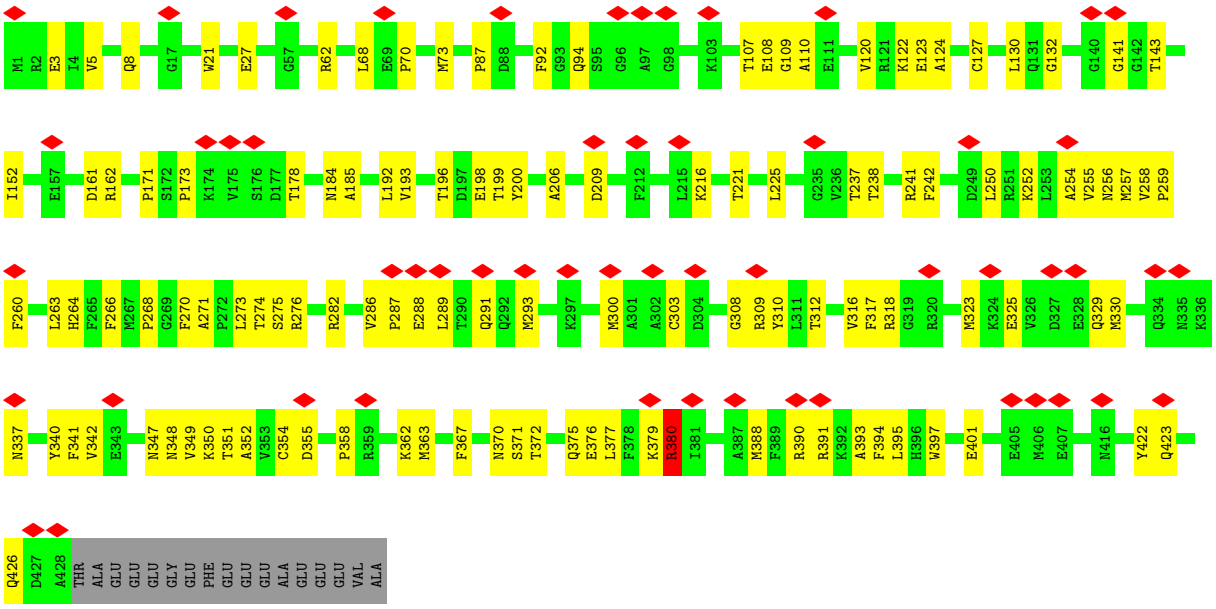
- Molecule 41: Tubulin beta-4B chain

Chain UD:



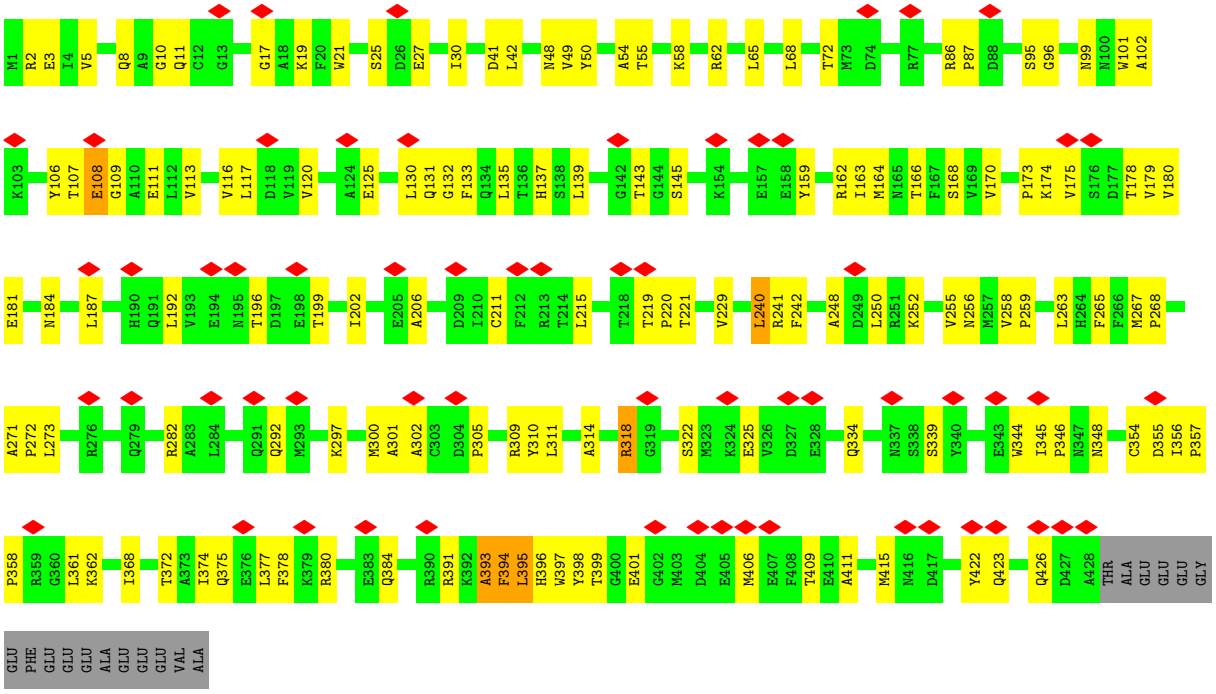
- Molecule 41: Tubulin beta-4B chain

Chain UF:



- Molecule 41: Tubulin beta-4B chain

Chain UH:



- Molecule 41: Tubulin beta-4B chain

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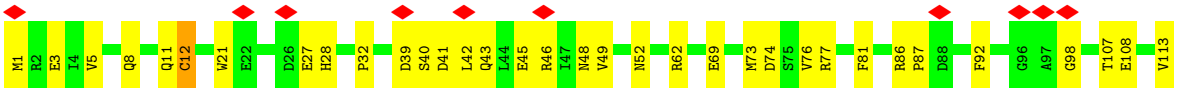
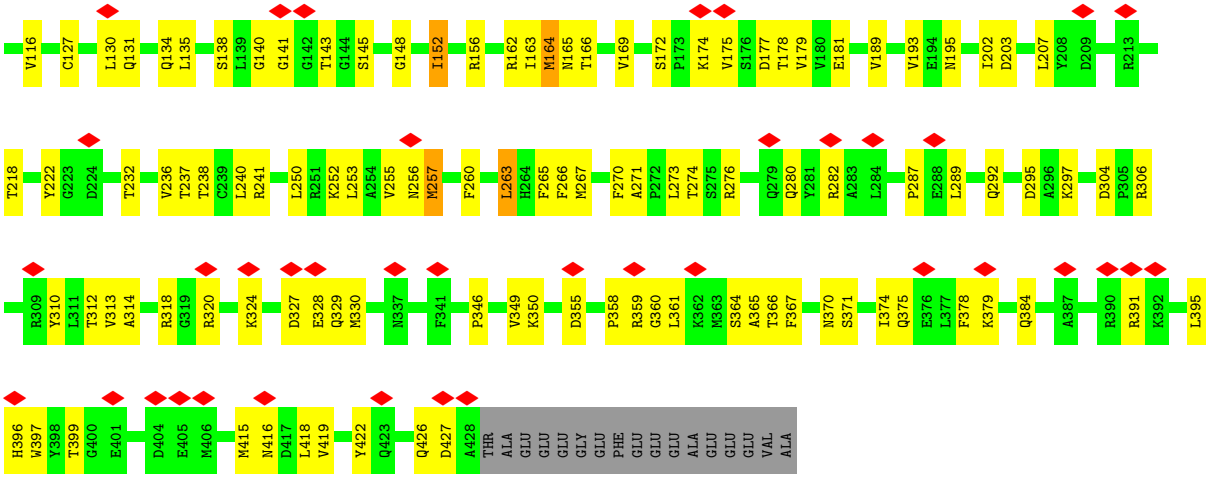
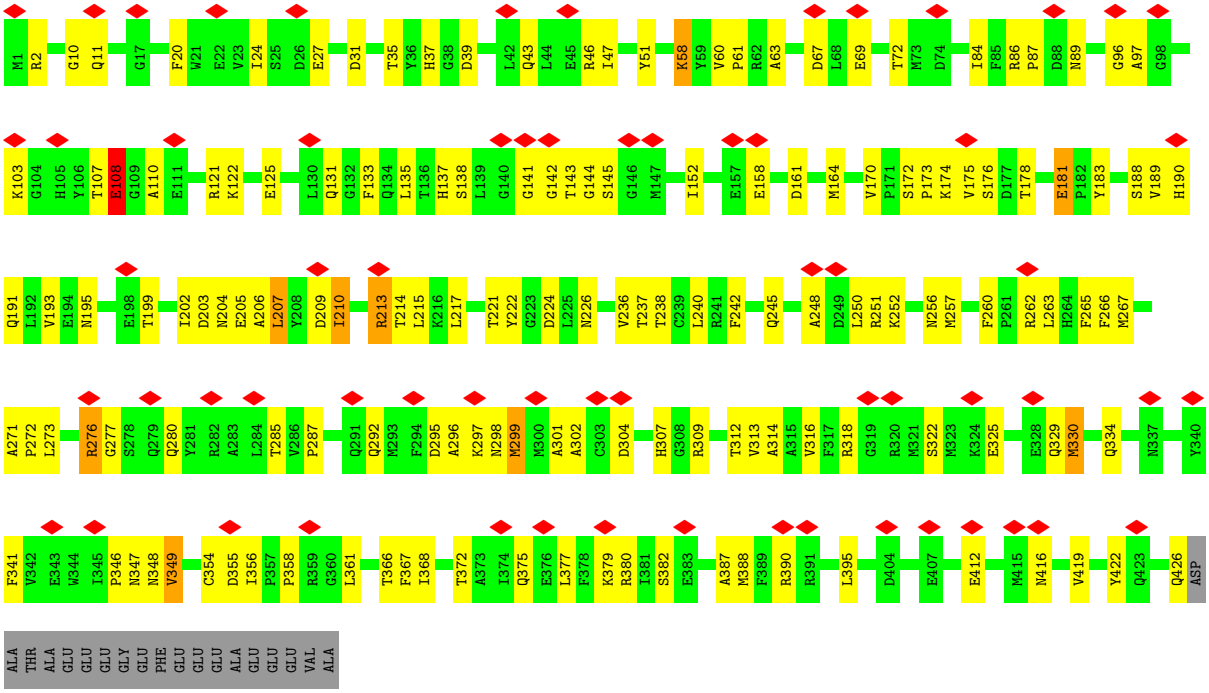




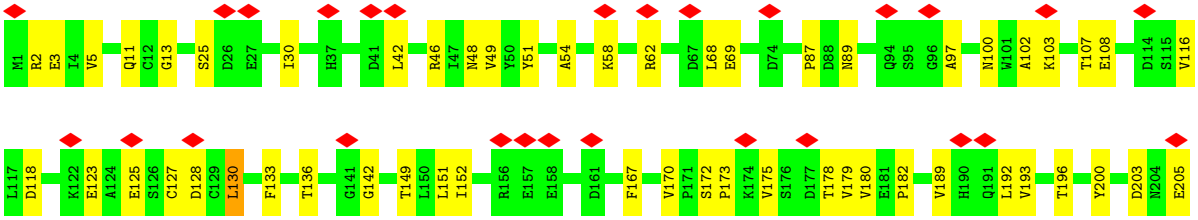
- Molecule 41: Tubulin beta-4B chain

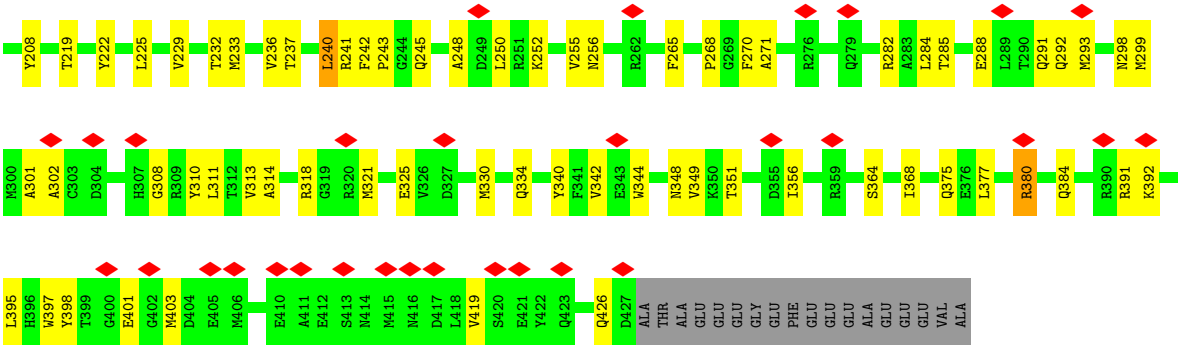
Chain UL:



- Molecule 41: Tubulin beta-4B chain

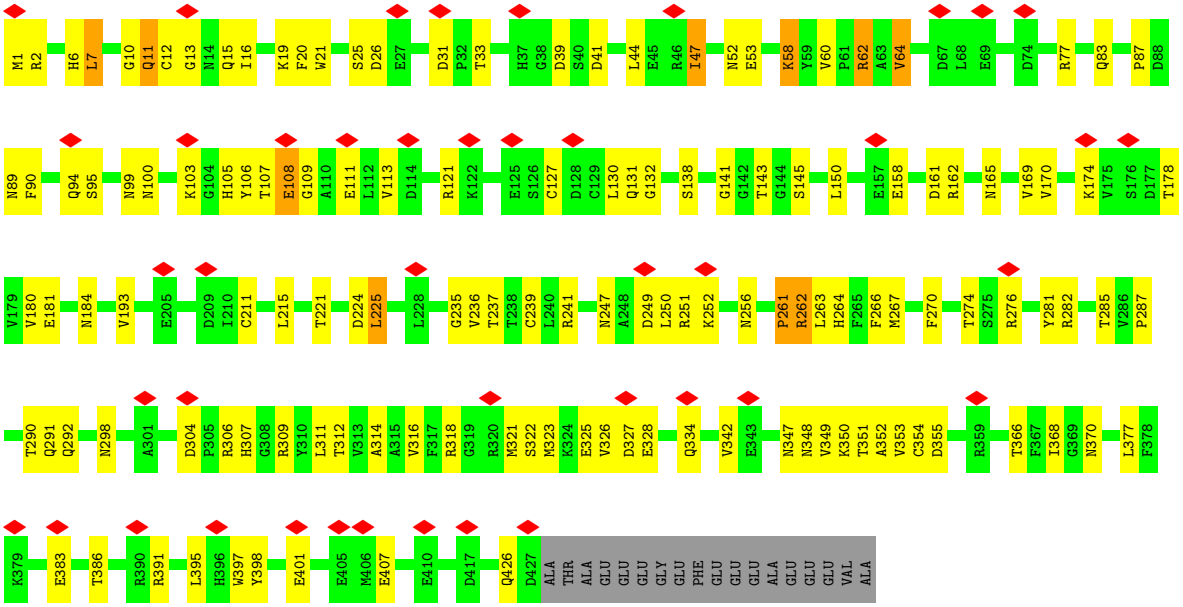
Chain VD:





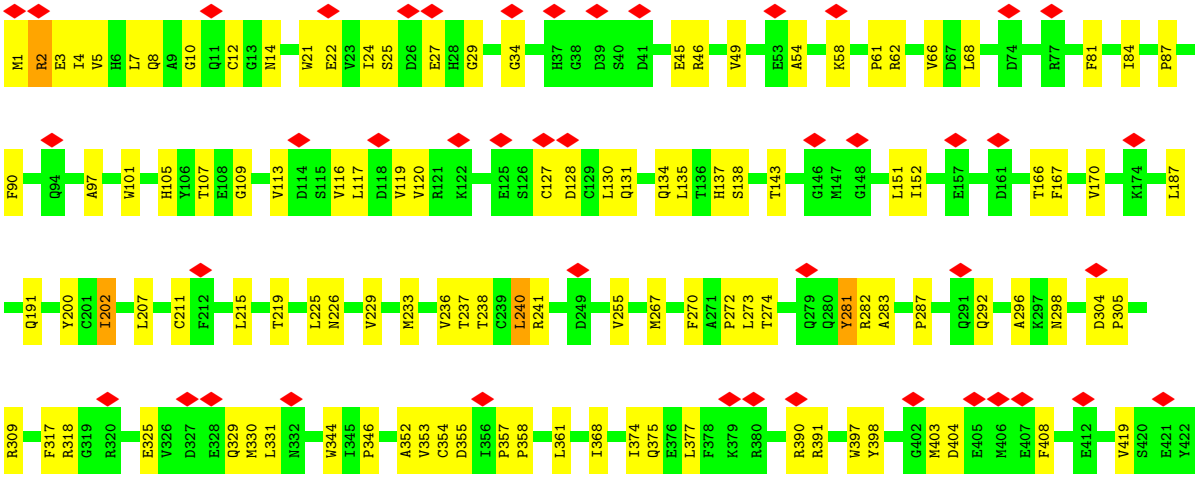
- Molecule 41: Tubulin beta-4B chain

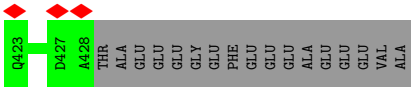
Chain VF:



- Molecule 41: Tubulin beta-4B chain

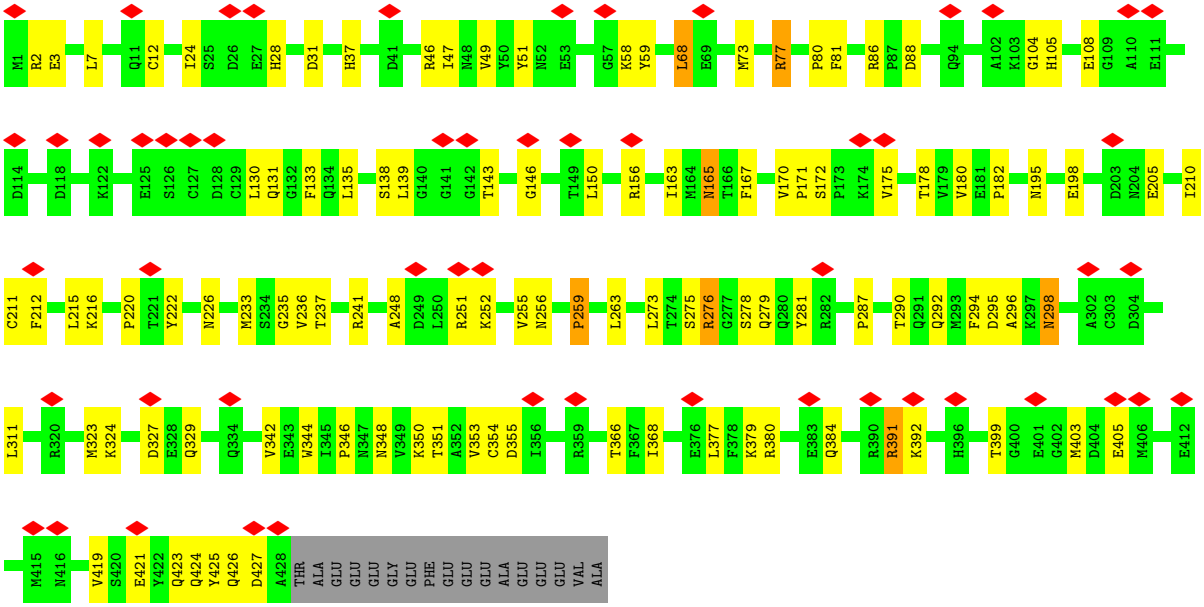
Chain VH:





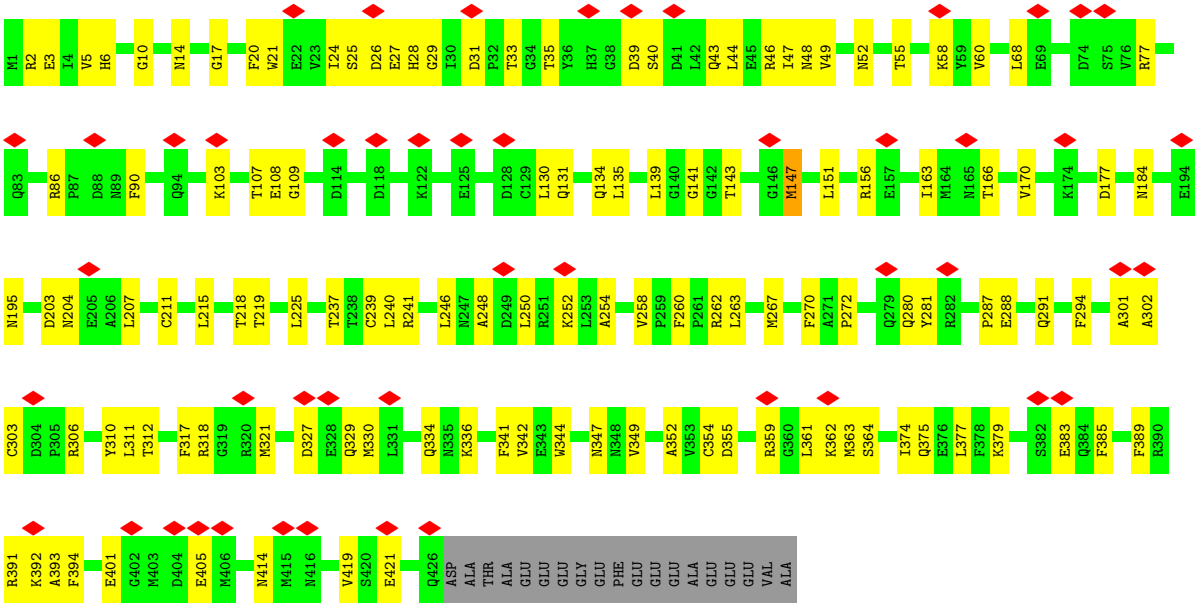
• Molecule 41: Tubulin beta-4B chain

Chain VJ:



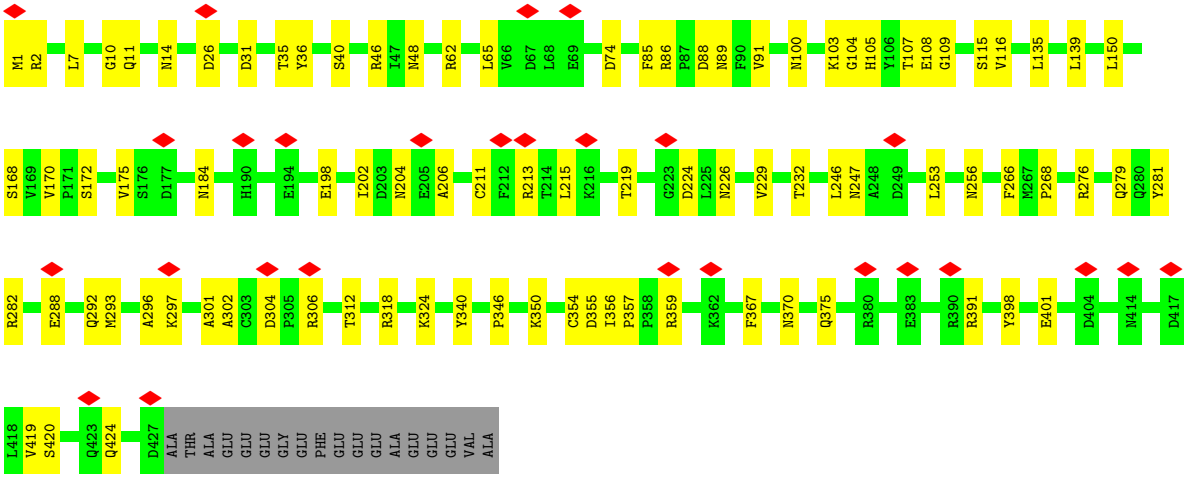
• Molecule 41: Tubulin beta-4B chain

Chain VL:



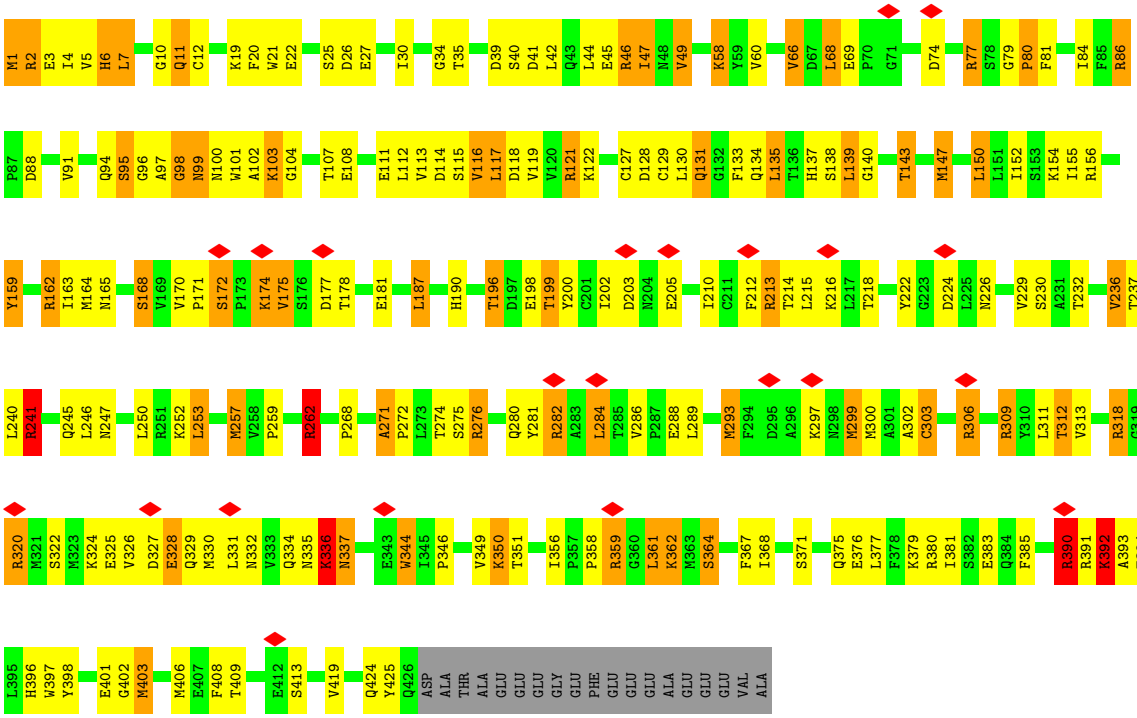
• Molecule 41: Tubulin beta-4B chain

Chain WD:



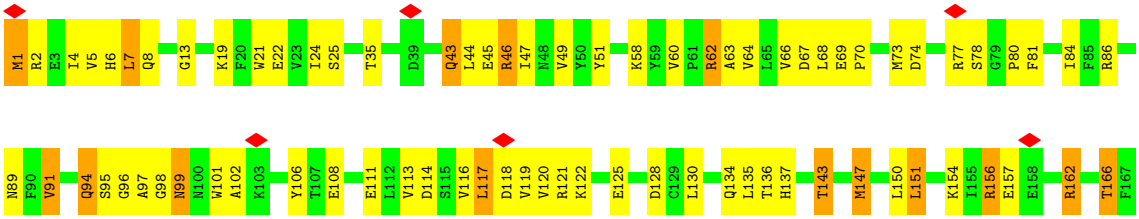
- Molecule 41: Tubulin beta-4B chain

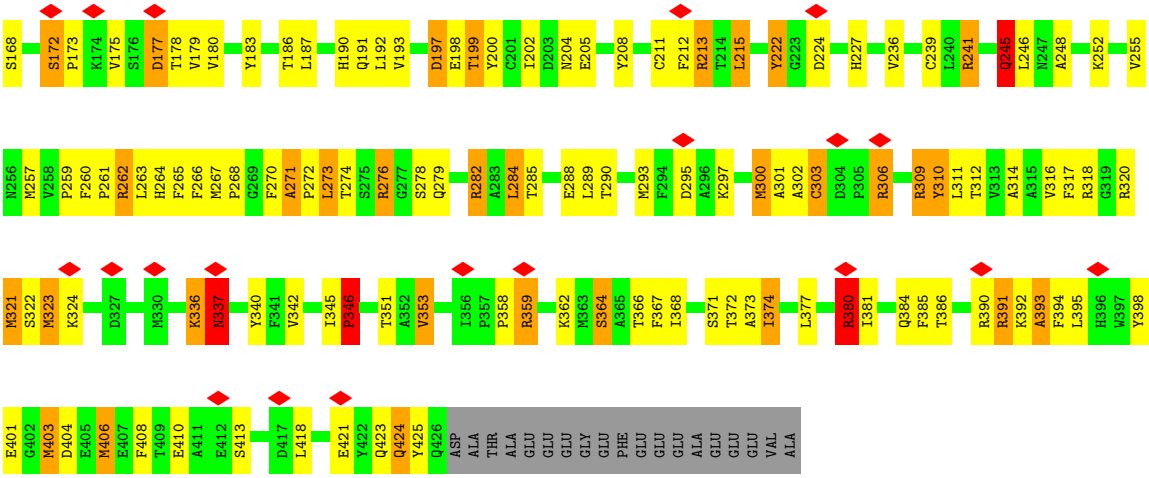
Chain WF:



- Molecule 41: Tubulin beta-4B chain

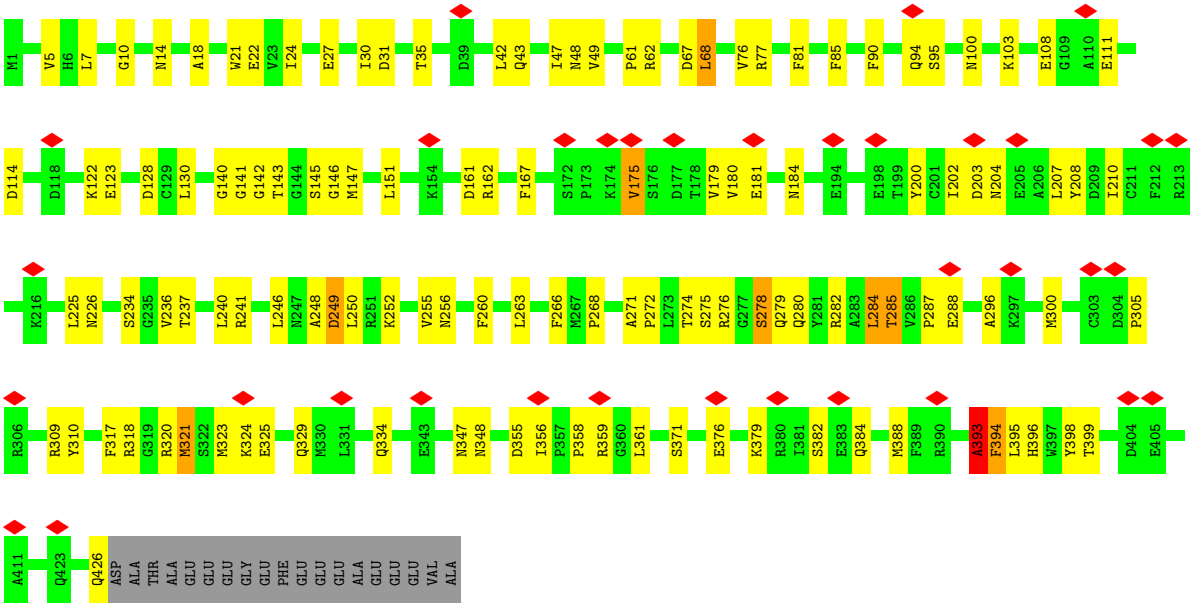
Chain WH:





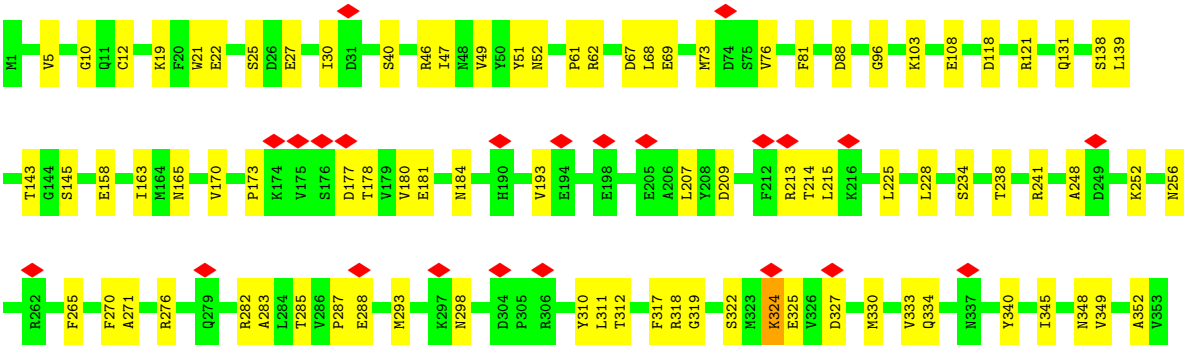
• Molecule 41: Tubulin beta-4B chain

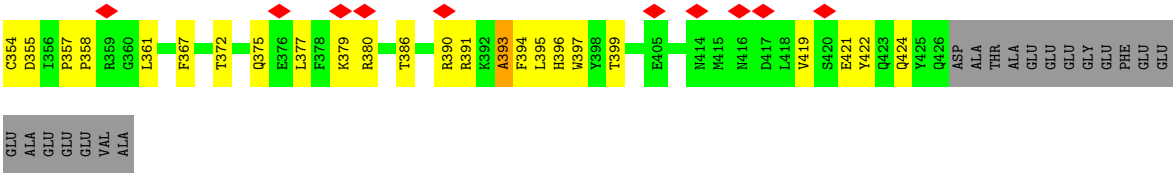
Chain WJ:



• Molecule 41: Tubulin beta-4B chain

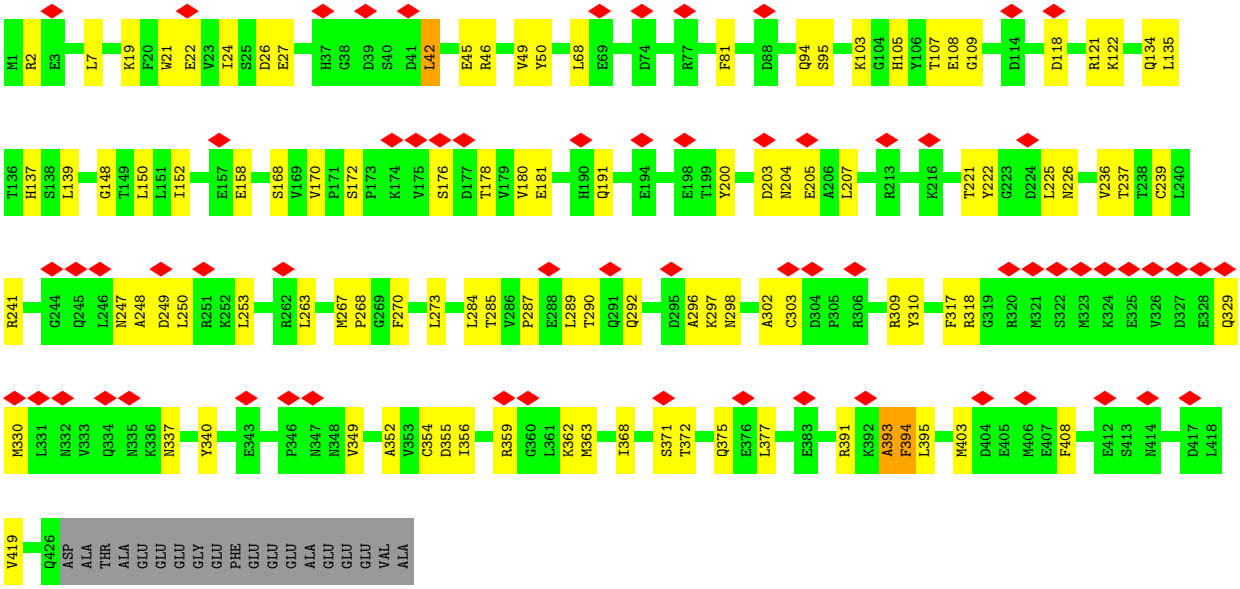
Chain WL:





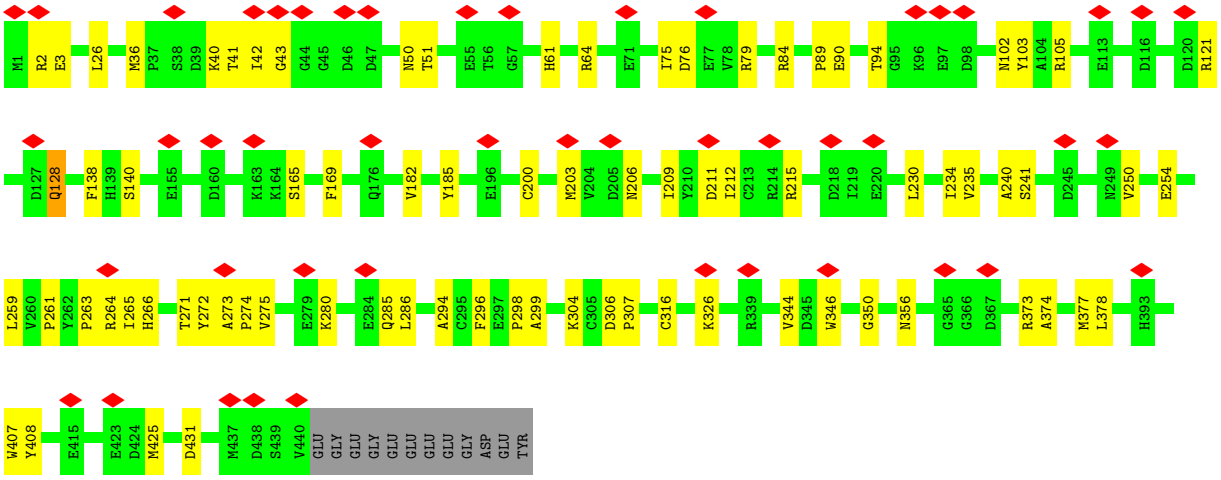
• Molecule 41: Tubulin beta-4B chain

Chain WN:



• Molecule 42: Tubulin alpha-1D chain

Chain AC:



• Molecule 42: Tubulin alpha-1D chain

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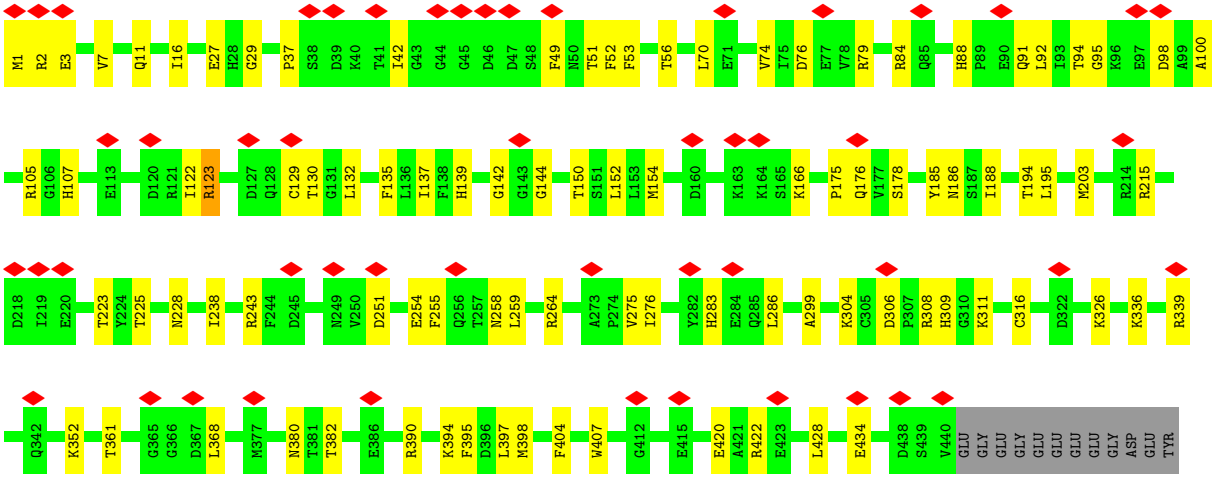
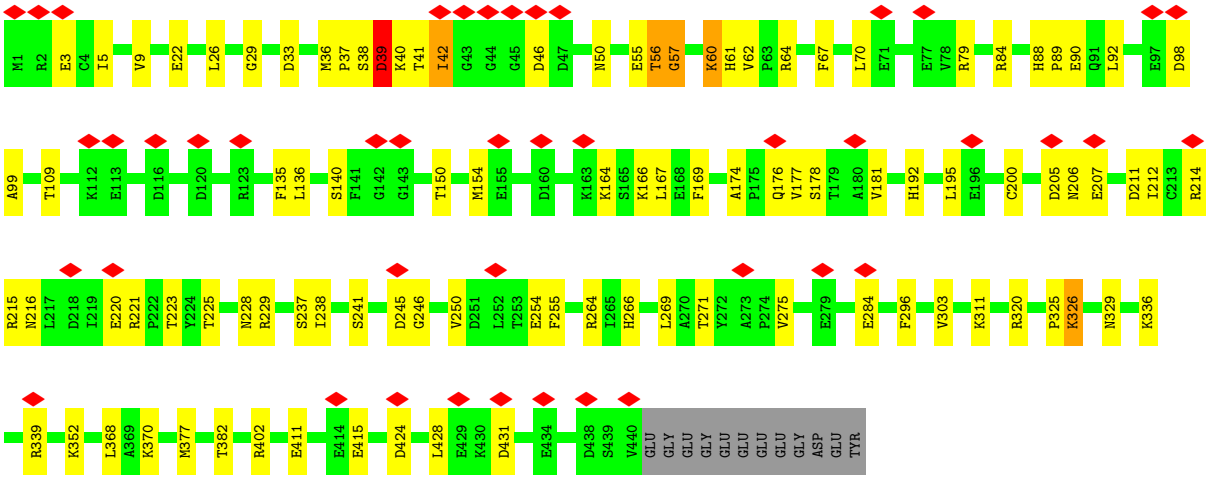


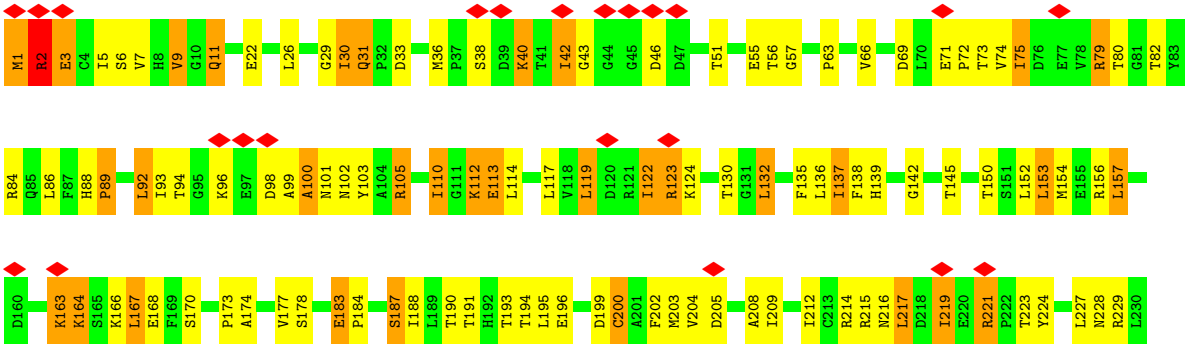
- Molecule 42: Tubulin alpha-1D chain

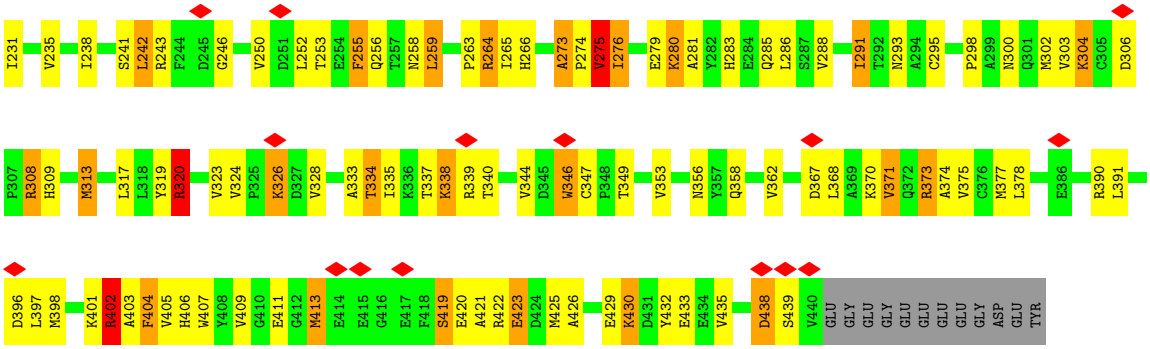
Chain AG:



- Molecule 42: Tubulin alpha-1D chain

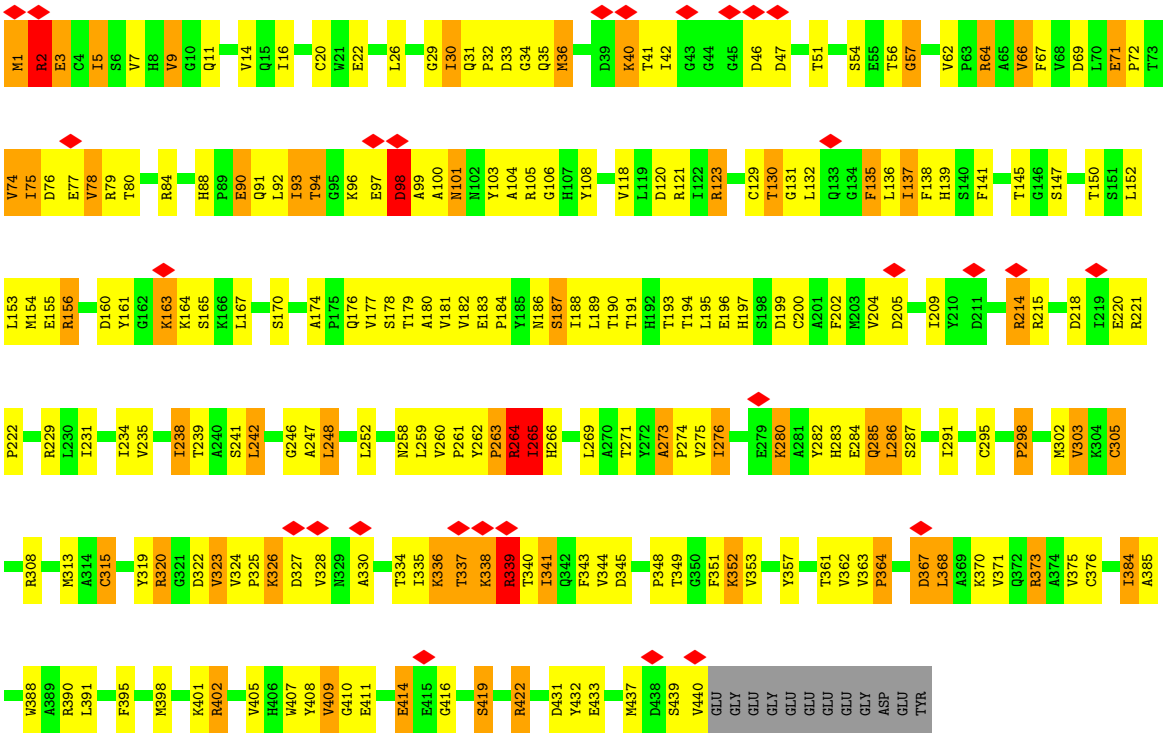
Chain AI:





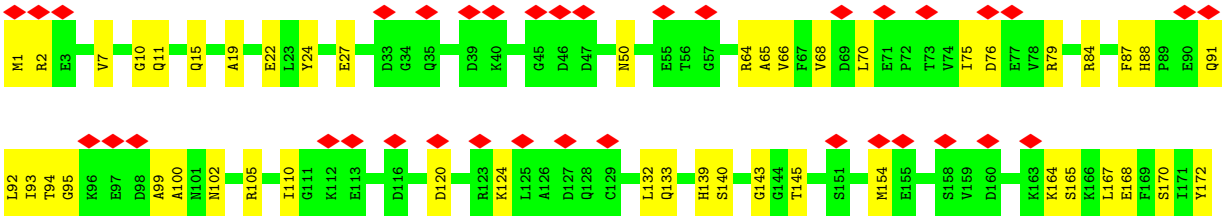
- Molecule 42: Tubulin alpha-1D chain

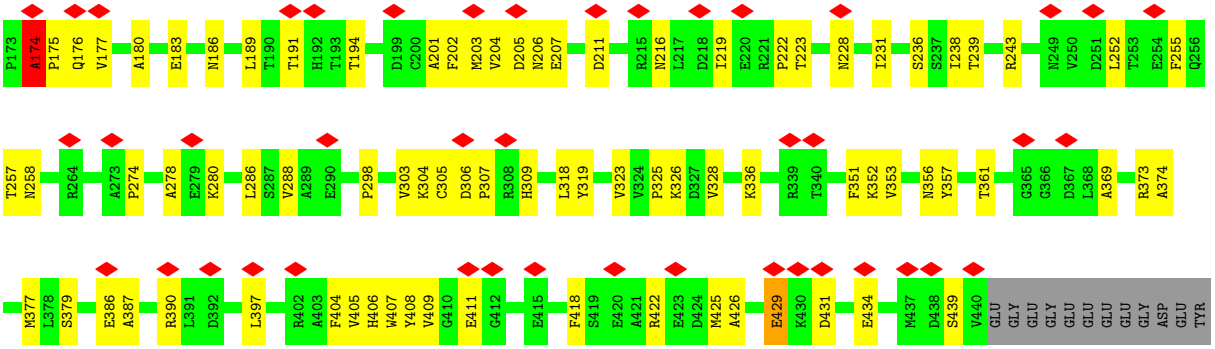
Chain AK:



- Molecule 42: Tubulin alpha-1D chain

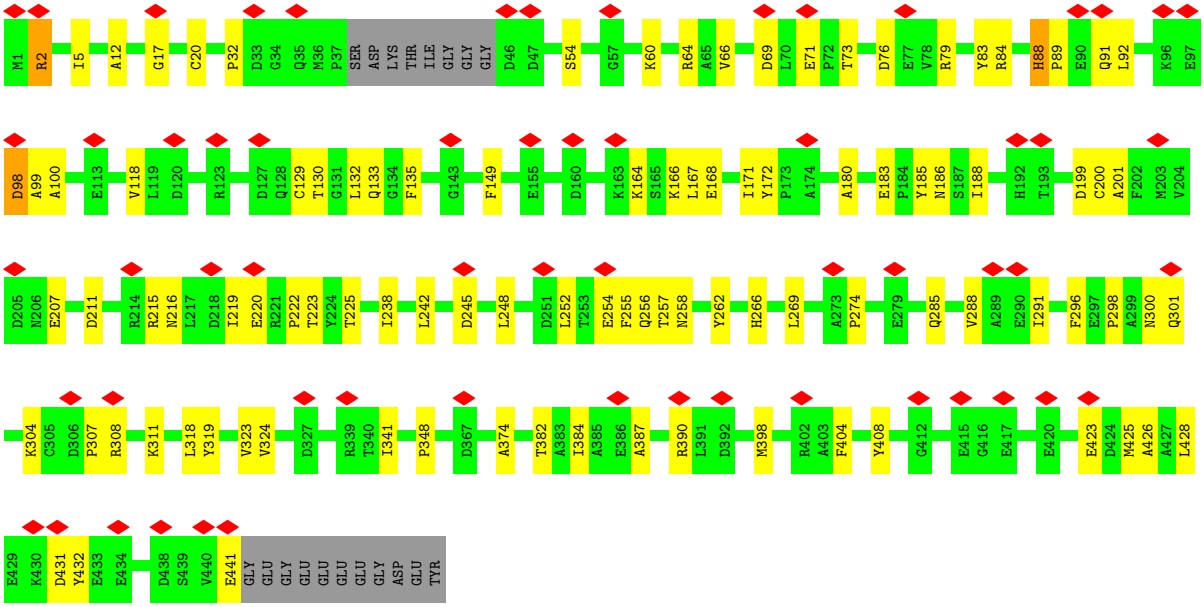
Chain BC:





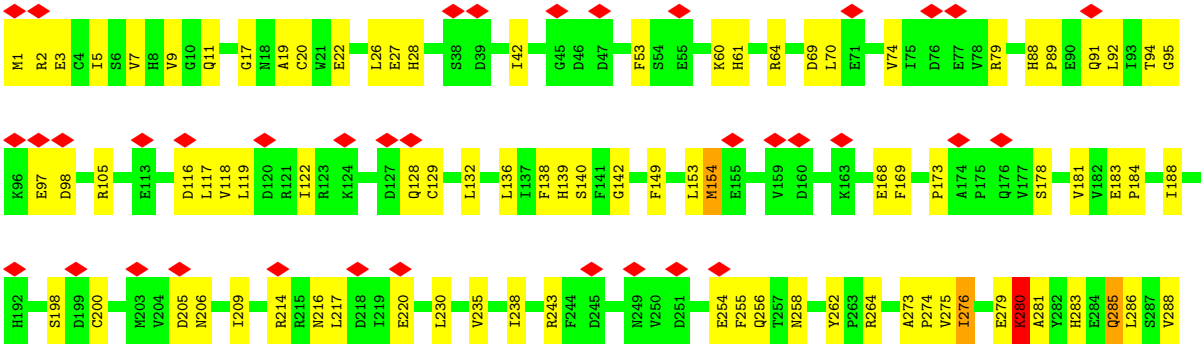
• Molecule 42: Tubulin alpha-1D chain

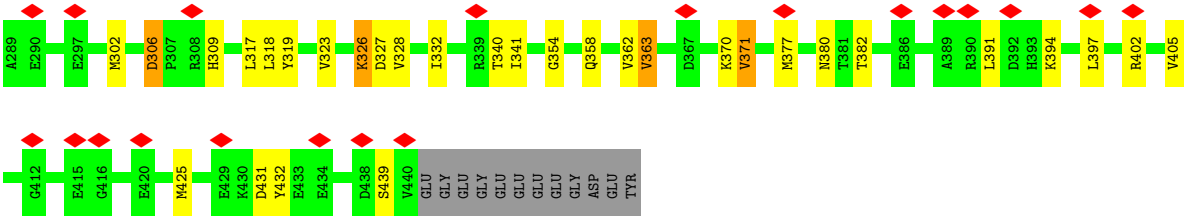
Chain BE:



• Molecule 42: Tubulin alpha-1D chain

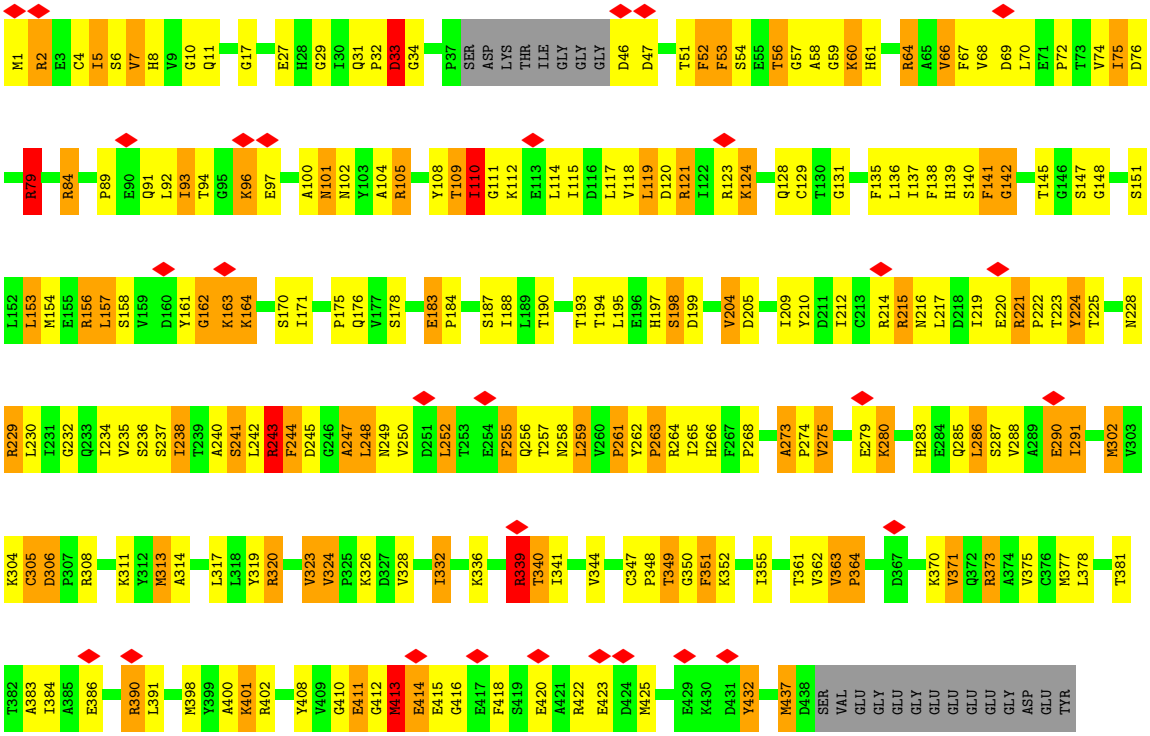
Chain BG:





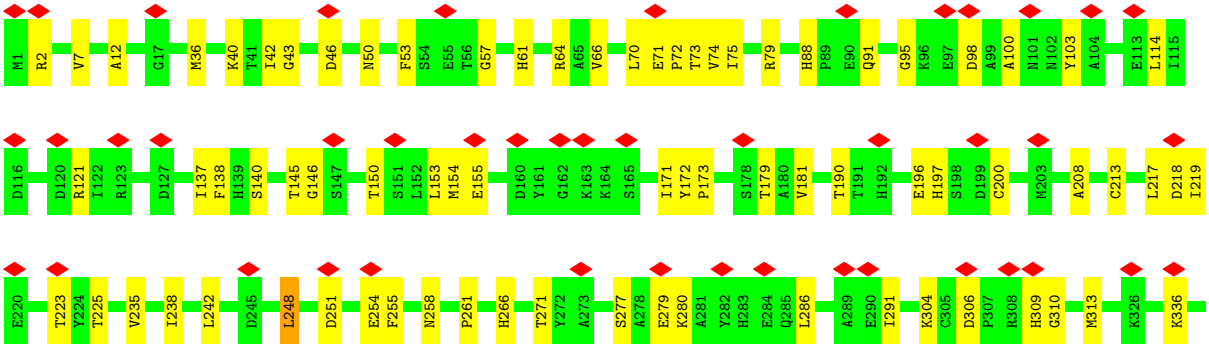
- Molecule 42: Tubulin alpha-1D chain

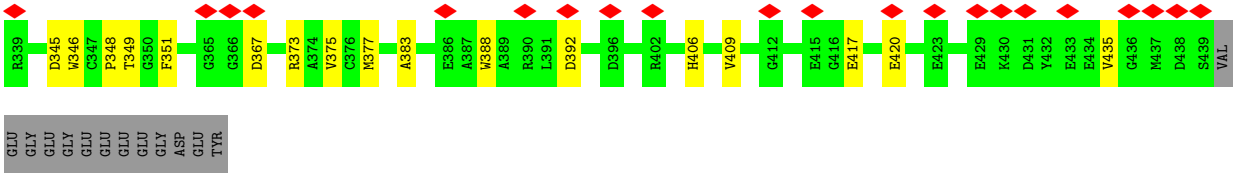
Chain BI:



- Molecule 42: Tubulin alpha-1D chain

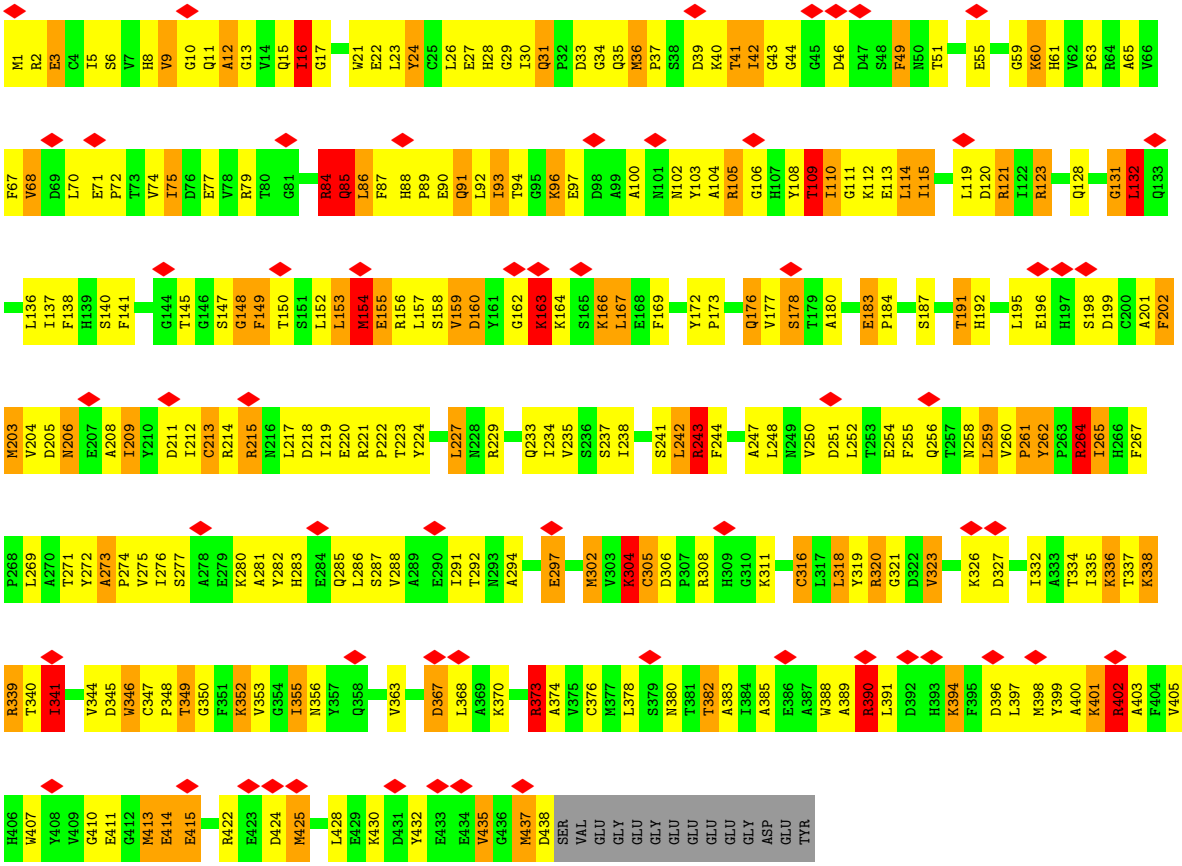
Chain BK:





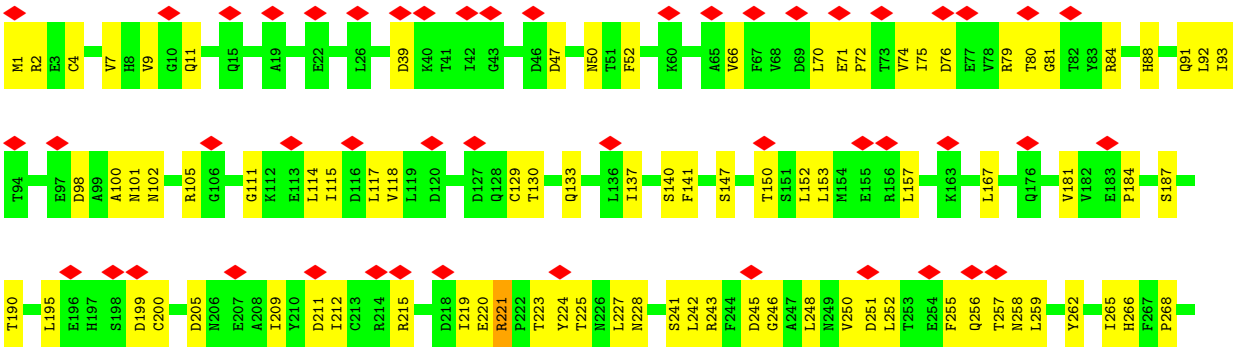
• Molecule 42: Tubulin alpha-1D chain

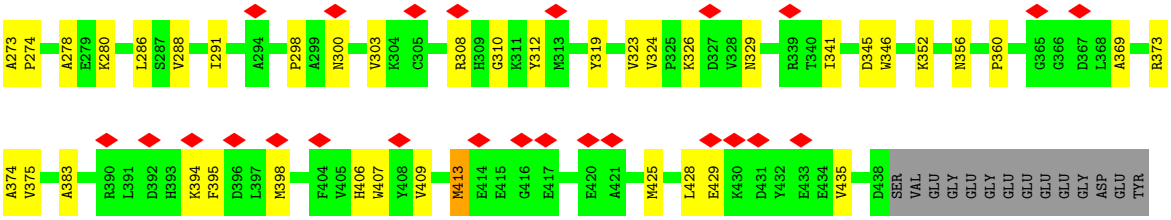
Chain CC:



• Molecule 42: Tubulin alpha-1D chain

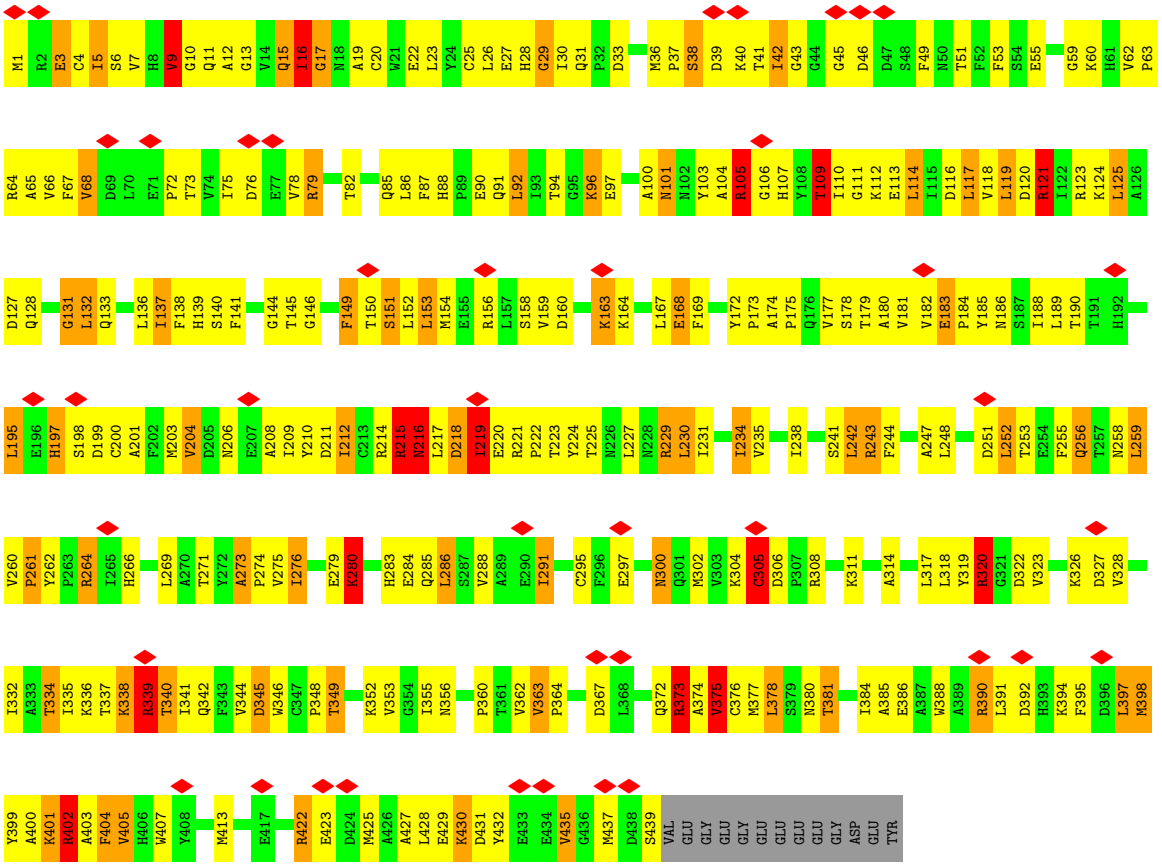
Chain CE:





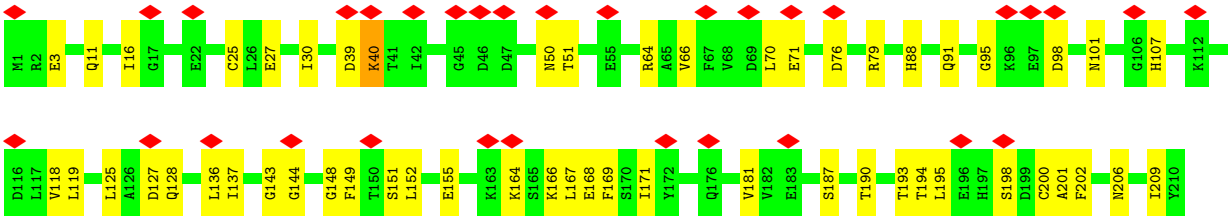
• Molecule 42: Tubulin alpha-1D chain

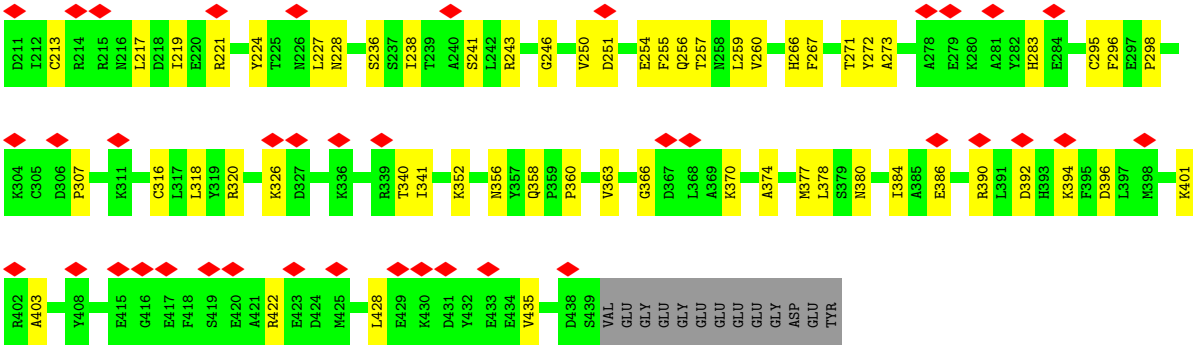
Chain CG:



• Molecule 42: Tubulin alpha-1D chain

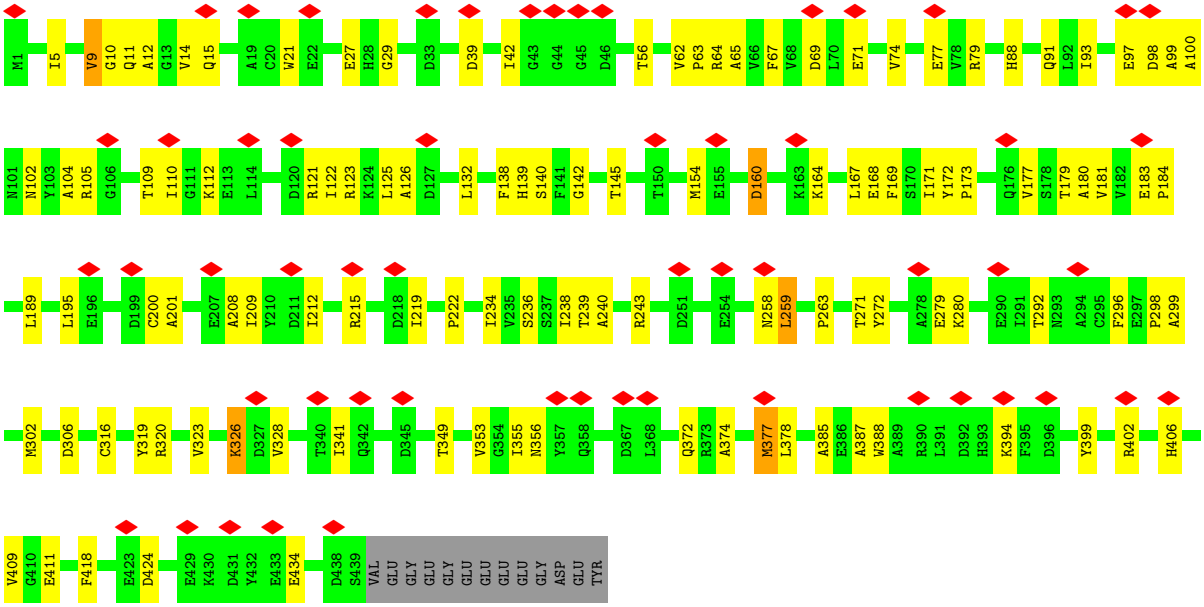
Chain CI:





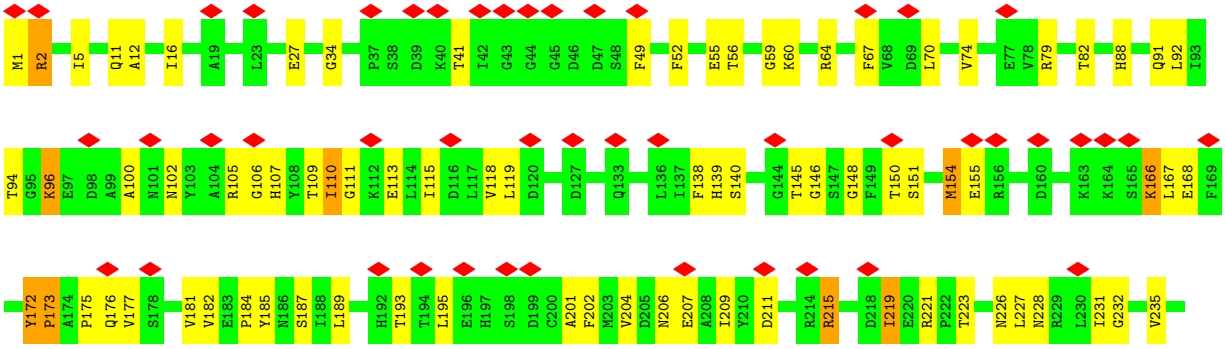
• Molecule 42: Tubulin alpha-1D chain

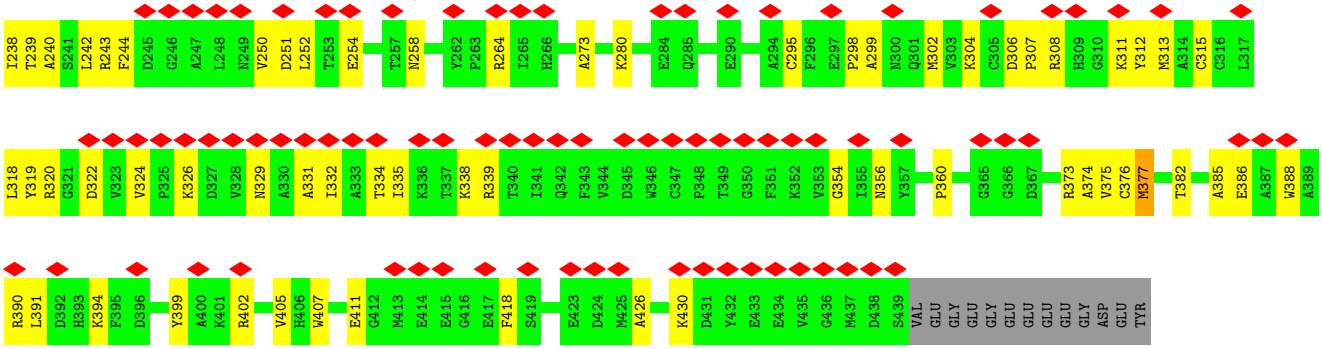
Chain CK:



• Molecule 42: Tubulin alpha-1D chain

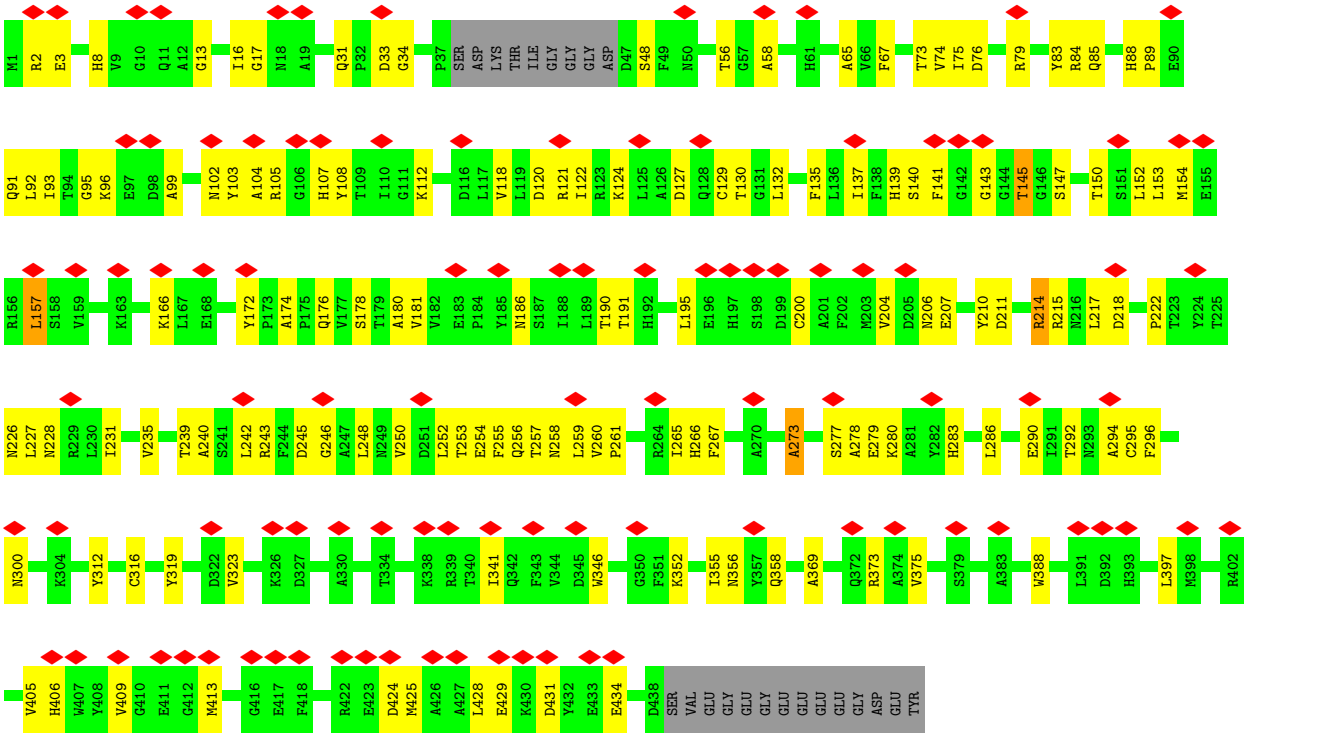
Chain CM:





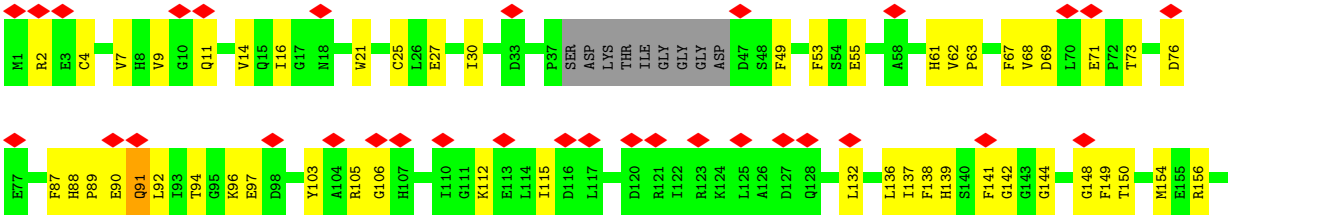
- Molecule 42: Tubulin alpha-1D chain

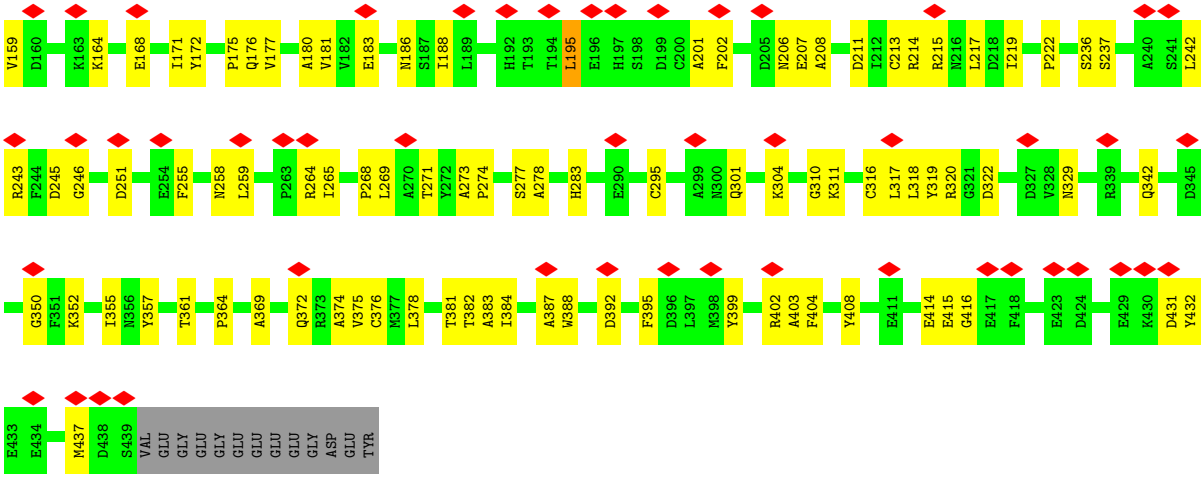
Chain DC:



- Molecule 42: Tubulin alpha-1D chain

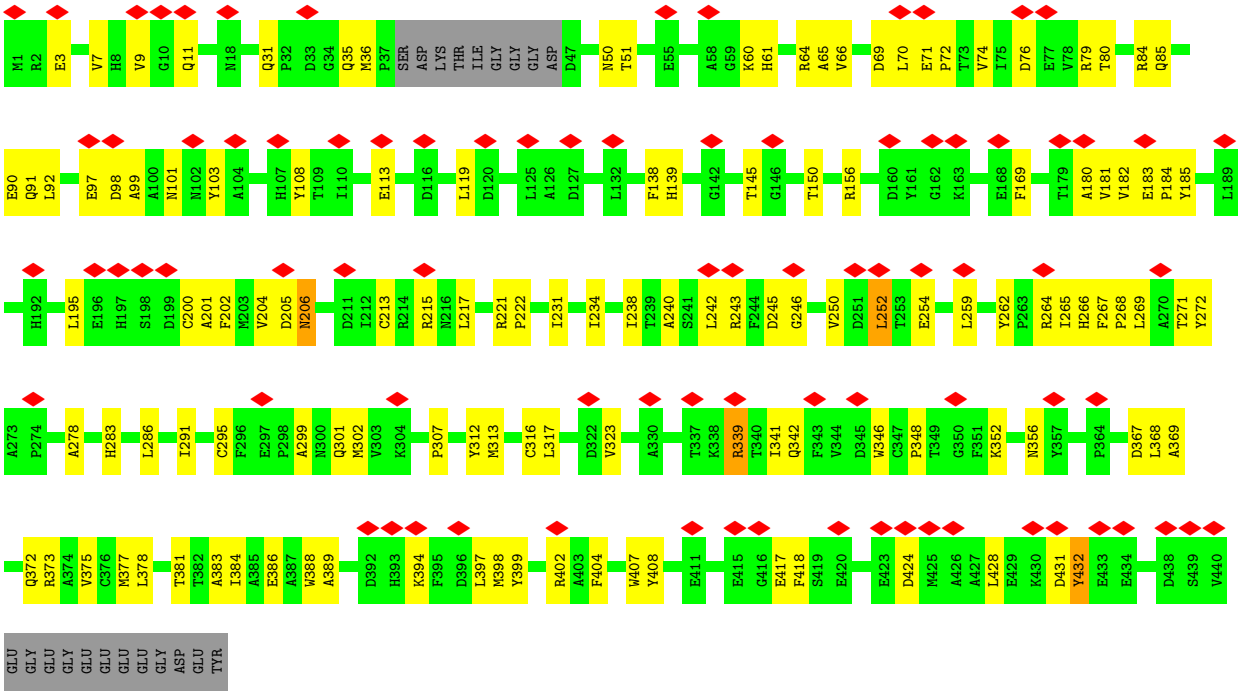
Chain DE:





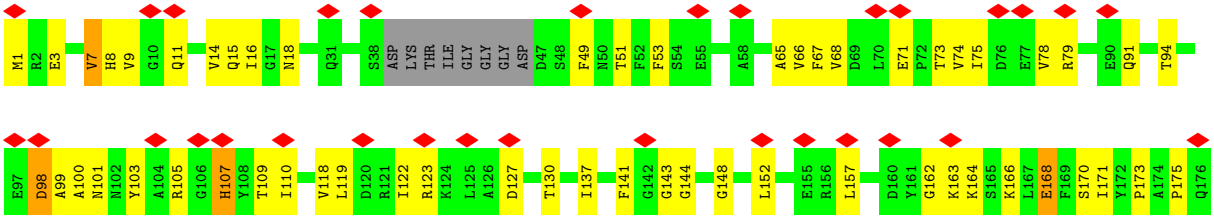
- Molecule 42: Tubulin alpha-1D chain

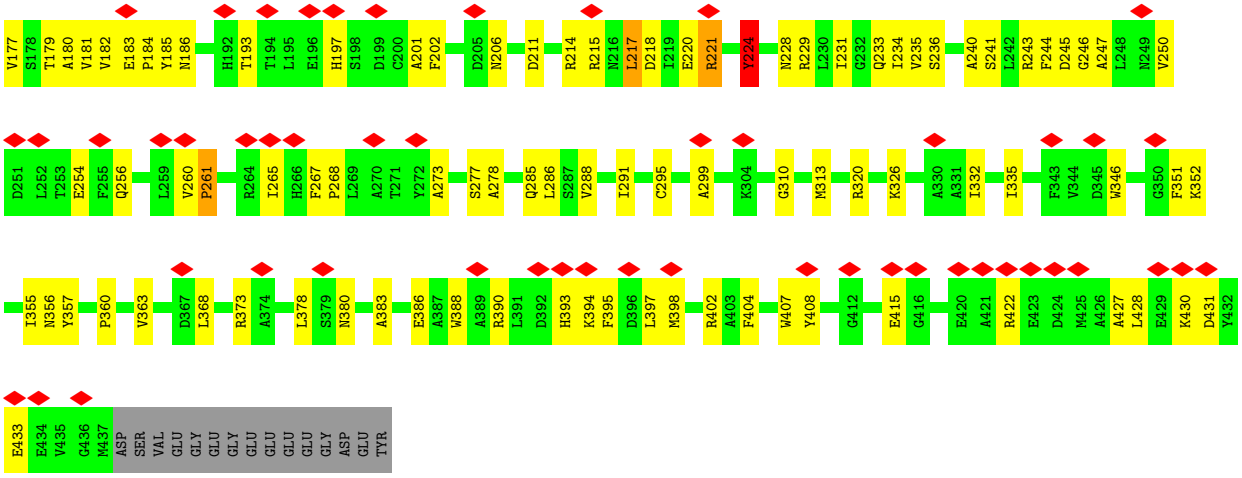
Chain DG:



- Molecule 42: Tubulin alpha-1D chain

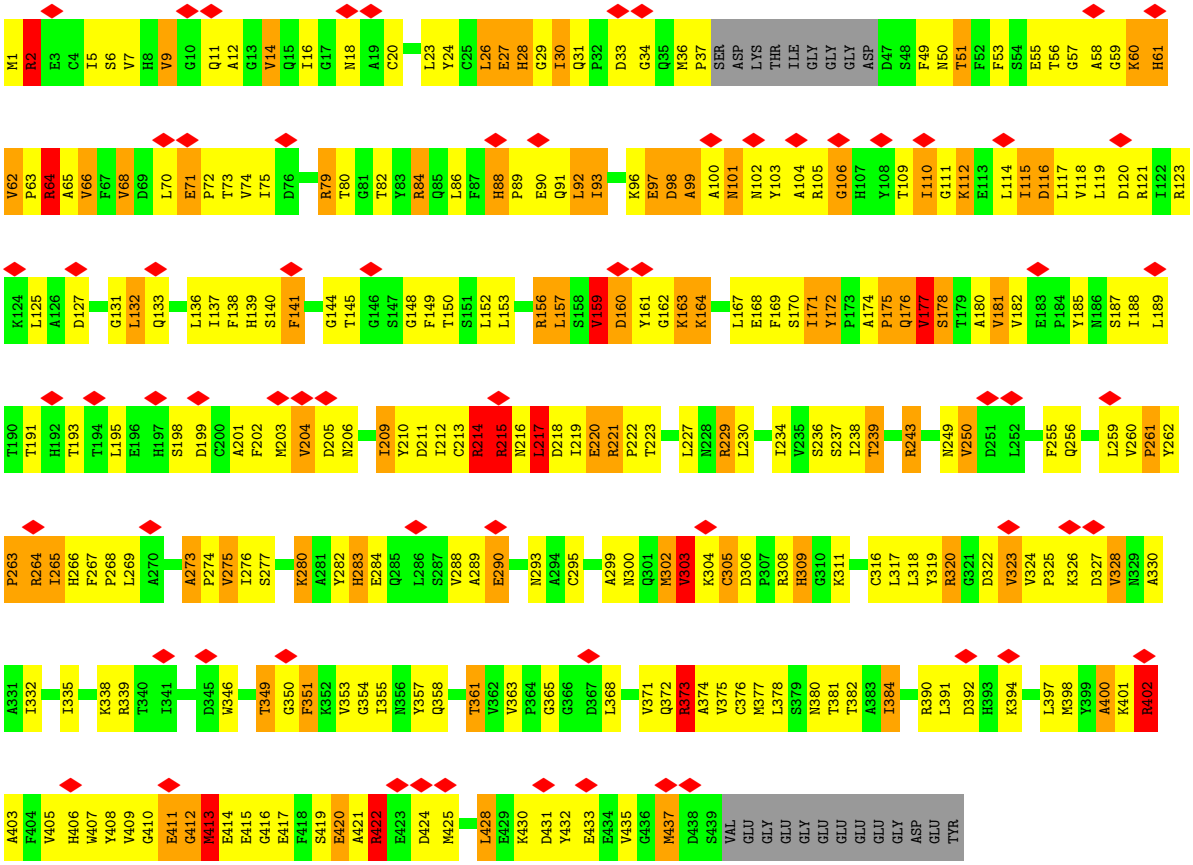
Chain DI:





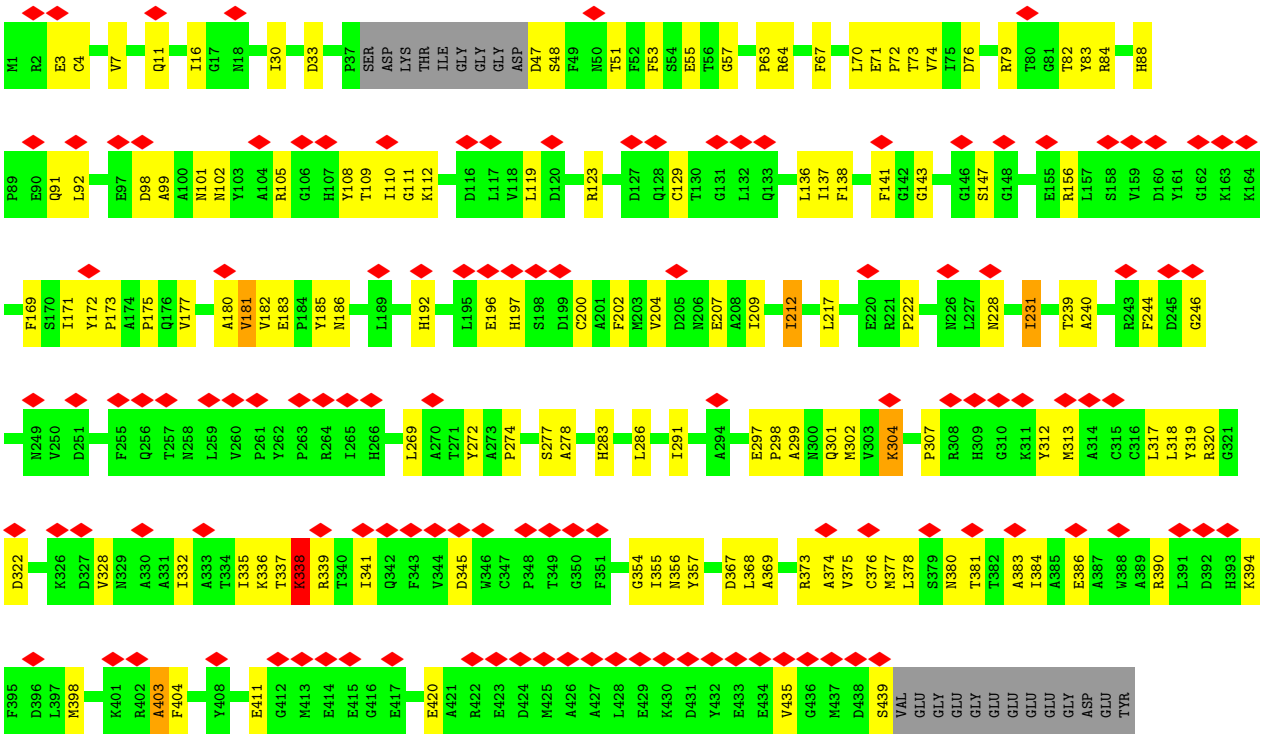
- Molecule 42: Tubulin alpha-1D chain

Chain DK:



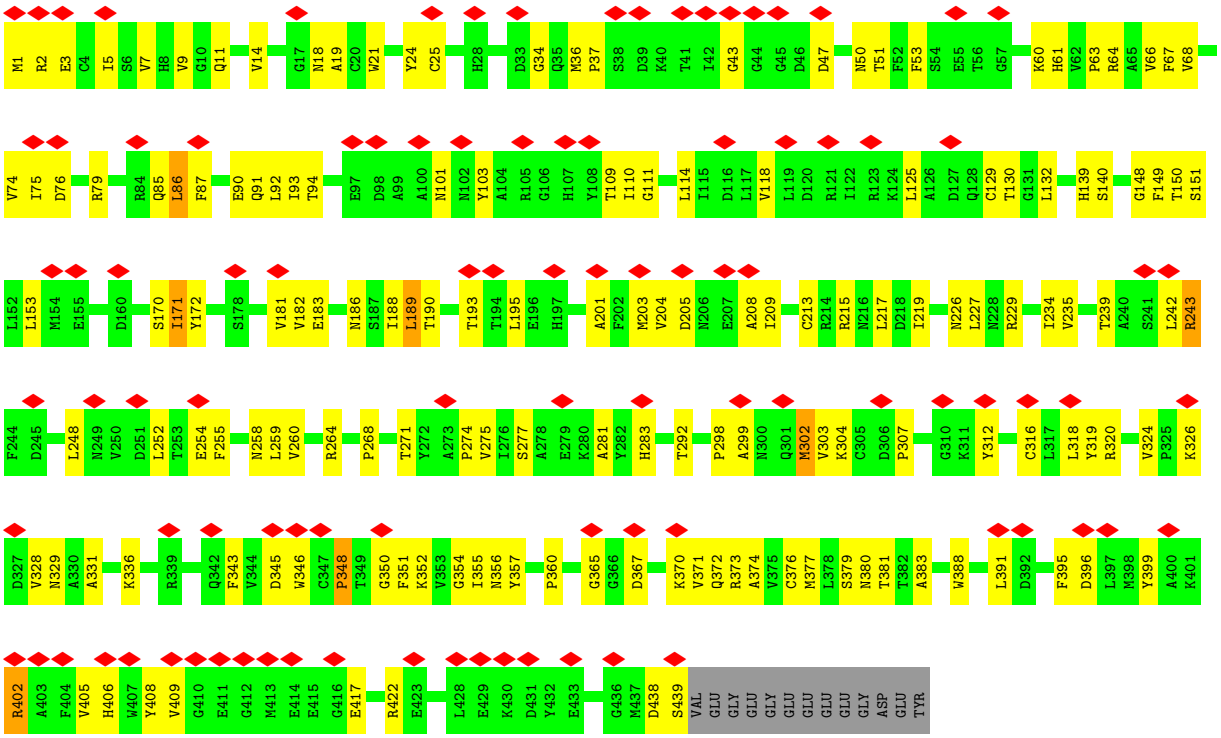
- Molecule 42: Tubulin alpha-1D chain

Chain DM:



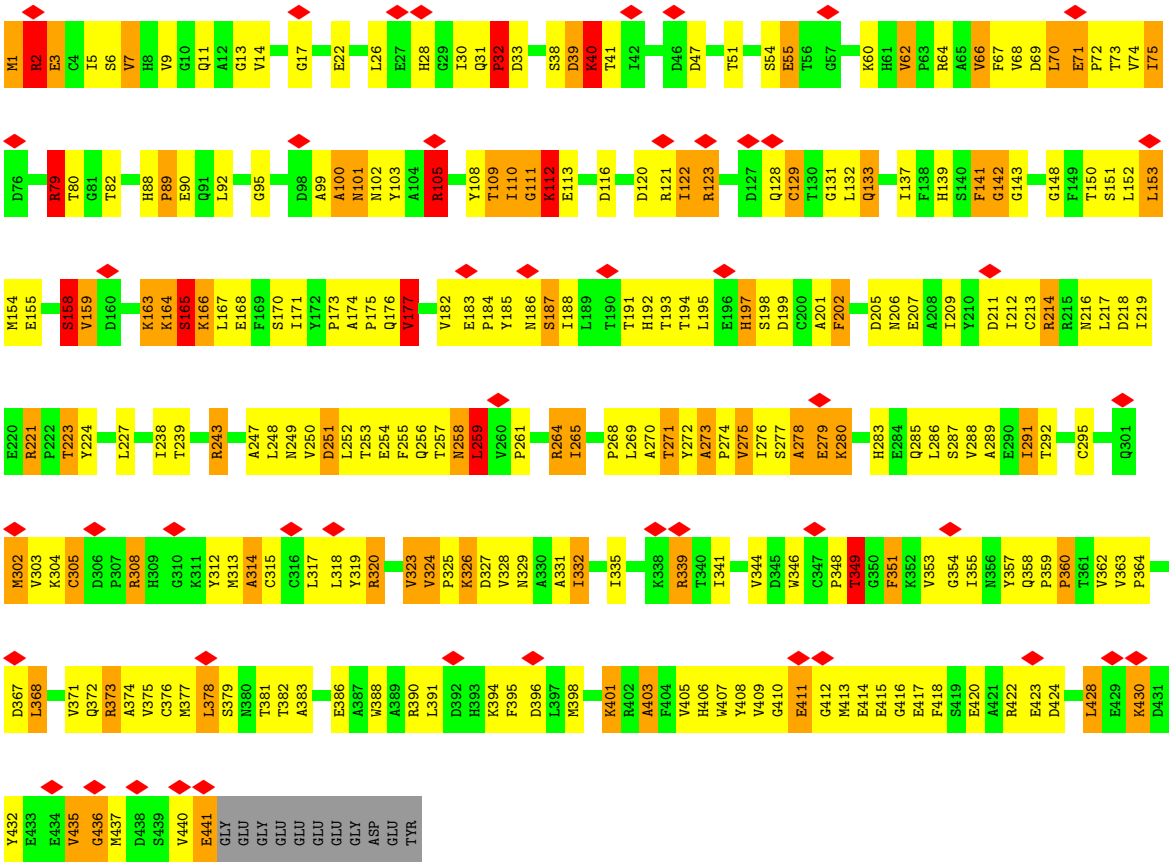
- Molecule 42: Tubulin alpha-1D chain

Chain EC:



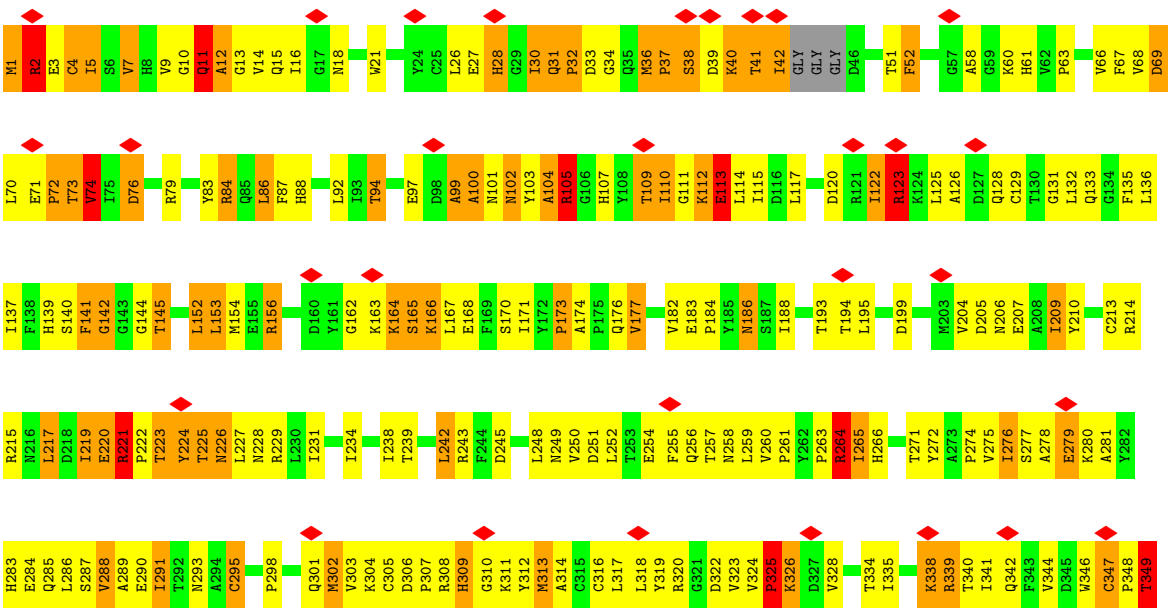
- Molecule 42: Tubulin alpha-1D chain

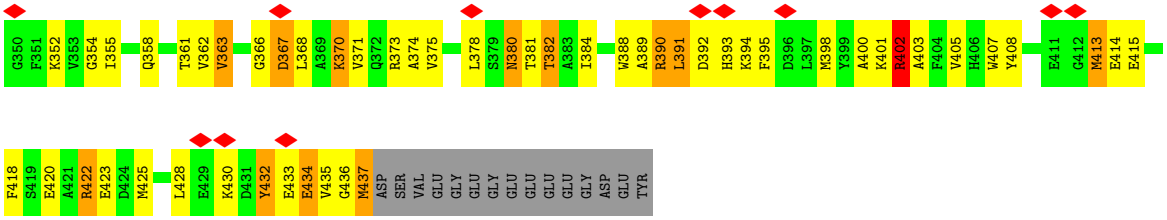
Chain EE:



- Molecule 42: Tubulin alpha-1D chain

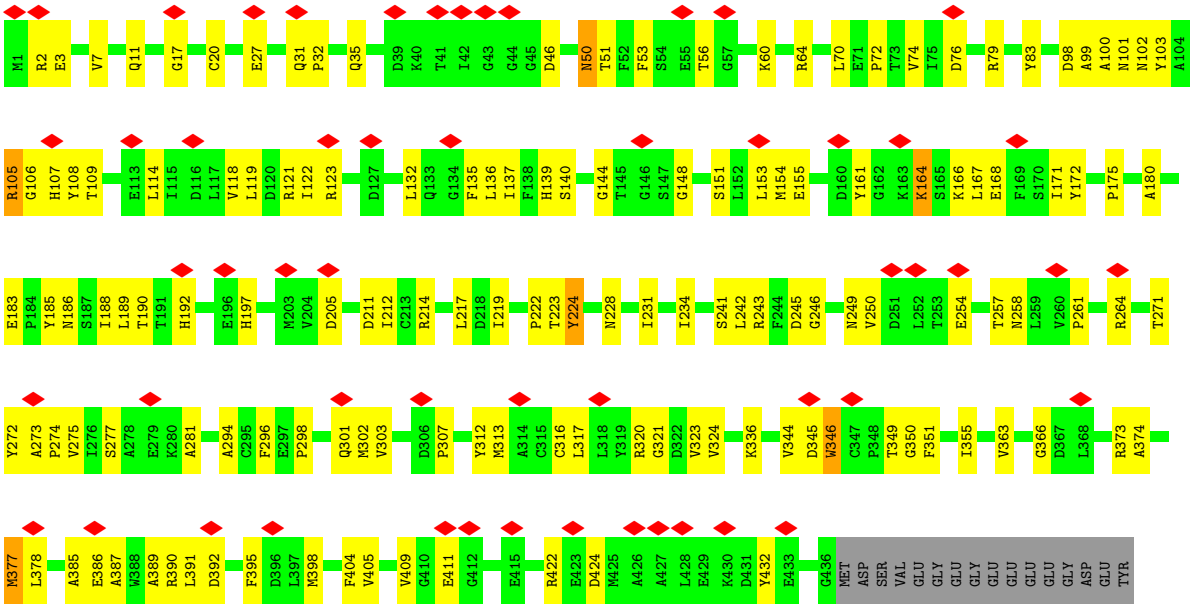
Chain EG:





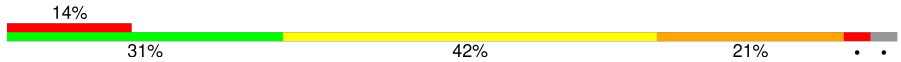
• Molecule 42: Tubulin alpha-1D chain

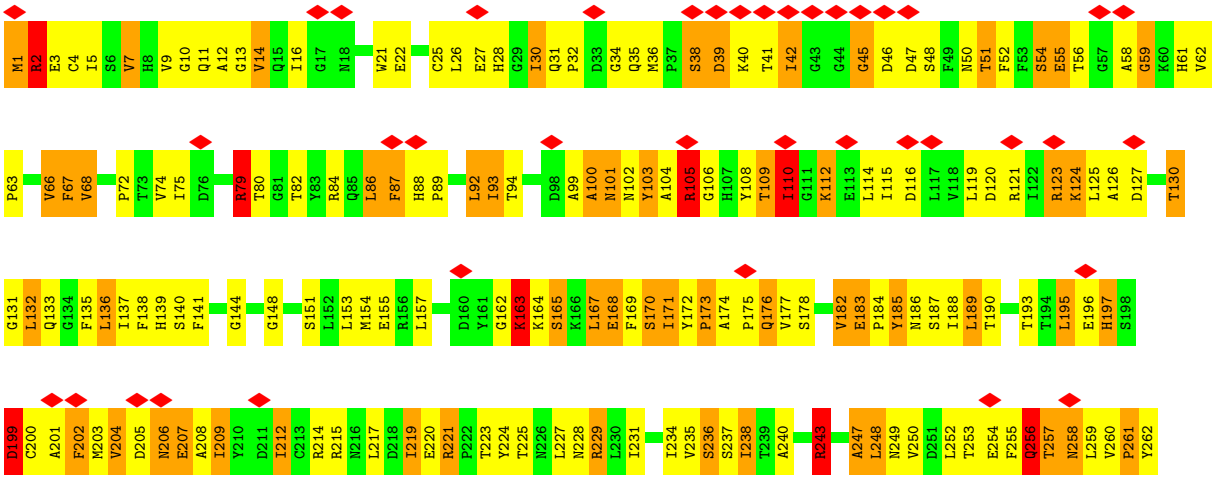
Chain EI:

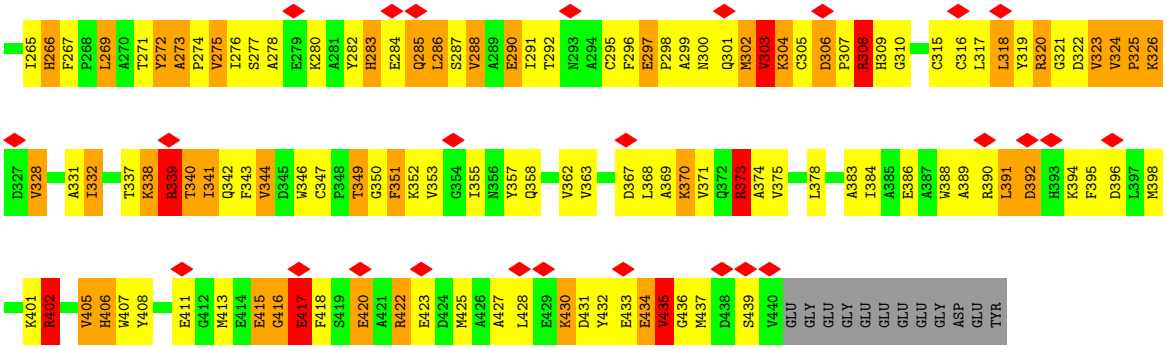


• Molecule 42: Tubulin alpha-1D chain

Chain EK:

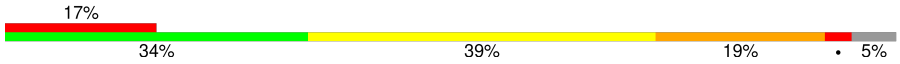


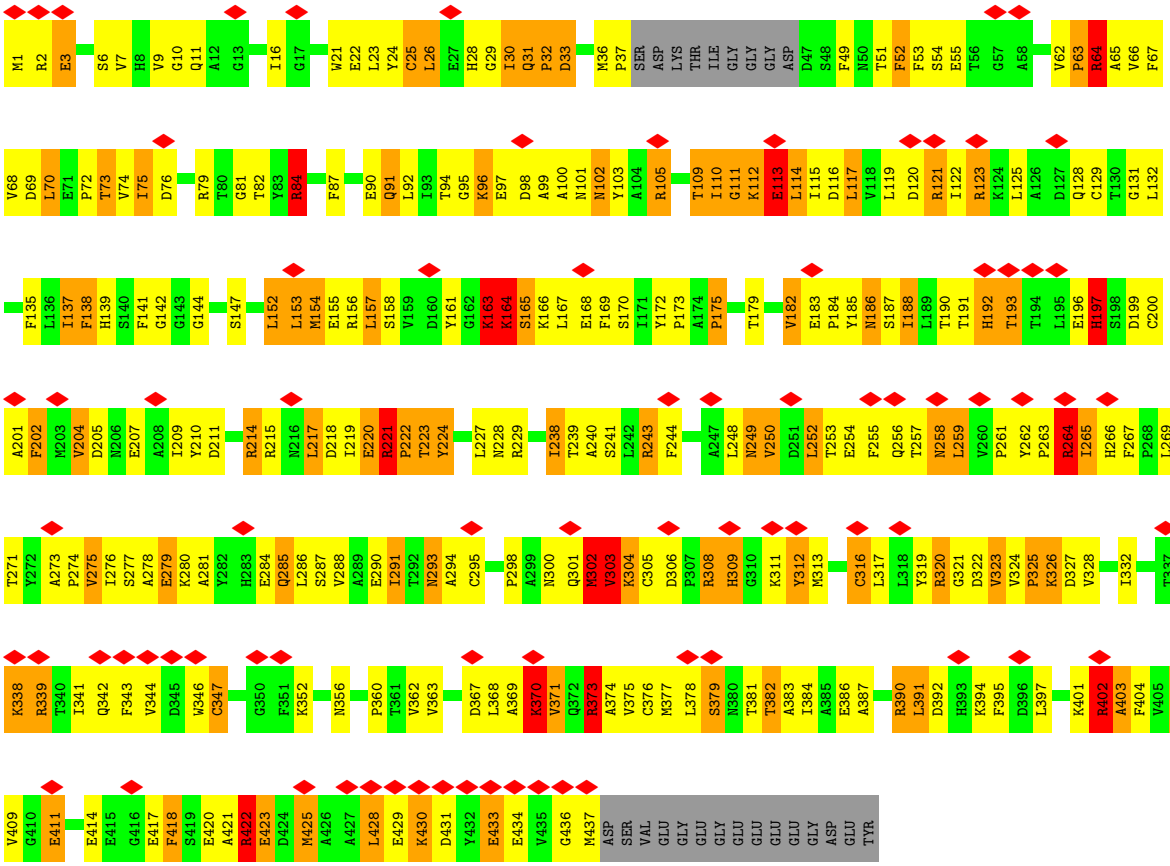




- Molecule 42: Tubulin alpha-1D chain

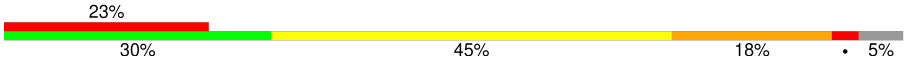
Chain EM:

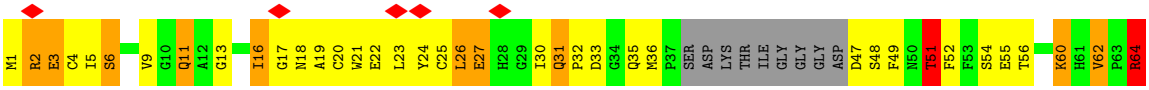


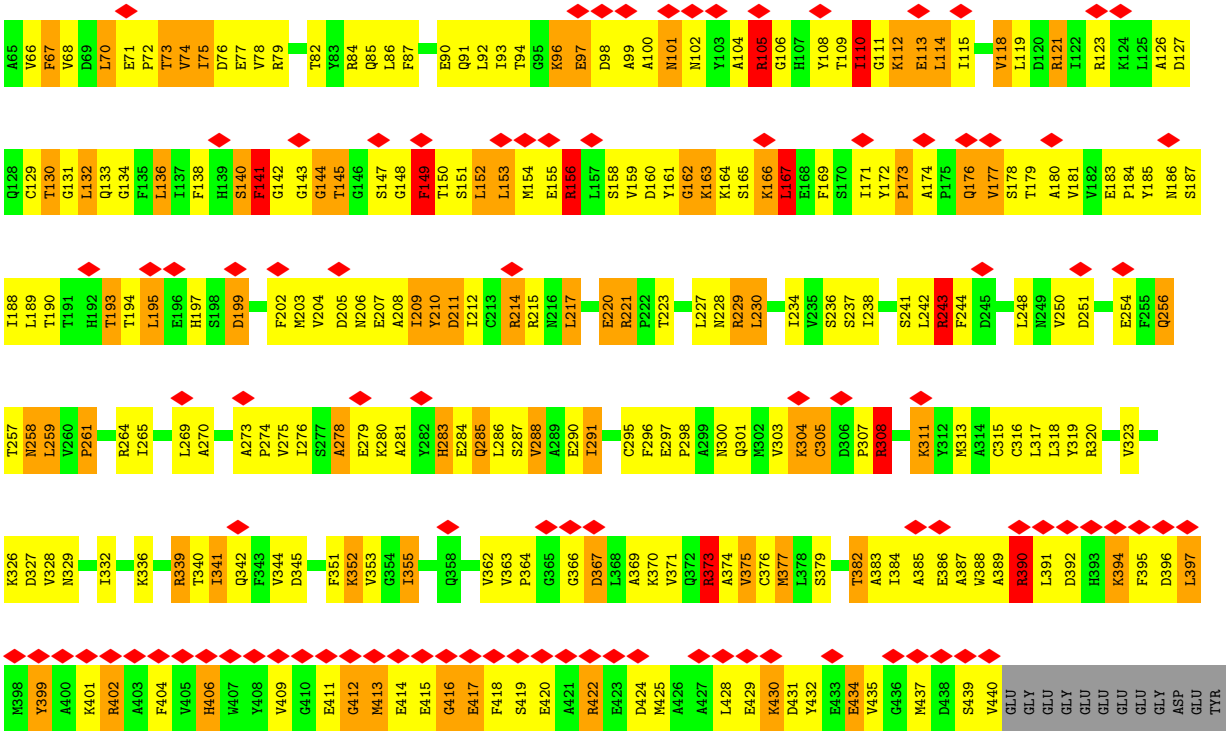


- Molecule 42: Tubulin alpha-1D chain

Chain FC:

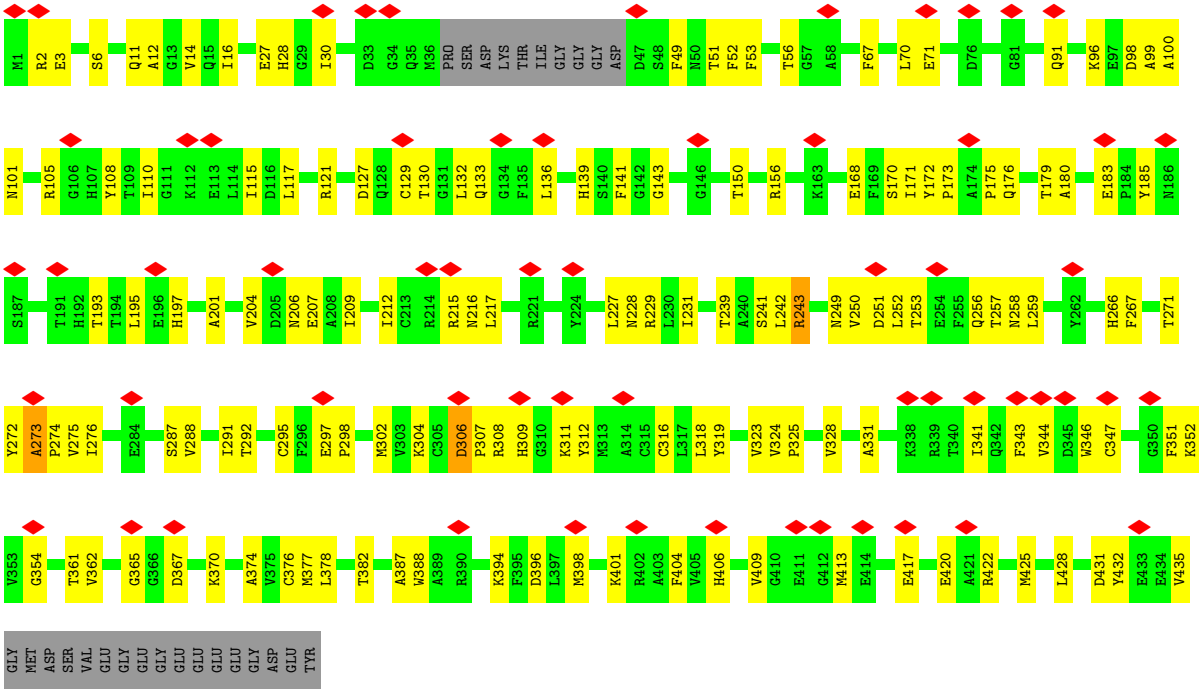






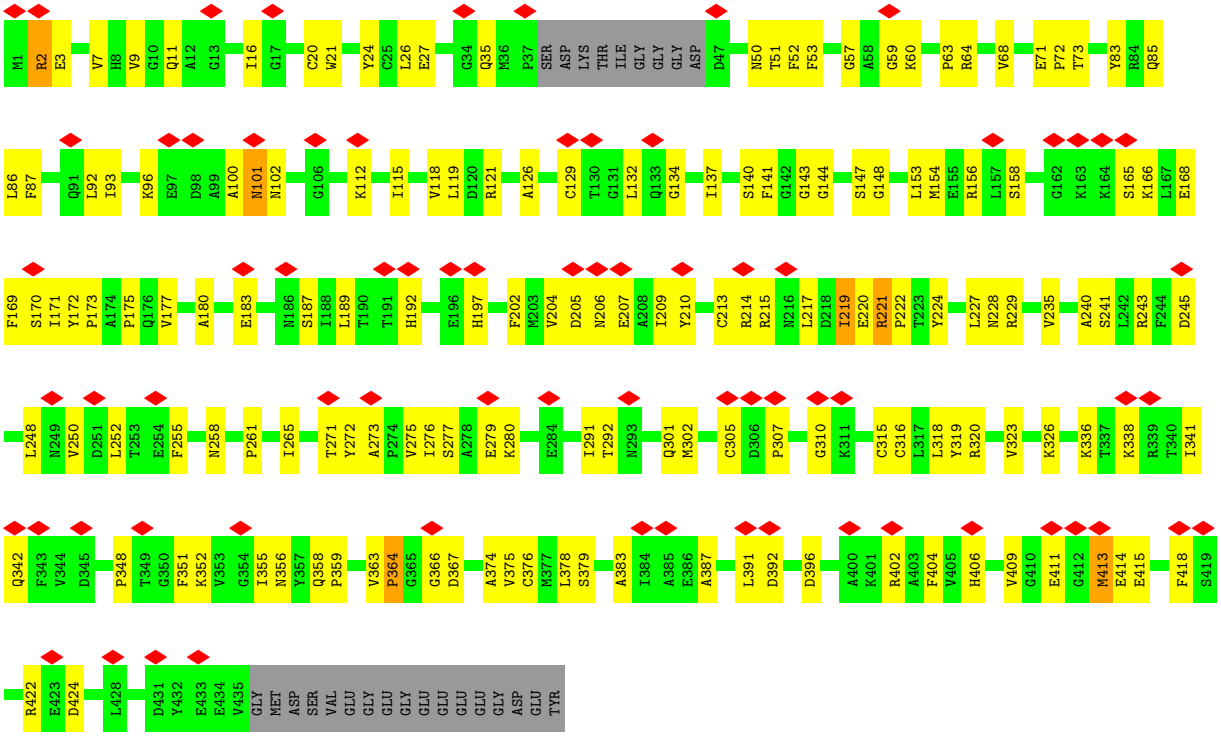
- Molecule 42: Tubulin alpha-1D chain

Chain FE:



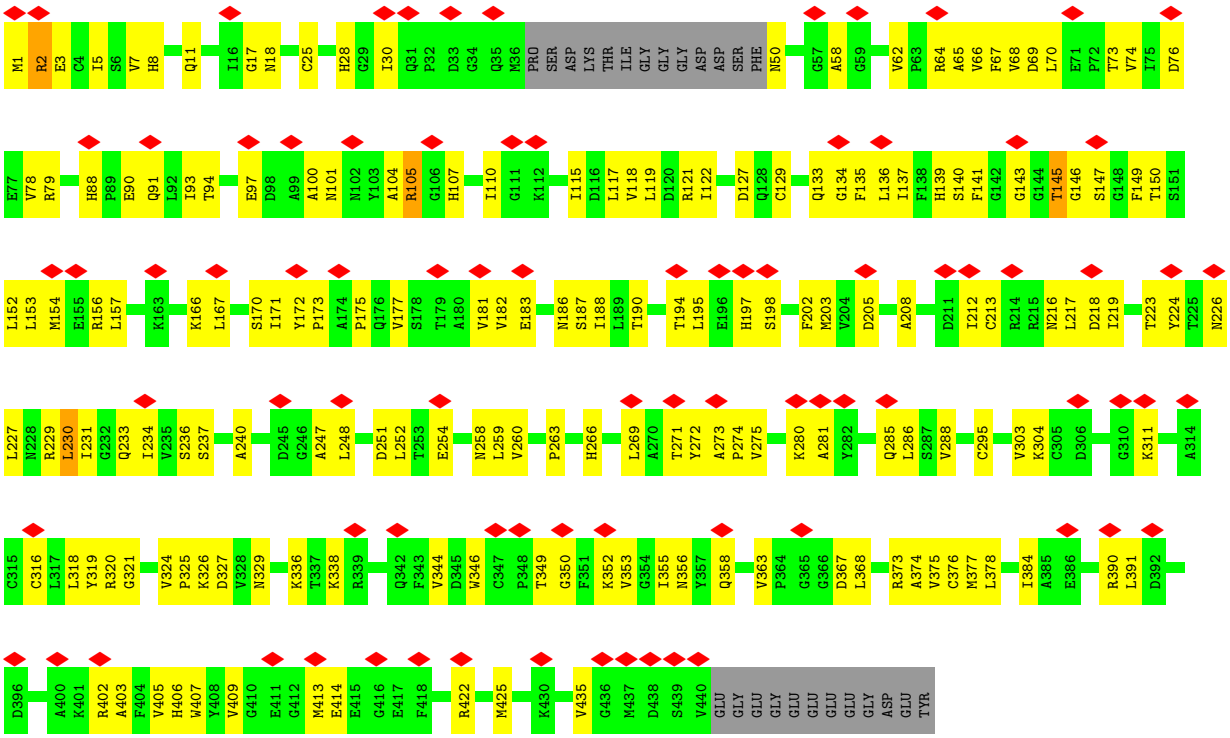
- Molecule 42: Tubulin alpha-1D chain

Chain FG:



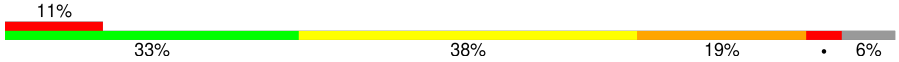
- Molecule 42: Tubulin alpha-1D chain

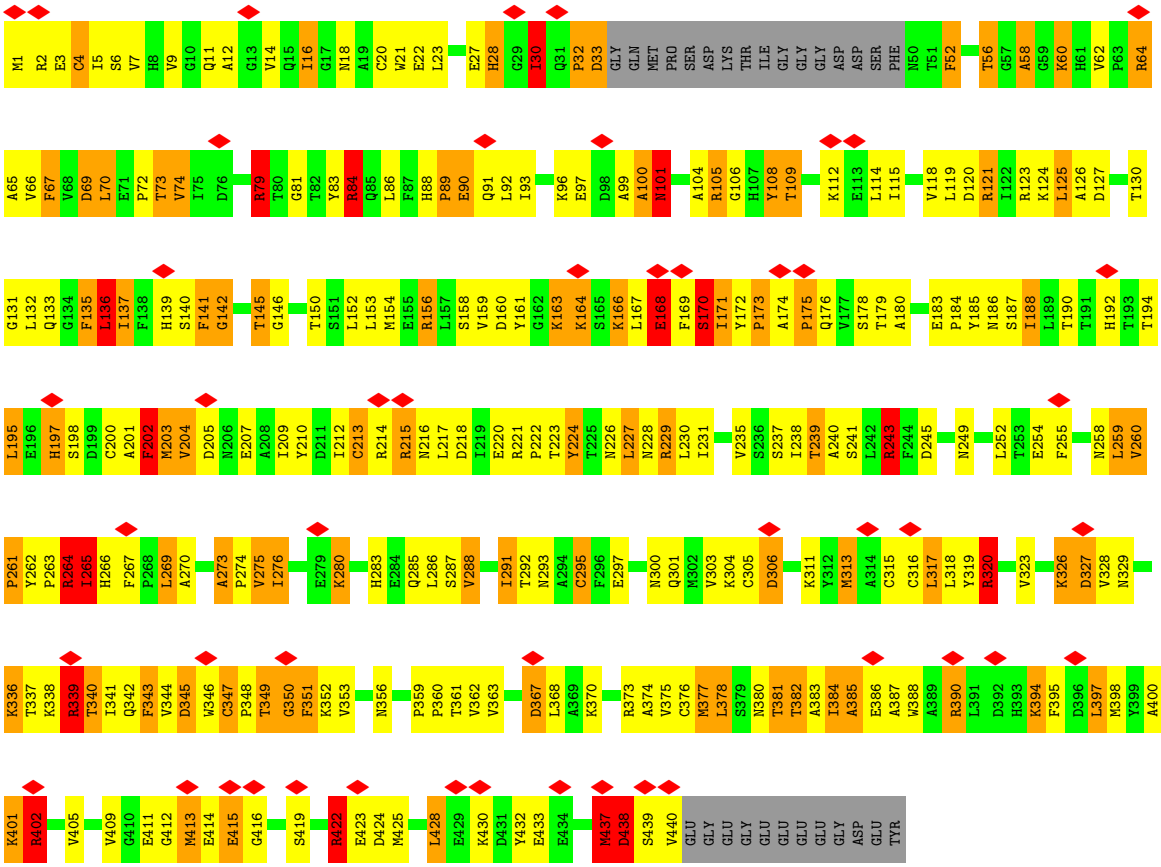
Chain FI:



- Molecule 42: Tubulin alpha-1D chain

Chain FK:





- Molecule 42: Tubulin alpha-1D chain

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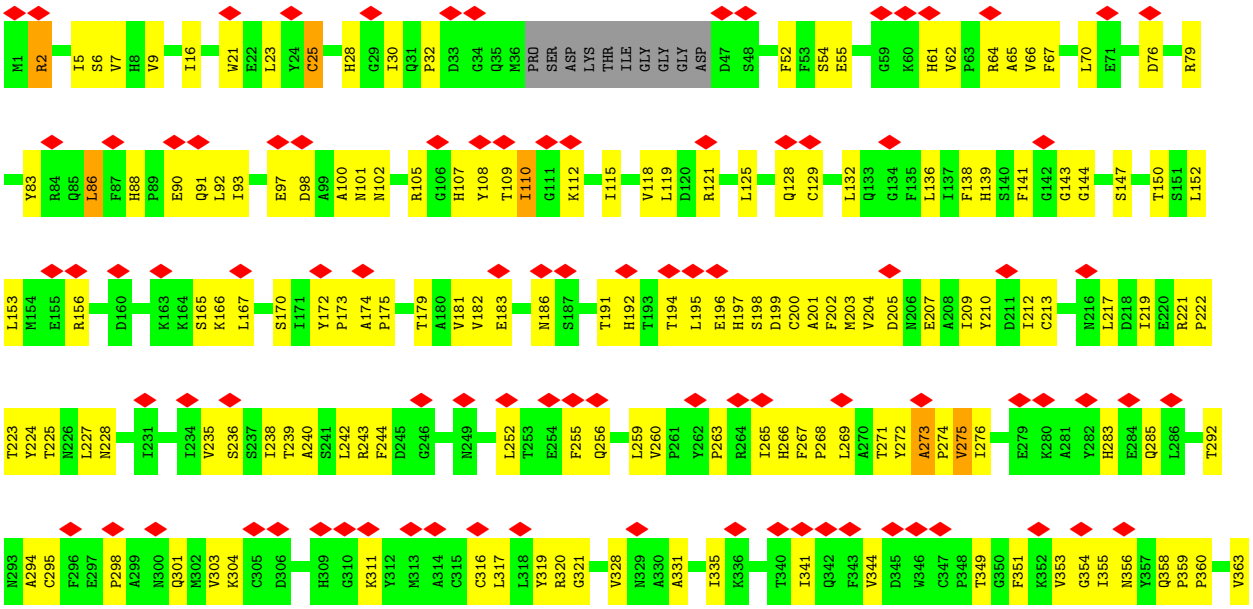

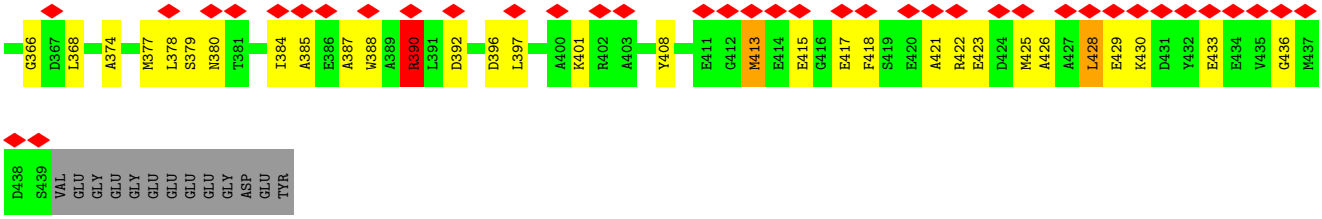

- Molecule 42: Tubulin alpha-1D chain

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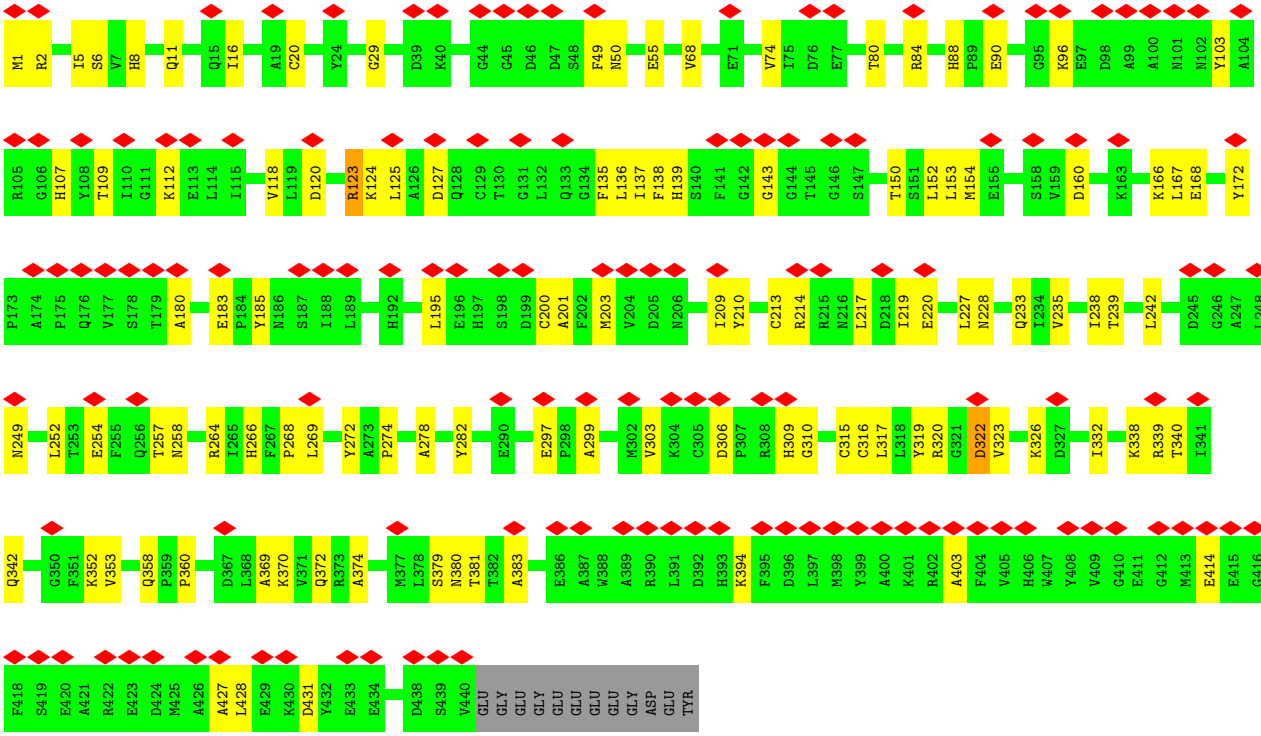
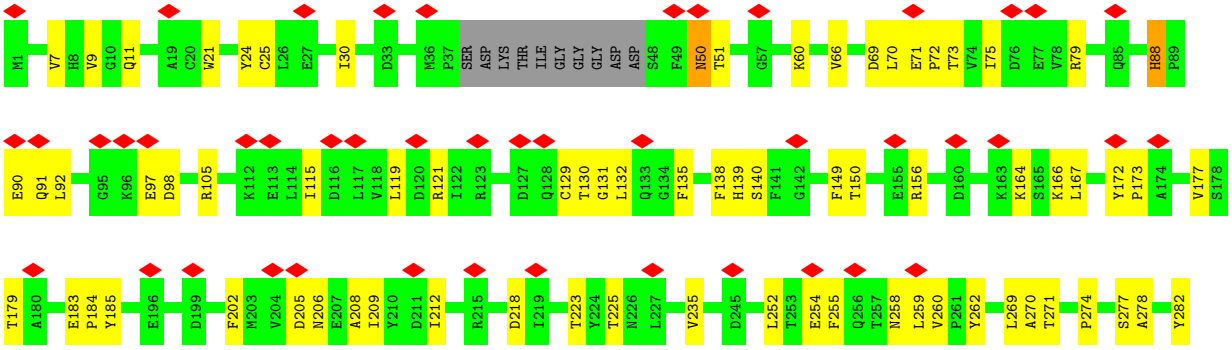
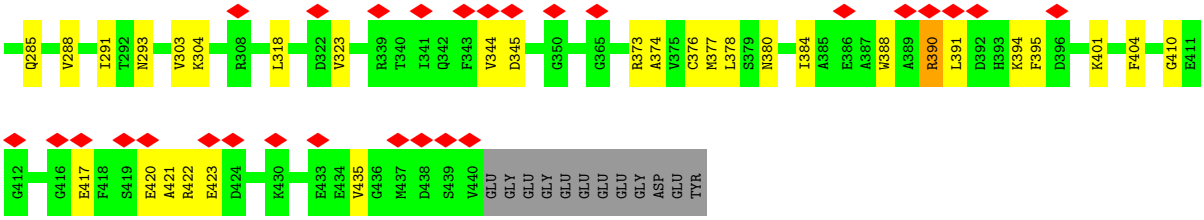


- Molecule 42: Tubulin alpha-1D chain

Chain GE:





• Molecule 42: Tubulin alpha-1D chain

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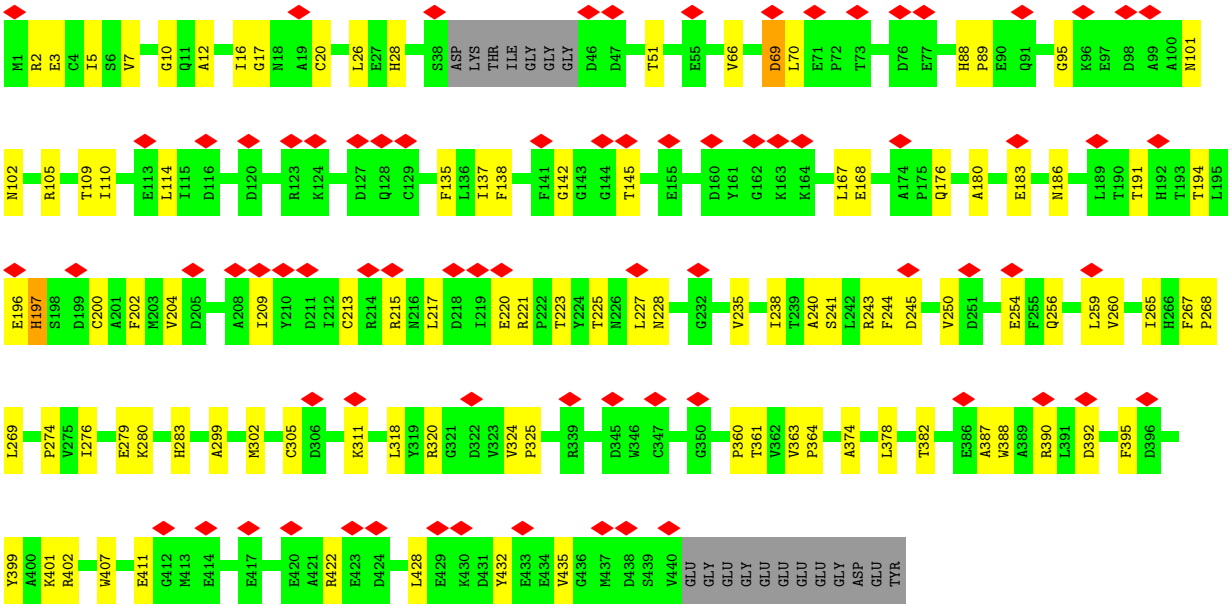

• Molecule 42: Tubulin alpha-1D chain

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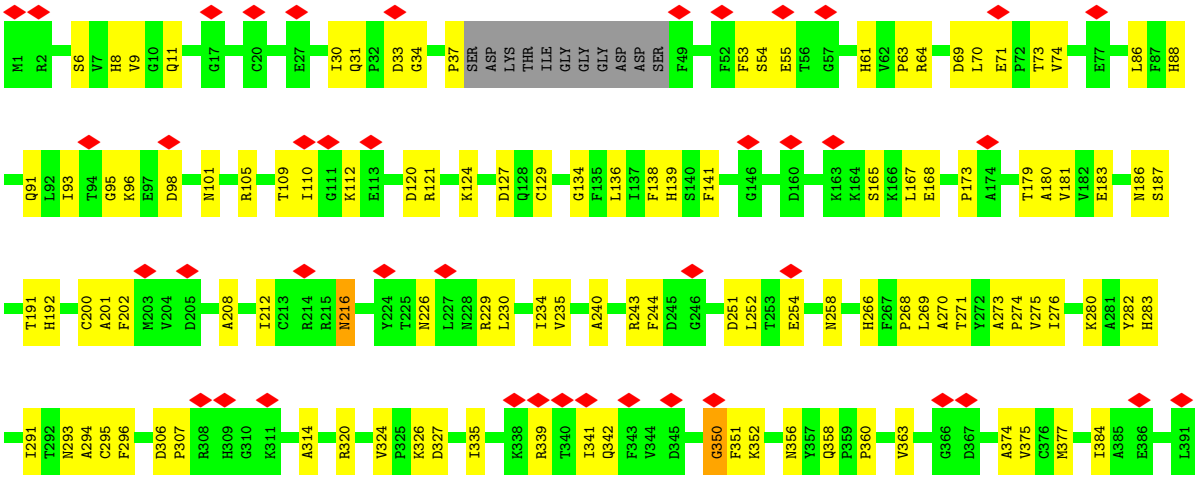

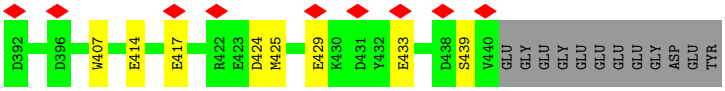

• Molecule 42: Tubulin alpha-1D chain

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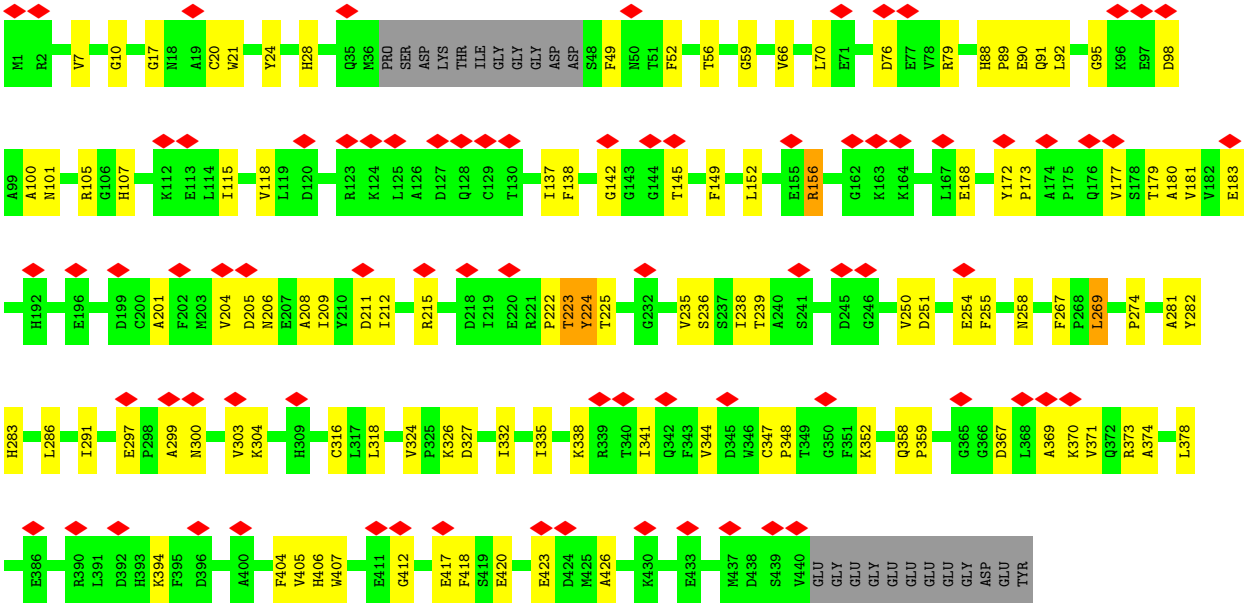
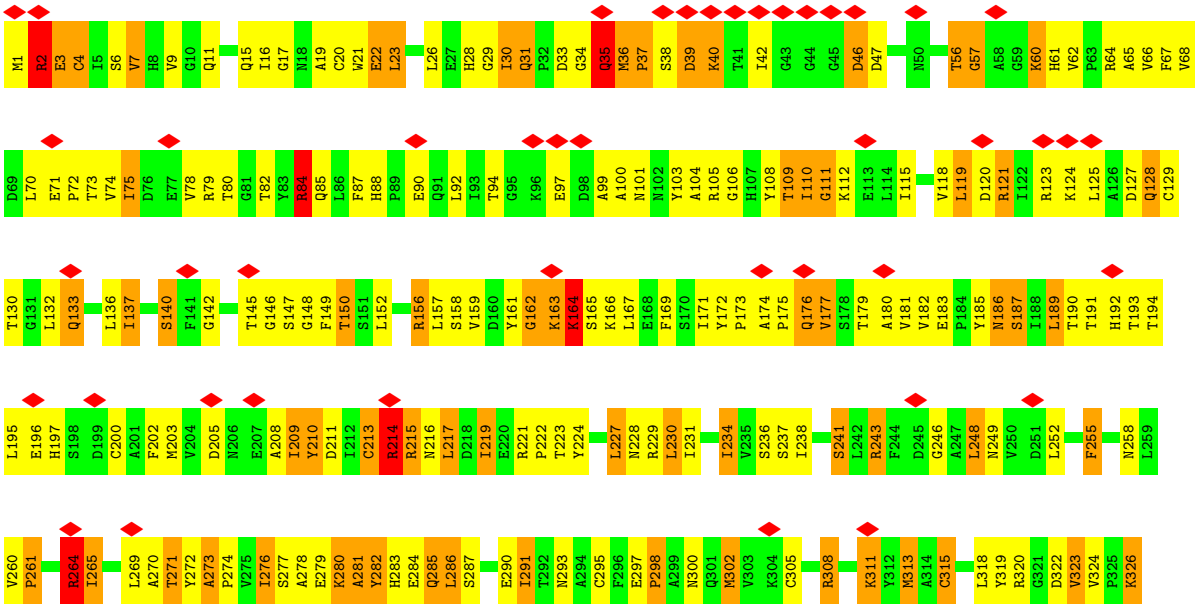
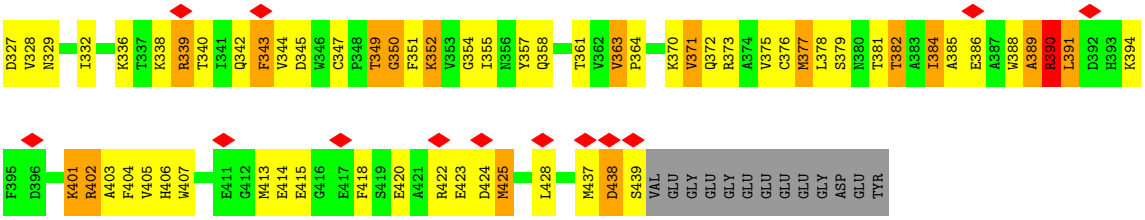


• Molecule 42: Tubulin alpha-1D chain

Chain GM:





• Molecule 42: Tubulin alpha-1D chain

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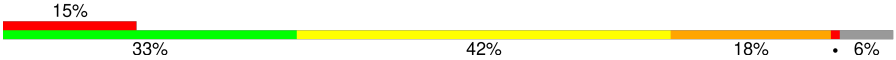

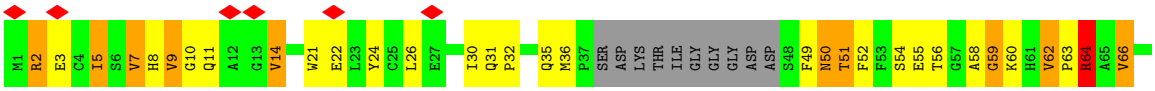

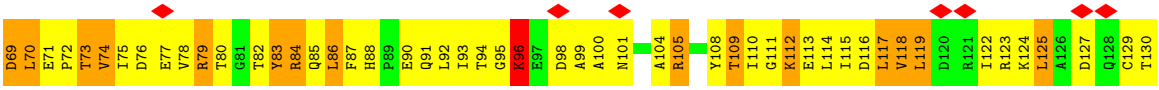

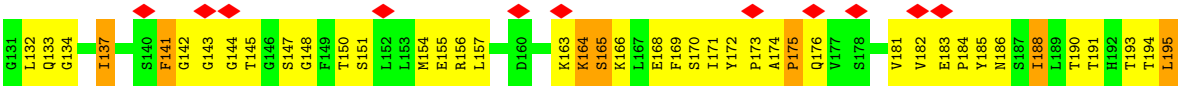

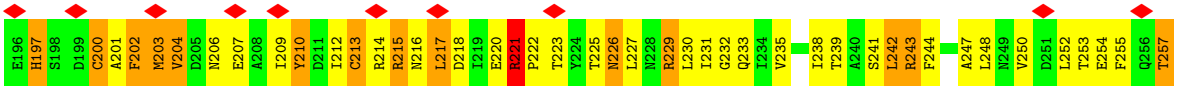

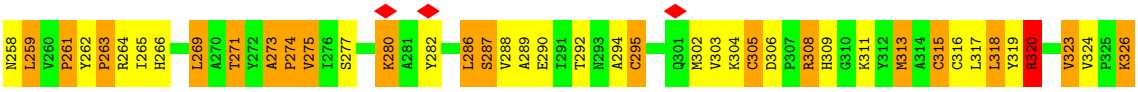

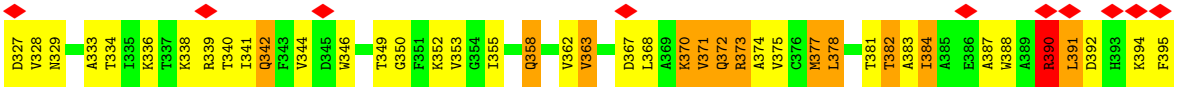

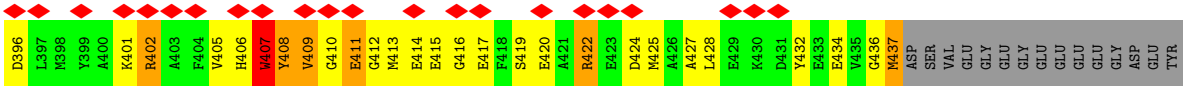

• Molecule 42: Tubulin alpha-1D chain

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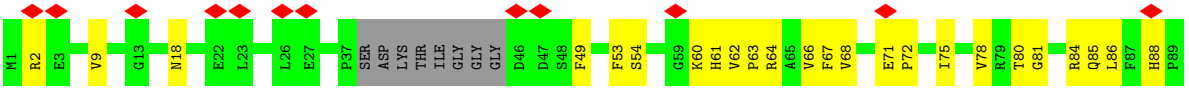
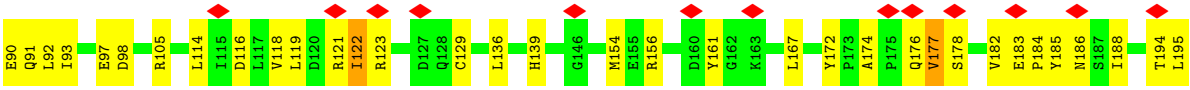
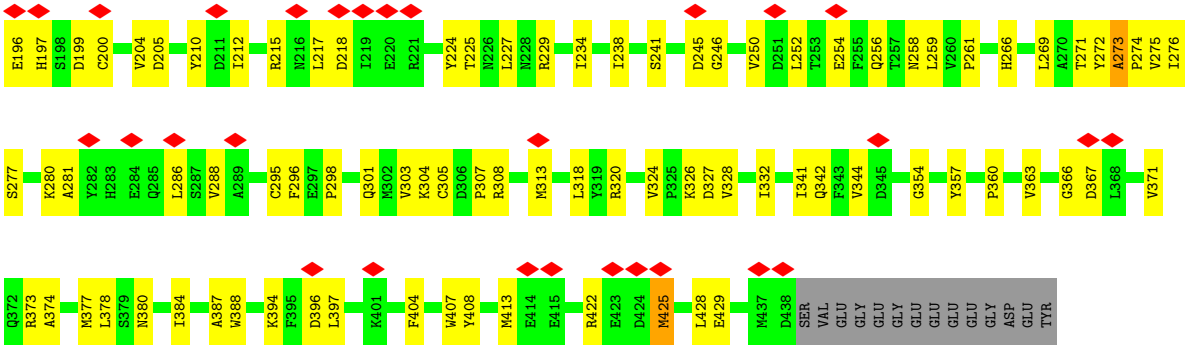
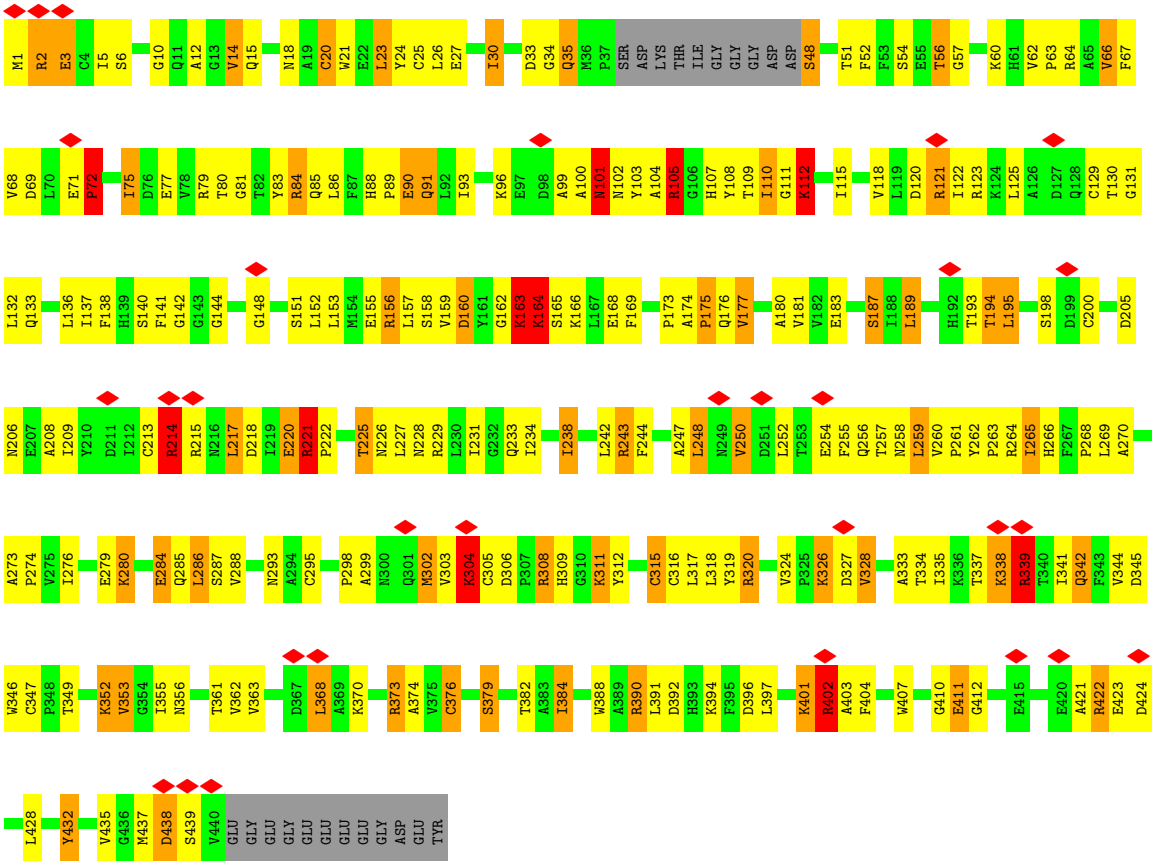






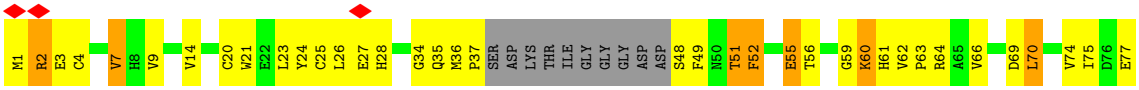
• Molecule 42: Tubulin alpha-1D chain

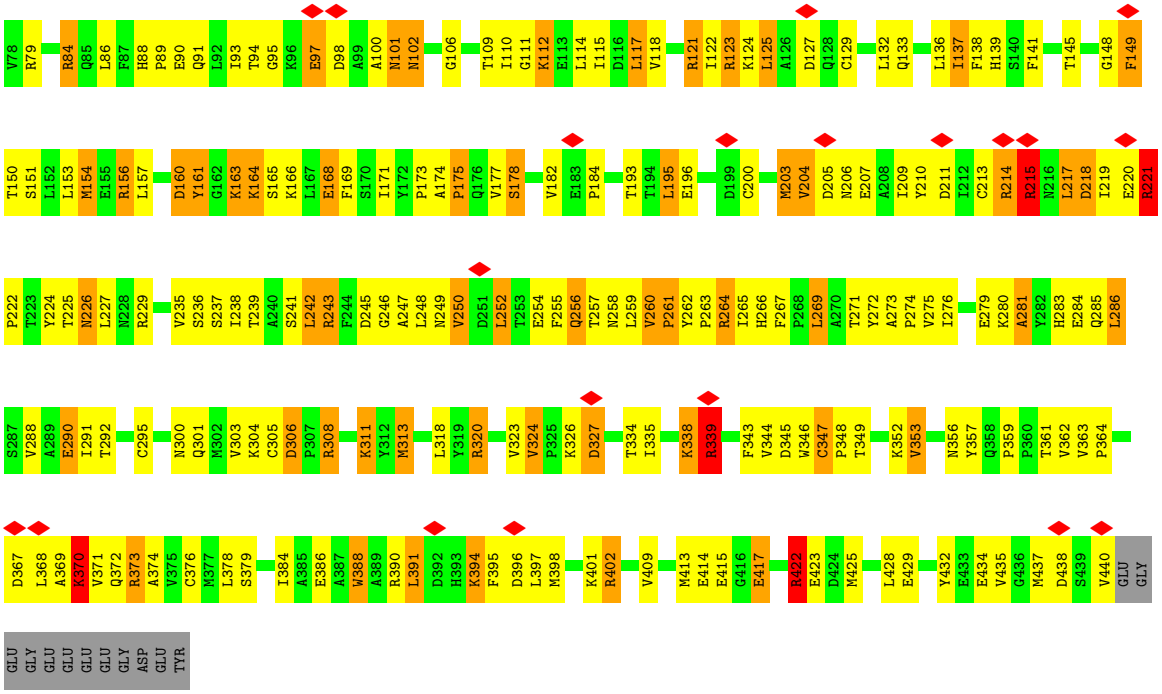
Chain HG:



• Molecule 42: Tubulin alpha-1D chain

Chain HI:





- Molecule 42: Tubulin alpha-1D chain

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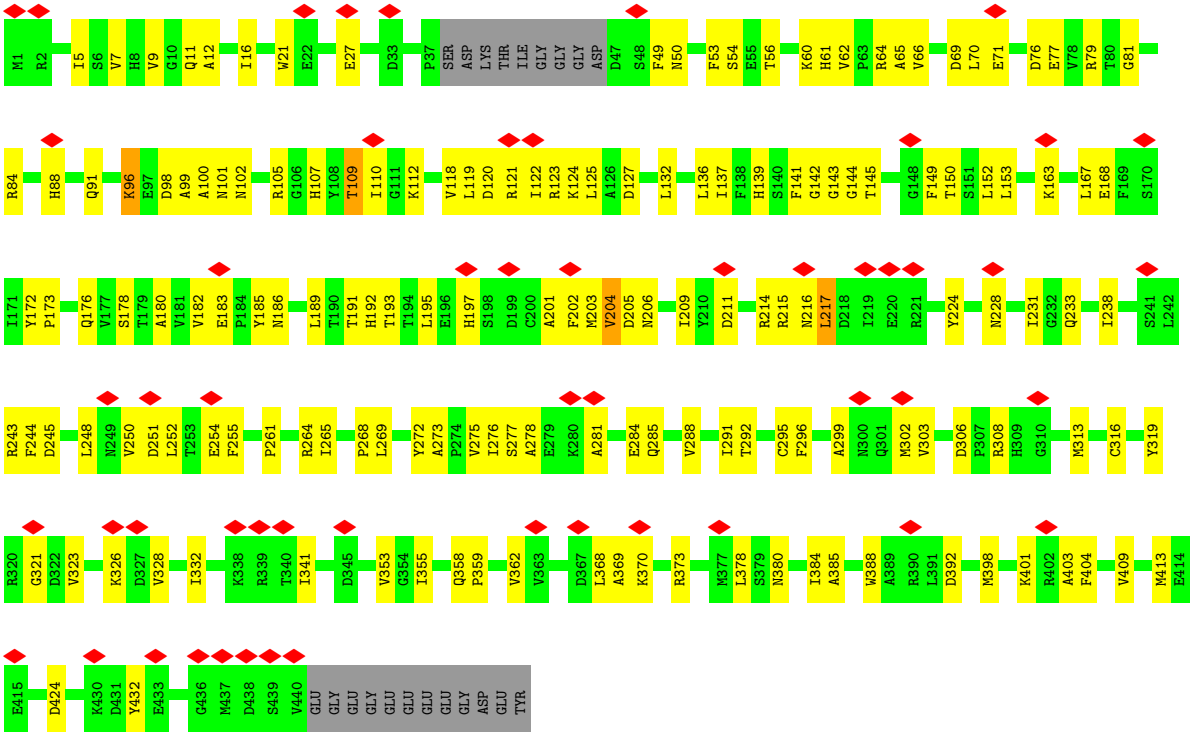
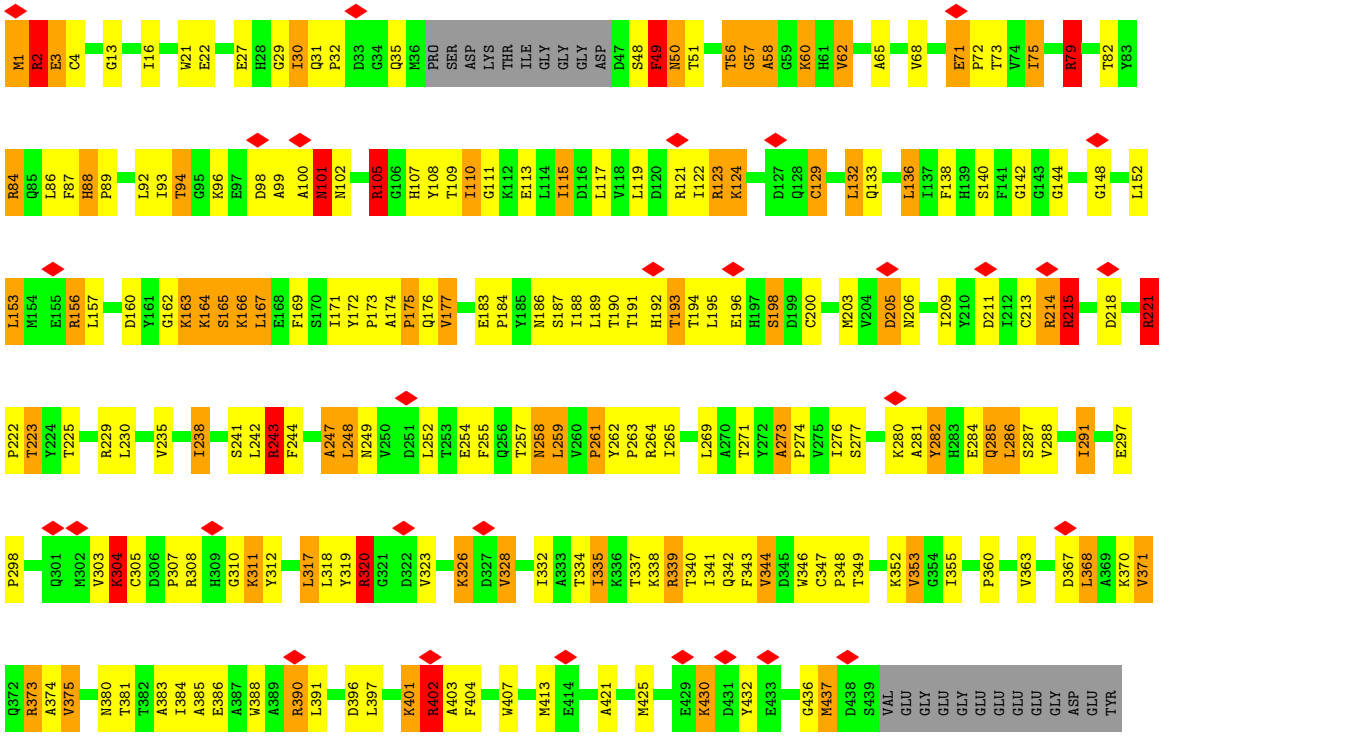


- Molecule 42: Tubulin alpha-1D chain

Chain HM:



- Molecule 42: Tubulin alpha-1D chain

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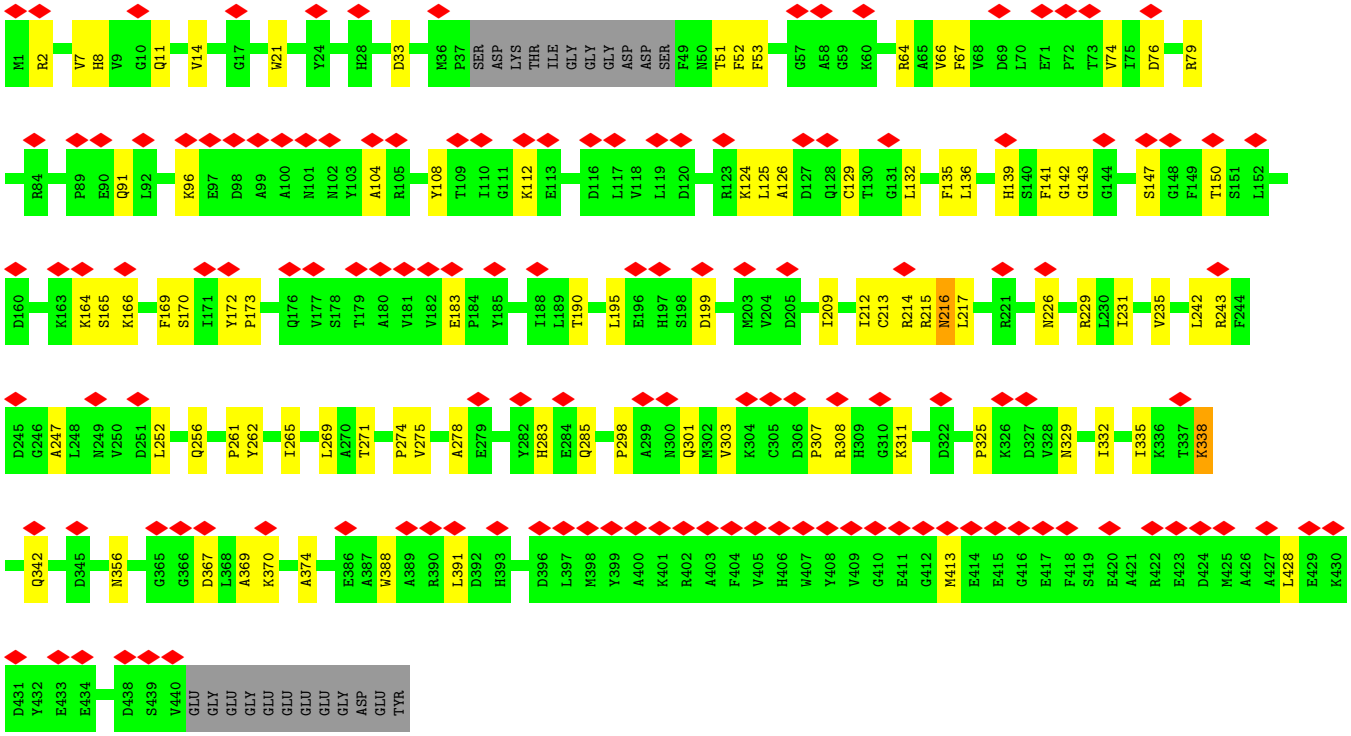
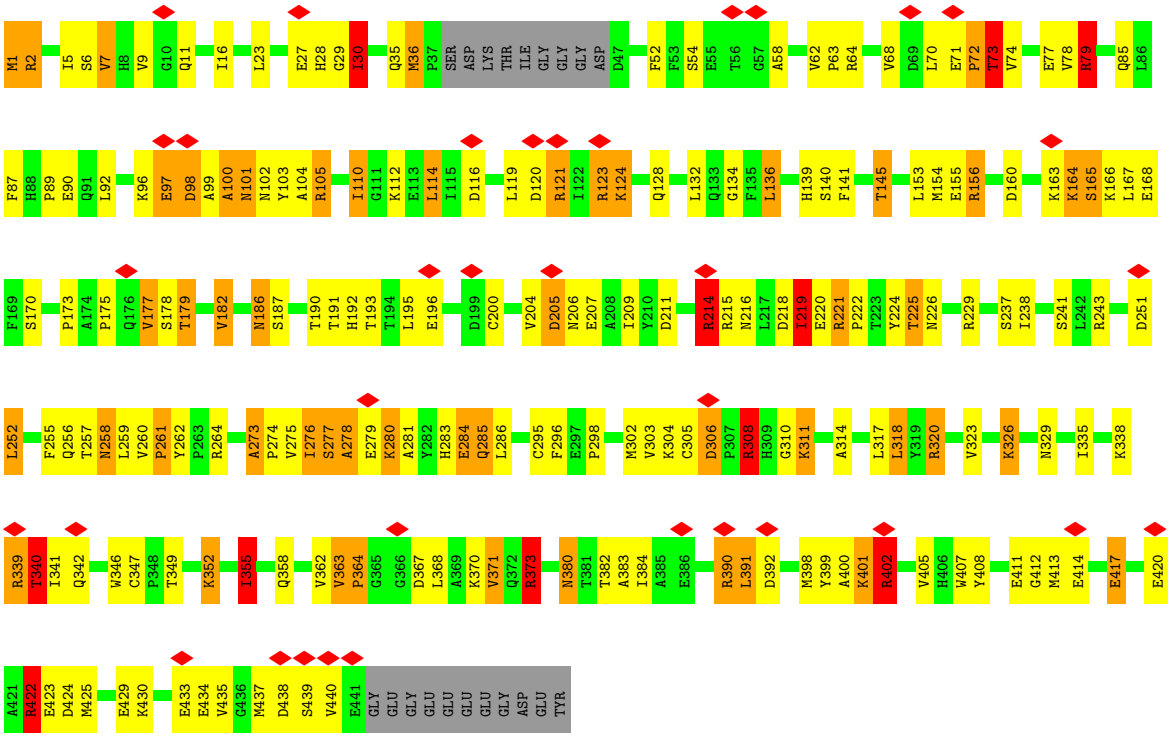


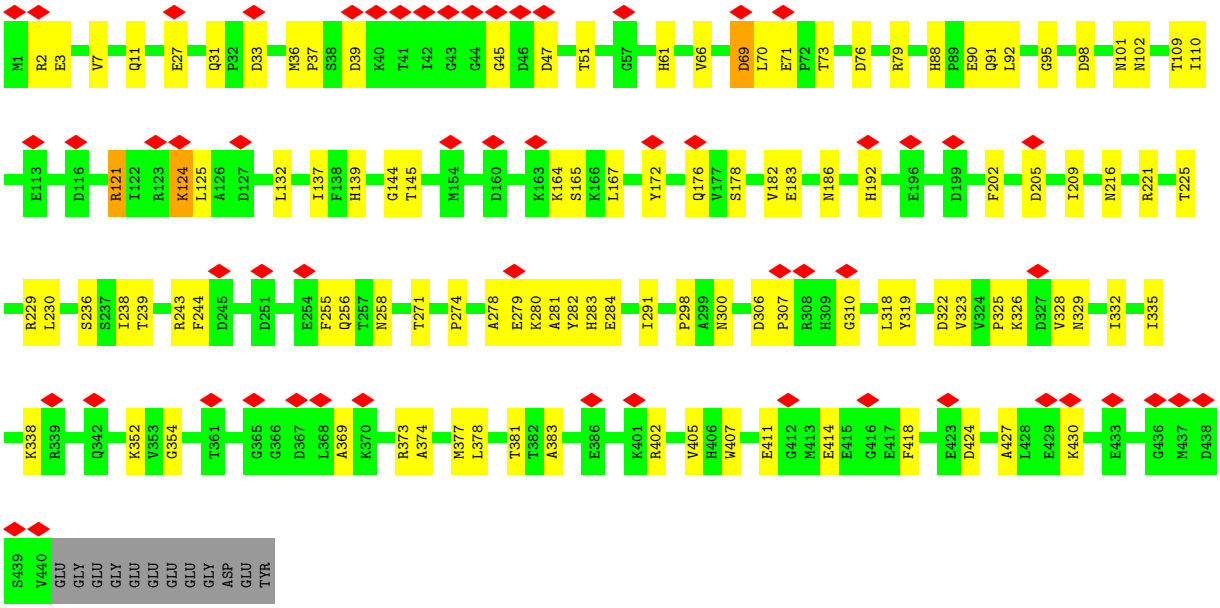
- Molecule 42: Tubulin alpha-1D chain

Chain IE:



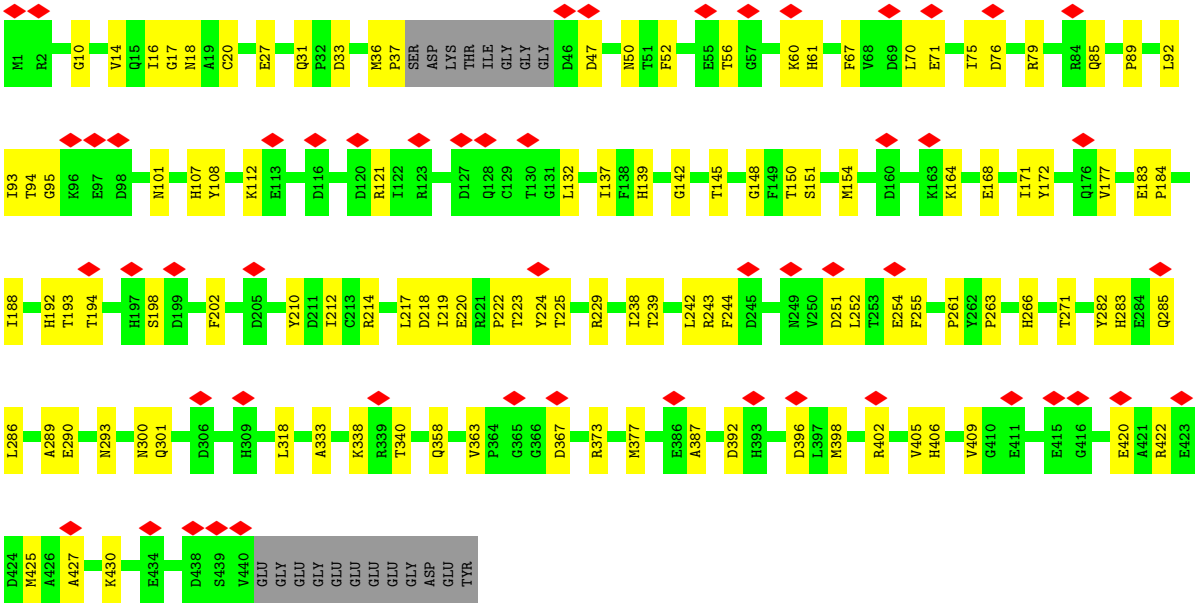
- Molecule 42: Tubulin alpha-1D chain

Chain IG:



- Molecule 42: Tubulin alpha-1D chain

Chain II:



- Molecule 42: Tubulin alpha-1D chain

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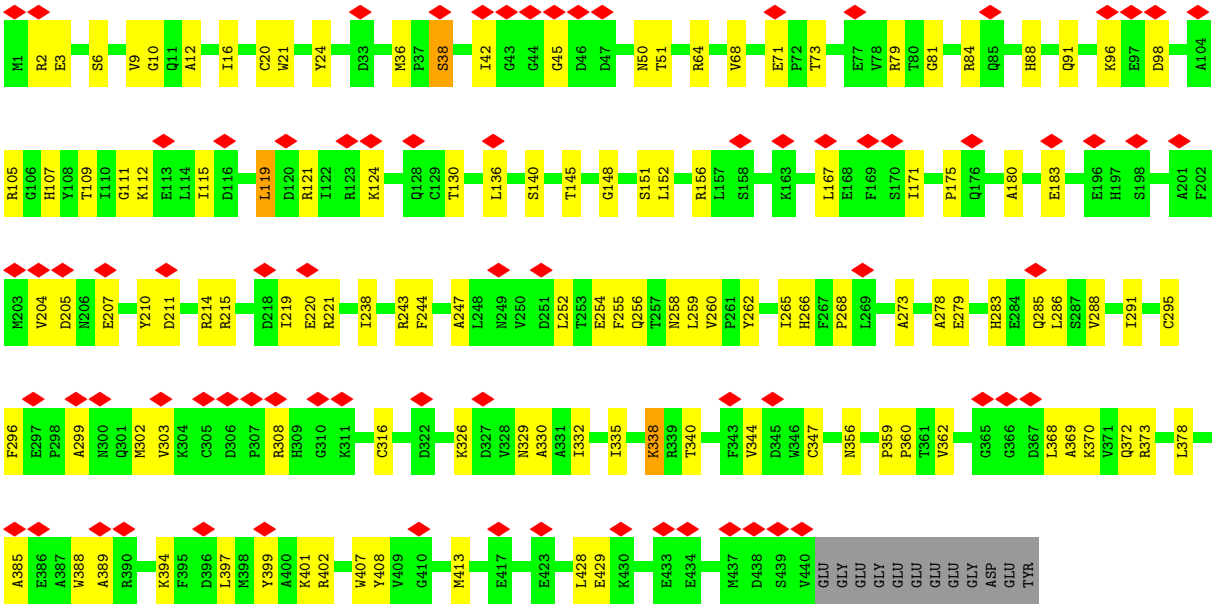
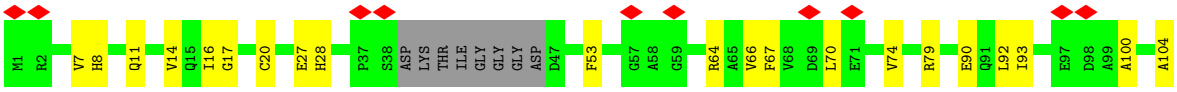
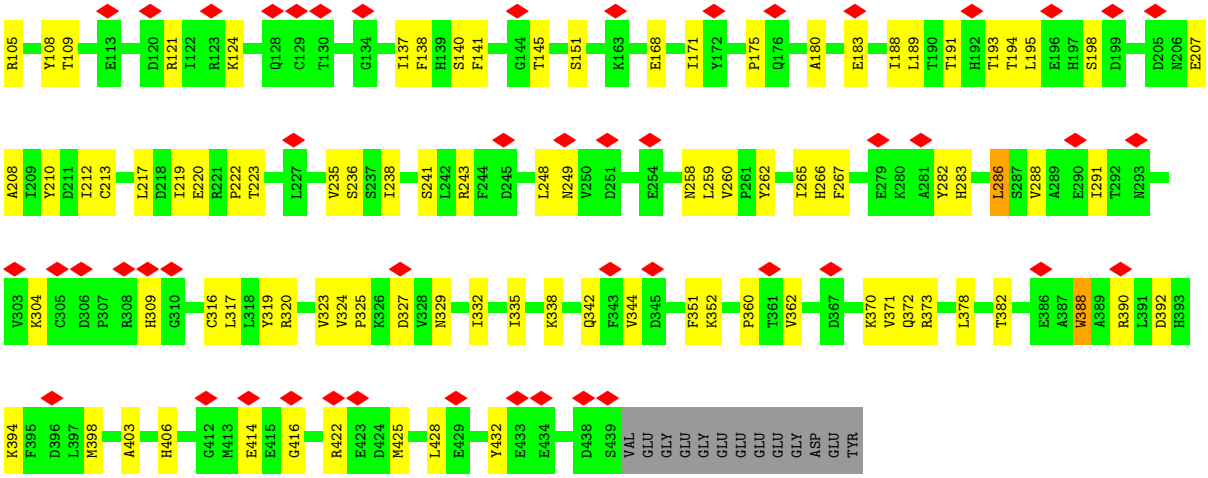


- Molecule 42: Tubulin alpha-1D chain

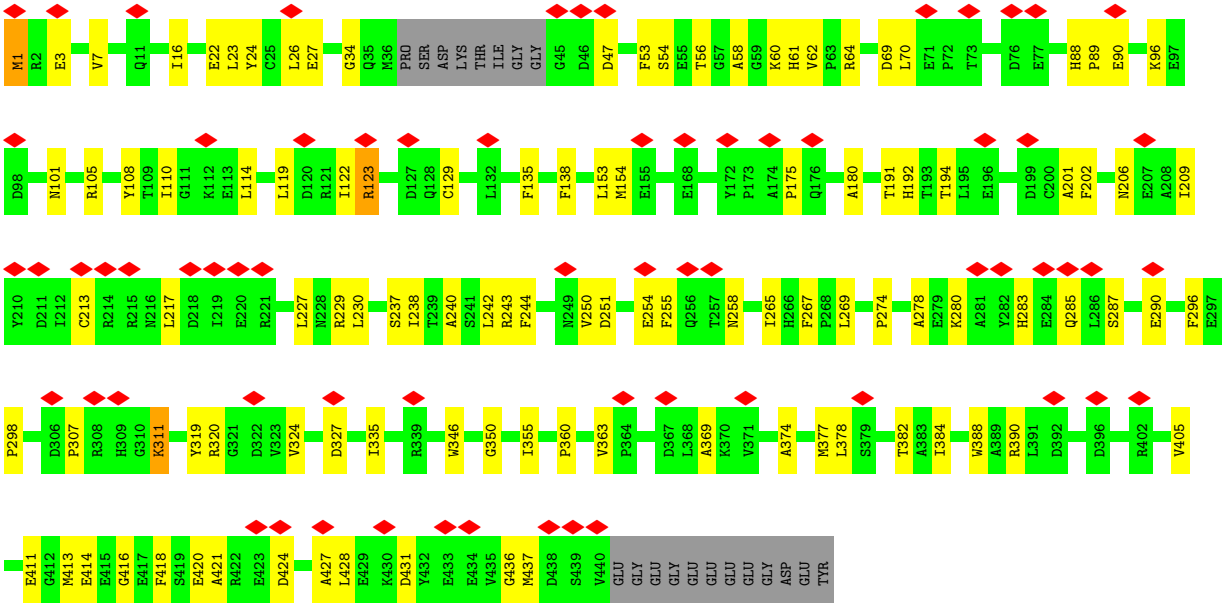
Chain IM:





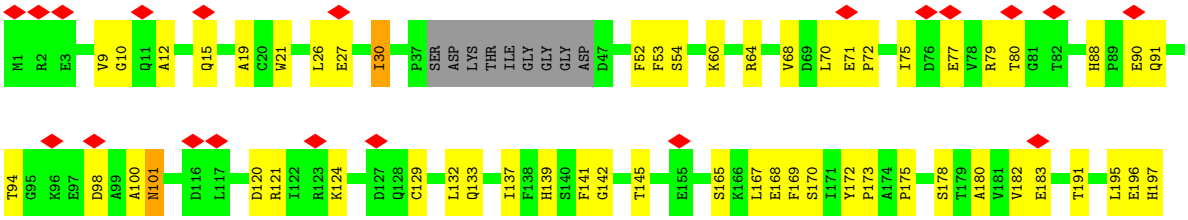
- Molecule 42: Tubulin alpha-1D chain

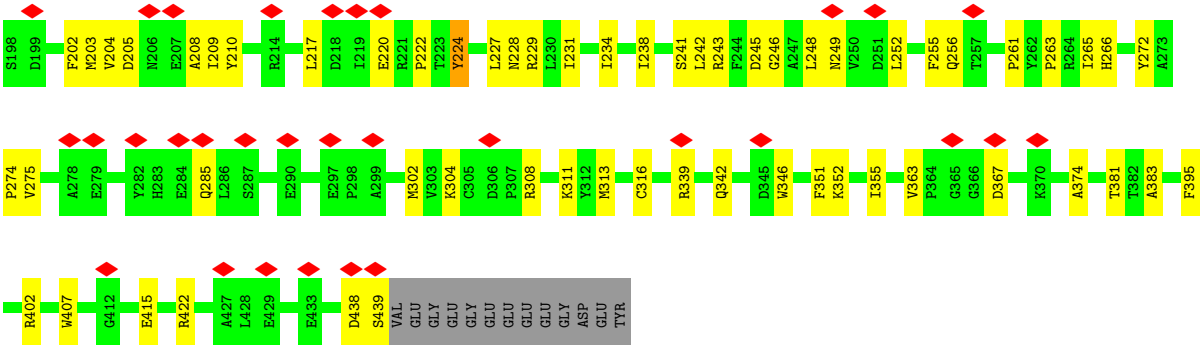
Chain JC:



- Molecule 42: Tubulin alpha-1D chain

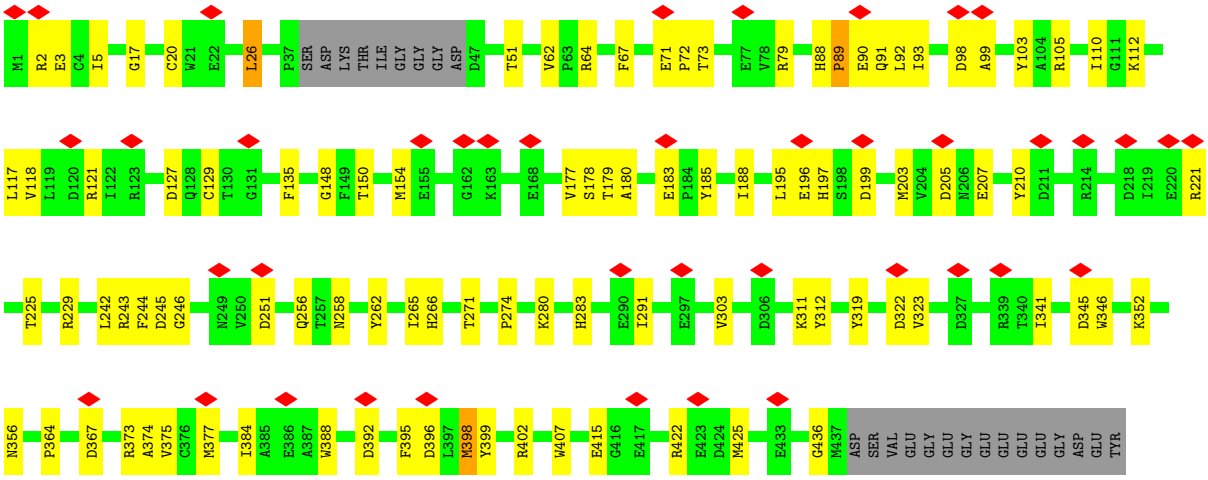
Chain JE:





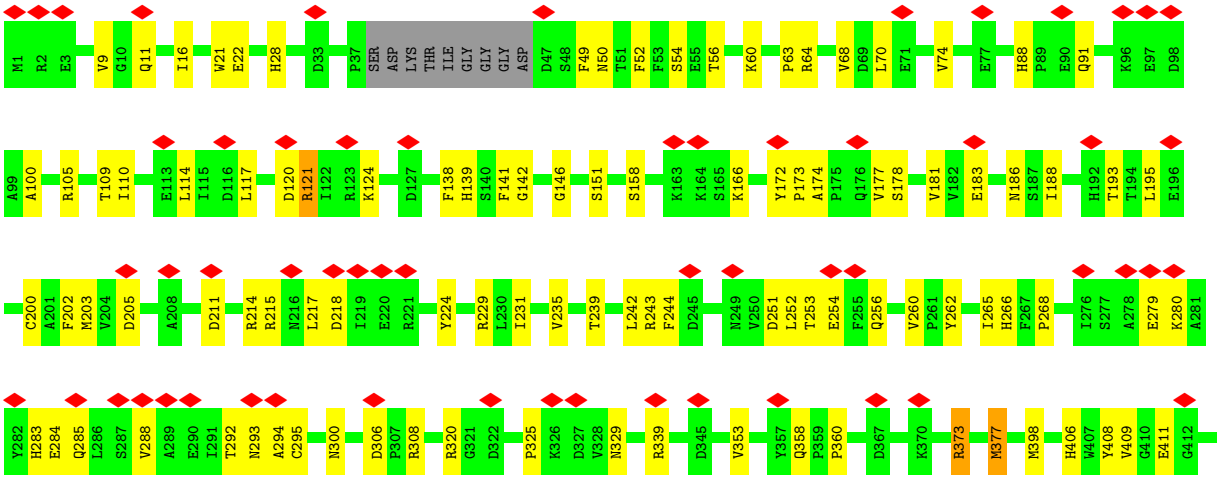
• Molecule 42: Tubulin alpha-1D chain

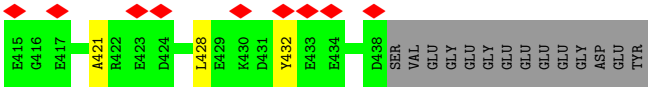
Chain JG:



• Molecule 42: Tubulin alpha-1D chain

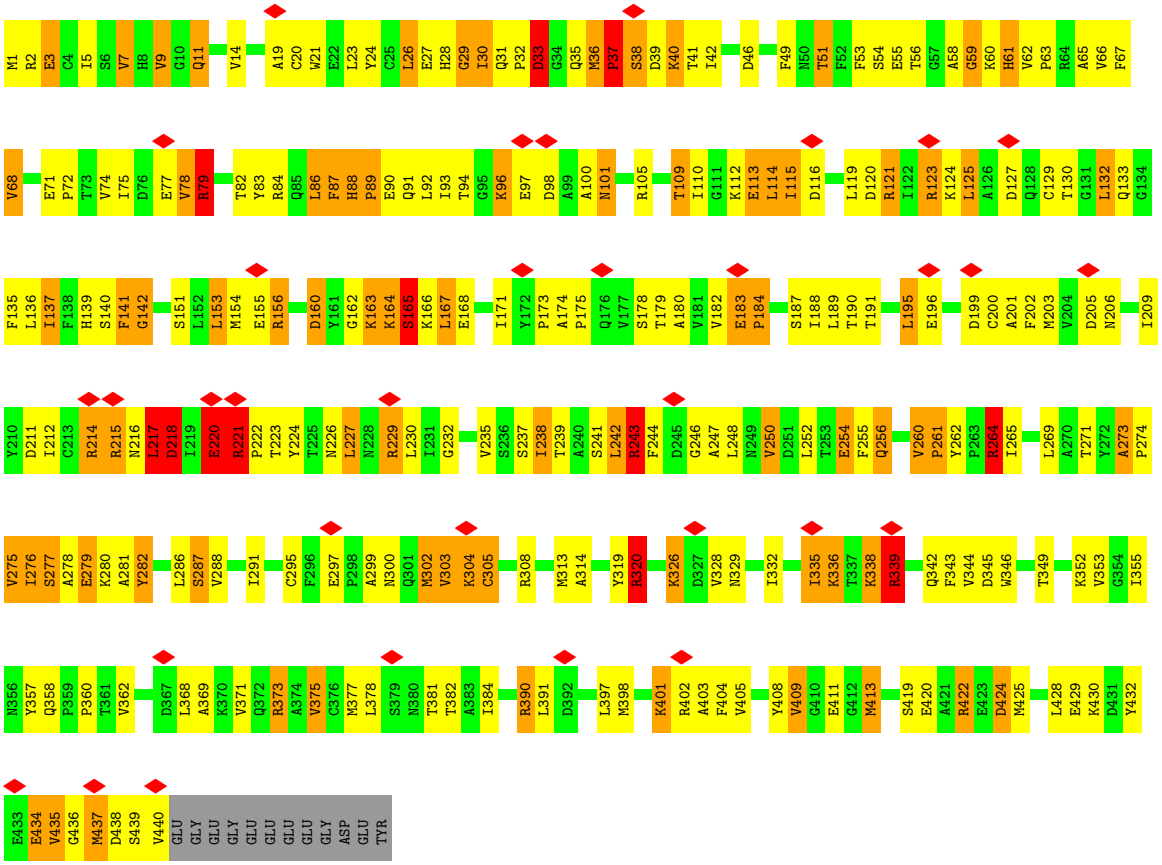
Chain JI:





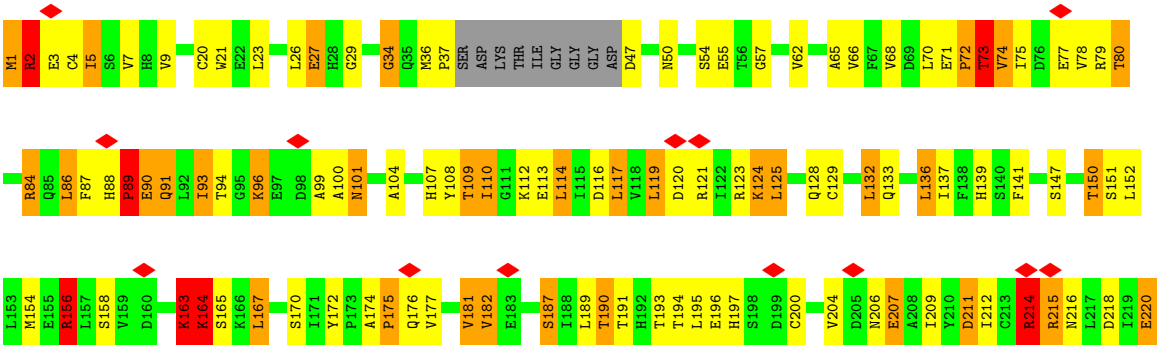
• Molecule 42: Tubulin alpha-1D chain

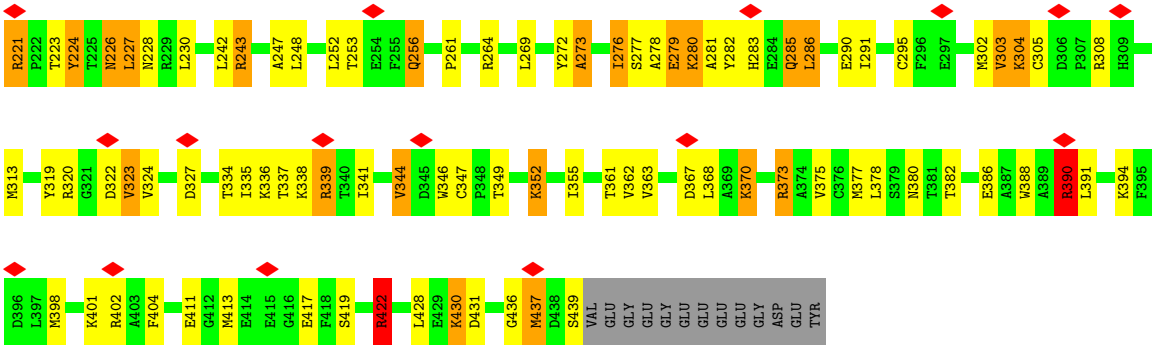
Chain JK:



• Molecule 42: Tubulin alpha-1D chain

Chain JM:





• Molecule 42: Tubulin alpha-1D chain

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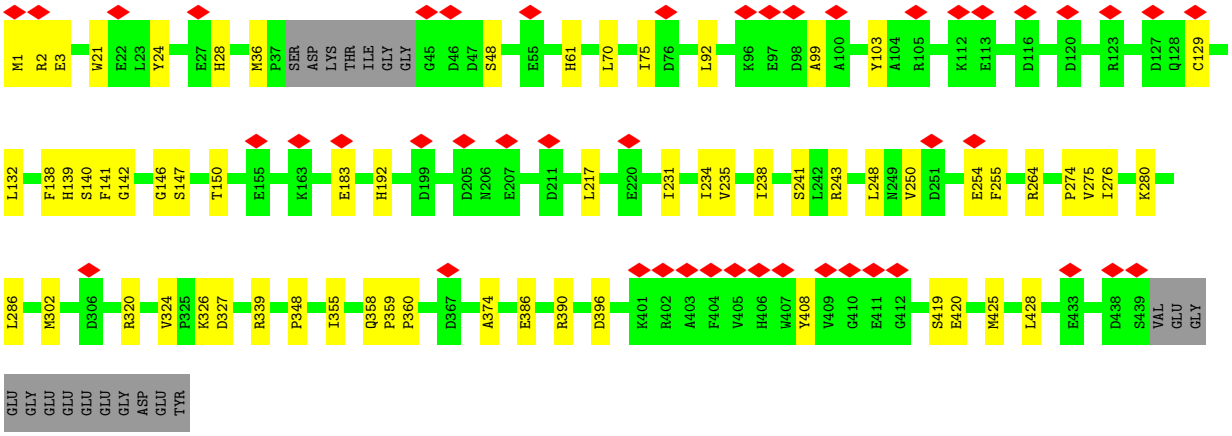
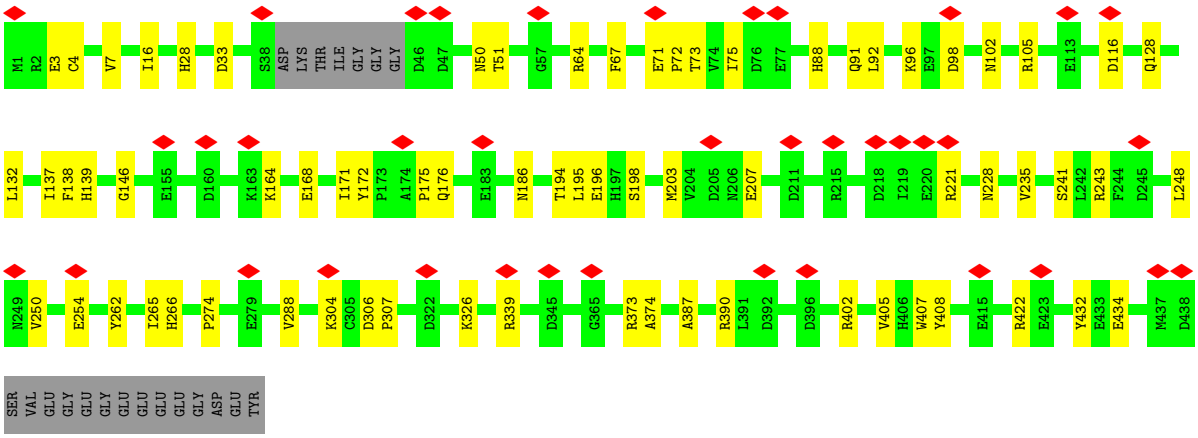


• Molecule 42: Tubulin alpha-1D chain

Chain KE:



• Molecule 42: Tubulin alpha-1D chain

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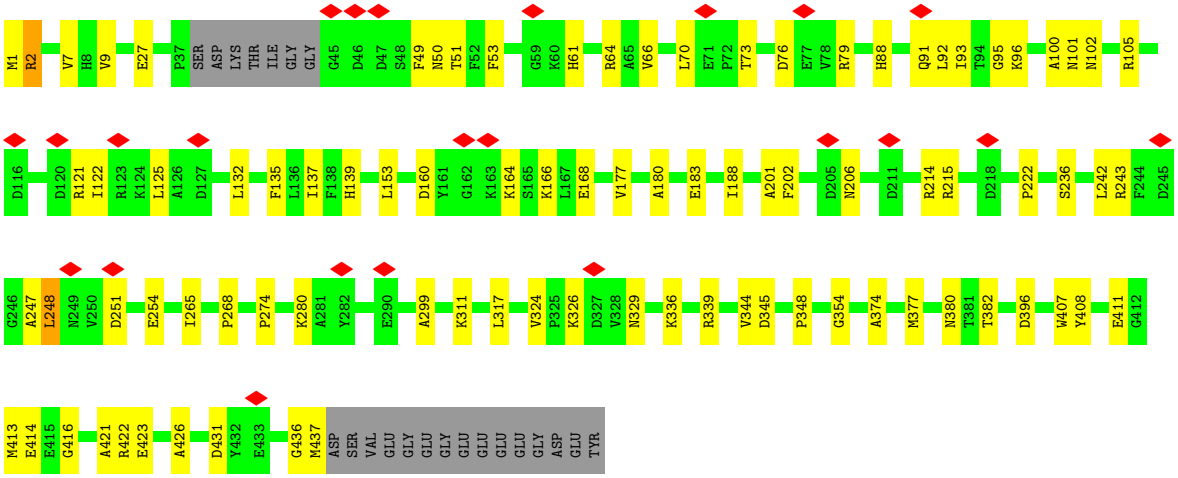

- Molecule 42: Tubulin alpha-1D chain

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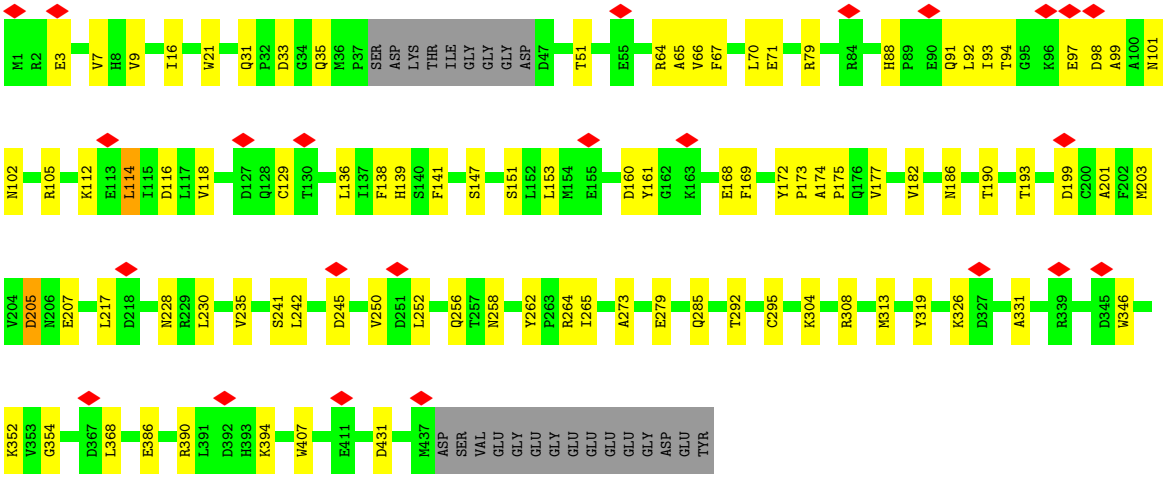

- Molecule 42: Tubulin alpha-1D chain

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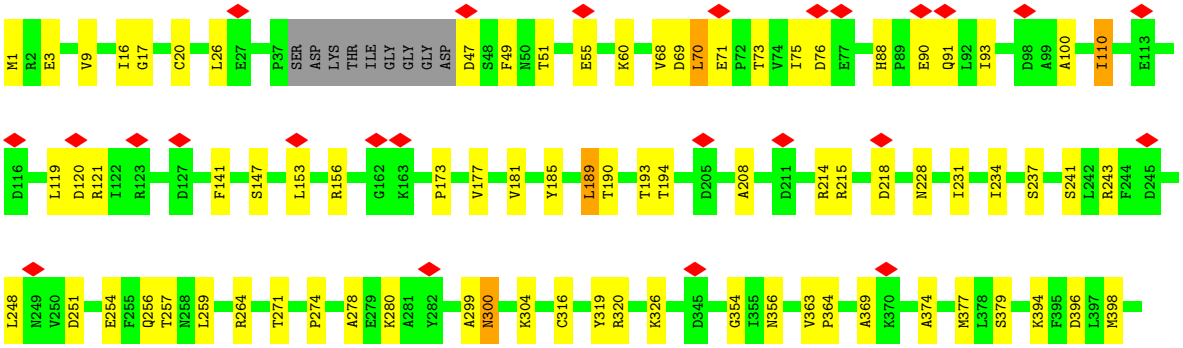

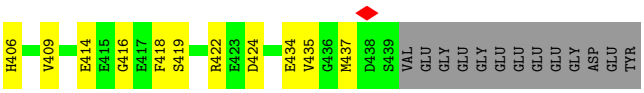

• Molecule 42: Tubulin alpha-1D chain

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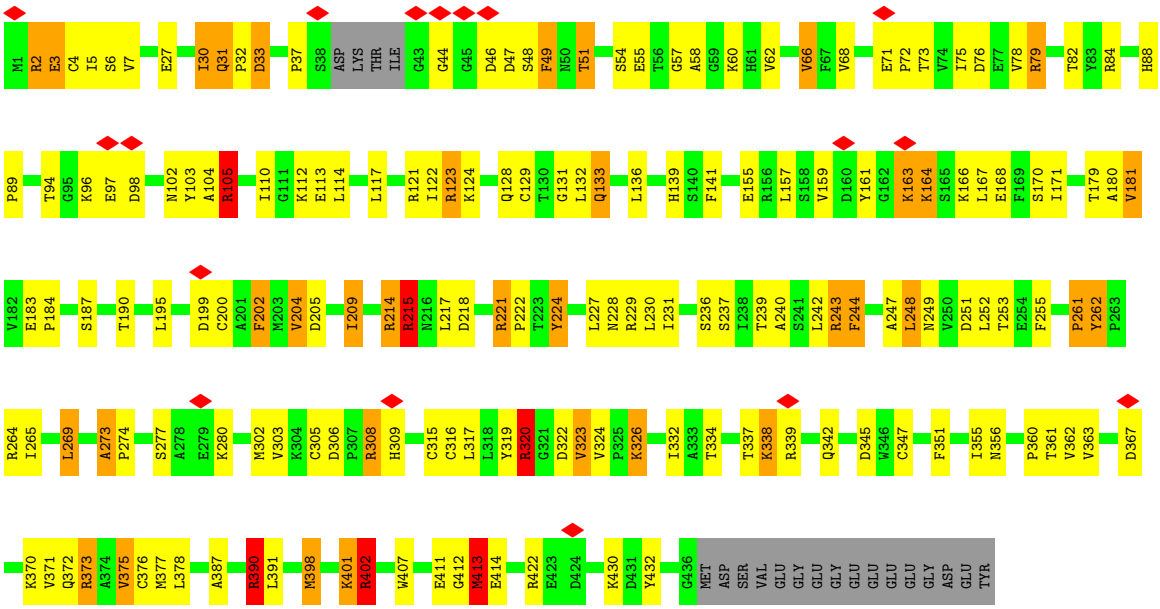

• Molecule 42: Tubulin alpha-1D chain

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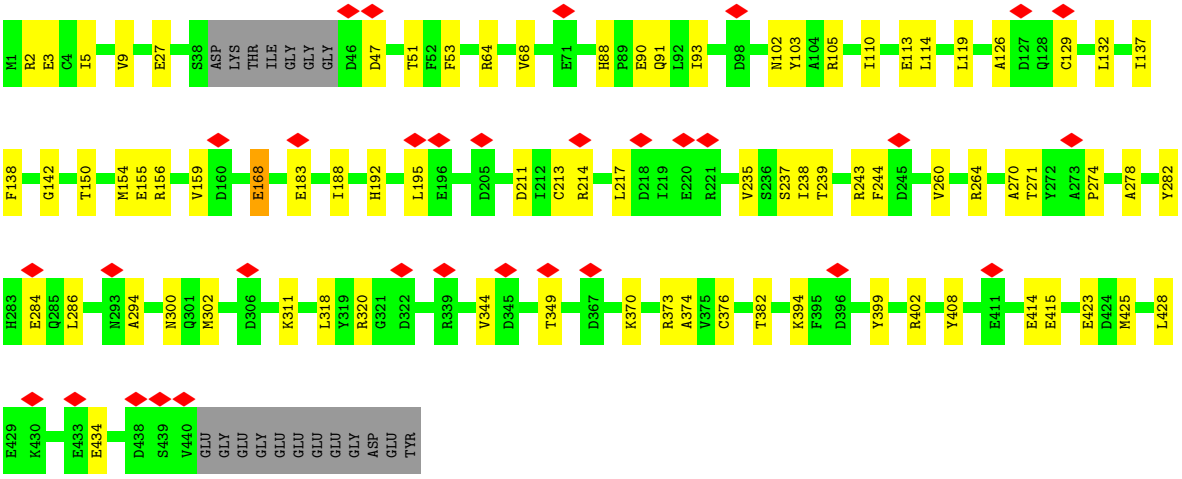

• Molecule 42: Tubulin alpha-1D chain

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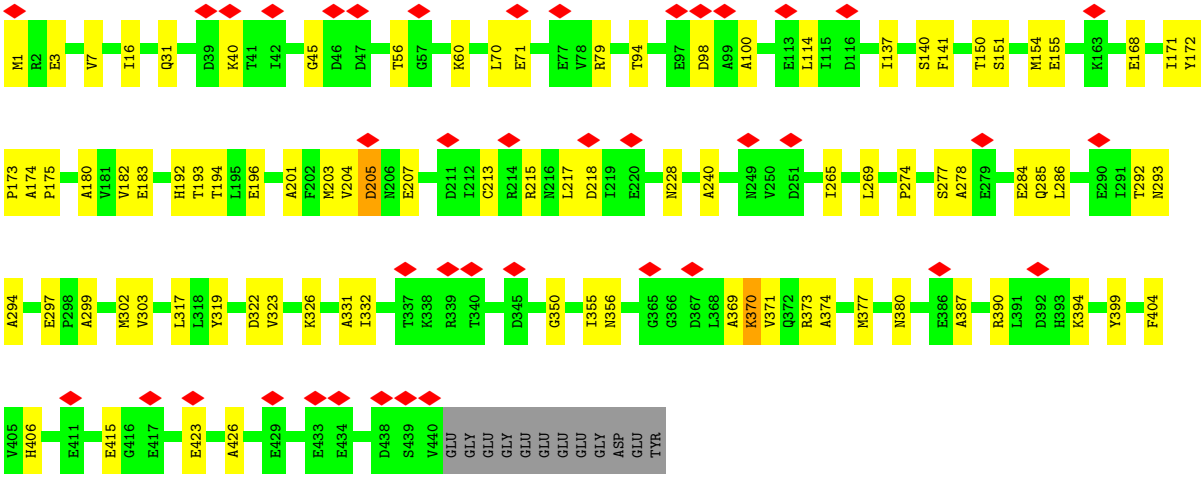

- Molecule 42: Tubulin alpha-1D chain

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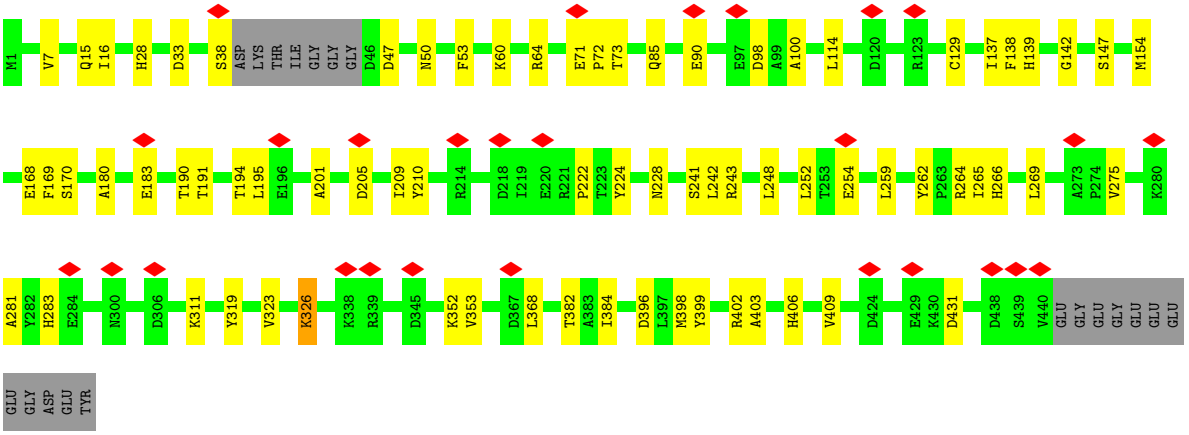

- Molecule 42: Tubulin alpha-1D chain

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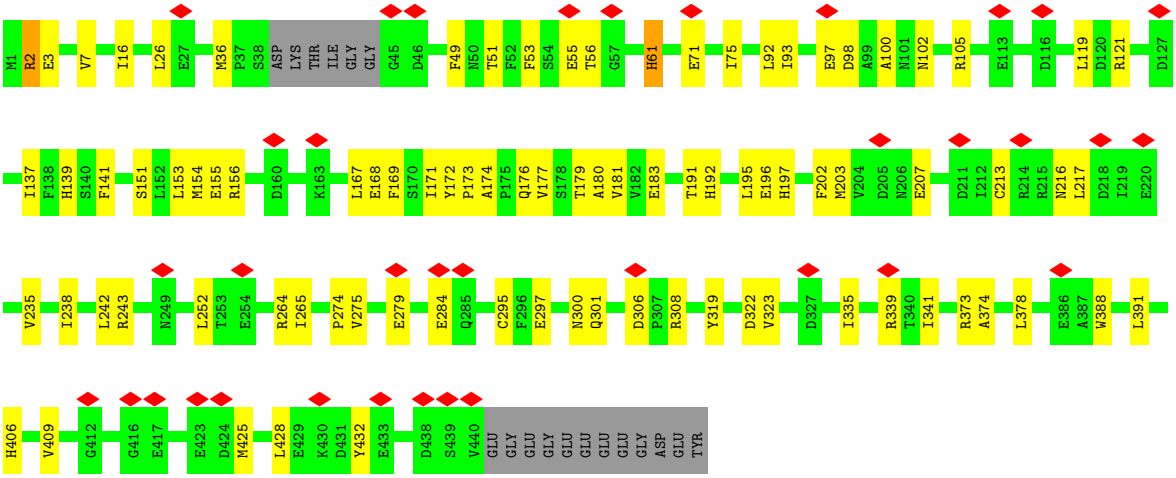

- Molecule 42: Tubulin alpha-1D chain

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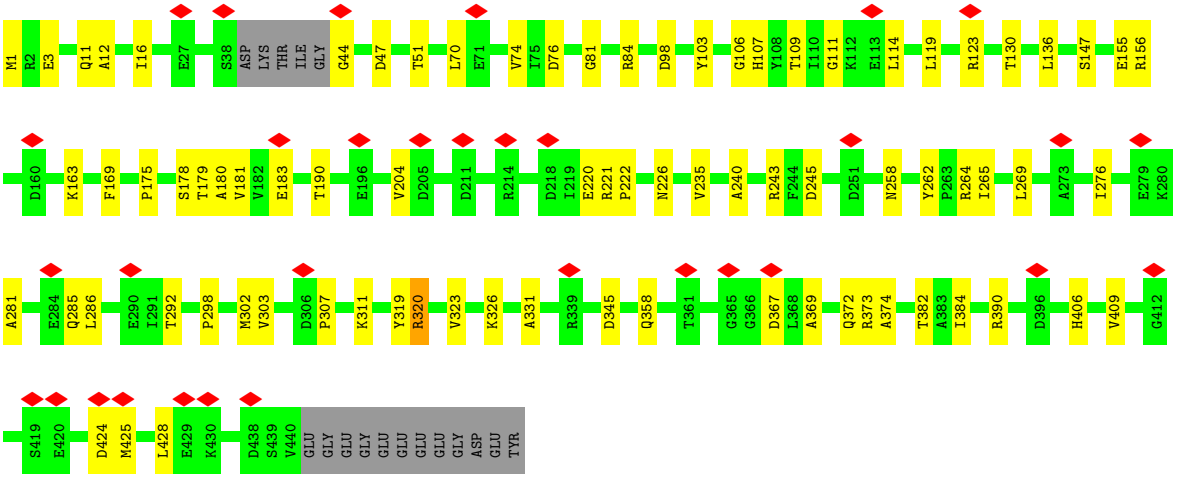
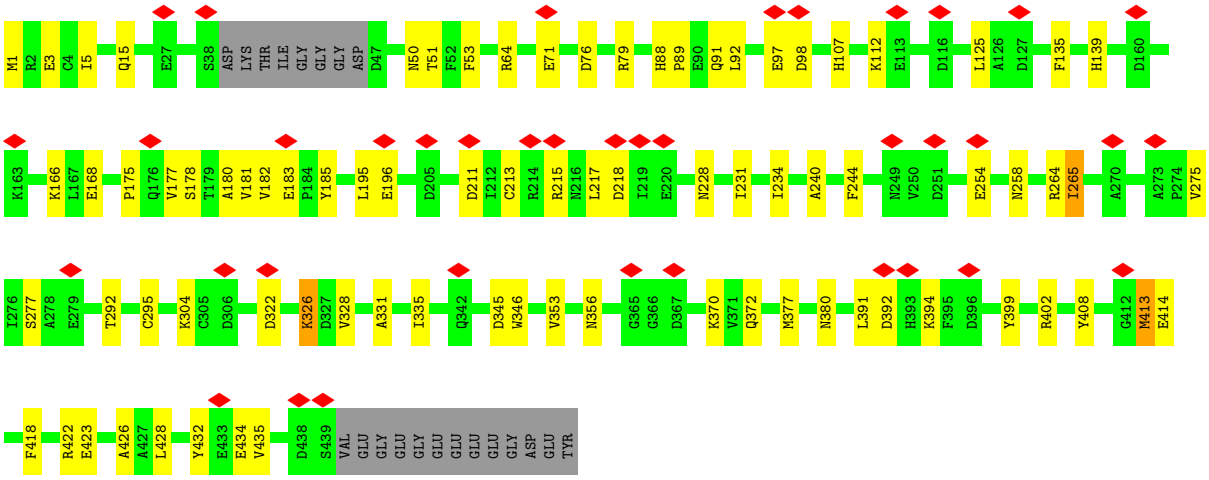


- Molecule 42: Tubulin alpha-1D chain

Chain LM:



- Molecule 42: Tubulin alpha-1D chain

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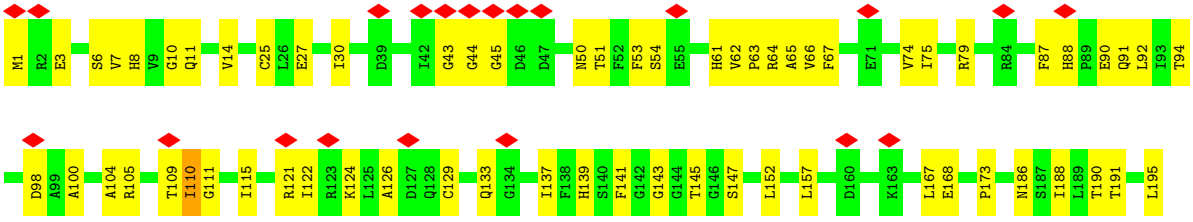

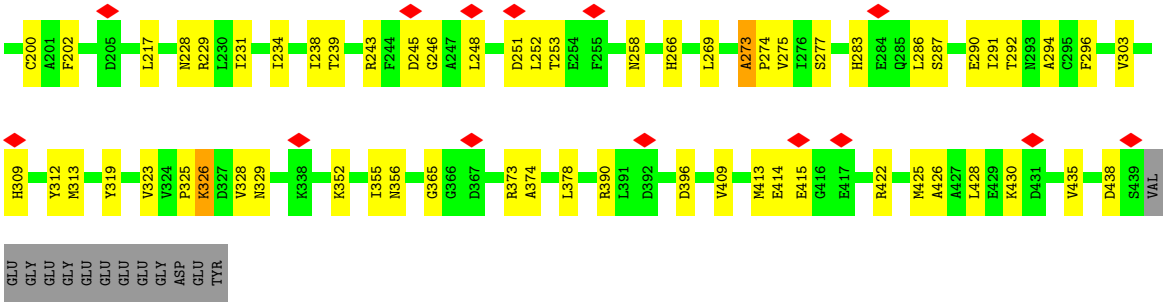

• Molecule 42: Tubulin alpha-1D chain

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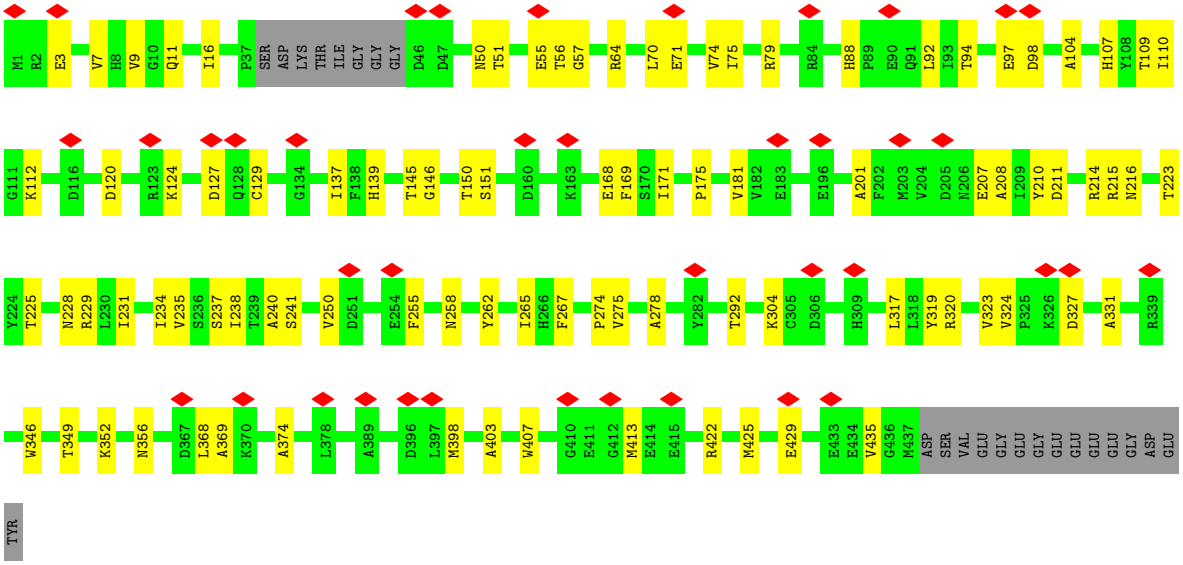

• Molecule 42: Tubulin alpha-1D chain

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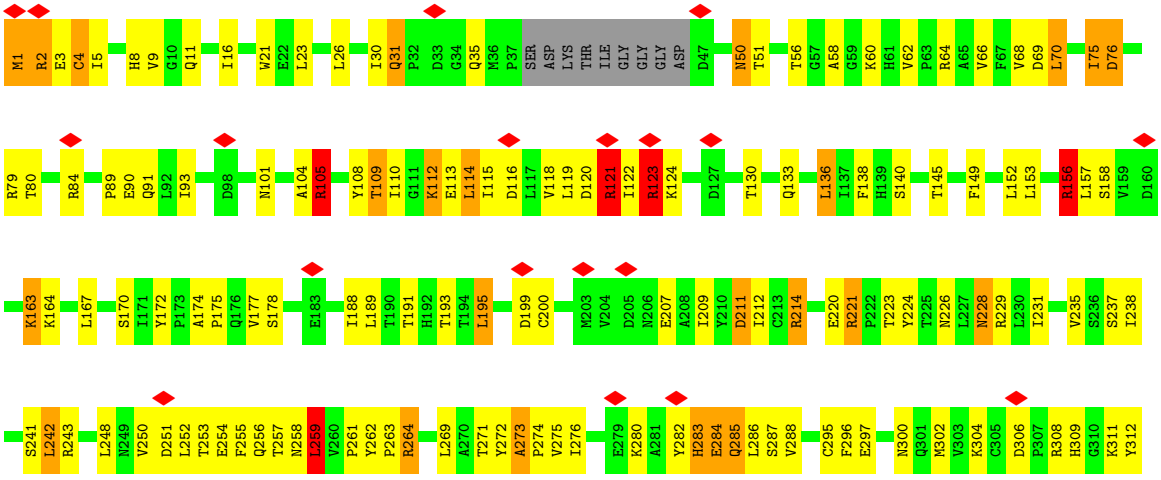

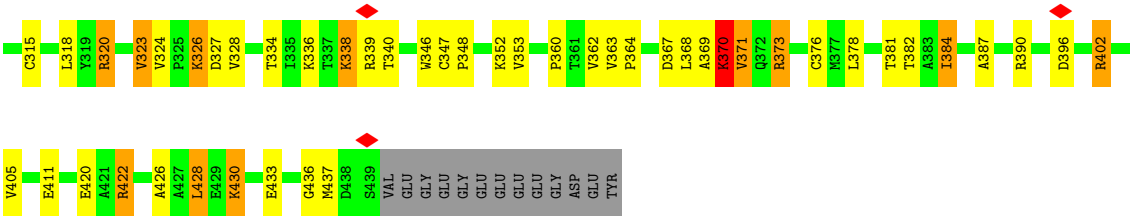

• Molecule 42: Tubulin alpha-1D chain

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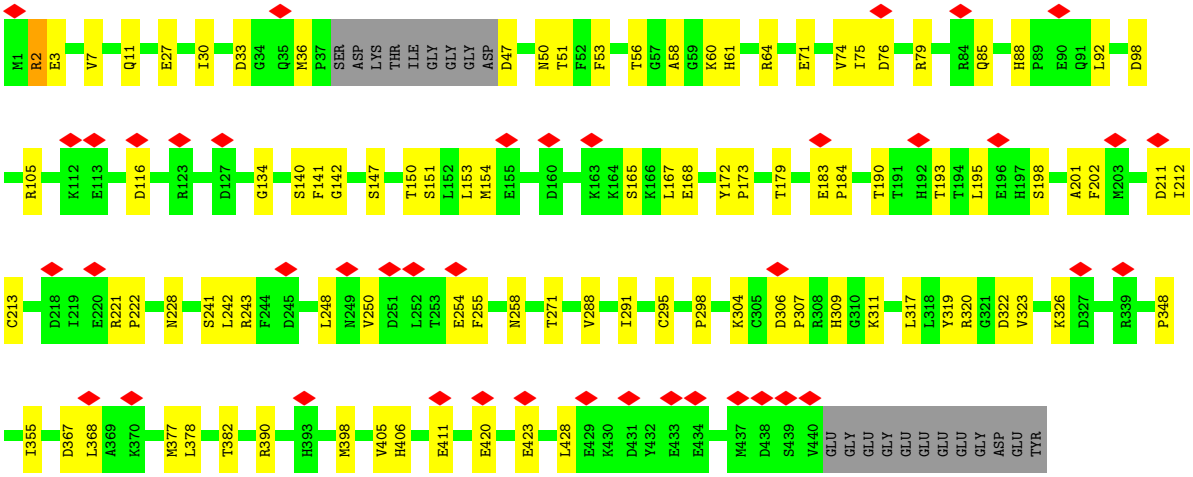

• Molecule 42: Tubulin alpha-1D chain

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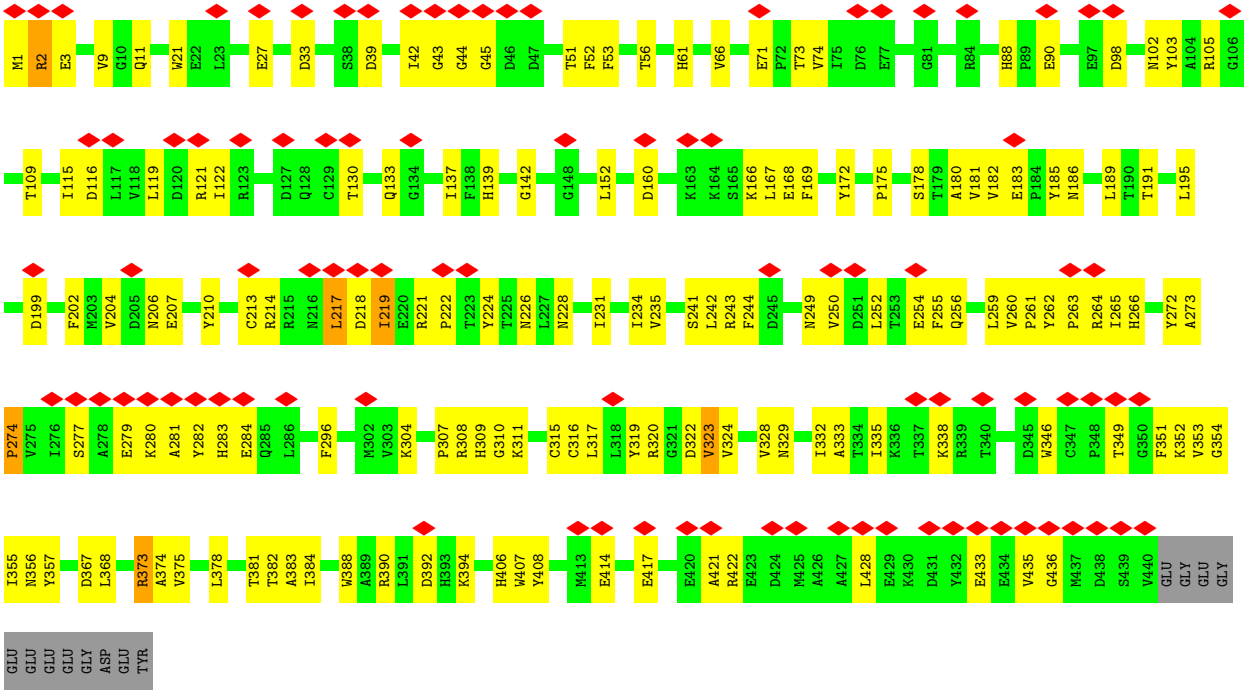

- Molecule 42: Tubulin alpha-1D chain

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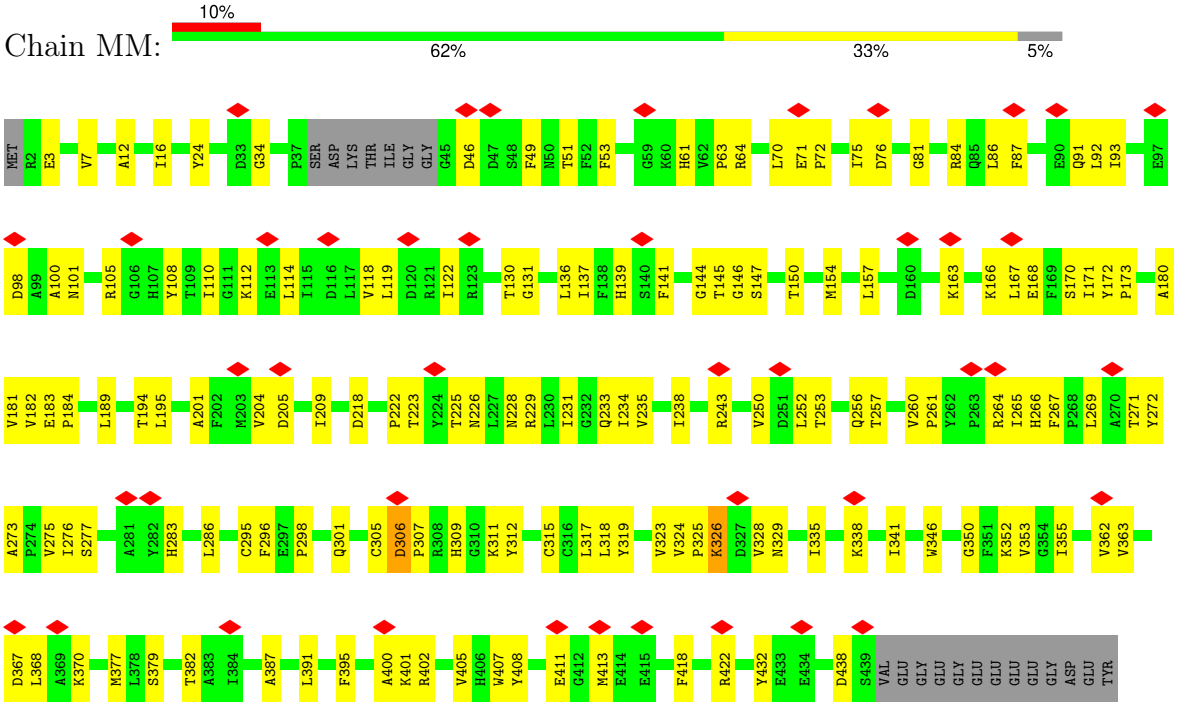

- Molecule 42: Tubulin alpha-1D chain

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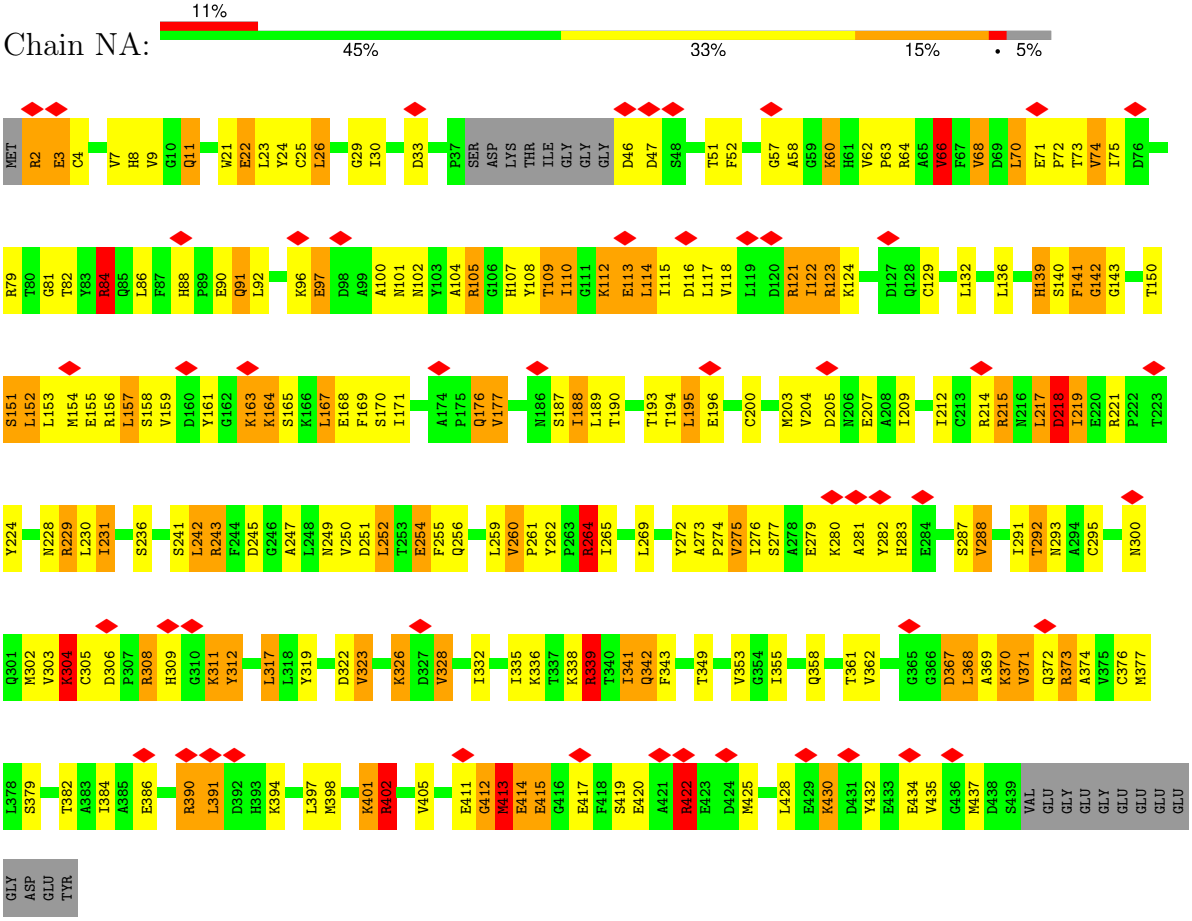

• Molecule 42: Tubulin alpha-1D chain

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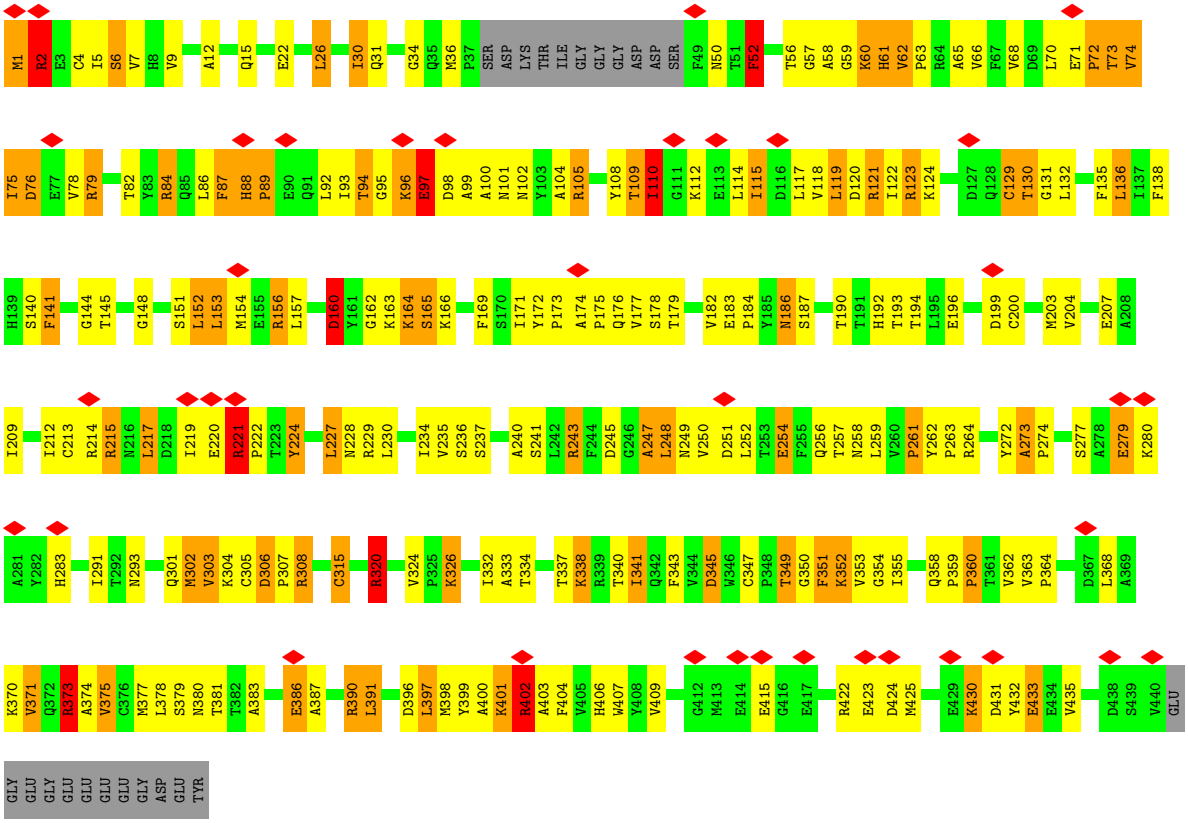

• Molecule 42: Tubulin alpha-1D chain

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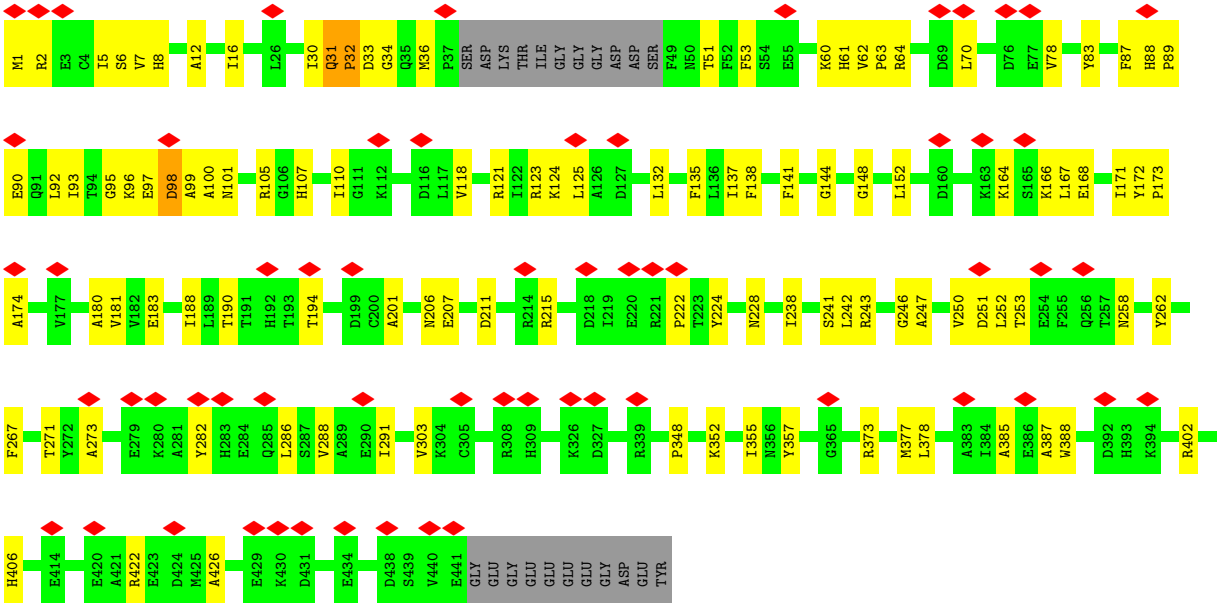

- Molecule 42: Tubulin alpha-1D chain

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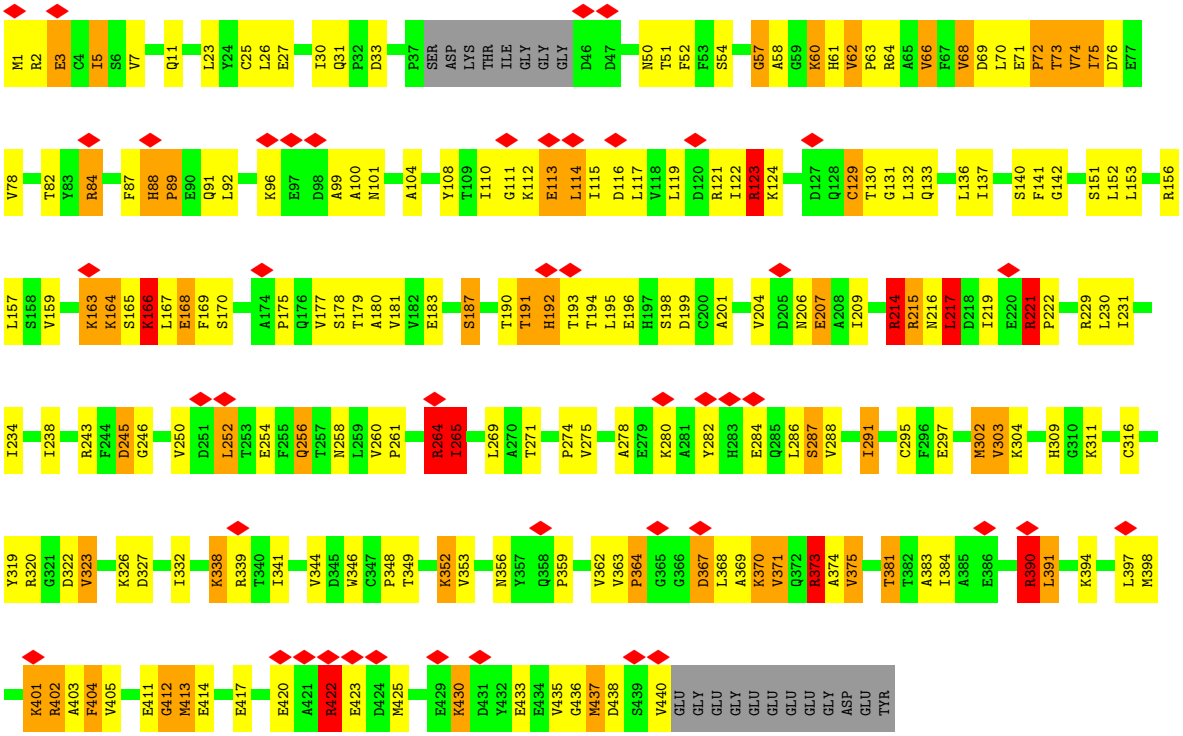

- Molecule 42: Tubulin alpha-1D chain

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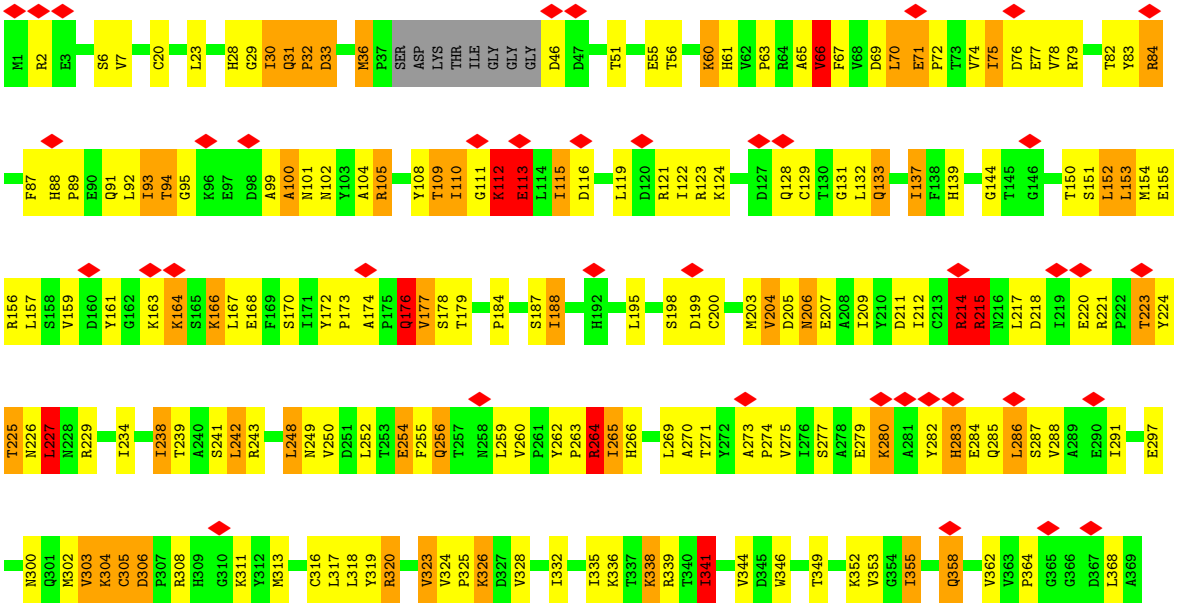

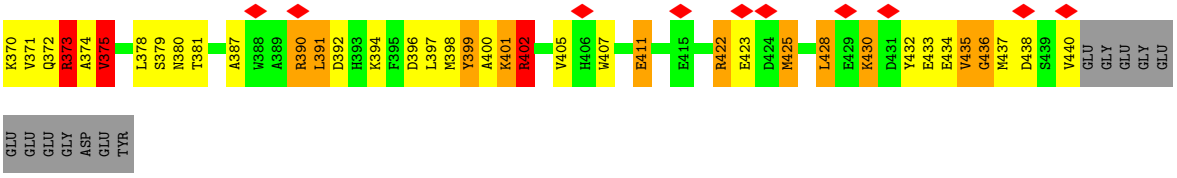

• Molecule 42: Tubulin alpha-1D chain

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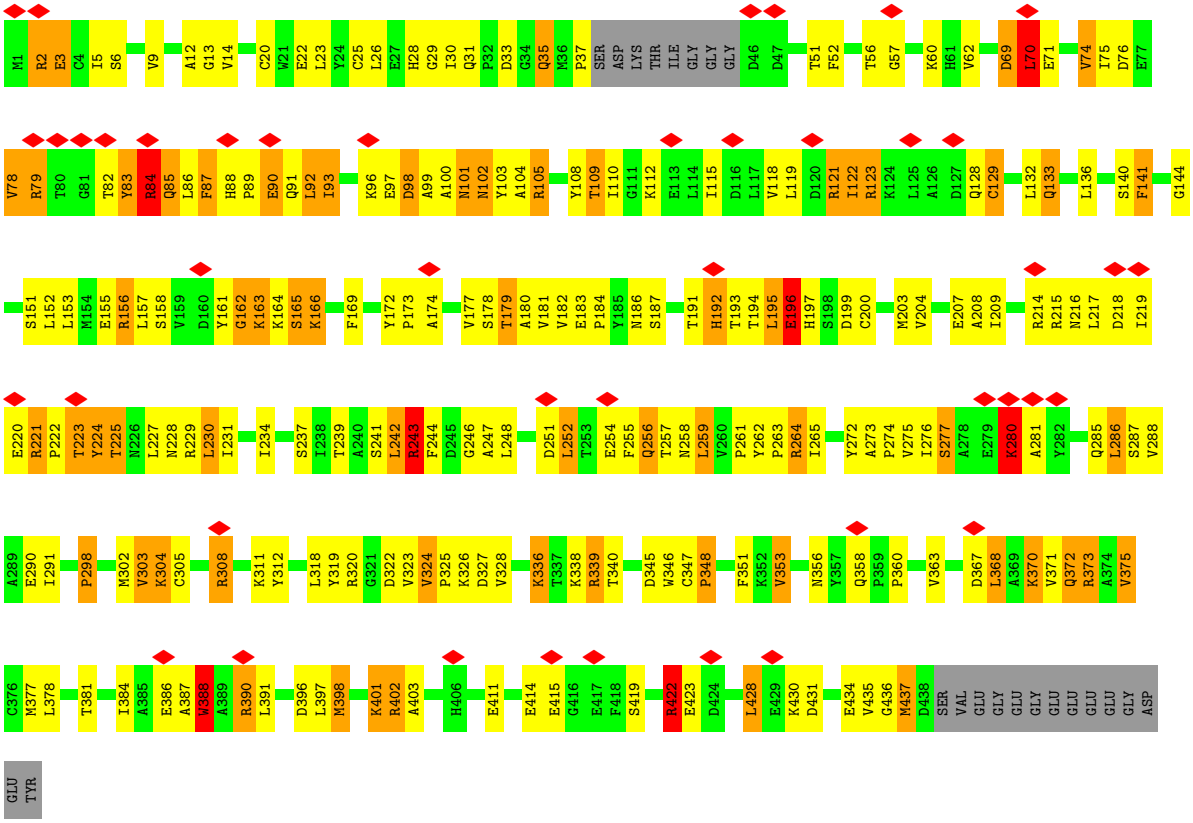
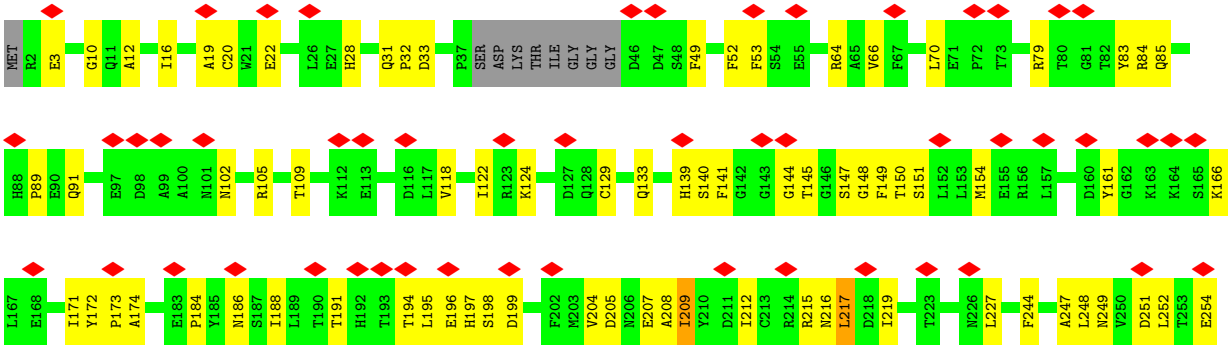
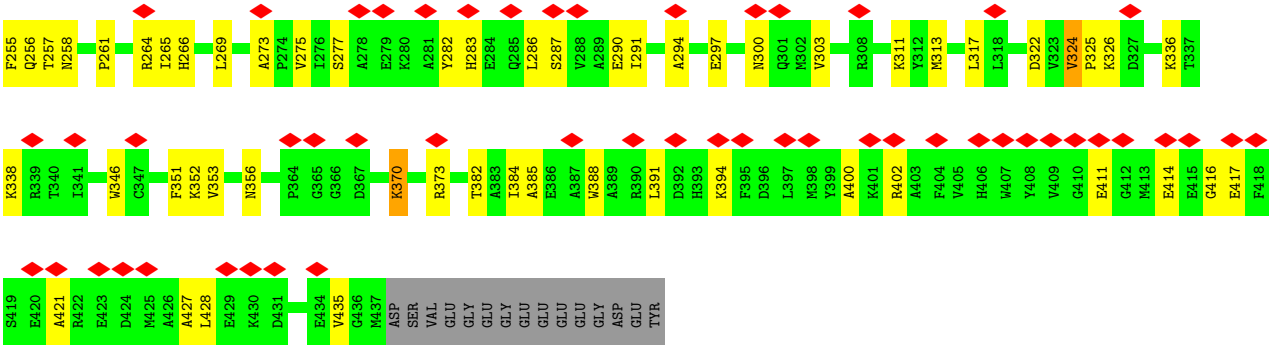


• Molecule 42: Tubulin alpha-1D chain

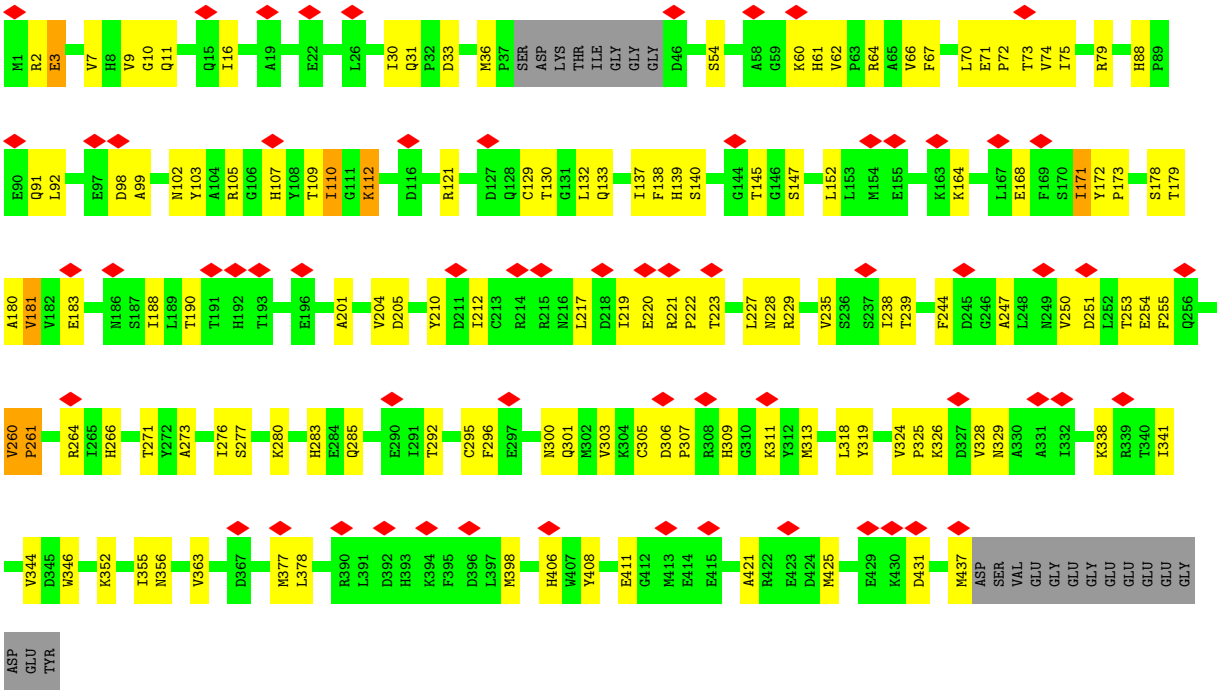
Chain OA:





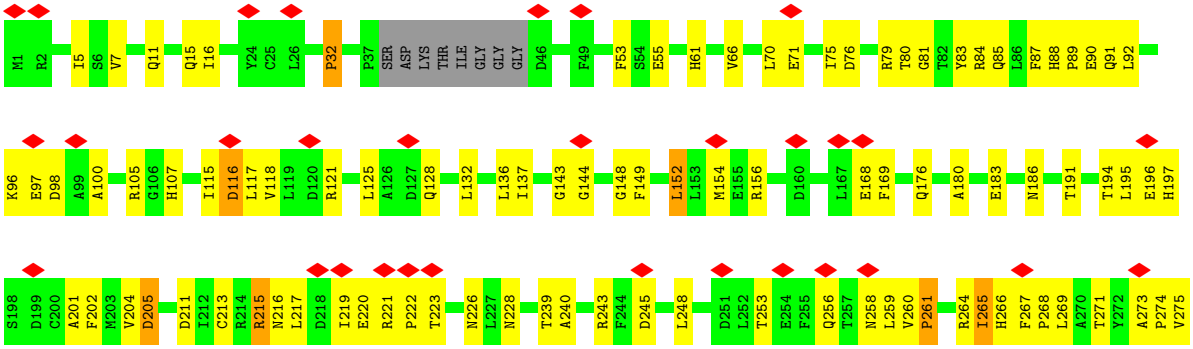
• Molecule 42: Tubulin alpha-1D chain

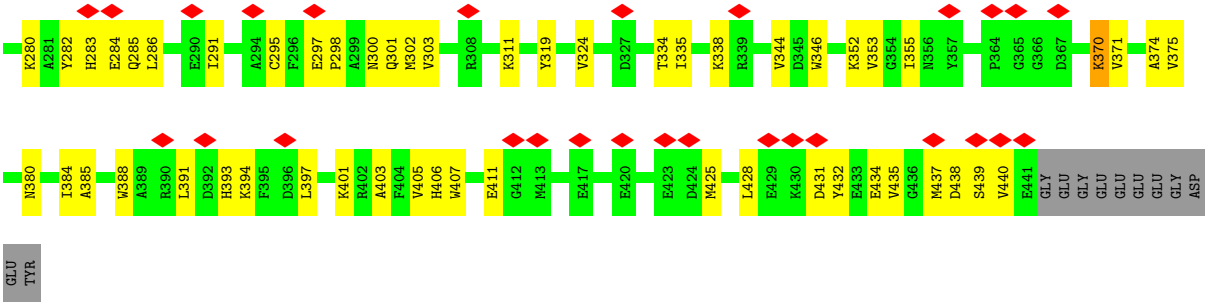
Chain OC:



• Molecule 42: Tubulin alpha-1D chain

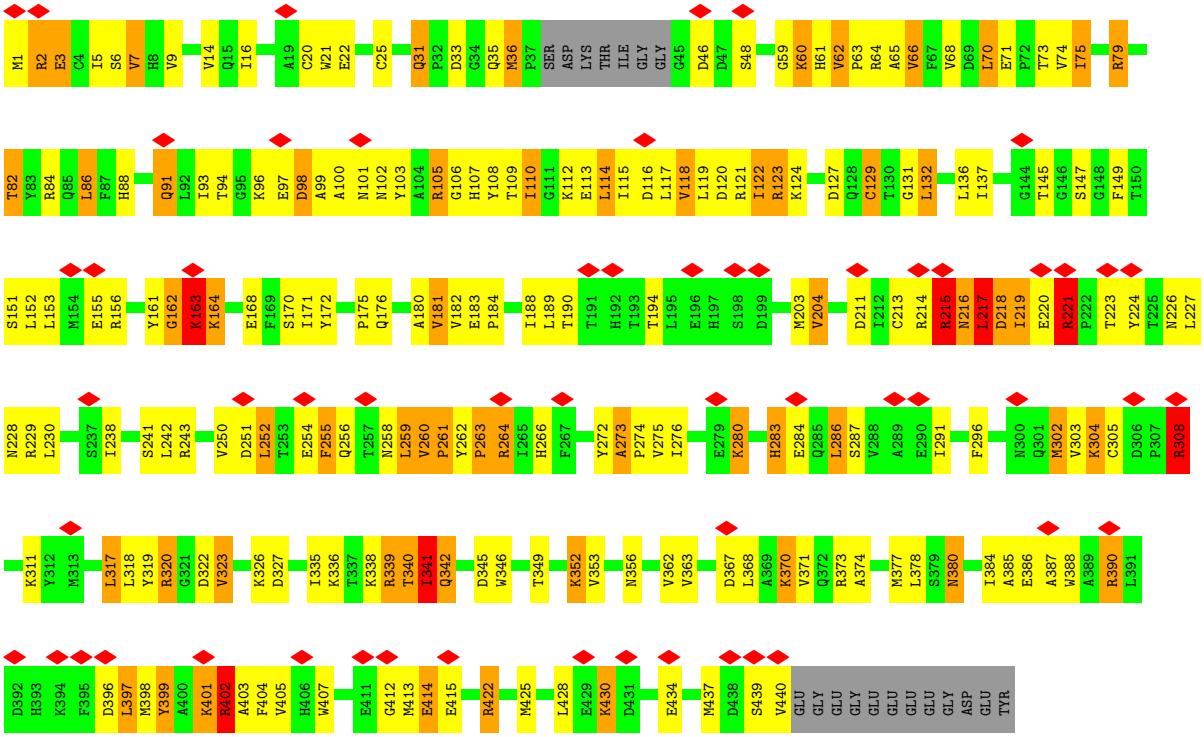
Chain OE:





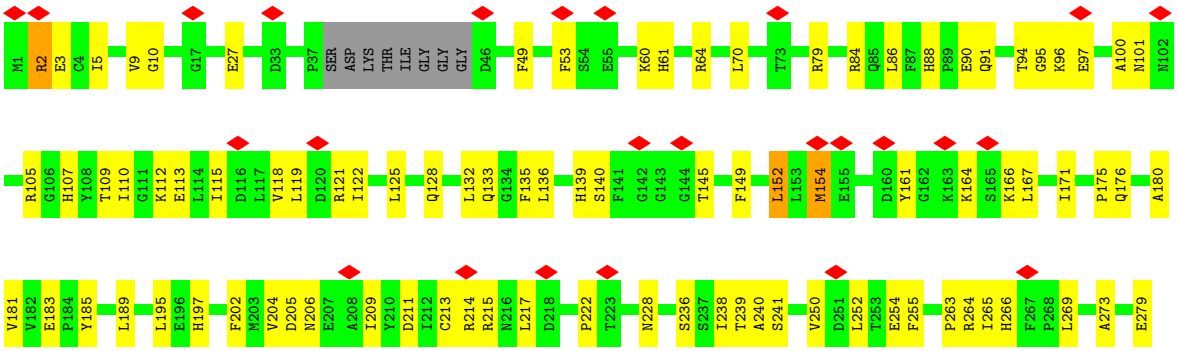
• Molecule 42: Tubulin alpha-1D chain

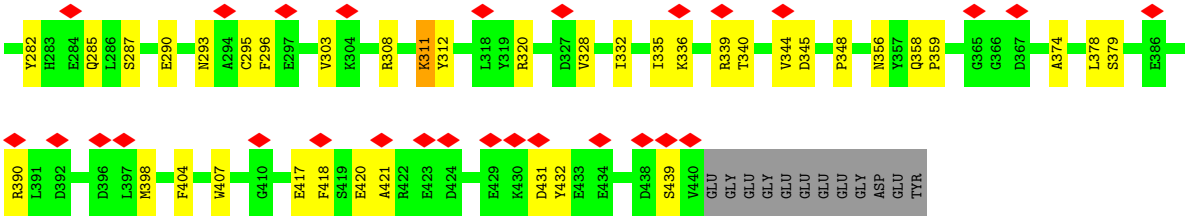
Chain OG:



• Molecule 42: Tubulin alpha-1D chain

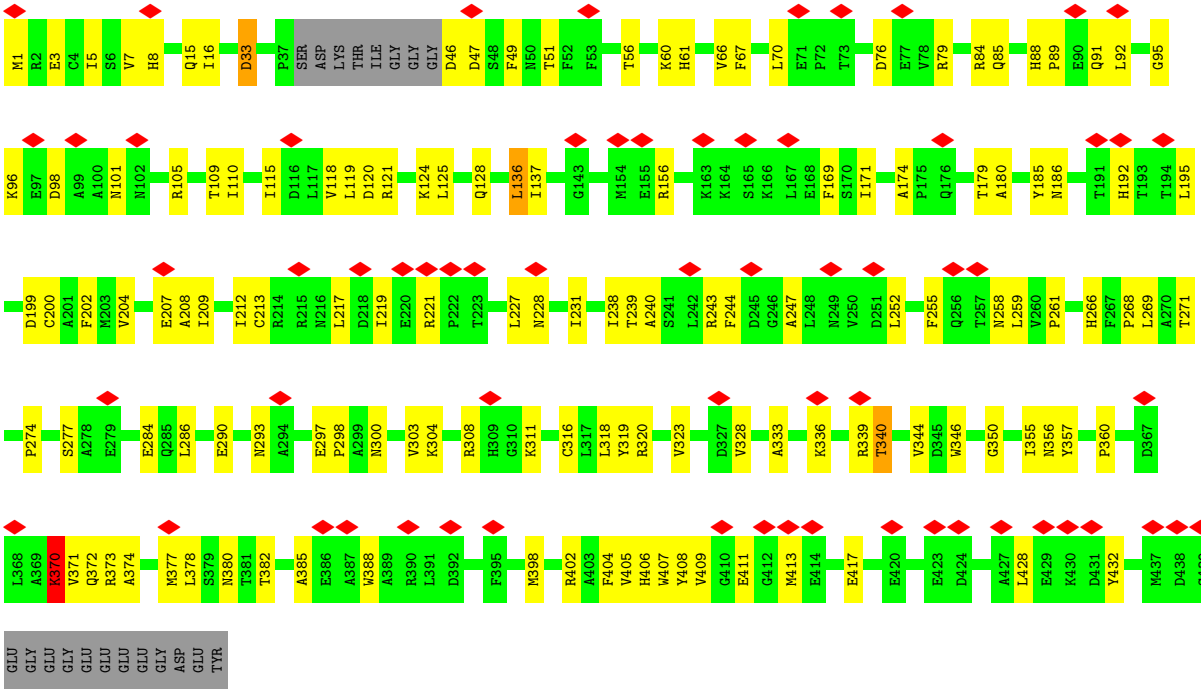
Chain OI:





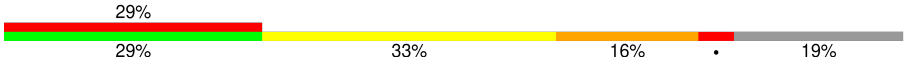
• Molecule 42: Tubulin alpha-1D chain

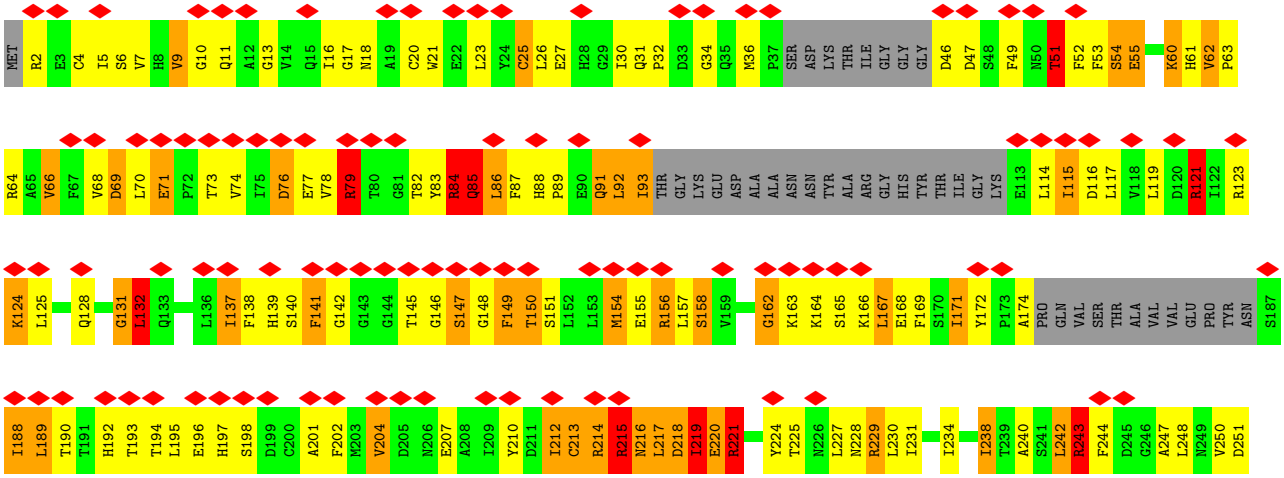
Chain OK:

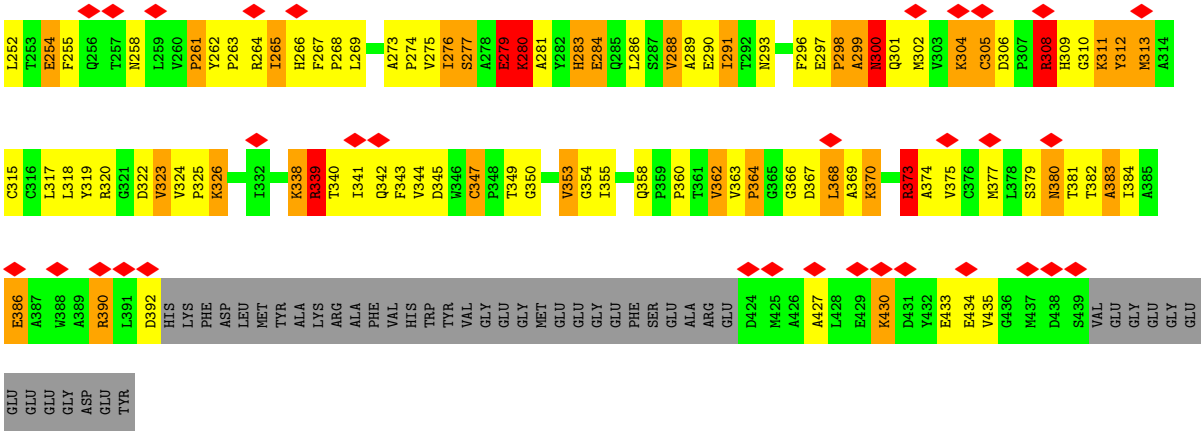


• Molecule 42: Tubulin alpha-1D chain

Chain PA:

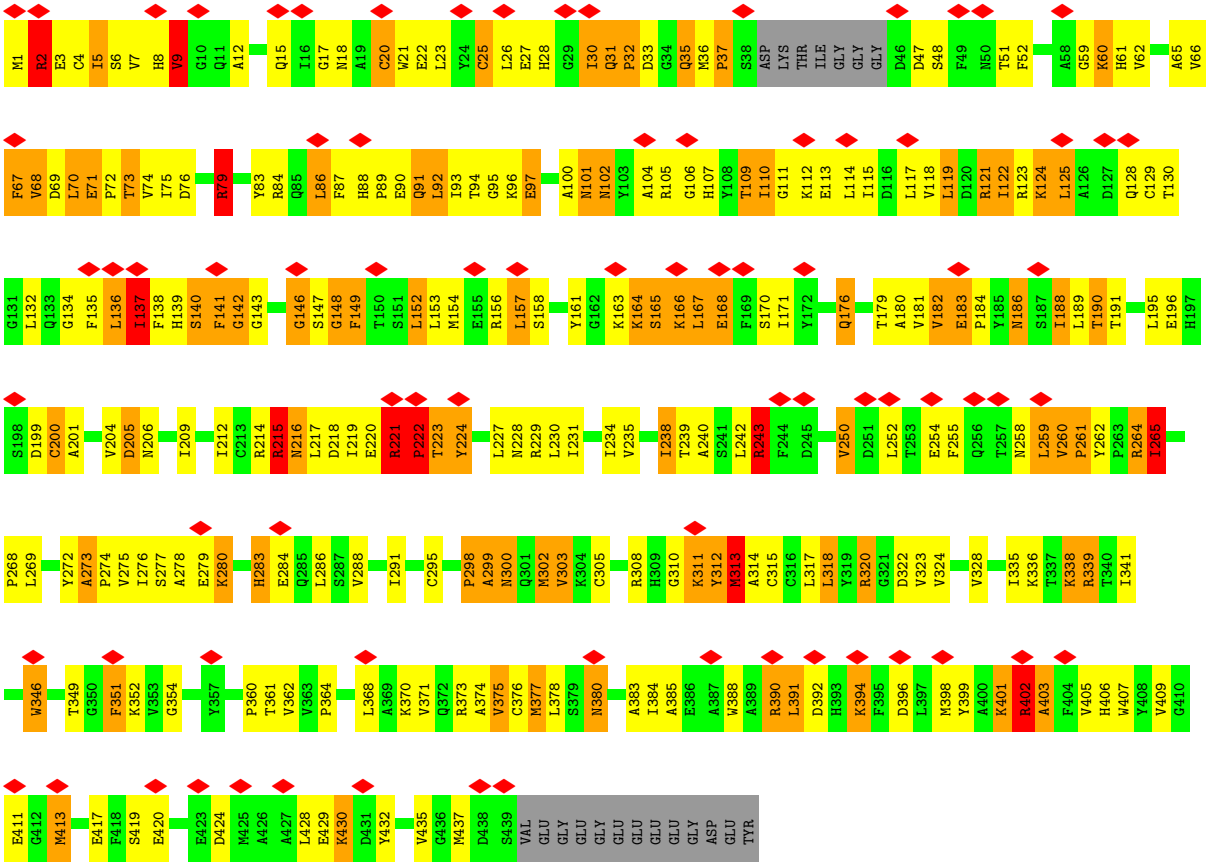






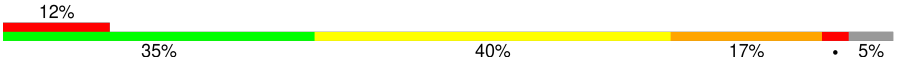
• Molecule 42: Tubulin alpha-1D chain

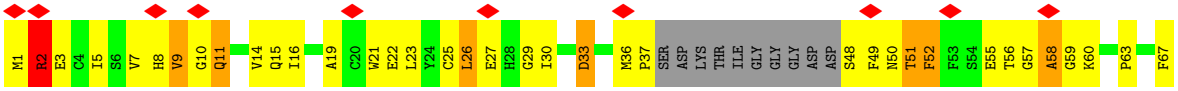
Chain PC:

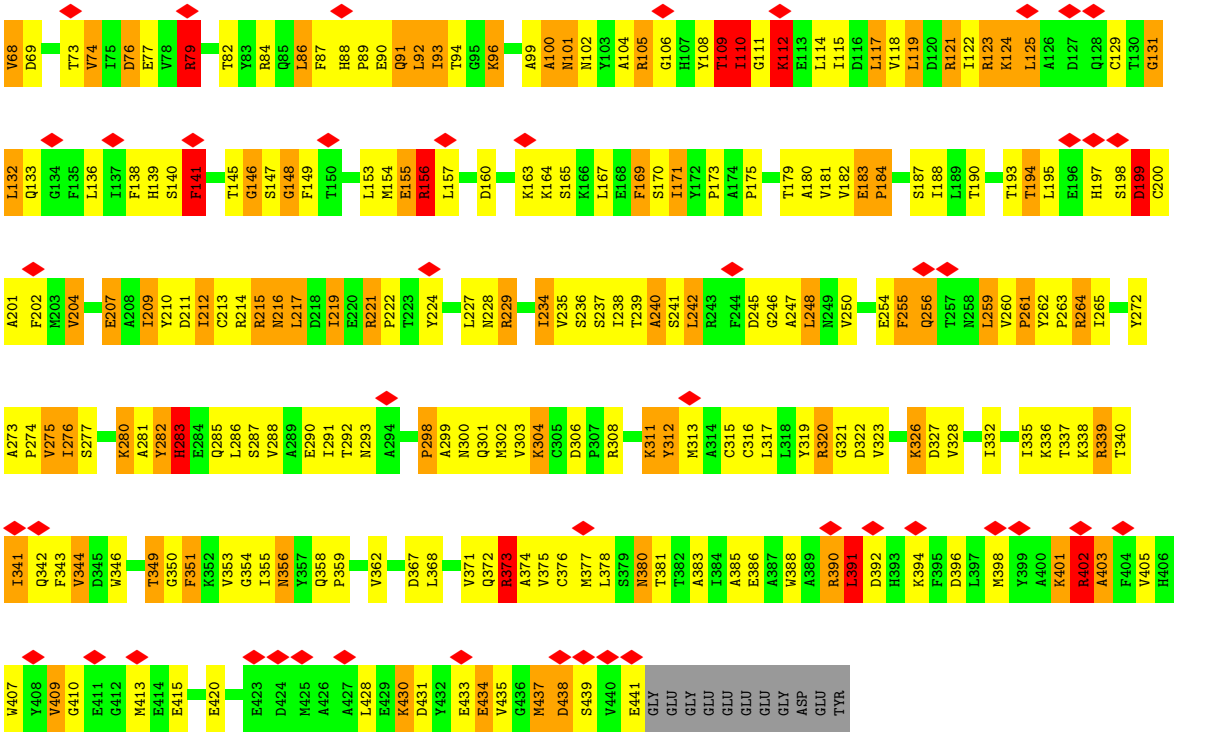


• Molecule 42: Tubulin alpha-1D chain

Chain PE:

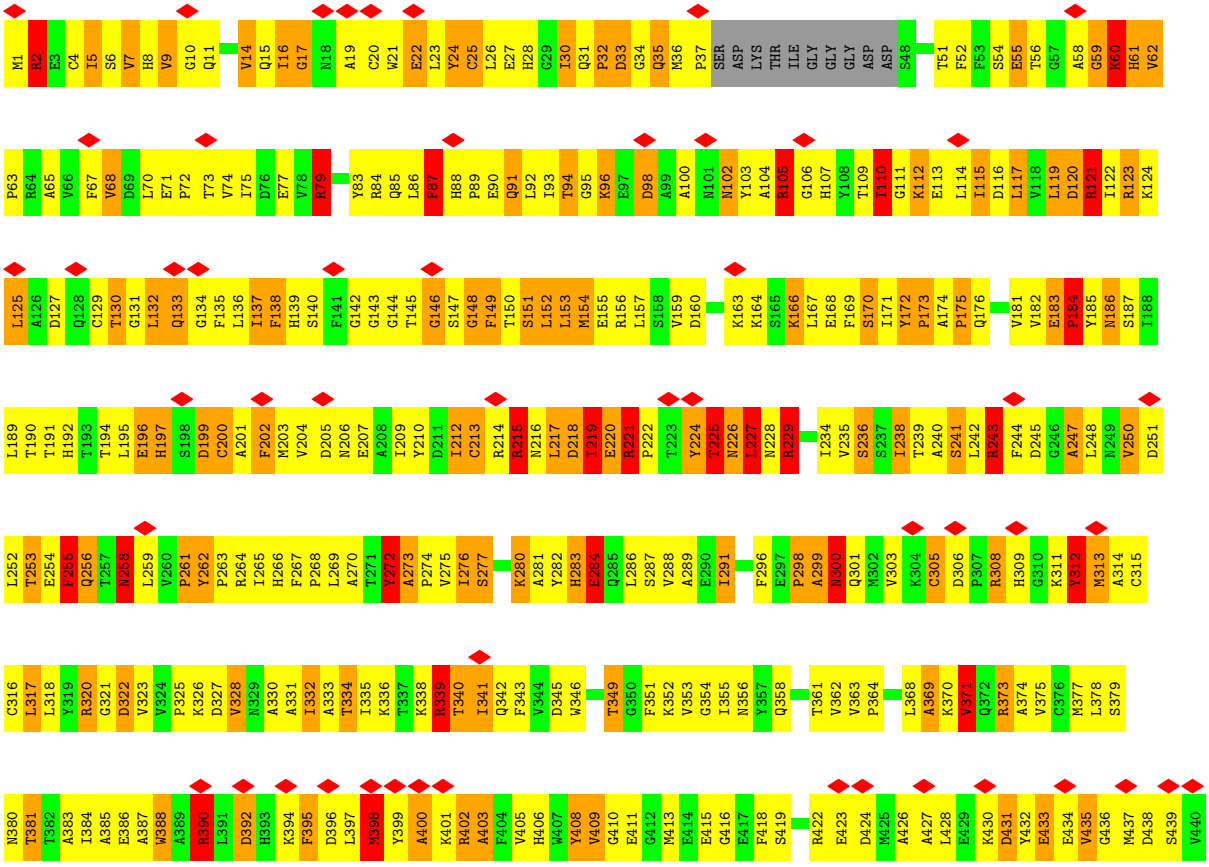






• Molecule 42: Tubulin alpha-1D chain

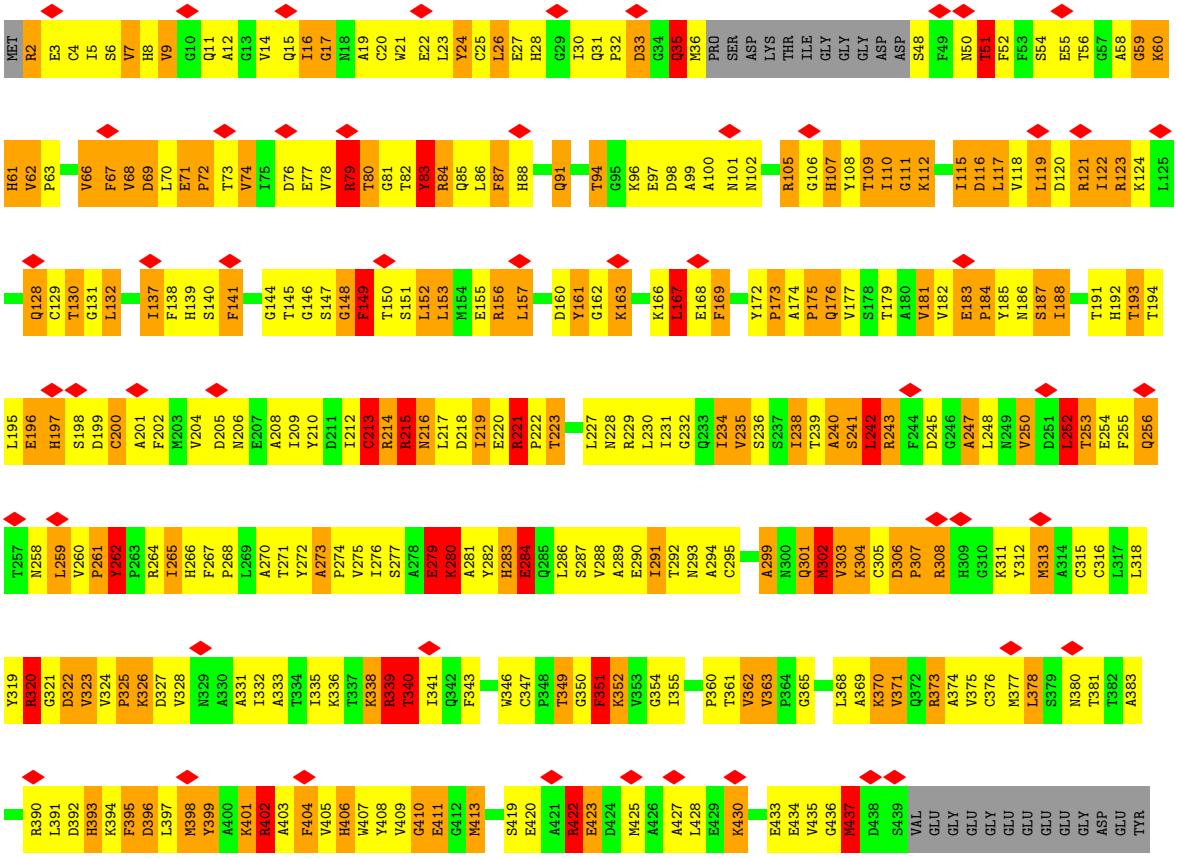
Chain PG:



GLU GLY GLU GLY GLU GLU GLU GLU GLY ASP GLU TYR

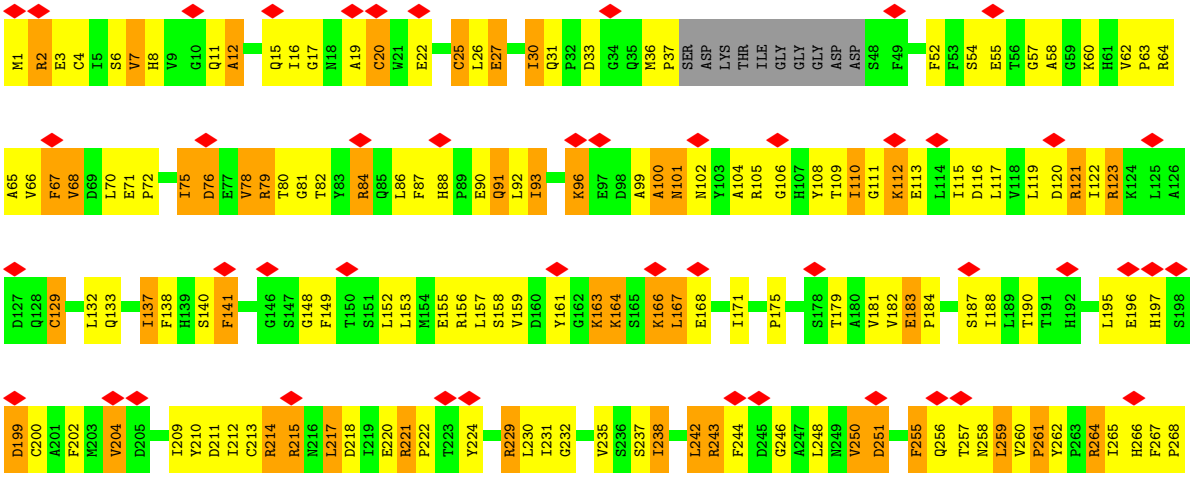
- Molecule 42: Tubulin alpha-1D chain

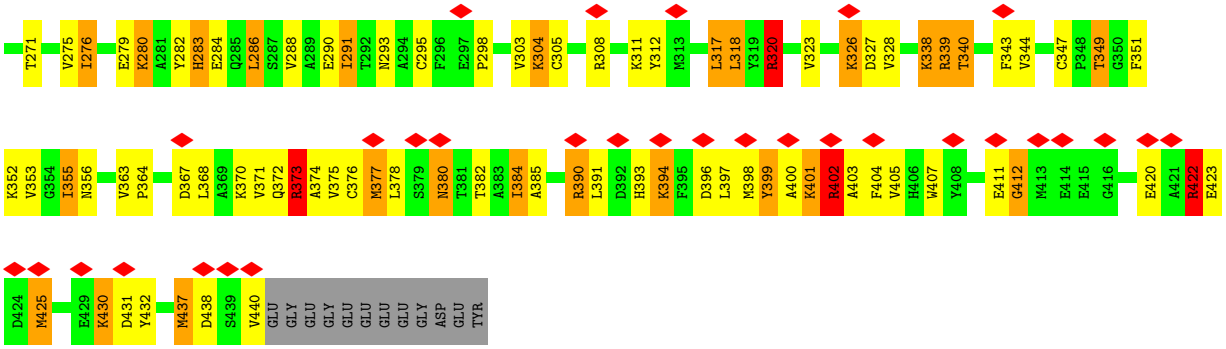
Chain PI:



- Molecule 42: Tubulin alpha-1D chain

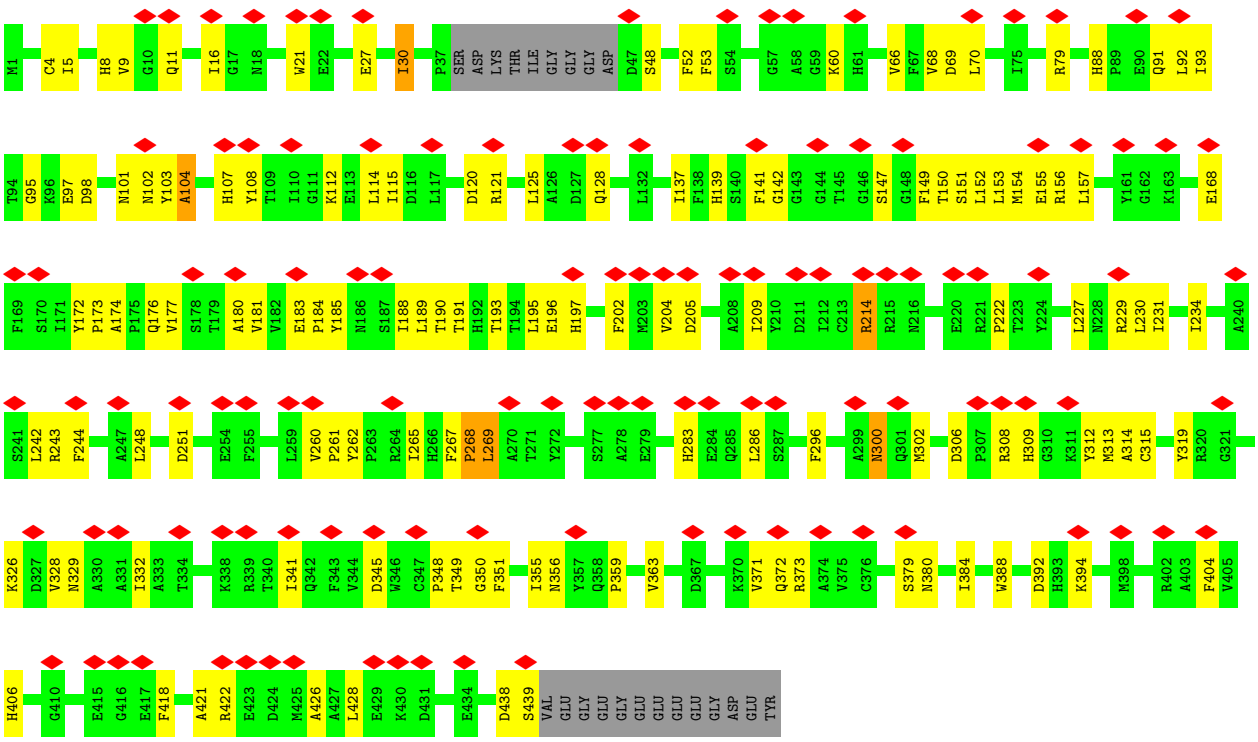
Chain PK:





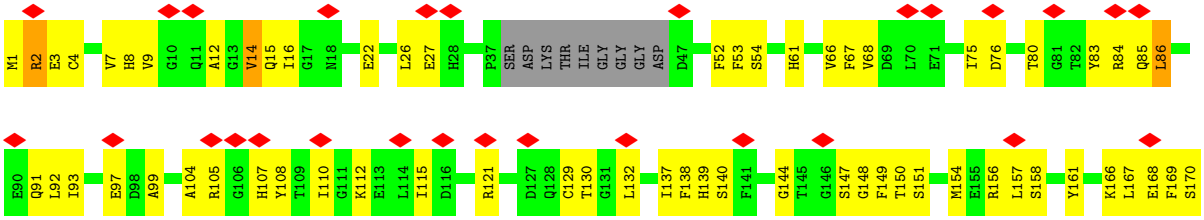
- Molecule 42: Tubulin alpha-1D chain

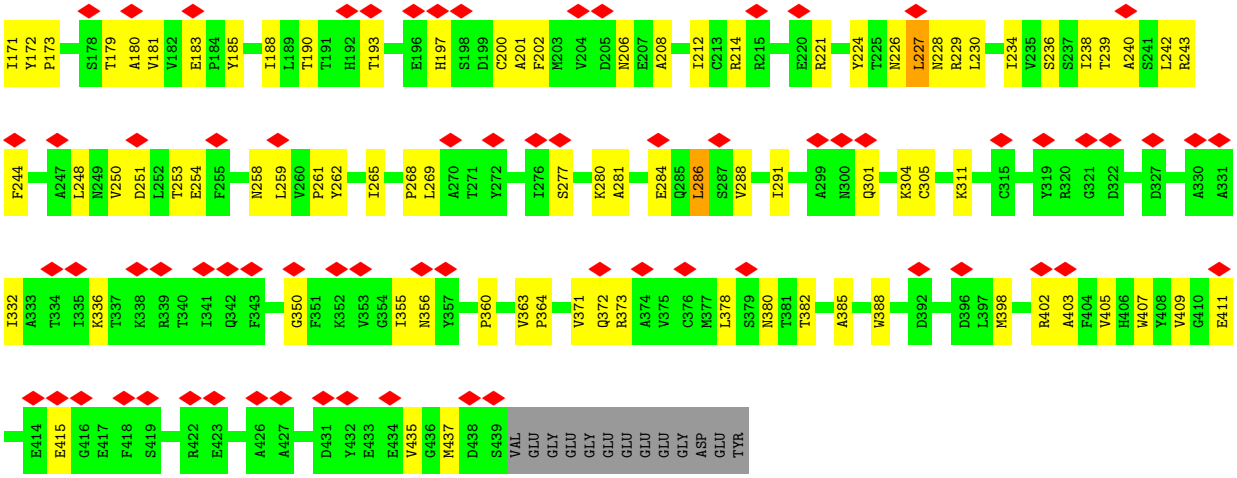
Chain QC:



- Molecule 42: Tubulin alpha-1D chain

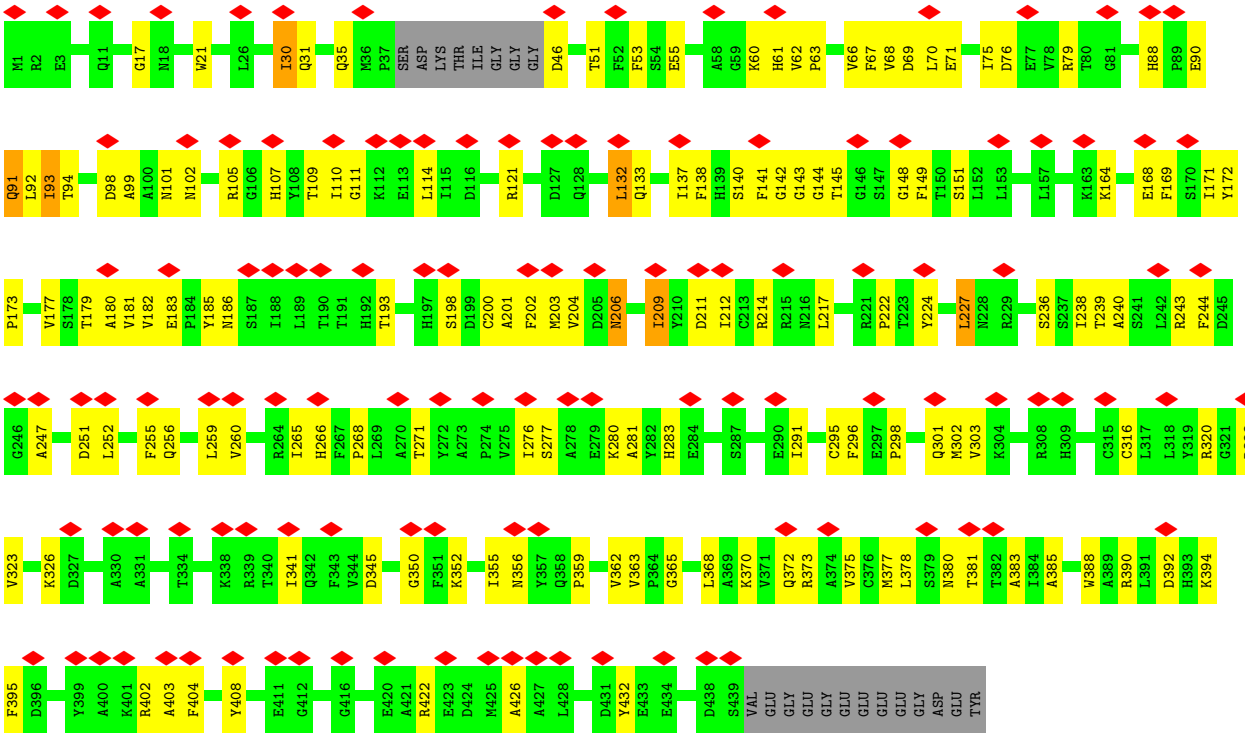
Chain QE:





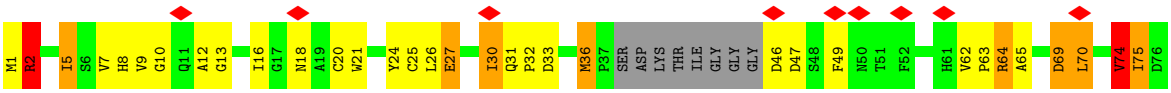
- Molecule 42: Tubulin alpha-1D chain

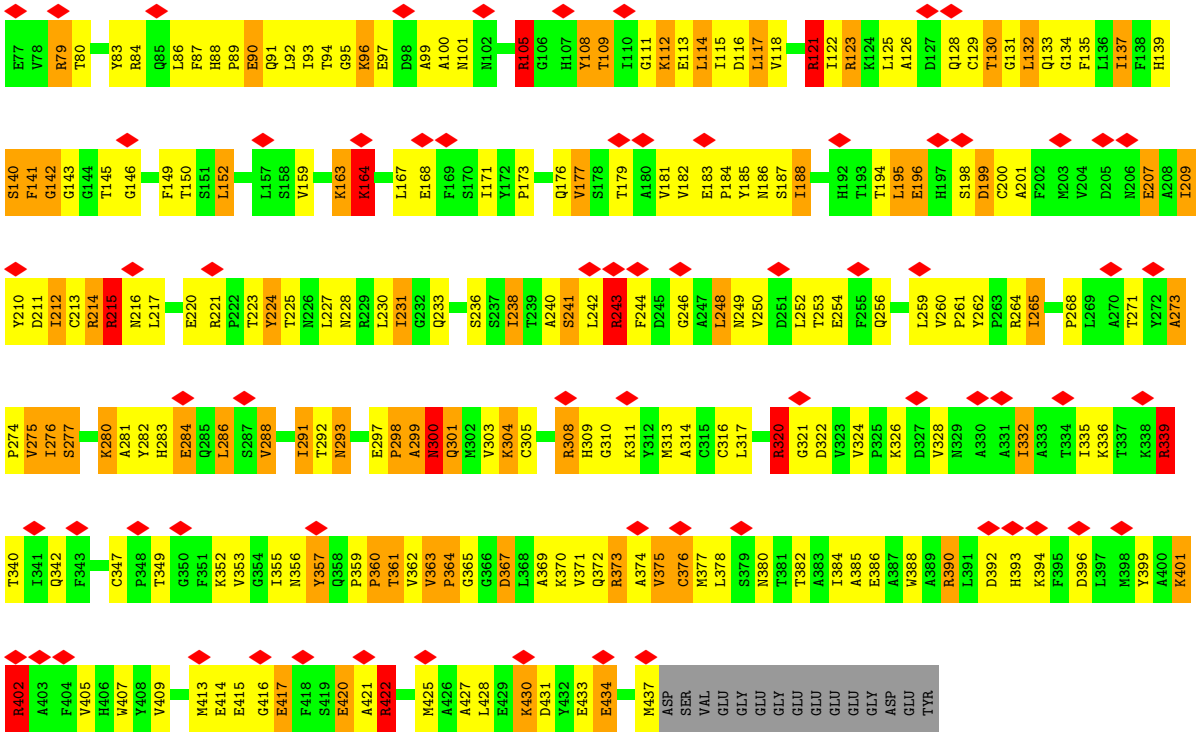
Chain QG:



- Molecule 42: Tubulin alpha-1D chain

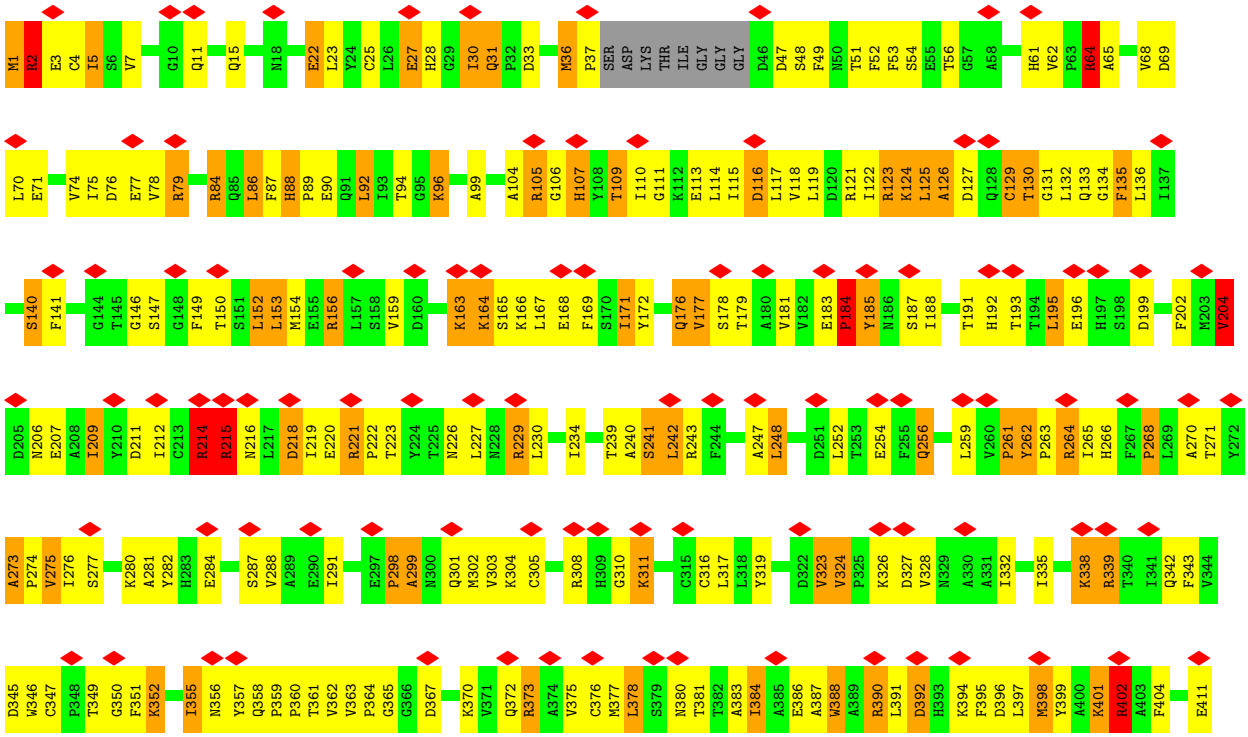
Chain QI:

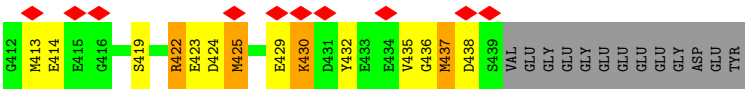




- Molecule 42: Tubulin alpha-1D chain

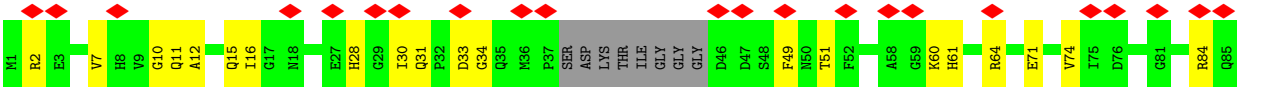
Chain QK:

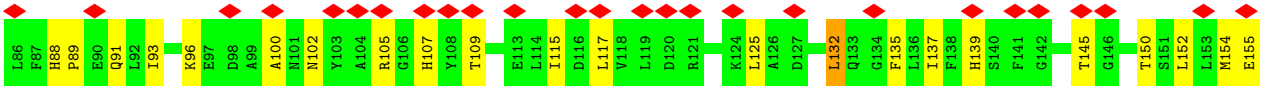


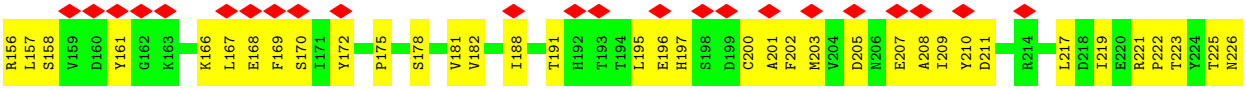


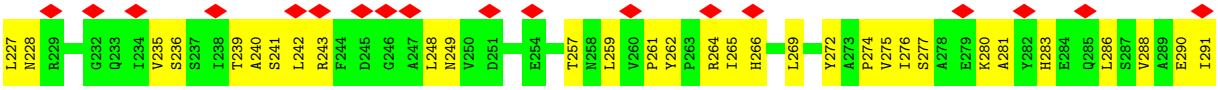
• Molecule 42: Tubulin alpha-1D chain

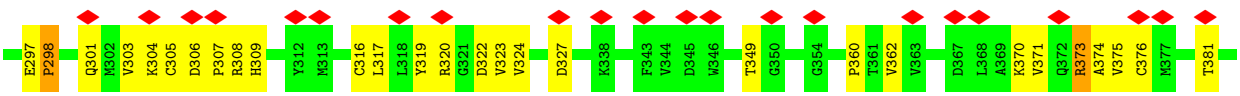
Chain RC:

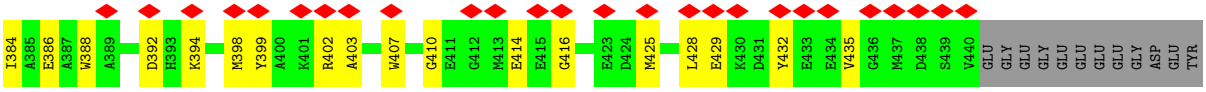






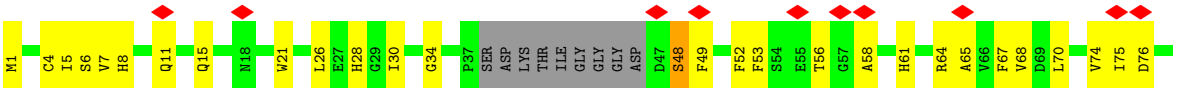


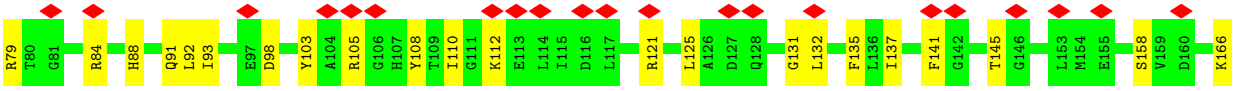


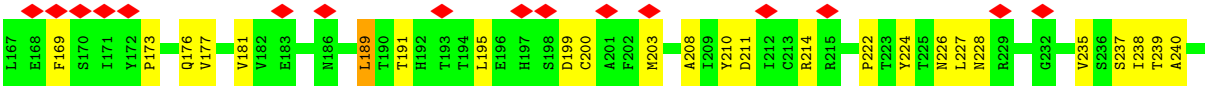


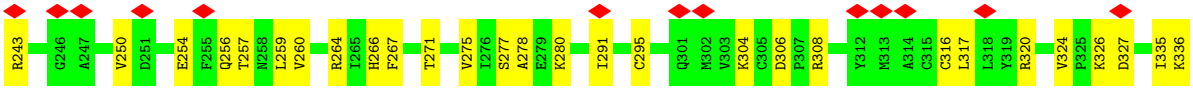
• Molecule 42: Tubulin alpha-1D chain

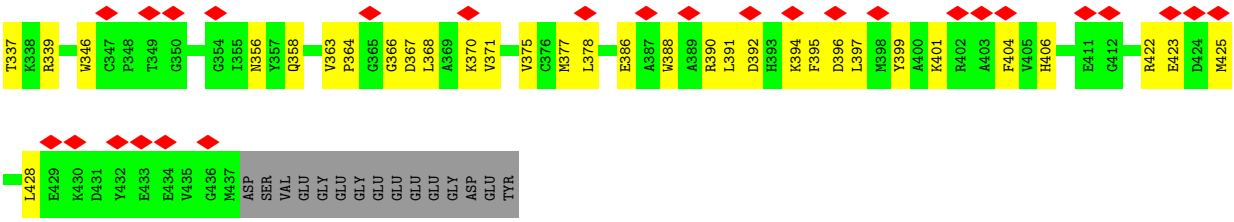
Chain RE:





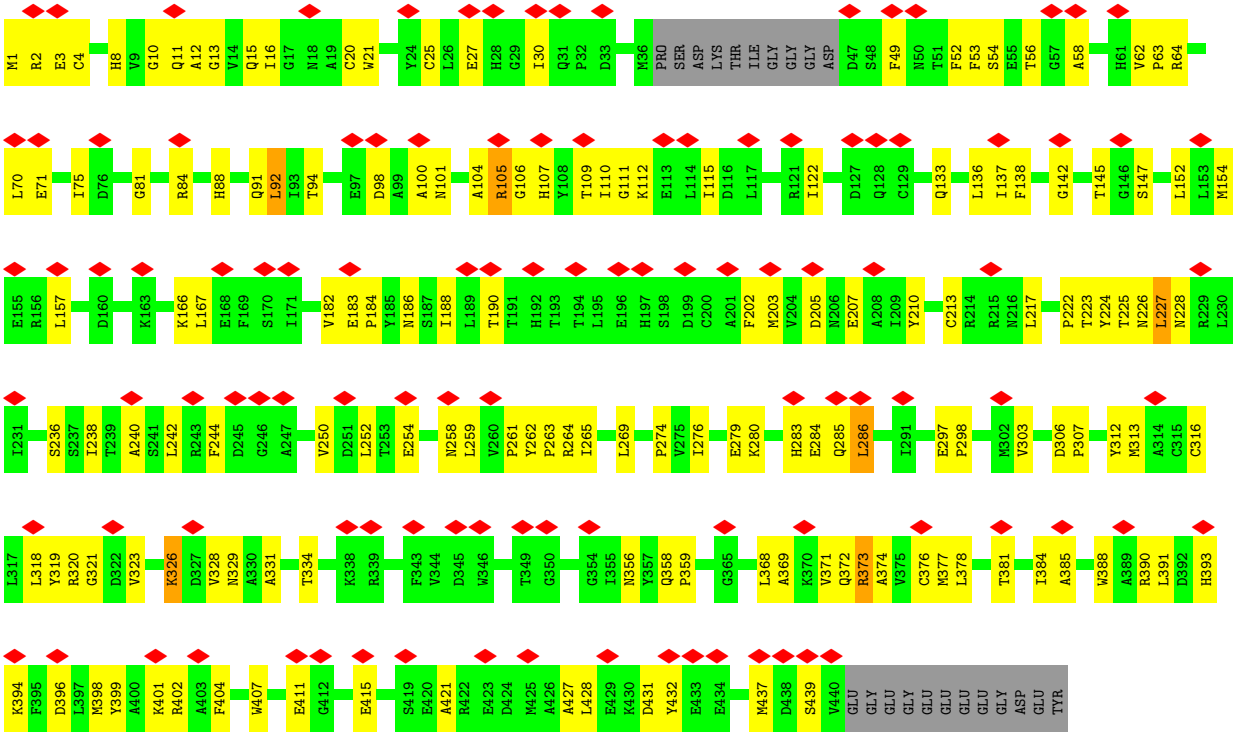






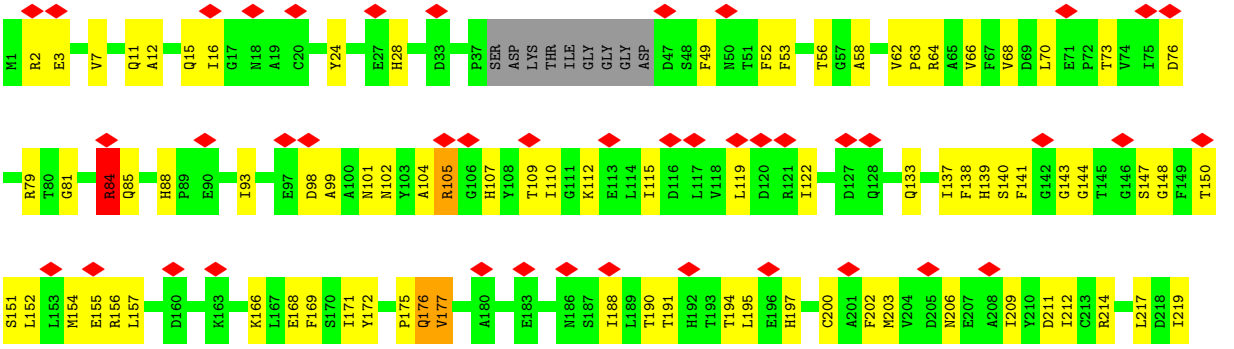
- Molecule 42: Tubulin alpha-1D chain

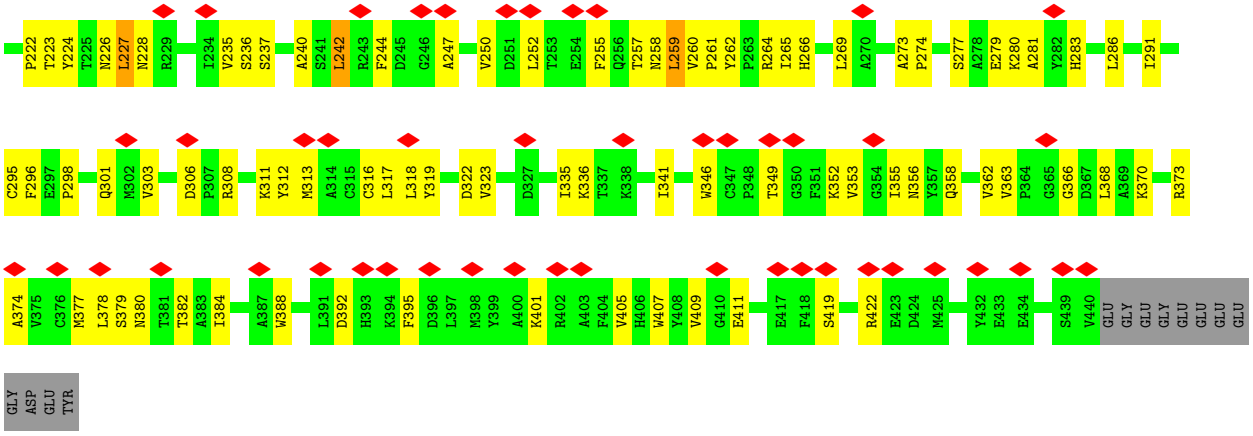
Chain RG:



- Molecule 42: Tubulin alpha-1D chain

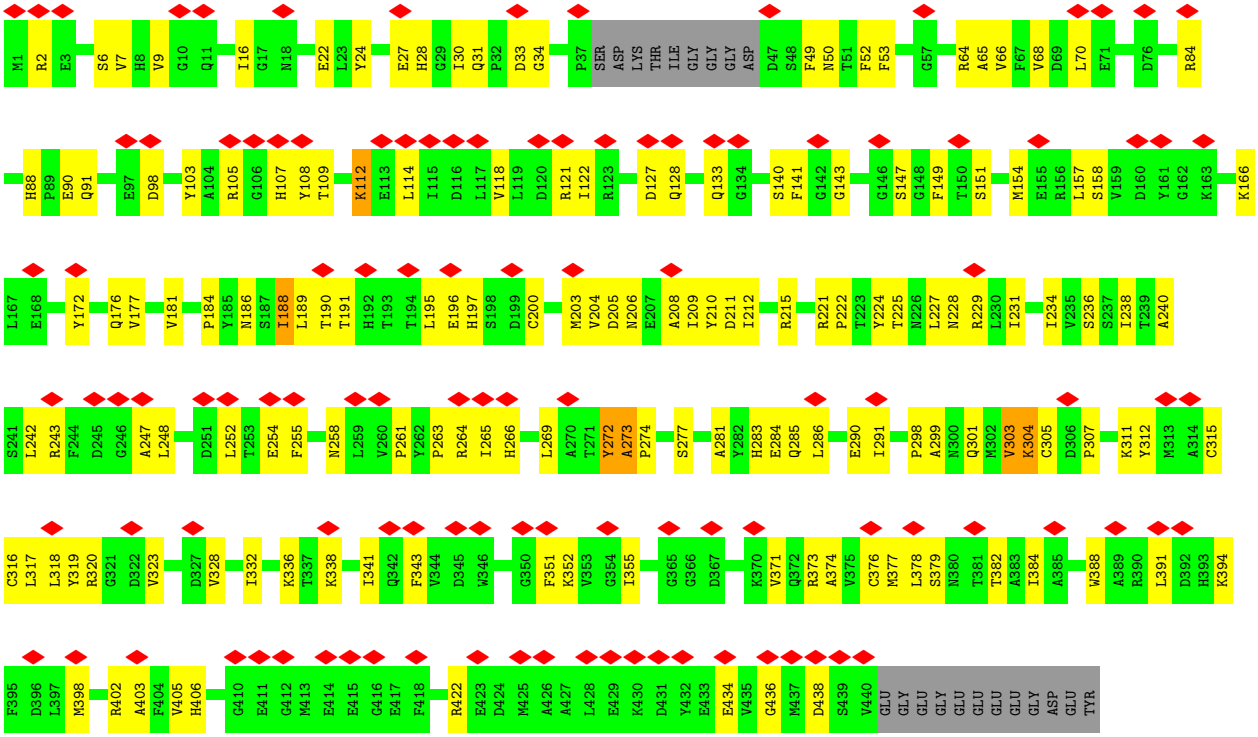
Chain RI:





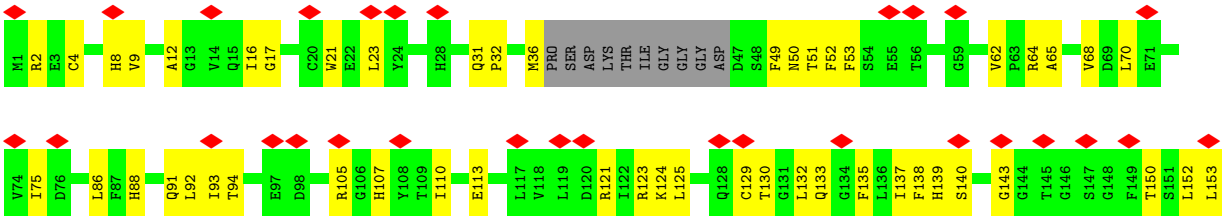
- Molecule 42: Tubulin alpha-1D chain

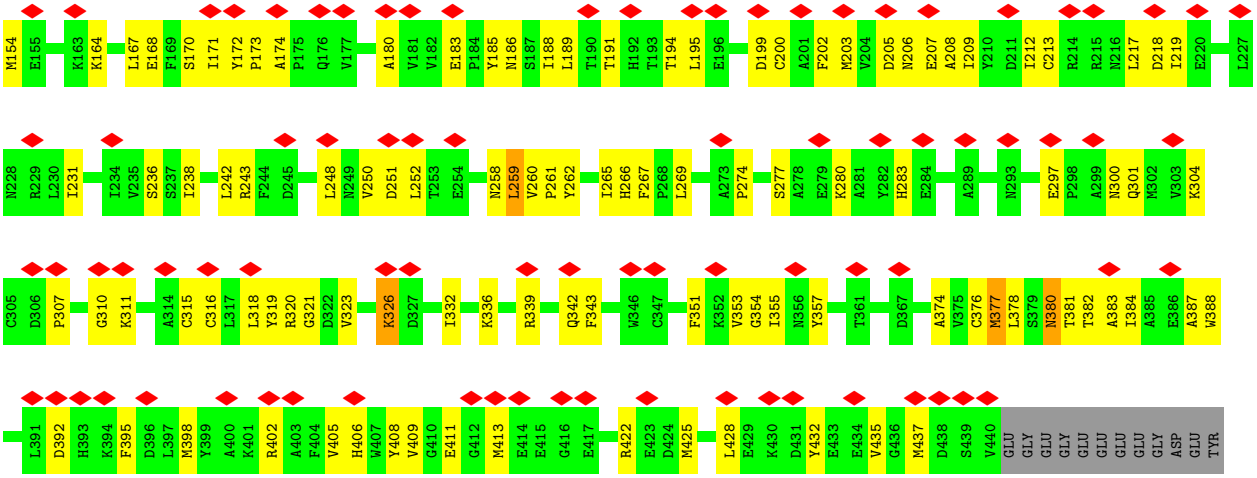
Chain RK:



- Molecule 42: Tubulin alpha-1D chain

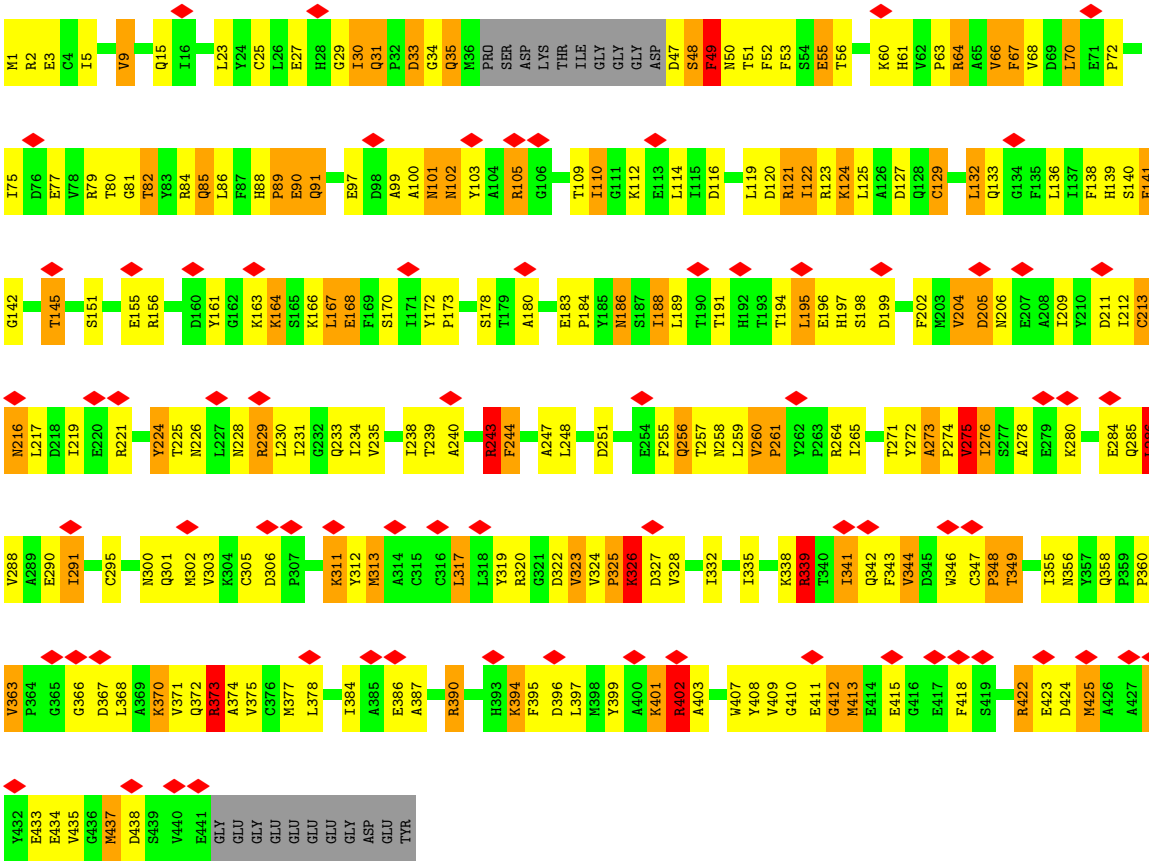
Chain SC:





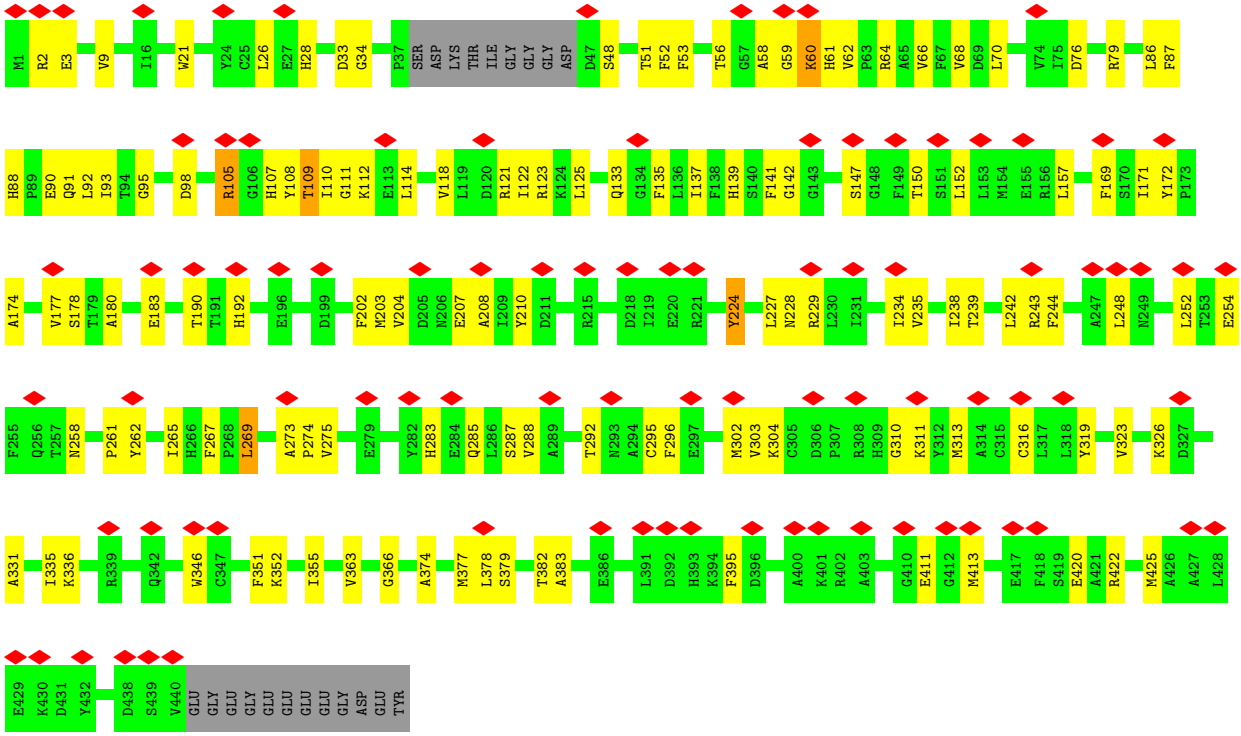
- Molecule 42: Tubulin alpha-1D chain

Chain SE:



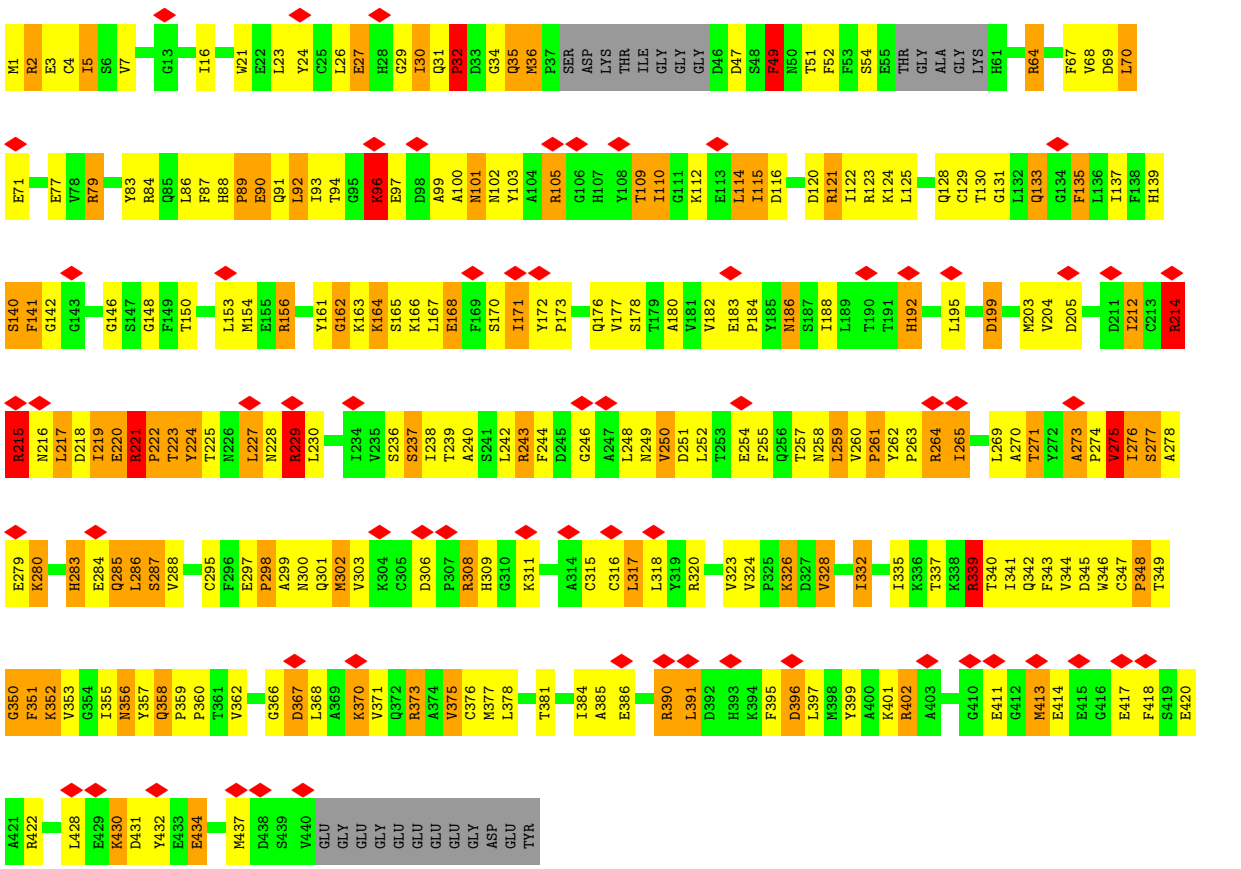
- Molecule 42: Tubulin alpha-1D chain

Chain SG:



- Molecule 42: Tubulin alpha-1D chain

Chain SI: 14% 40% 35% 17% 6%



- Molecule 42: Tubulin alpha-1D chain

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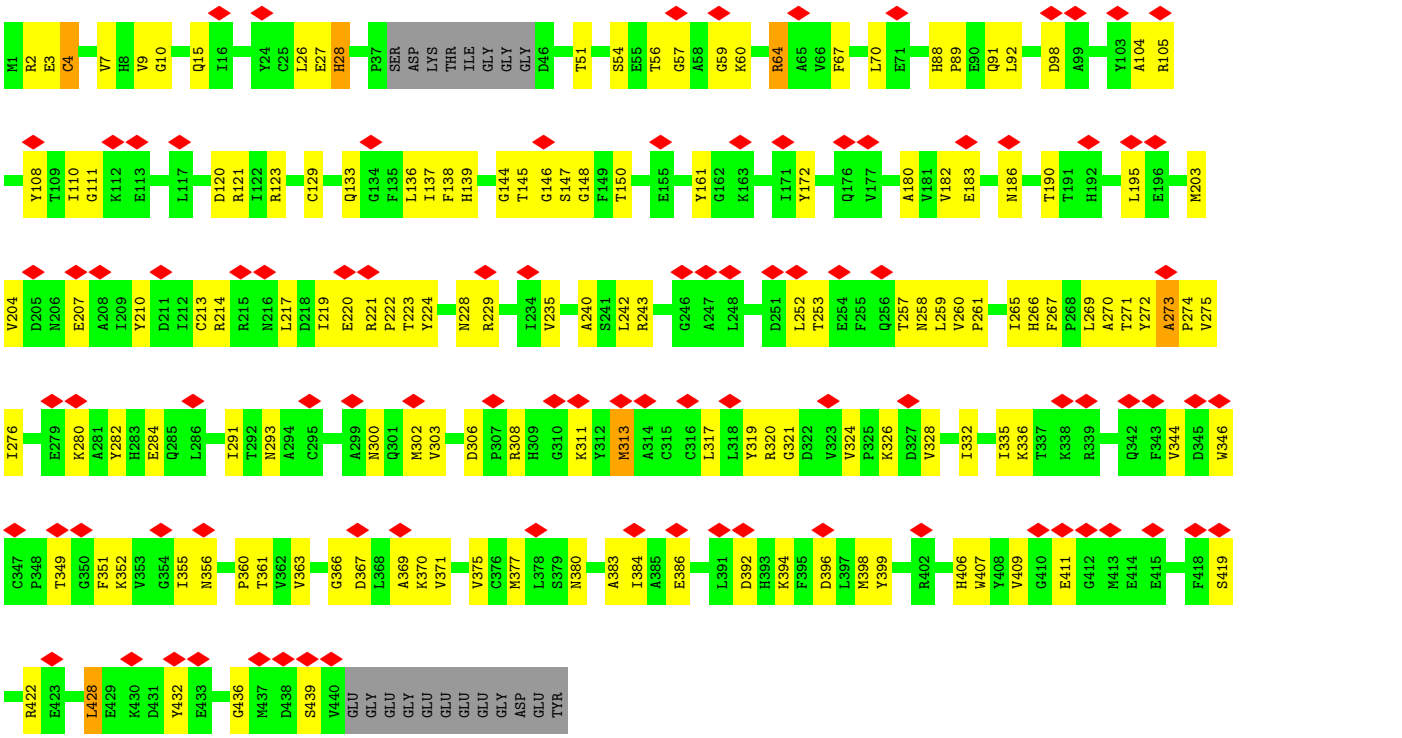
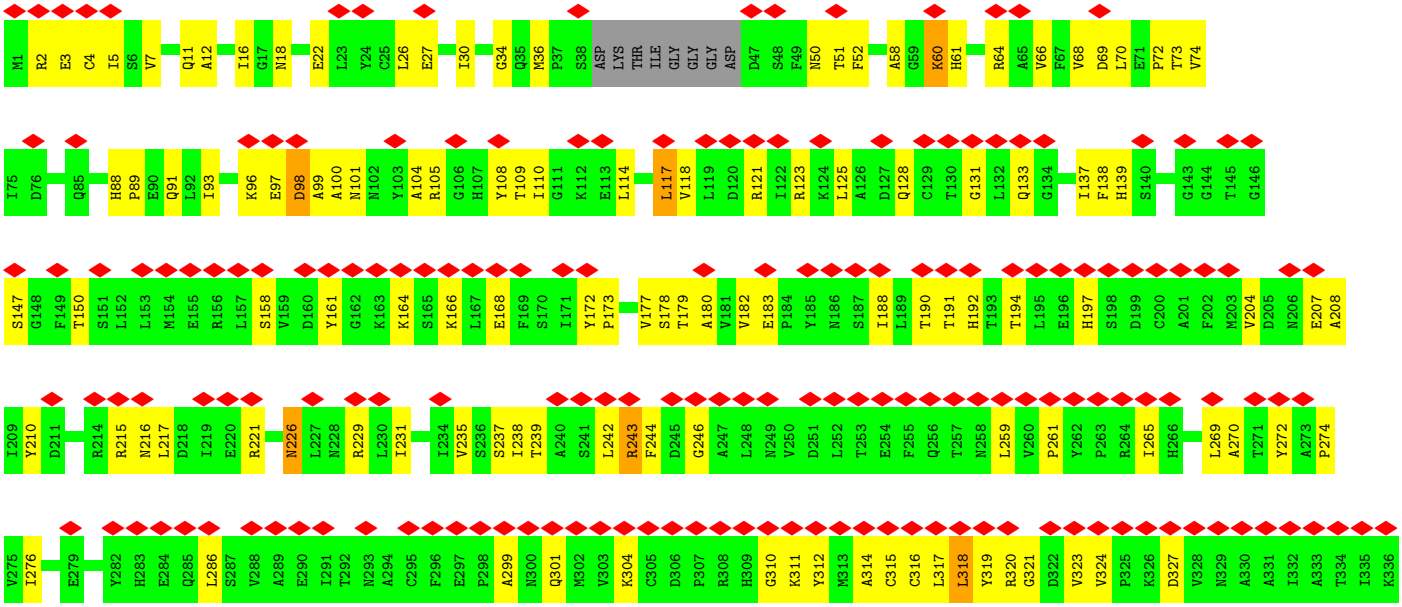
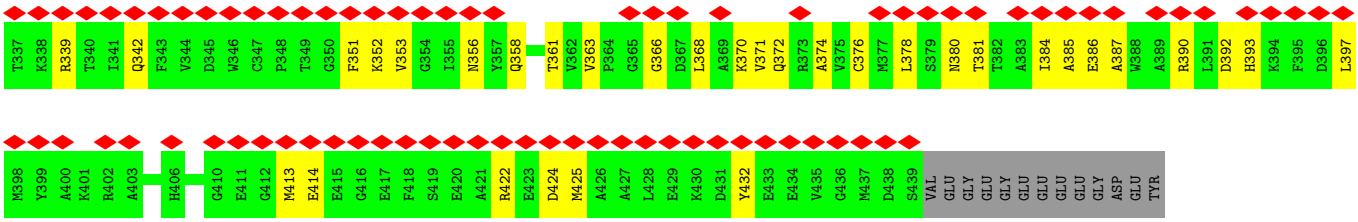


- Molecule 42: Tubulin alpha-1D chain

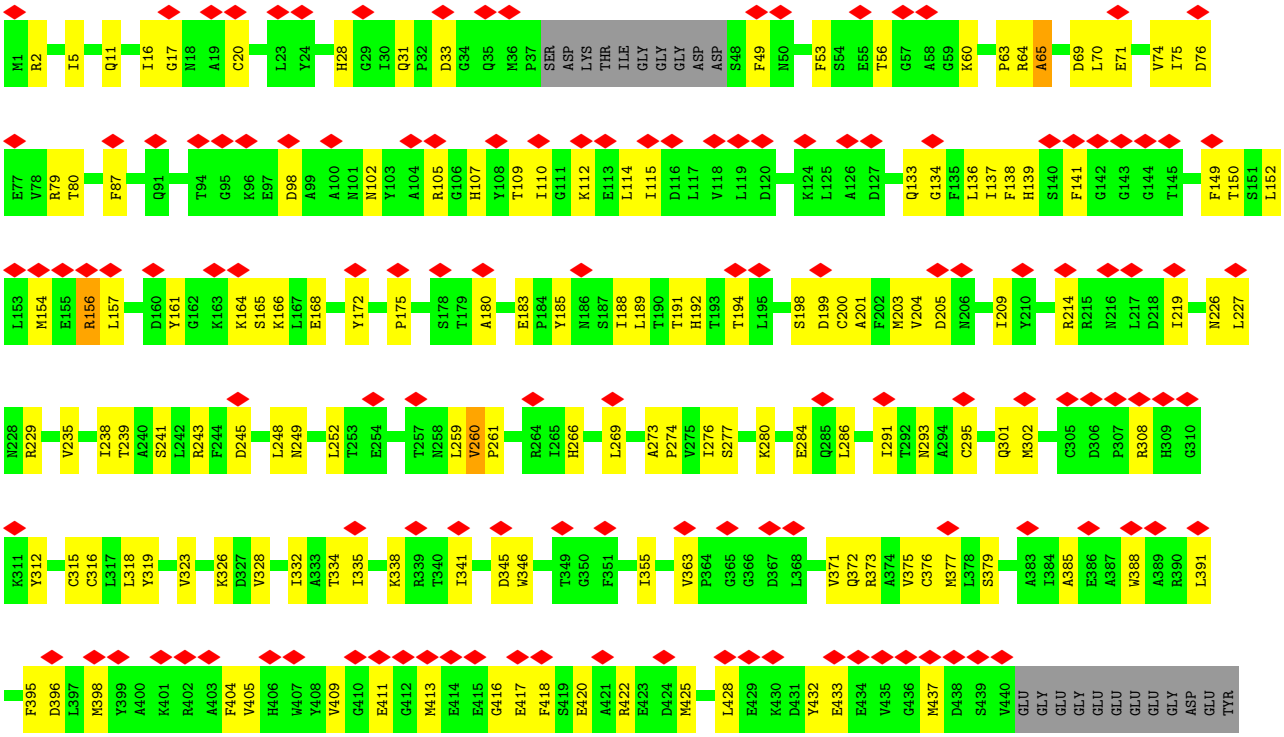
Chain SM:





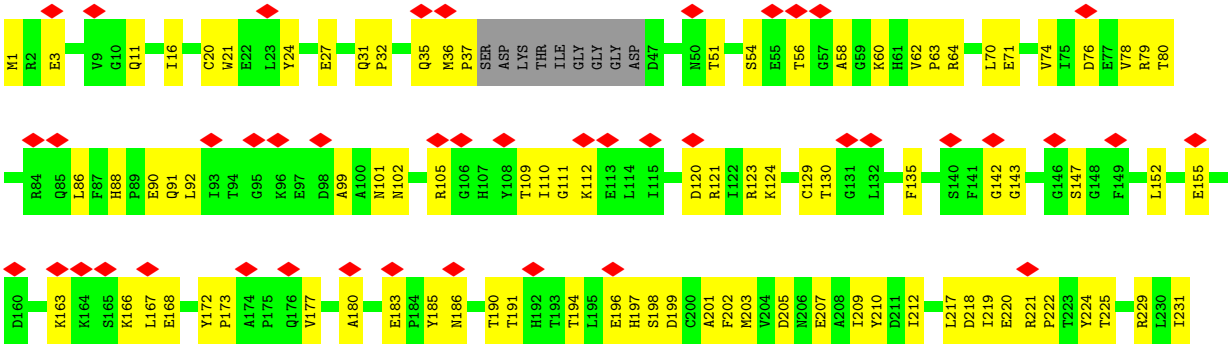
- Molecule 42: Tubulin alpha-1D chain

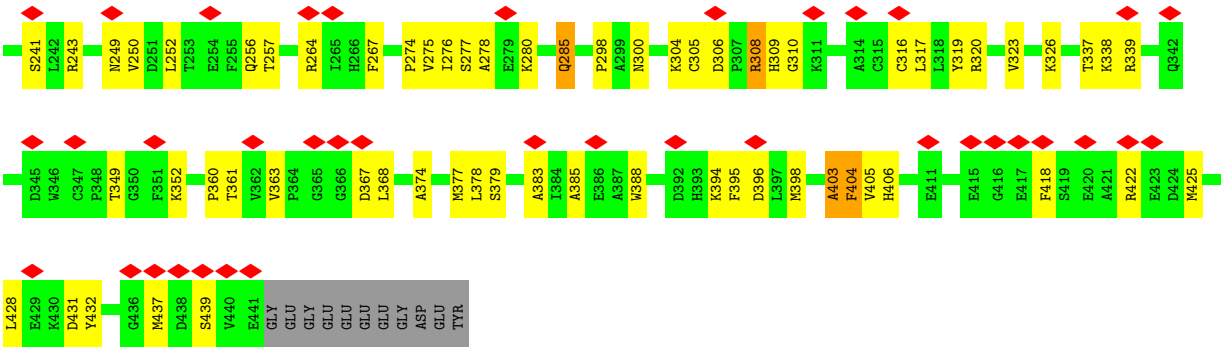
Chain TC:



- Molecule 42: Tubulin alpha-1D chain

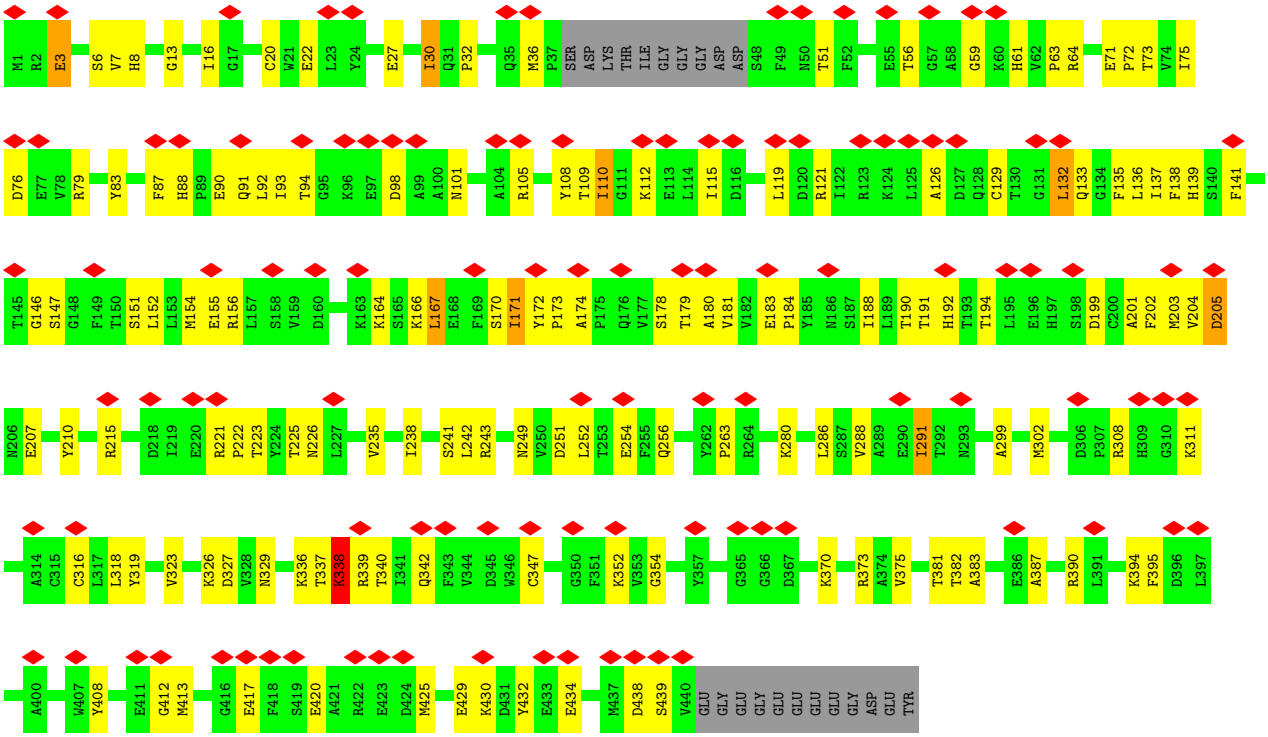
Chain TE:





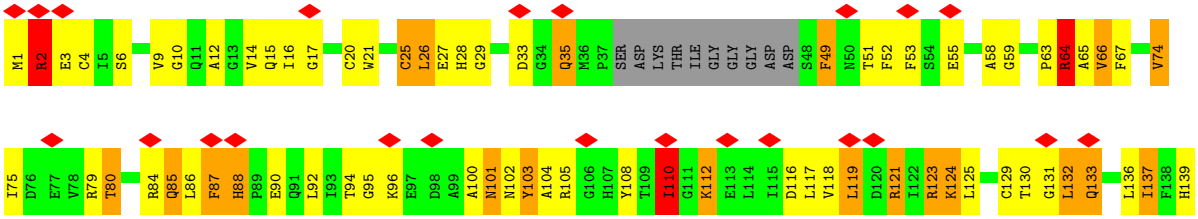
- Molecule 42: Tubulin alpha-1D chain

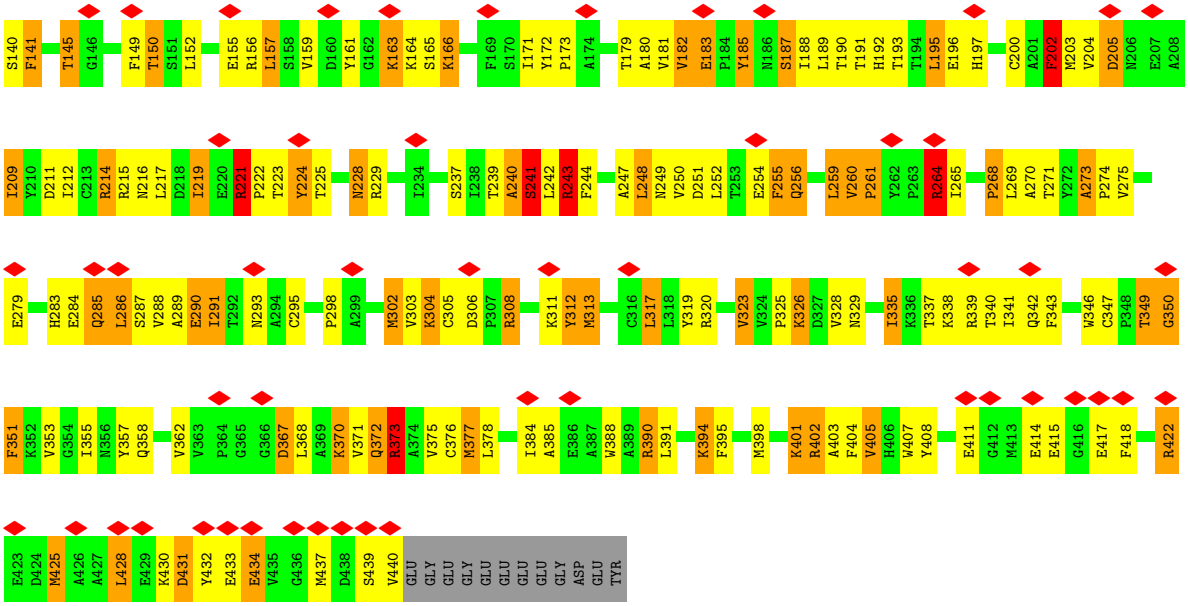
Chain TG:



- Molecule 42: Tubulin alpha-1D chain

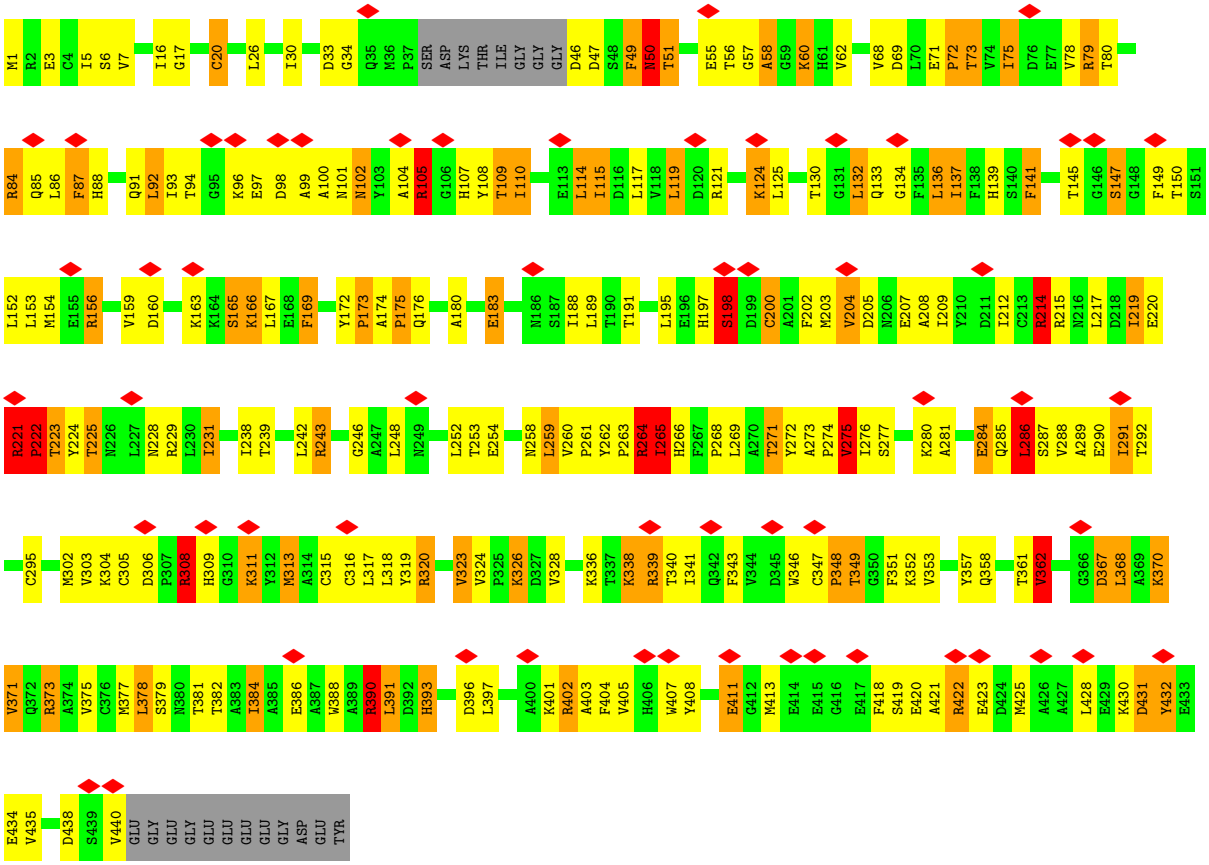
Chain TI:





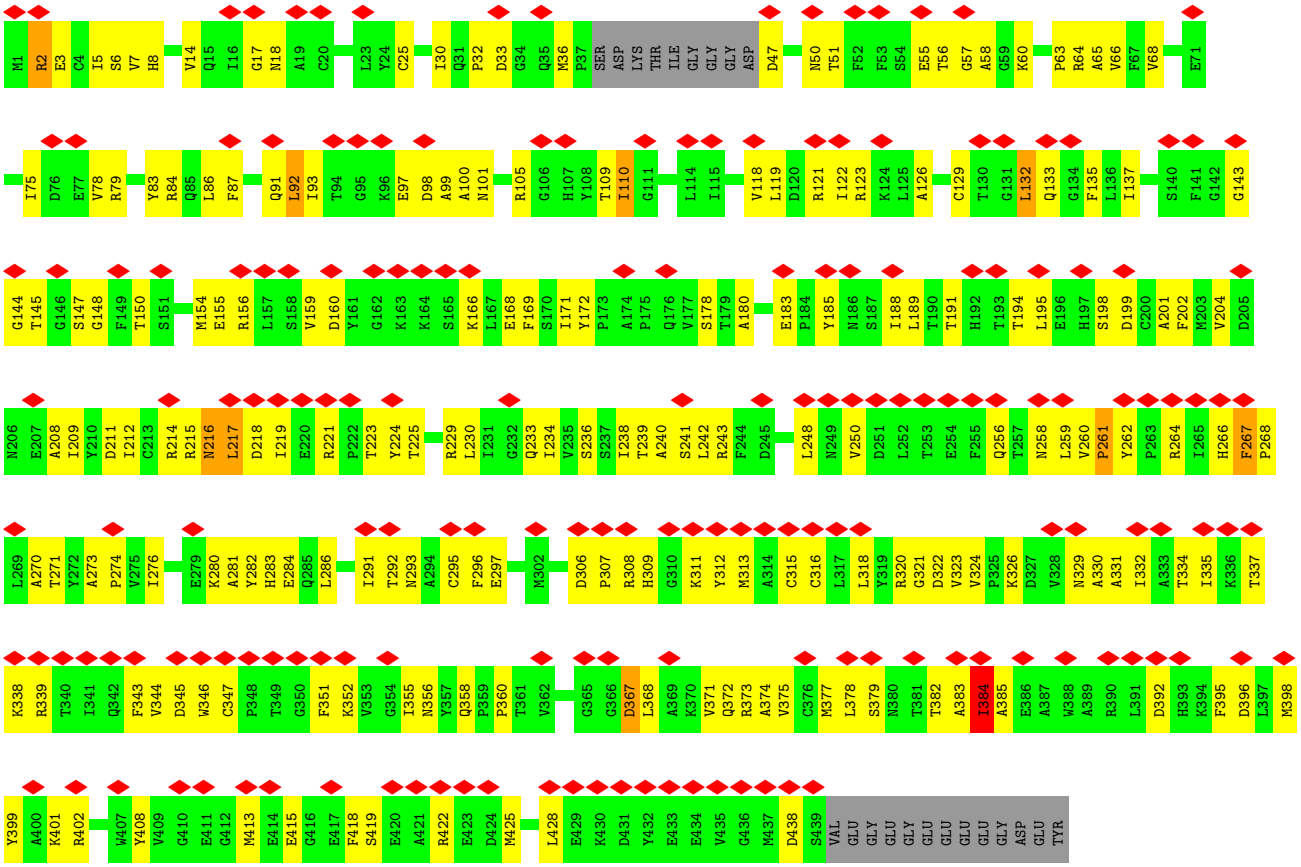
- Molecule 42: Tubulin alpha-1D chain

Chain TK:



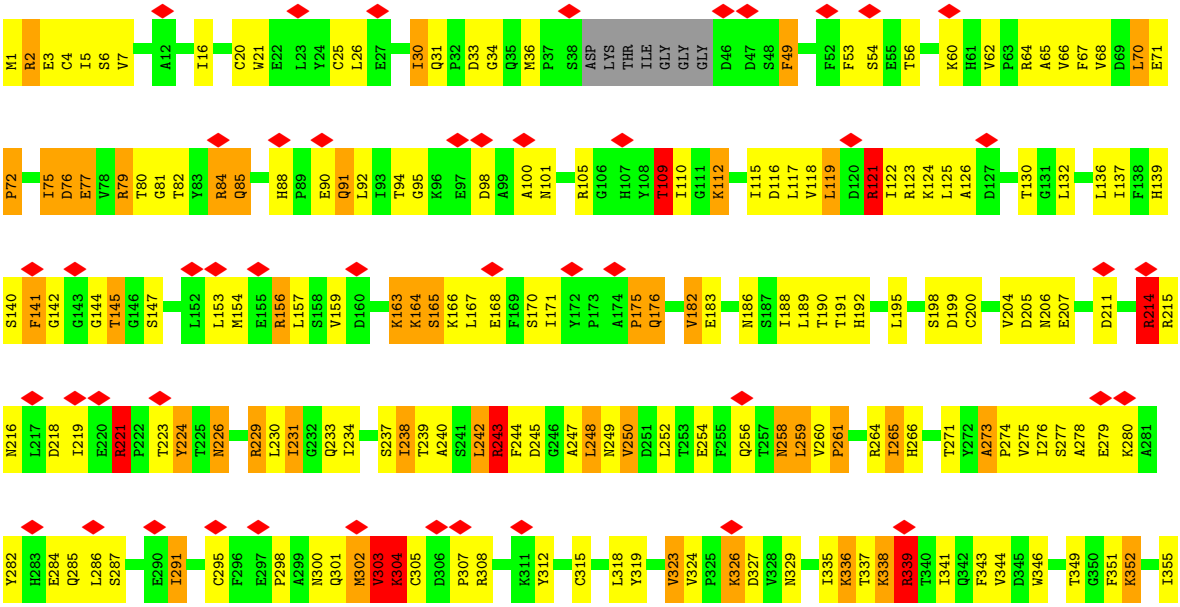
- Molecule 42: Tubulin alpha-1D chain

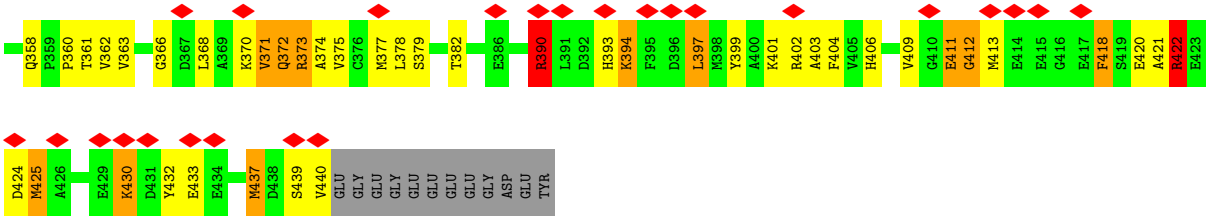
Chain TM:



- Molecule 42: Tubulin alpha-1D chain

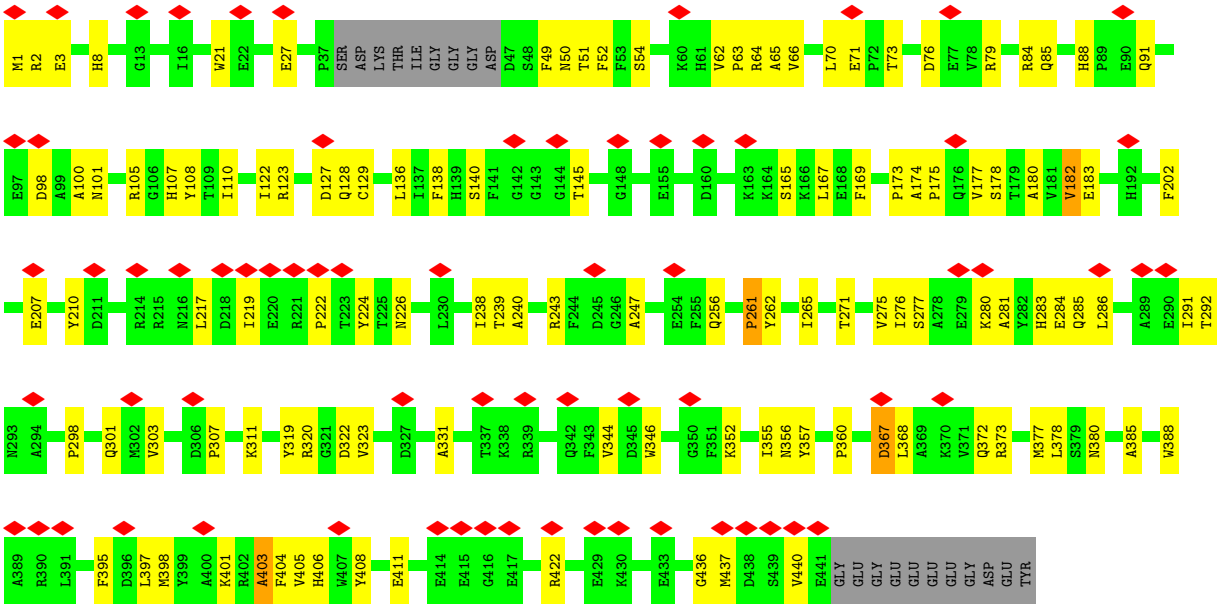
Chain UC:





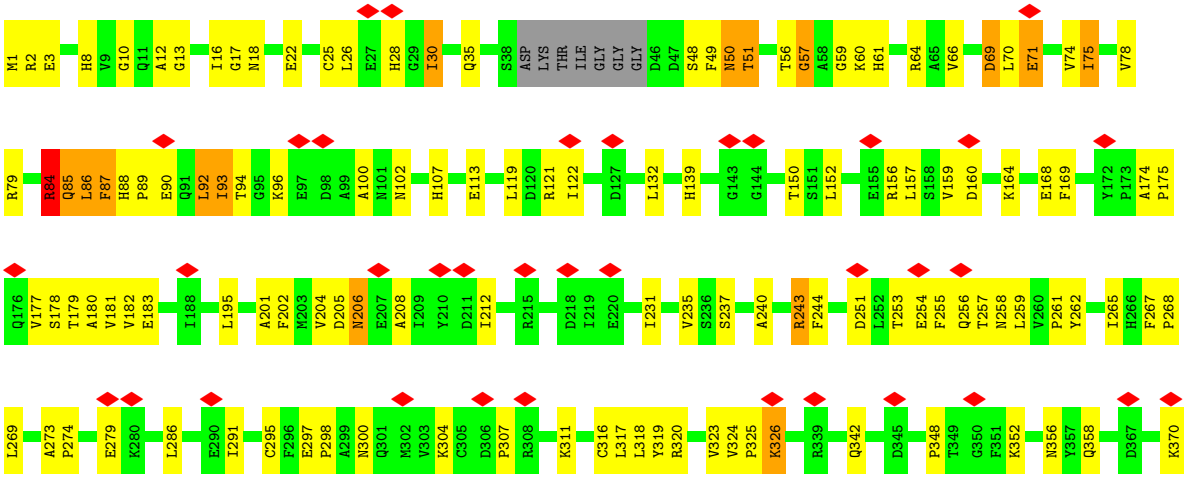
• Molecule 42: Tubulin alpha-1D chain

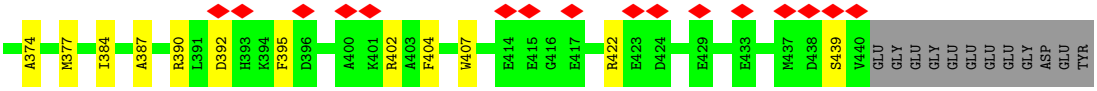
Chain UE:



• Molecule 42: Tubulin alpha-1D chain

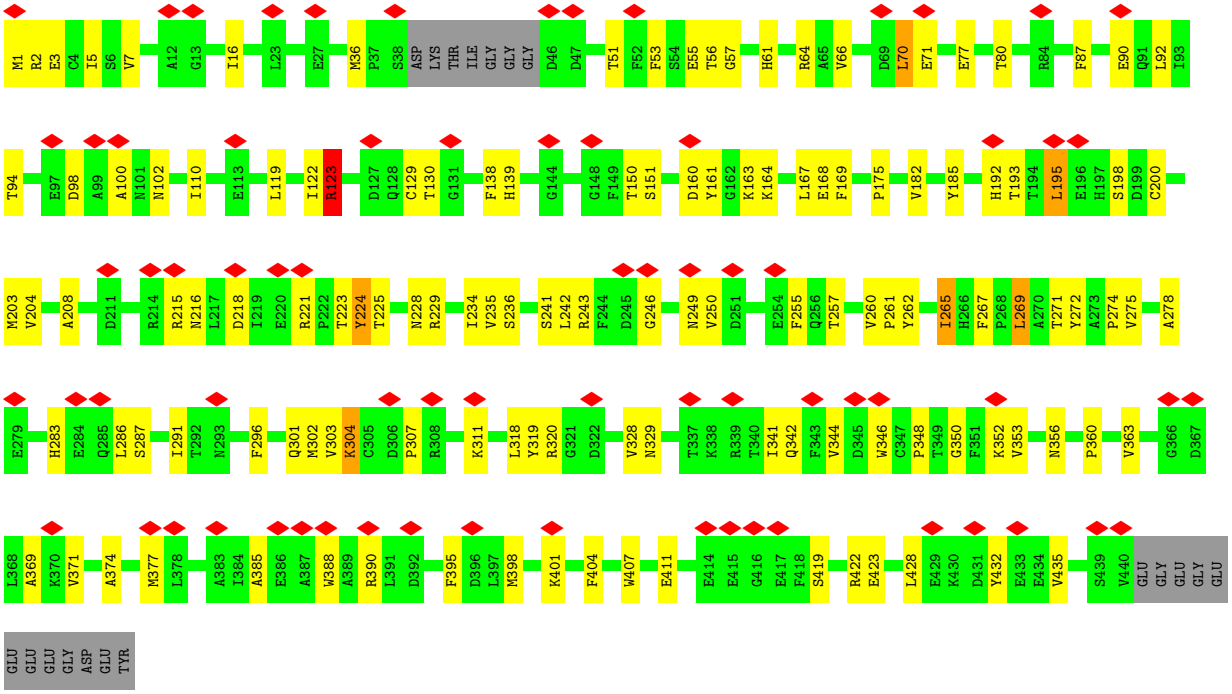
Chain UG:





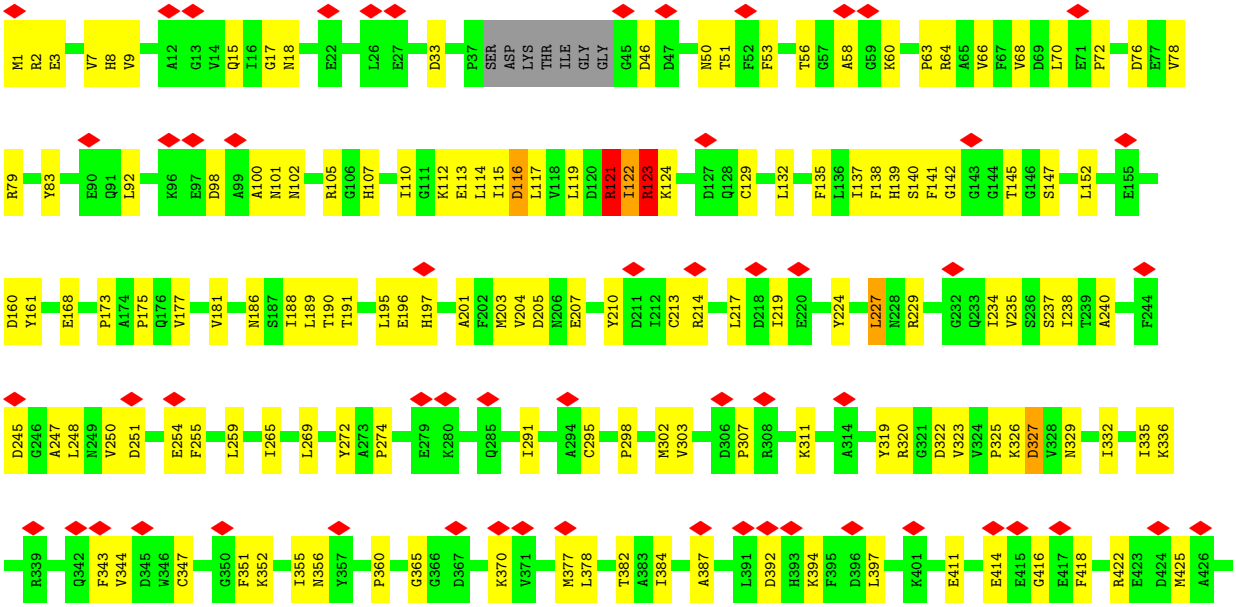
- Molecule 42: Tubulin alpha-1D chain

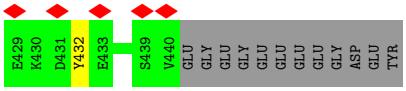
Chain UI:



- Molecule 42: Tubulin alpha-1D chain

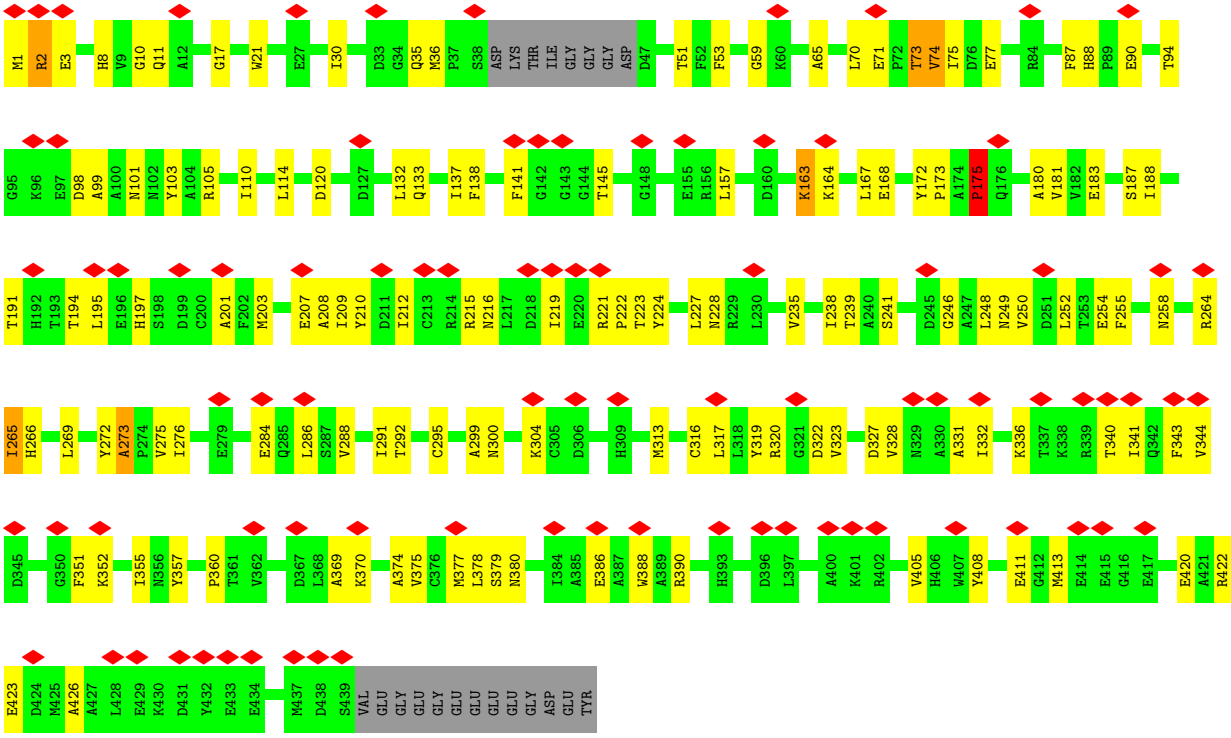
Chain UK:





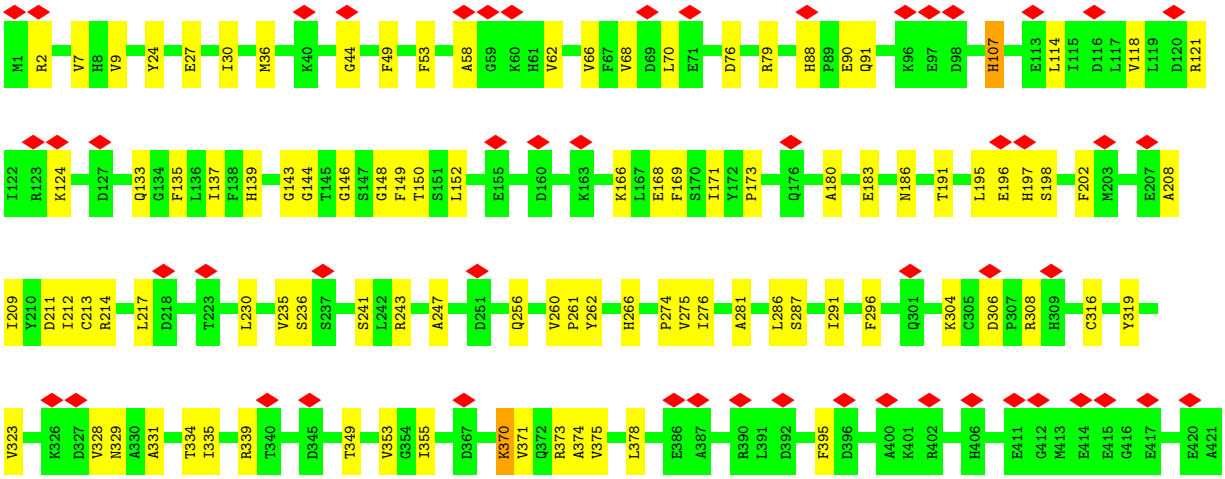
• Molecule 42: Tubulin alpha-1D chain

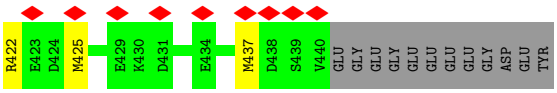
Chain UM:



• Molecule 42: Tubulin alpha-1D chain

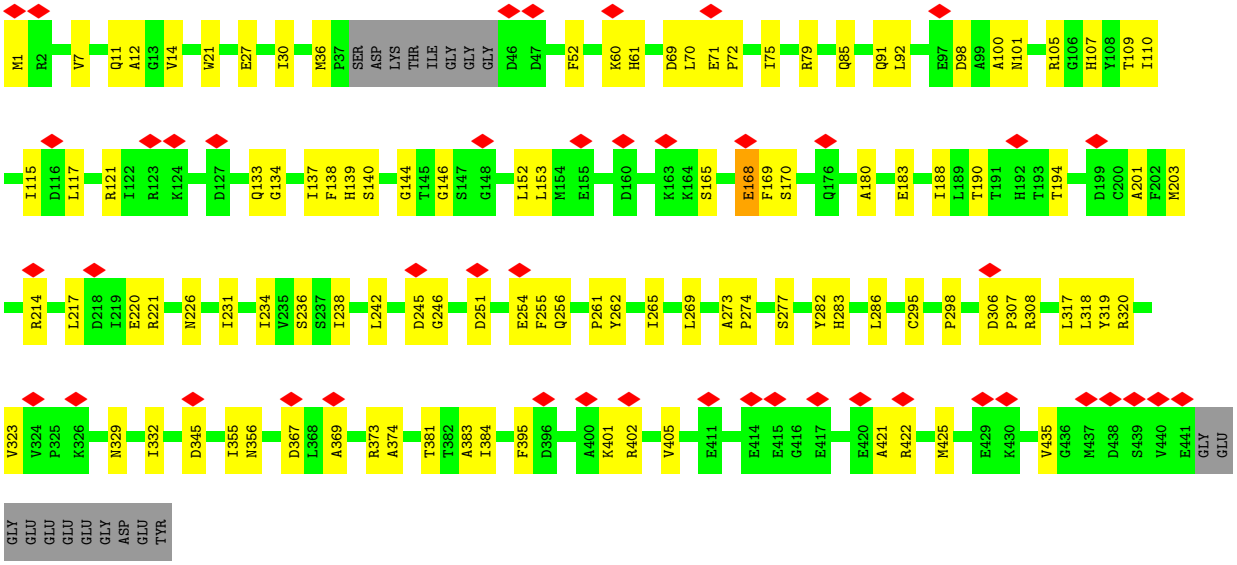
Chain VC:





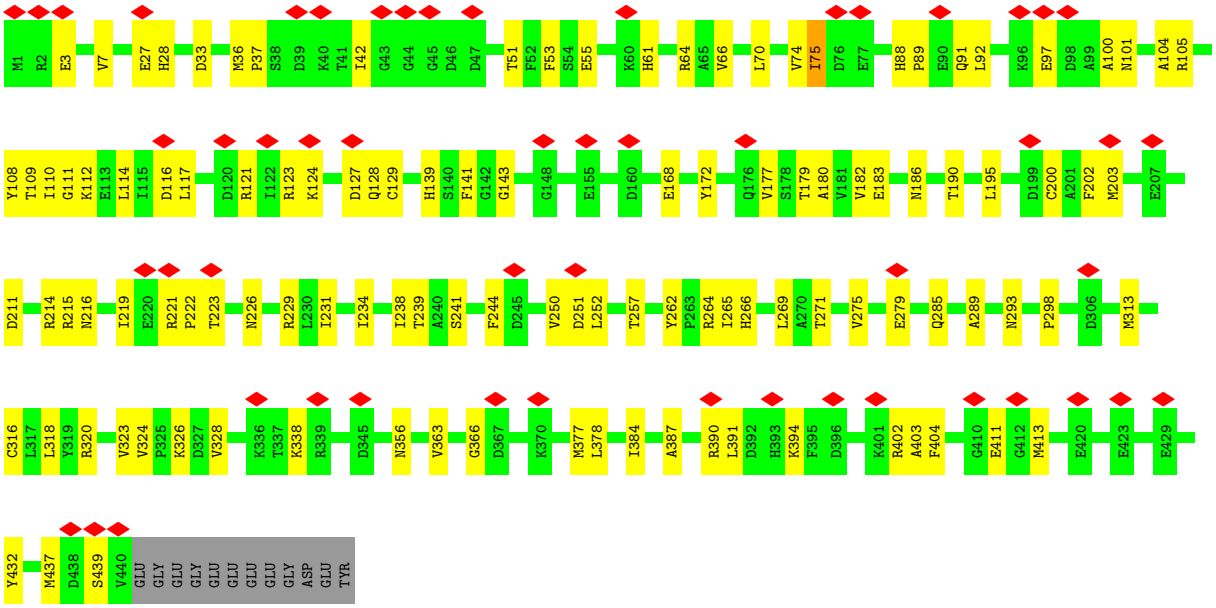
• Molecule 42: Tubulin alpha-1D chain

Chain VE:



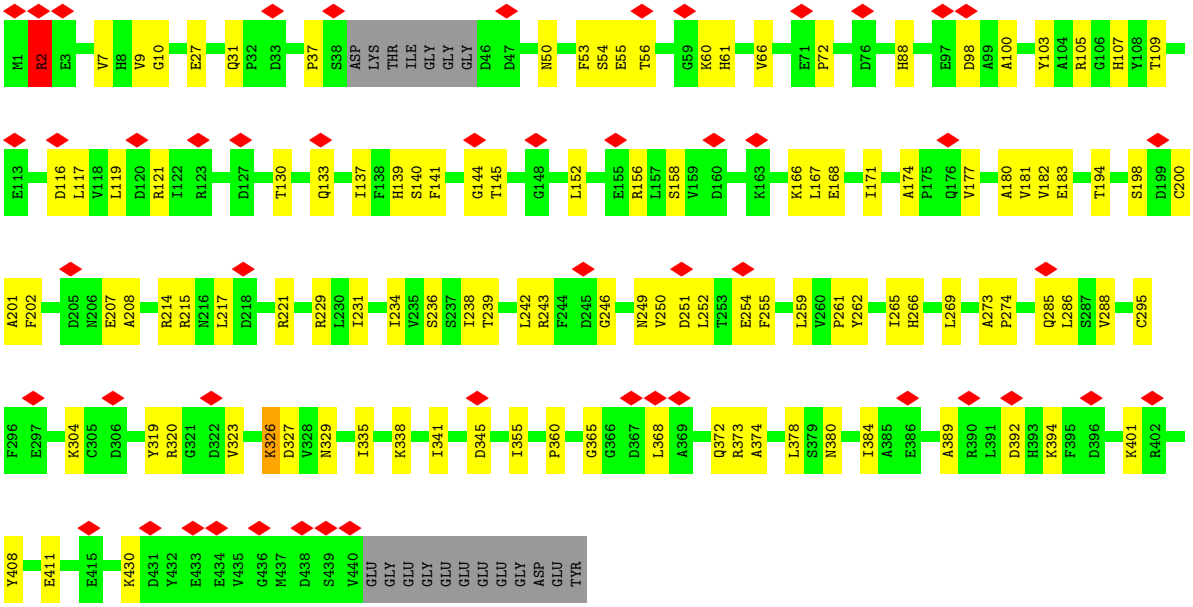
• Molecule 42: Tubulin alpha-1D chain

Chain VG:



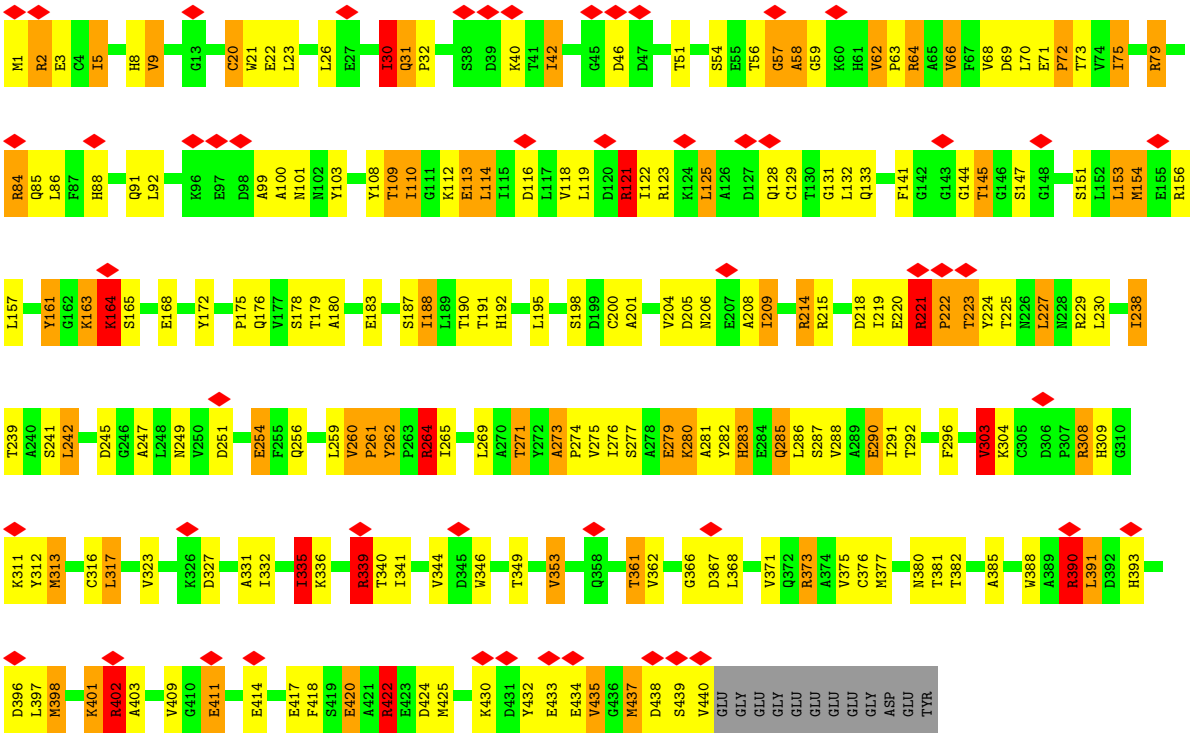
• Molecule 42: Tubulin alpha-1D chain

Chain VI:



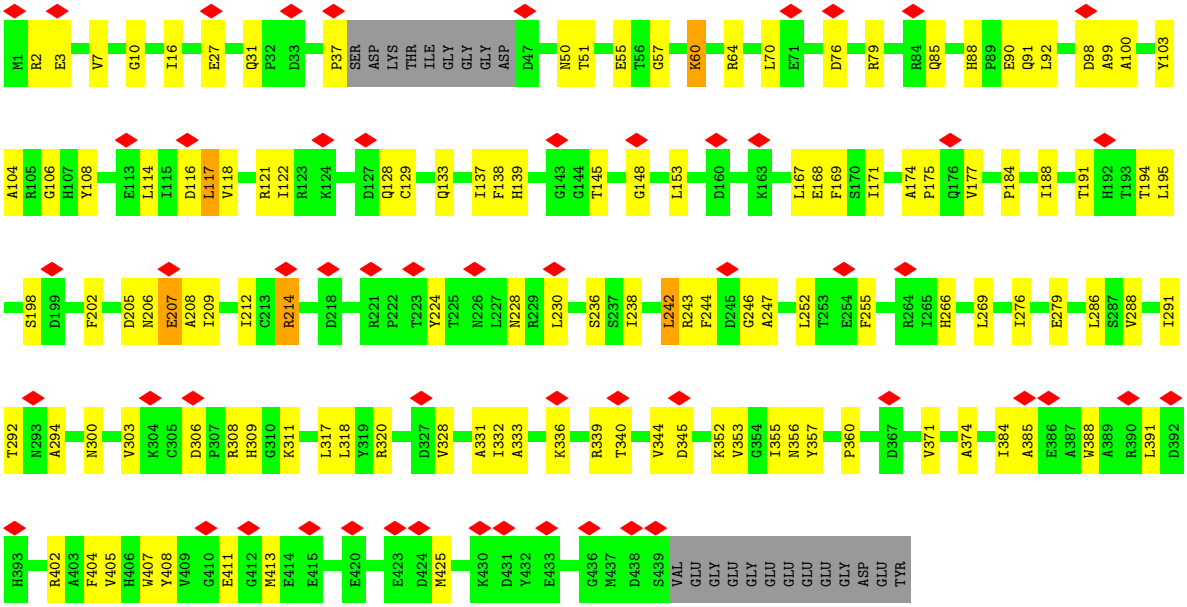
- Molecule 42: Tubulin alpha-1D chain

Chain VK:



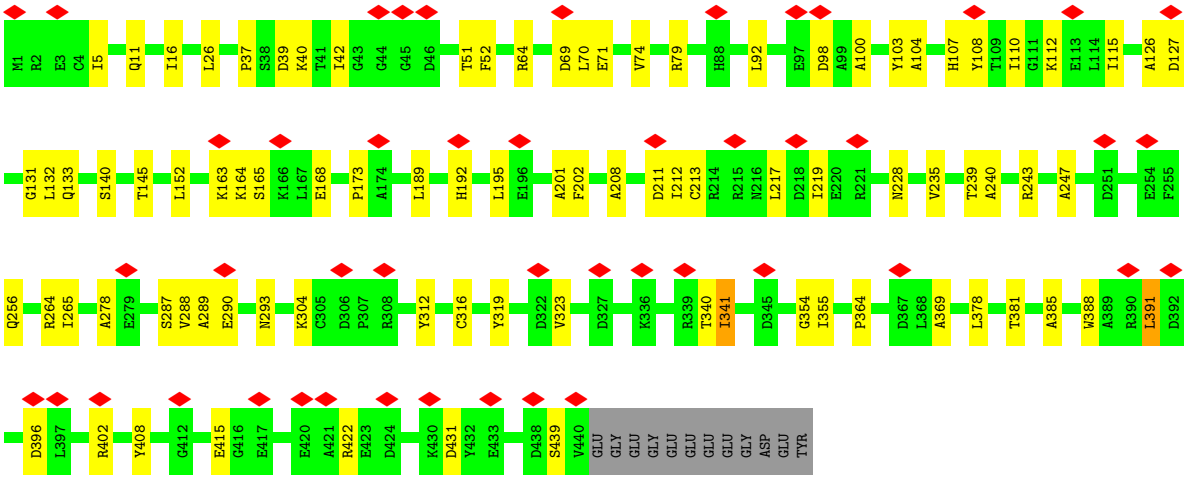
- Molecule 42: Tubulin alpha-1D chain

Chain VM:



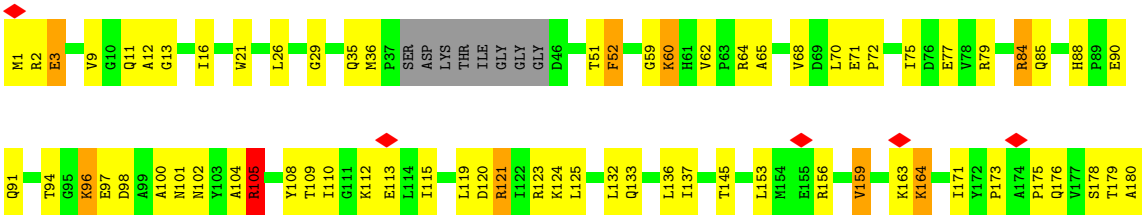
- Molecule 42: Tubulin alpha-1D chain

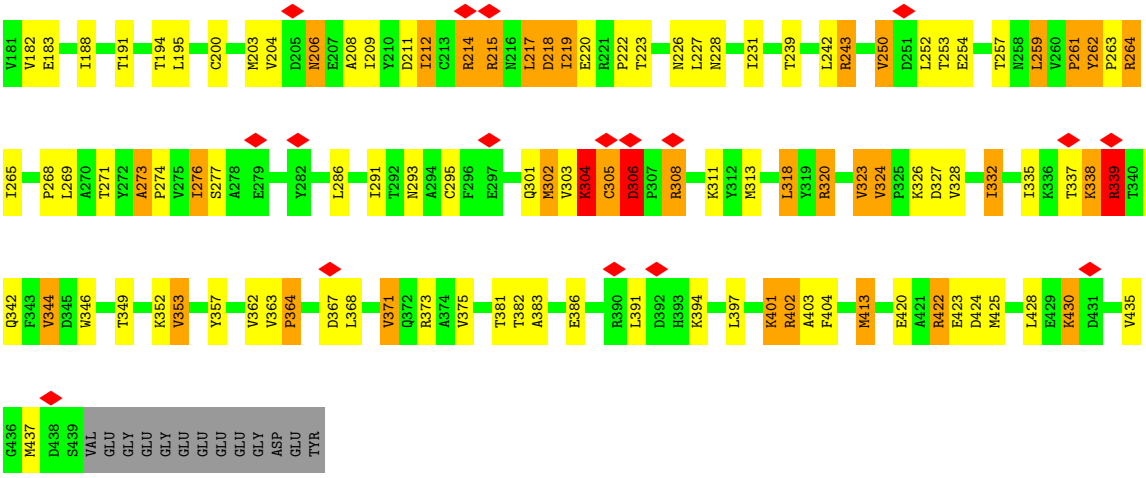
Chain WC:



- Molecule 42: Tubulin alpha-1D chain

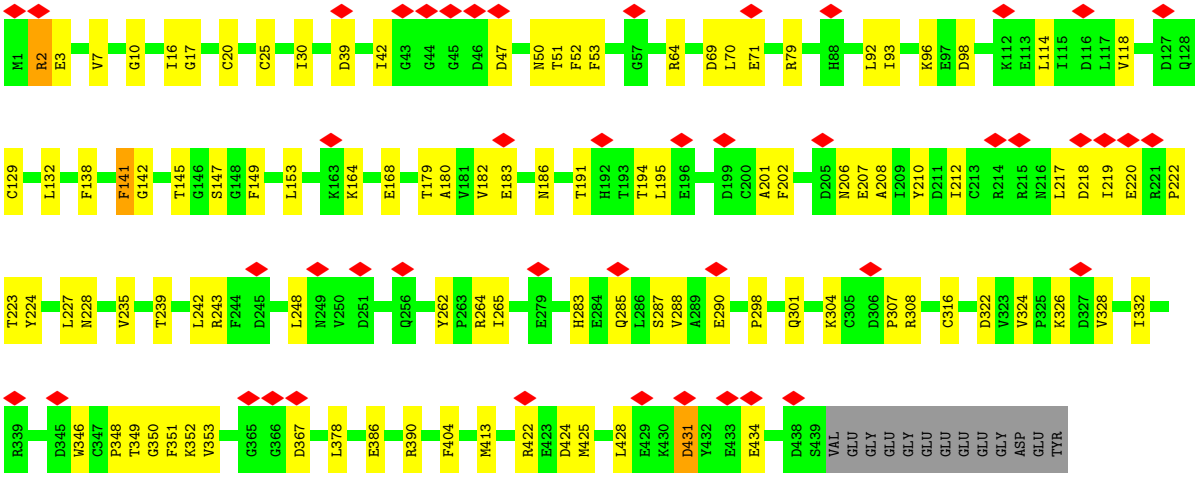
Chain WE:





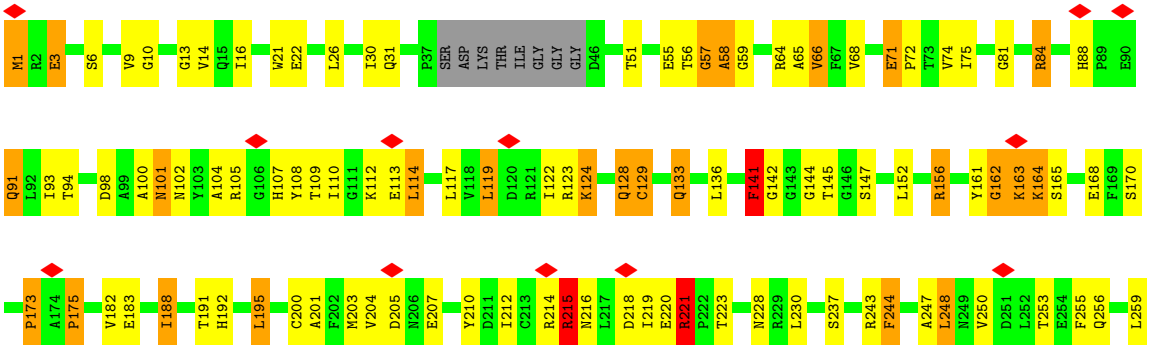
- Molecule 42: Tubulin alpha-1D chain

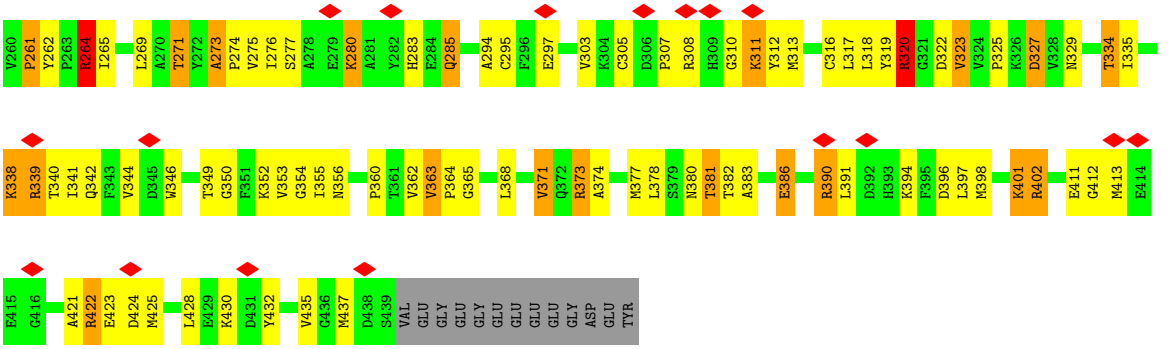
Chain WG:



- Molecule 42: Tubulin alpha-1D chain

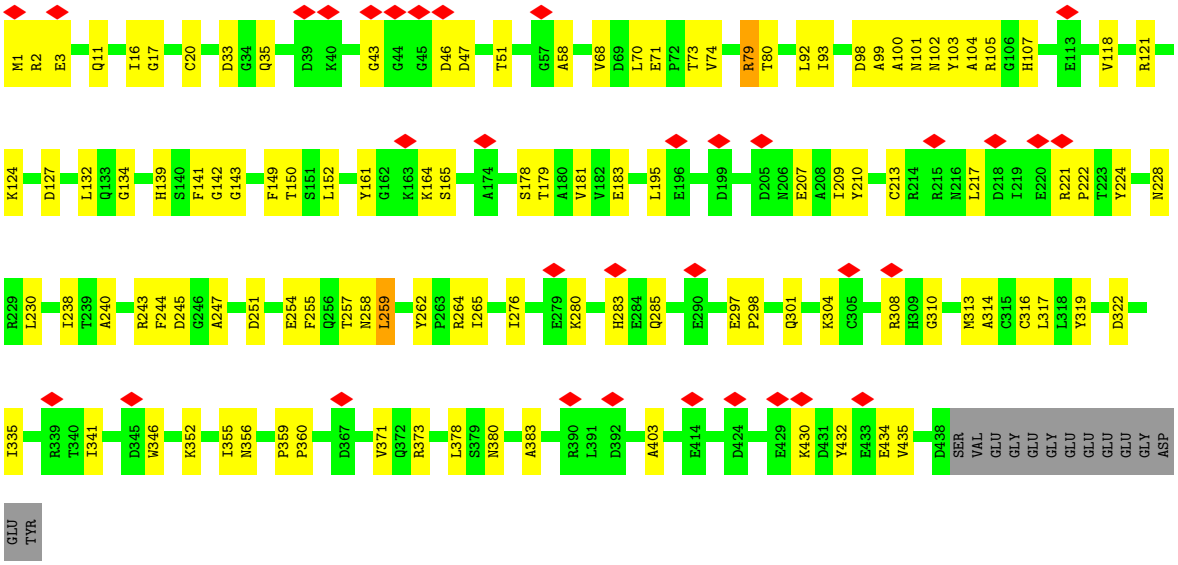
Chain WI:





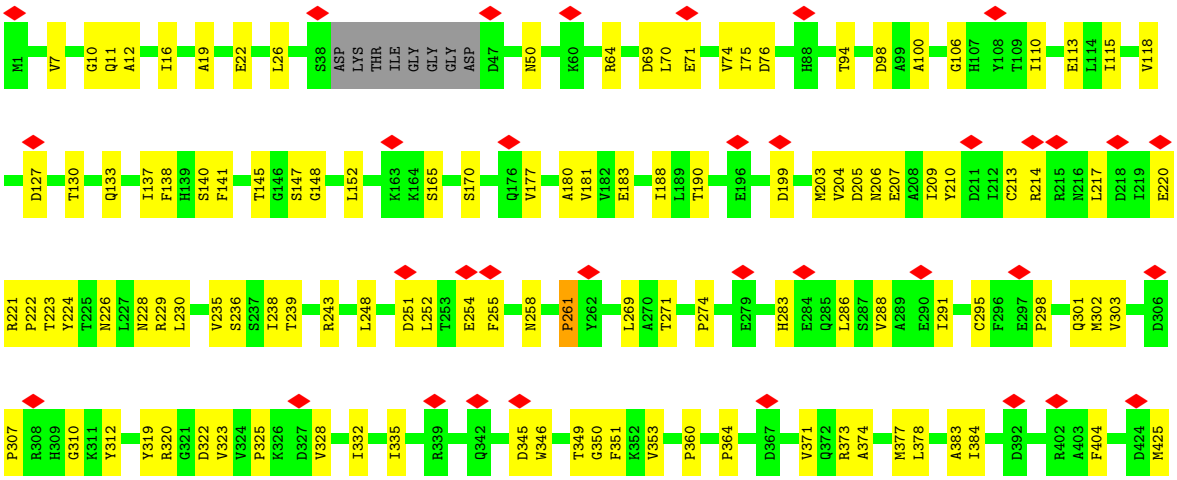
• Molecule 42: Tubulin alpha-1D chain

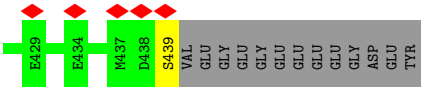
Chain WK:



• Molecule 42: Tubulin alpha-1D chain

Chain WM:




E429
E434
M437
D438
S439
VAL
GLU
GLY
GLU
GLY
GLU
GLU
GLU
GLU
GLY
ASP
GLU
TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153589	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.542	Depositor
Minimum map value	0.000	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	686.08, 686.08, 686.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	1A	0.22	0/2435	0.37	0/3389
2	1D	0.44	0/1114	0.73	1/1488 (0.1%)
2	1E	0.45	0/1577	0.83	3/2102 (0.1%)
2	1F	0.30	0/701	0.73	0/930
3	1H	0.36	0/693	0.60	0/922
3	1I	0.34	0/3271	0.69	2/4333 (0.0%)
4	1K	0.34	0/1405	0.69	3/1922 (0.2%)
4	1L	0.36	0/276	0.66	0/372
5	1N	0.37	0/921	0.70	2/1253 (0.2%)
5	1O	0.30	0/938	0.60	0/1276
5	1P	0.32	0/957	0.61	0/1302
6	1R	0.32	0/801	0.63	0/1073
7	1T	0.31	0/2105	0.64	0/2851
7	1U	0.32	0/2105	0.72	2/2851 (0.1%)
8	1W	0.65	0/1166	0.66	0/1565
8	1X	0.30	0/1565	0.65	1/2111 (0.0%)
8	1Y	0.30	0/1565	0.65	2/2111 (0.1%)
8	1Z	0.31	0/1565	0.77	4/2111 (0.2%)
8	2A	0.41	0/1565	0.71	2/2111 (0.1%)
8	2B	4.82	8/1565 (0.5%)	1.03	9/2111 (0.4%)
9	2D	3.11	6/3746 (0.2%)	0.75	11/5066 (0.2%)
9	2E	0.26	0/832	0.51	0/1122
10	2F	0.30	0/646	0.57	0/871
10	2G	0.33	0/646	0.62	0/871
10	2H	0.30	0/646	0.63	0/871
11	2J	0.35	0/1359	0.78	4/1811 (0.2%)
11	2K	0.39	0/2567	0.77	3/3392 (0.1%)
11	2L	0.33	0/2344	0.76	4/3111 (0.1%)
11	2M	0.40	2/1598 (0.1%)	0.78	5/2115 (0.2%)
12	2O	0.41	1/4812 (0.0%)	0.74	5/6515 (0.1%)
12	2P	0.36	0/4812	0.73	8/6515 (0.1%)
12	2Q	0.38	1/4812 (0.0%)	0.72	4/6515 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
13	2S	0.30	0/2089	0.66	1/2798 (0.0%)
13	2T	0.43	0/1706	0.67	0/2257
14	2V	0.25	0/298	0.57	0/402
14	2W	0.31	0/1800	0.71	1/2430 (0.0%)
14	2X	0.30	0/1754	0.69	3/2370 (0.1%)
14	2Y	0.32	0/1359	0.70	2/1842 (0.1%)
15	3A	0.42	0/1525	0.75	2/2064 (0.1%)
16	3C	0.44	0/1739	0.75	2/2338 (0.1%)
16	3D	0.32	0/547	0.59	0/739
17	3F	0.21	0/516	0.37	0/713
18	3H	0.24	0/480	0.43	0/668
19	3J	0.41	1/3656 (0.0%)	0.74	5/4945 (0.1%)
19	3K	0.35	0/3747	0.70	4/5069 (0.1%)
19	3L	0.35	0/3823	0.73	8/5172 (0.2%)
20	3N	0.35	0/2452	0.75	7/3310 (0.2%)
20	3O	0.33	0/4889	0.70	6/6578 (0.1%)
20	3P	0.31	0/4895	0.63	2/6590 (0.0%)
20	3Q	0.30	0/2450	0.63	0/3282
21	3S	0.42	0/573	0.54	0/771
21	3T	0.31	0/1982	0.64	3/2659 (0.1%)
21	3U	0.30	0/1982	0.62	3/2659 (0.1%)
21	3V	0.31	0/1733	0.59	2/2322 (0.1%)
22	3X	0.31	0/1047	0.62	0/1413
22	3Y	0.50	0/1153	0.77	1/1557 (0.1%)
22	3Z	0.96	4/1093 (0.4%)	1.35	7/1474 (0.5%)
22	4A	0.39	0/867	0.66	0/1170
22	4B	0.32	0/856	0.59	0/1153
22	4C	0.28	0/685	0.54	0/920
23	4D	0.36	0/1019	0.69	0/1379
24	4F	0.49	0/1268	0.64	0/1685
24	4G	0.38	0/2909	0.71	1/3853 (0.0%)
25	4I	0.28	0/2575	0.58	2/3508 (0.1%)
25	4J	0.36	0/3011	0.68	1/4065 (0.0%)
26	4K	0.37	0/1114	0.78	4/1495 (0.3%)
26	4L	0.36	0/1933	0.75	2/2595 (0.1%)
26	4M	0.29	0/886	0.72	3/1189 (0.3%)
27	4O	0.31	0/1810	0.61	0/2446
27	4P	0.29	0/1810	0.62	1/2446 (0.0%)
27	4Q	0.38	1/1810 (0.1%)	0.70	2/2446 (0.1%)
27	4R	0.67	0/1810	0.65	0/2446
27	4S	0.29	0/1810	0.63	1/2446 (0.0%)
27	4T	0.40	0/1810	0.60	1/2446 (0.0%)
28	4V	0.34	0/312	0.66	0/424

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
28	4W	0.33	0/676	0.69	0/918
29	4Y	0.59	2/802 (0.2%)	0.74	1/1094 (0.1%)
30	5A	0.30	0/2949	0.65	1/3937 (0.0%)
30	5B	0.26	0/136	0.57	0/183
31	5D	0.25	0/1284	0.53	0/1731
31	5E	0.36	0/1278	0.59	0/1724
31	5F	0.26	0/1301	0.52	0/1753
31	5G	0.28	0/1284	0.62	1/1731 (0.1%)
31	5H	0.38	3/1284 (0.2%)	0.55	0/1731
31	5I	0.24	0/1284	0.46	0/1731
31	5J	0.27	0/1284	0.51	0/1731
32	5L	0.40	0/951	0.67	2/1279 (0.2%)
32	5M	0.32	0/3270	0.63	1/4403 (0.0%)
32	5N	0.30	0/3270	0.64	5/4403 (0.1%)
32	5O	0.64	0/2445	0.63	0/3290
33	5Q	0.36	0/917	0.67	0/1244
33	5R	0.42	3/3290 (0.1%)	0.68	4/4434 (0.1%)
33	5S	0.47	0/3290	0.64	2/4434 (0.0%)
33	5T	0.63	0/2523	0.66	0/3388
33	5V	0.41	0/2541	0.80	2/3414 (0.1%)
33	5W	0.36	0/3378	0.73	3/4552 (0.1%)
33	5X	0.41	0/3378	0.79	10/4552 (0.2%)
33	5Y	0.45	0/892	0.71	0/1210
34	6A	0.64	0/2272	0.72	0/3060
34	6B	0.40	0/3230	0.71	3/4355 (0.1%)
34	6C	0.65	0/3241	0.63	0/4369
34	6D	0.63	0/999	0.63	0/1347
34	6E	0.67	1/489 (0.2%)	0.65	0/656
34	6F	0.37	0/2930	0.66	2/3947 (0.1%)
34	6G	0.34	0/3432	0.65	6/4630 (0.1%)
34	6H	0.40	0/3031	0.72	8/4086 (0.2%)
34	6I	0.47	0/542	0.68	0/734
34	6J	0.33	0/571	0.68	2/780 (0.3%)
34	6K	0.32	0/3071	0.64	0/4147
34	6L	0.39	1/3462 (0.0%)	0.61	1/4675 (0.0%)
34	6M	0.34	0/2957	0.63	1/3983 (0.0%)
34	6N	0.32	0/447	0.74	1/600 (0.2%)
35	6P	0.34	0/1520	0.61	1/2050 (0.0%)
35	6Q	0.45	4/3415 (0.1%)	0.66	3/4600 (0.1%)
35	6R	0.46	1/3415 (0.0%)	0.74	4/4600 (0.1%)
35	6S	0.47	0/2076	0.63	1/2791 (0.0%)
35	6T	0.35	0/1936	0.72	2/2601 (0.1%)
35	6U	0.34	0/3465	0.67	2/4671 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	6V	0.41	0/3625	0.69	4/4886 (0.1%)
35	6W	0.42	0/1799	0.69	2/2427 (0.1%)
36	6Y	0.31	0/1318	0.64	1/1783 (0.1%)
36	6Z	0.28	0/1318	0.55	0/1783
37	7C	0.43	0/923	0.96	1/1247 (0.1%)
37	7D	0.41	0/642	0.90	3/877 (0.3%)
37	7E	0.34	0/640	0.72	0/862
37	7F	0.48	0/539	0.60	0/731
38	7H	0.40	0/657	0.88	1/892 (0.1%)
38	7I	0.51	0/245	0.71	0/333
39	7K	0.41	0/900	0.64	0/1209
39	7L	0.32	0/396	0.68	1/538 (0.2%)
40	7N	0.38	0/534	0.76	2/721 (0.3%)
41	AB	0.37	0/3500	0.69	5/4742 (0.1%)
41	AD	0.35	1/3500 (0.0%)	0.62	2/4742 (0.0%)
41	AF	0.31	0/3500	0.62	1/4742 (0.0%)
41	AH	0.66	0/3500	0.67	0/4742
41	AJ	0.38	0/3500	0.59	0/4742
41	AL	0.65	0/3500	0.70	0/4742
41	BB	0.33	0/3431	0.67	3/4649 (0.1%)
41	BD	0.66	0/3431	0.68	0/4649
41	BF	0.31	0/3436	0.59	0/4656
41	BH	0.37	1/3431 (0.0%)	0.62	1/4649 (0.0%)
41	BJ	0.37	0/3431	0.66	5/4649 (0.1%)
41	BL	2.79	6/3415 (0.2%)	0.71	6/4628 (0.1%)
41	CB	0.39	3/3423 (0.1%)	0.72	7/4638 (0.2%)
41	CD	0.66	0/3423	0.68	0/4638
41	CF	0.66	0/3436	0.69	0/4656
41	CH	0.36	0/3431	0.71	9/4649 (0.2%)
41	CJ	0.66	0/3436	0.68	0/4656
41	CL	0.37	0/3415	0.70	3/4628 (0.1%)
41	DB	0.43	0/3423	0.81	5/4638 (0.1%)
41	DD	0.40	0/3423	0.74	3/4638 (0.1%)
41	DF	0.44	0/3423	0.83	10/4638 (0.2%)
41	DH	0.67	0/3423	0.70	0/4638
41	DJ	0.66	0/3423	0.69	0/4638
41	DL	0.47	0/3415	0.74	4/4628 (0.1%)
41	ED	0.66	0/3423	0.69	0/4638
41	EF	0.39	0/3423	0.77	7/4638 (0.2%)
41	EH	0.38	0/3436	0.82	6/4656 (0.1%)
41	EJ	0.49	3/3423 (0.1%)	0.84	11/4638 (0.2%)
41	EL	0.49	0/3415	0.78	8/4628 (0.2%)
41	FD	0.66	0/3431	0.68	0/4649

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
41	FF	0.41	1/3423 (0.0%)	0.73	5/4638 (0.1%)
41	FH	0.42	0/3423	0.77	4/4638 (0.1%)
41	FJ	0.41	0/3423	0.73	5/4638 (0.1%)
41	FL	0.66	0/3415	0.68	0/4628
41	GD	0.65	0/3431	0.70	0/4649
41	GF	0.36	1/3436 (0.0%)	0.71	6/4656 (0.1%)
41	GH	0.38	0/3436	0.72	4/4656 (0.1%)
41	GJ	0.65	0/3436	0.68	0/4656
41	GL	0.32	0/3415	0.66	1/4628 (0.0%)
41	HB	0.41	1/3423 (0.0%)	0.75	6/4638 (0.1%)
41	HD	0.65	0/3431	0.66	0/4649
41	HF	0.41	0/3436	0.74	4/4656 (0.1%)
41	HH	0.40	0/3431	0.74	7/4649 (0.2%)
41	HJ	0.65	0/3436	0.67	0/4656
41	HL	0.37	0/3415	0.71	3/4628 (0.1%)
41	ID	0.33	0/3431	0.66	1/4649 (0.0%)
41	IF	0.36	1/3436 (0.0%)	0.64	0/4656
41	IH	0.34	0/3431	0.64	2/4649 (0.0%)
41	IJ	0.45	3/3436 (0.1%)	0.67	3/4656 (0.1%)
41	IL	0.38	0/3423	0.69	3/4638 (0.1%)
41	IN	0.62	1/3436 (0.0%)	1.07	15/4656 (0.3%)
41	JD	0.46	1/3431 (0.0%)	0.72	7/4649 (0.2%)
41	JF	0.35	0/3423	0.70	7/4638 (0.2%)
41	JH	0.37	0/3423	0.70	2/4638 (0.0%)
41	JJ	0.35	0/3423	0.72	5/4638 (0.1%)
41	JL	0.65	0/3423	0.68	0/4638
41	KD	0.36	0/3436	0.75	12/4656 (0.3%)
41	KF	0.34	0/3431	0.59	1/4649 (0.0%)
41	KH	0.32	0/3443	0.59	1/4666 (0.0%)
41	KJ	0.33	0/3423	0.62	3/4638 (0.1%)
41	KL	0.33	0/3443	0.61	2/4666 (0.0%)
41	KN	0.32	0/3436	0.61	0/4656
41	LD	0.65	0/3431	0.69	0/4649
41	LF	0.30	0/3436	0.57	0/4656
41	LH	0.32	0/3436	0.59	0/4656
41	LJ	0.35	0/3436	0.63	5/4656 (0.1%)
41	LL	0.32	0/3423	0.63	4/4638 (0.1%)
41	LN	0.29	0/3436	0.59	2/4656 (0.0%)
41	MD	0.65	0/3423	0.69	0/4638
41	MF	0.65	0/3436	0.69	0/4656
41	MH	0.31	0/3436	0.62	0/4656
41	MJ	0.36	0/3423	0.65	3/4638 (0.1%)
41	ML	0.40	0/3423	0.74	4/4638 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
41	MN	0.66	0/3423	0.69	0/4638
41	NB	0.65	0/3436	0.70	0/4656
41	ND	0.65	0/3431	0.71	0/4649
41	NF	0.66	0/3431	0.70	1/4649 (0.0%)
41	NH	0.65	0/3436	0.69	1/4656 (0.0%)
41	NJ	0.41	0/3436	0.69	1/4656 (0.0%)
41	NL	0.38	0/3188	0.76	8/4316 (0.2%)
41	OB	0.66	0/3414	0.67	0/4626
41	OD	0.39	0/3401	0.78	6/4608 (0.1%)
41	OF	0.43	0/3414	0.76	9/4626 (0.2%)
41	OH	0.65	0/3436	0.71	0/4656
41	OJ	0.65	0/3436	0.69	0/4656
41	OL	0.39	0/3401	0.76	5/4608 (0.1%)
41	PB	0.65	0/3431	0.72	1/4649 (0.0%)
41	PD	0.65	0/3431	0.71	0/4649
41	PF	0.65	0/3436	0.71	0/4656
41	PH	0.67	0/3436	1.07	16/4656 (0.3%)
41	PJ	0.65	0/3436	1.03	5/4656 (0.1%)
41	PL	0.64	0/3415	0.70	0/4628
41	QB	0.39	0/3436	0.78	8/4656 (0.2%)
41	QD	0.39	1/3431 (0.0%)	0.81	9/4649 (0.2%)
41	QF	0.39	0/3436	0.76	7/4656 (0.2%)
41	QH	0.65	0/3436	0.74	0/4656
41	QJ	0.65	0/3436	0.74	1/4656 (0.0%)
41	QL	0.65	0/3423	0.71	0/4638
41	RB	0.39	1/3436 (0.0%)	0.79	8/4656 (0.2%)
41	RD	0.65	0/3431	0.71	0/4649
41	RF	0.66	0/3436	0.74	0/4656
41	RH	0.43	0/3436	0.74	3/4656 (0.1%)
41	RJ	0.66	0/3436	0.71	0/4656
41	RL	0.41	0/3423	0.81	8/4638 (0.2%)
41	SD	0.44	1/3431 (0.0%)	0.91	10/4649 (0.2%)
41	SF	0.65	0/3436	0.71	0/4656
41	SH	0.43	3/3436 (0.1%)	0.83	9/4656 (0.2%)
41	SJ	0.42	1/3436 (0.0%)	0.79	6/4656 (0.1%)
41	SL	0.65	0/3423	0.71	0/4638
41	TD	0.38	0/3431	0.81	12/4649 (0.3%)
41	TF	0.46	2/3436 (0.1%)	0.82	3/4656 (0.1%)
41	TH	0.38	0/3436	0.77	8/4656 (0.2%)
41	TJ	0.44	0/3436	0.76	4/4656 (0.1%)
41	TL	0.42	1/3423 (0.0%)	0.82	10/4638 (0.2%)
41	UD	0.42	0/3431	0.73	5/4649 (0.1%)
41	UF	0.39	0/3436	0.72	2/4656 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
41	UH	0.39	0/3436	0.74	6/4656 (0.1%)
41	UJ	0.43	0/3436	0.87	12/4656 (0.3%)
41	UL	0.54	5/3423 (0.1%)	0.79	5/4638 (0.1%)
41	VD	0.38	0/3431	0.74	4/4649 (0.1%)
41	VF	0.42	0/3431	0.70	5/4649 (0.1%)
41	VH	0.40	0/3436	0.72	3/4656 (0.1%)
41	VJ	0.43	0/3436	0.73	3/4656 (0.1%)
41	VL	0.34	0/3423	0.67	4/4638 (0.1%)
41	WD	0.36	0/3431	0.68	3/4649 (0.1%)
41	WF	0.65	0/3423	0.70	0/4638
41	WH	0.65	0/3423	0.69	0/4638
41	WJ	0.36	0/3423	0.65	4/4638 (0.1%)
41	WL	0.36	0/3423	0.67	2/4638 (0.0%)
41	WN	0.36	0/3423	0.67	2/4638 (0.0%)
42	AC	0.31	0/3515	0.61	1/4771 (0.0%)
42	AE	0.36	0/3515	0.64	3/4771 (0.1%)
42	AG	0.38	0/3515	0.62	1/4771 (0.0%)
42	AI	0.66	0/3515	0.65	0/4771
42	AK	0.66	0/3515	0.69	0/4771
42	BC	0.36	1/3515 (0.0%)	0.68	3/4771 (0.1%)
42	BE	0.35	0/3473	0.66	3/4714 (0.1%)
42	BG	0.39	1/3515 (0.0%)	0.67	5/4771 (0.1%)
42	BI	0.65	0/3451	0.68	0/4684
42	BK	0.32	0/3508	0.63	2/4761 (0.0%)
42	CC	0.66	0/3502	0.68	0/4753
42	CE	0.34	0/3502	0.66	5/4753 (0.1%)
42	CG	0.66	0/3508	0.69	0/4761
42	CI	0.33	0/3508	0.65	1/4761 (0.0%)
42	CK	0.40	0/3508	0.72	8/4761 (0.2%)
42	CM	0.71	6/3508 (0.2%)	0.90	12/4761 (0.3%)
42	DC	0.43	0/3443	0.77	4/4673 (0.1%)
42	DE	0.39	1/3449 (0.0%)	0.77	8/4681 (0.2%)
42	DG	0.41	1/3456 (0.0%)	0.72	1/4691 (0.0%)
42	DI	0.40	0/3441	0.76	7/4670 (0.1%)
42	DK	0.66	0/3449	0.69	0/4681
42	DM	0.44	2/3449 (0.1%)	0.81	7/4681 (0.1%)
42	EC	0.45	1/3508 (0.0%)	0.83	6/4761 (0.1%)
42	EE	0.67	0/3524	0.68	0/4783
42	EG	0.66	0/3481	0.70	0/4724
42	EI	0.84	7/3486 (0.2%)	0.81	11/4732 (0.2%)
42	EK	0.66	0/3515	0.69	1/4771 (0.0%)
42	EM	0.66	0/3435	0.67	1/4662 (0.0%)
42	FC	0.66	0/3456	0.65	0/4691

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
42	FE	0.43	0/3415	0.73	2/4635 (0.0%)
42	FG	0.41	1/3423 (0.0%)	0.72	5/4647 (0.1%)
42	FI	0.40	0/3422	0.68	2/4644 (0.0%)
42	FK	0.67	0/3401	0.67	0/4617
42	FM	0.44	1/3441 (0.0%)	0.75	6/4669 (0.1%)
42	GC	0.34	0/3515	0.66	2/4771 (0.0%)
42	GE	0.35	0/3448	0.64	1/4680 (0.0%)
42	GG	0.35	0/3470	0.65	2/4710 (0.0%)
42	GI	0.36	0/3442	0.66	1/4672 (0.0%)
42	GK	0.33	0/3440	0.68	2/4668 (0.0%)
42	GM	0.66	0/3508	0.66	0/4761
42	HC	0.65	0/3427	0.65	0/4651
42	HE	0.42	0/3451	0.73	6/4684 (0.1%)
42	HG	0.66	0/3448	0.67	0/4680
42	HI	0.66	0/3448	0.69	0/4680
42	HK	0.45	0/3456	0.74	2/4691 (0.0%)
42	HM	0.66	0/3441	0.66	2/4669 (0.0%)
42	IC	0.34	0/3442	0.65	1/4672 (0.0%)
42	IE	0.65	0/3465	0.69	0/4703
42	IG	0.37	1/3515 (0.0%)	0.67	3/4771 (0.1%)
42	II	0.36	0/3464	0.65	0/4702
42	IK	0.38	0/3515	0.71	2/4771 (0.0%)
42	IM	0.40	1/3455 (0.0%)	0.68	3/4689 (0.1%)
42	JC	0.41	0/3460	0.75	7/4695 (0.1%)
42	JE	0.41	1/3449 (0.0%)	0.67	4/4681 (0.1%)
42	JG	0.35	0/3435	0.66	5/4662 (0.1%)
42	JI	0.36	0/3443	0.69	2/4673 (0.0%)
42	JK	0.66	0/3515	0.67	0/4771
42	JM	0.65	0/3449	0.69	0/4681
42	KC	0.31	0/3461	0.57	0/4697
42	KE	0.30	0/3457	0.59	1/4692 (0.0%)
42	KG	0.33	0/3447	0.61	4/4678 (0.1%)
42	KI	0.33	0/3435	0.62	4/4662 (0.1%)
42	KK	0.35	0/3449	0.62	6/4681 (0.1%)
42	KM	0.65	0/3453	0.68	0/4686
42	LC	0.35	1/3470 (0.0%)	0.60	3/4710 (0.1%)
42	LE	0.31	0/3515	0.60	2/4771 (0.0%)
42	LG	0.34	1/3470 (0.0%)	0.59	3/4710 (0.1%)
42	LI	0.33	1/3474 (0.0%)	0.62	4/4715 (0.1%)
42	LK	0.32	0/3478	0.61	2/4720 (0.0%)
42	LM	0.38	0/3455	0.62	3/4689 (0.1%)
42	MC	0.39	0/3508	0.68	3/4761 (0.1%)
42	ME	0.34	0/3443	0.63	0/4673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
42	MG	0.65	0/3449	0.68	0/4681
42	MI	0.32	0/3456	0.61	2/4691 (0.0%)
42	MK	0.50	1/3515 (0.0%)	0.80	9/4771 (0.2%)
42	MM	0.40	0/3453	0.73	4/4687 (0.1%)
42	NA	0.65	0/3449	0.69	0/4682
42	NC	0.66	0/3442	0.67	0/4672
42	NE	0.34	0/3451	0.69	2/4684 (0.0%)
42	NG	0.65	0/3464	0.70	0/4702
42	NI	0.65	0/3464	0.71	0/4702
42	NK	0.65	0/3451	0.71	0/4684
42	OA	0.40	0/3435	0.77	6/4663 (0.1%)
42	OC	0.41	2/3443 (0.1%)	0.74	3/4673 (0.1%)
42	OE	0.52	2/3473 (0.1%)	0.85	9/4714 (0.2%)
42	OG	0.65	0/3468	0.69	0/4707
42	OI	0.41	0/3464	0.74	4/4702 (0.1%)
42	OK	0.36	0/3457	0.73	4/4692 (0.1%)
42	PA	0.65	0/2931	0.70	0/3977
42	PC	0.66	0/3463	0.73	0/4700
42	PE	0.64	0/3457	0.72	0/4692
42	PG	0.66	0/3448	1.14	22/4680 (0.5%)
42	PI	0.66	0/3425	1.04	14/4648 (0.3%)
42	PK	0.65	0/3448	0.70	0/4680
42	QC	0.46	1/3449 (0.0%)	0.90	4/4681 (0.1%)
42	QE	0.39	0/3449	0.82	8/4681 (0.2%)
42	QG	0.42	0/3457	0.78	5/4692 (0.1%)
42	QI	0.65	0/3443	0.73	0/4673
42	QK	0.65	0/3457	0.71	0/4692
42	RC	0.68	3/3464 (0.1%)	0.90	10/4702 (0.2%)
42	RE	0.42	0/3435	0.74	1/4662 (0.0%)
42	RG	0.46	1/3448 (0.0%)	0.78	5/4679 (0.1%)
42	RI	0.39	0/3456	0.78	5/4691 (0.1%)
42	RK	0.41	0/3456	0.78	5/4691 (0.1%)
42	SC	0.39	0/3448	0.76	2/4679 (0.0%)
42	SE	0.65	0/3457	0.72	0/4691
42	SG	0.46	0/3456	0.81	7/4691 (0.1%)
42	SI	0.65	0/3434	0.71	0/4661
42	SK	0.42	2/3464 (0.1%)	0.77	3/4702 (0.1%)
42	SM	0.40	0/3455	0.78	5/4689 (0.1%)
42	TC	0.75	3/3448 (0.1%)	0.90	7/4680 (0.1%)
42	TE	0.42	0/3465	0.73	4/4703 (0.1%)
42	TG	0.38	1/3448 (0.0%)	0.79	10/4680 (0.2%)
42	TI	0.66	0/3448	0.73	1/4680 (0.0%)
42	TK	0.66	0/3464	0.71	0/4702

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
42	TM	0.42	1/3449 (0.0%)	0.80	9/4681 (0.2%)
42	UC	0.65	0/3470	0.70	0/4710
42	UE	0.44	1/3465 (0.0%)	0.77	0/4703
42	UG	0.45	0/3470	0.72	4/4710 (0.1%)
42	UI	0.37	0/3470	0.71	5/4710 (0.1%)
42	UK	0.46	0/3468	0.78	7/4707 (0.1%)
42	UM	0.42	0/3455	0.77	6/4689 (0.1%)
42	VC	0.35	0/3515	0.68	3/4771 (0.1%)
42	VE	0.45	3/3473 (0.1%)	0.72	4/4714 (0.1%)
42	VG	0.42	2/3515 (0.1%)	0.67	2/4771 (0.0%)
42	VI	0.37	0/3470	0.68	3/4710 (0.1%)
42	VK	0.65	0/3515	0.69	0/4771
42	VM	0.40	1/3449 (0.0%)	0.70	3/4681 (0.1%)
42	WC	0.36	0/3515	0.66	2/4771 (0.0%)
42	WE	0.65	0/3457	0.70	0/4692
42	WG	0.38	0/3508	0.69	4/4761 (0.1%)
42	WI	0.65	0/3457	0.68	0/4692
42	WK	0.32	0/3502	0.63	2/4753 (0.0%)
42	WM	0.34	0/3455	0.72	5/4689 (0.1%)
All	All	0.56	129/1148355 (0.0%)	0.71	1083/1555321 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1D	0	4
2	1E	0	4
3	1I	0	1
6	1R	0	1
7	1T	0	1
7	1U	0	1
8	1W	0	10
8	1X	0	1
8	2A	0	5
8	2B	0	1
9	2D	0	3
11	2J	0	1
11	2K	0	4
11	2M	0	1
12	2O	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	2P	0	1
13	2S	0	1
13	2T	0	6
14	2V	0	1
14	2W	0	2
14	2X	0	1
15	3A	0	3
16	3C	0	3
19	3J	0	2
19	3K	0	1
19	3L	0	2
20	3N	0	3
20	3O	0	3
20	3Q	0	1
21	3U	0	1
22	3Y	0	3
22	4B	0	1
24	4F	0	7
27	4R	0	6
27	4T	0	2
28	4W	0	1
29	4Y	0	1
30	5A	0	1
31	5D	0	1
32	5O	0	20
33	5R	0	1
33	5S	0	14
33	5T	0	17
33	5V	0	5
33	5W	0	2
33	5X	0	2
33	5Y	0	5
34	6A	0	18
34	6B	0	5
34	6C	0	20
34	6D	0	8
34	6E	0	5
34	6F	0	1
34	6H	0	4
34	6L	0	1
35	6R	0	8
35	6S	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
35	6V	0	7
35	6W	0	2
36	6Z	0	1
37	7C	0	3
37	7D	0	1
37	7F	0	1
38	7H	0	2
41	AH	0	17
41	AL	0	18
41	BD	0	19
41	CD	0	17
41	CF	0	17
41	CH	0	2
41	CJ	0	19
41	CL	0	1
41	DF	0	1
41	DH	0	18
41	DJ	0	17
41	DL	0	4
41	ED	0	18
41	EF	0	1
41	EH	0	3
41	EJ	0	3
41	EL	0	5
41	FD	0	17
41	FF	0	4
41	FH	0	1
41	FL	0	20
41	GD	0	20
41	GF	0	2
41	GJ	0	20
41	GL	0	1
41	HB	0	2
41	HD	0	15
41	HF	0	1
41	HH	0	2
41	HJ	0	17
41	HL	0	2
41	ID	0	1
41	IF	0	1
41	IJ	0	2
41	IL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	IN	0	15
41	JD	0	2
41	JL	0	18
41	KD	0	2
41	KJ	0	1
41	KN	0	1
41	LD	0	15
41	LJ	0	1
41	MD	0	18
41	MF	0	21
41	MH	0	1
41	MJ	0	1
41	ML	0	1
41	MN	0	19
41	NB	0	18
41	ND	0	15
41	NF	0	17
41	NH	0	20
41	NJ	0	1
41	NL	0	1
41	OB	0	17
41	OD	0	1
41	OF	0	1
41	OH	0	19
41	OJ	0	16
41	OL	0	3
41	PB	0	18
41	PD	0	21
41	PF	0	15
41	PH	0	19
41	PJ	0	18
41	PL	0	17
41	QB	0	1
41	QD	0	1
41	QF	0	1
41	QH	0	21
41	QJ	0	16
41	QL	0	18
41	RB	0	2
41	RD	0	21
41	RF	0	15
41	RH	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	RJ	0	18
41	RL	0	1
41	SD	0	2
41	SF	0	17
41	SH	0	4
41	SJ	0	2
41	SL	0	17
41	TD	0	1
41	TF	0	1
41	TH	0	2
41	TJ	0	4
41	UD	0	1
41	UF	0	2
41	UH	0	1
41	UL	0	1
41	VD	0	1
41	VF	0	1
41	VH	0	1
41	VJ	0	4
41	WD	0	1
41	WF	0	17
41	WH	0	19
41	WJ	0	3
42	AI	0	18
42	AK	0	16
42	BC	0	1
42	BE	0	1
42	BI	0	20
42	CC	0	14
42	CG	0	16
42	CK	0	3
42	CM	0	2
42	DC	0	3
42	DG	0	1
42	DI	0	3
42	DK	0	18
42	DM	0	1
42	EC	0	3
42	EE	0	14
42	EG	0	10
42	EI	0	2
42	EK	0	14

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	EM	0	17
42	FC	0	19
42	FE	0	1
42	FG	0	1
42	FI	0	1
42	FK	0	18
42	FM	0	1
42	GC	0	2
42	GE	0	1
42	GK	0	2
42	GM	0	15
42	HC	0	17
42	HG	0	15
42	HI	0	17
42	HK	0	1
42	HM	0	19
42	IC	0	1
42	IE	0	17
42	IG	0	1
42	IK	0	1
42	IM	0	1
42	JC	0	2
42	JI	0	4
42	JK	0	17
42	JM	0	16
42	KM	0	16
42	LI	0	1
42	LK	0	1
42	MC	0	1
42	MG	0	17
42	MM	0	2
42	NA	0	15
42	NC	0	15
42	NE	0	1
42	NG	0	13
42	NI	0	12
42	NK	0	17
42	OA	0	1
42	OC	0	1
42	OE	0	1
42	OG	0	21
42	PA	0	15

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	PC	0	17
42	PE	0	17
42	PG	0	18
42	PI	0	16
42	PK	0	20
42	QC	0	1
42	QE	0	2
42	QI	0	19
42	QK	0	19
42	RI	0	1
42	RK	0	1
42	SC	0	1
42	SE	0	15
42	SG	0	2
42	SI	0	18
42	SK	0	1
42	SM	0	1
42	TC	0	1
42	TG	0	2
42	TI	0	15
42	TK	0	16
42	TM	0	1
42	UC	0	16
42	UE	0	2
42	UG	0	3
42	UI	0	1
42	UK	0	4
42	VC	0	1
42	VG	0	1
42	VI	0	1
42	VK	0	18
42	VM	0	1
42	WC	0	1
42	WE	0	17
42	WI	0	16
42	WK	0	1
All	All	0	1942

The worst 5 of 129 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2D	567	TYR	CD2-CE2	104.46	2.96	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2B	15	TYR	CD1-CE1	103.98	2.95	1.39
9	2D	567	TYR	CD1-CE1	101.76	2.92	1.39
8	2B	15	TYR	CD2-CE2	101.38	2.91	1.39
41	BL	281	TYR	CD2-CE2	89.68	2.73	1.39

The worst 5 of 1083 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	TC	261	PRO	N-CD-CG	-32.13	55.01	103.20
41	IN	276	ARG	CD-NE-CZ	29.54	164.96	123.60
8	2B	164	ARG	CD-NE-CZ	28.16	163.03	123.60
42	CM	173	PRO	CB-CG-CD	-27.29	0.07	106.50
42	QC	268	PRO	N-CD-CG	-27.15	62.48	103.20

There are no chirality outliers.

5 of 1942 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1D	150	ARG	Sidechain
2	1D	151	ARG	Sidechain
2	1D	187	ARG	Sidechain
2	1D	222	ARG	Sidechain
2	1E	150	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	2437	0	1166	0	0
2	1D	1109	0	1132	15	0
2	1E	1569	0	1624	24	0
2	1F	698	0	735	12	0
3	1H	685	0	684	3	0
3	1I	3234	0	3300	13	0
4	1K	1348	0	1323	11	0
4	1L	269	0	267	3	0
5	1N	894	0	894	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1O	910	0	914	10	0
5	1P	928	0	925	5	0
6	1R	785	0	787	5	0
7	1T	2055	0	2024	11	0
7	1U	2055	0	2024	11	0
8	1W	1143	0	1162	0	0
8	1X	1532	0	1559	8	0
8	1Y	1532	0	1559	5	0
8	1Z	1532	0	1559	5	0
8	2A	1532	0	1559	11	0
8	2B	1532	0	1559	5	0
9	2D	3649	0	3628	96	0
9	2E	816	0	802	4	0
10	2F	631	0	605	7	0
10	2G	631	0	605	5	0
10	2H	631	0	605	9	0
11	2J	1349	0	1408	8	0
11	2K	2554	0	2614	12	0
11	2L	2330	0	2400	18	0
11	2M	1589	0	1624	7	0
12	2O	4713	0	4699	6	0
12	2P	4713	0	4699	5	0
12	2Q	4713	0	4699	8	0
13	2S	2081	0	1873	19	0
13	2T	1694	0	1714	13	0
14	2V	287	0	270	3	0
14	2W	1756	0	1756	11	0
14	2X	1711	0	1706	13	0
14	2Y	1327	0	1334	13	0
15	3A	1487	0	1428	17	0
16	3C	1693	0	1653	36	0
16	3D	531	0	532	8	0
17	3F	520	0	221	0	0
18	3H	481	0	216	0	0
19	3J	3563	0	3513	49	0
19	3K	3652	0	3604	77	0
19	3L	3726	0	3675	74	0
20	3N	2388	0	2308	60	0
20	3O	4781	0	4714	95	0
20	3P	4787	0	4707	88	0
20	3Q	2409	0	2414	26	0
21	3S	563	0	565	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	3T	1939	0	2008	29	0
21	3U	1939	0	2008	27	0
21	3V	1696	0	1761	28	0
22	3X	1014	0	974	19	0
22	3Y	1116	0	1085	41	0
22	3Z	1059	0	1008	31	0
22	4A	840	0	810	30	0
22	4B	830	0	795	16	0
22	4C	667	0	637	24	0
23	4D	992	0	974	27	0
24	4F	1261	0	1276	44	0
24	4G	2883	0	2934	54	0
25	4I	2533	0	2088	32	0
25	4J	2947	0	2927	60	0
26	4K	1102	0	1103	27	0
26	4L	1911	0	1935	45	0
26	4M	876	0	903	22	0
27	4O	1767	0	1777	32	0
27	4P	1767	0	1777	22	0
27	4Q	1767	0	1777	34	0
27	4R	1767	0	1777	62	0
27	4S	1767	0	1777	15	0
27	4T	1767	0	1777	31	0
28	4V	304	0	287	14	0
28	4W	654	0	616	16	0
29	4Y	775	0	745	23	0
30	5A	2915	0	2907	67	0
30	5B	133	0	110	6	0
31	5D	1260	0	1246	24	0
31	5E	1254	0	1235	23	0
31	5F	1277	0	1270	8	0
31	5G	1260	0	1246	29	0
31	5H	1260	0	1246	17	0
31	5I	1260	0	1246	6	0
31	5J	1260	0	1246	25	0
32	5L	943	0	978	22	0
32	5M	3231	0	3294	69	0
32	5N	3231	0	3294	56	0
32	5O	2414	0	2445	71	0
33	5Q	901	0	878	25	0
33	5R	3250	0	3272	65	0
33	5S	3250	0	3272	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	5T	2498	0	2529	78	0
33	5V	2513	0	2534	97	0
33	5W	3336	0	3348	95	0
33	5X	3336	0	3348	92	0
33	5Y	877	0	846	12	0
34	6A	2240	0	2185	123	0
34	6B	3189	0	3161	102	0
34	6C	3200	0	3174	116	0
34	6D	992	0	1015	43	0
34	6E	487	0	509	28	0
34	6F	2896	0	2894	62	0
34	6G	3386	0	3351	74	0
34	6H	2989	0	2948	70	0
34	6I	531	0	508	8	0
34	6J	553	0	512	13	0
34	6K	3022	0	2962	56	0
34	6L	3411	0	3370	87	0
34	6M	2923	0	2929	69	0
34	6N	445	0	463	14	0
35	6P	1491	0	1389	21	0
35	6Q	3364	0	3303	60	0
35	6R	3364	0	3303	66	0
35	6S	2057	0	2109	48	0
35	6T	1917	0	1965	51	0
35	6U	3413	0	3327	76	0
35	6V	3571	0	3522	99	0
35	6W	1766	0	1683	59	0
36	6Y	1300	0	1065	13	0
36	6Z	1300	0	1065	11	0
37	7C	898	0	885	65	0
37	7D	618	0	637	25	0
37	7E	625	0	614	30	0
37	7F	519	0	497	26	0
38	7H	637	0	600	44	0
38	7I	238	0	215	14	0
39	7K	878	0	850	11	0
39	7L	382	0	368	7	0
40	7N	524	0	492	13	0
41	AB	3424	0	3291	83	0
41	AD	3424	0	3293	79	0
41	AF	3424	0	3291	67	0
41	AH	3424	0	3293	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	AJ	3424	0	3293	66	0
41	AL	3424	0	3293	73	0
41	BB	3356	0	3237	57	0
41	BD	3356	0	3240	134	0
41	BF	3361	0	3245	62	0
41	BH	3356	0	3240	78	0
41	BJ	3356	0	3240	77	0
41	BL	3340	0	3223	77	0
41	CB	3348	0	3236	84	0
41	CD	3348	0	3236	125	0
41	CF	3361	0	3245	153	0
41	CH	3356	0	3240	92	0
41	CJ	3361	0	3245	146	0
41	CL	3340	0	3224	108	0
41	DB	3348	0	3234	110	0
41	DD	3348	0	3235	99	0
41	DF	3348	0	3236	101	0
41	DH	3348	0	3236	239	0
41	DJ	3348	0	3236	261	0
41	DL	3340	0	3223	122	0
41	ED	3348	0	3236	206	0
41	EF	3348	0	3236	115	0
41	EH	3361	0	3243	106	0
41	EJ	3348	0	3235	120	0
41	EL	3340	0	3224	117	0
41	FD	3356	0	3240	169	0
41	FF	3348	0	3234	108	0
41	FH	3348	0	3236	125	0
41	FJ	3348	0	3236	146	0
41	FL	3340	0	3223	185	0
41	GD	3356	0	3240	109	0
41	GF	3361	0	3244	75	0
41	GH	3361	0	3245	80	0
41	GJ	3361	0	3245	148	0
41	GL	3340	0	3224	72	0
41	HB	3348	0	3236	81	0
41	HD	3356	0	3240	165	0
41	HF	3361	0	3245	101	0
41	HH	3356	0	3238	108	0
41	HJ	3361	0	3245	157	0
41	HL	3340	0	3224	84	0
41	ID	3356	0	3240	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	IF	3361	0	3244	96	0
41	IH	3356	0	3240	68	0
41	IJ	3361	0	3245	76	0
41	IL	3348	0	3236	98	0
41	IN	3361	0	3245	187	0
41	JD	3356	0	3239	84	0
41	JF	3348	0	3236	71	0
41	JH	3348	0	3235	80	0
41	JJ	3348	0	3236	89	0
41	JL	3348	0	3236	90	0
41	KD	3361	0	3244	93	0
41	KF	3356	0	3239	67	0
41	KH	3368	0	3252	73	0
41	KJ	3348	0	3235	66	0
41	KL	3368	0	3252	74	0
41	KN	3361	0	3245	59	0
41	LD	3356	0	3240	78	0
41	LF	3361	0	3243	45	0
41	LH	3361	0	3245	54	0
41	LJ	3361	0	3245	57	0
41	LL	3348	0	3236	66	0
41	LN	3361	0	3245	62	0
41	MD	3348	0	3236	132	0
41	MF	3361	0	3245	90	0
41	MH	3361	0	3245	59	0
41	MJ	3348	0	3236	78	0
41	ML	3348	0	3236	111	0
41	MN	3348	0	3236	130	0
41	NB	3361	0	3245	111	0
41	ND	3356	0	3240	107	0
41	NF	3356	0	3240	95	0
41	NH	3361	0	3245	96	0
41	NJ	3361	0	3245	79	0
41	NL	3118	0	3001	81	0
41	OB	3339	0	3228	179	0
41	OD	3327	0	3218	100	0
41	OF	3339	0	3227	92	0
41	OH	3361	0	3245	107	0
41	OJ	3361	0	3245	113	0
41	OL	3327	0	3219	95	0
41	PB	3356	0	3240	150	0
41	PD	3356	0	3240	129	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	PF	3361	0	3245	137	0
41	PH	3361	0	3245	258	0
41	PJ	3361	0	3245	216	0
41	PL	3340	0	3224	177	0
41	QB	3361	0	3245	104	0
41	QD	3356	0	3240	108	0
41	QF	3361	0	3244	106	0
41	QH	3361	0	3245	168	0
41	QJ	3361	0	3245	161	0
41	QL	3348	0	3236	188	0
41	RB	3361	0	3244	113	0
41	RD	3356	0	3240	158	0
41	RF	3361	0	3245	188	0
41	RH	3361	0	3245	101	0
41	RJ	3361	0	3245	153	0
41	RL	3348	0	3236	88	0
41	SD	3356	0	3239	107	0
41	SF	3361	0	3245	140	0
41	SH	3361	0	3243	118	0
41	SJ	3361	0	3244	88	0
41	SL	3348	0	3236	159	0
41	TD	3356	0	3240	103	0
41	TF	3361	0	3245	110	0
41	TH	3361	0	3245	107	0
41	TJ	3361	0	3245	121	0
41	TL	3348	0	3236	114	0
41	UD	3356	0	3238	107	0
41	UF	3361	0	3244	83	0
41	UH	3361	0	3245	96	0
41	UJ	3361	0	3243	109	0
41	UL	3348	0	3236	113	0
41	VD	3356	0	3240	87	0
41	VF	3356	0	3240	94	0
41	VH	3361	0	3244	87	0
41	VJ	3361	0	3244	70	0
41	VL	3348	0	3236	88	0
41	WD	3356	0	3240	60	0
41	WF	3348	0	3236	97	0
41	WH	3348	0	3236	86	0
41	WJ	3348	0	3236	85	0
41	WL	3348	0	3236	75	0
41	WN	3348	0	3236	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	AC	3437	0	3349	55	0
42	AE	3437	0	3349	63	0
42	AG	3437	0	3349	75	0
42	AI	3437	0	3349	131	0
42	AK	3437	0	3349	133	0
42	BC	3437	0	3349	92	0
42	BE	3396	0	3305	70	0
42	BG	3437	0	3349	75	0
42	BI	3374	0	3285	136	0
42	BK	3430	0	3340	68	0
42	CC	3424	0	3335	166	0
42	CE	3424	0	3335	89	0
42	CG	3430	0	3340	181	0
42	CI	3430	0	3340	88	0
42	CK	3430	0	3340	79	0
42	CM	3430	0	3340	94	0
42	DC	3366	0	3281	99	0
42	DE	3372	0	3286	100	0
42	DG	3379	0	3295	83	0
42	DI	3364	0	3282	114	0
42	DK	3372	0	3286	203	0
42	DM	3372	0	3285	92	0
42	EC	3430	0	3340	110	0
42	EE	3446	0	3355	177	0
42	EG	3404	0	3321	211	0
42	EI	3408	0	3322	105	0
42	EK	3437	0	3349	223	0
42	EM	3358	0	3277	187	0
42	FC	3379	0	3295	170	0
42	FE	3339	0	3258	115	0
42	FG	3346	0	3264	104	0
42	FI	3347	0	3270	125	0
42	FK	3326	0	3250	206	0
42	FM	3365	0	3279	140	0
42	GC	3437	0	3349	82	0
42	GE	3371	0	3291	74	0
42	GG	3393	0	3304	71	0
42	GI	3365	0	3285	86	0
42	GK	3364	0	3283	106	0
42	GM	3430	0	3340	155	0
42	HC	3350	0	3273	188	0
42	HE	3374	0	3285	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	HG	3371	0	3291	176	0
42	HI	3371	0	3291	151	0
42	HK	3379	0	3295	127	0
42	HM	3365	0	3279	143	0
42	IC	3365	0	3286	63	0
42	IE	3388	0	3301	99	0
42	IG	3437	0	3349	78	0
42	II	3387	0	3299	80	0
42	IK	3437	0	3348	96	0
42	IM	3378	0	3291	80	0
42	JC	3384	0	3295	72	0
42	JE	3372	0	3285	76	0
42	JG	3358	0	3277	64	0
42	JI	3366	0	3281	70	0
42	JK	3437	0	3349	157	0
42	JM	3372	0	3286	91	0
42	KC	3384	0	3293	41	0
42	KE	3380	0	3290	52	0
42	KG	3370	0	3284	66	0
42	KI	3358	0	3277	59	0
42	KK	3372	0	3286	63	0
42	KM	3376	0	3286	75	0
42	LC	3393	0	3304	57	0
42	LE	3437	0	3349	63	0
42	LG	3393	0	3304	51	0
42	LI	3397	0	3307	54	0
42	LK	3401	0	3310	56	0
42	LM	3378	0	3291	57	0
42	MC	3430	0	3340	94	0
42	ME	3366	0	3281	60	0
42	MG	3372	0	3286	82	0
42	MI	3379	0	3295	63	0
42	MK	3437	0	3349	125	0
42	MM	3376	0	3281	116	0
42	NA	3372	0	3278	98	0
42	NC	3365	0	3286	156	0
42	NE	3374	0	3292	70	0
42	NG	3387	0	3299	93	0
42	NI	3387	0	3299	126	0
42	NK	3374	0	3285	125	0
42	OA	3358	0	3269	95	0
42	OC	3366	0	3281	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	OE	3396	0	3305	114	0
42	OG	3391	0	3302	95	0
42	OI	3387	0	3299	91	0
42	OK	3380	0	3289	102	0
42	PA	2872	0	2816	166	0
42	PC	3386	0	3295	170	0
42	PE	3380	0	3297	149	0
42	PG	3371	0	3291	257	0
42	PI	3349	0	3263	244	0
42	PK	3371	0	3291	137	0
42	QC	3372	0	3286	105	0
42	QE	3372	0	3285	105	0
42	QG	3380	0	3290	119	0
42	QI	3366	0	3281	163	0
42	QK	3380	0	3290	139	0
42	RC	3387	0	3299	109	0
42	RE	3358	0	3275	100	0
42	RG	3372	0	3288	119	0
42	RI	3379	0	3295	117	0
42	RK	3379	0	3295	127	0
42	SC	3372	0	3288	127	0
42	SE	3381	0	3294	149	0
42	SG	3379	0	3295	96	0
42	SI	3358	0	3267	144	0
42	SK	3387	0	3298	119	0
42	SM	3378	0	3291	118	0
42	TC	3371	0	3291	101	0
42	TE	3388	0	3301	110	0
42	TG	3371	0	3290	119	0
42	TI	3371	0	3291	152	0
42	TK	3387	0	3299	137	0
42	TM	3372	0	3286	154	0
42	UC	3393	0	3304	118	0
42	UE	3388	0	3301	100	0
42	UG	3393	0	3304	95	0
42	UI	3393	0	3303	97	0
42	UK	3391	0	3302	95	0
42	UM	3378	0	3291	99	0
42	VC	3437	0	3349	64	0
42	VE	3396	0	3305	77	0
42	VG	3437	0	3349	83	0
42	VI	3393	0	3304	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	VK	3437	0	3349	115	0
42	VM	3372	0	3286	86	0
42	WC	3437	0	3349	54	0
42	WE	3380	0	3290	88	0
42	WG	3430	0	3340	70	0
42	WI	3380	0	3290	88	0
42	WK	3424	0	3335	72	0
42	WM	3378	0	3291	81	0
43	AB	28	0	11	0	0
43	AD	28	0	12	0	0
43	AF	28	0	12	1	0
43	AH	28	0	12	0	0
43	AJ	28	0	12	1	0
43	AL	28	0	12	0	0
43	BB	28	0	10	0	0
43	BD	28	0	12	0	0
43	BF	28	0	12	1	0
43	BH	28	0	12	0	0
43	BJ	28	0	12	1	0
43	BL	28	0	12	0	0
43	CB	28	0	12	2	0
43	CD	28	0	12	0	0
43	CF	28	0	12	3	0
43	CH	28	0	12	0	0
43	CJ	28	0	12	1	0
43	CL	28	0	12	0	0
43	DB	28	0	12	0	0
43	DD	28	0	12	2	0
43	DF	28	0	12	1	0
43	DH	28	0	12	3	0
43	DJ	28	0	12	1	0
43	DL	28	0	11	1	0
43	ED	28	0	12	2	0
43	EF	28	0	12	2	0
43	EH	28	0	12	3	0
43	EJ	28	0	11	1	0
43	EL	28	0	12	0	0
43	FD	28	0	12	3	0
43	FF	28	0	10	2	0
43	FH	28	0	12	3	0
43	FJ	28	0	12	0	0
43	FL	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	GD	28	0	12	0	0
43	GF	28	0	12	3	0
43	GH	28	0	12	0	0
43	GJ	28	0	12	1	0
43	GL	28	0	12	2	0
43	HB	28	0	12	1	0
43	HD	28	0	12	2	0
43	HF	28	0	12	0	0
43	HH	28	0	11	4	0
43	HJ	28	0	12	0	0
43	HL	28	0	12	0	0
43	ID	28	0	12	3	0
43	IF	28	0	12	3	0
43	IH	28	0	11	2	0
43	IJ	28	0	12	2	0
43	IL	28	0	11	2	0
43	IN	28	0	12	0	0
43	JD	28	0	11	1	0
43	JF	28	0	12	2	0
43	JH	28	0	12	3	0
43	JJ	28	0	12	0	0
43	JL	28	0	12	1	0
43	KD	28	0	12	1	0
43	KF	28	0	12	0	0
43	KG	28	0	11	1	0
43	KJ	28	0	12	0	0
43	KL	28	0	12	0	0
43	KN	28	0	12	1	0
43	LD	28	0	12	1	0
43	LF	28	0	12	1	0
43	LH	28	0	12	1	0
43	LJ	28	0	12	0	0
43	LL	28	0	12	2	0
43	LN	28	0	12	2	0
43	MD	28	0	12	2	0
43	MF	28	0	12	0	0
43	MH	28	0	12	1	0
43	MJ	28	0	12	0	0
43	ML	28	0	12	2	0
43	MN	28	0	12	1	0
43	NB	28	0	12	0	0
43	ND	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	NF	28	0	12	0	0
43	NH	28	0	12	0	0
43	NJ	28	0	12	1	0
43	NL	28	0	12	1	0
43	OB	28	0	12	0	0
43	OD	28	0	12	1	0
43	OF	28	0	12	0	0
43	OH	28	0	12	1	0
43	OJ	28	0	12	1	0
43	OL	28	0	11	0	0
43	PB	28	0	12	1	0
43	PD	28	0	12	0	0
43	PF	28	0	12	0	0
43	PH	28	0	12	2	0
43	PJ	28	0	12	2	0
43	PL	28	0	12	1	0
43	QB	28	0	12	3	0
43	QD	28	0	12	0	0
43	QF	28	0	12	1	0
43	QH	28	0	12	1	0
43	QJ	28	0	12	2	0
43	QL	28	0	12	2	0
43	RB	28	0	12	2	0
43	RD	28	0	12	1	0
43	RF	28	0	12	1	0
43	RH	28	0	12	0	0
43	RJ	28	0	12	2	0
43	RL	28	0	12	0	0
43	SD	28	0	12	0	0
43	SF	28	0	12	2	0
43	SH	28	0	12	0	0
43	SJ	28	0	11	1	0
43	SL	28	0	12	3	0
43	TD	28	0	12	1	0
43	TF	28	0	12	0	0
43	TH	28	0	11	1	0
43	TJ	28	0	12	1	0
43	TL	28	0	12	0	0
43	UD	28	0	12	0	0
43	UF	28	0	12	0	0
43	UH	28	0	12	0	0
43	UJ	28	0	10	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	UL	28	0	12	1	0
43	VD	28	0	12	1	0
43	VF	28	0	12	0	0
43	VH	28	0	12	1	0
43	VJ	28	0	12	0	0
43	VL	28	0	12	1	0
43	WD	28	0	12	2	0
43	WF	28	0	12	2	0
43	WH	28	0	12	0	0
43	WJ	28	0	12	1	0
43	WL	28	0	12	0	0
43	WN	28	0	12	2	0
44	AB	1	0	0	0	0
44	AE	1	0	0	0	0
44	AG	1	0	0	0	0
44	AI	1	0	0	0	0
44	AK	1	0	0	0	0
44	BC	1	0	0	0	0
44	BE	1	0	0	0	0
44	BG	1	0	0	0	0
44	BI	1	0	0	0	0
44	BK	1	0	0	0	0
44	CC	1	0	0	0	0
44	CE	1	0	0	0	0
44	CI	1	0	0	0	0
44	CK	1	0	0	0	0
44	CM	1	0	0	0	0
44	DM	1	0	0	0	0
44	EK	1	0	0	0	0
44	FC	1	0	0	0	0
44	FD	1	0	0	0	0
44	FG	1	0	0	0	0
44	FI	1	0	0	0	0
44	FK	1	0	0	0	0
44	FL	1	0	0	0	0
44	GC	1	0	0	0	0
44	GE	1	0	0	0	0
44	GG	1	0	0	0	0
44	GI	1	0	0	0	0
44	GK	1	0	0	0	0
44	GM	1	0	0	0	0
44	HC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	HE	1	0	0	0	0
44	HG	1	0	0	0	0
44	HI	1	0	0	0	0
44	HK	1	0	0	0	0
44	HM	1	0	0	0	0
44	IC	1	0	0	0	0
44	IE	1	0	0	0	0
44	IG	1	0	0	0	0
44	IK	1	0	0	0	0
44	IL	1	0	0	0	0
44	JC	1	0	0	0	0
44	JE	1	0	0	0	0
44	JG	1	0	0	0	0
44	JI	1	0	0	0	0
44	JK	1	0	0	0	0
44	JM	1	0	0	0	0
44	KC	1	0	0	0	0
44	KE	1	0	0	0	0
44	KG	1	0	0	0	0
44	KI	1	0	0	0	0
44	KK	1	0	0	0	0
44	KM	1	0	0	0	0
44	LC	1	0	0	0	0
44	LD	1	0	0	0	0
44	LG	1	0	0	0	0
44	LI	1	0	0	0	0
44	LK	1	0	0	0	0
44	LM	1	0	0	0	0
44	MC	1	0	0	0	0
44	ME	1	0	0	0	0
44	MH	1	0	0	0	0
44	MK	1	0	0	0	0
44	MM	1	0	0	0	0
44	NA	1	0	0	0	0
44	NB	1	0	0	0	0
44	NE	1	0	0	0	0
44	NG	1	0	0	0	0
44	NI	1	0	0	0	0
44	NK	1	0	0	0	0
44	OA	1	0	0	0	0
44	OC	1	0	0	0	0
44	OE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	OI	1	0	0	0	0
44	OK	1	0	0	0	0
44	PC	1	0	0	0	0
44	PE	1	0	0	0	0
44	PG	1	0	0	0	0
44	PI	1	0	0	0	0
44	SC	1	0	0	0	0
44	SD	1	0	0	0	0
44	SF	1	0	0	0	0
44	SH	1	0	0	0	0
44	SJ	1	0	0	0	0
44	TC	1	0	0	0	0
44	TD	1	0	0	0	0
44	TF	1	0	0	0	0
44	TI	1	0	0	0	0
44	TK	1	0	0	0	0
44	TL	1	0	0	0	0
44	UE	1	0	0	0	0
44	UG	1	0	0	0	0
44	UI	1	0	0	0	0
44	UK	1	0	0	0	0
44	UM	1	0	0	0	0
44	VC	1	0	0	0	0
44	VE	1	0	0	0	0
44	VG	1	0	0	0	0
44	VI	1	0	0	0	0
44	VJ	1	0	0	0	0
44	VM	1	0	0	0	0
44	WC	1	0	0	0	0
44	WD	1	0	0	0	0
44	WG	1	0	0	0	0
44	WI	1	0	0	0	0
44	WK	1	0	0	0	0
44	WM	1	0	0	0	0
45	AC	32	0	12	2	0
45	AE	32	0	12	2	0
45	AF	32	0	12	3	0
45	AI	32	0	12	1	0
45	AK	32	0	12	0	0
45	BC	32	0	12	1	0
45	BE	32	0	12	0	0
45	BG	32	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	BI	32	0	12	1	0
45	BK	32	0	12	2	0
45	CC	32	0	12	0	0
45	CE	32	0	12	4	0
45	CG	32	0	12	4	0
45	CI	32	0	11	4	0
45	CK	32	0	12	2	0
45	CM	32	0	12	4	0
45	DC	32	0	11	4	0
45	DE	32	0	12	2	0
45	DG	32	0	12	0	0
45	DI	32	0	12	2	0
45	DK	32	0	12	1	0
45	DM	32	0	11	0	0
45	EC	32	0	12	1	0
45	EE	32	0	12	1	0
45	EG	32	0	12	6	0
45	EI	32	0	12	2	0
45	EK	32	0	12	2	0
45	EM	32	0	12	0	0
45	FC	32	0	12	2	0
45	FE	32	0	12	1	0
45	FF	32	0	12	1	0
45	FI	32	0	12	2	0
45	FK	32	0	12	5	0
45	FM	32	0	12	1	0
45	GC	32	0	11	3	0
45	GE	32	0	12	3	0
45	GF	32	0	11	0	0
45	GI	32	0	10	0	0
45	GK	32	0	12	2	0
45	GM	32	0	12	3	0
45	HC	32	0	12	3	0
45	HE	32	0	12	1	0
45	HG	32	0	12	2	0
45	HI	32	0	12	1	0
45	HK	32	0	12	2	0
45	HM	32	0	12	0	0
45	IC	32	0	12	0	0
45	IE	32	0	12	2	0
45	IG	32	0	12	0	0
45	II	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	IK	32	0	11	1	0
45	IM	32	0	12	0	0
45	JC	32	0	11	0	0
45	JE	32	0	12	2	0
45	JG	32	0	12	1	0
45	JI	32	0	12	1	0
45	JK	32	0	12	3	0
45	JM	32	0	12	3	0
45	KC	32	0	12	1	0
45	KE	32	0	12	1	0
45	KG	32	0	12	1	0
45	KI	32	0	12	0	0
45	KK	32	0	12	1	0
45	KM	32	0	12	0	0
45	LC	32	0	12	0	0
45	LE	32	0	12	3	0
45	LF	32	0	11	1	0
45	LI	32	0	12	1	0
45	LK	32	0	12	0	0
45	LM	32	0	12	0	0
45	MC	32	0	12	1	0
45	ME	32	0	12	1	0
45	MG	32	0	12	0	0
45	MI	32	0	12	2	0
45	MK	32	0	12	0	0
45	MM	32	0	12	4	0
45	NA	32	0	12	2	0
45	NC	32	0	12	3	0
45	NE	32	0	12	1	0
45	NG	32	0	12	0	0
45	NI	32	0	12	1	0
45	NK	32	0	12	2	0
45	OA	32	0	12	2	0
45	OC	32	0	12	1	0
45	OE	32	0	12	2	0
45	OG	32	0	12	0	0
45	OI	32	0	12	2	0
45	OK	32	0	12	1	0
45	PA	32	0	12	3	0
45	PC	32	0	12	1	0
45	PE	32	0	12	3	0
45	PG	32	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	PI	32	0	12	3	0
45	PK	32	0	12	5	0
45	QC	32	0	12	1	0
45	QE	32	0	12	0	0
45	QG	32	0	12	2	0
45	QI	32	0	12	1	0
45	QK	32	0	12	2	0
45	RC	32	0	12	0	0
45	RE	32	0	10	0	0
45	RG	32	0	12	3	0
45	RI	32	0	12	2	0
45	RK	32	0	12	2	0
45	SC	32	0	12	0	0
45	SE	32	0	12	3	0
45	SG	32	0	12	0	0
45	SI	32	0	12	2	0
45	SK	32	0	12	0	0
45	SM	32	0	12	3	0
45	TC	32	0	12	0	0
45	TE	32	0	12	3	0
45	TG	32	0	12	2	0
45	TI	32	0	12	1	0
45	TK	32	0	12	0	0
45	TM	32	0	12	2	0
45	UC	32	0	12	4	0
45	UE	32	0	12	1	0
45	UG	32	0	12	0	0
45	UI	32	0	12	1	0
45	UK	32	0	12	1	0
45	UM	32	0	12	1	0
45	VC	32	0	12	1	0
45	VE	32	0	12	1	0
45	VG	32	0	12	0	0
45	VI	32	0	12	1	0
45	VK	32	0	12	0	0
45	VM	32	0	12	4	0
45	WC	32	0	12	2	0
45	WE	32	0	12	2	0
45	WG	32	0	12	1	0
45	WI	32	0	12	0	0
45	WK	32	0	12	3	0
45	WM	32	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1132145	0	1096916	29327	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 13.

The worst 5 of 29327 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)
42:EI:346:TRP:CH2	42:EI:346:TRP:CZ3	1.87	1.57
41:EJ:391:ARG:CB	41:EJ:391:ARG:CG	1.76	1.57
41:BL:281:TYR:CD2	41:BL:281:TYR:CG	1.96	1.53
41:BL:281:TYR:CG	41:BL:281:TYR:CD1	1.96	1.51
41:EJ:391:ARG:CG	41:EJ:391:ARG:CD	1.84	1.51

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	1A	489/1044 (47%)	425 (87%)	56 (12%)	8 (2%)	8 36
2	1D	130/687 (19%)	123 (95%)	5 (4%)	2 (2%)	8 37
2	1E	183/687 (27%)	174 (95%)	9 (5%)	0	100 100
2	1F	81/687 (12%)	79 (98%)	2 (2%)	0	100 100
3	1H	81/547 (15%)	78 (96%)	3 (4%)	0	100 100
3	1I	375/547 (69%)	364 (97%)	11 (3%)	0	100 100
4	1K	157/196 (80%)	135 (86%)	22 (14%)	0	100 100
4	1L	30/196 (15%)	27 (90%)	3 (10%)	0	100 100
5	1N	112/196 (57%)	101 (90%)	10 (9%)	1 (1%)	14 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1O	114/196 (58%)	111 (97%)	3 (3%)	0	100	100
5	1P	116/196 (59%)	108 (93%)	8 (7%)	0	100	100
6	1R	89/101 (88%)	89 (100%)	0	0	100	100
7	1T	251/321 (78%)	227 (90%)	23 (9%)	1 (0%)	30	63
7	1U	251/321 (78%)	210 (84%)	37 (15%)	4 (2%)	8	36
8	1W	126/193 (65%)	89 (71%)	32 (25%)	5 (4%)	2	19
8	1X	182/193 (94%)	172 (94%)	10 (6%)	0	100	100
8	1Y	182/193 (94%)	173 (95%)	9 (5%)	0	100	100
8	1Z	182/193 (94%)	169 (93%)	13 (7%)	0	100	100
8	2A	182/193 (94%)	164 (90%)	18 (10%)	0	100	100
8	2B	182/193 (94%)	168 (92%)	14 (8%)	0	100	100
9	2D	449/877 (51%)	377 (84%)	69 (15%)	3 (1%)	19	53
9	2E	99/877 (11%)	97 (98%)	2 (2%)	0	100	100
10	2F	75/170 (44%)	68 (91%)	7 (9%)	0	100	100
10	2G	75/170 (44%)	69 (92%)	6 (8%)	0	100	100
10	2H	75/170 (44%)	65 (87%)	10 (13%)	0	100	100
11	2J	160/549 (29%)	154 (96%)	5 (3%)	1 (1%)	22	55
11	2K	292/549 (53%)	288 (99%)	4 (1%)	0	100	100
11	2L	273/549 (50%)	252 (92%)	20 (7%)	1 (0%)	30	63
11	2M	182/549 (33%)	173 (95%)	9 (5%)	0	100	100
12	2O	607/623 (97%)	531 (88%)	72 (12%)	4 (1%)	19	53
12	2P	607/623 (97%)	515 (85%)	88 (14%)	4 (1%)	19	53
12	2Q	607/623 (97%)	505 (83%)	101 (17%)	1 (0%)	44	75
13	2S	279/514 (54%)	265 (95%)	13 (5%)	1 (0%)	30	63
13	2T	197/514 (38%)	186 (94%)	9 (5%)	2 (1%)	13	45
14	2V	32/284 (11%)	30 (94%)	2 (6%)	0	100	100
14	2W	207/284 (73%)	163 (79%)	42 (20%)	2 (1%)	13	45
14	2X	202/284 (71%)	186 (92%)	13 (6%)	3 (2%)	8	37
14	2Y	161/284 (57%)	138 (86%)	21 (13%)	2 (1%)	11	42
15	3A	179/232 (77%)	142 (79%)	33 (18%)	4 (2%)	5	30
16	3C	209/309 (68%)	175 (84%)	31 (15%)	3 (1%)	9	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	3D	67/309 (22%)	61 (91%)	6 (9%)	0	100	100
17	3F	97/212 (46%)	86 (89%)	9 (9%)	2 (2%)	5	31
18	3H	95/1410 (7%)	88 (93%)	7 (7%)	0	100	100
19	3J	425/640 (66%)	371 (87%)	50 (12%)	4 (1%)	14	48
19	3K	437/640 (68%)	376 (86%)	58 (13%)	3 (1%)	19	53
19	3L	446/640 (70%)	386 (86%)	60 (14%)	0	100	100
20	3N	278/733 (38%)	246 (88%)	31 (11%)	1 (0%)	30	63
20	3O	561/733 (76%)	486 (87%)	71 (13%)	4 (1%)	19	53
20	3P	563/733 (77%)	527 (94%)	36 (6%)	0	100	100
20	3Q	280/733 (38%)	252 (90%)	25 (9%)	3 (1%)	12	44
21	3S	68/259 (26%)	63 (93%)	5 (7%)	0	100	100
21	3T	231/259 (89%)	217 (94%)	14 (6%)	0	100	100
21	3U	231/259 (89%)	214 (93%)	17 (7%)	0	100	100
21	3V	199/259 (77%)	191 (96%)	8 (4%)	0	100	100
22	3X	119/274 (43%)	109 (92%)	10 (8%)	0	100	100
22	3Y	132/274 (48%)	104 (79%)	25 (19%)	3 (2%)	5	29
22	3Z	125/274 (46%)	103 (82%)	21 (17%)	1 (1%)	16	50
22	4A	99/274 (36%)	95 (96%)	4 (4%)	0	100	100
22	4B	99/274 (36%)	91 (92%)	8 (8%)	0	100	100
22	4C	79/274 (29%)	74 (94%)	5 (6%)	0	100	100
23	4D	114/135 (84%)	100 (88%)	11 (10%)	3 (3%)	4	27
24	4F	149/495 (30%)	141 (95%)	8 (5%)	0	100	100
24	4G	333/495 (67%)	321 (96%)	11 (3%)	1 (0%)	37	68
25	4I	370/377 (98%)	346 (94%)	24 (6%)	0	100	100
25	4J	370/377 (98%)	345 (93%)	24 (6%)	1 (0%)	37	68
26	4K	130/621 (21%)	128 (98%)	2 (2%)	0	100	100
26	4L	226/621 (36%)	217 (96%)	8 (4%)	1 (0%)	30	63
26	4M	102/621 (16%)	101 (99%)	1 (1%)	0	100	100
27	4O	217/257 (84%)	202 (93%)	15 (7%)	0	100	100
27	4P	217/257 (84%)	204 (94%)	13 (6%)	0	100	100
27	4Q	217/257 (84%)	205 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	4R	217/257 (84%)	162 (75%)	38 (18%)	17 (8%)	1	8
27	4S	217/257 (84%)	205 (94%)	12 (6%)	0	100	100
27	4T	217/257 (84%)	197 (91%)	17 (8%)	3 (1%)	9	39
28	4V	35/136 (26%)	30 (86%)	5 (14%)	0	100	100
28	4W	77/136 (57%)	70 (91%)	6 (8%)	1 (1%)	10	40
29	4Y	94/120 (78%)	81 (86%)	12 (13%)	1 (1%)	12	44
30	5A	348/377 (92%)	324 (93%)	20 (6%)	4 (1%)	12	44
30	5B	14/377 (4%)	11 (79%)	3 (21%)	0	100	100
31	5D	155/169 (92%)	146 (94%)	8 (5%)	1 (1%)	22	55
31	5E	155/169 (92%)	137 (88%)	14 (9%)	4 (3%)	4	27
31	5F	157/169 (93%)	148 (94%)	9 (6%)	0	100	100
31	5G	155/169 (92%)	148 (96%)	7 (4%)	0	100	100
31	5H	155/169 (92%)	148 (96%)	6 (4%)	1 (1%)	22	55
31	5I	155/169 (92%)	149 (96%)	5 (3%)	1 (1%)	22	55
31	5J	155/169 (92%)	147 (95%)	6 (4%)	2 (1%)	10	40
32	5L	114/418 (27%)	111 (97%)	3 (3%)	0	100	100
32	5M	390/418 (93%)	373 (96%)	17 (4%)	0	100	100
32	5N	390/418 (93%)	377 (97%)	13 (3%)	0	100	100
32	5O	287/418 (69%)	243 (85%)	34 (12%)	10 (4%)	3	23
33	5Q	105/430 (24%)	100 (95%)	4 (4%)	1 (1%)	13	45
33	5R	397/430 (92%)	384 (97%)	11 (3%)	2 (0%)	25	59
33	5S	397/430 (92%)	358 (90%)	28 (7%)	11 (3%)	4	26
33	5T	302/430 (70%)	273 (90%)	24 (8%)	5 (2%)	7	35
33	5V	304/430 (71%)	281 (92%)	21 (7%)	2 (1%)	19	53
33	5W	406/430 (94%)	384 (95%)	22 (5%)	0	100	100
33	5X	406/430 (94%)	387 (95%)	18 (4%)	1 (0%)	44	75
33	5Y	103/430 (24%)	99 (96%)	4 (4%)	0	100	100
34	6A	267/490 (54%)	199 (74%)	64 (24%)	4 (2%)	8	37
34	6B	390/490 (80%)	363 (93%)	22 (6%)	5 (1%)	10	40
34	6C	391/490 (80%)	312 (80%)	68 (17%)	11 (3%)	4	26
34	6D	121/490 (25%)	92 (76%)	27 (22%)	2 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	6E	57/490 (12%)	49 (86%)	6 (10%)	2 (4%)	3	23
34	6F	356/490 (73%)	339 (95%)	17 (5%)	0	100	100
34	6G	414/490 (84%)	404 (98%)	10 (2%)	0	100	100
34	6H	364/490 (74%)	339 (93%)	22 (6%)	3 (1%)	16	50
34	6I	61/490 (12%)	58 (95%)	3 (5%)	0	100	100
34	6J	61/490 (12%)	60 (98%)	1 (2%)	0	100	100
34	6K	365/490 (74%)	358 (98%)	7 (2%)	0	100	100
34	6L	414/490 (84%)	393 (95%)	17 (4%)	4 (1%)	13	45
34	6M	359/490 (73%)	353 (98%)	6 (2%)	0	100	100
34	6N	52/490 (11%)	50 (96%)	2 (4%)	0	100	100
35	6P	176/447 (39%)	175 (99%)	1 (1%)	0	100	100
35	6Q	408/447 (91%)	398 (98%)	10 (2%)	0	100	100
35	6R	408/447 (91%)	394 (97%)	13 (3%)	1 (0%)	44	75
35	6S	250/447 (56%)	233 (93%)	14 (6%)	3 (1%)	11	42
35	6T	232/447 (52%)	224 (97%)	8 (3%)	0	100	100
35	6U	417/447 (93%)	395 (95%)	20 (5%)	2 (0%)	25	59
35	6V	433/447 (97%)	392 (90%)	33 (8%)	8 (2%)	7	34
35	6W	209/447 (47%)	188 (90%)	17 (8%)	4 (2%)	6	33
36	6Y	188/683 (28%)	161 (86%)	24 (13%)	3 (2%)	8	36
36	6Z	188/683 (28%)	171 (91%)	17 (9%)	0	100	100
37	7C	107/254 (42%)	63 (59%)	38 (36%)	6 (6%)	1	14
37	7D	76/254 (30%)	60 (79%)	13 (17%)	3 (4%)	2	20
37	7E	73/254 (29%)	53 (73%)	20 (27%)	0	100	100
37	7F	55/254 (22%)	36 (66%)	17 (31%)	2 (4%)	3	21
38	7H	73/274 (27%)	47 (64%)	22 (30%)	4 (6%)	1	14
38	7I	28/274 (10%)	24 (86%)	4 (14%)	0	100	100
39	7K	103/147 (70%)	83 (81%)	18 (18%)	2 (2%)	6	33
39	7L	44/147 (30%)	39 (89%)	4 (9%)	1 (2%)	5	29
40	7N	54/484 (11%)	45 (83%)	9 (17%)	0	100	100
41	AB	434/445 (98%)	388 (89%)	44 (10%)	2 (0%)	25	59
41	AD	434/445 (98%)	415 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	AF	434/445 (98%)	418 (96%)	15 (4%)	1 (0%)	44	75
41	AH	434/445 (98%)	347 (80%)	68 (16%)	19 (4%)	2	17
41	AJ	434/445 (98%)	419 (96%)	15 (4%)	0	100	100
41	AL	434/445 (98%)	350 (81%)	66 (15%)	18 (4%)	2	19
41	BB	425/445 (96%)	400 (94%)	25 (6%)	0	100	100
41	BD	425/445 (96%)	325 (76%)	83 (20%)	17 (4%)	2	19
41	BF	426/445 (96%)	411 (96%)	15 (4%)	0	100	100
41	BH	425/445 (96%)	408 (96%)	15 (4%)	2 (0%)	25	59
41	BJ	425/445 (96%)	407 (96%)	18 (4%)	0	100	100
41	BL	423/445 (95%)	401 (95%)	22 (5%)	0	100	100
41	CB	424/445 (95%)	395 (93%)	29 (7%)	0	100	100
41	CD	424/445 (95%)	309 (73%)	91 (22%)	24 (6%)	1	13
41	CF	426/445 (96%)	314 (74%)	89 (21%)	23 (5%)	1	14
41	CH	425/445 (96%)	390 (92%)	33 (8%)	2 (0%)	25	59
41	CJ	426/445 (96%)	315 (74%)	85 (20%)	26 (6%)	1	12
41	CL	423/445 (95%)	383 (90%)	40 (10%)	0	100	100
41	DB	424/445 (95%)	370 (87%)	52 (12%)	2 (0%)	25	59
41	DD	424/445 (95%)	376 (89%)	46 (11%)	2 (0%)	25	59
41	DF	424/445 (95%)	365 (86%)	55 (13%)	4 (1%)	14	48
41	DH	424/445 (95%)	272 (64%)	111 (26%)	41 (10%)	0	6
41	DJ	424/445 (95%)	261 (62%)	120 (28%)	43 (10%)	0	6
41	DL	423/445 (95%)	353 (84%)	58 (14%)	12 (3%)	4	26
41	ED	424/445 (95%)	266 (63%)	121 (28%)	37 (9%)	0	7
41	EF	424/445 (95%)	377 (89%)	44 (10%)	3 (1%)	19	53
41	EH	426/445 (96%)	357 (84%)	65 (15%)	4 (1%)	14	48
41	EJ	424/445 (95%)	374 (88%)	45 (11%)	5 (1%)	11	42
41	EL	423/445 (95%)	352 (83%)	66 (16%)	5 (1%)	11	42
41	FD	425/445 (96%)	290 (68%)	101 (24%)	34 (8%)	1	8
41	FF	424/445 (95%)	379 (89%)	41 (10%)	4 (1%)	14	48
41	FH	424/445 (95%)	378 (89%)	44 (10%)	2 (0%)	25	59
41	FJ	424/445 (95%)	396 (93%)	28 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	FL	423/445 (95%)	289 (68%)	103 (24%)	31 (7%)	1	9
41	GD	425/445 (96%)	321 (76%)	78 (18%)	26 (6%)	1	12
41	GF	426/445 (96%)	404 (95%)	22 (5%)	0	100	100
41	GH	426/445 (96%)	391 (92%)	35 (8%)	0	100	100
41	GJ	426/445 (96%)	321 (75%)	85 (20%)	20 (5%)	2	17
41	GL	423/445 (95%)	399 (94%)	24 (6%)	0	100	100
41	HB	424/445 (95%)	360 (85%)	59 (14%)	5 (1%)	11	42
41	HD	425/445 (96%)	303 (71%)	91 (21%)	31 (7%)	1	9
41	HF	426/445 (96%)	385 (90%)	39 (9%)	2 (0%)	25	59
41	HH	425/445 (96%)	384 (90%)	39 (9%)	2 (0%)	25	59
41	HJ	426/445 (96%)	310 (73%)	98 (23%)	18 (4%)	2	18
41	HL	423/445 (95%)	373 (88%)	48 (11%)	2 (0%)	25	59
41	ID	425/445 (96%)	403 (95%)	21 (5%)	1 (0%)	44	75
41	IF	426/445 (96%)	406 (95%)	20 (5%)	0	100	100
41	IH	425/445 (96%)	404 (95%)	20 (5%)	1 (0%)	44	75
41	IJ	426/445 (96%)	411 (96%)	15 (4%)	0	100	100
41	IL	424/445 (95%)	406 (96%)	18 (4%)	0	100	100
41	IN	426/445 (96%)	303 (71%)	92 (22%)	31 (7%)	1	9
41	JD	425/445 (96%)	384 (90%)	41 (10%)	0	100	100
41	JF	424/445 (95%)	403 (95%)	21 (5%)	0	100	100
41	JH	424/445 (95%)	405 (96%)	19 (4%)	0	100	100
41	JJ	424/445 (95%)	400 (94%)	24 (6%)	0	100	100
41	JL	424/445 (95%)	346 (82%)	68 (16%)	10 (2%)	5	29
41	KD	426/445 (96%)	406 (95%)	19 (4%)	1 (0%)	44	75
41	KF	425/445 (96%)	410 (96%)	15 (4%)	0	100	100
41	KH	427/445 (96%)	414 (97%)	13 (3%)	0	100	100
41	KJ	424/445 (95%)	410 (97%)	14 (3%)	0	100	100
41	KL	427/445 (96%)	407 (95%)	20 (5%)	0	100	100
41	KN	426/445 (96%)	407 (96%)	17 (4%)	2 (0%)	25	59
41	LD	425/445 (96%)	366 (86%)	51 (12%)	8 (2%)	6	33
41	LF	426/445 (96%)	411 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	LH	426/445 (96%)	409 (96%)	17 (4%)	0	100	100
41	LJ	426/445 (96%)	408 (96%)	18 (4%)	0	100	100
41	LL	424/445 (95%)	406 (96%)	18 (4%)	0	100	100
41	LN	426/445 (96%)	407 (96%)	19 (4%)	0	100	100
41	MD	424/445 (95%)	326 (77%)	79 (19%)	19 (4%)	2	17
41	MF	426/445 (96%)	345 (81%)	68 (16%)	13 (3%)	3	25
41	MH	426/445 (96%)	413 (97%)	13 (3%)	0	100	100
41	MJ	424/445 (95%)	405 (96%)	19 (4%)	0	100	100
41	ML	424/445 (95%)	393 (93%)	30 (7%)	1 (0%)	44	75
41	MN	424/445 (95%)	328 (77%)	74 (18%)	22 (5%)	1	14
41	NB	426/445 (96%)	318 (75%)	83 (20%)	25 (6%)	1	13
41	ND	425/445 (96%)	324 (76%)	82 (19%)	19 (4%)	2	17
41	NF	425/445 (96%)	323 (76%)	77 (18%)	25 (6%)	1	13
41	NH	426/445 (96%)	316 (74%)	93 (22%)	17 (4%)	2	19
41	NJ	426/445 (96%)	382 (90%)	42 (10%)	2 (0%)	25	59
41	NL	388/445 (87%)	343 (88%)	42 (11%)	3 (1%)	16	50
41	OB	423/445 (95%)	278 (66%)	102 (24%)	43 (10%)	0	5
41	OD	422/445 (95%)	370 (88%)	51 (12%)	1 (0%)	44	75
41	OF	423/445 (95%)	368 (87%)	51 (12%)	4 (1%)	14	48
41	OH	426/445 (96%)	308 (72%)	94 (22%)	24 (6%)	1	14
41	OJ	426/445 (96%)	305 (72%)	103 (24%)	18 (4%)	2	18
41	OL	422/445 (95%)	365 (86%)	55 (13%)	2 (0%)	25	59
41	PB	425/445 (96%)	287 (68%)	108 (25%)	30 (7%)	1	9
41	PD	425/445 (96%)	306 (72%)	92 (22%)	27 (6%)	1	11
41	PF	426/445 (96%)	298 (70%)	100 (24%)	28 (7%)	1	11
41	PH	426/445 (96%)	240 (56%)	119 (28%)	67 (16%)	0	2
41	PJ	426/445 (96%)	267 (63%)	112 (26%)	47 (11%)	0	5
41	PL	423/445 (95%)	255 (60%)	123 (29%)	45 (11%)	0	5
41	QB	426/445 (96%)	350 (82%)	73 (17%)	3 (1%)	19	53
41	QD	425/445 (96%)	370 (87%)	53 (12%)	2 (0%)	25	59
41	QF	426/445 (96%)	375 (88%)	46 (11%)	5 (1%)	11	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	QH	426/445 (96%)	278 (65%)	115 (27%)	33 (8%)	1	8
41	QJ	426/445 (96%)	280 (66%)	100 (24%)	46 (11%)	0	5
41	QL	424/445 (95%)	258 (61%)	122 (29%)	44 (10%)	0	5
41	RB	426/445 (96%)	376 (88%)	49 (12%)	1 (0%)	44	75
41	RD	425/445 (96%)	289 (68%)	109 (26%)	27 (6%)	1	11
41	RF	426/445 (96%)	277 (65%)	117 (28%)	32 (8%)	1	9
41	RH	426/445 (96%)	361 (85%)	63 (15%)	2 (0%)	25	59
41	RJ	426/445 (96%)	275 (65%)	119 (28%)	32 (8%)	1	9
41	RL	424/445 (95%)	371 (88%)	48 (11%)	5 (1%)	11	42
41	SD	425/445 (96%)	377 (89%)	46 (11%)	2 (0%)	25	59
41	SF	426/445 (96%)	277 (65%)	119 (28%)	30 (7%)	1	9
41	SH	426/445 (96%)	361 (85%)	60 (14%)	5 (1%)	11	42
41	SJ	426/445 (96%)	373 (88%)	50 (12%)	3 (1%)	19	53
41	SL	424/445 (95%)	290 (68%)	102 (24%)	32 (8%)	1	9
41	TD	425/445 (96%)	367 (86%)	58 (14%)	0	100	100
41	TF	426/445 (96%)	365 (86%)	56 (13%)	5 (1%)	11	42
41	TH	426/445 (96%)	367 (86%)	51 (12%)	8 (2%)	6	33
41	TJ	426/445 (96%)	370 (87%)	54 (13%)	2 (0%)	25	59
41	TL	424/445 (95%)	363 (86%)	57 (13%)	4 (1%)	14	48
41	UD	425/445 (96%)	382 (90%)	41 (10%)	2 (0%)	25	59
41	UF	426/445 (96%)	375 (88%)	47 (11%)	4 (1%)	14	48
41	UH	426/445 (96%)	374 (88%)	49 (12%)	3 (1%)	19	53
41	UJ	426/445 (96%)	372 (87%)	53 (12%)	1 (0%)	44	75
41	UL	424/445 (95%)	378 (89%)	43 (10%)	3 (1%)	19	53
41	VD	425/445 (96%)	392 (92%)	33 (8%)	0	100	100
41	VF	425/445 (96%)	384 (90%)	39 (9%)	2 (0%)	25	59
41	VH	426/445 (96%)	386 (91%)	40 (9%)	0	100	100
41	VJ	426/445 (96%)	380 (89%)	42 (10%)	4 (1%)	14	48
41	VL	424/445 (95%)	390 (92%)	33 (8%)	1 (0%)	44	75
41	WD	425/445 (96%)	377 (89%)	45 (11%)	3 (1%)	19	53
41	WF	424/445 (95%)	341 (80%)	71 (17%)	12 (3%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	WH	424/445 (95%)	353 (83%)	58 (14%)	13 (3%)	3	25
41	WJ	424/445 (95%)	385 (91%)	35 (8%)	4 (1%)	14	48
41	WL	424/445 (95%)	379 (89%)	41 (10%)	4 (1%)	14	48
41	WN	424/445 (95%)	378 (89%)	44 (10%)	2 (0%)	25	59
42	AC	438/452 (97%)	424 (97%)	13 (3%)	1 (0%)	44	75
42	AE	438/452 (97%)	414 (94%)	24 (6%)	0	100	100
42	AG	438/452 (97%)	409 (93%)	26 (6%)	3 (1%)	19	53
42	AI	438/452 (97%)	367 (84%)	60 (14%)	11 (2%)	4	28
42	AK	438/452 (97%)	346 (79%)	75 (17%)	17 (4%)	2	20
42	BC	438/452 (97%)	409 (93%)	29 (7%)	0	100	100
42	BE	429/452 (95%)	414 (96%)	15 (4%)	0	100	100
42	BG	438/452 (97%)	405 (92%)	32 (7%)	1 (0%)	44	75
42	BI	426/452 (94%)	323 (76%)	72 (17%)	31 (7%)	1	9
42	BK	437/452 (97%)	408 (93%)	29 (7%)	0	100	100
42	CC	436/452 (96%)	289 (66%)	110 (25%)	37 (8%)	0	7
42	CE	436/452 (96%)	417 (96%)	19 (4%)	0	100	100
42	CG	437/452 (97%)	303 (69%)	105 (24%)	29 (7%)	1	11
42	CI	437/452 (97%)	409 (94%)	27 (6%)	1 (0%)	44	75
42	CK	437/452 (97%)	393 (90%)	43 (10%)	1 (0%)	44	75
42	CM	437/452 (97%)	390 (89%)	42 (10%)	5 (1%)	12	44
42	DC	425/452 (94%)	370 (87%)	52 (12%)	3 (1%)	19	53
42	DE	426/452 (94%)	366 (86%)	57 (13%)	3 (1%)	19	53
42	DG	427/452 (94%)	366 (86%)	59 (14%)	2 (0%)	25	59
42	DI	425/452 (94%)	379 (89%)	41 (10%)	5 (1%)	11	42
42	DK	426/452 (94%)	265 (62%)	120 (28%)	41 (10%)	0	6
42	DM	426/452 (94%)	357 (84%)	63 (15%)	6 (1%)	9	39
42	EC	437/452 (97%)	387 (89%)	48 (11%)	2 (0%)	25	59
42	EE	439/452 (97%)	299 (68%)	107 (24%)	33 (8%)	1	9
42	EG	430/452 (95%)	277 (64%)	112 (26%)	41 (10%)	0	6
42	EI	434/452 (96%)	384 (88%)	50 (12%)	0	100	100
42	EK	438/452 (97%)	274 (63%)	121 (28%)	43 (10%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
42	EM	424/452 (94%)	264 (62%)	123 (29%)	37 (9%)	0 7
42	FC	427/452 (94%)	276 (65%)	122 (29%)	29 (7%)	1 10
42	FE	421/452 (93%)	378 (90%)	42 (10%)	1 (0%)	44 75
42	FG	422/452 (93%)	386 (92%)	36 (8%)	0	100 100
42	FI	423/452 (94%)	370 (88%)	51 (12%)	2 (0%)	25 59
42	FK	420/452 (93%)	274 (65%)	107 (26%)	39 (9%)	0 6
42	FM	425/452 (94%)	382 (90%)	42 (10%)	1 (0%)	44 75
42	GC	438/452 (97%)	417 (95%)	21 (5%)	0	100 100
42	GE	426/452 (94%)	406 (95%)	19 (4%)	1 (0%)	44 75
42	GG	429/452 (95%)	411 (96%)	18 (4%)	0	100 100
42	GI	425/452 (94%)	387 (91%)	37 (9%)	1 (0%)	44 75
42	GK	425/452 (94%)	395 (93%)	29 (7%)	1 (0%)	44 75
42	GM	437/452 (97%)	322 (74%)	83 (19%)	32 (7%)	1 9
42	HC	423/452 (94%)	282 (67%)	106 (25%)	35 (8%)	0 7
42	HE	426/452 (94%)	388 (91%)	35 (8%)	3 (1%)	19 53
42	HG	426/452 (94%)	317 (74%)	81 (19%)	28 (7%)	1 11
42	HI	426/452 (94%)	327 (77%)	80 (19%)	19 (4%)	2 17
42	HK	427/452 (94%)	389 (91%)	37 (9%)	1 (0%)	44 75
42	HM	425/452 (94%)	313 (74%)	88 (21%)	24 (6%)	1 14
42	IC	425/452 (94%)	405 (95%)	20 (5%)	0	100 100
42	IE	428/452 (95%)	326 (76%)	82 (19%)	20 (5%)	2 17
42	IG	438/452 (97%)	409 (93%)	28 (6%)	1 (0%)	44 75
42	II	428/452 (95%)	404 (94%)	24 (6%)	0	100 100
42	IK	438/452 (97%)	404 (92%)	33 (8%)	1 (0%)	44 75
42	IM	427/452 (94%)	402 (94%)	25 (6%)	0	100 100
42	JC	428/452 (95%)	402 (94%)	26 (6%)	0	100 100
42	JE	426/452 (94%)	402 (94%)	23 (5%)	1 (0%)	44 75
42	JG	424/452 (94%)	406 (96%)	18 (4%)	0	100 100
42	JI	425/452 (94%)	393 (92%)	32 (8%)	0	100 100
42	JK	438/452 (97%)	326 (74%)	82 (19%)	30 (7%)	1 10
42	JM	426/452 (94%)	332 (78%)	74 (17%)	20 (5%)	2 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	KC	428/452 (95%)	406 (95%)	22 (5%)	0	100	100
42	KE	427/452 (94%)	404 (95%)	23 (5%)	0	100	100
42	KG	426/452 (94%)	411 (96%)	15 (4%)	0	100	100
42	KI	424/452 (94%)	408 (96%)	16 (4%)	0	100	100
42	KK	426/452 (94%)	407 (96%)	19 (4%)	0	100	100
42	KM	428/452 (95%)	360 (84%)	57 (13%)	11 (3%)	4	27
42	LC	429/452 (95%)	417 (97%)	12 (3%)	0	100	100
42	LE	438/452 (97%)	416 (95%)	22 (5%)	0	100	100
42	LG	429/452 (95%)	416 (97%)	13 (3%)	0	100	100
42	LI	430/452 (95%)	414 (96%)	15 (4%)	1 (0%)	44	75
42	LK	431/452 (95%)	419 (97%)	12 (3%)	0	100	100
42	LM	427/452 (94%)	407 (95%)	20 (5%)	0	100	100
42	MC	437/452 (97%)	410 (94%)	25 (6%)	2 (0%)	25	59
42	ME	425/452 (94%)	404 (95%)	21 (5%)	0	100	100
42	MG	426/452 (94%)	348 (82%)	69 (16%)	9 (2%)	5	31
42	MI	427/452 (94%)	402 (94%)	25 (6%)	0	100	100
42	MK	438/452 (97%)	394 (90%)	42 (10%)	2 (0%)	25	59
42	MM	427/452 (94%)	392 (92%)	35 (8%)	0	100	100
42	NA	426/452 (94%)	324 (76%)	76 (18%)	26 (6%)	1	12
42	NC	425/452 (94%)	295 (69%)	94 (22%)	36 (8%)	0	7
42	NE	426/452 (94%)	373 (88%)	48 (11%)	5 (1%)	11	42
42	NG	428/452 (95%)	316 (74%)	88 (21%)	24 (6%)	1	14
42	NI	428/452 (95%)	318 (74%)	87 (20%)	23 (5%)	1	14
42	NK	426/452 (94%)	292 (68%)	105 (25%)	29 (7%)	1	10
42	OA	424/452 (94%)	362 (85%)	62 (15%)	0	100	100
42	OC	425/452 (94%)	370 (87%)	52 (12%)	3 (1%)	19	53
42	OE	429/452 (95%)	372 (87%)	55 (13%)	2 (0%)	25	59
42	OG	429/452 (95%)	309 (72%)	99 (23%)	21 (5%)	2	16
42	OI	428/452 (95%)	382 (89%)	45 (10%)	1 (0%)	44	75
42	OK	427/452 (94%)	366 (86%)	60 (14%)	1 (0%)	44	75
42	PA	358/452 (79%)	230 (64%)	101 (28%)	27 (8%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	PC	428/452 (95%)	280 (65%)	108 (25%)	40 (9%)	0	6
42	PE	427/452 (94%)	275 (64%)	112 (26%)	40 (9%)	0	6
42	PG	426/452 (94%)	250 (59%)	122 (29%)	54 (13%)	0	3
42	PI	423/452 (94%)	236 (56%)	131 (31%)	56 (13%)	0	3
42	PK	426/452 (94%)	301 (71%)	103 (24%)	22 (5%)	1	14
42	QC	426/452 (94%)	365 (86%)	59 (14%)	2 (0%)	25	59
42	QE	426/452 (94%)	357 (84%)	68 (16%)	1 (0%)	44	75
42	QG	427/452 (94%)	351 (82%)	75 (18%)	1 (0%)	44	75
42	QI	425/452 (94%)	279 (66%)	120 (28%)	26 (6%)	1	12
42	QK	427/452 (94%)	285 (67%)	115 (27%)	27 (6%)	1	12
42	RC	428/452 (95%)	366 (86%)	60 (14%)	2 (0%)	25	59
42	RE	424/452 (94%)	366 (86%)	56 (13%)	2 (0%)	25	59
42	RG	426/452 (94%)	363 (85%)	61 (14%)	2 (0%)	25	59
42	RI	427/452 (94%)	368 (86%)	55 (13%)	4 (1%)	14	48
42	RK	427/452 (94%)	367 (86%)	56 (13%)	4 (1%)	14	48
42	SC	426/452 (94%)	367 (86%)	57 (13%)	2 (0%)	25	59
42	SE	427/452 (94%)	291 (68%)	98 (23%)	38 (9%)	0	7
42	SG	427/452 (94%)	364 (85%)	62 (14%)	1 (0%)	44	75
42	SI	421/452 (93%)	274 (65%)	118 (28%)	29 (7%)	1	10
42	SK	428/452 (95%)	369 (86%)	57 (13%)	2 (0%)	25	59
42	SM	427/452 (94%)	365 (86%)	60 (14%)	2 (0%)	25	59
42	TC	426/452 (94%)	369 (87%)	53 (12%)	4 (1%)	14	48
42	TE	428/452 (95%)	364 (85%)	60 (14%)	4 (1%)	14	48
42	TG	426/452 (94%)	348 (82%)	77 (18%)	1 (0%)	44	75
42	TI	426/452 (94%)	286 (67%)	113 (26%)	27 (6%)	1	12
42	TK	428/452 (95%)	303 (71%)	96 (22%)	29 (7%)	1	10
42	TM	426/452 (94%)	339 (80%)	82 (19%)	5 (1%)	11	42
42	UC	429/452 (95%)	307 (72%)	99 (23%)	23 (5%)	1	14
42	UE	428/452 (95%)	366 (86%)	59 (14%)	3 (1%)	19	53
42	UG	429/452 (95%)	368 (86%)	57 (13%)	4 (1%)	14	48
42	UI	429/452 (95%)	382 (89%)	42 (10%)	5 (1%)	11	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
42	UK	429/452 (95%)	373 (87%)	54 (13%)	2 (0%)	25 59
42	UM	427/452 (94%)	380 (89%)	44 (10%)	3 (1%)	19 53
42	VC	438/452 (97%)	399 (91%)	38 (9%)	1 (0%)	44 75
42	VE	429/452 (95%)	397 (92%)	30 (7%)	2 (0%)	25 59
42	VG	438/452 (97%)	393 (90%)	44 (10%)	1 (0%)	44 75
42	VI	429/452 (95%)	391 (91%)	38 (9%)	0	100 100
42	VK	438/452 (97%)	337 (77%)	79 (18%)	22 (5%)	1 15
42	VM	426/452 (94%)	389 (91%)	37 (9%)	0	100 100
42	WC	438/452 (97%)	393 (90%)	45 (10%)	0	100 100
42	WE	427/452 (94%)	341 (80%)	69 (16%)	17 (4%)	2 19
42	WG	437/452 (97%)	400 (92%)	35 (8%)	2 (0%)	25 59
42	WI	427/452 (94%)	343 (80%)	62 (14%)	22 (5%)	1 14
42	WK	436/452 (96%)	390 (89%)	44 (10%)	2 (0%)	25 59
42	WM	427/452 (94%)	402 (94%)	23 (5%)	2 (0%)	25 59
All	All	141324/170864 (83%)	120912 (86%)	17406 (12%)	3006 (2%)	8 31

5 of 3006 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	619	SER
1	1A	807	VAL
1	1A	850	PRO
2	1D	146	VAL
5	1N	86	ALA

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
2	1D	123/611 (20%)	105 (85%)	18 (15%)	2 15
2	1E	176/611 (29%)	157 (89%)	19 (11%)	5 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1F	78/611 (13%)	78 (100%)	0	100	100
3	1H	72/486 (15%)	72 (100%)	0	100	100
3	1I	342/486 (70%)	338 (99%)	4 (1%)	67	82
4	1K	147/182 (81%)	145 (99%)	2 (1%)	62	79
4	1L	31/182 (17%)	31 (100%)	0	100	100
5	1N	95/168 (56%)	95 (100%)	0	100	100
5	1O	97/168 (58%)	97 (100%)	0	100	100
5	1P	99/168 (59%)	98 (99%)	1 (1%)	73	84
6	1R	83/92 (90%)	83 (100%)	0	100	100
7	1T	223/281 (79%)	221 (99%)	2 (1%)	75	86
7	1U	223/281 (79%)	221 (99%)	2 (1%)	75	86
8	1W	128/180 (71%)	82 (64%)	46 (36%)	0	1
8	1X	172/180 (96%)	171 (99%)	1 (1%)	84	91
8	1Y	172/180 (96%)	169 (98%)	3 (2%)	56	75
8	1Z	172/180 (96%)	172 (100%)	0	100	100
8	2A	172/180 (96%)	159 (92%)	13 (8%)	11	35
8	2B	172/180 (96%)	172 (100%)	0	100	100
9	2D	392/750 (52%)	390 (100%)	2 (0%)	86	92
9	2E	91/750 (12%)	91 (100%)	0	100	100
10	2F	69/152 (45%)	68 (99%)	1 (1%)	62	79
10	2G	69/152 (45%)	69 (100%)	0	100	100
10	2H	69/152 (45%)	67 (97%)	2 (3%)	37	63
11	2J	150/495 (30%)	149 (99%)	1 (1%)	81	89
11	2K	268/495 (54%)	254 (95%)	14 (5%)	19	47
11	2L	256/495 (52%)	251 (98%)	5 (2%)	50	71
11	2M	162/495 (33%)	160 (99%)	2 (1%)	67	82
12	2O	515/527 (98%)	513 (100%)	2 (0%)	89	94
12	2P	515/527 (98%)	513 (100%)	2 (0%)	89	94
12	2Q	515/527 (98%)	513 (100%)	2 (0%)	89	94
13	2S	175/469 (37%)	172 (98%)	3 (2%)	56	75
13	2T	183/469 (39%)	147 (80%)	36 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	2V	29/252 (12%)	29 (100%)	0	100	100
14	2W	189/252 (75%)	188 (100%)	1 (0%)	86	92
14	2X	184/252 (73%)	184 (100%)	0	100	100
14	2Y	144/252 (57%)	143 (99%)	1 (1%)	81	89
15	3A	165/208 (79%)	161 (98%)	4 (2%)	44	68
16	3C	182/264 (69%)	176 (97%)	6 (3%)	33	60
16	3D	58/264 (22%)	58 (100%)	0	100	100
19	3J	391/574 (68%)	389 (100%)	2 (0%)	86	92
19	3K	400/574 (70%)	398 (100%)	2 (0%)	86	92
19	3L	409/574 (71%)	406 (99%)	3 (1%)	81	89
20	3N	264/672 (39%)	262 (99%)	2 (1%)	79	87
20	3O	532/672 (79%)	530 (100%)	2 (0%)	89	94
20	3P	532/672 (79%)	529 (99%)	3 (1%)	84	91
20	3Q	268/672 (40%)	266 (99%)	2 (1%)	81	89
21	3S	62/238 (26%)	62 (100%)	0	100	100
21	3T	218/238 (92%)	216 (99%)	2 (1%)	75	86
21	3U	218/238 (92%)	215 (99%)	3 (1%)	62	79
21	3V	191/238 (80%)	191 (100%)	0	100	100
22	3X	106/231 (46%)	106 (100%)	0	100	100
22	3Y	116/231 (50%)	107 (92%)	9 (8%)	10	34
22	3Z	108/231 (47%)	108 (100%)	0	100	100
22	4A	89/231 (38%)	89 (100%)	0	100	100
22	4B	87/231 (38%)	87 (100%)	0	100	100
22	4C	70/231 (30%)	70 (100%)	0	100	100
23	4D	107/121 (88%)	107 (100%)	0	100	100
24	4F	131/450 (29%)	104 (79%)	27 (21%)	1	5
24	4G	306/450 (68%)	304 (99%)	2 (1%)	81	89
25	4I	191/324 (59%)	190 (100%)	1 (0%)	86	92
25	4J	319/324 (98%)	312 (98%)	7 (2%)	47	69
26	4K	118/551 (21%)	117 (99%)	1 (1%)	79	87
26	4L	206/551 (37%)	205 (100%)	1 (0%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	4M	95/551 (17%)	95 (100%)	0	100	100
27	4O	192/227 (85%)	192 (100%)	0	100	100
27	4P	192/227 (85%)	191 (100%)	1 (0%)	86	92
27	4Q	192/227 (85%)	192 (100%)	0	100	100
27	4R	192/227 (85%)	140 (73%)	52 (27%)	0	2
27	4S	192/227 (85%)	192 (100%)	0	100	100
27	4T	192/227 (85%)	180 (94%)	12 (6%)	15	42
28	4V	36/122 (30%)	36 (100%)	0	100	100
28	4W	70/122 (57%)	69 (99%)	1 (1%)	62	79
29	4Y	91/114 (80%)	91 (100%)	0	100	100
30	5A	311/335 (93%)	308 (99%)	3 (1%)	73	84
30	5B	14/335 (4%)	14 (100%)	0	100	100
31	5D	145/154 (94%)	145 (100%)	0	100	100
31	5E	144/154 (94%)	135 (94%)	9 (6%)	15	42
31	5F	147/154 (96%)	147 (100%)	0	100	100
31	5G	145/154 (94%)	144 (99%)	1 (1%)	81	89
31	5H	145/154 (94%)	144 (99%)	1 (1%)	81	89
31	5I	145/154 (94%)	145 (100%)	0	100	100
31	5J	145/154 (94%)	145 (100%)	0	100	100
32	5L	103/382 (27%)	103 (100%)	0	100	100
32	5M	363/382 (95%)	357 (98%)	6 (2%)	56	75
32	5N	363/382 (95%)	360 (99%)	3 (1%)	79	87
32	5O	274/382 (72%)	174 (64%)	100 (36%)	0	1
33	5Q	103/386 (27%)	103 (100%)	0	100	100
33	5R	357/386 (92%)	356 (100%)	1 (0%)	91	96
33	5S	357/386 (92%)	301 (84%)	56 (16%)	2	13
33	5T	271/386 (70%)	159 (59%)	112 (41%)	0	0
33	5V	271/386 (70%)	257 (95%)	14 (5%)	19	47
33	5W	366/386 (95%)	360 (98%)	6 (2%)	58	75
33	5X	366/386 (95%)	364 (100%)	2 (0%)	86	92
33	5Y	99/386 (26%)	93 (94%)	6 (6%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	6A	249/444 (56%)	151 (61%)	98 (39%)	0	1
34	6B	354/444 (80%)	324 (92%)	30 (8%)	8	32
34	6C	355/444 (80%)	225 (63%)	130 (37%)	0	1
34	6D	110/444 (25%)	69 (63%)	41 (37%)	0	1
34	6E	55/444 (12%)	43 (78%)	12 (22%)	1	4
34	6F	320/444 (72%)	308 (96%)	12 (4%)	28	57
34	6G	378/444 (85%)	376 (100%)	2 (0%)	86	92
34	6H	333/444 (75%)	330 (99%)	3 (1%)	75	86
34	6I	63/444 (14%)	63 (100%)	0	100	100
34	6J	63/444 (14%)	63 (100%)	0	100	100
34	6K	335/444 (76%)	334 (100%)	1 (0%)	91	96
34	6L	378/444 (85%)	362 (96%)	16 (4%)	25	54
34	6M	323/444 (73%)	323 (100%)	0	100	100
34	6N	50/444 (11%)	50 (100%)	0	100	100
35	6P	158/394 (40%)	158 (100%)	0	100	100
35	6Q	363/394 (92%)	362 (100%)	1 (0%)	91	96
35	6R	363/394 (92%)	334 (92%)	29 (8%)	10	33
35	6S	226/394 (57%)	202 (89%)	24 (11%)	5	24
35	6T	209/394 (53%)	208 (100%)	1 (0%)	86	92
35	6U	365/394 (93%)	364 (100%)	1 (0%)	91	96
35	6V	386/394 (98%)	360 (93%)	26 (7%)	13	40
35	6W	189/394 (48%)	178 (94%)	11 (6%)	17	44
36	6Y	97/593 (16%)	96 (99%)	1 (1%)	73	84
36	6Z	97/593 (16%)	96 (99%)	1 (1%)	73	84
37	7C	98/215 (46%)	97 (99%)	1 (1%)	73	84
37	7D	66/215 (31%)	66 (100%)	0	100	100
37	7E	65/215 (30%)	65 (100%)	0	100	100
37	7F	56/215 (26%)	50 (89%)	6 (11%)	5	24
38	7H	66/239 (28%)	66 (100%)	0	100	100
38	7I	25/239 (10%)	24 (96%)	1 (4%)	27	55
39	7K	93/126 (74%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	7L	41/126 (32%)	41 (100%)	0	100	100
40	7N	62/397 (16%)	62 (100%)	0	100	100
41	AB	373/380 (98%)	371 (100%)	2 (0%)	86	92
41	AD	373/380 (98%)	372 (100%)	1 (0%)	91	96
41	AF	373/380 (98%)	372 (100%)	1 (0%)	91	96
41	AH	373/380 (98%)	268 (72%)	105 (28%)	0	2
41	AJ	373/380 (98%)	373 (100%)	0	100	100
41	AL	373/380 (98%)	267 (72%)	106 (28%)	0	2
41	BB	367/380 (97%)	367 (100%)	0	100	100
41	BD	367/380 (97%)	245 (67%)	122 (33%)	0	1
41	BF	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	BH	367/380 (97%)	363 (99%)	4 (1%)	70	83
41	BJ	367/380 (97%)	365 (100%)	2 (0%)	86	92
41	BL	365/380 (96%)	361 (99%)	4 (1%)	70	83
41	CB	366/380 (96%)	366 (100%)	0	100	100
41	CD	366/380 (96%)	225 (62%)	141 (38%)	0	1
41	CF	367/380 (97%)	229 (62%)	138 (38%)	0	1
41	CH	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	CJ	367/380 (97%)	238 (65%)	129 (35%)	0	1
41	CL	365/380 (96%)	364 (100%)	1 (0%)	91	96
41	DB	366/380 (96%)	364 (100%)	2 (0%)	86	92
41	DD	366/380 (96%)	366 (100%)	0	100	100
41	DF	366/380 (96%)	366 (100%)	0	100	100
41	DH	366/380 (96%)	246 (67%)	120 (33%)	0	1
41	DJ	366/380 (96%)	242 (66%)	124 (34%)	0	1
41	DL	365/380 (96%)	344 (94%)	21 (6%)	17	44
41	ED	366/380 (96%)	258 (70%)	108 (30%)	0	2
41	EF	366/380 (96%)	366 (100%)	0	100	100
41	EH	367/380 (97%)	365 (100%)	2 (0%)	86	92
41	EJ	366/380 (96%)	363 (99%)	3 (1%)	79	87
41	EL	365/380 (96%)	344 (94%)	21 (6%)	17	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	FD	367/380 (97%)	233 (64%)	134 (36%)	0	1
41	FF	366/380 (96%)	356 (97%)	10 (3%)	40	65
41	FH	366/380 (96%)	366 (100%)	0	100	100
41	FJ	366/380 (96%)	363 (99%)	3 (1%)	79	87
41	FL	365/380 (96%)	237 (65%)	128 (35%)	0	1
41	GD	367/380 (97%)	250 (68%)	117 (32%)	0	2
41	GF	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	GH	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	GJ	367/380 (97%)	249 (68%)	118 (32%)	0	1
41	GL	365/380 (96%)	365 (100%)	0	100	100
41	HB	366/380 (96%)	359 (98%)	7 (2%)	52	73
41	HD	367/380 (97%)	251 (68%)	116 (32%)	0	2
41	HF	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	HH	367/380 (97%)	364 (99%)	3 (1%)	79	87
41	HJ	367/380 (97%)	245 (67%)	122 (33%)	0	1
41	HL	365/380 (96%)	364 (100%)	1 (0%)	91	96
41	ID	367/380 (97%)	367 (100%)	0	100	100
41	IF	367/380 (97%)	367 (100%)	0	100	100
41	IH	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	IJ	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	IL	366/380 (96%)	365 (100%)	1 (0%)	91	96
41	IN	367/380 (97%)	257 (70%)	110 (30%)	0	2
41	JD	367/380 (97%)	357 (97%)	10 (3%)	40	65
41	JF	366/380 (96%)	365 (100%)	1 (0%)	91	96
41	JH	366/380 (96%)	364 (100%)	2 (0%)	86	92
41	JJ	366/380 (96%)	365 (100%)	1 (0%)	91	96
41	JL	366/380 (96%)	258 (70%)	108 (30%)	0	2
41	KD	367/380 (97%)	365 (100%)	2 (0%)	86	92
41	KF	367/380 (97%)	367 (100%)	0	100	100
41	KH	368/380 (97%)	367 (100%)	1 (0%)	91	96
41	KJ	366/380 (96%)	366 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	KL	368/380 (97%)	368 (100%)	0	100	100
41	KN	367/380 (97%)	364 (99%)	3 (1%)	79	87
41	LD	367/380 (97%)	276 (75%)	91 (25%)	0	3
41	LF	367/380 (97%)	365 (100%)	2 (0%)	86	92
41	LH	367/380 (97%)	367 (100%)	0	100	100
41	LJ	367/380 (97%)	365 (100%)	2 (0%)	86	92
41	LL	366/380 (96%)	366 (100%)	0	100	100
41	LN	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	MD	366/380 (96%)	246 (67%)	120 (33%)	0	1
41	MF	367/380 (97%)	224 (61%)	143 (39%)	0	1
41	MH	367/380 (97%)	367 (100%)	0	100	100
41	MJ	366/380 (96%)	365 (100%)	1 (0%)	91	96
41	ML	366/380 (96%)	365 (100%)	1 (0%)	91	96
41	MN	366/380 (96%)	232 (63%)	134 (37%)	0	1
41	NB	367/380 (97%)	257 (70%)	110 (30%)	0	2
41	ND	367/380 (97%)	237 (65%)	130 (35%)	0	1
41	NF	367/380 (97%)	239 (65%)	128 (35%)	0	1
41	NH	367/380 (97%)	244 (66%)	123 (34%)	0	1
41	NJ	367/380 (97%)	362 (99%)	5 (1%)	62	79
41	NL	339/380 (89%)	337 (99%)	2 (1%)	84	91
41	OB	365/380 (96%)	247 (68%)	118 (32%)	0	1
41	OD	364/380 (96%)	364 (100%)	0	100	100
41	OF	365/380 (96%)	358 (98%)	7 (2%)	52	73
41	OH	367/380 (97%)	244 (66%)	123 (34%)	0	1
41	OJ	367/380 (97%)	236 (64%)	131 (36%)	0	1
41	OL	364/380 (96%)	364 (100%)	0	100	100
41	PB	367/380 (97%)	231 (63%)	136 (37%)	0	1
41	PD	367/380 (97%)	236 (64%)	131 (36%)	0	1
41	PF	367/380 (97%)	242 (66%)	125 (34%)	0	1
41	PH	367/380 (97%)	222 (60%)	145 (40%)	0	1
41	PJ	367/380 (97%)	216 (59%)	151 (41%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	PL	365/380 (96%)	228 (62%)	137 (38%)	0	1
41	QB	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	QD	367/380 (97%)	367 (100%)	0	100	100
41	QF	367/380 (97%)	365 (100%)	2 (0%)	86	92
41	QH	367/380 (97%)	237 (65%)	130 (35%)	0	1
41	QJ	367/380 (97%)	225 (61%)	142 (39%)	0	1
41	QL	366/380 (96%)	241 (66%)	125 (34%)	0	1
41	RB	367/380 (97%)	367 (100%)	0	100	100
41	RD	367/380 (97%)	230 (63%)	137 (37%)	0	1
41	RF	367/380 (97%)	215 (59%)	152 (41%)	0	0
41	RH	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	RJ	367/380 (97%)	238 (65%)	129 (35%)	0	1
41	RL	366/380 (96%)	364 (100%)	2 (0%)	86	92
41	SD	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	SF	367/380 (97%)	246 (67%)	121 (33%)	0	1
41	SH	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	SJ	367/380 (97%)	362 (99%)	5 (1%)	62	79
41	SL	366/380 (96%)	239 (65%)	127 (35%)	0	1
41	TD	367/380 (97%)	365 (100%)	2 (0%)	86	92
41	TF	367/380 (97%)	367 (100%)	0	100	100
41	TH	367/380 (97%)	363 (99%)	4 (1%)	70	83
41	TJ	367/380 (97%)	358 (98%)	9 (2%)	42	67
41	TL	366/380 (96%)	366 (100%)	0	100	100
41	UD	367/380 (97%)	360 (98%)	7 (2%)	52	73
41	UF	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	UH	367/380 (97%)	365 (100%)	2 (0%)	86	92
41	UJ	367/380 (97%)	366 (100%)	1 (0%)	91	96
41	UL	366/380 (96%)	353 (96%)	13 (4%)	30	58
41	VD	367/380 (97%)	367 (100%)	0	100	100
41	VF	367/380 (97%)	352 (96%)	15 (4%)	26	54
41	VH	367/380 (97%)	365 (100%)	2 (0%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	VJ	367/380 (97%)	361 (98%)	6 (2%)	58	75
41	VL	366/380 (96%)	366 (100%)	0	100	100
41	WD	367/380 (97%)	367 (100%)	0	100	100
41	WF	366/380 (96%)	239 (65%)	127 (35%)	0	1
41	WH	366/380 (96%)	264 (72%)	102 (28%)	0	2
41	WJ	366/380 (96%)	359 (98%)	7 (2%)	52	73
41	WL	366/380 (96%)	364 (100%)	2 (0%)	86	92
41	WN	366/380 (96%)	365 (100%)	1 (0%)	91	96
42	AC	370/379 (98%)	367 (99%)	3 (1%)	79	87
42	AE	370/379 (98%)	369 (100%)	1 (0%)	91	96
42	AG	370/379 (98%)	362 (98%)	8 (2%)	47	69
42	AI	370/379 (98%)	265 (72%)	105 (28%)	0	2
42	AK	370/379 (98%)	262 (71%)	108 (29%)	0	2
42	BC	370/379 (98%)	369 (100%)	1 (0%)	91	96
42	BE	366/379 (97%)	362 (99%)	4 (1%)	70	83
42	BG	370/379 (98%)	358 (97%)	12 (3%)	34	61
42	BI	363/379 (96%)	259 (71%)	104 (29%)	0	2
42	BK	369/379 (97%)	369 (100%)	0	100	100
42	CC	368/379 (97%)	240 (65%)	128 (35%)	0	1
42	CE	368/379 (97%)	368 (100%)	0	100	100
42	CG	369/379 (97%)	239 (65%)	130 (35%)	0	1
42	CI	369/379 (97%)	369 (100%)	0	100	100
42	CK	369/379 (97%)	369 (100%)	0	100	100
42	CM	369/379 (97%)	368 (100%)	1 (0%)	91	96
42	DC	362/379 (96%)	359 (99%)	3 (1%)	79	87
42	DE	363/379 (96%)	363 (100%)	0	100	100
42	DG	364/379 (96%)	362 (100%)	2 (0%)	86	92
42	DI	362/379 (96%)	362 (100%)	0	100	100
42	DK	363/379 (96%)	258 (71%)	105 (29%)	0	2
42	DM	363/379 (96%)	363 (100%)	0	100	100
42	EC	369/379 (97%)	368 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	EE	371/379 (98%)	260 (70%)	111 (30%)	0	2
42	EG	367/379 (97%)	258 (70%)	109 (30%)	0	2
42	EI	366/379 (97%)	365 (100%)	1 (0%)	91	96
42	EK	370/379 (98%)	232 (63%)	138 (37%)	0	1
42	EM	361/379 (95%)	228 (63%)	133 (37%)	0	1
42	FC	364/379 (96%)	217 (60%)	147 (40%)	0	1
42	FE	359/379 (95%)	359 (100%)	0	100	100
42	FG	360/379 (95%)	354 (98%)	6 (2%)	56	75
42	FI	360/379 (95%)	357 (99%)	3 (1%)	79	87
42	FK	358/379 (94%)	219 (61%)	139 (39%)	0	1
42	FM	362/379 (96%)	360 (99%)	2 (1%)	84	91
42	GC	370/379 (98%)	368 (100%)	2 (0%)	86	92
42	GE	363/379 (96%)	362 (100%)	1 (0%)	91	96
42	GG	366/379 (97%)	364 (100%)	2 (0%)	86	92
42	GI	362/379 (96%)	361 (100%)	1 (0%)	91	96
42	GK	362/379 (96%)	361 (100%)	1 (0%)	91	96
42	GM	369/379 (97%)	232 (63%)	137 (37%)	0	1
42	HC	360/379 (95%)	230 (64%)	130 (36%)	0	1
42	HE	363/379 (96%)	361 (99%)	2 (1%)	84	91
42	HG	363/379 (96%)	256 (70%)	107 (30%)	0	2
42	HI	363/379 (96%)	230 (63%)	133 (37%)	0	1
42	HK	364/379 (96%)	360 (99%)	4 (1%)	70	83
42	HM	362/379 (96%)	256 (71%)	106 (29%)	0	2
42	IC	362/379 (96%)	357 (99%)	5 (1%)	62	79
42	IE	365/379 (96%)	233 (64%)	132 (36%)	0	1
42	IG	370/379 (98%)	370 (100%)	0	100	100
42	II	365/379 (96%)	365 (100%)	0	100	100
42	IK	370/379 (98%)	369 (100%)	1 (0%)	91	96
42	IM	364/379 (96%)	364 (100%)	0	100	100
42	JC	364/379 (96%)	363 (100%)	1 (0%)	91	96
42	JE	363/379 (96%)	360 (99%)	3 (1%)	79	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	JG	361/379 (95%)	359 (99%)	2 (1%)	84	91
42	JI	362/379 (96%)	362 (100%)	0	100	100
42	JK	370/379 (98%)	233 (63%)	137 (37%)	0	1
42	JM	363/379 (96%)	240 (66%)	123 (34%)	0	1
42	KC	364/379 (96%)	363 (100%)	1 (0%)	91	96
42	KE	364/379 (96%)	364 (100%)	0	100	100
42	KG	362/379 (96%)	361 (100%)	1 (0%)	91	96
42	KI	361/379 (95%)	360 (100%)	1 (0%)	91	96
42	KK	363/379 (96%)	362 (100%)	1 (0%)	91	96
42	KM	362/379 (96%)	265 (73%)	97 (27%)	0	2
42	LC	366/379 (97%)	365 (100%)	1 (0%)	91	96
42	LE	370/379 (98%)	368 (100%)	2 (0%)	86	92
42	LG	366/379 (97%)	366 (100%)	0	100	100
42	LI	366/379 (97%)	365 (100%)	1 (0%)	91	96
42	LK	366/379 (97%)	366 (100%)	0	100	100
42	LM	364/379 (96%)	364 (100%)	0	100	100
42	MC	369/379 (97%)	367 (100%)	2 (0%)	86	92
42	ME	362/379 (96%)	361 (100%)	1 (0%)	91	96
42	MG	363/379 (96%)	262 (72%)	101 (28%)	0	2
42	MI	364/379 (96%)	363 (100%)	1 (0%)	91	96
42	MK	370/379 (98%)	367 (99%)	3 (1%)	79	87
42	MM	363/379 (96%)	363 (100%)	0	100	100
42	NA	363/379 (96%)	224 (62%)	139 (38%)	0	1
42	NC	362/379 (96%)	252 (70%)	110 (30%)	0	2
42	NE	363/379 (96%)	361 (99%)	2 (1%)	84	91
42	NG	365/379 (96%)	241 (66%)	124 (34%)	0	1
42	NI	365/379 (96%)	235 (64%)	130 (36%)	0	1
42	NK	363/379 (96%)	246 (68%)	117 (32%)	0	1
42	OA	361/379 (95%)	360 (100%)	1 (0%)	91	96
42	OC	362/379 (96%)	362 (100%)	0	100	100
42	OE	366/379 (97%)	363 (99%)	3 (1%)	79	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	OG	365/379 (96%)	239 (66%)	126 (34%)	0	1
42	OI	365/379 (96%)	364 (100%)	1 (0%)	91	96
42	OK	364/379 (96%)	363 (100%)	1 (0%)	91	96
42	PA	314/379 (83%)	196 (62%)	118 (38%)	0	1
42	PC	365/379 (96%)	234 (64%)	131 (36%)	0	1
42	PE	364/379 (96%)	238 (65%)	126 (35%)	0	1
42	PG	363/379 (96%)	227 (62%)	136 (38%)	0	1
42	PI	360/379 (95%)	222 (62%)	138 (38%)	0	1
42	PK	363/379 (96%)	248 (68%)	115 (32%)	0	2
42	QC	363/379 (96%)	362 (100%)	1 (0%)	91	96
42	QE	363/379 (96%)	360 (99%)	3 (1%)	79	87
42	QG	364/379 (96%)	363 (100%)	1 (0%)	91	96
42	QI	362/379 (96%)	238 (66%)	124 (34%)	0	1
42	QK	364/379 (96%)	243 (67%)	121 (33%)	0	1
42	RC	365/379 (96%)	363 (100%)	2 (0%)	86	92
42	RE	361/379 (95%)	360 (100%)	1 (0%)	91	96
42	RG	363/379 (96%)	361 (99%)	2 (1%)	84	91
42	RI	364/379 (96%)	363 (100%)	1 (0%)	91	96
42	RK	364/379 (96%)	363 (100%)	1 (0%)	91	96
42	SC	363/379 (96%)	361 (99%)	2 (1%)	84	91
42	SE	364/379 (96%)	258 (71%)	106 (29%)	0	2
42	SG	364/379 (96%)	363 (100%)	1 (0%)	91	96
42	SI	363/379 (96%)	231 (64%)	132 (36%)	0	1
42	SK	365/379 (96%)	364 (100%)	1 (0%)	91	96
42	SM	364/379 (96%)	362 (100%)	2 (0%)	86	92
42	TC	363/379 (96%)	362 (100%)	1 (0%)	91	96
42	TE	365/379 (96%)	364 (100%)	1 (0%)	91	96
42	TG	363/379 (96%)	363 (100%)	0	100	100
42	TI	363/379 (96%)	239 (66%)	124 (34%)	0	1
42	TK	365/379 (96%)	248 (68%)	117 (32%)	0	1
42	TM	363/379 (96%)	361 (99%)	2 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	UC	366/379 (97%)	245 (67%)	121 (33%)	0 1
42	UE	365/379 (96%)	364 (100%)	1 (0%)	91 96
42	UG	366/379 (97%)	344 (94%)	22 (6%)	16 43
42	UI	366/379 (97%)	365 (100%)	1 (0%)	91 96
42	UK	365/379 (96%)	357 (98%)	8 (2%)	47 69
42	UM	364/379 (96%)	359 (99%)	5 (1%)	62 79
42	VC	370/379 (98%)	369 (100%)	1 (0%)	91 96
42	VE	366/379 (97%)	365 (100%)	1 (0%)	91 96
42	VG	370/379 (98%)	369 (100%)	1 (0%)	91 96
42	VI	366/379 (97%)	364 (100%)	2 (0%)	86 92
42	VK	370/379 (98%)	253 (68%)	117 (32%)	0 2
42	VM	363/379 (96%)	363 (100%)	0	100 100
42	WC	370/379 (98%)	370 (100%)	0	100 100
42	WE	364/379 (96%)	274 (75%)	90 (25%)	0 3
42	WG	369/379 (97%)	367 (100%)	2 (0%)	86 92
42	WI	364/379 (96%)	269 (74%)	95 (26%)	0 3
42	WK	368/379 (97%)	367 (100%)	1 (0%)	91 96
42	WM	364/379 (96%)	364 (100%)	0	100 100
All	All	121565/144487 (84%)	109251 (90%)	12314 (10%)	9 26

5 of 12314 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	NI	167	LEU
41	PH	390	ARG
41	OB	19	LYS
42	NI	137	ILE
41	PB	209	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1108 such sidechains are listed below:

Mol	Chain	Res	Type
42	RG	11	GLN
42	SE	61	HIS
41	RF	426	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	UG	101	ASN
42	FM	380	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 370 ligands modelled in this entry, 106 are monoatomic - leaving 264 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	$\#\|Z\| > 2$
43	GDP	LD	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.11	2 (6%)
45	GTP	EM	501	-	29,34,34	1.22	1 (3%)	35,54,54	1.31	6 (17%)
43	GDP	JL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.18	4 (13%)
45	GTP	IK	501	44	29,34,34	1.36	4 (13%)	35,54,54	1.66	6 (17%)
43	GDP	HF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.14	3 (10%)
45	GTP	AE	501	44	29,34,34	1.19	2 (6%)	35,54,54	1.35	4 (11%)
43	GDP	WL	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
43	GDP	UF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.13	2 (6%)
45	GTP	UG	501	44	29,34,34	1.19	2 (6%)	35,54,54	1.31	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	GDP	KL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
45	GTP	BC	501	44	29,34,34	1.32	3 (10%)	35,54,54	1.29	4 (11%)
45	GTP	NE	501	44	29,34,34	1.14	2 (6%)	35,54,54	1.38	5 (14%)
43	GDP	LN	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.08	1 (3%)
43	GDP	BD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.10	2 (6%)
43	GDP	SD	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.10	2 (6%)
43	GDP	EH	501	-	25,30,30	1.05	1 (4%)	30,47,47	2.09	5 (16%)
43	GDP	RB	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.17	2 (6%)
43	GDP	NF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	1 (3%)
45	GTP	PE	501	44	29,34,34	1.25	2 (6%)	35,54,54	1.43	6 (17%)
45	GTP	PA	501	-	29,34,34	1.25	1 (3%)	35,54,54	1.41	5 (14%)
43	GDP	BF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	2 (6%)
45	GTP	GE	501	44	29,34,34	1.23	2 (6%)	35,54,54	1.38	5 (14%)
45	GTP	LF	502	44	29,34,34	1.24	3 (10%)	35,54,54	1.39	4 (11%)
45	GTP	TE	501	44	29,34,34	1.27	2 (6%)	35,54,54	1.52	6 (17%)
43	GDP	DJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	1 (3%)
43	GDP	BB	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.30	6 (20%)
43	GDP	ND	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.03	1 (3%)
43	GDP	OL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.22	3 (10%)
45	GTP	BE	501	44	29,34,34	1.24	2 (6%)	35,54,54	1.31	4 (11%)
43	GDP	HH	501	-	25,30,30	1.13	2 (8%)	30,47,47	1.76	4 (13%)
43	GDP	PB	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.26	4 (13%)
45	GTP	FE	501	44	29,34,34	1.25	2 (6%)	35,54,54	1.38	5 (14%)
45	GTP	CE	501	44	29,34,34	1.26	1 (3%)	35,54,54	1.26	4 (11%)
43	GDP	HL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	3 (10%)
43	GDP	LJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	3 (10%)
45	GTP	VC	501	44	29,34,34	1.27	2 (6%)	35,54,54	1.38	5 (14%)
45	GTP	WG	501	44	29,34,34	1.22	2 (6%)	35,54,54	1.35	5 (14%)
45	GTP	JC	501	44	29,34,34	1.20	1 (3%)	35,54,54	1.33	3 (8%)
43	GDP	JD	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
43	GDP	SJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.15	1 (3%)
45	GTP	DK	501	-	29,34,34	1.29	4 (13%)	35,54,54	1.53	7 (20%)
43	GDP	LH	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	3 (10%)
45	GTP	II	501	-	29,34,34	1.25	2 (6%)	35,54,54	1.29	3 (8%)
45	GTP	LM	501	44	29,34,34	1.27	2 (6%)	35,54,54	1.34	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	GDP	VD	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.11	2 (6%)
43	GDP	FD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.13	2 (6%)
43	GDP	CL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
43	GDP	OJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.27	3 (10%)
43	GDP	BJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
43	GDP	KN	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
45	GTP	CG	501	-	29,34,34	1.22	1 (3%)	35,54,54	1.27	5 (14%)
43	GDP	JF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.11	2 (6%)
43	GDP	QJ	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.28	5 (16%)
45	GTP	KG	501	44	29,34,34	1.29	3 (10%)	35,54,54	1.28	4 (11%)
45	GTP	JM	501	44	29,34,34	1.20	2 (6%)	35,54,54	1.26	4 (11%)
45	GTP	GM	501	44	29,34,34	1.19	2 (6%)	35,54,54	1.31	4 (11%)
45	GTP	AC	501	44	29,34,34	1.21	2 (6%)	35,54,54	1.30	5 (14%)
45	GTP	VM	501	44	29,34,34	1.22	1 (3%)	35,54,54	1.42	6 (17%)
43	GDP	AJ	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.18	3 (10%)
43	GDP	TH	501	-	25,30,30	1.02	1 (4%)	30,47,47	1.09	2 (6%)
45	GTP	NI	501	44	29,34,34	1.22	1 (3%)	35,54,54	1.40	6 (17%)
43	GDP	OH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.05	2 (6%)
45	GTP	QC	501	-	29,34,34	1.28	2 (6%)	35,54,54	1.24	3 (8%)
45	GTP	LE	501	44	29,34,34	1.22	2 (6%)	35,54,54	1.39	5 (14%)
43	GDP	QB	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.12	2 (6%)
45	GTP	MK	501	44	29,34,34	1.26	2 (6%)	35,54,54	1.37	4 (11%)
45	GTP	TK	501	44	29,34,34	1.24	2 (6%)	35,54,54	1.33	6 (17%)
45	GTP	VI	501	44	29,34,34	1.27	2 (6%)	35,54,54	1.31	5 (14%)
45	GTP	AI	501	44	29,34,34	1.25	2 (6%)	35,54,54	1.32	4 (11%)
45	GTP	VK	501	44	29,34,34	1.28	2 (6%)	35,54,54	1.42	5 (14%)
43	GDP	MH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
45	GTP	PI	501	44	29,34,34	1.23	2 (6%)	35,54,54	1.33	4 (11%)
45	GTP	WM	501	44	29,34,34	1.21	2 (6%)	35,54,54	1.35	6 (17%)
43	GDP	OF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.14	2 (6%)
43	GDP	RJ	501	-	25,30,30	0.90	1 (4%)	30,47,47	1.39	4 (13%)
45	GTP	UI	501	44	29,34,34	1.11	1 (3%)	35,54,54	1.51	4 (11%)
43	GDP	FL	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.02	1 (3%)
45	GTP	SC	501	44	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
43	GDP	AL	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.18	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	GTP	PG	501	44	29,34,34	1.23	1 (3%)	35,54,54	1.30	3 (8%)
43	GDP	DB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.11	3 (10%)
45	GTP	EK	501	44	29,34,34	1.23	2 (6%)	35,54,54	1.31	3 (8%)
45	GTP	VE	501	44	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
43	GDP	HJ	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	3 (10%)
43	GDP	CF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.24	4 (13%)
45	GTP	IE	501	44	29,34,34	1.25	2 (6%)	35,54,54	1.38	7 (20%)
43	GDP	WF	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.05	2 (6%)
45	GTP	FI	501	44	29,34,34	1.20	2 (6%)	35,54,54	1.28	4 (11%)
45	GTP	WI	501	44	29,34,34	1.21	2 (6%)	35,54,54	1.67	6 (17%)
45	GTP	SE	501	44	29,34,34	1.20	2 (6%)	35,54,54	1.39	5 (14%)
45	GTP	BK	501	44	29,34,34	1.20	3 (10%)	35,54,54	1.50	6 (17%)
45	GTP	MI	501	44	29,34,34	1.22	1 (3%)	35,54,54	1.22	3 (8%)
43	GDP	PD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.21	4 (13%)
45	GTP	OA	501	44	29,34,34	1.33	5 (17%)	35,54,54	1.29	5 (14%)
43	GDP	FF	501	-	25,30,30	1.29	2 (8%)	30,47,47	1.61	5 (16%)
43	GDP	HD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
45	GTP	RI	501	-	29,34,34	1.12	2 (6%)	35,54,54	1.74	6 (17%)
43	GDP	ED	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
45	GTP	SG	501	44	29,34,34	1.26	2 (6%)	35,54,54	1.49	6 (17%)
45	GTP	JG	501	44	29,34,34	1.29	3 (10%)	35,54,54	1.34	5 (14%)
45	GTP	KE	501	44	29,34,34	1.27	2 (6%)	35,54,54	1.31	5 (14%)
43	GDP	RF	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.15	2 (6%)
45	GTP	RE	501	-	29,34,34	1.27	2 (6%)	35,54,54	1.43	7 (20%)
45	GTP	EG	501	-	29,34,34	1.31	2 (6%)	35,54,54	1.32	4 (11%)
43	GDP	AF	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.12	2 (6%)
43	GDP	DH	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.31	3 (10%)
43	GDP	KF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	2 (6%)
45	GTP	WE	501	44	29,34,34	1.25	2 (6%)	35,54,54	1.24	4 (11%)
45	GTP	QI	501	-	29,34,34	1.21	2 (6%)	35,54,54	1.27	4 (11%)
43	GDP	VL	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	3 (10%)
43	GDP	MJ	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.13	3 (10%)
45	GTP	LK	501	44	29,34,34	1.29	4 (13%)	35,54,54	1.30	6 (17%)
45	GTP	GF	502	44	29,34,34	1.26	2 (6%)	35,54,54	1.35	5 (14%)
45	GTP	HC	501	44	29,34,34	1.25	2 (6%)	35,54,54	1.40	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	GDP	NB	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.10	2 (6%)
45	GTP	PK	501	-	29,34,34	1.25	2 (6%)	35,54,54	1.30	4 (11%)
45	GTP	DG	501	-	29,34,34	1.24	2 (6%)	35,54,54	1.43	5 (14%)
43	GDP	GD	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
45	GTP	RC	501	-	29,34,34	1.20	2 (6%)	35,54,54	1.24	4 (11%)
45	GTP	AF	502	44	29,34,34	1.25	2 (6%)	35,54,54	1.38	7 (20%)
43	GDP	KJ	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.11	2 (6%)
45	GTP	NC	501	44	29,34,34	1.19	2 (6%)	35,54,54	1.34	4 (11%)
45	GTP	UE	501	44	29,34,34	1.22	2 (6%)	35,54,54	1.36	6 (17%)
43	GDP	NJ	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	2 (6%)
43	GDP	JH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.26	3 (10%)
43	GDP	UD	501	-	25,30,30	0.91	1 (4%)	30,47,47	1.09	2 (6%)
43	GDP	GH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	1 (3%)
45	GTP	AK	501	44	29,34,34	1.23	2 (6%)	35,54,54	1.34	4 (11%)
43	GDP	EL	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.13	3 (10%)
43	GDP	CD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
43	GDP	TD	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.24	3 (10%)
45	GTP	TM	501	44	29,34,34	1.18	2 (6%)	35,54,54	1.42	7 (20%)
45	GTP	WK	501	44	29,34,34	1.25	2 (6%)	35,54,54	1.34	4 (11%)
43	GDP	IH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.13	3 (10%)
43	GDP	RH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.13	1 (3%)
43	GDP	QL	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.12	2 (6%)
45	GTP	LC	501	44	29,34,34	1.24	2 (6%)	35,54,54	1.31	4 (11%)
45	GTP	KM	501	44	29,34,34	1.22	2 (6%)	35,54,54	1.31	4 (11%)
45	GTP	RK	501	-	29,34,34	1.20	2 (6%)	35,54,54	1.39	4 (11%)
45	GTP	EE	501	-	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
45	GTP	KI	501	44	29,34,34	1.22	2 (6%)	35,54,54	1.32	5 (14%)
43	GDP	SH	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	3 (10%)
45	GTP	VG	501	44	29,34,34	1.29	2 (6%)	35,54,54	1.31	5 (14%)
43	GDP	AH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
43	GDP	FH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.03	2 (6%)
45	GTP	HK	501	44	29,34,34	1.31	2 (6%)	35,54,54	1.42	6 (17%)
45	GTP	PC	501	44	29,34,34	1.29	2 (6%)	35,54,54	1.39	6 (17%)
45	GTP	OI	501	44	29,34,34	1.24	2 (6%)	35,54,54	1.37	6 (17%)
43	GDP	NH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	GTP	FC	501	44	29,34,34	1.30	4 (13%)	35,54,54	1.40	4 (11%)
45	GTP	GK	501	44	29,34,34	1.20	2 (6%)	35,54,54	1.33	5 (14%)
43	GDP	MN	501	-	25,30,30	0.92	1 (4%)	30,47,47	1.14	3 (10%)
45	GTP	UM	501	44	29,34,34	1.14	1 (3%)	35,54,54	1.39	4 (11%)
45	GTP	BI	501	44	29,34,34	1.25	2 (6%)	35,54,54	1.38	5 (14%)
43	GDP	EF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
43	GDP	PL	501	-	25,30,30	1.12	2 (8%)	30,47,47	1.14	3 (10%)
43	GDP	UJ	501	-	25,30,30	1.39	3 (12%)	30,47,47	1.69	6 (20%)
45	GTP	CI	501	44	29,34,34	1.26	2 (6%)	35,54,54	1.51	5 (14%)
45	GTP	QK	501	-	29,34,34	1.24	3 (10%)	35,54,54	1.41	4 (11%)
45	GTP	NK	501	44	29,34,34	1.33	4 (13%)	35,54,54	1.33	4 (11%)
43	GDP	IN	501	-	25,30,30	0.91	0	30,47,47	1.19	4 (13%)
43	GDP	IJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
43	GDP	MF	501	-	25,30,30	1.13	2 (8%)	30,47,47	1.25	2 (6%)
45	GTP	QE	501	-	29,34,34	1.11	3 (10%)	35,54,54	1.86	5 (14%)
43	GDP	WD	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.06	2 (6%)
45	GTP	IG	501	44	29,34,34	1.21	2 (6%)	35,54,54	1.32	4 (11%)
43	GDP	DD	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.24	4 (13%)
45	GTP	JK	501	44	29,34,34	1.23	2 (6%)	35,54,54	1.33	4 (11%)
43	GDP	GJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.14	3 (10%)
45	GTP	HI	501	44	29,34,34	1.30	3 (10%)	35,54,54	1.34	6 (17%)
45	GTP	JI	501	44	29,34,34	1.23	2 (6%)	35,54,54	1.31	4 (11%)
43	GDP	VH	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	2 (6%)
43	GDP	HB	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	2 (6%)
45	GTP	IC	501	44	29,34,34	1.26	1 (3%)	35,54,54	1.17	4 (11%)
45	GTP	ME	501	44	29,34,34	1.25	2 (6%)	35,54,54	1.40	5 (14%)
43	GDP	WH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
45	GTP	OC	501	44	29,34,34	1.19	2 (6%)	35,54,54	1.42	7 (20%)
43	GDP	UL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.15	2 (6%)
45	GTP	FK	501	44	29,34,34	1.34	4 (13%)	35,54,54	1.37	6 (17%)
43	GDP	JJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.16	3 (10%)
45	GTP	MG	501	-	29,34,34	1.23	2 (6%)	35,54,54	1.26	3 (8%)
43	GDP	WJ	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.15	2 (6%)
43	GDP	AB	501	-	25,30,30	0.90	1 (4%)	30,47,47	1.05	2 (6%)
43	GDP	VF	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	GDP	QH	501	-	25,30,30	1.02	1 (4%)	30,47,47	1.28	4 (13%)
43	GDP	MD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
43	GDP	PF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	3 (10%)
43	GDP	WN	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.03	1 (3%)
45	GTP	CC	501	44	29,34,34	1.27	3 (10%)	35,54,54	1.29	4 (11%)
45	GTP	QG	501	-	29,34,34	1.20	2 (6%)	35,54,54	1.40	5 (14%)
43	GDP	IL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.38	5 (16%)
43	GDP	DF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.20	2 (6%)
43	GDP	BL	501	-	25,30,30	1.03	2 (8%)	30,47,47	1.17	3 (10%)
43	GDP	VJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	3 (10%)
45	GTP	OG	501	-	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
43	GDP	BH	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.06	2 (6%)
45	GTP	EC	501	-	29,34,34	1.22	2 (6%)	35,54,54	1.32	4 (11%)
45	GTP	HM	501	44	29,34,34	1.29	4 (13%)	35,54,54	1.42	7 (20%)
43	GDP	GL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
45	GTP	SI	501	44	29,34,34	1.25	2 (6%)	35,54,54	1.26	4 (11%)
43	GDP	CJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
43	GDP	LF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
43	GDP	GF	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.06	2 (6%)
43	GDP	KG	503	-	25,30,30	0.97	1 (4%)	30,47,47	1.17	1 (3%)
43	GDP	PH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	3 (10%)
45	GTP	JE	501	44	29,34,34	1.42	4 (13%)	35,54,54	1.49	5 (14%)
45	GTP	EI	501	-	29,34,34	1.31	1 (3%)	35,54,54	1.28	5 (14%)
43	GDP	NL	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.17	2 (6%)
43	GDP	ML	501	-	25,30,30	0.92	1 (4%)	30,47,47	1.37	4 (13%)
45	GTP	DC	501	-	29,34,34	1.16	1 (3%)	35,54,54	1.33	5 (14%)
43	GDP	IF	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.17	3 (10%)
43	GDP	CB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
45	GTP	GC	501	44	29,34,34	1.31	3 (10%)	35,54,54	1.77	6 (17%)
45	GTP	HG	501	44	29,34,34	1.23	1 (3%)	35,54,54	1.28	5 (14%)
43	GDP	DL	501	-	25,30,30	0.92	1 (4%)	30,47,47	1.19	3 (10%)
45	GTP	LI	501	44	29,34,34	1.23	2 (6%)	35,54,54	1.34	4 (11%)
45	GTP	TC	501	44	29,34,34	1.23	2 (6%)	35,54,54	1.38	3 (8%)
43	GDP	LL	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
43	GDP	TF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	GDP	TL	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	3 (10%)
45	GTP	SM	501	-	29,34,34	1.22	2 (6%)	35,54,54	1.33	5 (14%)
43	GDP	QD	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
43	GDP	QF	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.10	2 (6%)
45	GTP	OE	501	44	29,34,34	1.23	2 (6%)	35,54,54	1.35	3 (8%)
45	GTP	UC	501	-	29,34,34	1.37	3 (10%)	35,54,54	1.41	5 (14%)
45	GTP	CM	501	44	29,34,34	1.18	1 (3%)	35,54,54	1.35	5 (14%)
45	GTP	NA	501	44	29,34,34	1.20	2 (6%)	35,54,54	1.41	6 (17%)
45	GTP	RG	501	-	29,34,34	1.23	2 (6%)	35,54,54	1.57	9 (25%)
45	GTP	DI	501	-	29,34,34	1.19	2 (6%)	35,54,54	1.31	4 (11%)
45	GTP	OK	501	44	29,34,34	1.34	4 (13%)	35,54,54	1.38	5 (14%)
45	GTP	SK	501	44	29,34,34	1.22	1 (3%)	35,54,54	1.42	5 (14%)
43	GDP	OB	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.13	3 (10%)
45	GTP	KC	501	44	29,34,34	1.19	2 (6%)	35,54,54	1.35	5 (14%)
43	GDP	SF	501	-	25,30,30	0.92	1 (4%)	30,47,47	1.12	2 (6%)
45	GTP	MC	501	44	29,34,34	1.26	2 (6%)	35,54,54	1.39	6 (17%)
43	GDP	AD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
45	GTP	GI	501	44	29,34,34	1.28	2 (6%)	35,54,54	1.53	6 (17%)
43	GDP	KD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
43	GDP	RD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
45	GTP	DM	501	44	29,34,34	1.24	3 (10%)	35,54,54	1.34	5 (14%)
45	GTP	HE	501	44	29,34,34	1.26	2 (6%)	35,54,54	1.32	3 (8%)
45	GTP	KK	501	44	29,34,34	1.27	1 (3%)	35,54,54	1.39	5 (14%)
45	GTP	IM	501	44	29,34,34	1.25	1 (3%)	35,54,54	1.35	4 (11%)
43	GDP	RL	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	3 (10%)
43	GDP	CH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
45	GTP	FM	501	44	29,34,34	1.27	2 (6%)	35,54,54	1.33	4 (11%)
45	GTP	TG	501	44	29,34,34	1.20	2 (6%)	35,54,54	1.25	4 (11%)
43	GDP	OD	501	-	25,30,30	1.03	2 (8%)	30,47,47	1.13	2 (6%)
45	GTP	CK	501	44	29,34,34	1.25	2 (6%)	35,54,54	1.42	6 (17%)
43	GDP	ID	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	3 (10%)
45	GTP	UK	501	44	29,34,34	1.30	3 (10%)	35,54,54	1.43	5 (14%)
43	GDP	SL	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.24	3 (10%)
45	GTP	FF	502	44	29,34,34	1.20	2 (6%)	35,54,54	1.32	4 (11%)
45	GTP	DE	501	-	29,34,34	1.24	3 (10%)	35,54,54	1.38	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	GDP	PJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	3 (10%)
43	GDP	FJ	501	-	25,30,30	0.92	1 (4%)	30,47,47	1.09	1 (3%)
43	GDP	TJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.11	2 (6%)
45	GTP	MM	501	44	29,34,34	1.19	2 (6%)	35,54,54	1.36	4 (11%)
45	GTP	BG	501	44	29,34,34	1.22	2 (6%)	35,54,54	1.33	5 (14%)
45	GTP	NG	501	44	29,34,34	1.17	1 (3%)	35,54,54	1.35	5 (14%)
45	GTP	WC	501	44	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
43	GDP	EJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.18	2 (6%)
43	GDP	UH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
45	GTP	TI	501	44	29,34,34	1.27	3 (10%)	35,54,54	1.33	4 (11%)

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
43	GDP	LD	501	-	-	4/12/32/32	0/3/3/3
45	GTP	EM	501	-	-	6/18/38/38	0/3/3/3
43	GDP	JL	501	-	-	0/12/32/32	0/3/3/3
45	GTP	IK	501	44	-	4/18/38/38	0/3/3/3
43	GDP	HF	501	-	-	2/12/32/32	0/3/3/3
45	GTP	AE	501	44	-	4/18/38/38	0/3/3/3
43	GDP	WL	501	-	-	2/12/32/32	0/3/3/3
43	GDP	UF	501	-	-	0/12/32/32	0/3/3/3
45	GTP	UG	501	44	-	4/18/38/38	0/3/3/3
43	GDP	KL	501	-	-	0/12/32/32	0/3/3/3
45	GTP	BC	501	44	-	4/18/38/38	0/3/3/3
45	GTP	NE	501	44	-	4/18/38/38	0/3/3/3
43	GDP	LN	501	-	-	3/12/32/32	0/3/3/3
43	GDP	BD	501	-	-	1/12/32/32	0/3/3/3
43	GDP	SD	501	-	-	1/12/32/32	0/3/3/3
43	GDP	EH	501	-	-	1/12/32/32	0/3/3/3
43	GDP	RB	501	-	-	1/12/32/32	0/3/3/3
43	GDP	NF	501	-	-	3/12/32/32	0/3/3/3
45	GTP	PE	501	44	-	5/18/38/38	0/3/3/3
45	GTP	PA	501	-	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	GDP	BF	501	-	-	2/12/32/32	0/3/3/3
45	GTP	GE	501	44	-	4/18/38/38	0/3/3/3
45	GTP	LF	502	44	-	9/18/38/38	0/3/3/3
45	GTP	TE	501	44	-	6/18/38/38	0/3/3/3
43	GDP	DJ	501	-	-	1/12/32/32	0/3/3/3
43	GDP	BB	501	-	-	3/12/32/32	0/3/3/3
43	GDP	ND	501	-	-	1/12/32/32	0/3/3/3
43	GDP	OL	501	-	-	2/12/32/32	0/3/3/3
45	GTP	BE	501	44	-	5/18/38/38	0/3/3/3
43	GDP	HH	501	-	-	6/12/32/32	0/3/3/3
43	GDP	PB	501	-	-	2/12/32/32	0/3/3/3
45	GTP	FE	501	44	-	4/18/38/38	0/3/3/3
45	GTP	CE	501	44	-	3/18/38/38	0/3/3/3
43	GDP	HL	501	-	-	2/12/32/32	0/3/3/3
43	GDP	LJ	501	-	-	6/12/32/32	0/3/3/3
45	GTP	VC	501	44	-	4/18/38/38	0/3/3/3
45	GTP	WG	501	44	-	5/18/38/38	0/3/3/3
45	GTP	JC	501	44	-	1/18/38/38	0/3/3/3
43	GDP	JD	501	-	-	0/12/32/32	0/3/3/3
43	GDP	SJ	501	-	-	3/12/32/32	0/3/3/3
45	GTP	DK	501	-	-	5/18/38/38	0/3/3/3
43	GDP	LH	501	-	-	3/12/32/32	0/3/3/3
45	GTP	II	501	-	-	3/18/38/38	0/3/3/3
45	GTP	LM	501	44	-	6/18/38/38	0/3/3/3
43	GDP	VD	501	-	-	5/12/32/32	0/3/3/3
43	GDP	FD	501	-	-	4/12/32/32	0/3/3/3
43	GDP	CL	501	-	-	2/12/32/32	0/3/3/3
43	GDP	OJ	501	-	-	2/12/32/32	0/3/3/3
43	GDP	BJ	501	-	-	2/12/32/32	0/3/3/3
43	GDP	KN	501	-	-	2/12/32/32	0/3/3/3
45	GTP	CG	501	-	-	5/18/38/38	0/3/3/3
43	GDP	JF	501	-	-	0/12/32/32	0/3/3/3
43	GDP	QJ	501	-	-	1/12/32/32	0/3/3/3
45	GTP	KG	501	44	-	5/18/38/38	0/3/3/3
45	GTP	JM	501	44	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	GTP	GM	501	44	-	5/18/38/38	0/3/3/3
45	GTP	AC	501	44	-	6/18/38/38	0/3/3/3
45	GTP	VM	501	44	-	5/18/38/38	0/3/3/3
43	GDP	AJ	501	-	-	2/12/32/32	0/3/3/3
43	GDP	TH	501	-	-	2/12/32/32	0/3/3/3
45	GTP	NI	501	44	-	7/18/38/38	0/3/3/3
43	GDP	OH	501	-	-	0/12/32/32	0/3/3/3
45	GTP	QC	501	-	-	8/18/38/38	0/3/3/3
45	GTP	LE	501	44	-	6/18/38/38	0/3/3/3
43	GDP	QB	501	-	-	1/12/32/32	0/3/3/3
45	GTP	MK	501	44	-	7/18/38/38	0/3/3/3
45	GTP	TK	501	44	-	3/18/38/38	0/3/3/3
45	GTP	VI	501	44	-	6/18/38/38	0/3/3/3
45	GTP	AI	501	44	-	7/18/38/38	0/3/3/3
45	GTP	VK	501	44	-	5/18/38/38	0/3/3/3
43	GDP	MH	501	-	-	2/12/32/32	0/3/3/3
45	GTP	PI	501	44	-	1/18/38/38	0/3/3/3
45	GTP	WM	501	44	-	6/18/38/38	0/3/3/3
43	GDP	OF	501	-	-	3/12/32/32	0/3/3/3
43	GDP	RJ	501	-	-	2/12/32/32	0/3/3/3
45	GTP	UI	501	44	-	7/18/38/38	0/3/3/3
43	GDP	FL	501	-	-	3/12/32/32	0/3/3/3
45	GTP	SC	501	44	-	4/18/38/38	0/3/3/3
43	GDP	AL	501	-	-	2/12/32/32	0/3/3/3
45	GTP	PG	501	44	-	8/18/38/38	0/3/3/3
43	GDP	DB	501	-	-	6/12/32/32	0/3/3/3
45	GTP	EK	501	44	-	3/18/38/38	0/3/3/3
45	GTP	VE	501	44	-	4/18/38/38	0/3/3/3
43	GDP	HJ	501	-	-	3/12/32/32	0/3/3/3
43	GDP	CF	501	-	-	3/12/32/32	0/3/3/3
45	GTP	IE	501	44	-	5/18/38/38	0/3/3/3
43	GDP	WF	501	-	-	1/12/32/32	0/3/3/3
45	GTP	FI	501	44	-	4/18/38/38	0/3/3/3
45	GTP	WI	501	44	-	2/18/38/38	0/3/3/3
45	GTP	SE	501	44	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	GTP	BK	501	44	-	8/18/38/38	0/3/3/3
45	GTP	MI	501	44	-	7/18/38/38	0/3/3/3
43	GDP	PD	501	-	-	3/12/32/32	0/3/3/3
45	GTP	OA	501	44	-	7/18/38/38	0/3/3/3
43	GDP	FF	501	-	-	3/12/32/32	0/3/3/3
43	GDP	HD	501	-	-	5/12/32/32	0/3/3/3
45	GTP	RI	501	-	-	5/18/38/38	0/3/3/3
43	GDP	ED	501	-	-	1/12/32/32	0/3/3/3
45	GTP	SG	501	44	-	4/18/38/38	0/3/3/3
45	GTP	JG	501	44	-	3/18/38/38	0/3/3/3
45	GTP	KE	501	44	-	6/18/38/38	0/3/3/3
43	GDP	RF	501	-	-	0/12/32/32	0/3/3/3
45	GTP	RE	501	-	-	7/18/38/38	0/3/3/3
45	GTP	EG	501	-	-	4/18/38/38	0/3/3/3
43	GDP	AF	501	-	-	3/12/32/32	0/3/3/3
43	GDP	DH	501	-	-	1/12/32/32	0/3/3/3
43	GDP	KF	501	-	-	3/12/32/32	0/3/3/3
45	GTP	WE	501	44	-	5/18/38/38	0/3/3/3
45	GTP	QI	501	-	-	6/18/38/38	0/3/3/3
43	GDP	VL	501	-	-	2/12/32/32	0/3/3/3
43	GDP	MJ	501	-	-	4/12/32/32	0/3/3/3
45	GTP	LK	501	44	-	9/18/38/38	0/3/3/3
45	GTP	GF	502	44	-	6/18/38/38	0/3/3/3
45	GTP	HC	501	44	-	6/18/38/38	0/3/3/3
43	GDP	NB	501	-	-	4/12/32/32	0/3/3/3
45	GTP	PK	501	-	-	3/18/38/38	0/3/3/3
45	GTP	DG	501	-	-	7/18/38/38	0/3/3/3
43	GDP	GD	501	-	-	3/12/32/32	0/3/3/3
45	GTP	RC	501	-	-	7/18/38/38	0/3/3/3
45	GTP	AF	502	44	-	7/18/38/38	0/3/3/3
43	GDP	KJ	501	-	-	1/12/32/32	0/3/3/3
45	GTP	NC	501	44	-	7/18/38/38	0/3/3/3
45	GTP	UE	501	44	-	4/18/38/38	0/3/3/3
43	GDP	NJ	501	-	-	2/12/32/32	0/3/3/3
43	GDP	JH	501	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	GDP	UD	501	-	-	4/12/32/32	0/3/3/3
43	GDP	GH	501	-	-	2/12/32/32	0/3/3/3
45	GTP	AK	501	44	-	7/18/38/38	0/3/3/3
43	GDP	EL	501	-	-	2/12/32/32	0/3/3/3
43	GDP	CD	501	-	-	2/12/32/32	0/3/3/3
43	GDP	TD	501	-	-	1/12/32/32	0/3/3/3
45	GTP	TM	501	44	-	4/18/38/38	0/3/3/3
45	GTP	WK	501	44	-	7/18/38/38	0/3/3/3
43	GDP	IH	501	-	-	3/12/32/32	0/3/3/3
43	GDP	RH	501	-	-	0/12/32/32	0/3/3/3
43	GDP	QL	501	-	-	3/12/32/32	0/3/3/3
45	GTP	LC	501	44	-	4/18/38/38	0/3/3/3
45	GTP	KM	501	44	-	2/18/38/38	0/3/3/3
45	GTP	RK	501	-	-	3/18/38/38	0/3/3/3
45	GTP	EE	501	-	-	4/18/38/38	0/3/3/3
45	GTP	KI	501	44	-	5/18/38/38	0/3/3/3
43	GDP	SH	501	-	-	0/12/32/32	0/3/3/3
45	GTP	VG	501	44	-	3/18/38/38	0/3/3/3
43	GDP	AH	501	-	-	5/12/32/32	0/3/3/3
43	GDP	FH	501	-	-	1/12/32/32	0/3/3/3
45	GTP	HK	501	44	-	7/18/38/38	0/3/3/3
45	GTP	PC	501	44	-	8/18/38/38	0/3/3/3
45	GTP	OI	501	44	-	6/18/38/38	0/3/3/3
43	GDP	NH	501	-	-	1/12/32/32	0/3/3/3
45	GTP	FC	501	44	-	7/18/38/38	0/3/3/3
45	GTP	GK	501	44	-	6/18/38/38	0/3/3/3
43	GDP	MN	501	-	-	4/12/32/32	0/3/3/3
45	GTP	UM	501	44	-	4/18/38/38	0/3/3/3
45	GTP	BI	501	44	-	6/18/38/38	0/3/3/3
43	GDP	EF	501	-	-	3/12/32/32	0/3/3/3
43	GDP	PL	501	-	-	1/12/32/32	0/3/3/3
43	GDP	UJ	501	-	-	4/12/32/32	0/3/3/3
45	GTP	CI	501	44	-	5/18/38/38	0/3/3/3
45	GTP	QK	501	-	-	6/18/38/38	0/3/3/3
45	GTP	NK	501	44	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	GDP	IN	501	-	-	1/12/32/32	0/3/3/3
43	GDP	IJ	501	-	-	1/12/32/32	0/3/3/3
43	GDP	MF	501	-	-	2/12/32/32	0/3/3/3
45	GTP	QE	501	-	-	6/18/38/38	0/3/3/3
43	GDP	WD	501	-	-	1/12/32/32	0/3/3/3
45	GTP	IG	501	44	-	6/18/38/38	0/3/3/3
43	GDP	DD	501	-	-	1/12/32/32	0/3/3/3
45	GTP	JK	501	44	-	9/18/38/38	0/3/3/3
43	GDP	GJ	501	-	-	0/12/32/32	0/3/3/3
45	GTP	HI	501	44	-	4/18/38/38	0/3/3/3
45	GTP	JI	501	44	-	1/18/38/38	0/3/3/3
43	GDP	VH	501	-	-	1/12/32/32	0/3/3/3
43	GDP	HB	501	-	-	4/12/32/32	0/3/3/3
45	GTP	IC	501	44	-	4/18/38/38	0/3/3/3
45	GTP	ME	501	44	-	5/18/38/38	0/3/3/3
43	GDP	WH	501	-	-	5/12/32/32	0/3/3/3
45	GTP	OC	501	44	-	8/18/38/38	0/3/3/3
43	GDP	UL	501	-	-	1/12/32/32	0/3/3/3
45	GTP	FK	501	44	-	7/18/38/38	0/3/3/3
43	GDP	JJ	501	-	-	1/12/32/32	0/3/3/3
45	GTP	MG	501	-	-	4/18/38/38	0/3/3/3
43	GDP	WJ	501	-	-	3/12/32/32	0/3/3/3
43	GDP	AB	501	-	-	3/12/32/32	0/3/3/3
43	GDP	VF	501	-	-	2/12/32/32	0/3/3/3
43	GDP	QH	501	-	-	2/12/32/32	0/3/3/3
43	GDP	MD	501	-	-	1/12/32/32	0/3/3/3
43	GDP	PF	501	-	-	2/12/32/32	0/3/3/3
43	GDP	WN	501	-	-	0/12/32/32	0/3/3/3
45	GTP	CC	501	44	-	7/18/38/38	0/3/3/3
45	GTP	QG	501	-	-	4/18/38/38	0/3/3/3
43	GDP	IL	501	-	-	6/12/32/32	0/3/3/3
43	GDP	DF	501	-	-	2/12/32/32	0/3/3/3
43	GDP	BL	501	-	-	1/12/32/32	0/3/3/3
43	GDP	VJ	501	-	-	1/12/32/32	0/3/3/3
45	GTP	OG	501	-	-	1/18/38/38	0/3/3/3
43	GDP	BH	501	-	-	4/12/32/32	0/3/3/3
45	GTP	EC	501	-	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	GTP	HM	501	44	-	8/18/38/38	0/3/3/3
43	GDP	GL	501	-	-	2/12/32/32	0/3/3/3
45	GTP	SI	501	44	-	6/18/38/38	0/3/3/3
43	GDP	CJ	501	-	-	2/12/32/32	0/3/3/3
43	GDP	LF	501	-	-	1/12/32/32	0/3/3/3
43	GDP	GF	501	-	-	5/12/32/32	0/3/3/3
43	GDP	KG	503	-	-	0/12/32/32	0/3/3/3
43	GDP	PH	501	-	-	2/12/32/32	0/3/3/3
45	GTP	JE	501	44	-	9/18/38/38	0/3/3/3
45	GTP	EI	501	-	-	3/18/38/38	0/3/3/3
43	GDP	NL	501	-	-	3/12/32/32	0/3/3/3
43	GDP	ML	501	-	-	0/12/32/32	0/3/3/3
45	GTP	DC	501	-	-	11/18/38/38	0/3/3/3
43	GDP	IF	501	-	-	1/12/32/32	0/3/3/3
43	GDP	CB	501	-	-	4/12/32/32	0/3/3/3
45	GTP	GC	501	44	-	5/18/38/38	0/3/3/3
45	GTP	HG	501	44	-	2/18/38/38	0/3/3/3
43	GDP	DL	501	-	-	5/12/32/32	0/3/3/3
45	GTP	LI	501	44	-	4/18/38/38	0/3/3/3
45	GTP	TC	501	44	-	3/18/38/38	0/3/3/3
43	GDP	LL	501	-	-	2/12/32/32	0/3/3/3
43	GDP	TF	501	-	-	1/12/32/32	0/3/3/3
43	GDP	TL	501	-	-	2/12/32/32	0/3/3/3
45	GTP	SM	501	-	-	5/18/38/38	0/3/3/3
43	GDP	QD	501	-	-	1/12/32/32	0/3/3/3
43	GDP	QF	501	-	-	2/12/32/32	0/3/3/3
45	GTP	OE	501	44	-	7/18/38/38	0/3/3/3
45	GTP	UC	501	-	-	6/18/38/38	0/3/3/3
45	GTP	CM	501	44	-	4/18/38/38	0/3/3/3
45	GTP	NA	501	44	-	5/18/38/38	0/3/3/3
45	GTP	RG	501	-	-	6/18/38/38	0/3/3/3
45	GTP	DI	501	-	-	4/18/38/38	0/3/3/3
45	GTP	OK	501	44	-	6/18/38/38	0/3/3/3
45	GTP	SK	501	44	-	6/18/38/38	0/3/3/3
43	GDP	OB	501	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	GTP	KC	501	44	-	5/18/38/38	0/3/3/3
43	GDP	SF	501	-	-	1/12/32/32	0/3/3/3
45	GTP	MC	501	44	-	6/18/38/38	0/3/3/3
43	GDP	AD	501	-	-	4/12/32/32	0/3/3/3
45	GTP	GI	501	44	-	2/18/38/38	0/3/3/3
43	GDP	KD	501	-	-	3/12/32/32	0/3/3/3
43	GDP	RD	501	-	-	1/12/32/32	0/3/3/3
45	GTP	DM	501	44	-	2/18/38/38	0/3/3/3
45	GTP	HE	501	44	-	4/18/38/38	0/3/3/3
45	GTP	KK	501	44	-	7/18/38/38	0/3/3/3
45	GTP	IM	501	44	-	6/18/38/38	0/3/3/3
43	GDP	RL	501	-	-	1/12/32/32	0/3/3/3
43	GDP	CH	501	-	-	3/12/32/32	0/3/3/3
45	GTP	FM	501	44	-	3/18/38/38	0/3/3/3
45	GTP	TG	501	44	-	2/18/38/38	0/3/3/3
43	GDP	OD	501	-	-	2/12/32/32	0/3/3/3
45	GTP	CK	501	44	-	5/18/38/38	0/3/3/3
43	GDP	ID	501	-	-	2/12/32/32	0/3/3/3
45	GTP	UK	501	44	-	6/18/38/38	0/3/3/3
43	GDP	SL	501	-	-	1/12/32/32	0/3/3/3
45	GTP	FF	502	44	-	6/18/38/38	0/3/3/3
45	GTP	DE	501	-	-	5/18/38/38	0/3/3/3
43	GDP	PJ	501	-	-	2/12/32/32	0/3/3/3
43	GDP	FJ	501	-	-	4/12/32/32	0/3/3/3
43	GDP	TJ	501	-	-	0/12/32/32	0/3/3/3
45	GTP	MM	501	44	-	6/18/38/38	0/3/3/3
45	GTP	BG	501	44	-	6/18/38/38	0/3/3/3
45	GTP	NG	501	44	-	7/18/38/38	0/3/3/3
45	GTP	WC	501	44	-	0/18/38/38	0/3/3/3
43	GDP	EJ	501	-	-	4/12/32/32	0/3/3/3
43	GDP	UH	501	-	-	2/12/32/32	0/3/3/3
45	GTP	TI	501	44	-	6/18/38/38	0/3/3/3

The worst 5 of 422 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	EI	501	GTP	C5-C6	-5.10	1.37	1.47
45	GC	501	GTP	C5-C6	-4.61	1.38	1.47
45	IC	501	GTP	C5-C6	-4.56	1.38	1.47
45	QC	501	GTP	C5-C6	-4.55	1.38	1.47
45	VG	501	GTP	C5-C6	-4.54	1.38	1.47

The worst 5 of 967 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	EH	501	GDP	O6-C6-N1	7.46	129.48	120.62
45	QE	501	GTP	O4'-C1'-N9	6.84	117.81	108.75
43	EH	501	GDP	O6-C6-C5	-6.51	111.42	124.32
43	HH	501	GDP	O4'-C1'-N9	6.49	117.35	108.75
45	RI	501	GTP	C4'-O4'-C1'	5.48	114.94	109.92

There are no chirality outliers.

5 of 974 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	AB	501	GDP	C5'-O5'-PA-O1A
43	AB	501	GDP	O4'-C4'-C5'-O5'
43	AB	501	GDP	C3'-C4'-C5'-O5'
43	AF	501	GDP	O4'-C4'-C5'-O5'
43	AF	501	GDP	C3'-C4'-C5'-O5'

There are no ring outliers.

178 monomers are involved in 336 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	LD	501	GDP	1	0
43	JL	501	GDP	1	0
45	IK	501	GTP	1	0
45	AE	501	GTP	2	0
45	BC	501	GTP	1	0
45	NE	501	GTP	1	0
43	LN	501	GDP	2	0
43	EH	501	GDP	3	0
43	RB	501	GDP	2	0
45	PE	501	GTP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	PA	501	GTP	3	0
43	BF	501	GDP	1	0
45	GE	501	GTP	3	0
45	LF	502	GTP	1	0
45	TE	501	GTP	3	0
43	DJ	501	GDP	1	0
43	HH	501	GDP	4	0
43	PB	501	GDP	1	0
45	FE	501	GTP	1	0
45	CE	501	GTP	4	0
45	VC	501	GTP	1	0
45	WG	501	GTP	1	0
43	JD	501	GDP	1	0
43	SJ	501	GDP	1	0
45	DK	501	GTP	1	0
43	LH	501	GDP	1	0
43	VD	501	GDP	1	0
43	FD	501	GDP	3	0
43	OJ	501	GDP	1	0
43	BJ	501	GDP	1	0
43	KN	501	GDP	1	0
45	CG	501	GTP	4	0
43	JF	501	GDP	2	0
43	QJ	501	GDP	2	0
45	KG	501	GTP	1	0
45	JM	501	GTP	3	0
45	GM	501	GTP	3	0
45	AC	501	GTP	2	0
45	VM	501	GTP	4	0
43	AJ	501	GDP	1	0
43	TH	501	GDP	1	0
45	NI	501	GTP	1	0
43	OH	501	GDP	1	0
45	QC	501	GTP	1	0
45	LE	501	GTP	3	0
43	QB	501	GDP	3	0
45	VI	501	GTP	1	0
45	AI	501	GTP	1	0
43	MH	501	GDP	1	0
45	PI	501	GTP	3	0
45	WM	501	GTP	2	0
43	RJ	501	GDP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	UI	501	GTP	1	0
45	PG	501	GTP	4	0
45	EK	501	GTP	2	0
45	VE	501	GTP	1	0
43	CF	501	GDP	3	0
45	IE	501	GTP	2	0
43	WF	501	GDP	2	0
45	FI	501	GTP	2	0
45	SE	501	GTP	3	0
45	BK	501	GTP	2	0
45	MI	501	GTP	2	0
45	OA	501	GTP	2	0
43	FF	501	GDP	2	0
43	HD	501	GDP	2	0
45	RI	501	GTP	2	0
43	ED	501	GDP	2	0
45	JG	501	GTP	1	0
45	KE	501	GTP	1	0
43	RF	501	GDP	1	0
45	EG	501	GTP	6	0
43	AF	501	GDP	1	0
43	DH	501	GDP	3	0
45	WE	501	GTP	2	0
45	QI	501	GTP	1	0
43	VL	501	GDP	1	0
45	HC	501	GTP	3	0
45	PK	501	GTP	5	0
45	AF	502	GTP	3	0
45	NC	501	GTP	3	0
45	UE	501	GTP	1	0
43	NJ	501	GDP	1	0
43	JH	501	GDP	3	0
43	TD	501	GDP	1	0
45	TM	501	GTP	2	0
45	WK	501	GTP	3	0
43	IH	501	GDP	2	0
43	QL	501	GDP	2	0
45	RK	501	GTP	2	0
45	EE	501	GTP	1	0
43	FH	501	GDP	3	0
45	HK	501	GTP	2	0
45	PC	501	GTP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	OI	501	GTP	2	0
45	FC	501	GTP	2	0
45	GK	501	GTP	2	0
43	MN	501	GDP	1	0
45	UM	501	GTP	1	0
45	BI	501	GTP	1	0
43	EF	501	GDP	2	0
43	PL	501	GDP	1	0
43	UJ	501	GDP	3	0
45	CI	501	GTP	4	0
45	QK	501	GTP	2	0
45	NK	501	GTP	2	0
43	IJ	501	GDP	2	0
43	WD	501	GDP	2	0
43	DD	501	GDP	2	0
45	JK	501	GTP	3	0
43	GJ	501	GDP	1	0
45	HI	501	GTP	1	0
45	JI	501	GTP	1	0
43	VH	501	GDP	1	0
43	HB	501	GDP	1	0
45	ME	501	GTP	1	0
45	OC	501	GTP	1	0
43	UL	501	GDP	1	0
45	FK	501	GTP	5	0
43	WJ	501	GDP	1	0
43	QH	501	GDP	1	0
43	MD	501	GDP	2	0
43	WN	501	GDP	2	0
45	QG	501	GTP	2	0
43	IL	501	GDP	2	0
43	DF	501	GDP	1	0
45	EC	501	GTP	1	0
43	GL	501	GDP	2	0
45	SI	501	GTP	2	0
43	CJ	501	GDP	1	0
43	LF	501	GDP	1	0
43	GF	501	GDP	3	0
43	KG	503	GDP	1	0
43	PH	501	GDP	2	0
45	JE	501	GTP	2	0
45	EI	501	GTP	2	0

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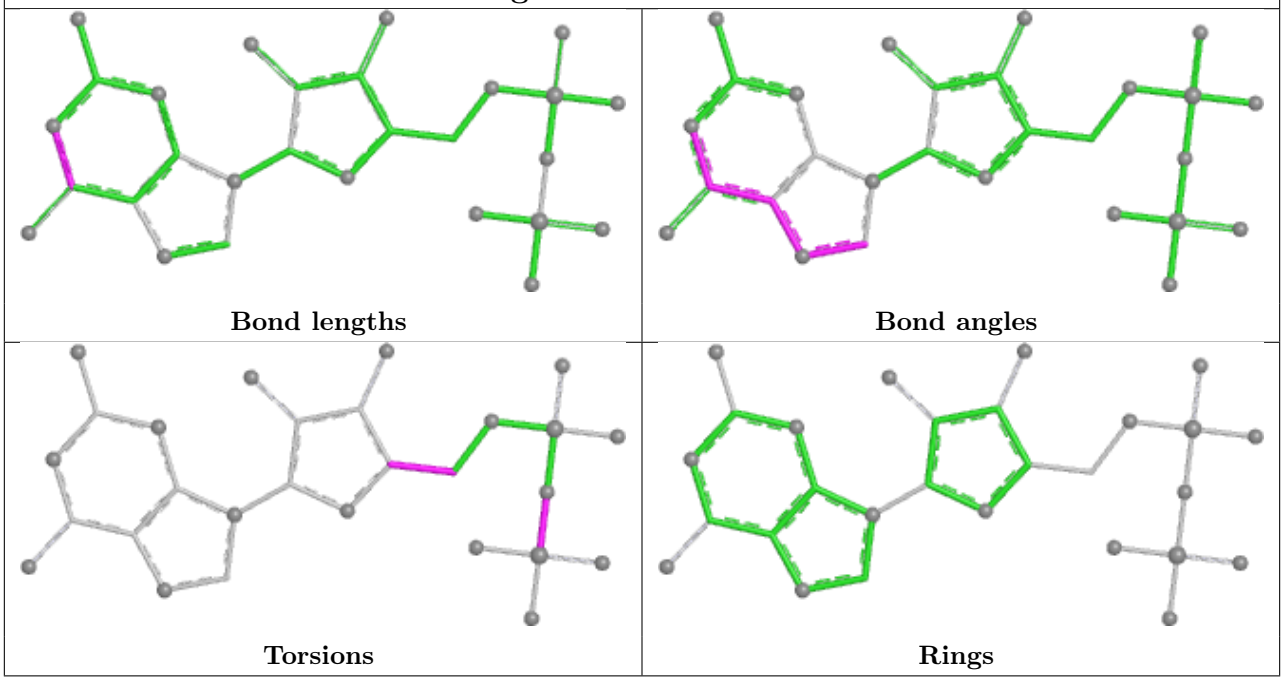
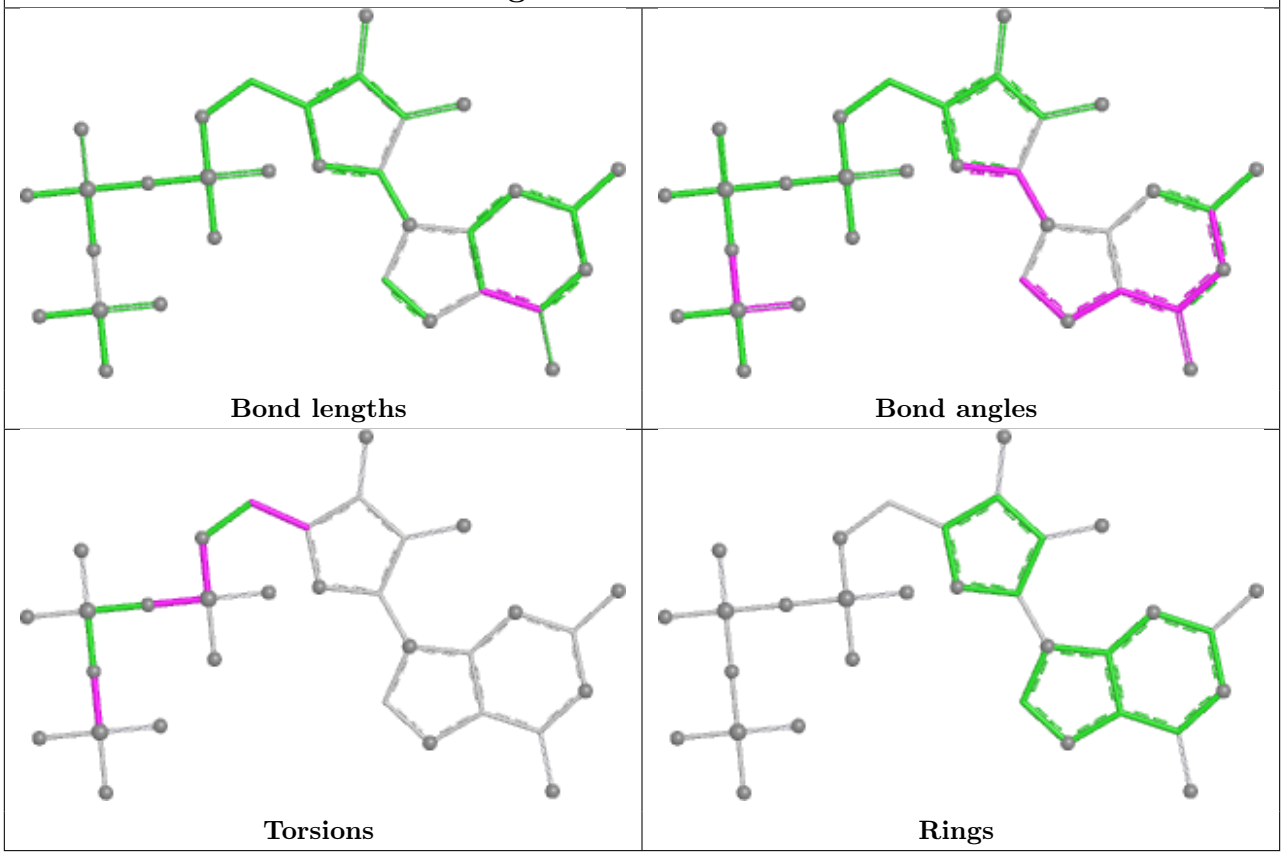
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	NL	501	GDP	1	0
43	ML	501	GDP	2	0
45	DC	501	GTP	4	0
43	IF	501	GDP	3	0
43	CB	501	GDP	2	0
45	GC	501	GTP	3	0
45	HG	501	GTP	2	0
43	DL	501	GDP	1	0
45	LI	501	GTP	1	0
43	LL	501	GDP	2	0
45	SM	501	GTP	3	0
43	QF	501	GDP	1	0
45	OE	501	GTP	2	0
45	UC	501	GTP	4	0
45	CM	501	GTP	4	0
45	NA	501	GTP	2	0
45	RG	501	GTP	3	0
45	DI	501	GTP	2	0
45	OK	501	GTP	1	0
45	KC	501	GTP	1	0
43	SF	501	GDP	2	0
45	MC	501	GTP	1	0
43	KD	501	GDP	1	0
43	RD	501	GDP	1	0
45	HE	501	GTP	1	0
45	KK	501	GTP	1	0
45	FM	501	GTP	1	0
45	TG	501	GTP	2	0
43	OD	501	GDP	1	0
45	CK	501	GTP	2	0
43	ID	501	GDP	3	0
45	UK	501	GTP	1	0
43	SL	501	GDP	3	0
45	FF	502	GTP	1	0
45	DE	501	GTP	2	0
43	PJ	501	GDP	2	0
43	TJ	501	GDP	1	0
45	MM	501	GTP	4	0
45	BG	501	GTP	2	0
45	WC	501	GTP	2	0
43	EJ	501	GDP	1	0
45	TI	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.

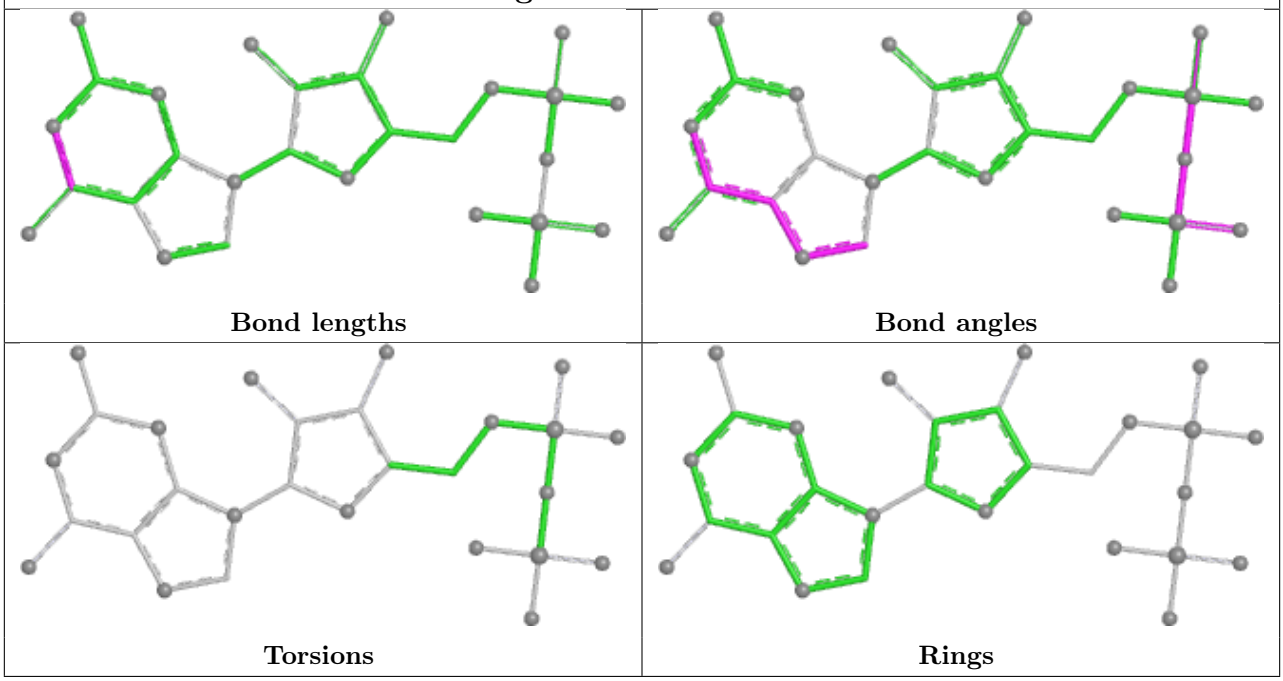
Ligand GDP LD 501



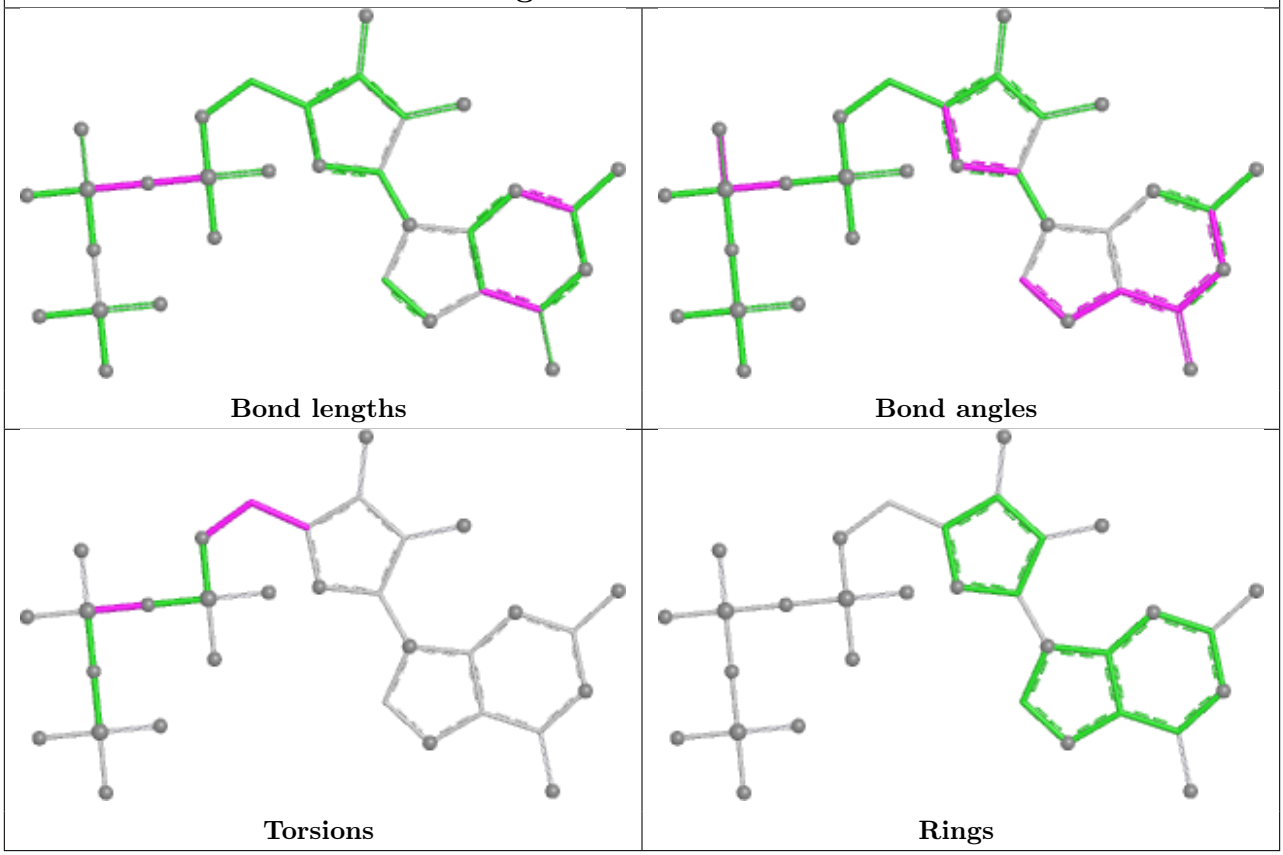
Ligand GTP EM 501



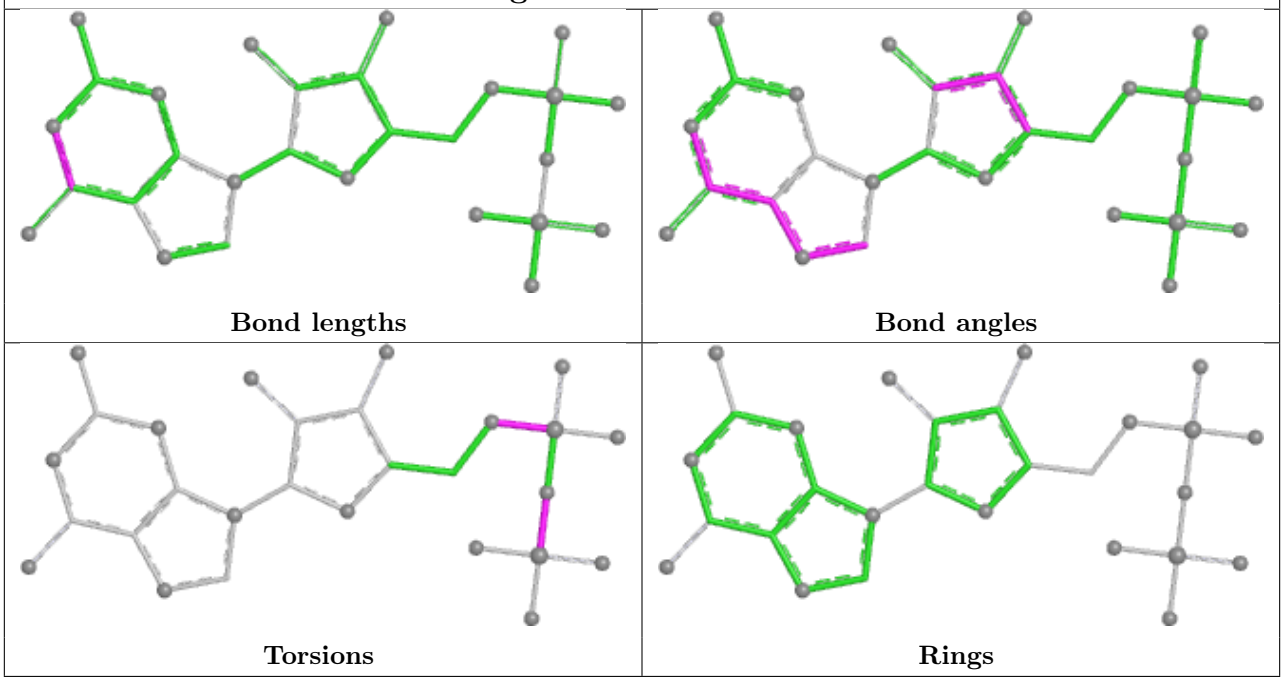
Ligand GDP JL 501



Ligand GTP IK 501



Ligand GDP HF 501



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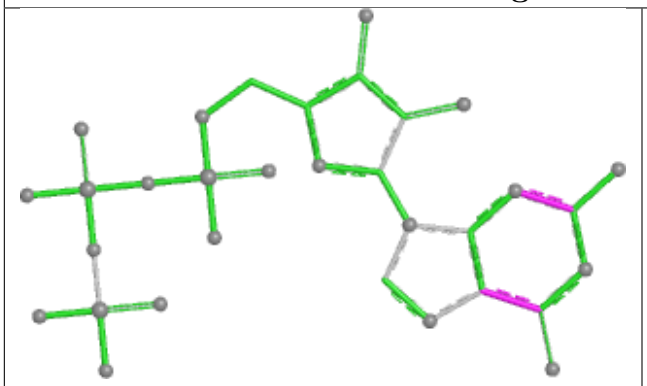
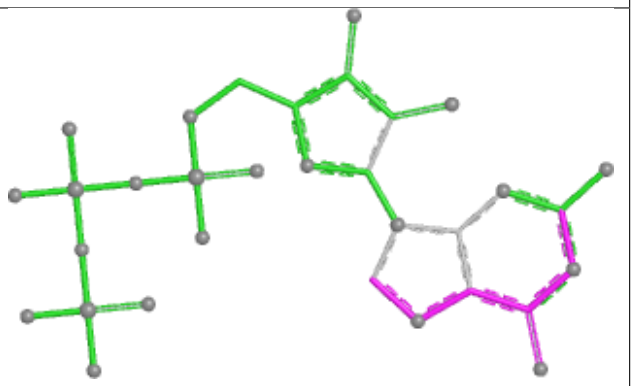
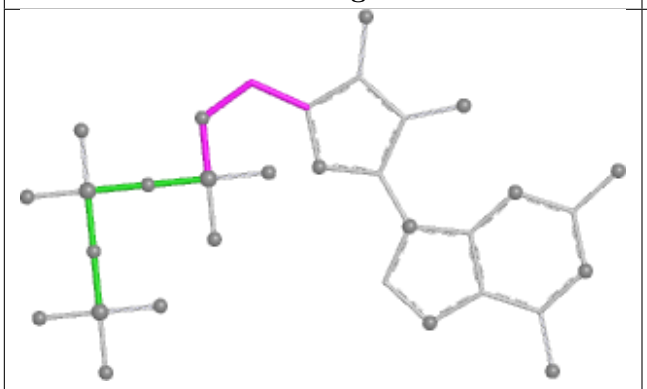


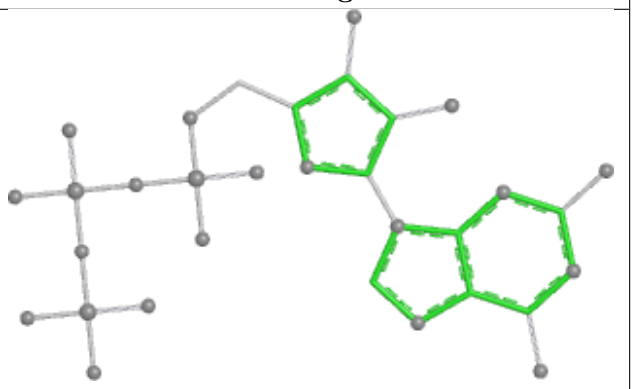
Bond lengths



Bond angles

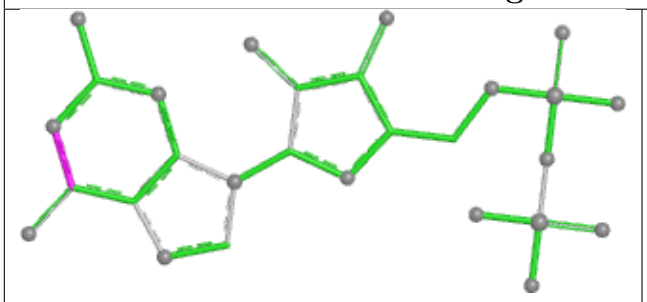


Torsions



Rings

Ligand GDP WL 501



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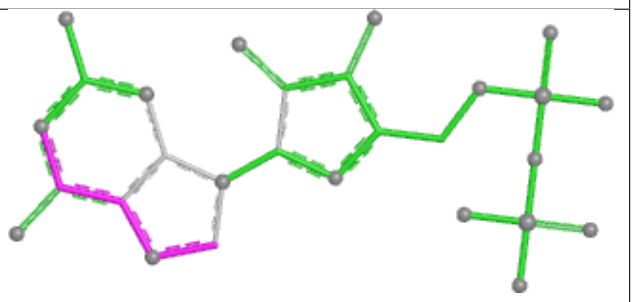

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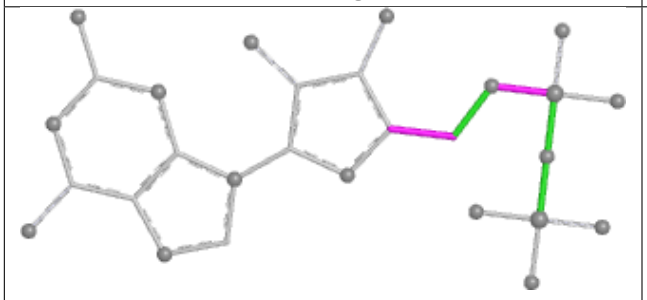

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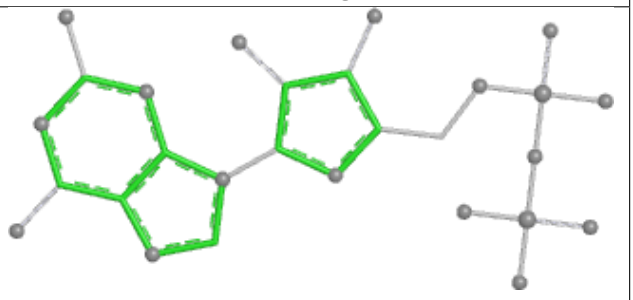
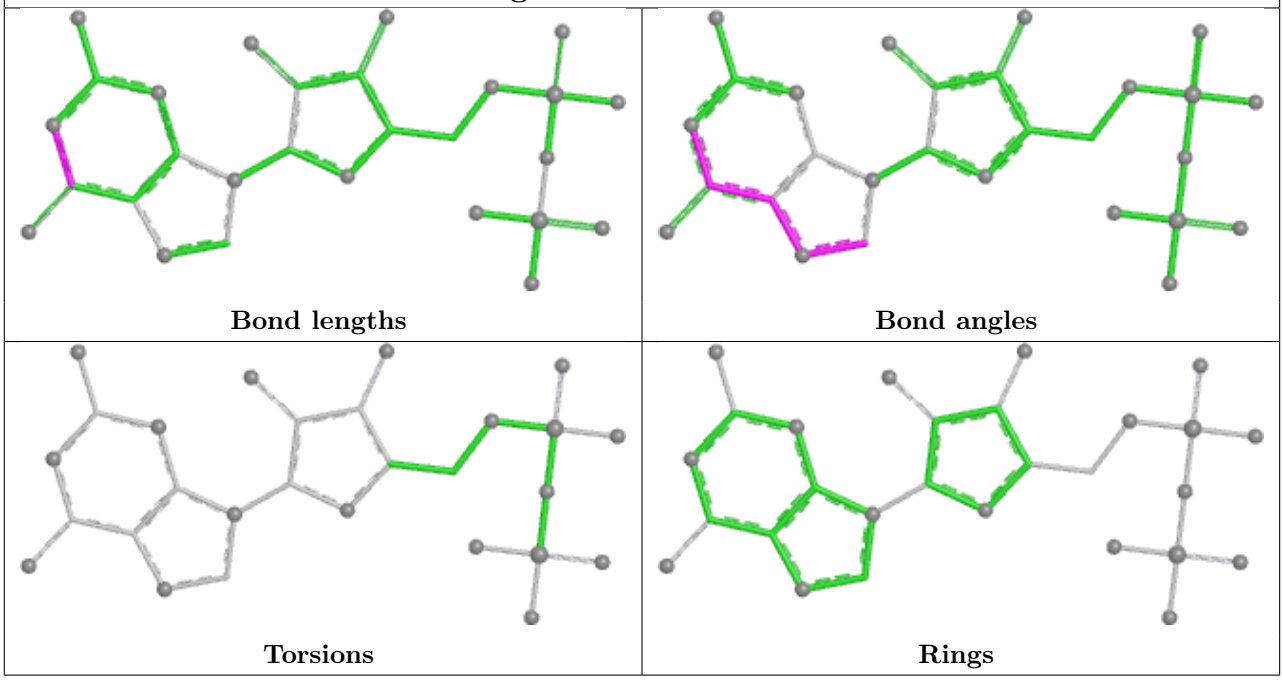


Rings

Ligand GDP UF 501



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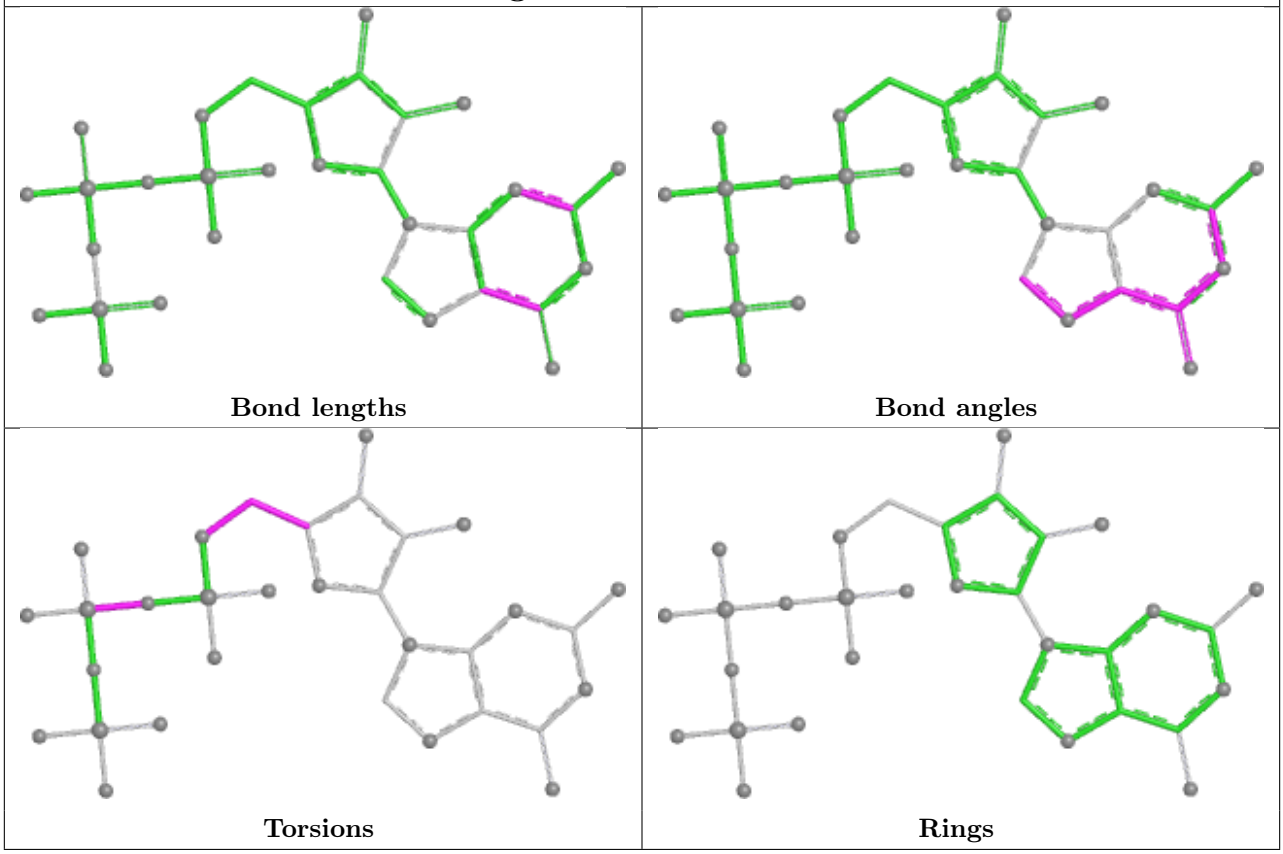

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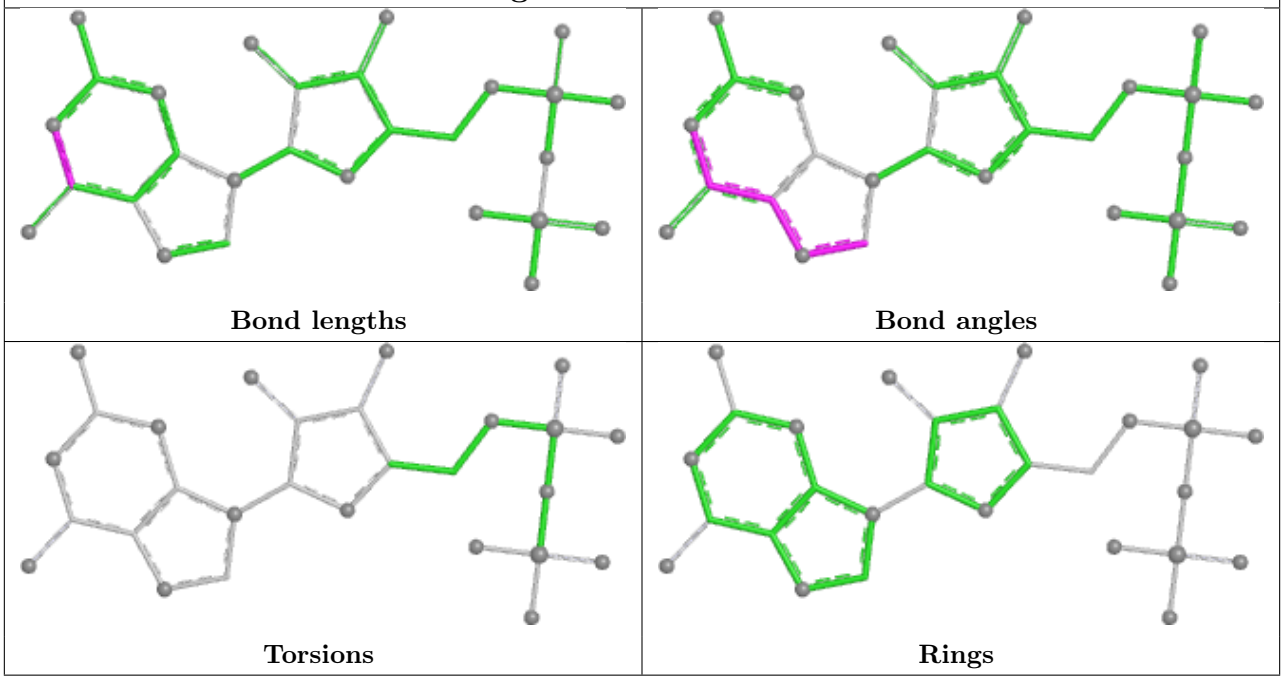

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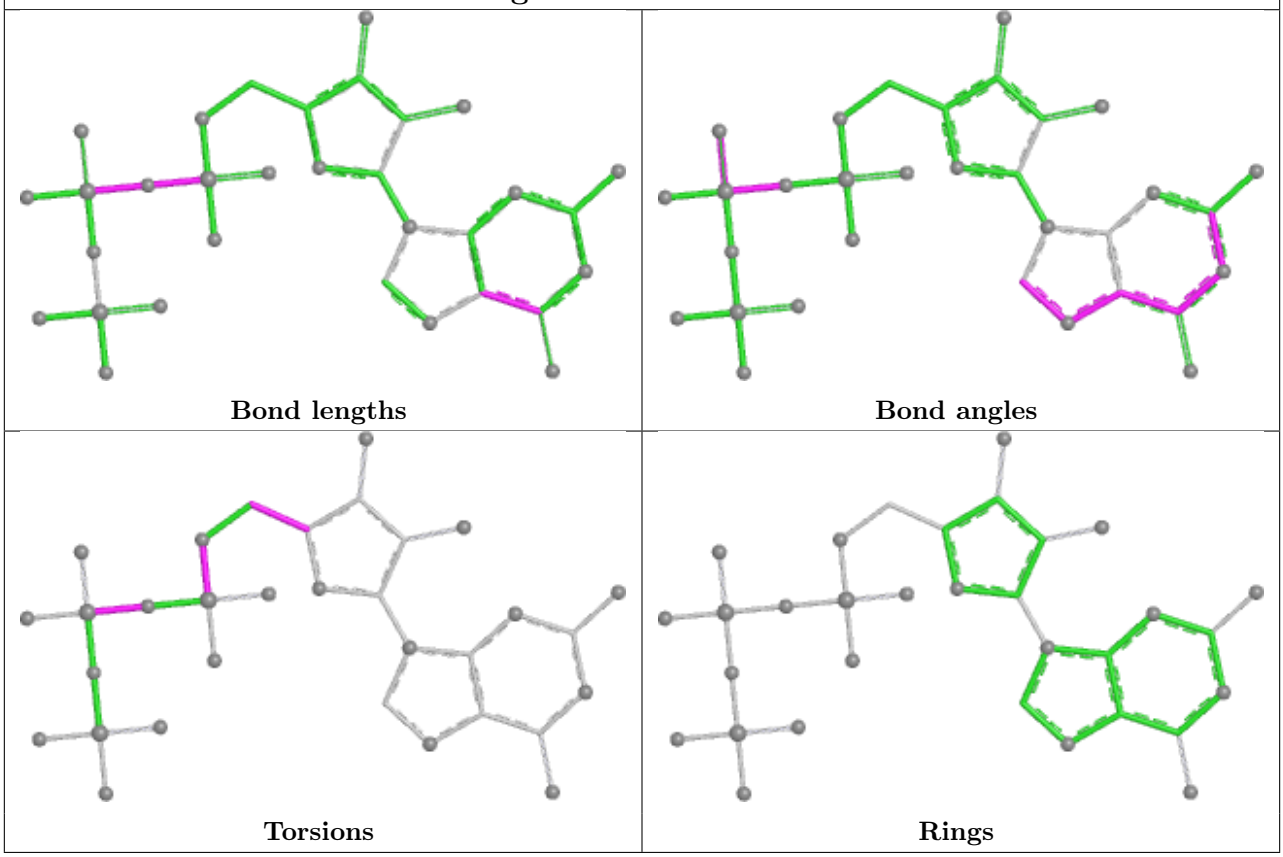

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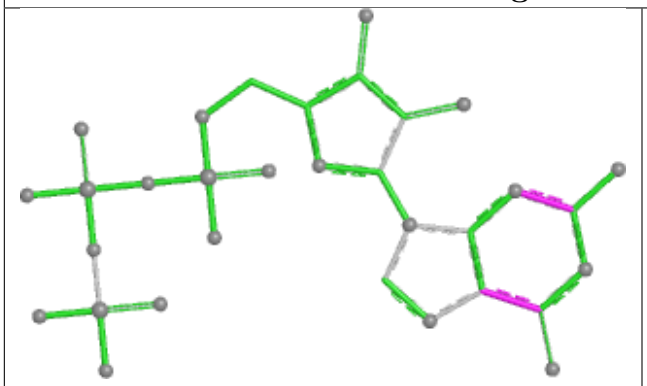
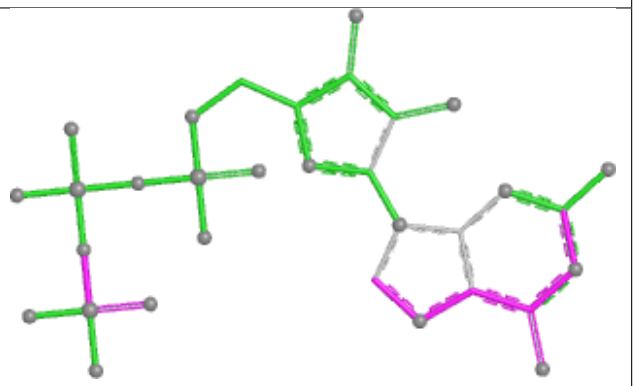
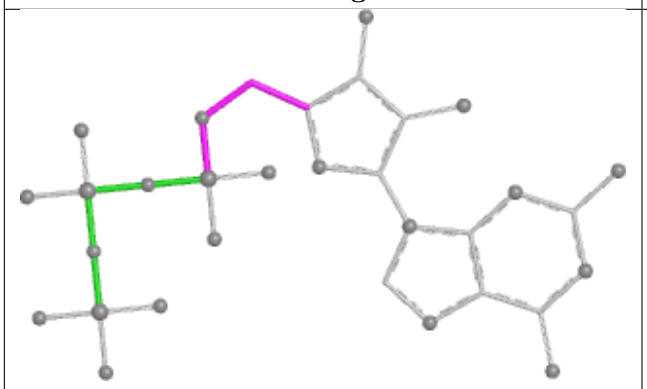


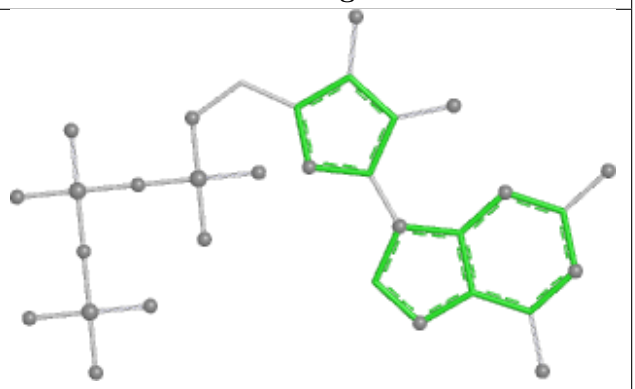
Bond lengths



Bond angles

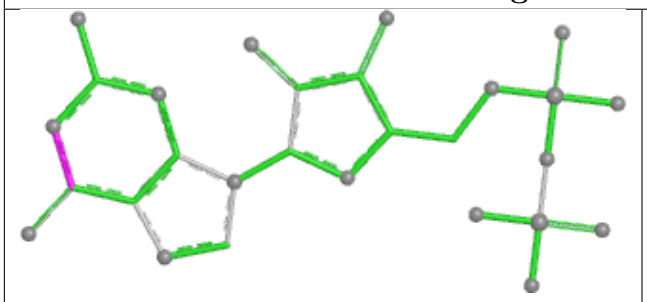


Torsions



Rings

Ligand GDP LN 501



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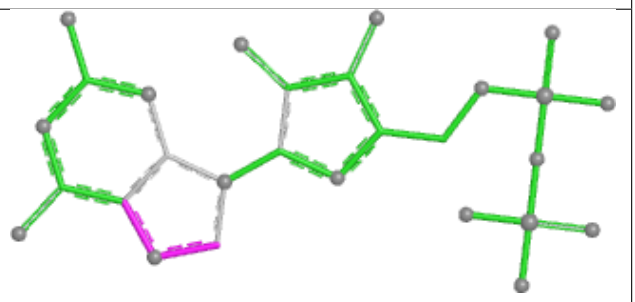
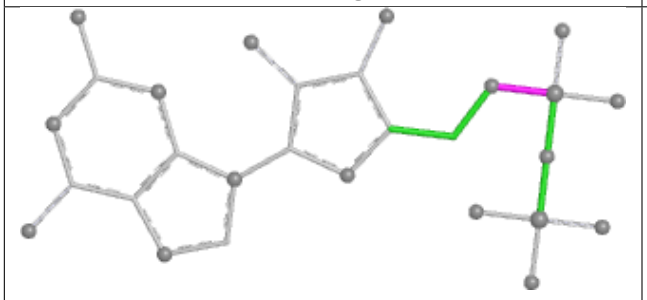


Bond angles



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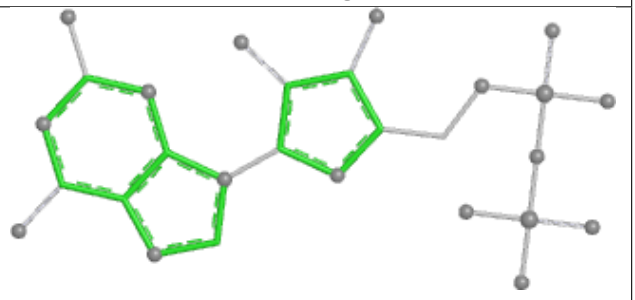

Rings

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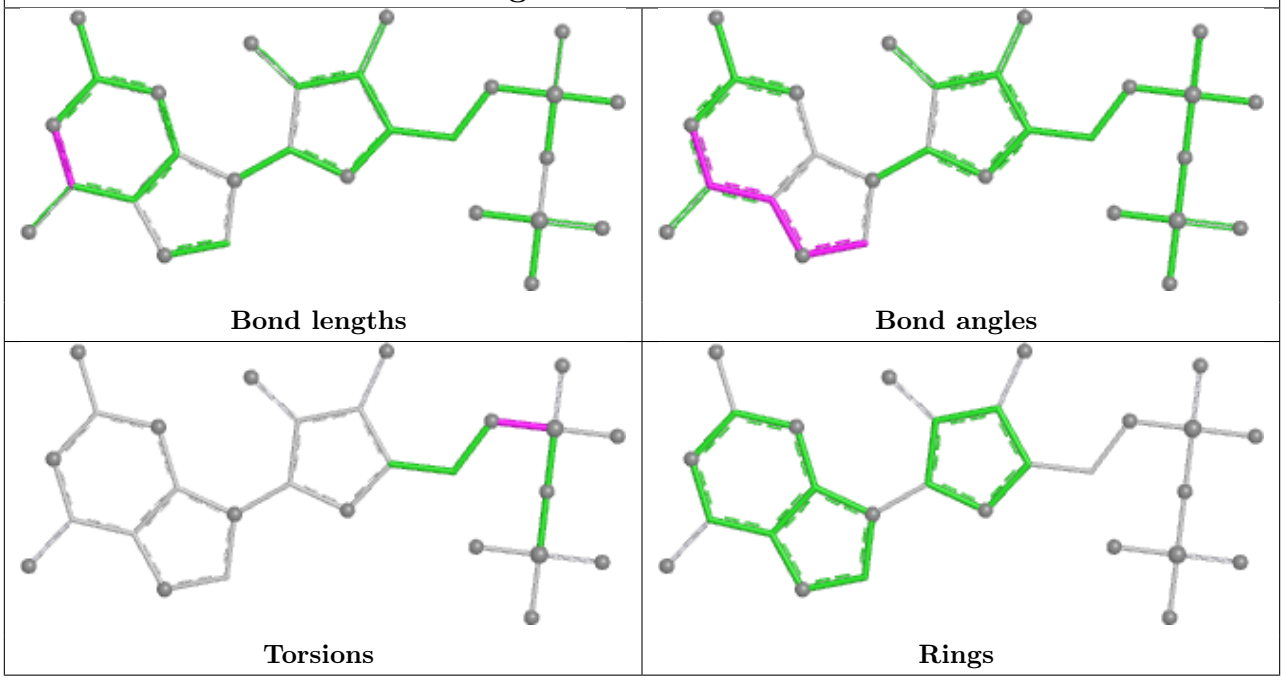

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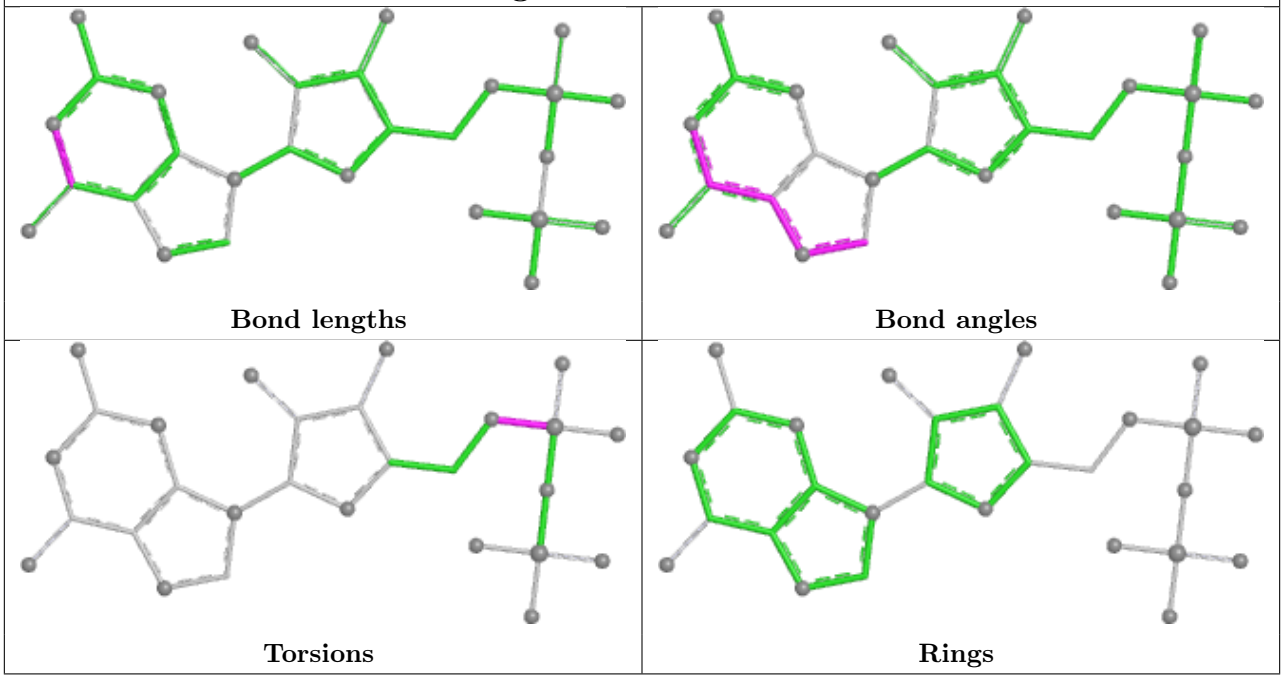

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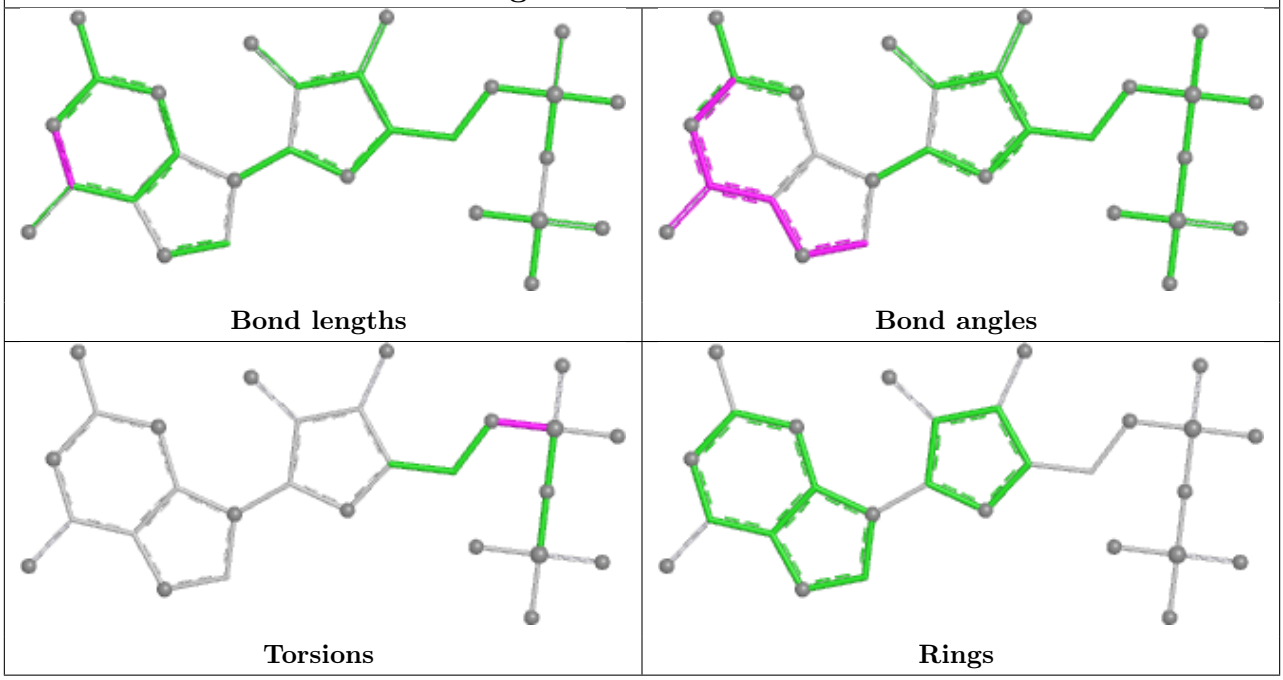

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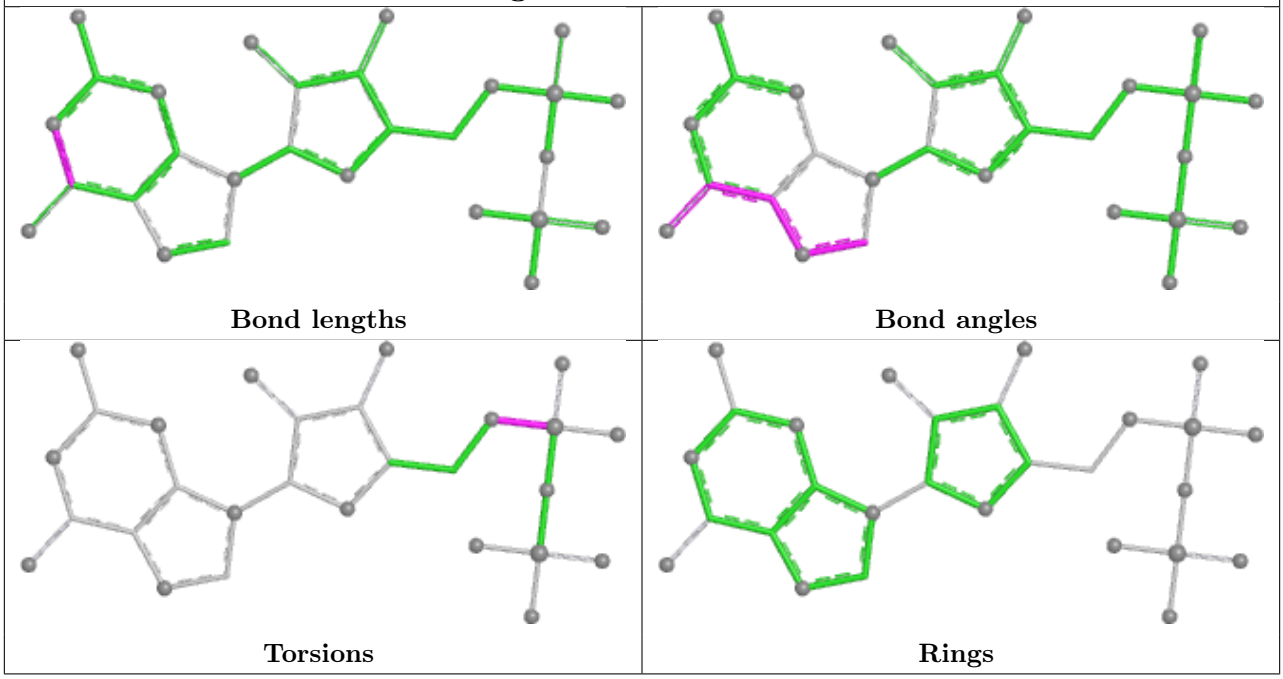

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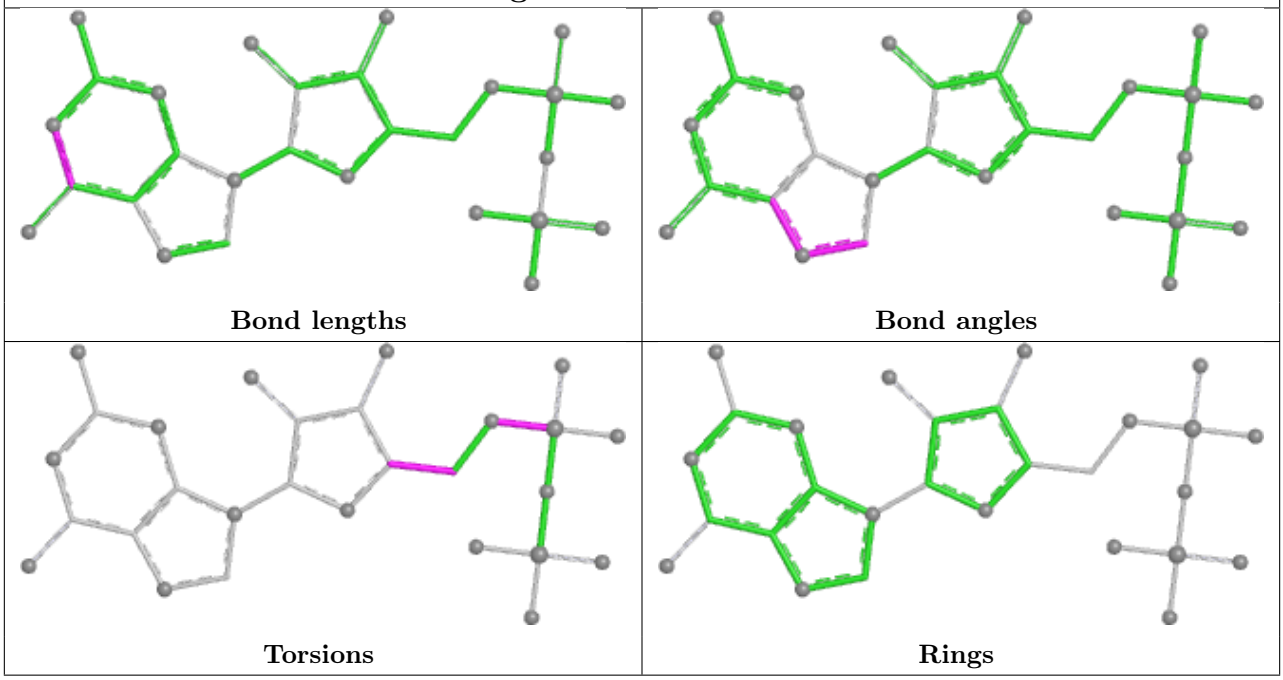

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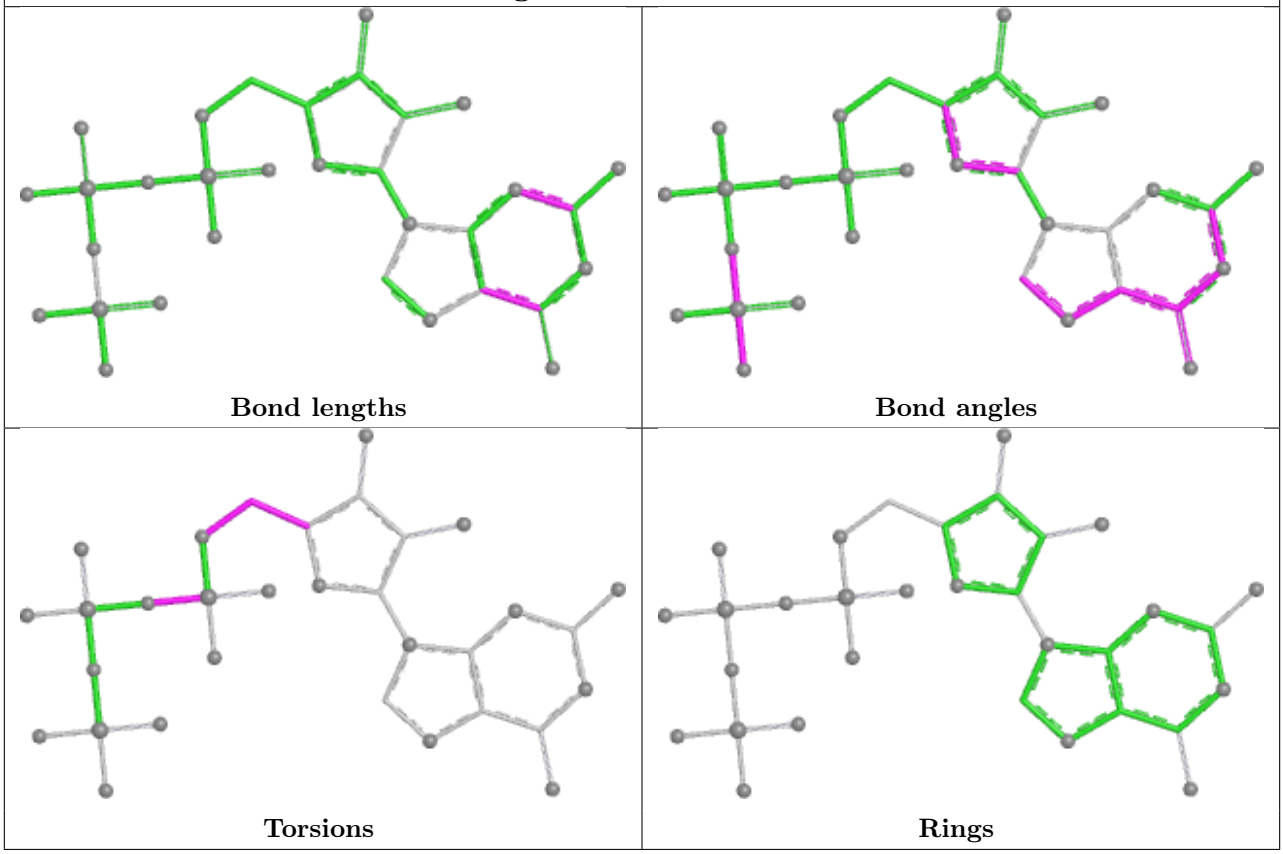

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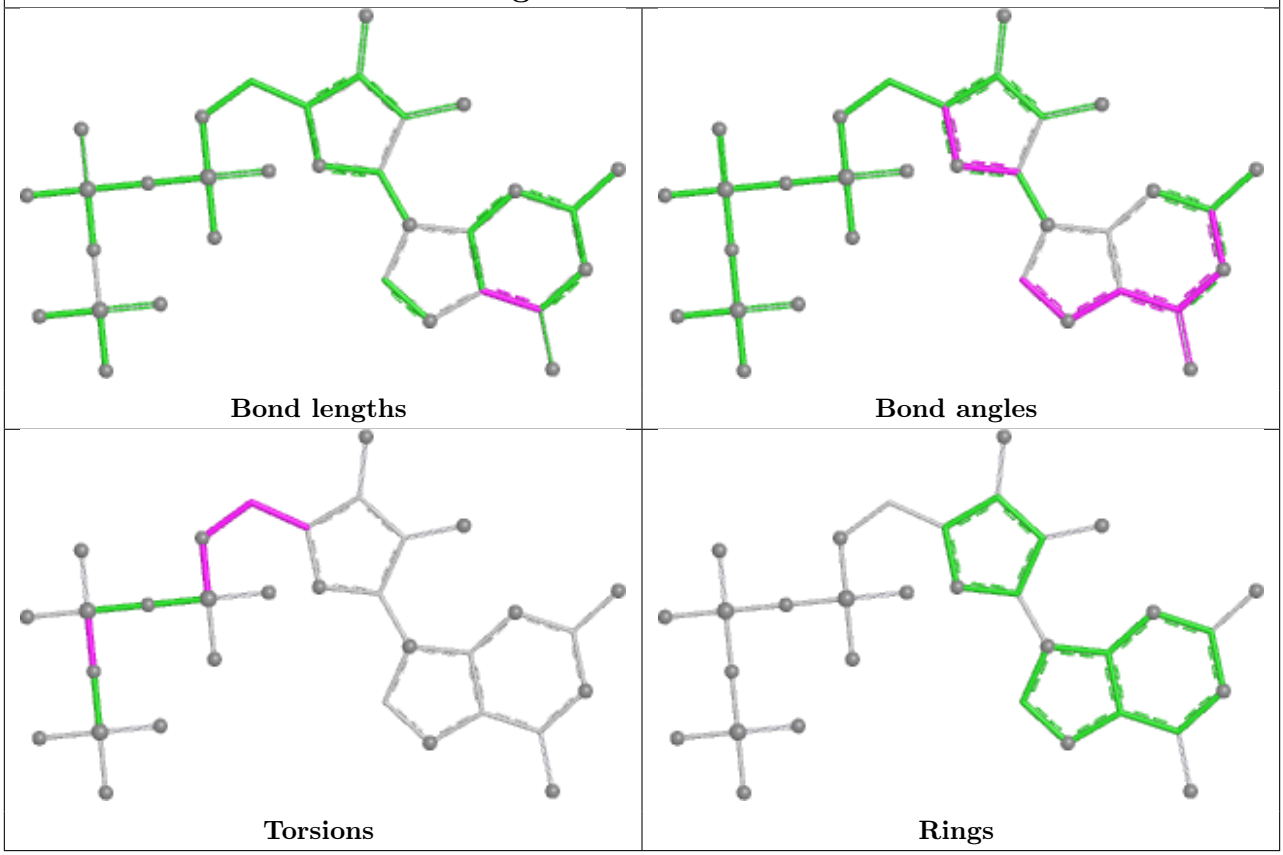

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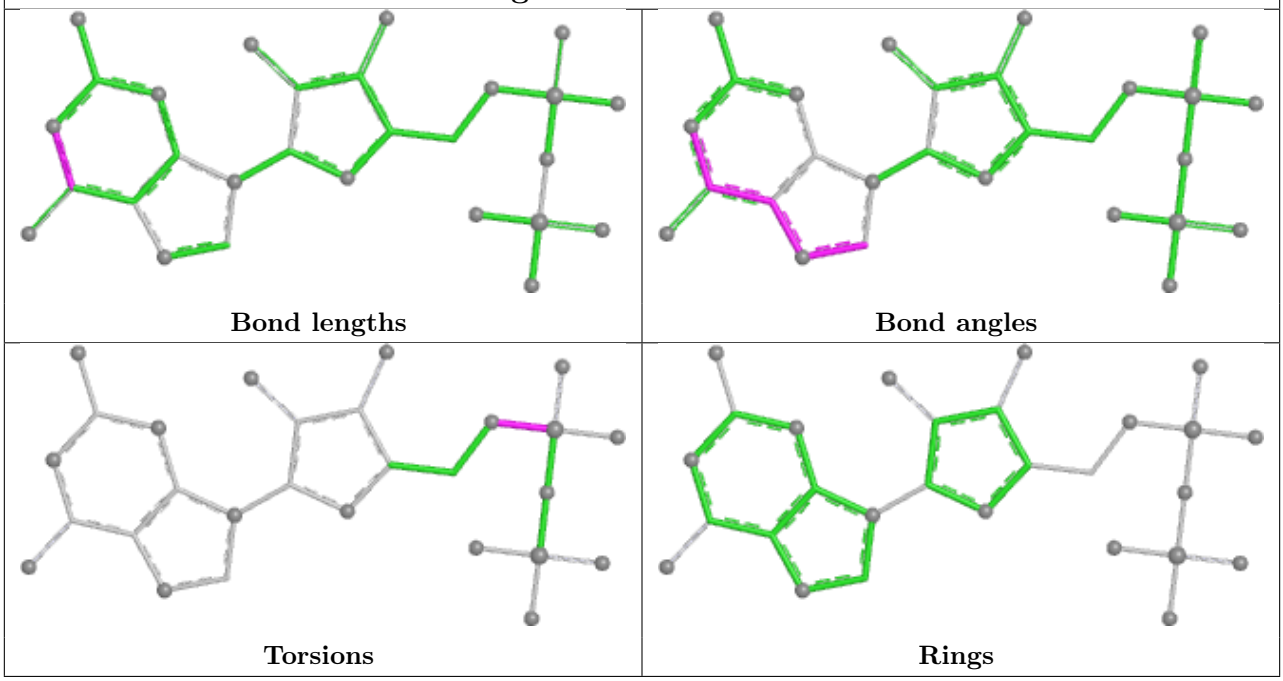

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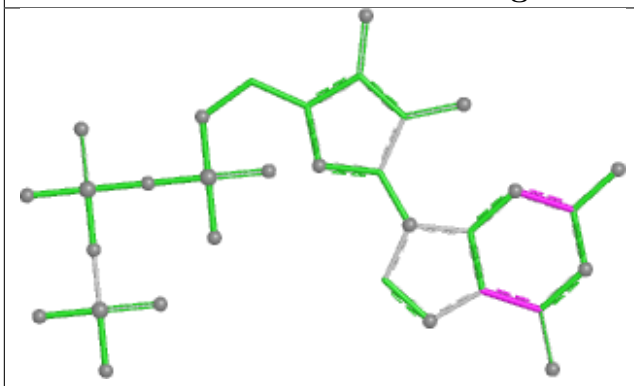
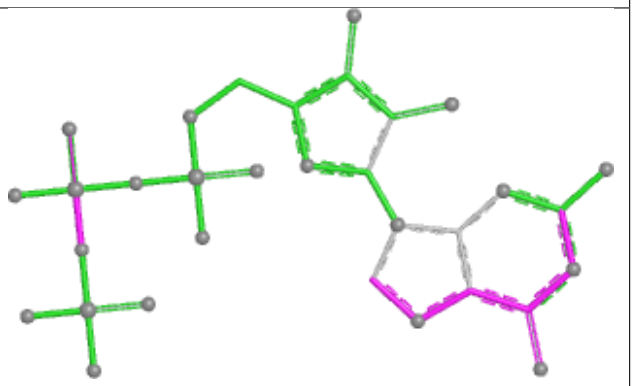
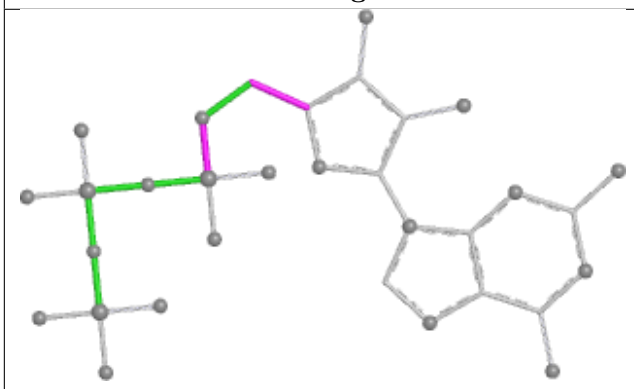


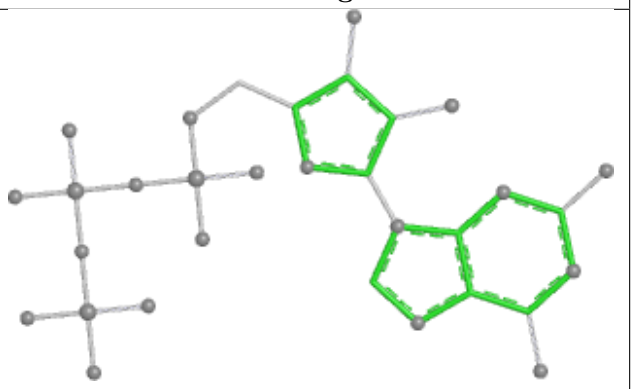
Bond lengths



Bond angles

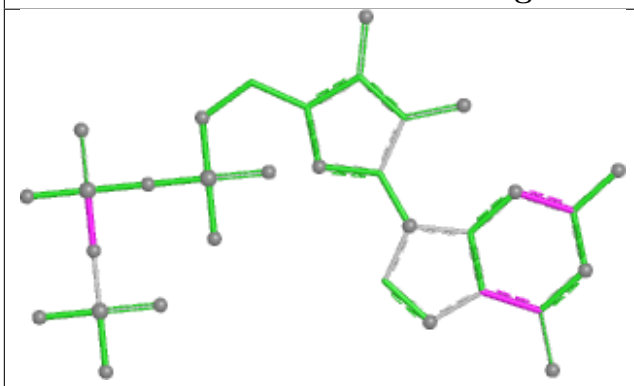


Torsions



Rings

Ligand GTP LF 502



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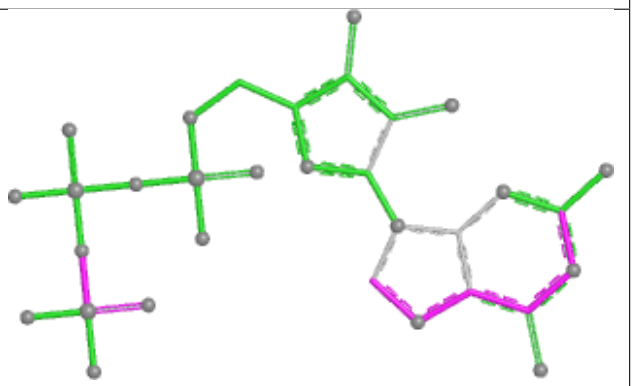

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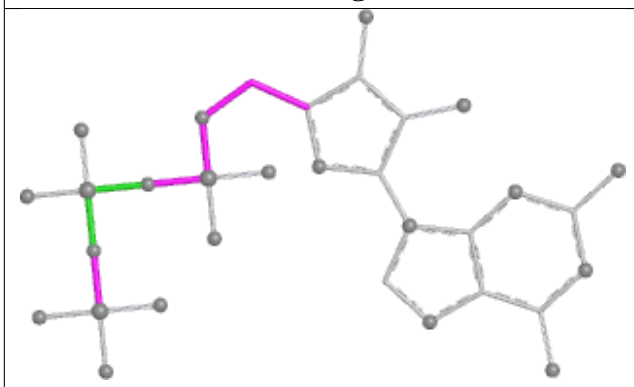
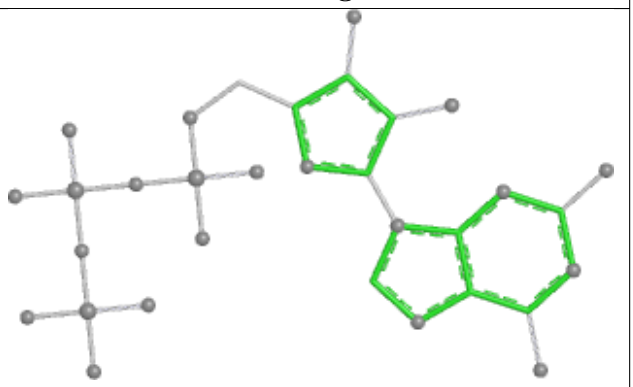
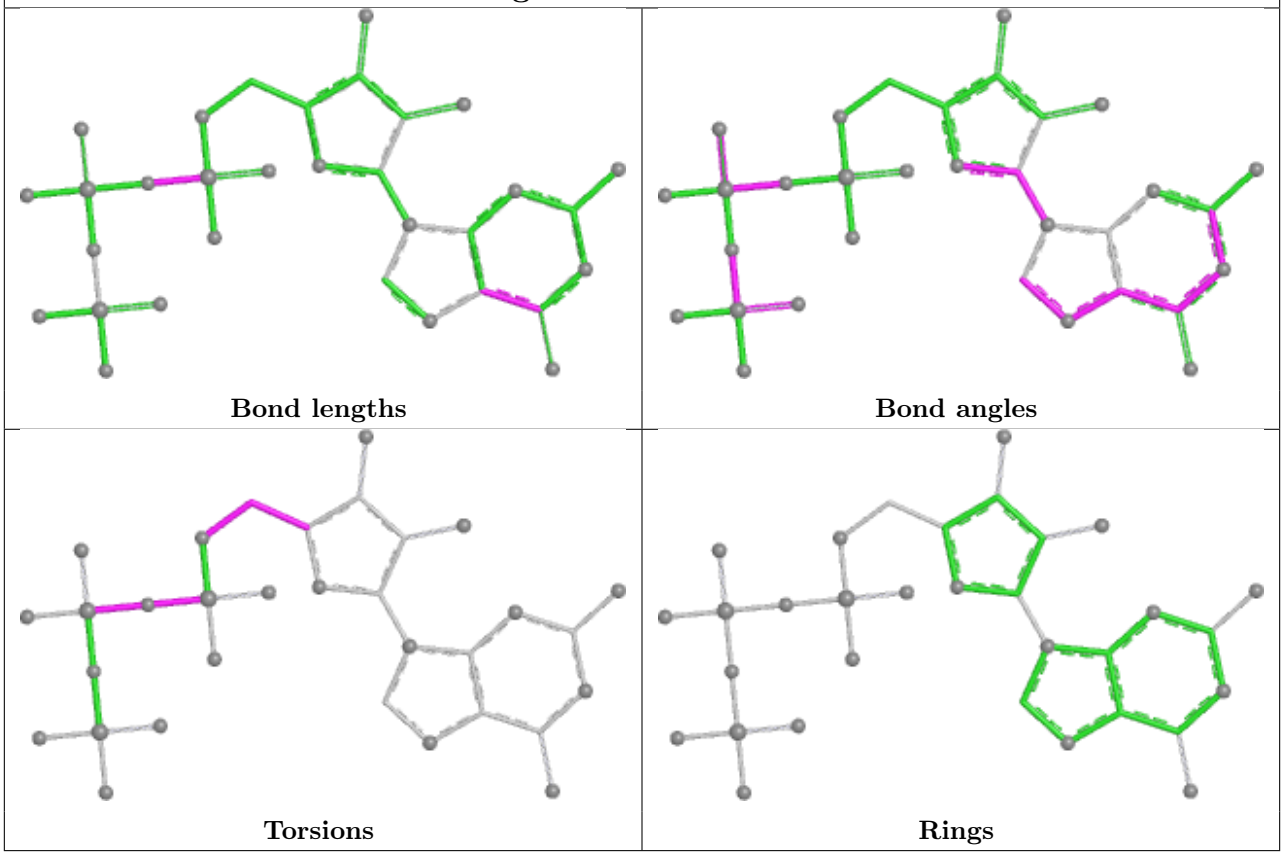


Torsions



Rings

Ligand GTP TE 501



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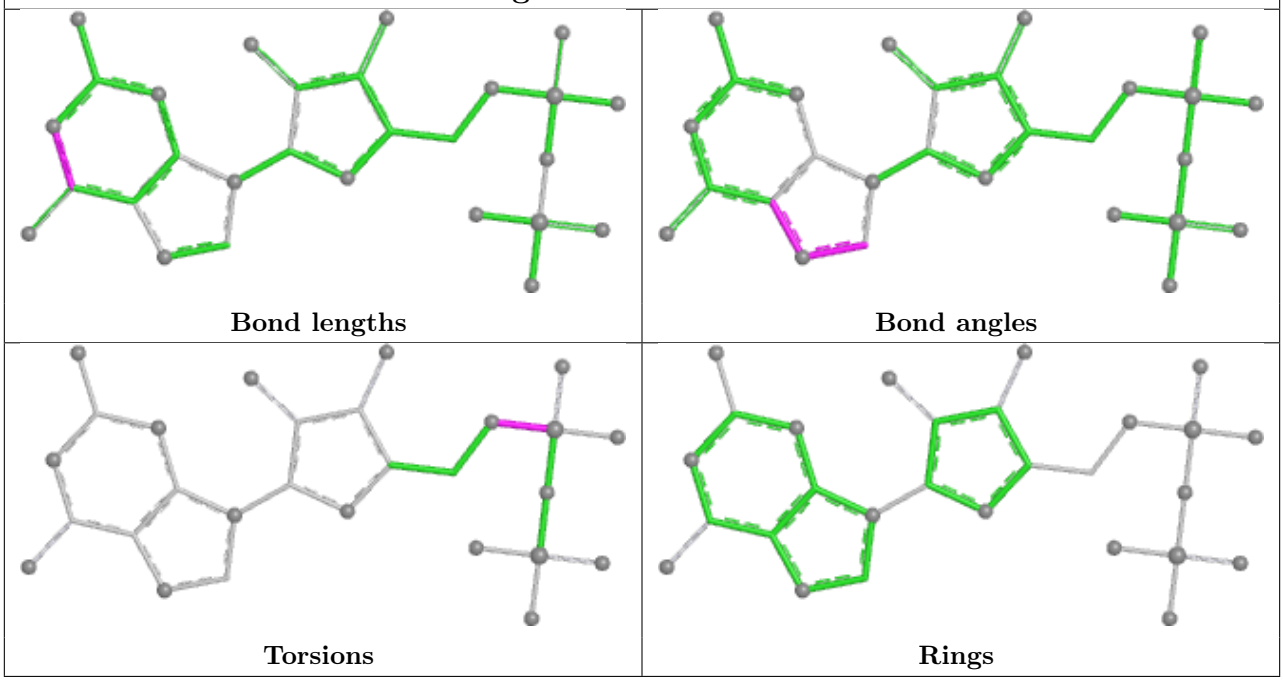

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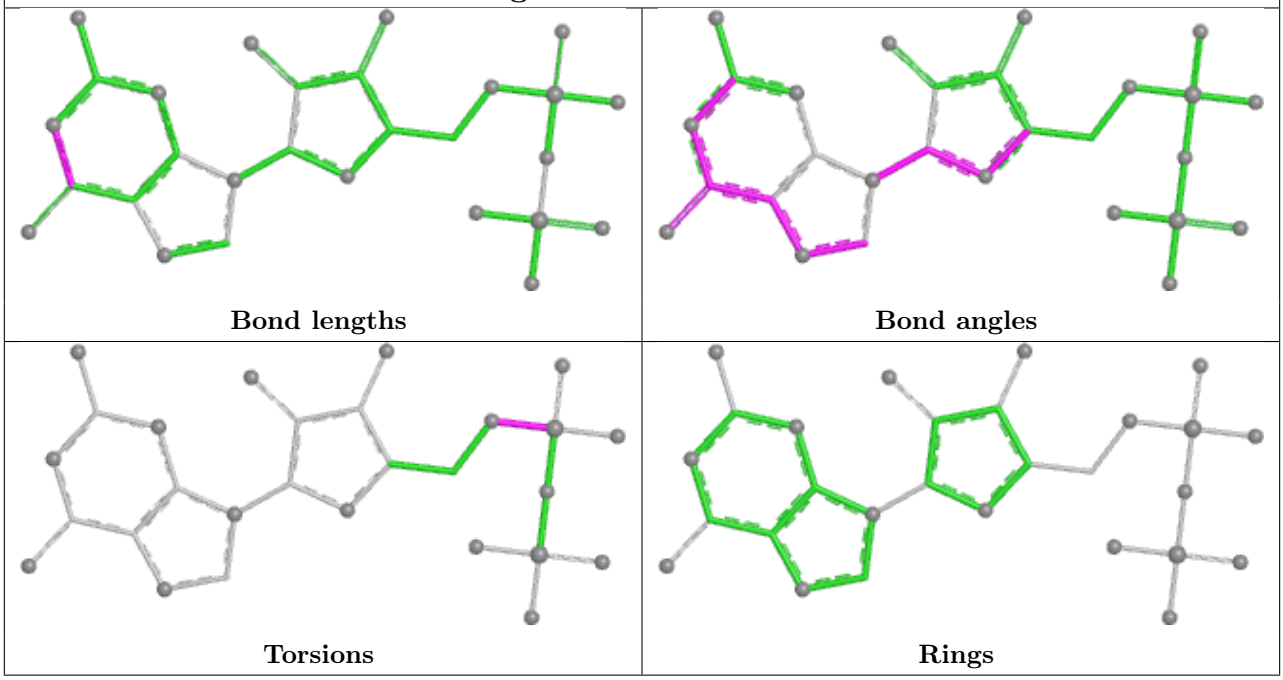

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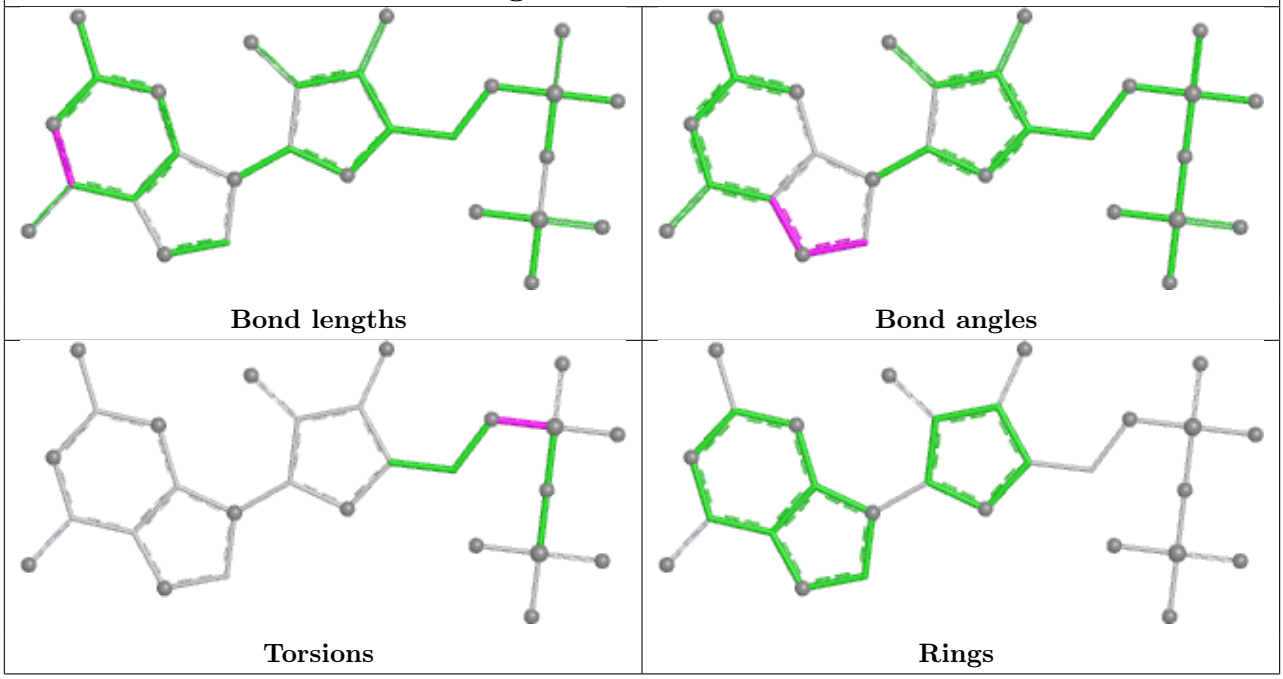
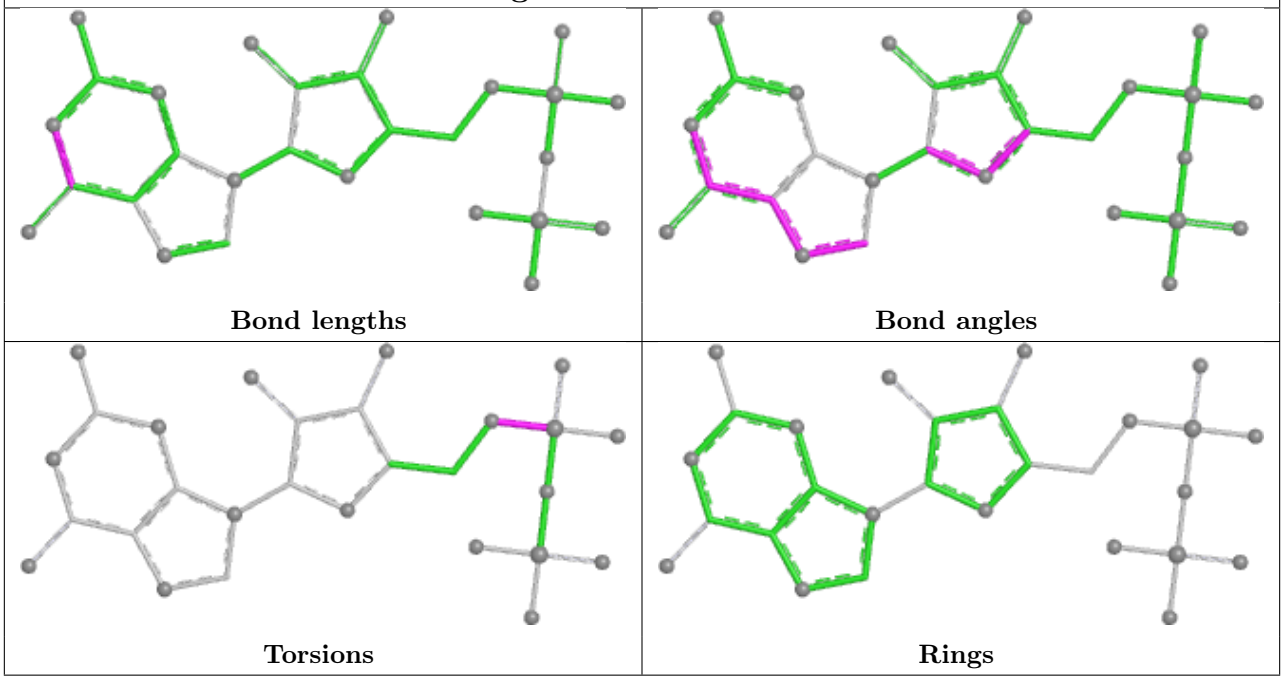
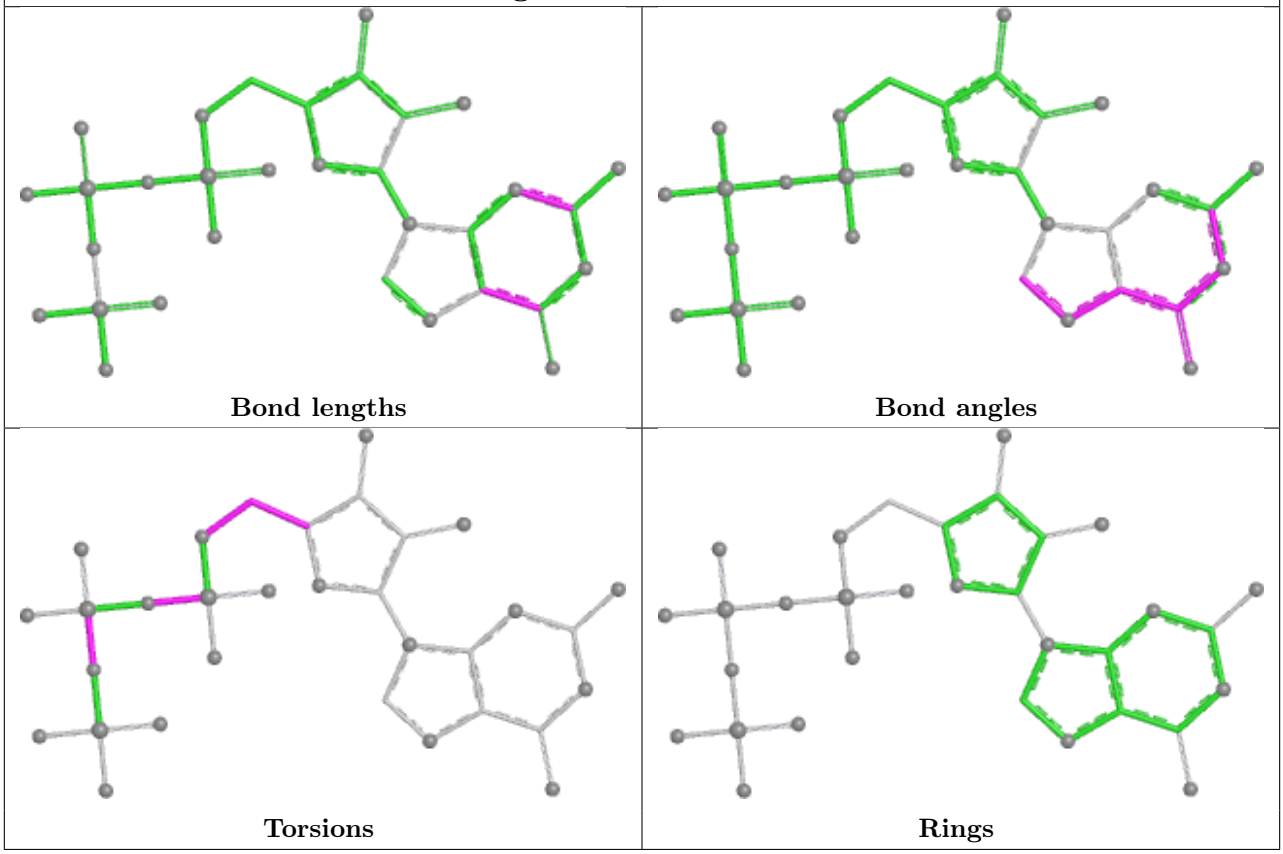


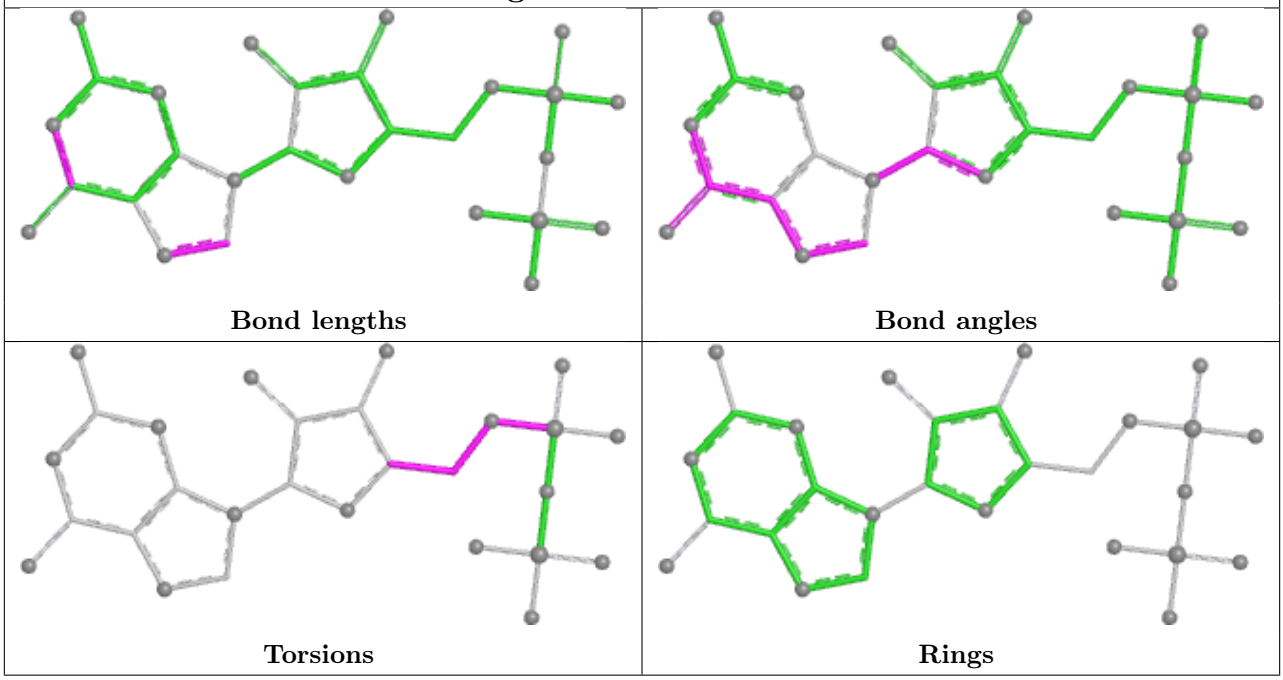
Ligand GDP OL 501



Ligand GTP BE 501



Ligand GDP HH 501



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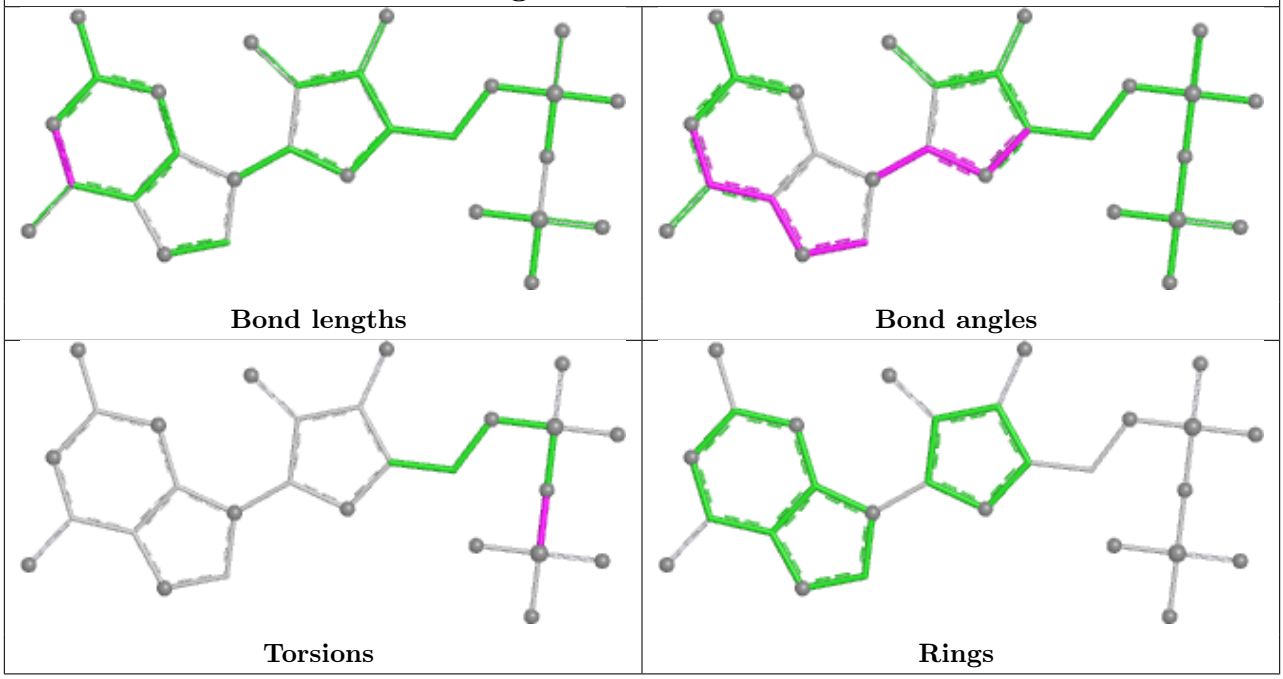

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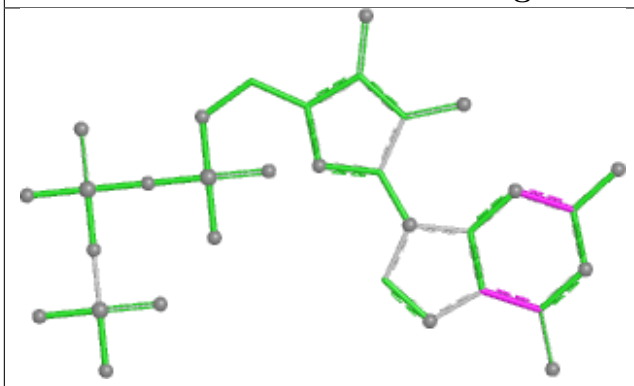
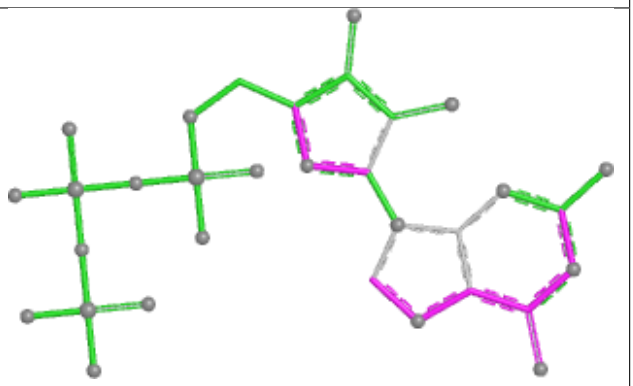
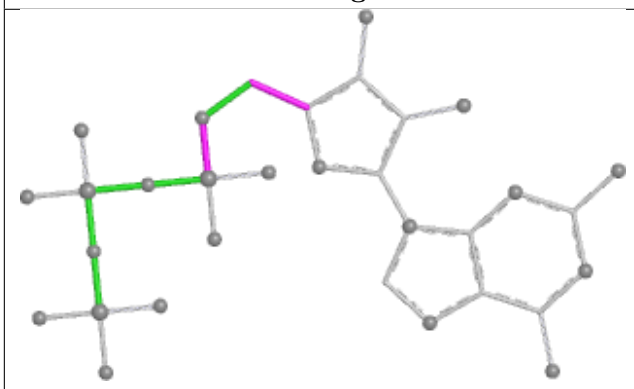


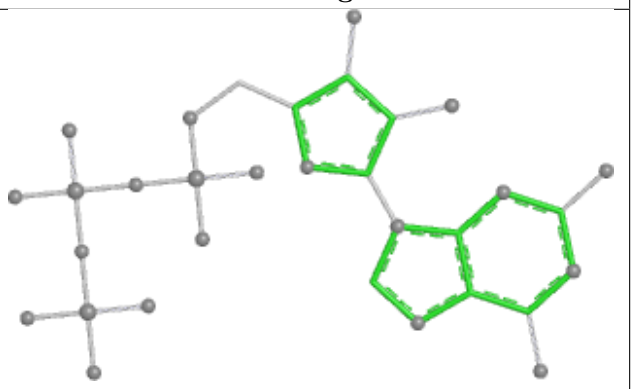
Bond lengths



Bond angles

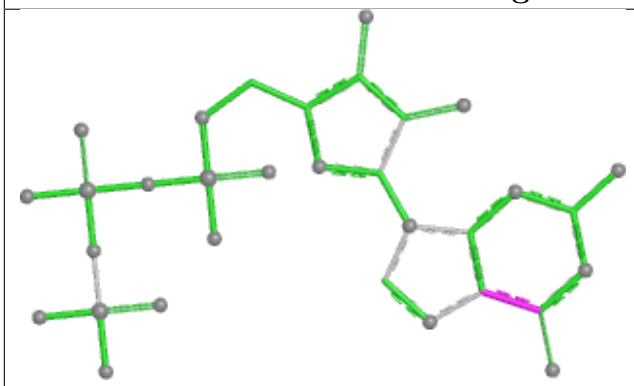


Torsions



Rings

Ligand GTP CE 501



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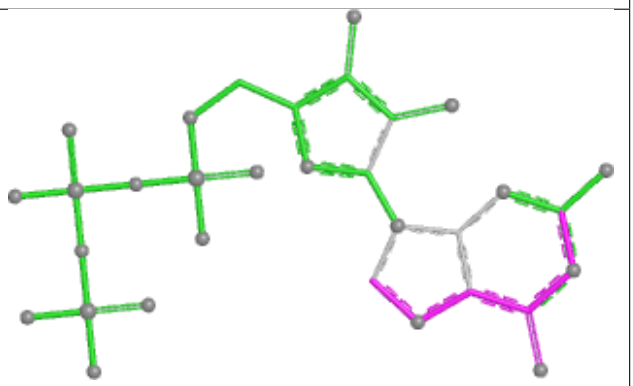

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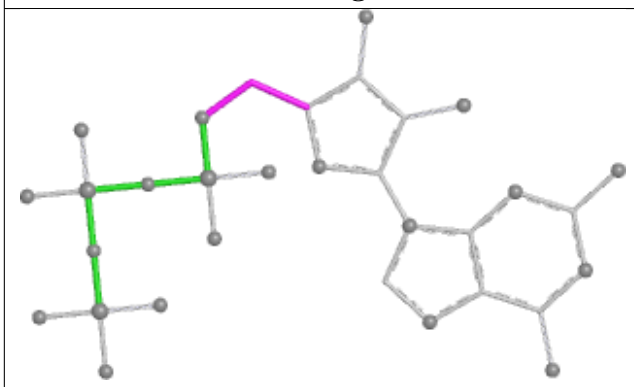
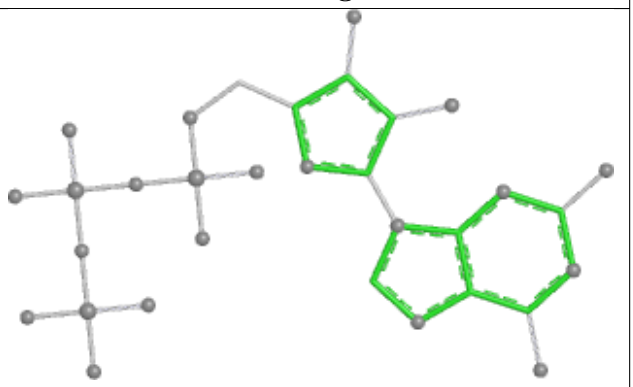
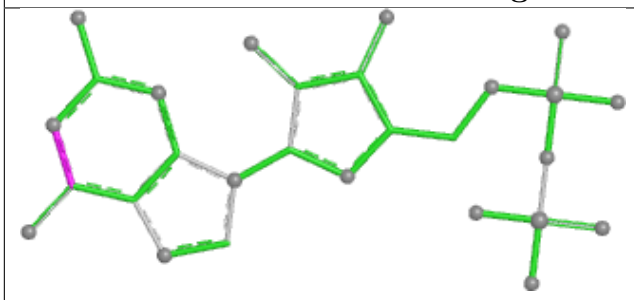


Torsions

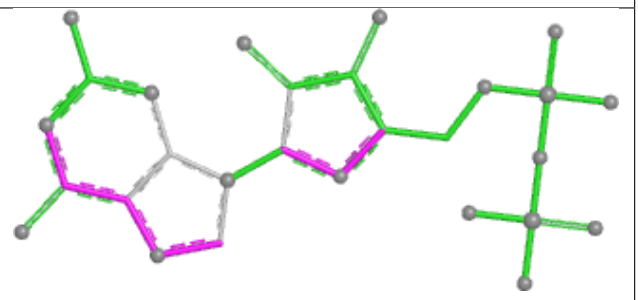


Rings

Ligand GDP HL 501



Bond lengths



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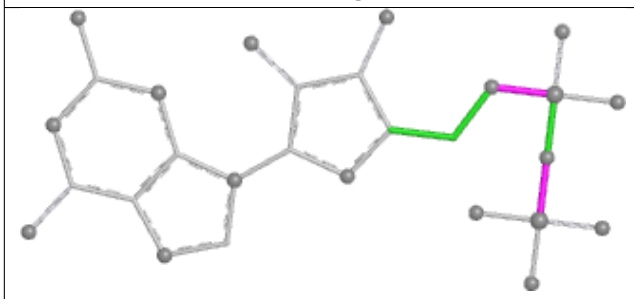

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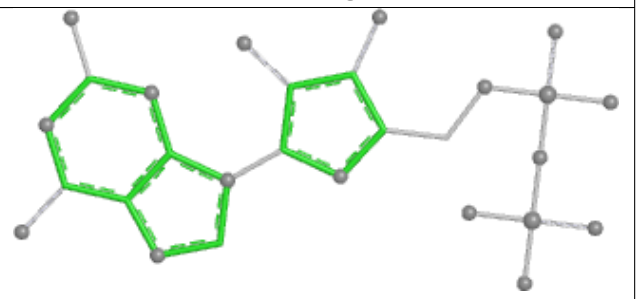
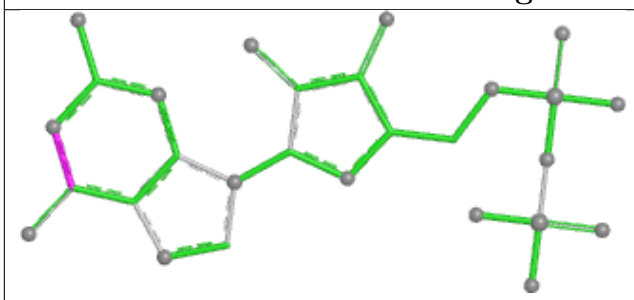


Rings

Ligand GDP LJ 501



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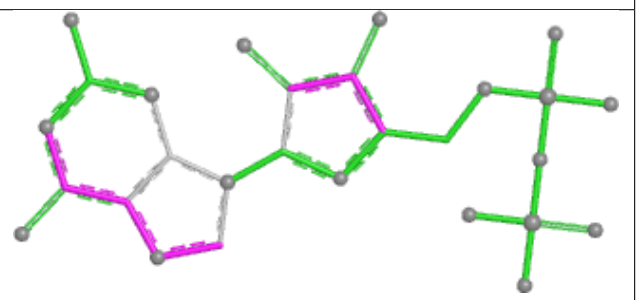

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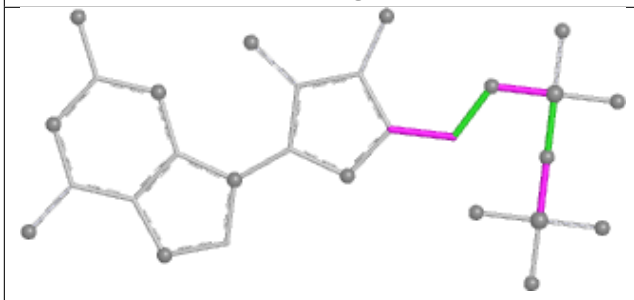

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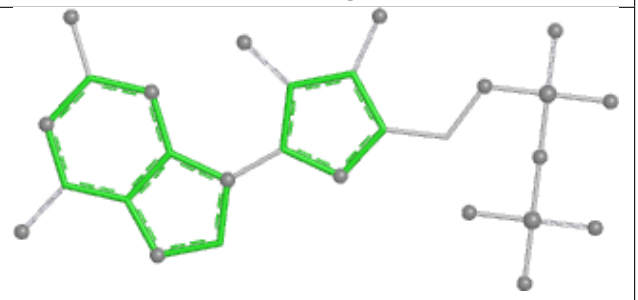

Rings

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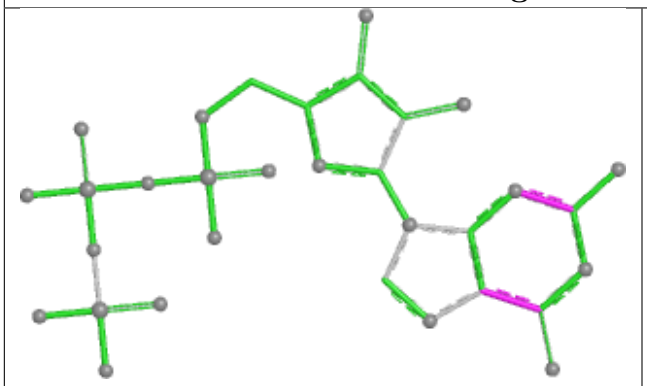

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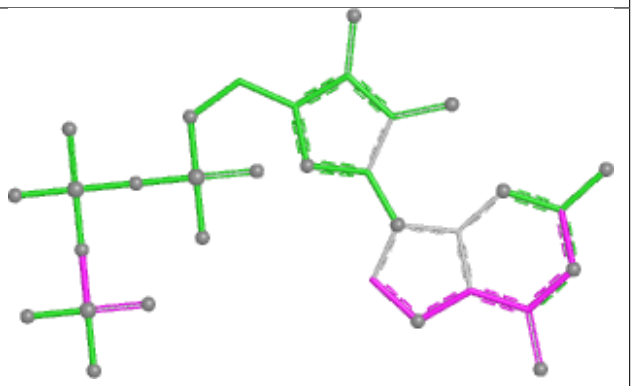

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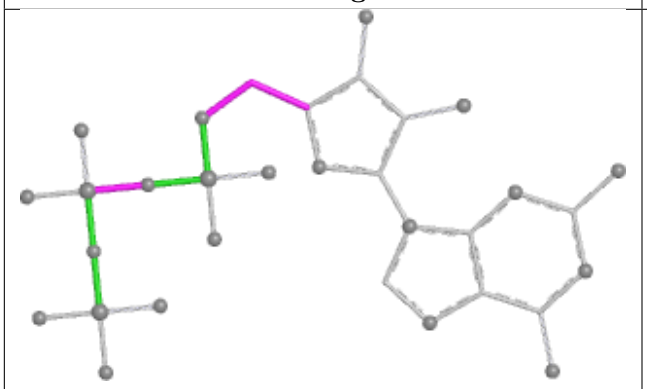

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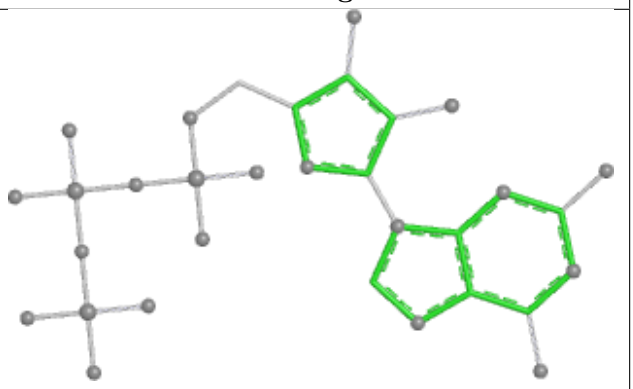
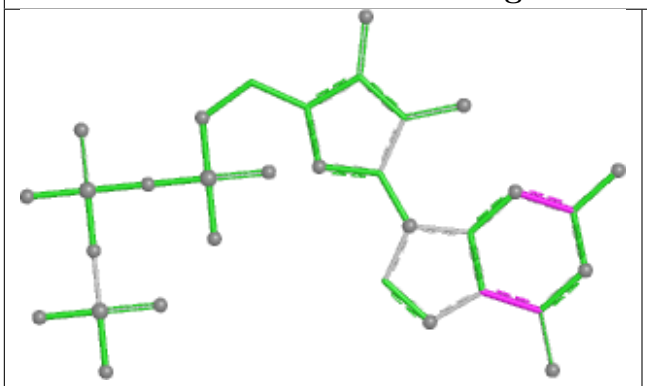


Rings

Ligand GTP WG 501



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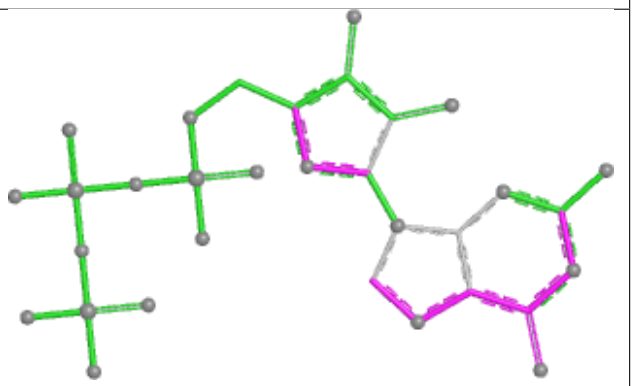

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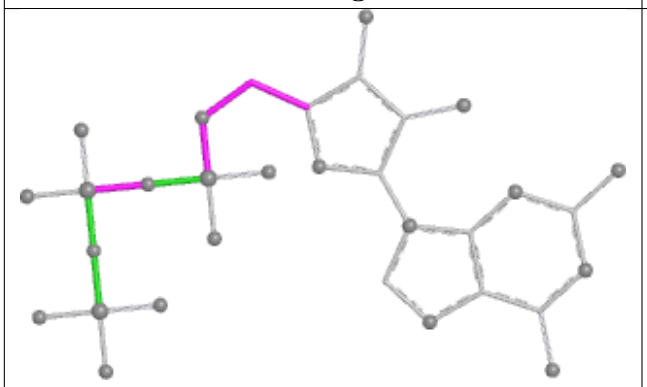

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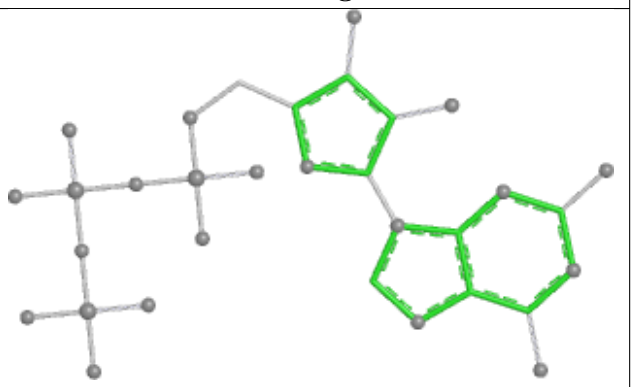
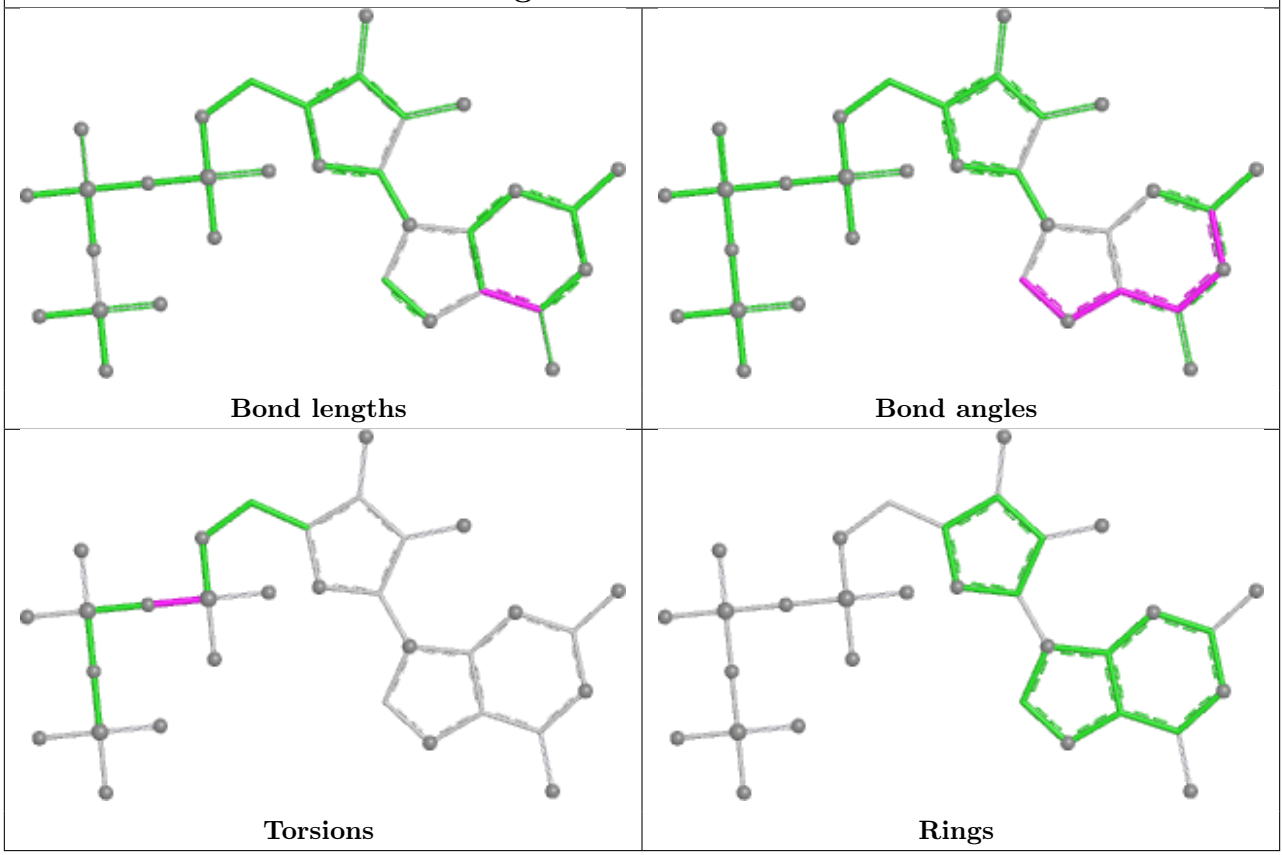


Rings

Ligand GTP JC 501



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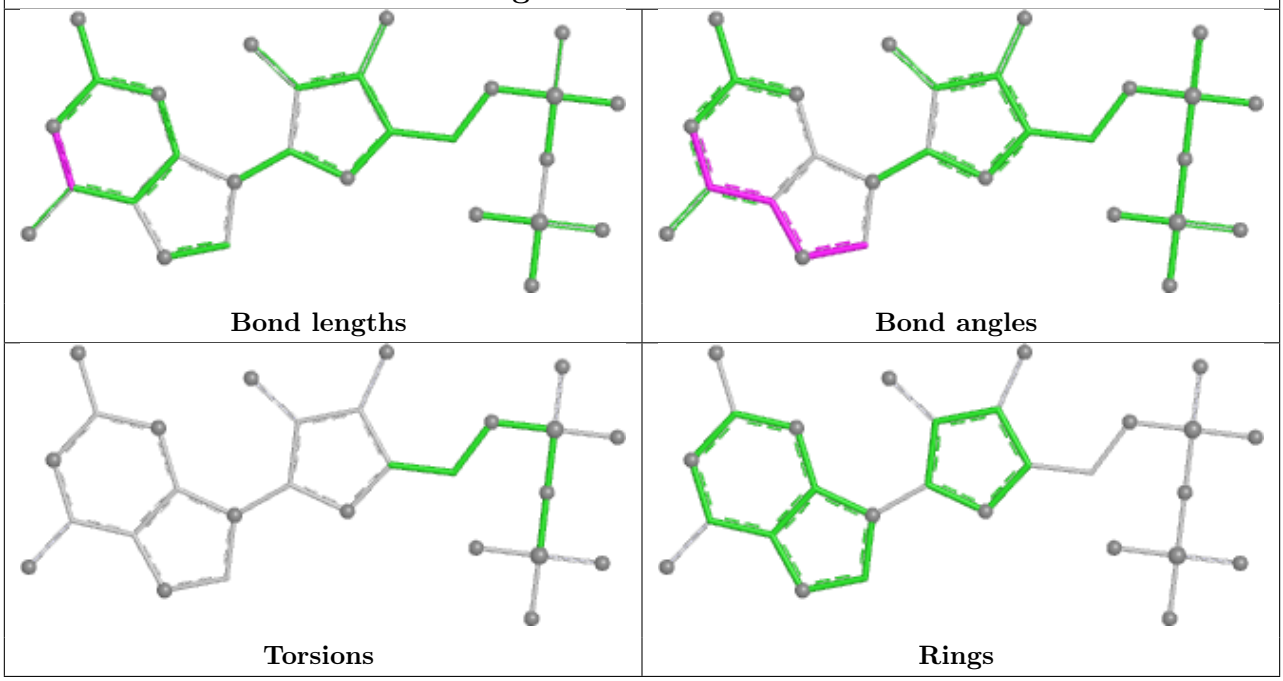

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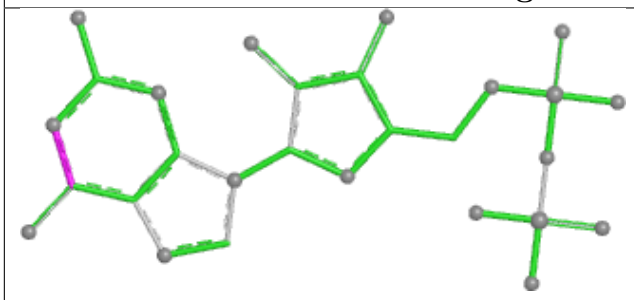

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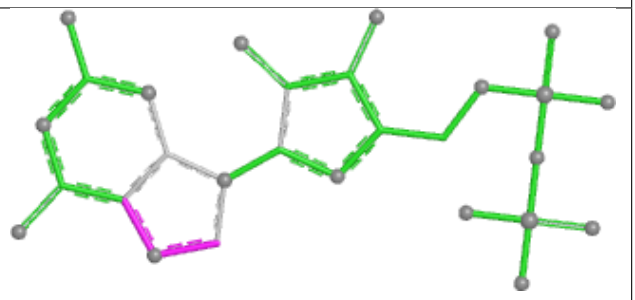
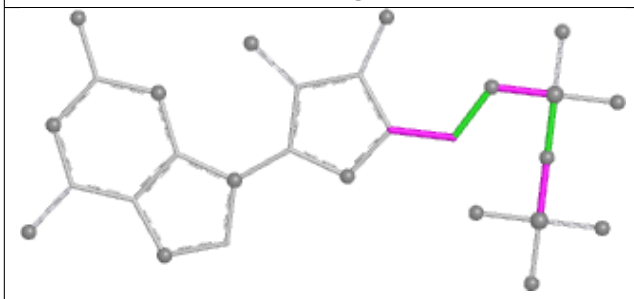


Bond angles



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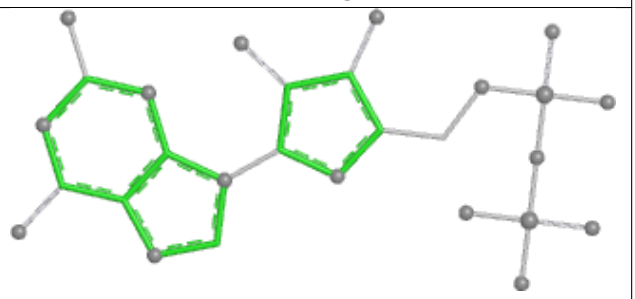
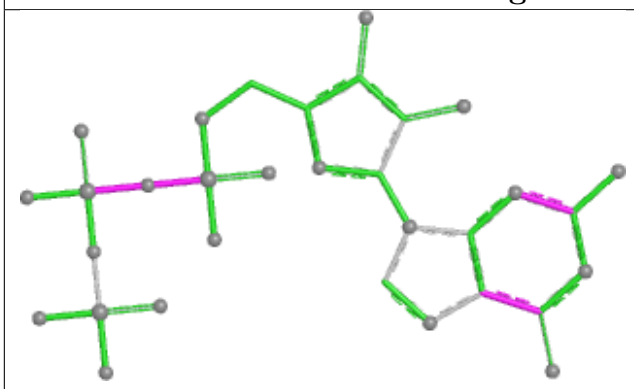


Rings

Ligand GTP DK 501



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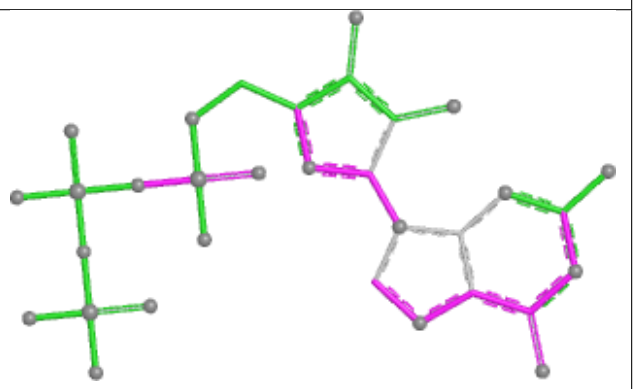

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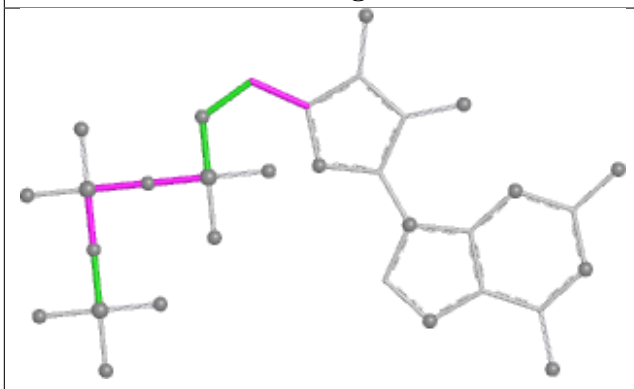

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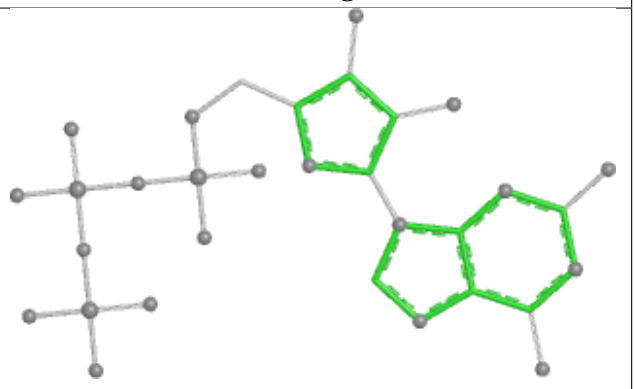

Rings

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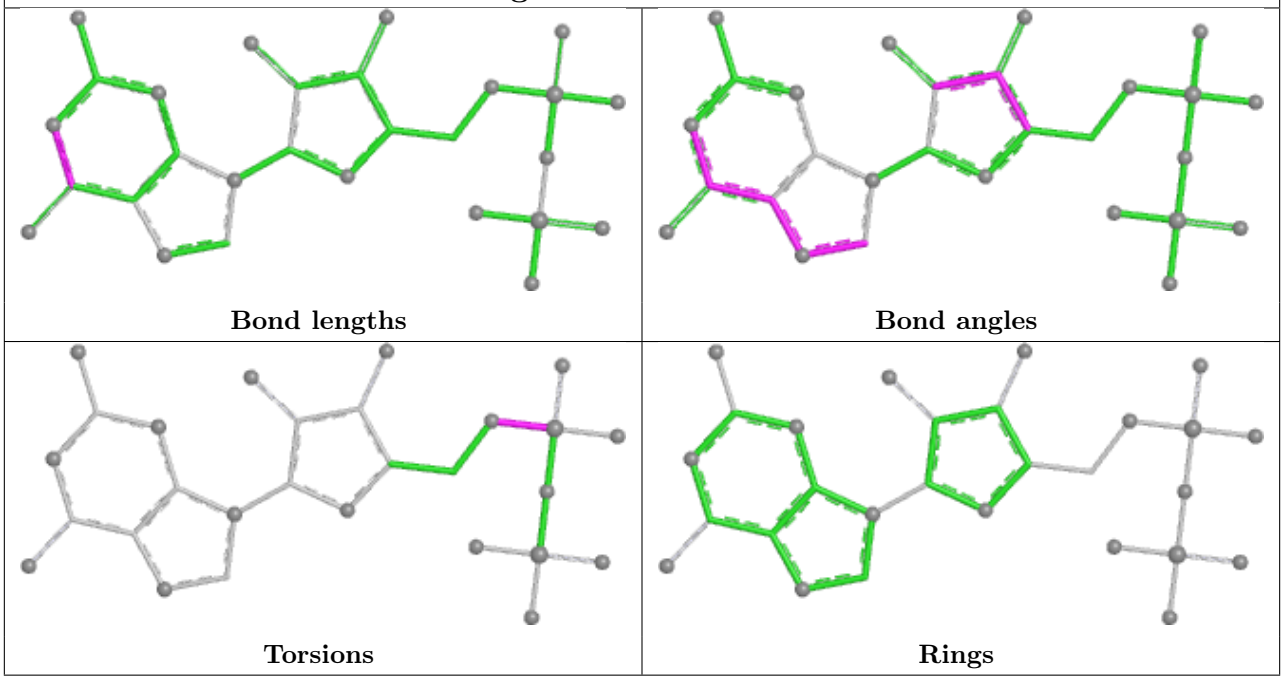
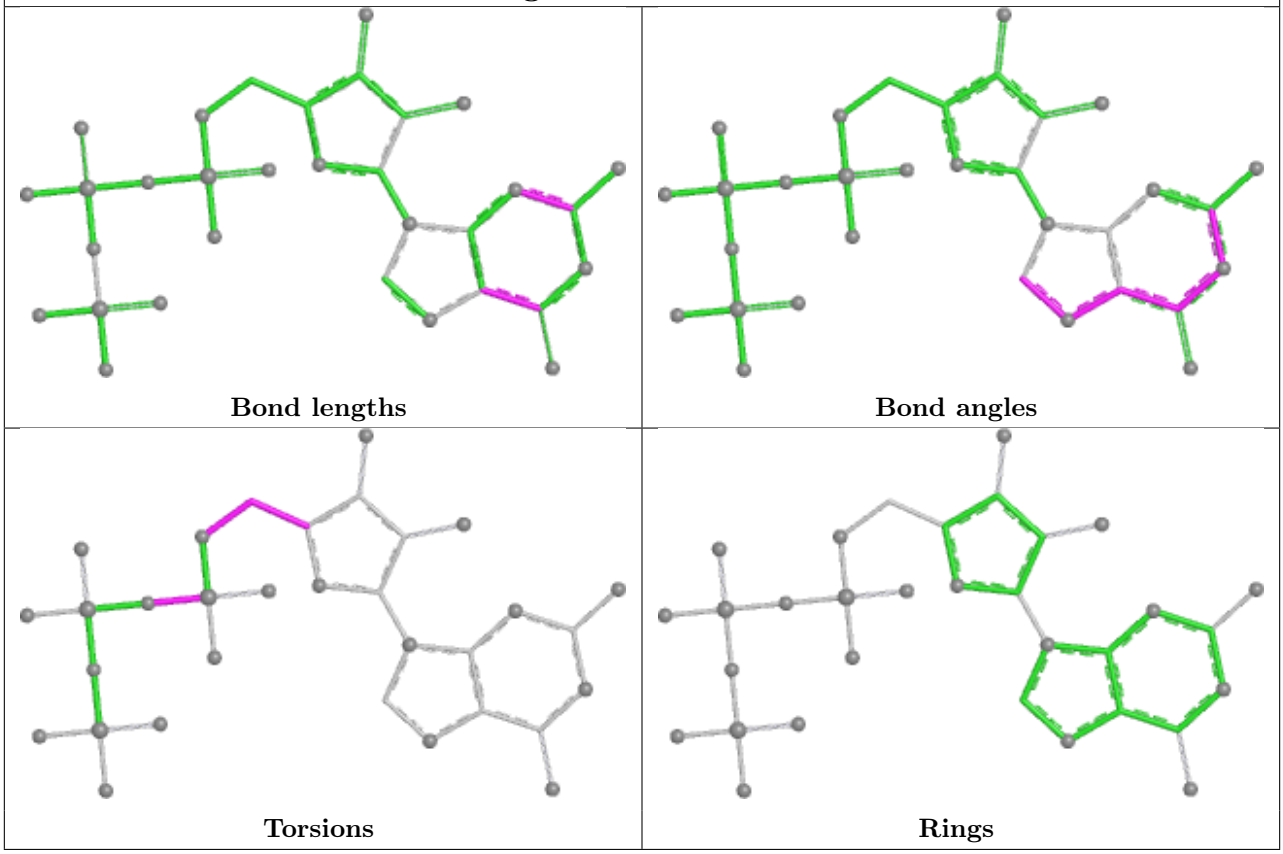
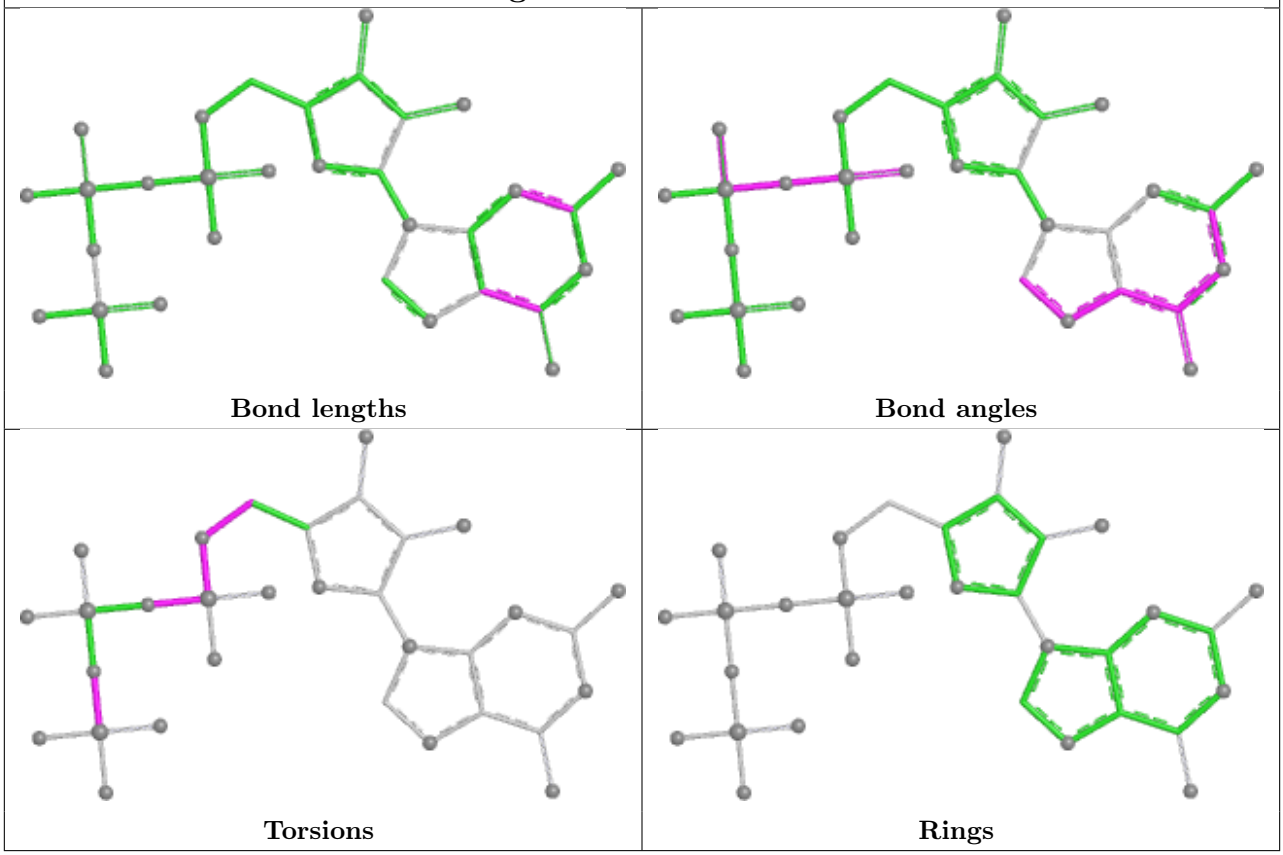


Ligand GTP II 501



Ligand GTP LM 501



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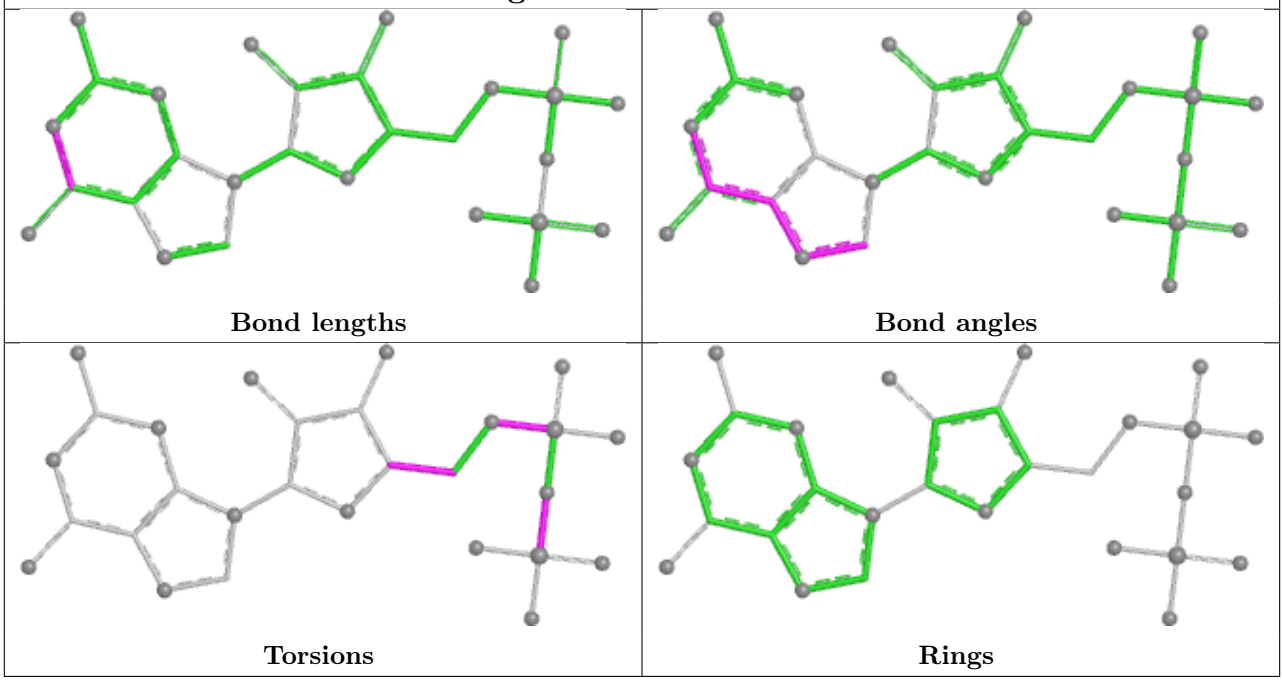

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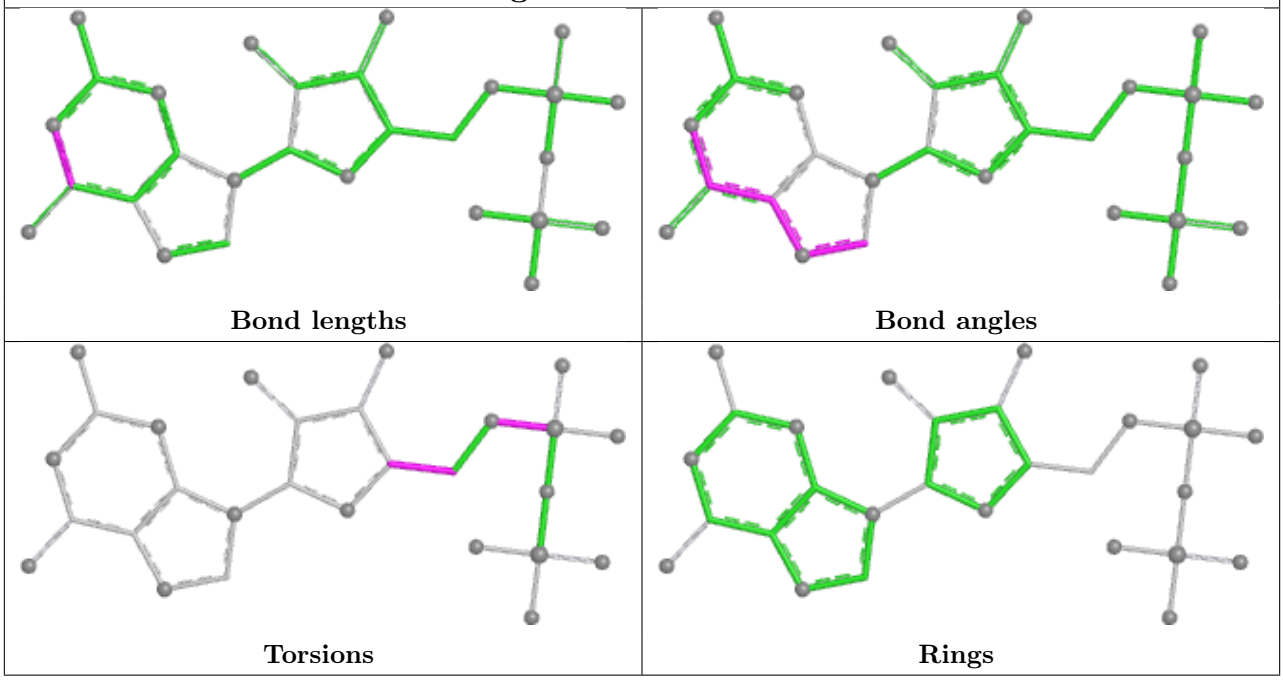
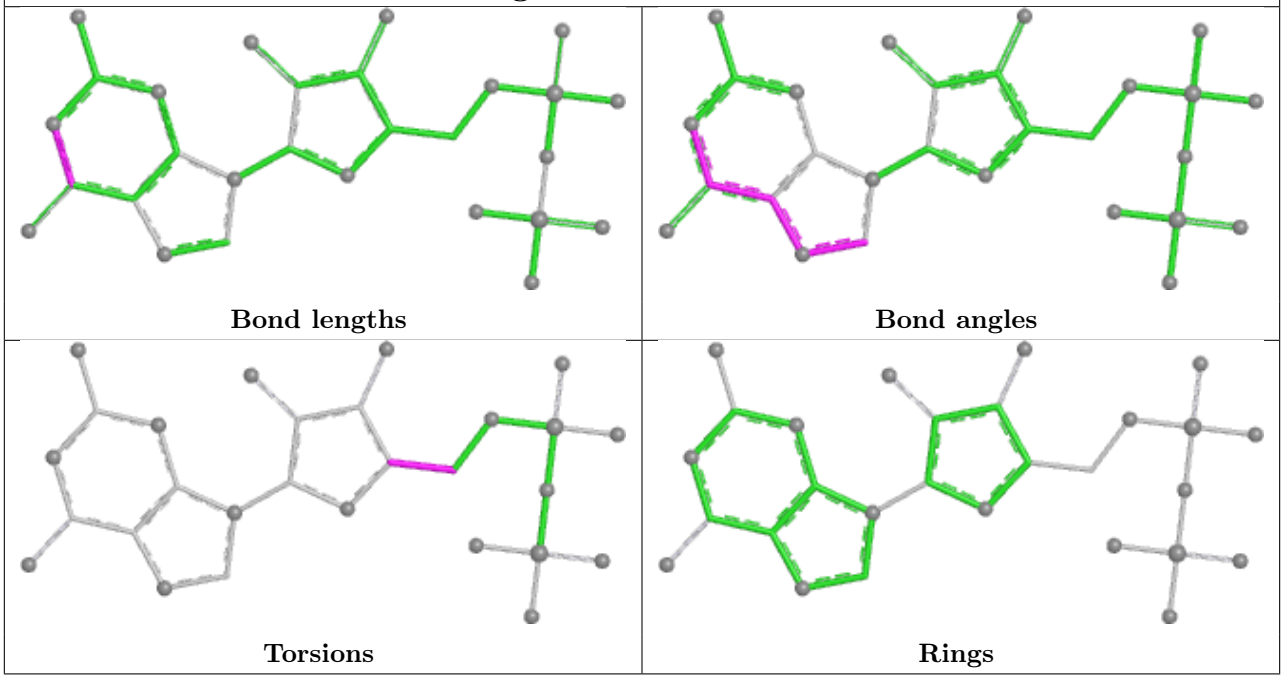
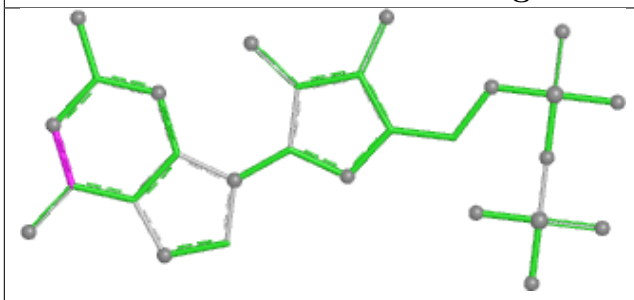


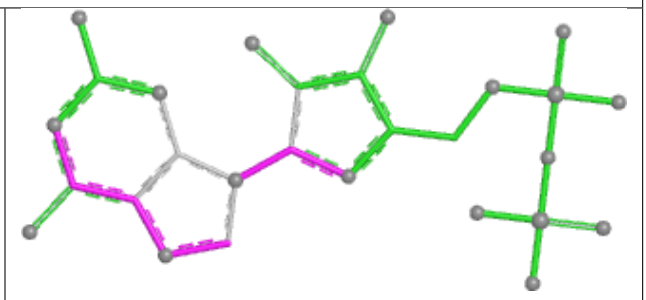
Ligand GDP CL 501



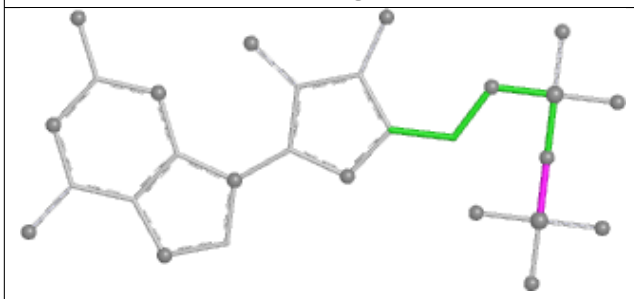
Ligand GDP OJ 501



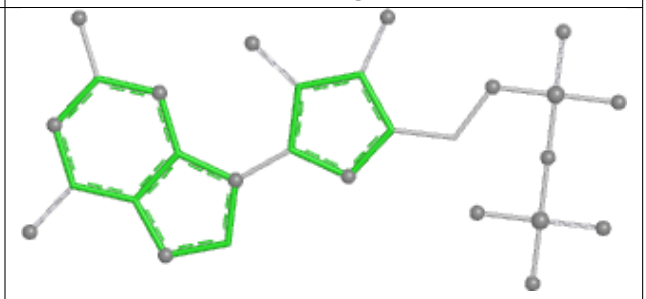
Bond lengths



Bond angles

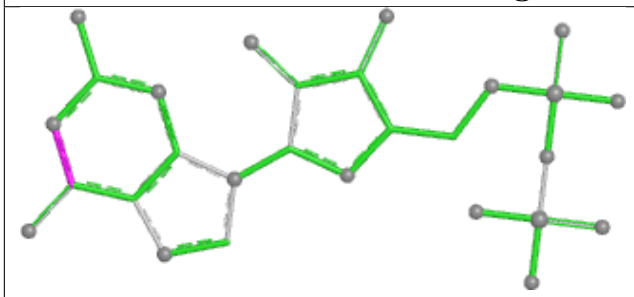


Torsions



Rings

Ligand GDP BJ 501



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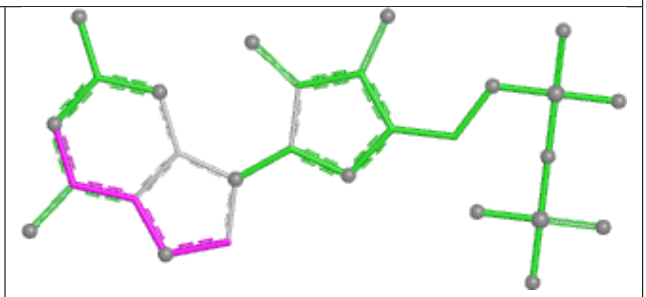
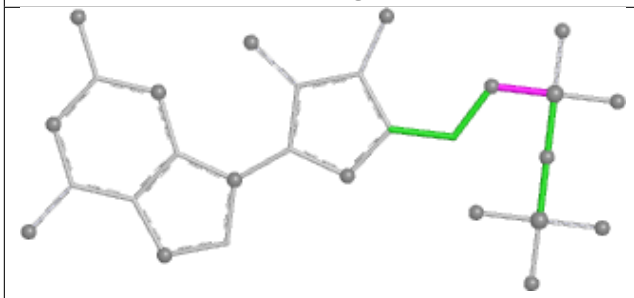


Bond angles



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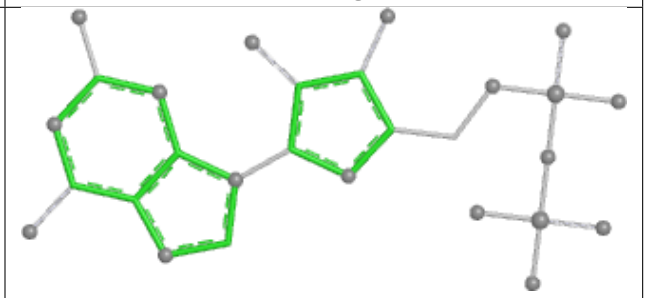
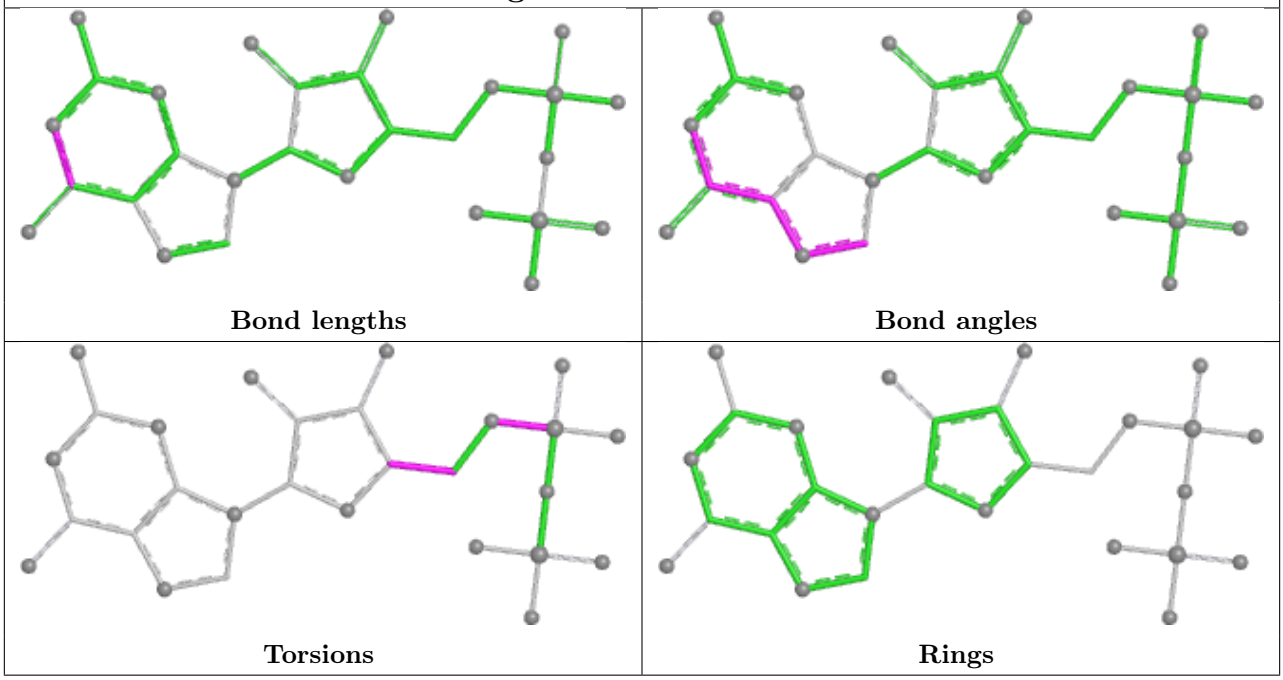


Rings

Ligand GDP KN 501



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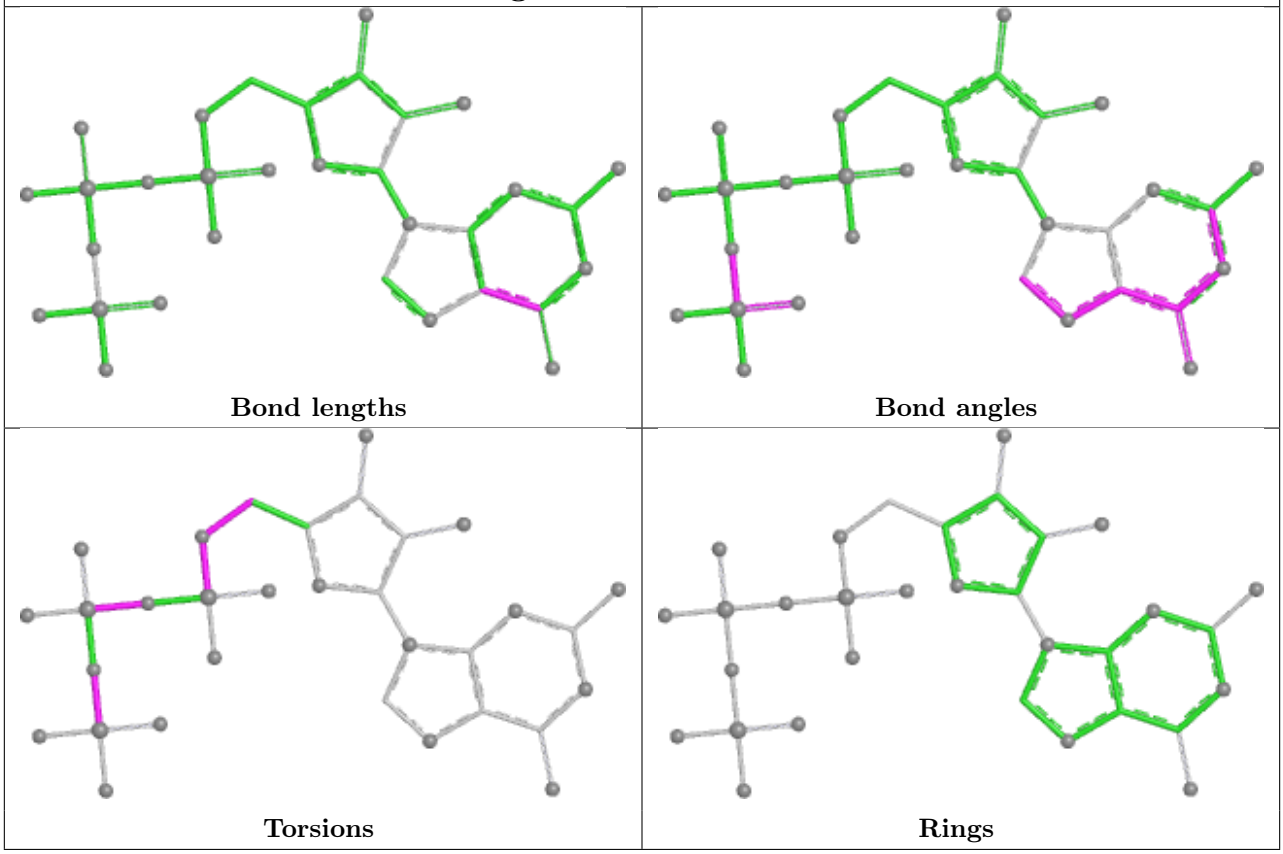

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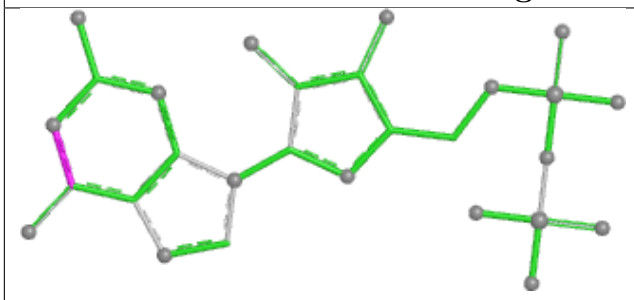
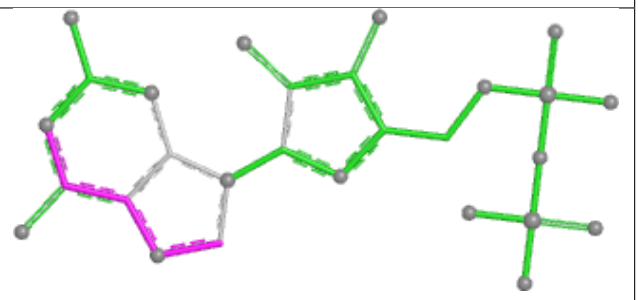
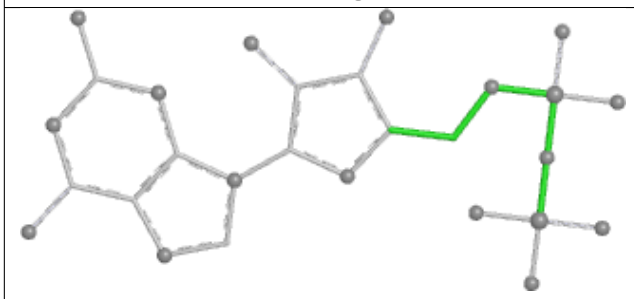


Bond lengths



Bond angles



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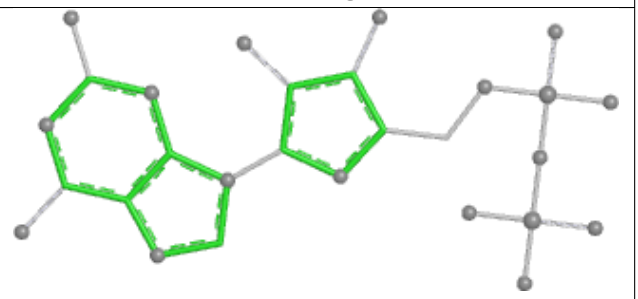
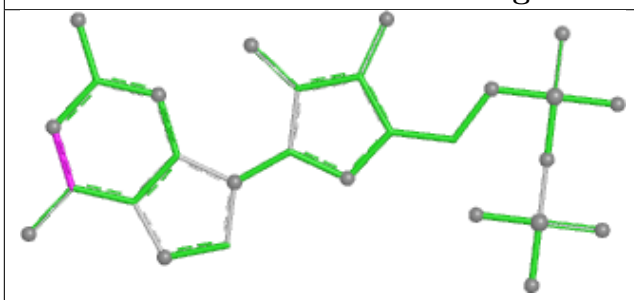


Rings

Ligand GDP QJ 501



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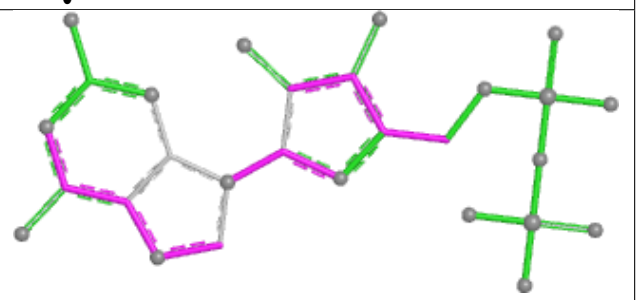

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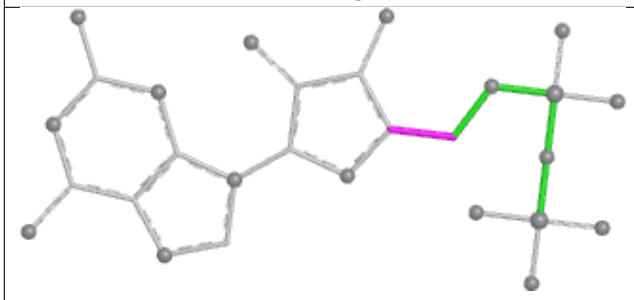

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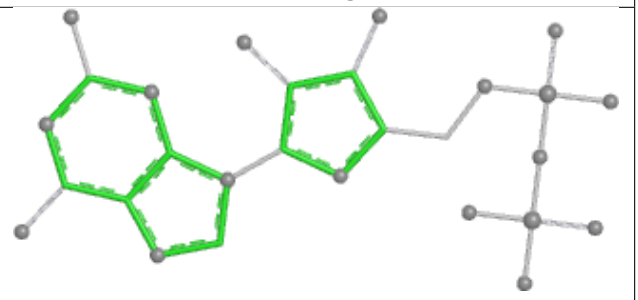
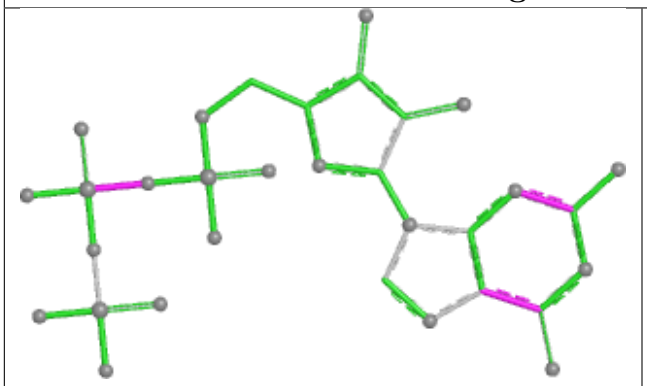


Rings

Ligand GTP KG 501



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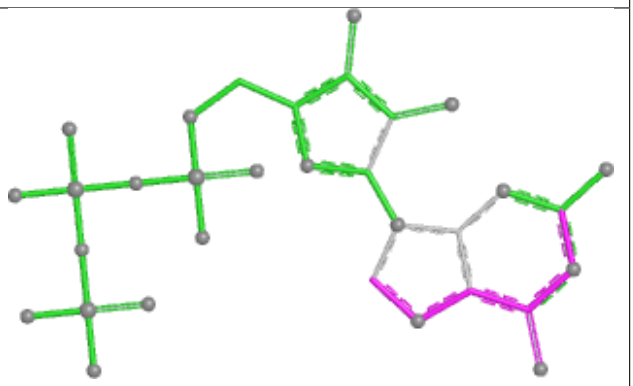

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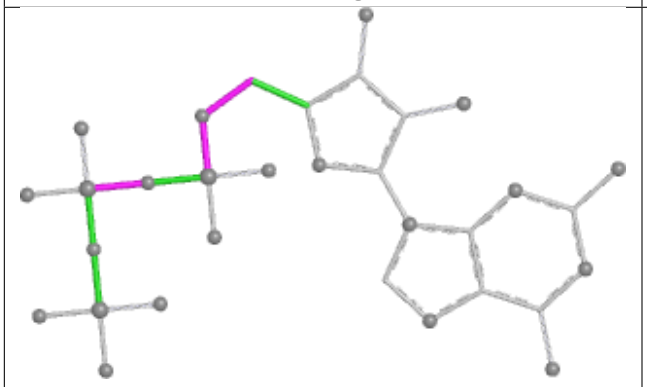
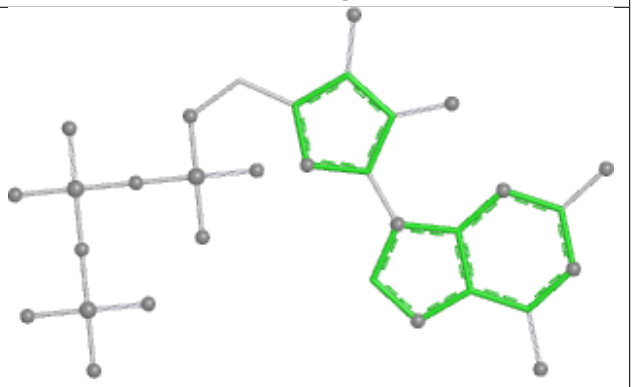
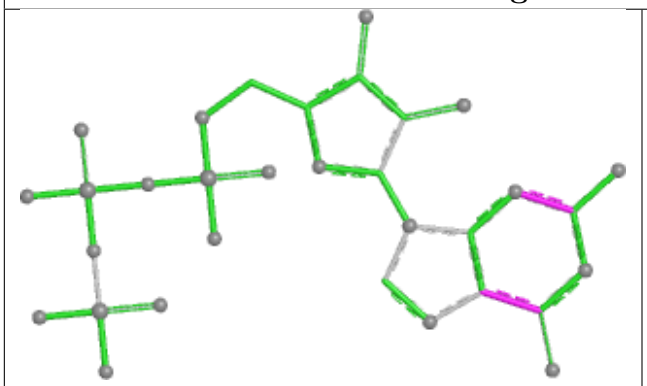


Torsions



Rings

Ligand GTP JM 501



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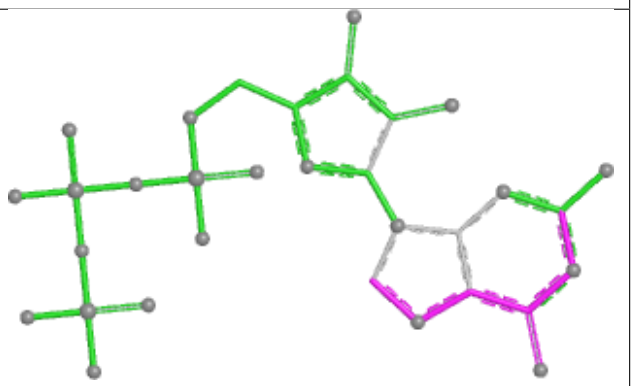
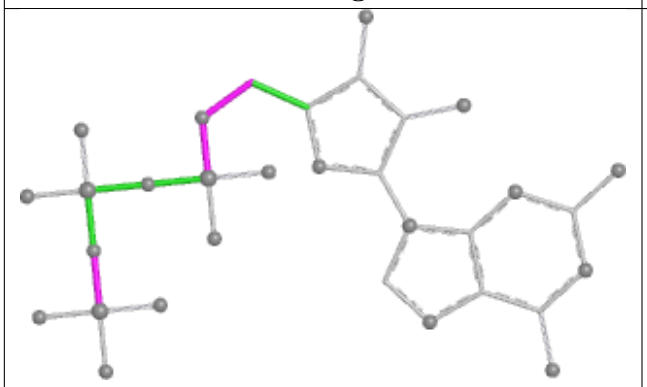


Bond angles



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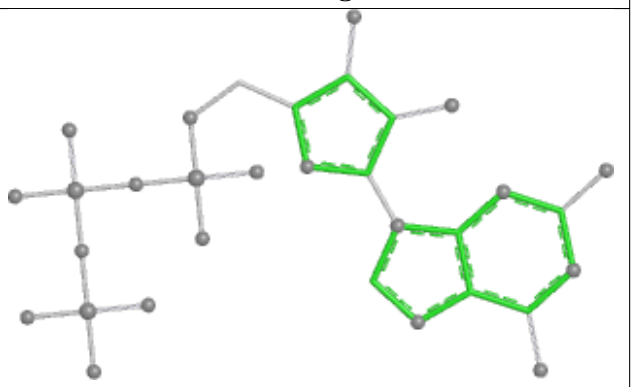
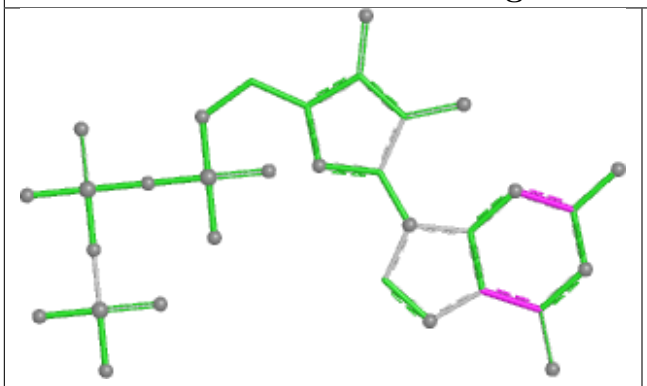


Rings

Ligand GTP GM 501



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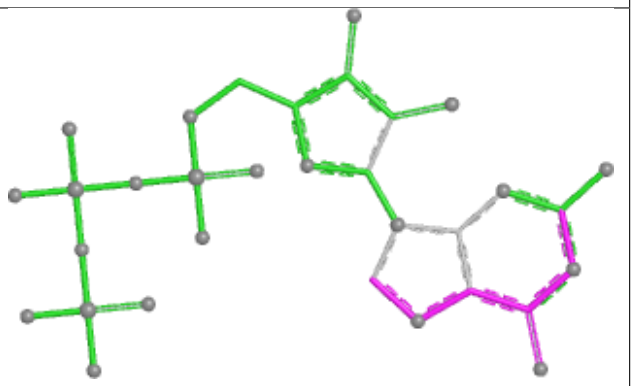
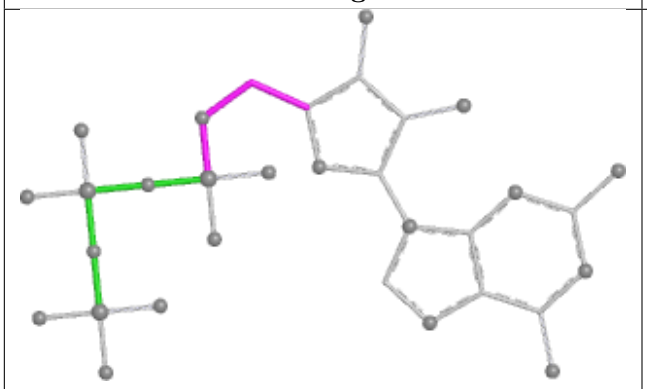


Bond angles



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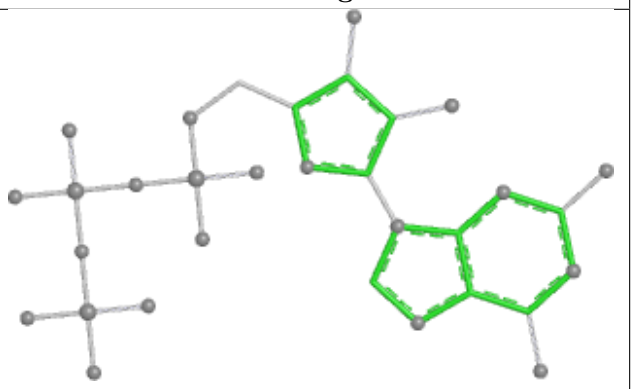
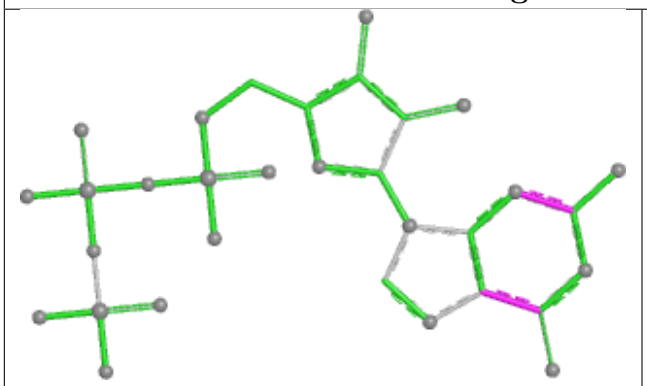


Rings

Ligand GTP AC 501



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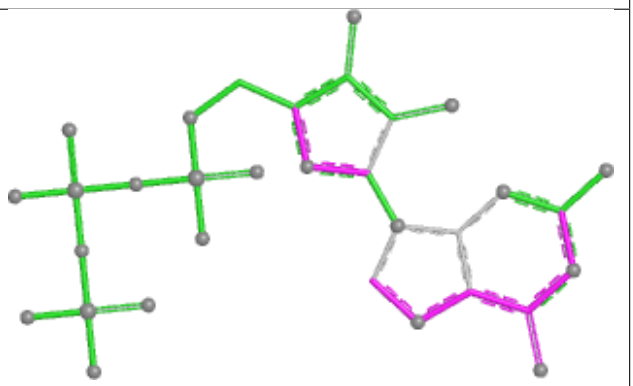
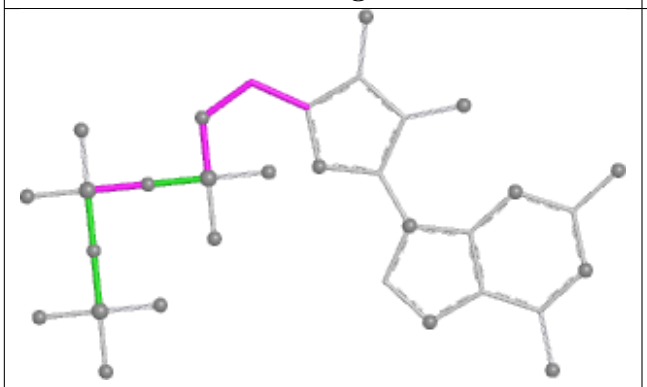
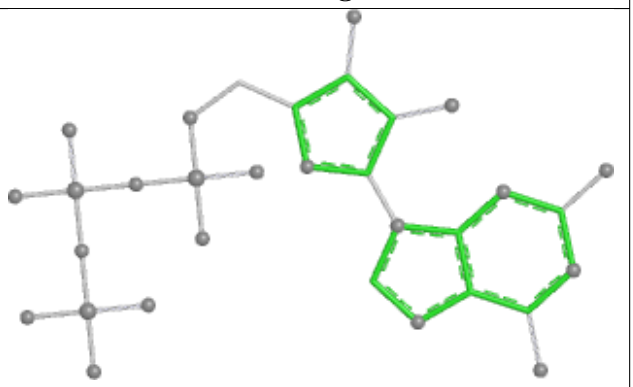


Bond angles

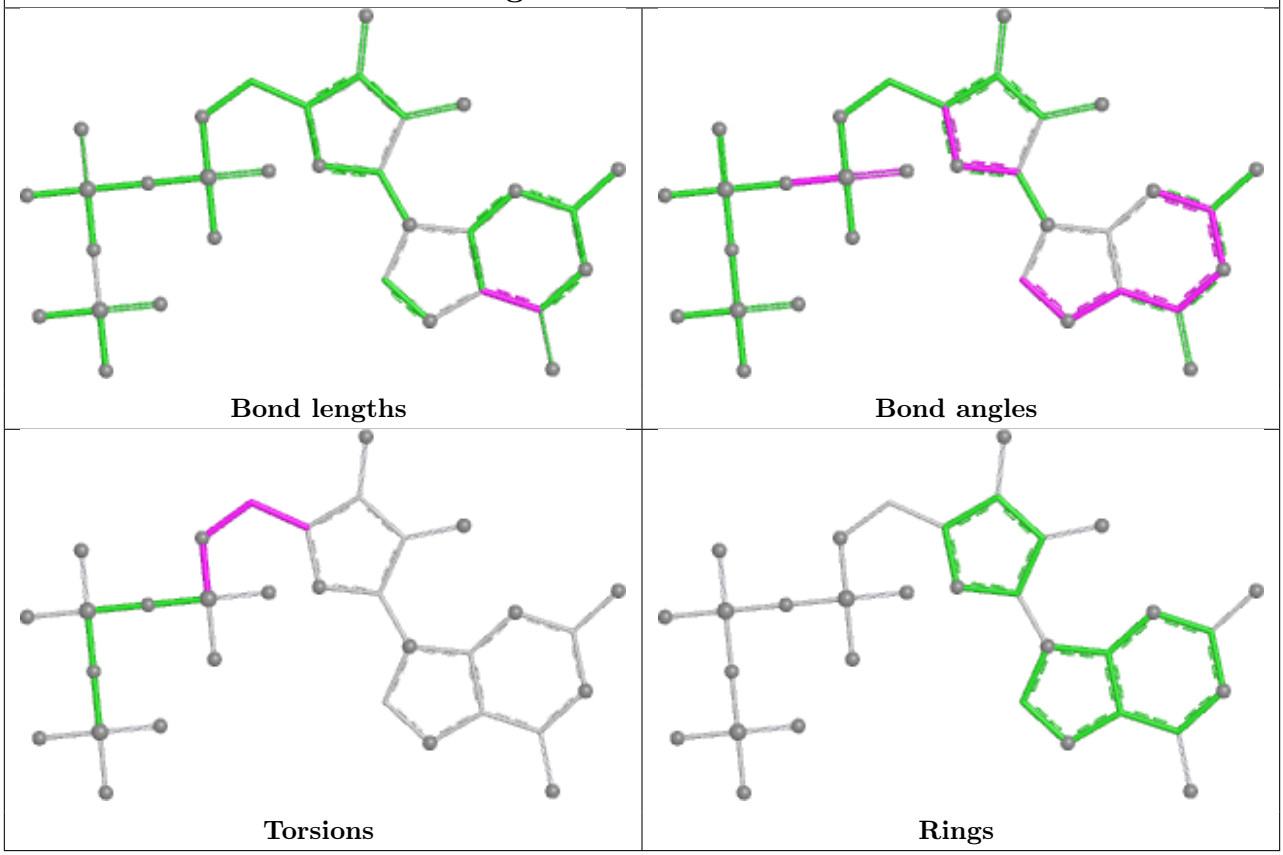


Torsions

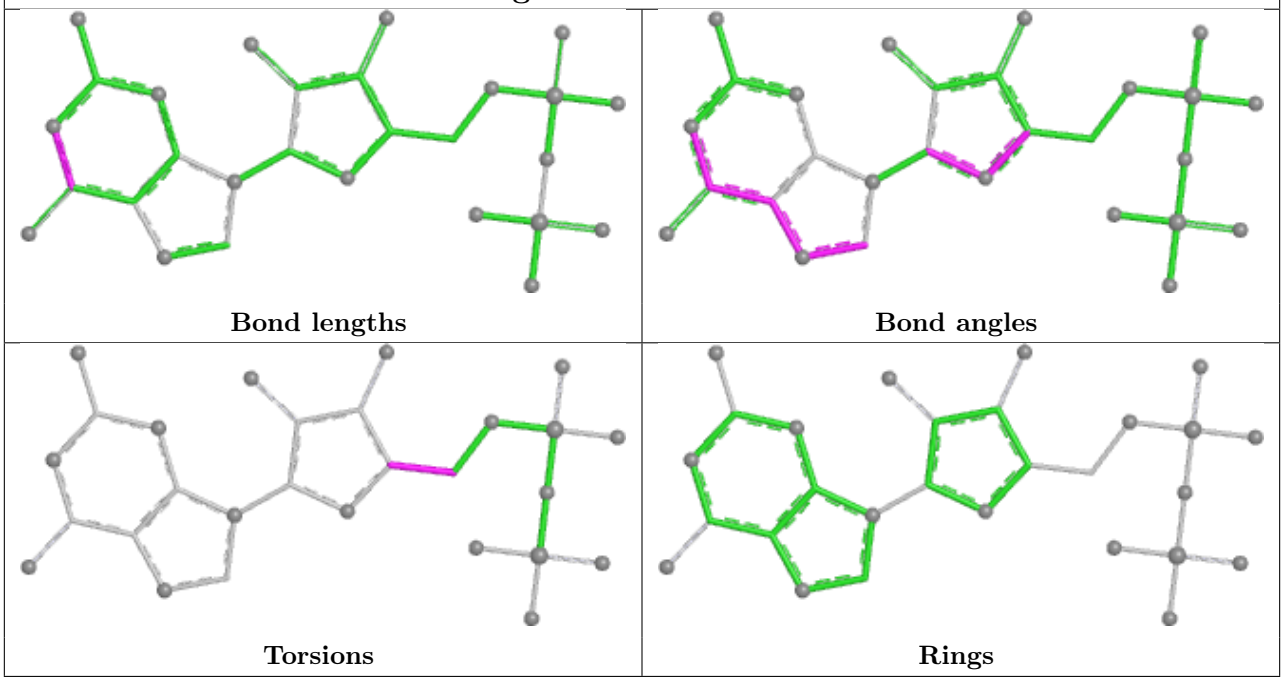


Rings

Ligand GTP VM 501



Ligand GDP AJ 501



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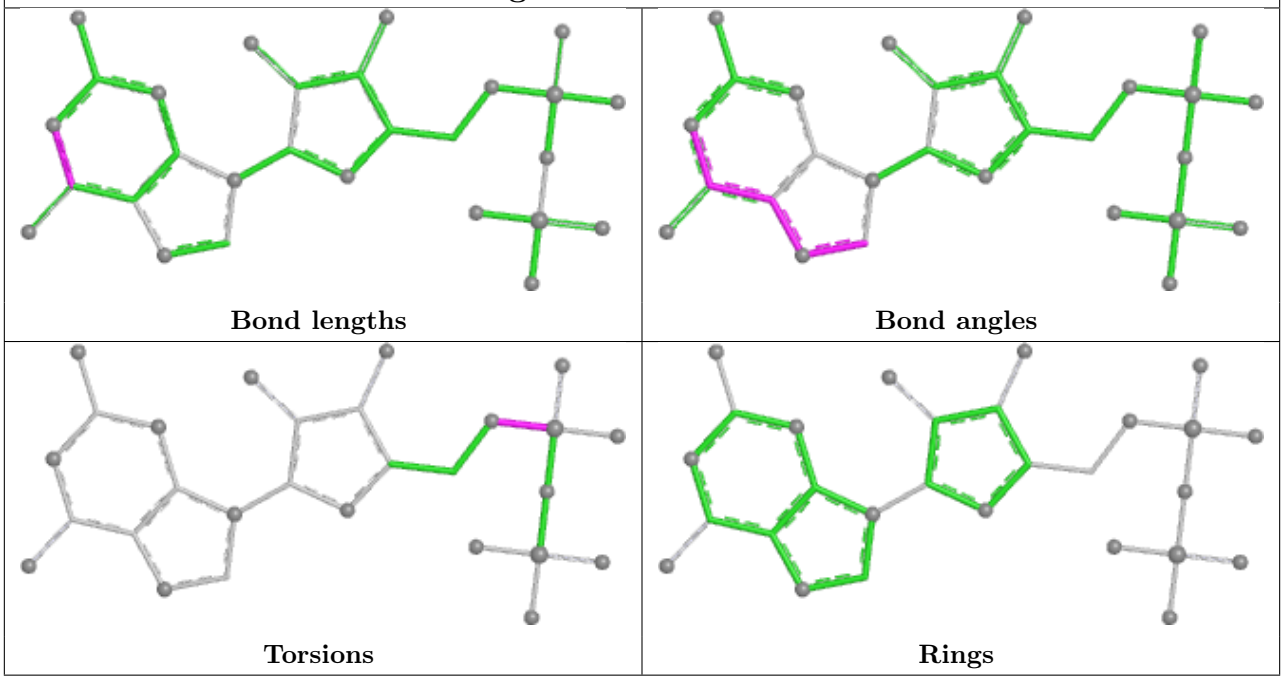

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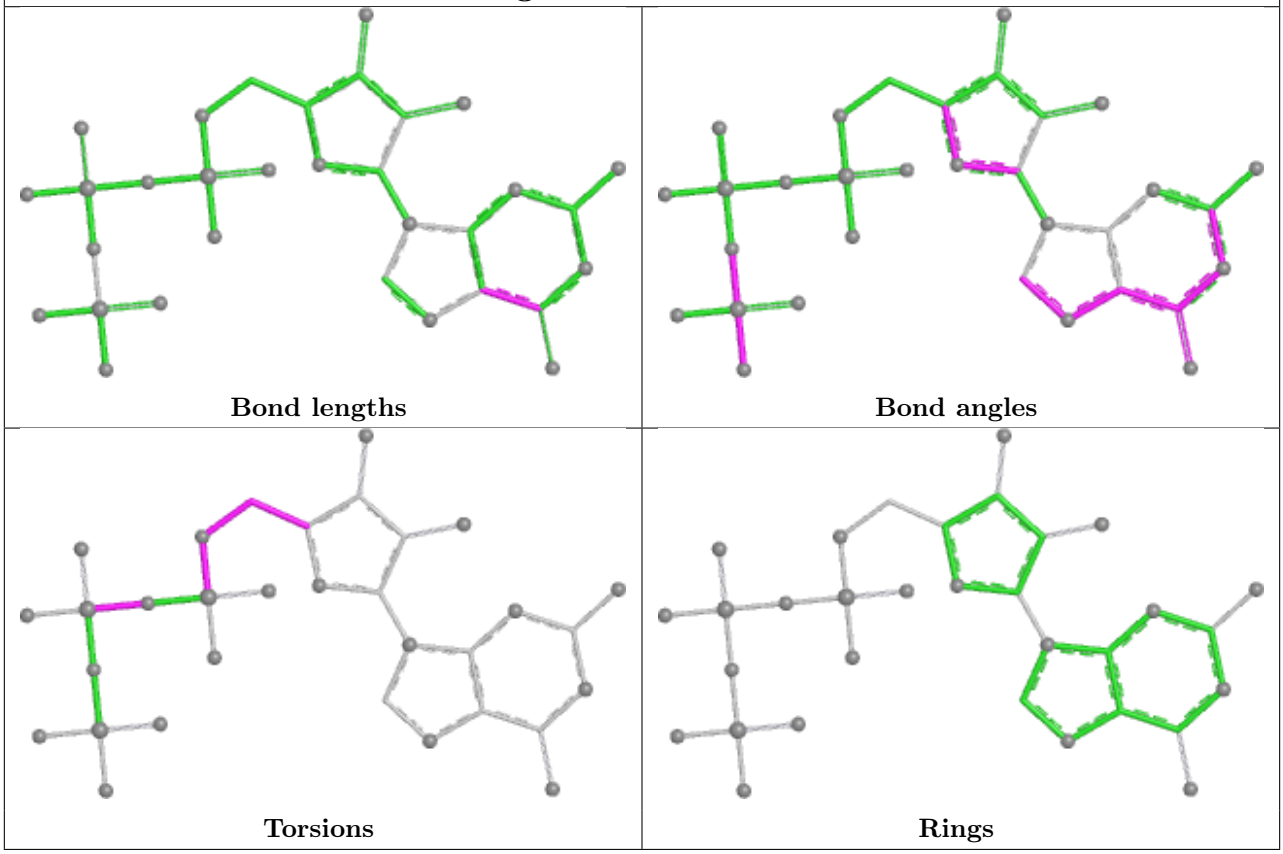

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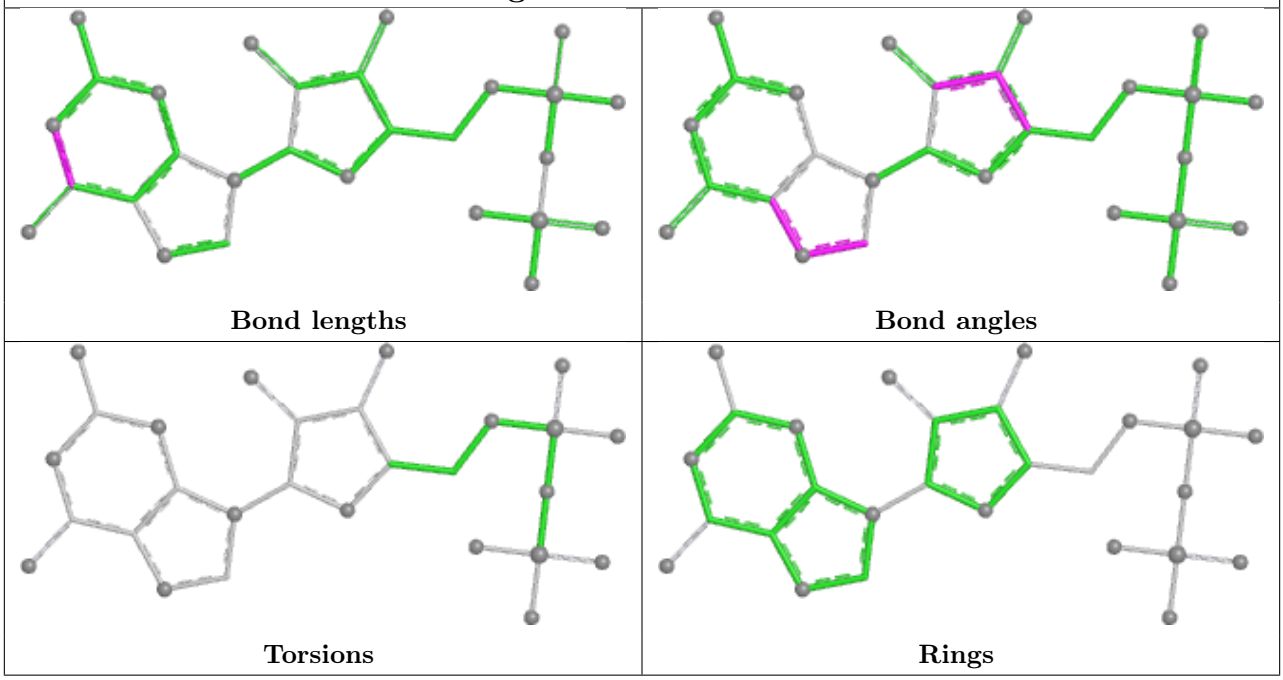

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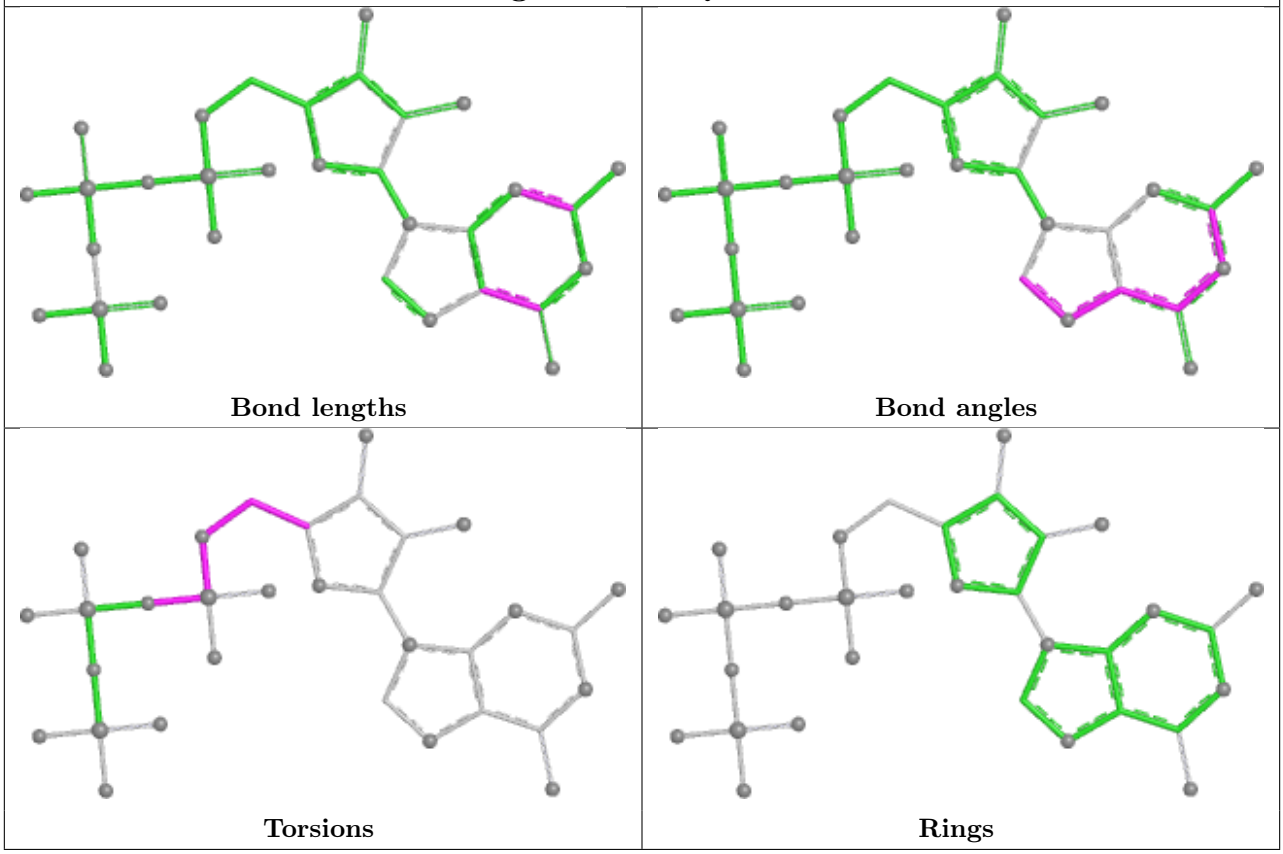

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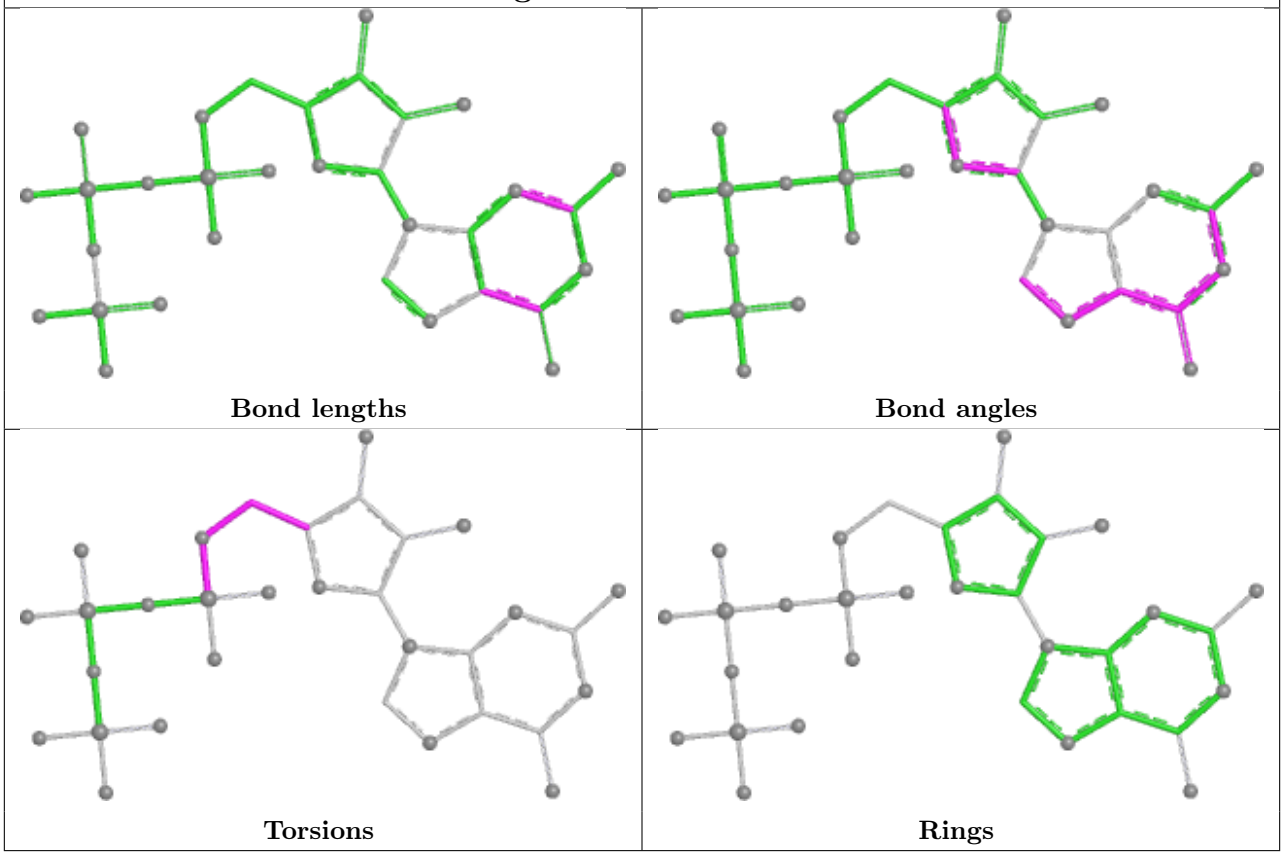

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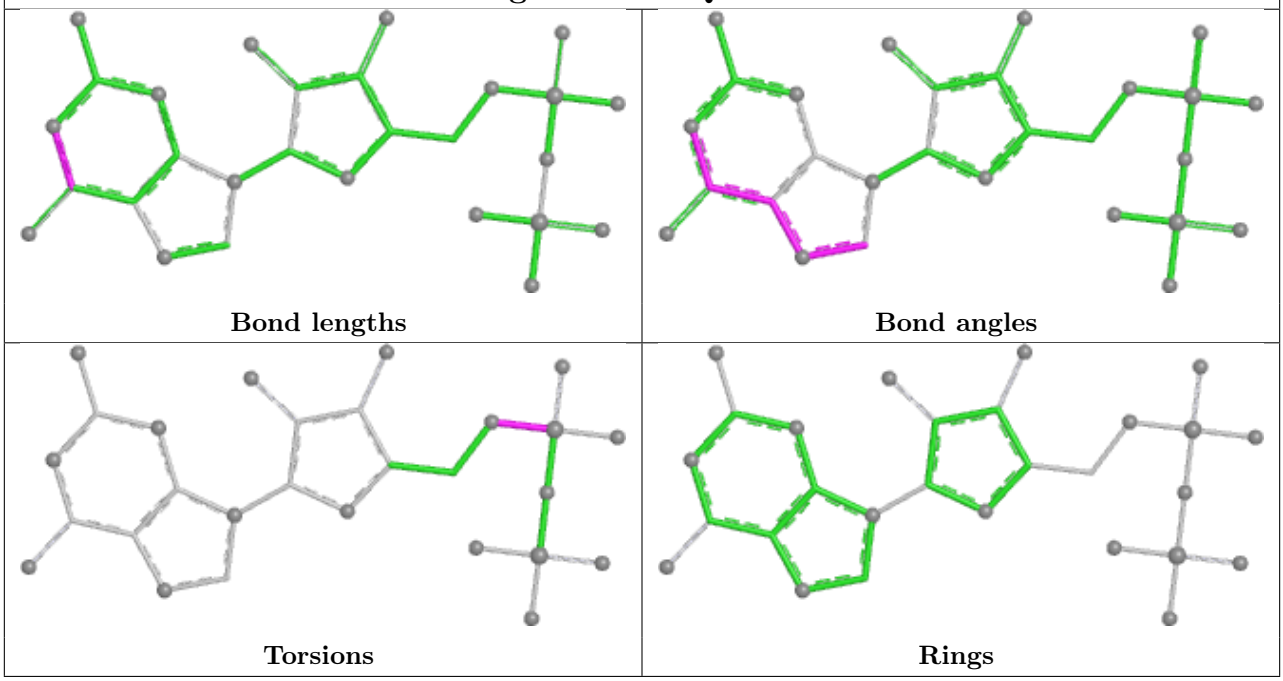

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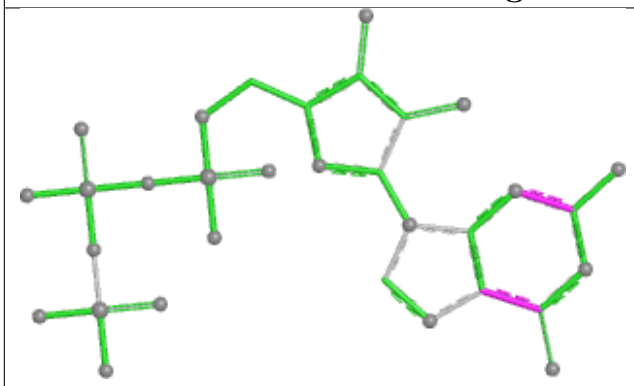
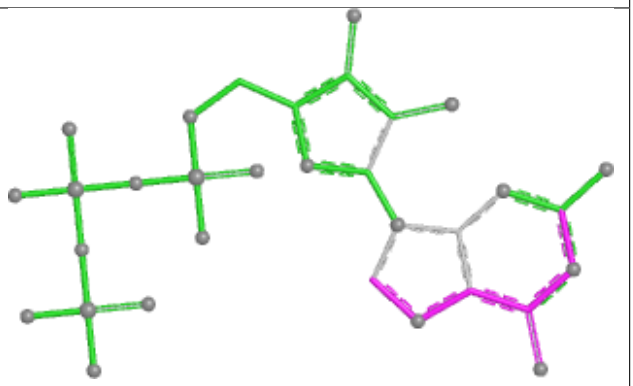
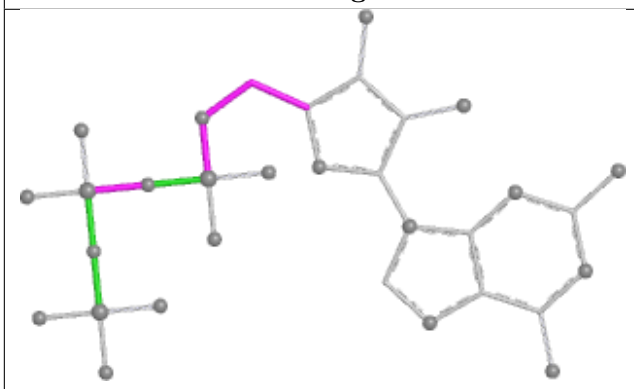


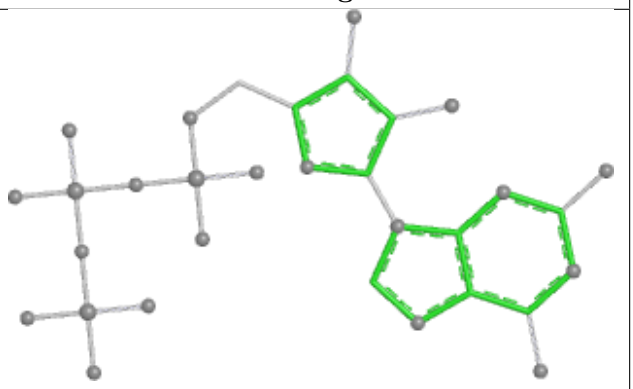
Bond lengths



Bond angles

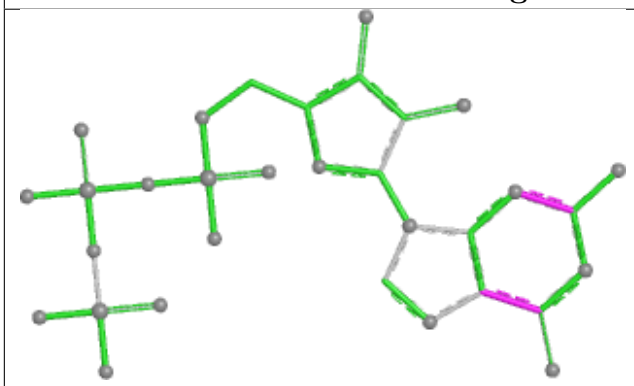


Torsions



Rings

Ligand GTP TK 501



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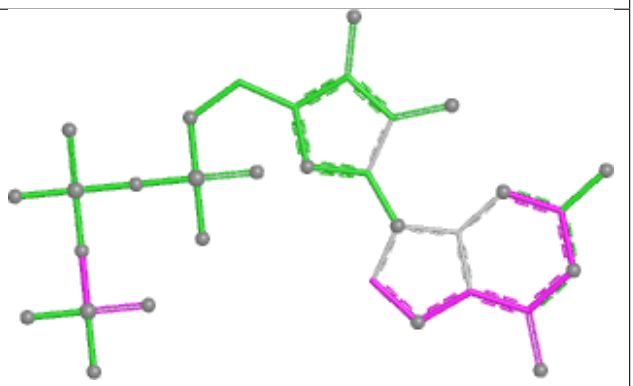

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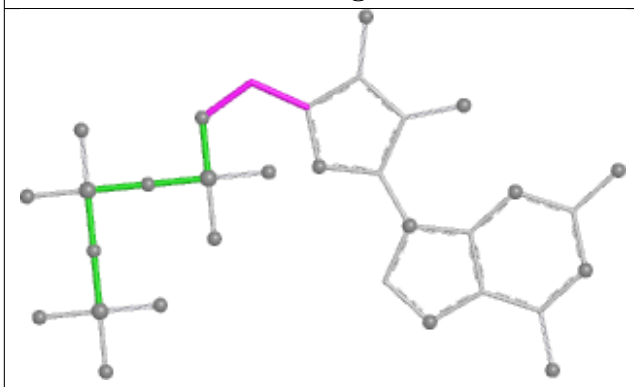

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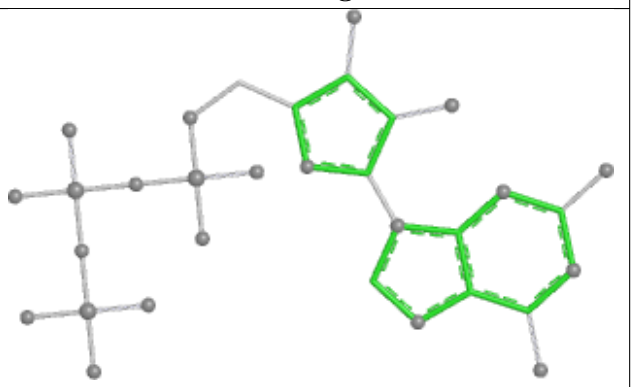
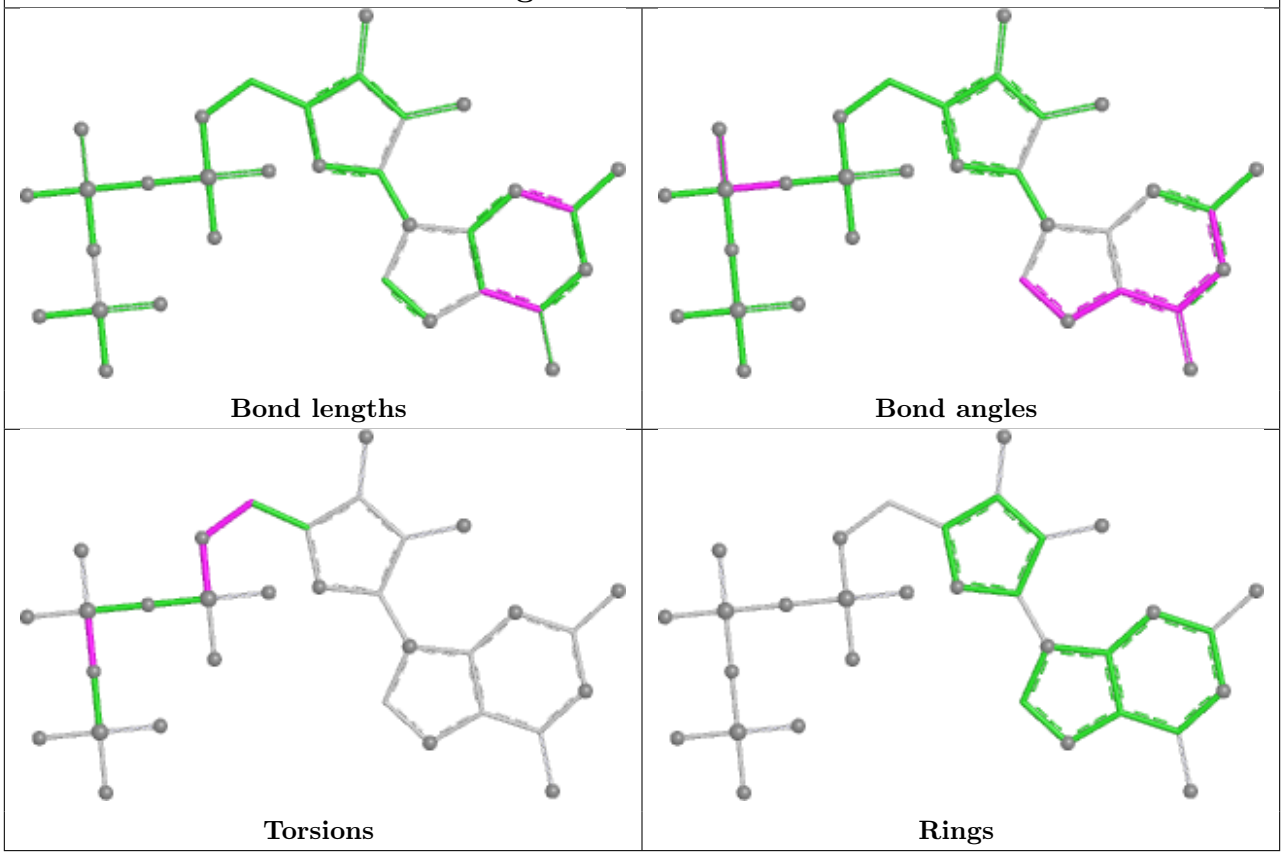
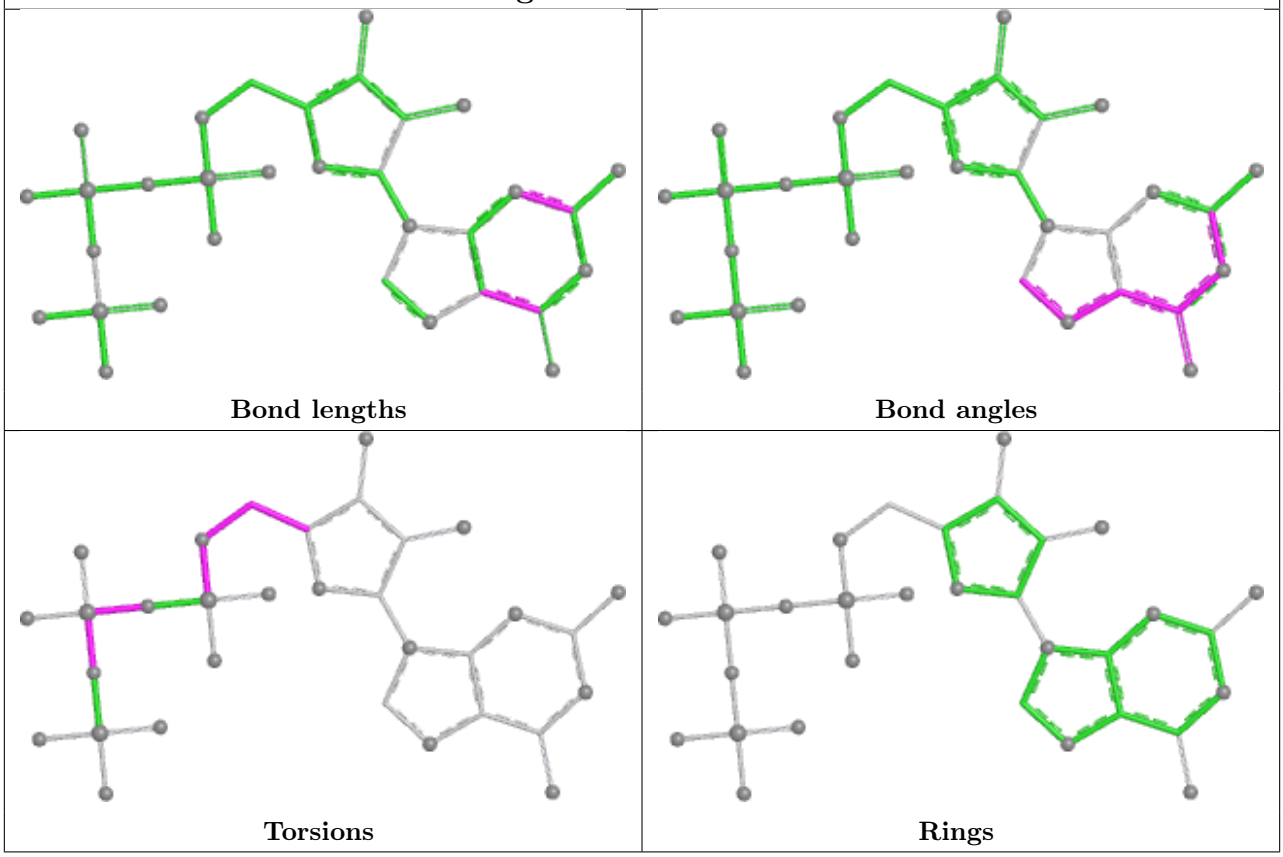


Rings

Ligand GTP VI 501



Ligand GTP AI 501



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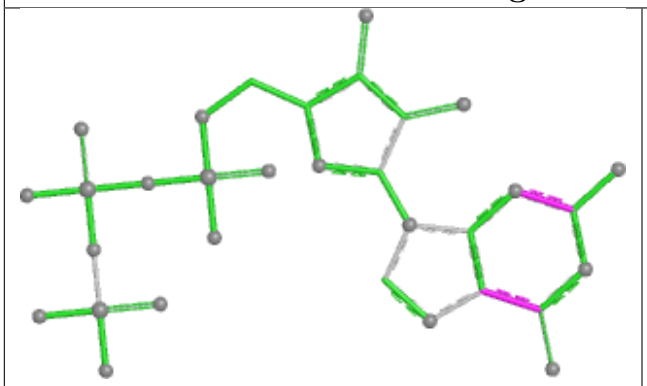

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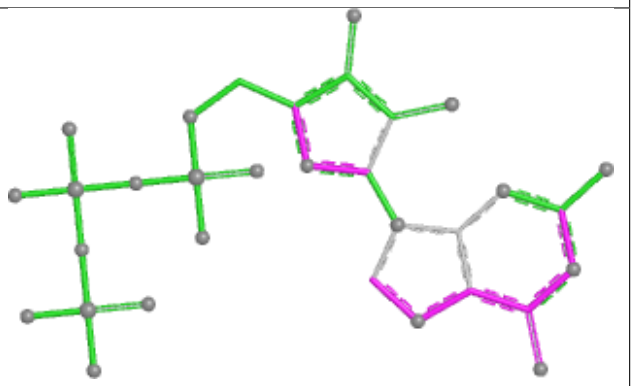
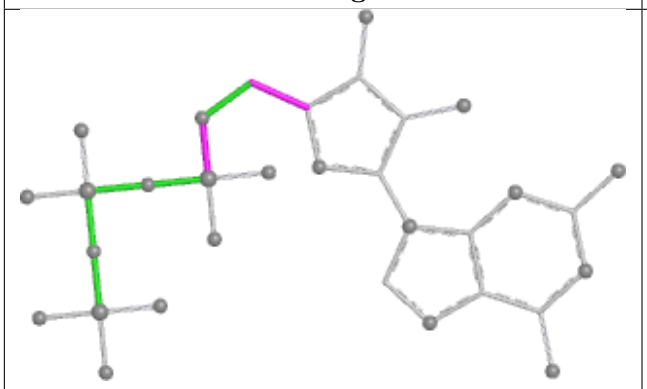


Bond angles



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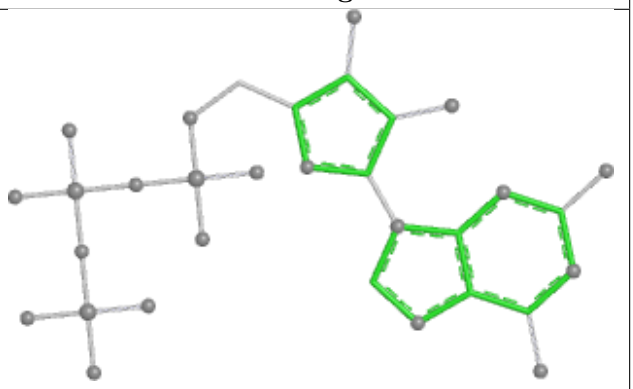
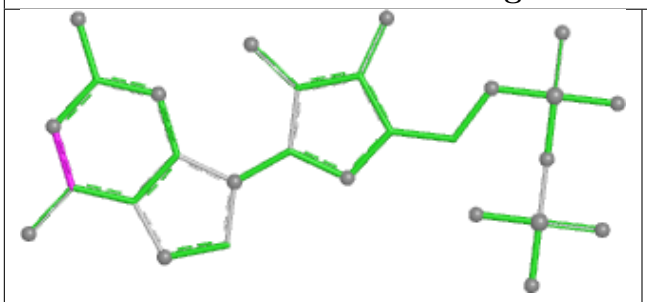


Rings

Ligand GDP MH 501



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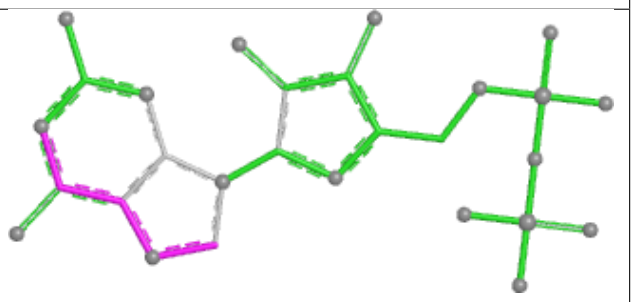
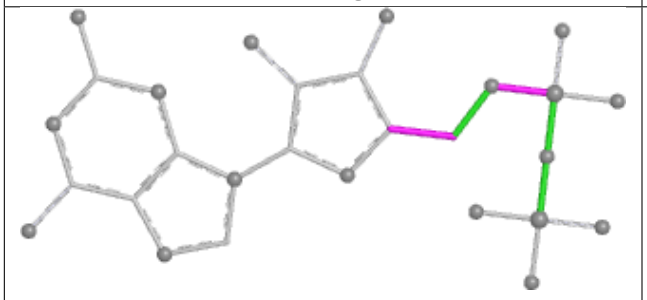


Bond angles



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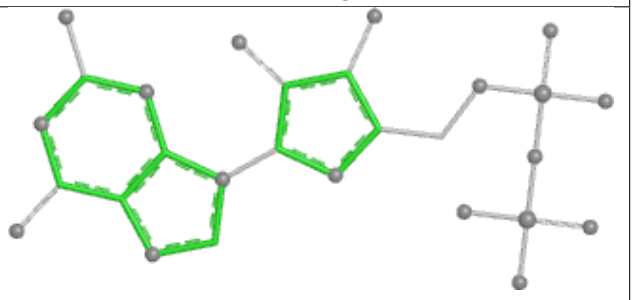
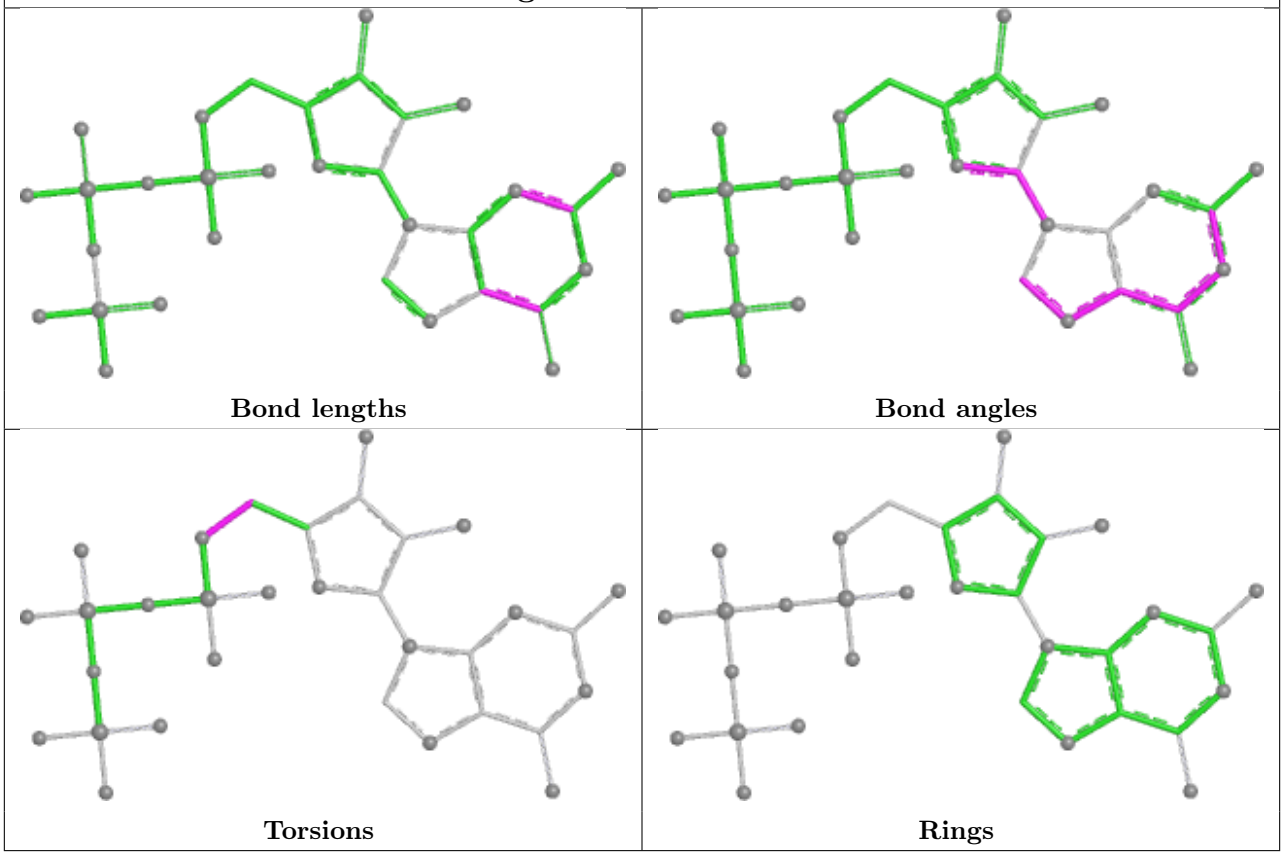


Rings

Ligand GTP PI 501



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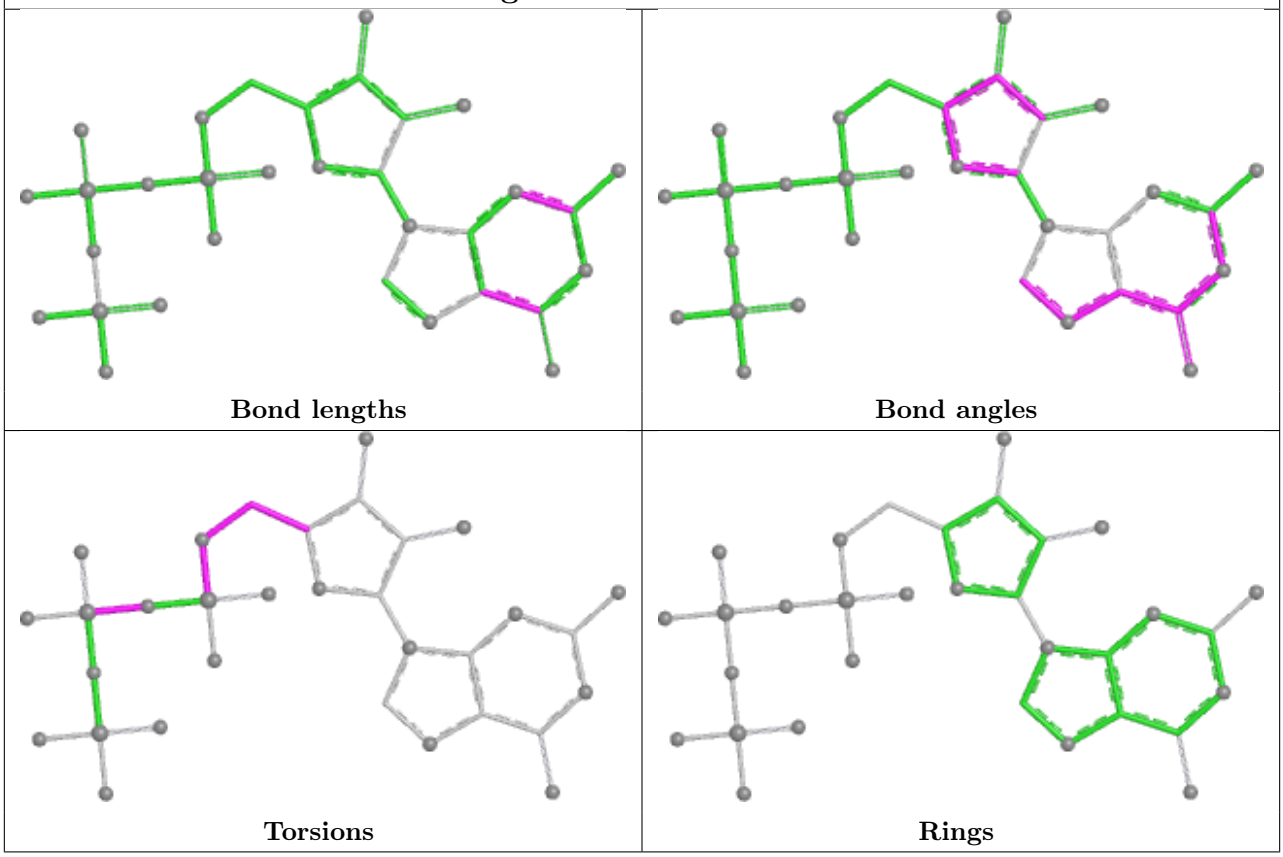
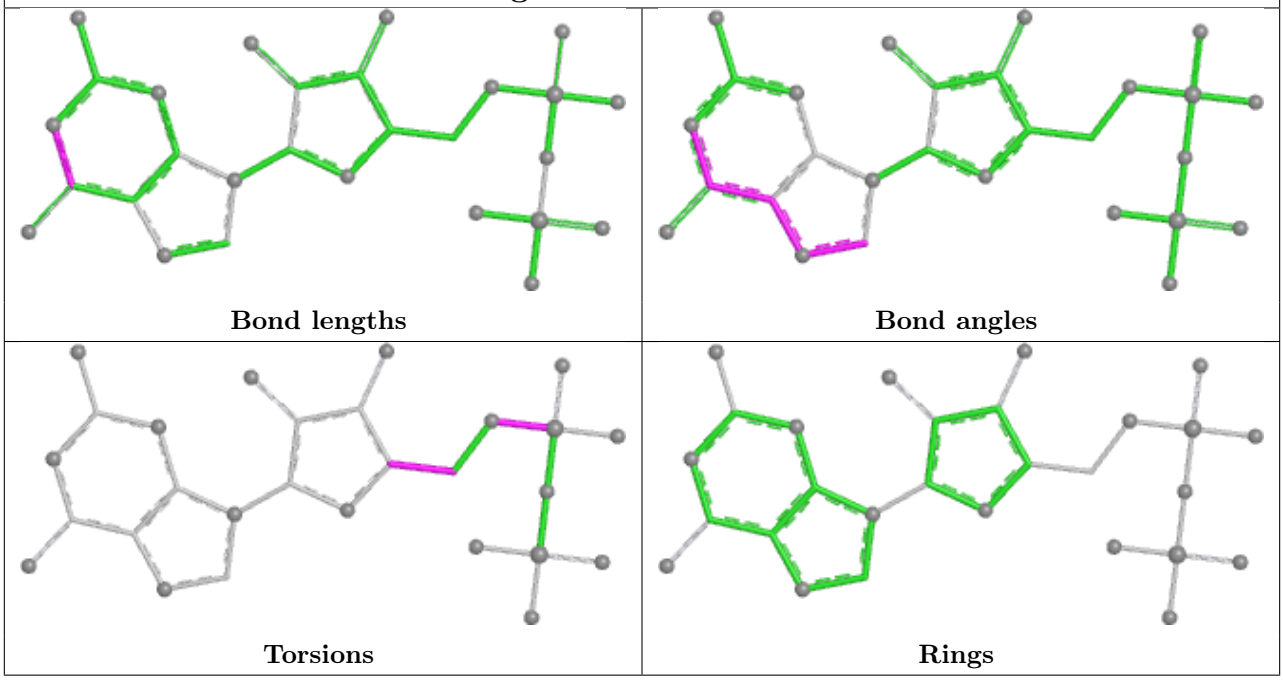
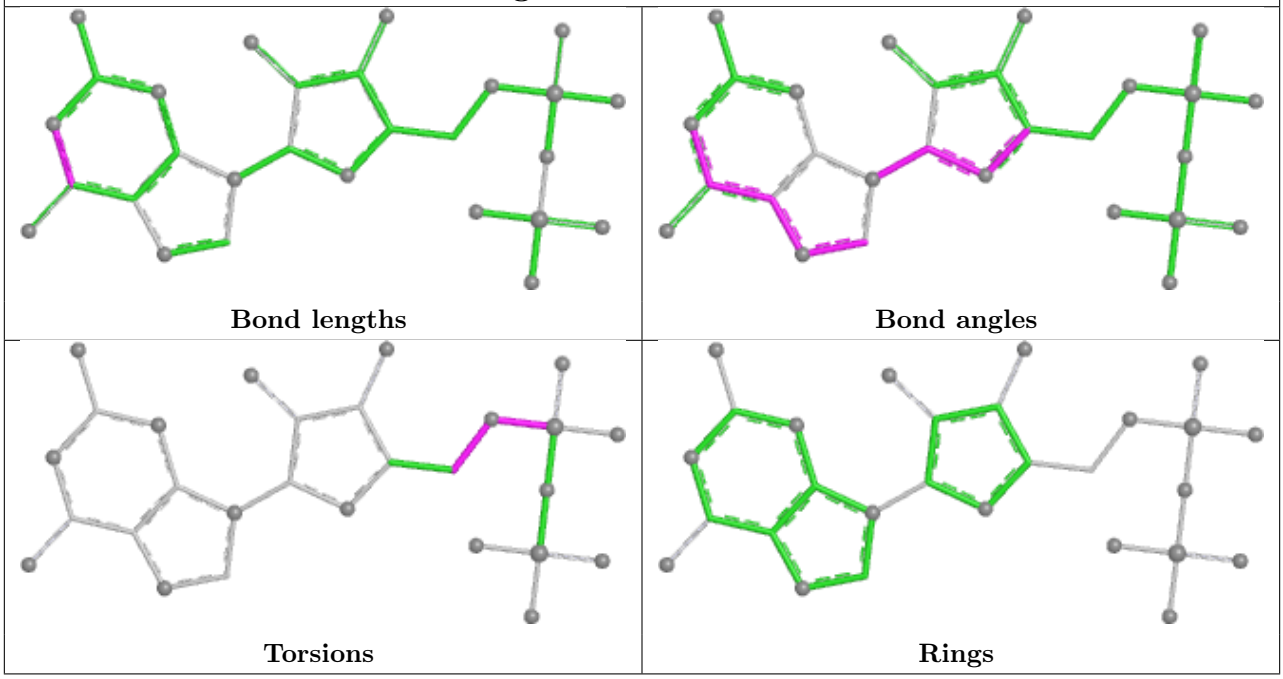


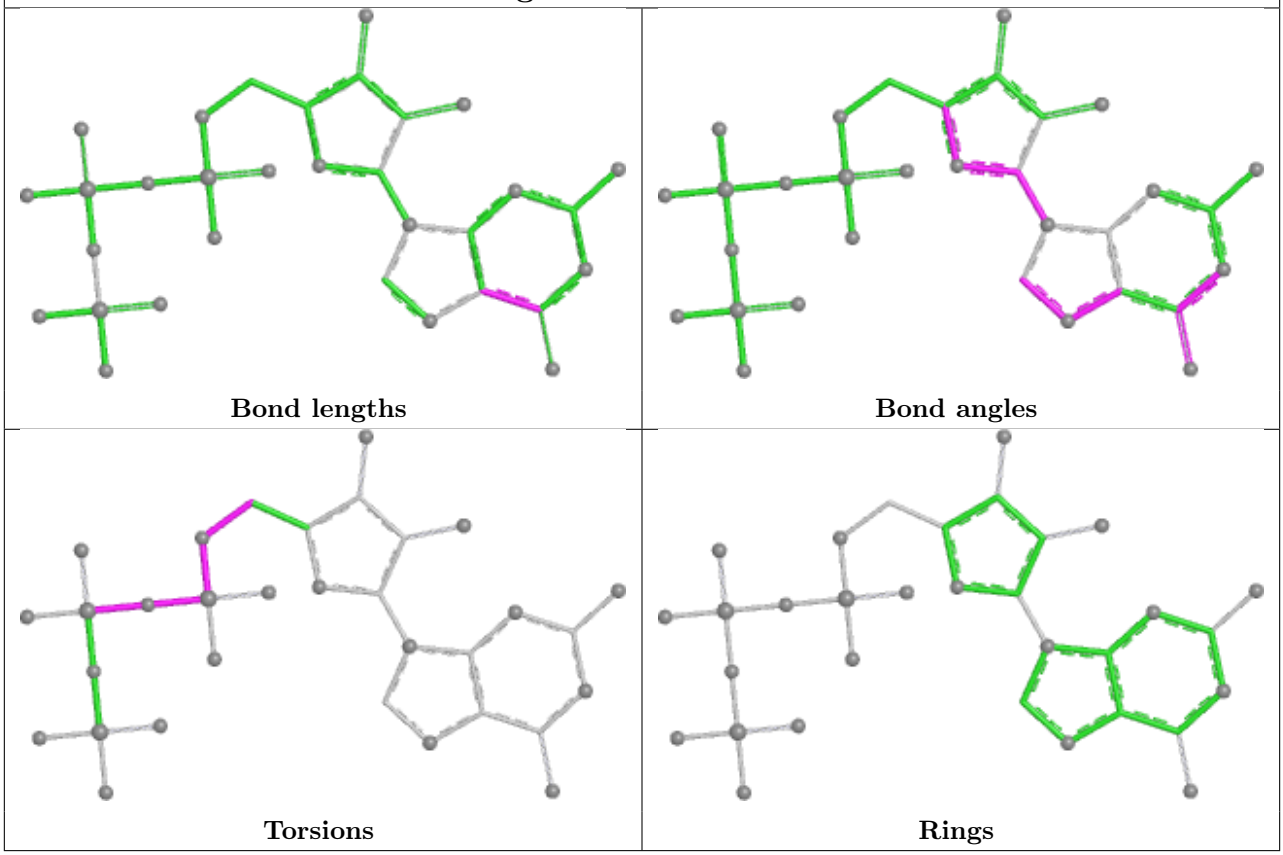
Ligand GDP OF 501



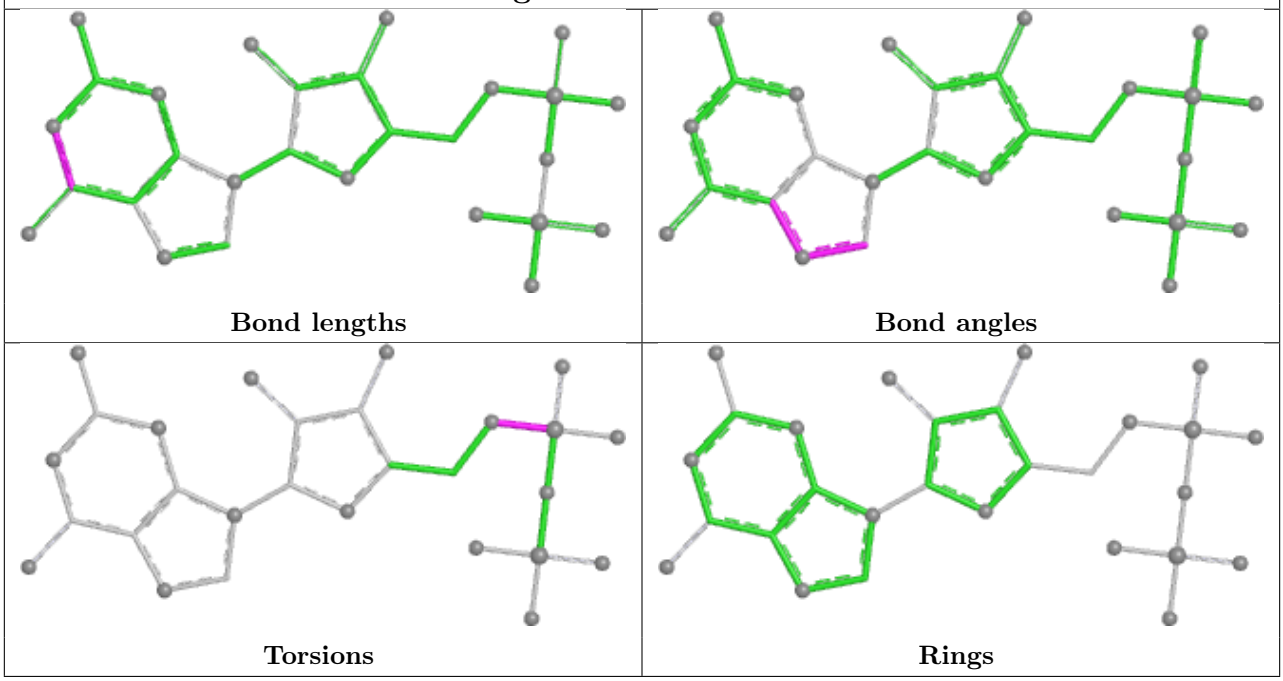
Ligand GDP RJ 501



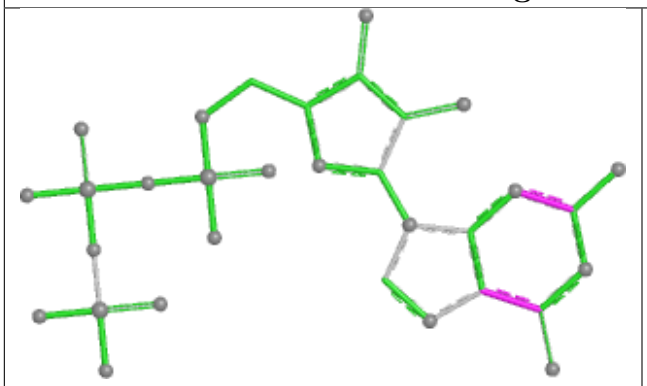
Ligand GTP UI 501



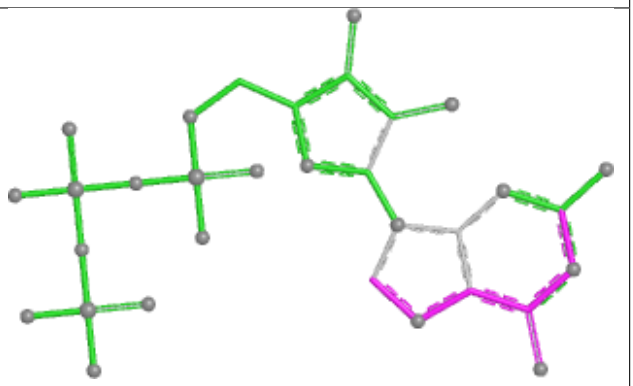
Ligand GDP FL 501



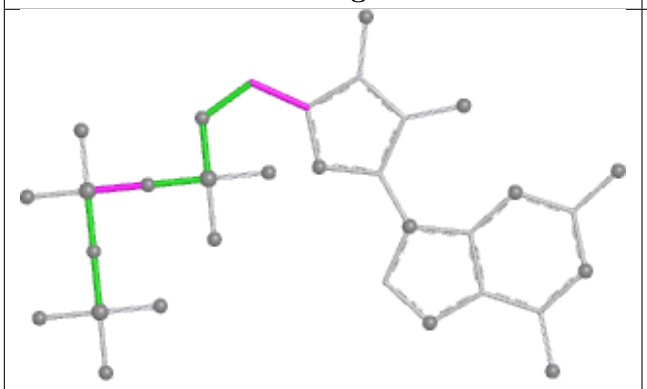
Ligand GTP SC 501



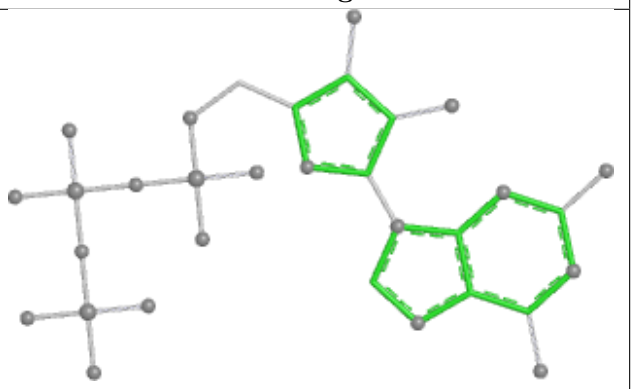
Bond lengths



Bond angles

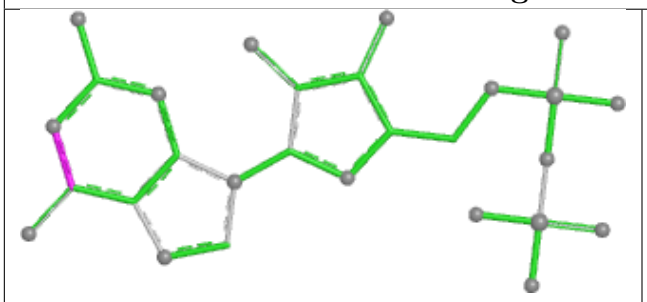


Torsions



Rings

Ligand GDP AL 501



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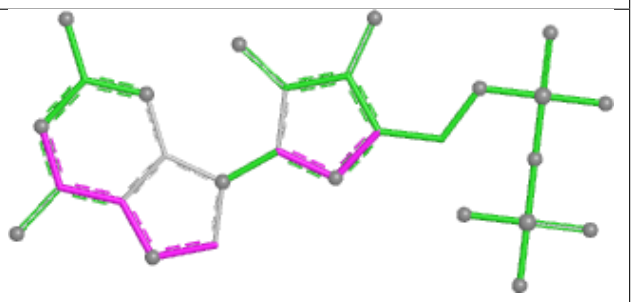
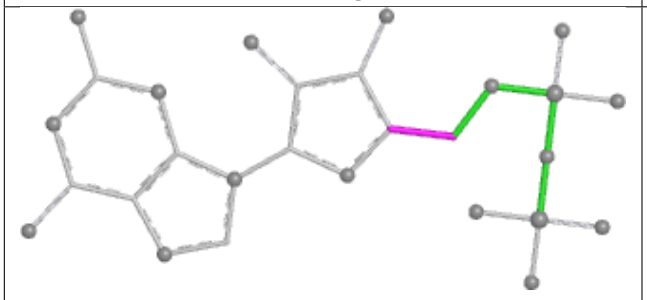


Bond angles



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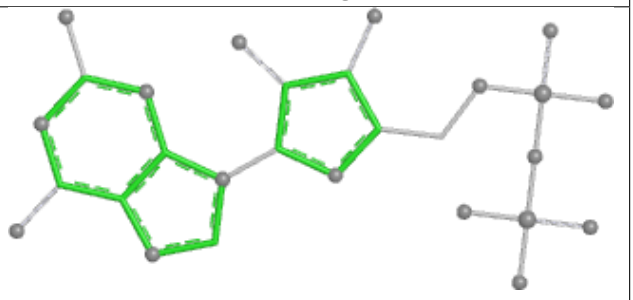
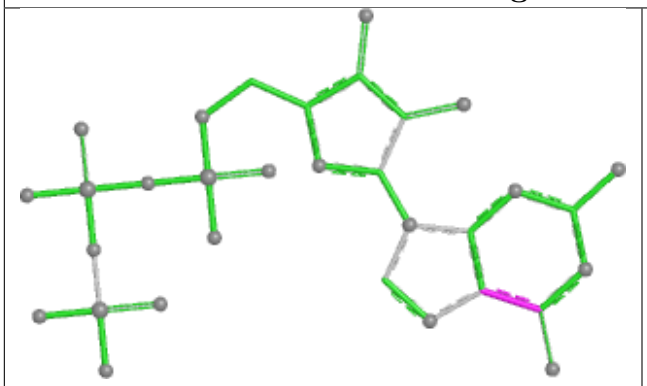
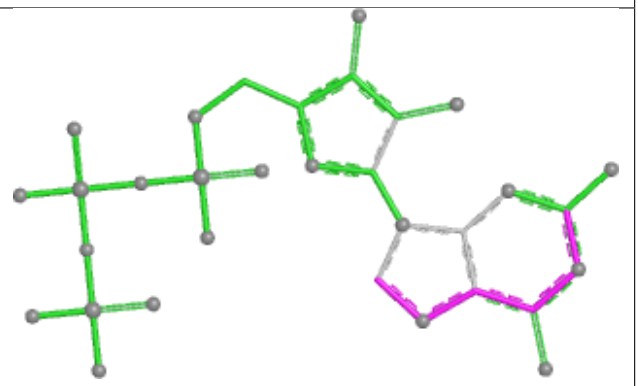


Rings

Ligand GTP PG 501



Bond lengths



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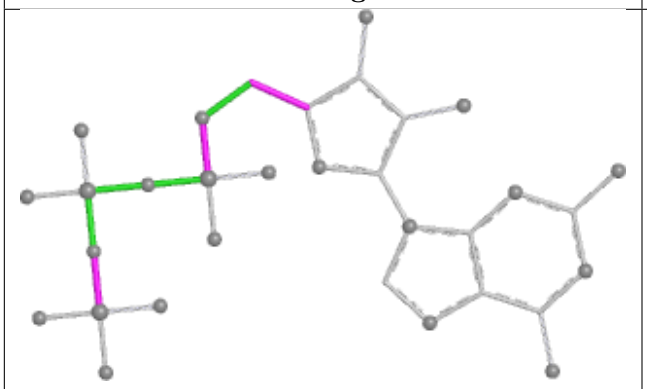
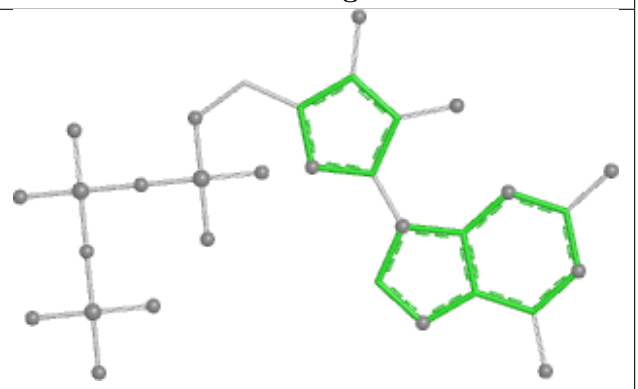
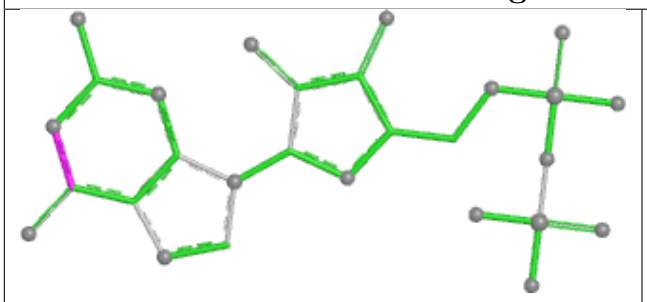


Torsions



Rings

Ligand GDP DB 501



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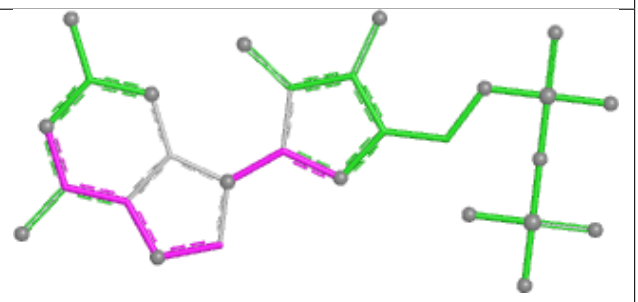

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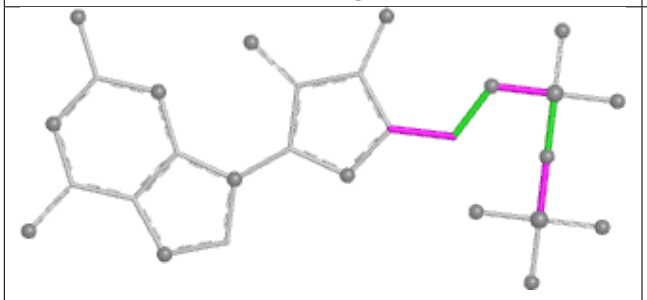

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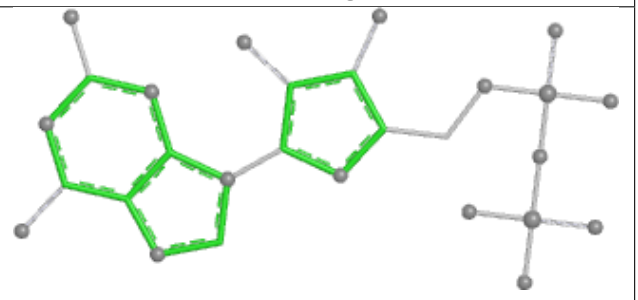

Rings

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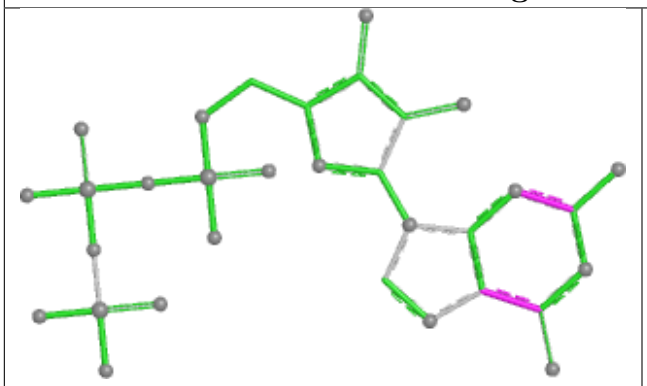

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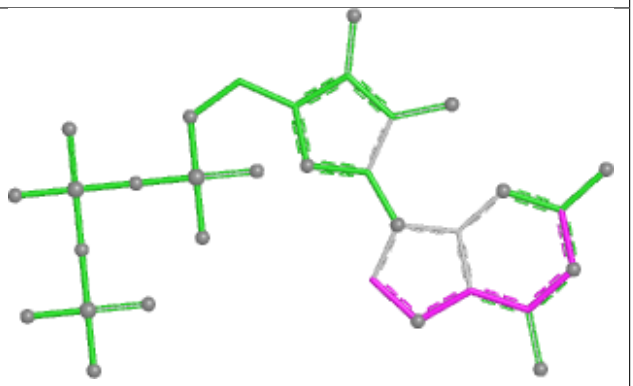

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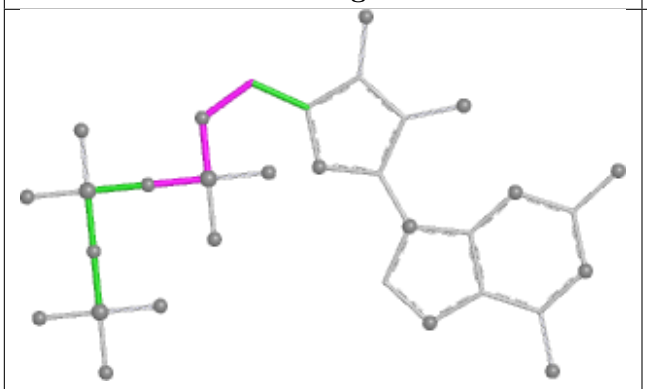

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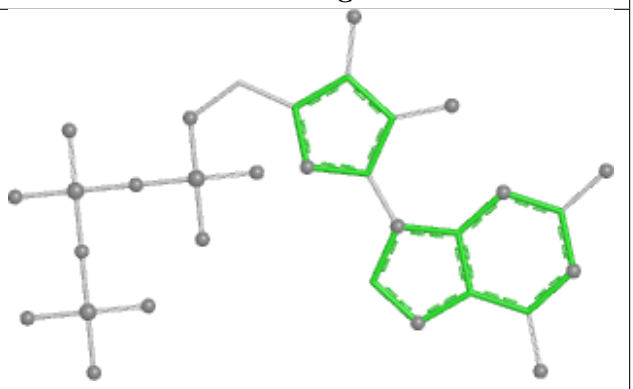

Rings

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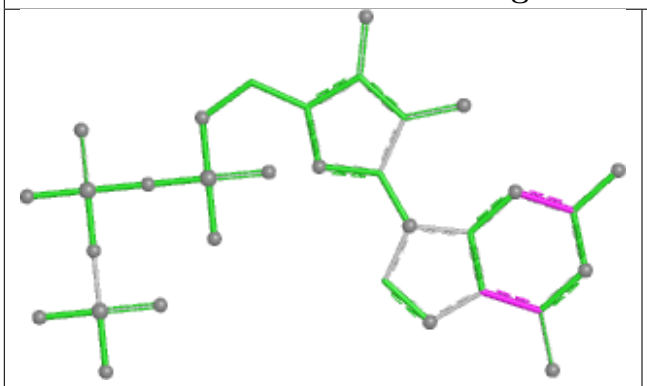

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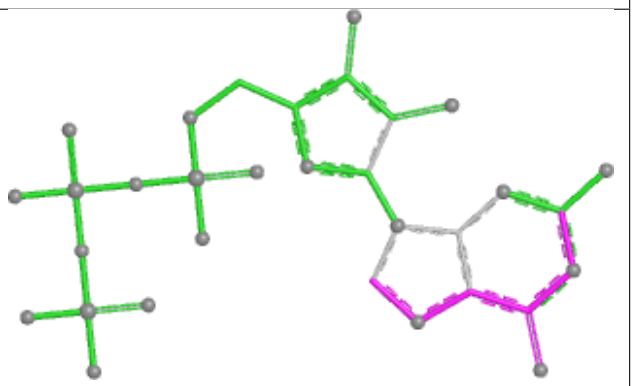

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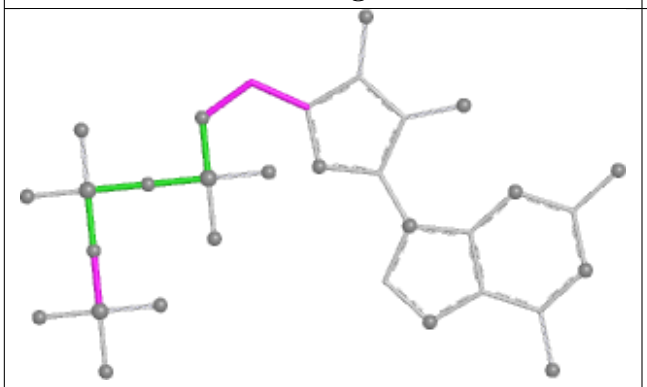

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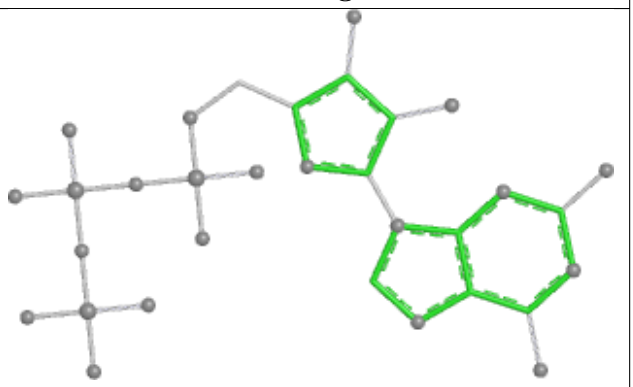
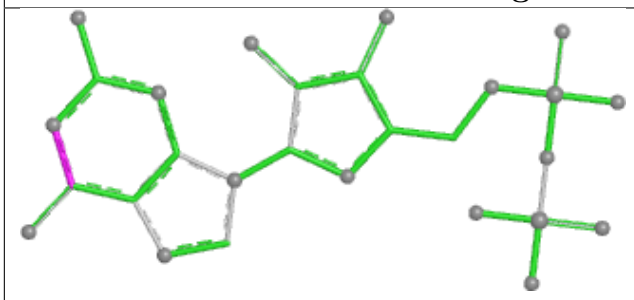


Rings

Ligand GDP HJ 501



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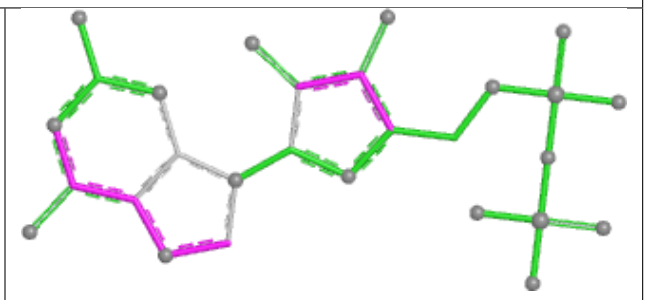

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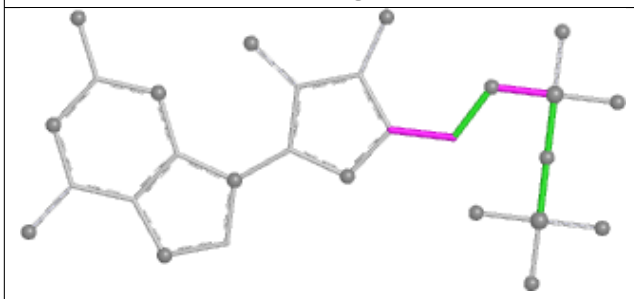

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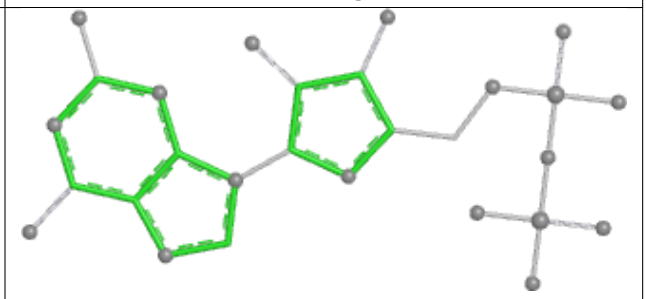
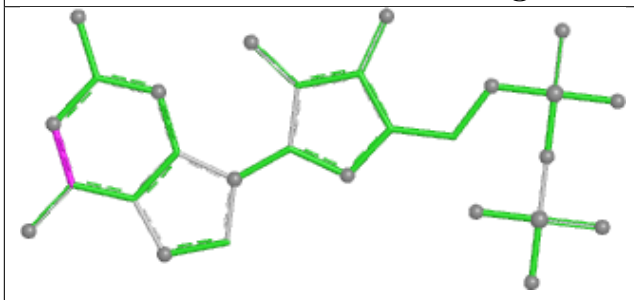


Rings

Ligand GDP CF 501



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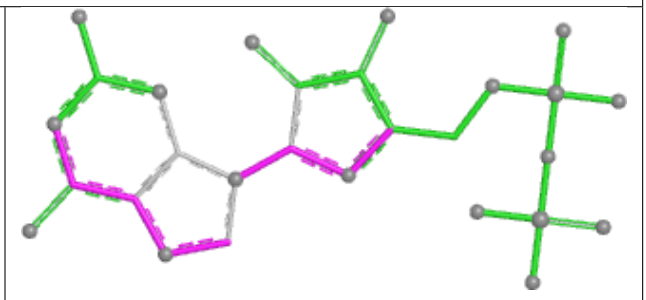

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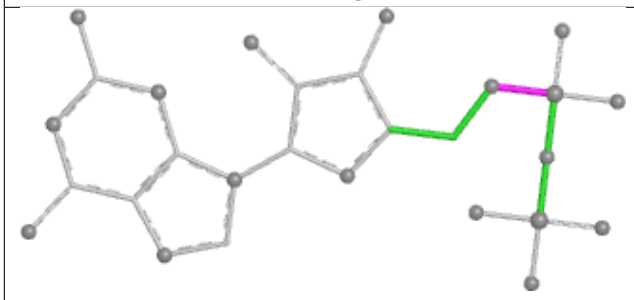

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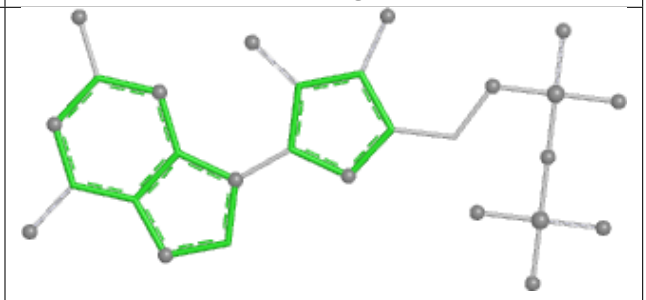

Rings

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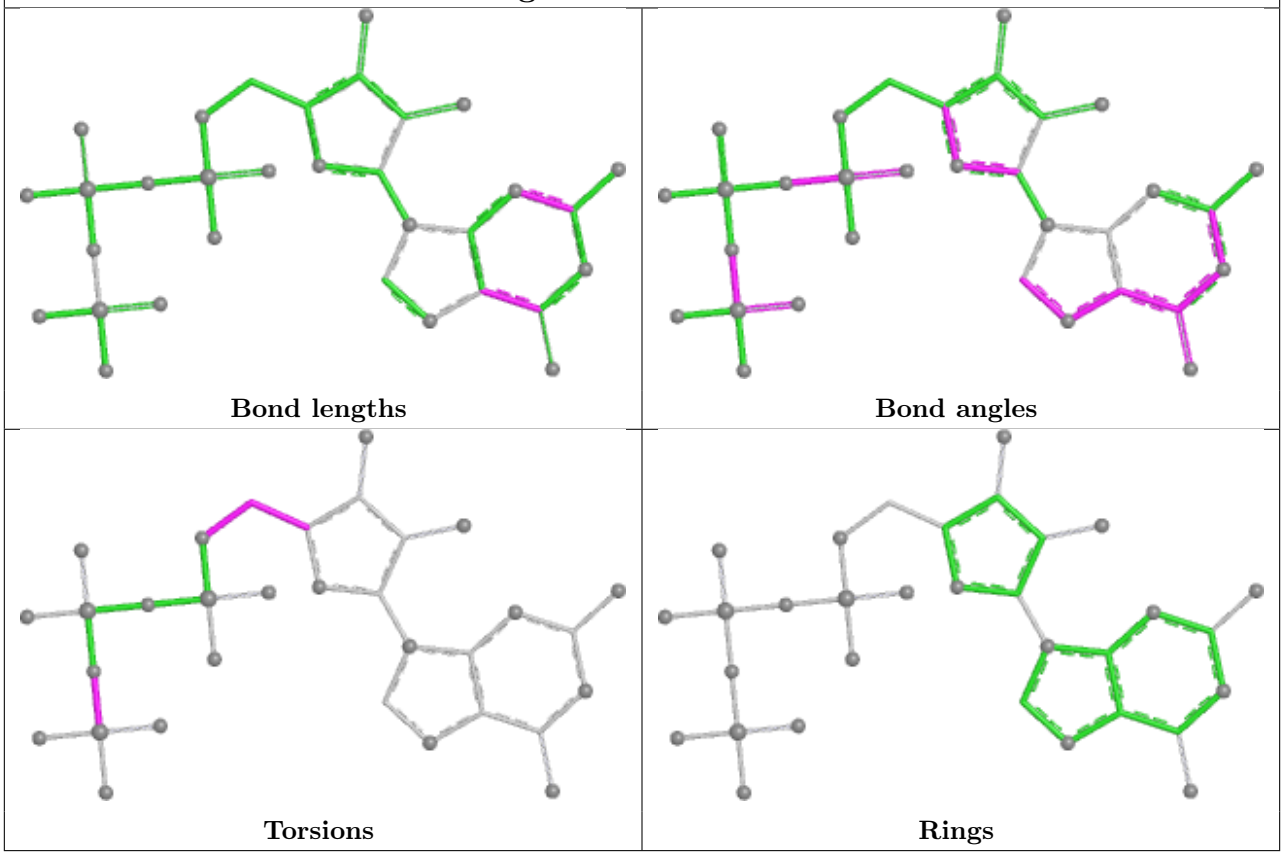

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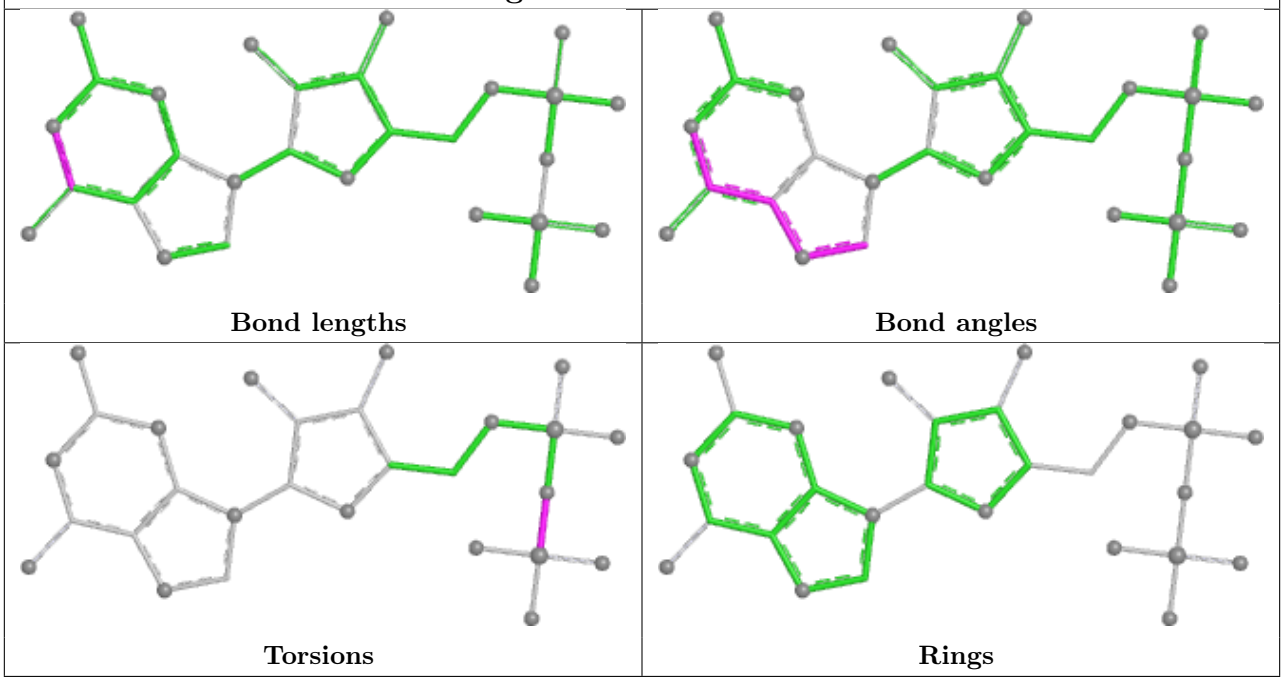

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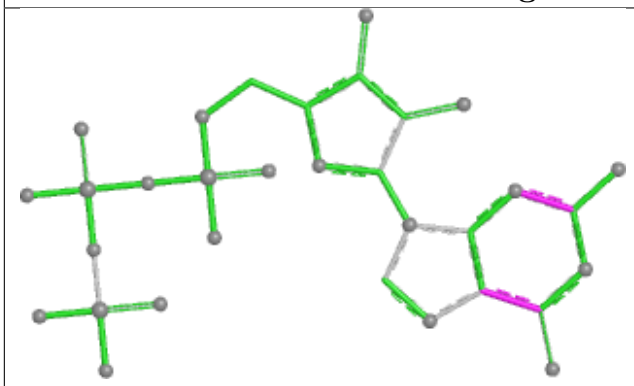

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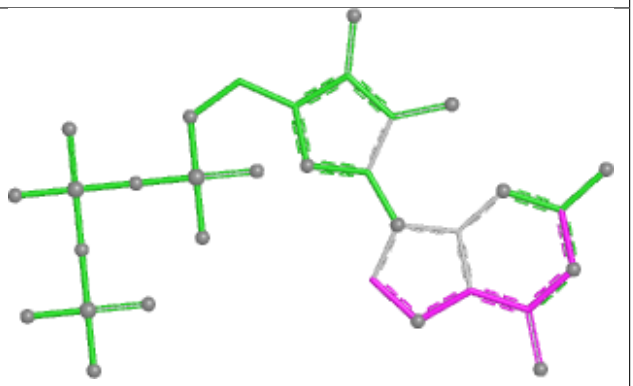

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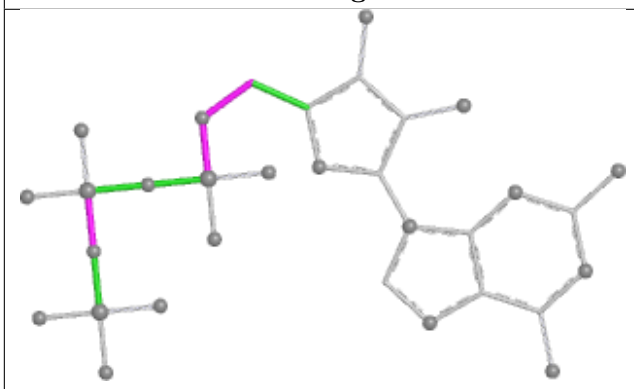

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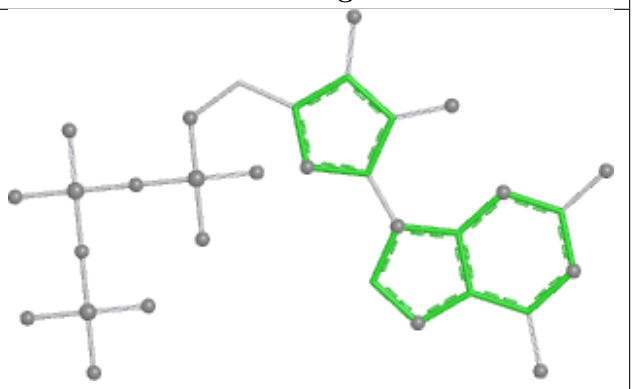

Rings

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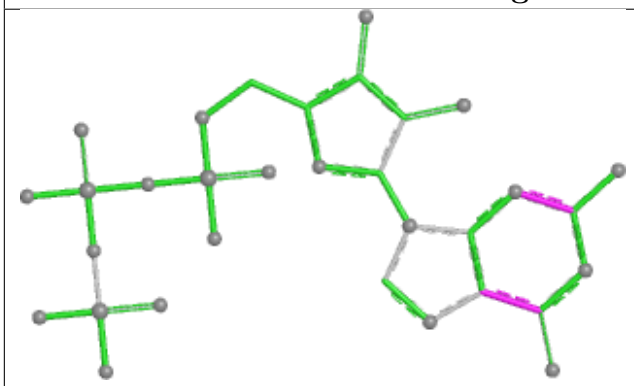

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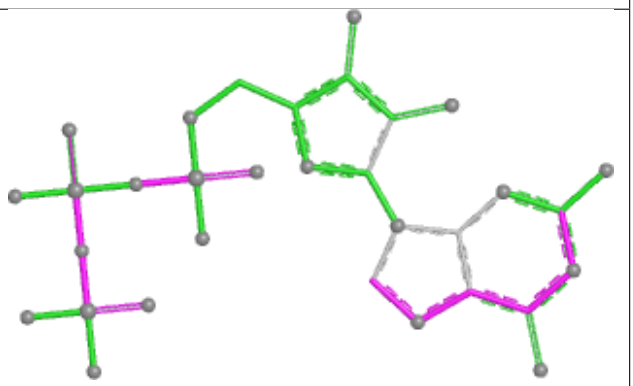

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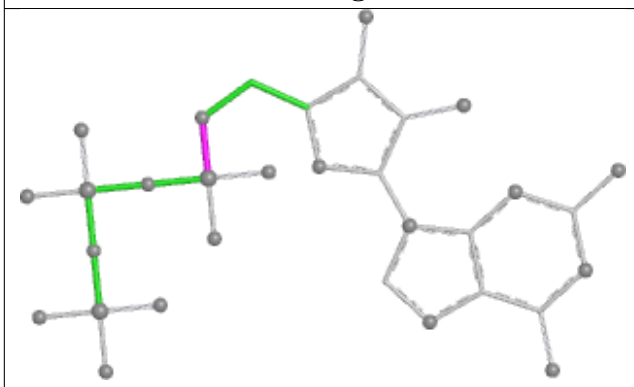

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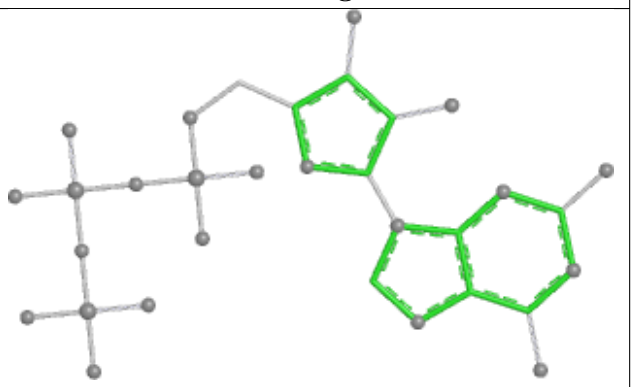
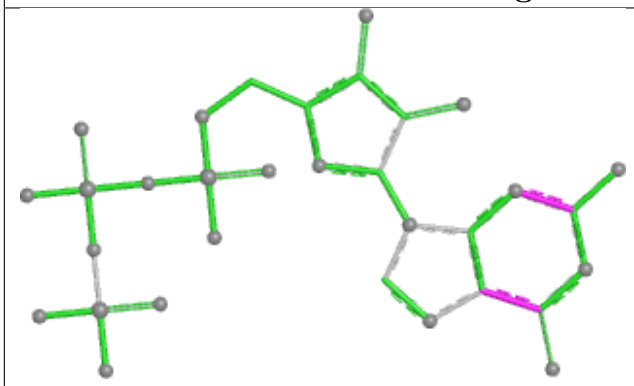


Rings

Ligand GTP SE 501



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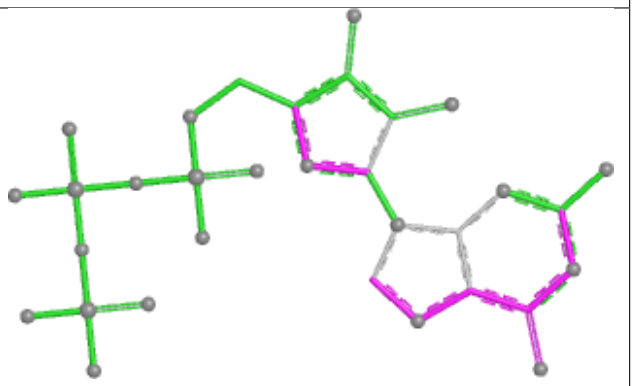
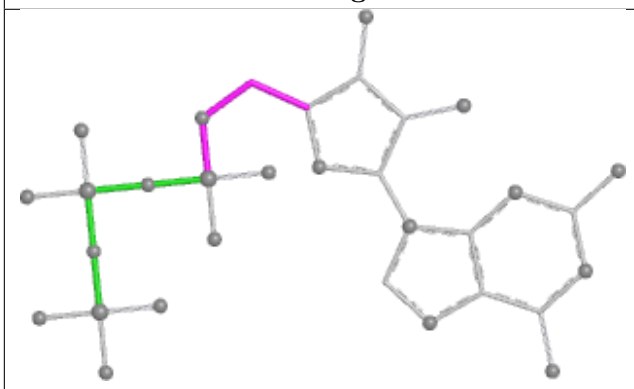


Bond angles



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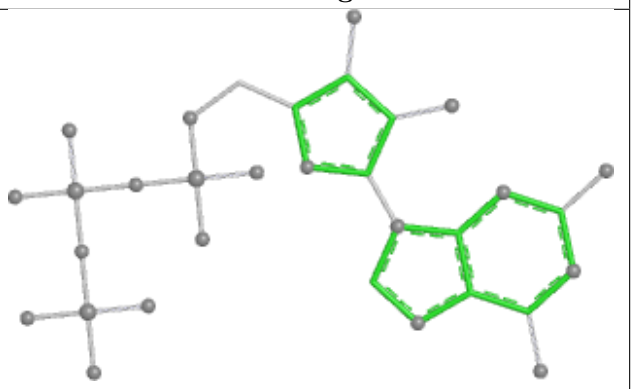
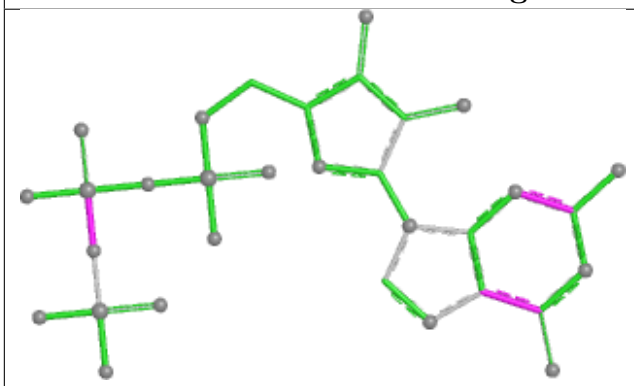


Rings

Ligand GTP BK 501



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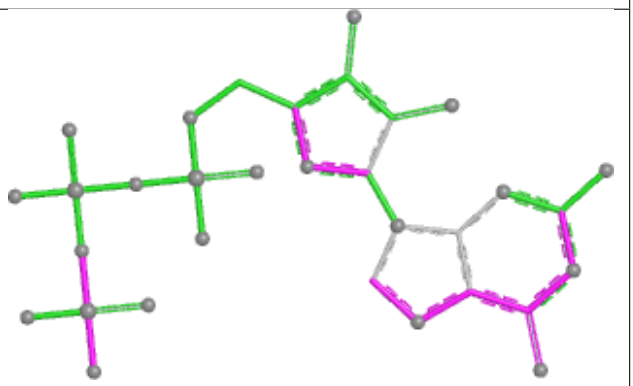

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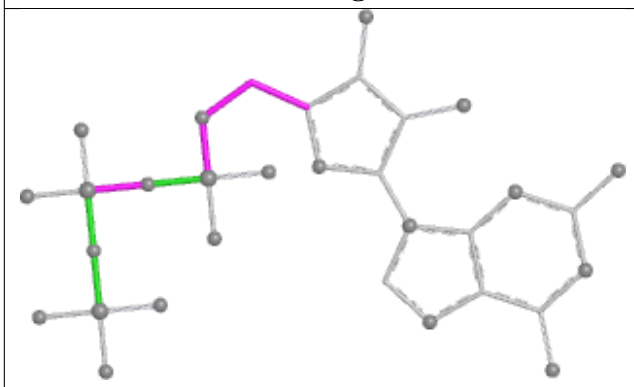

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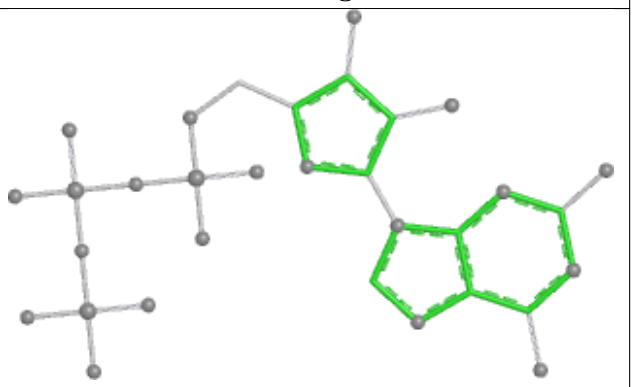

Rings

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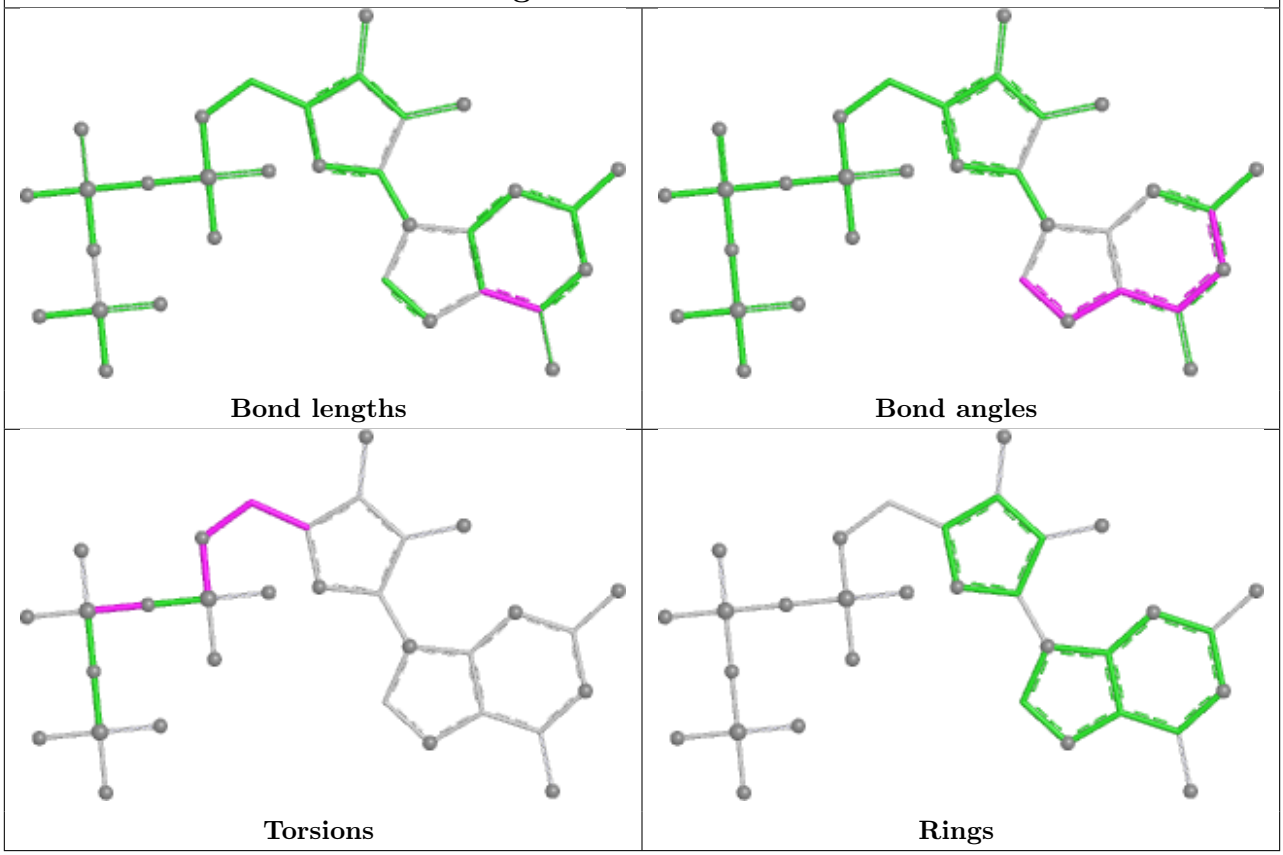

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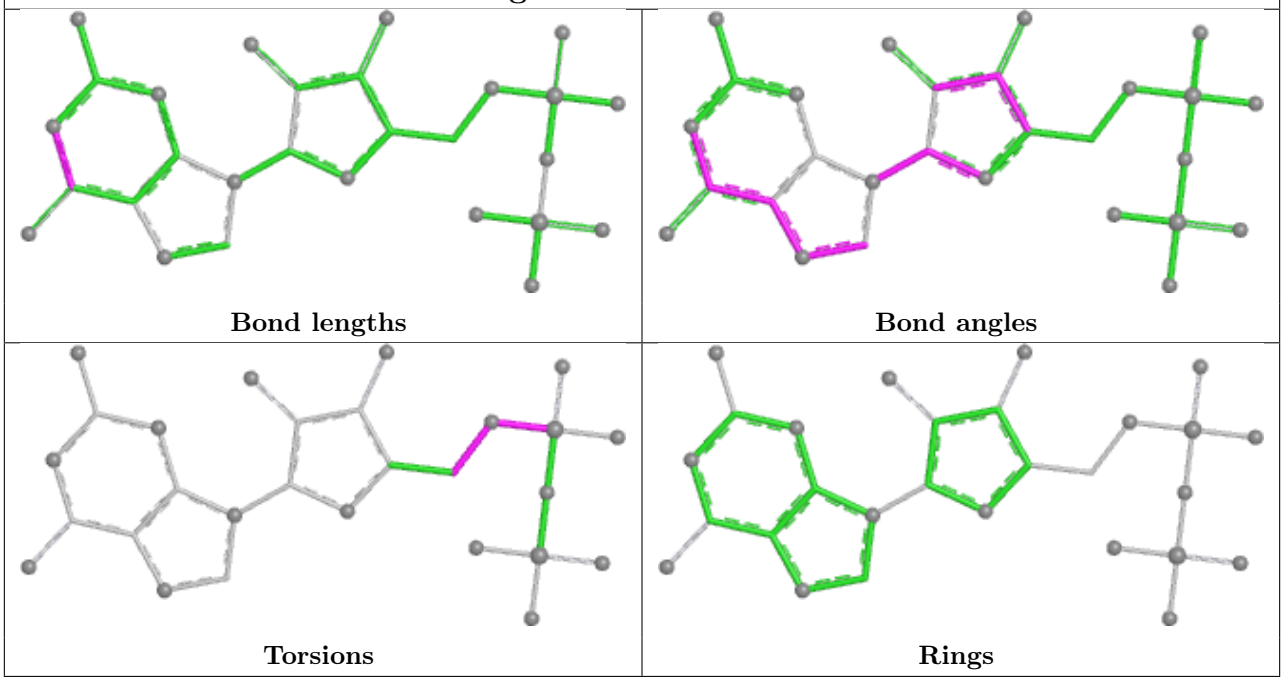

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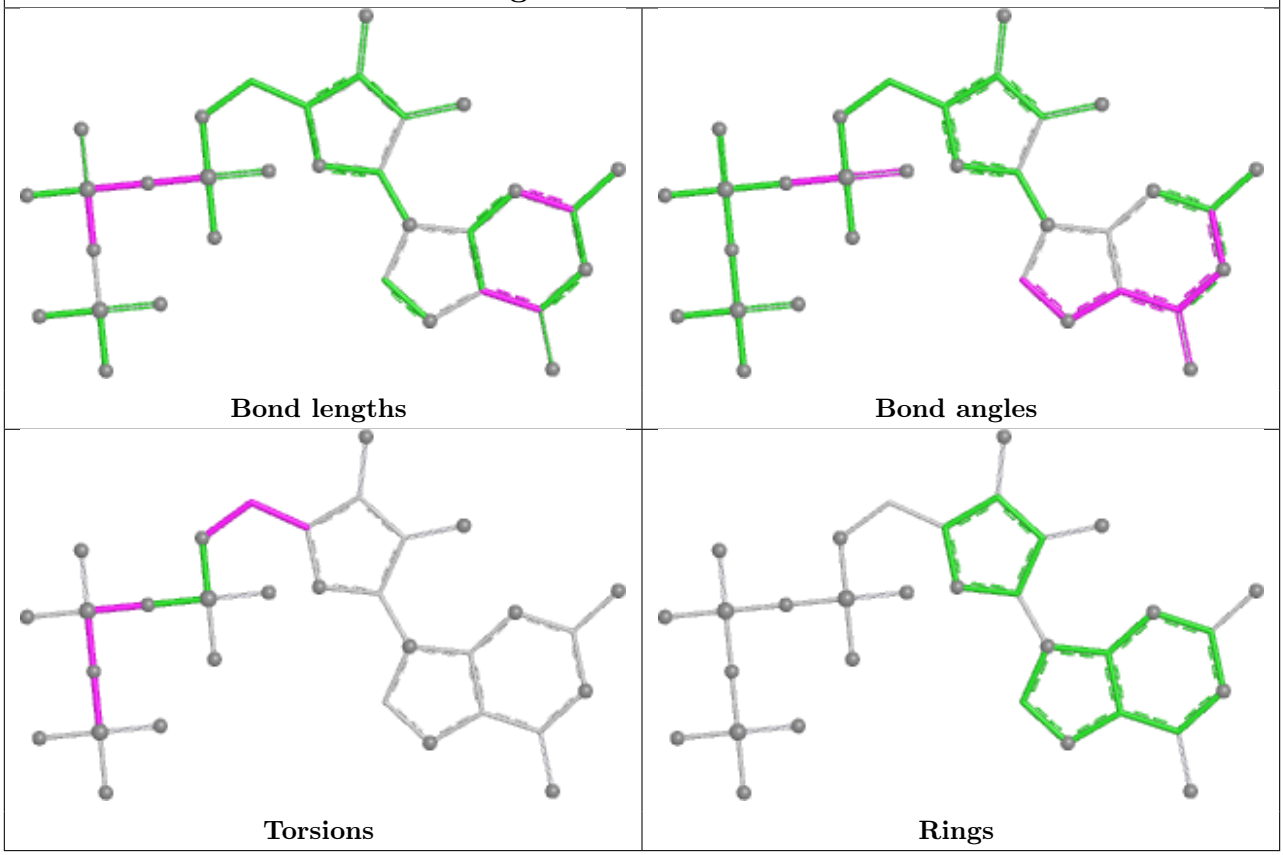

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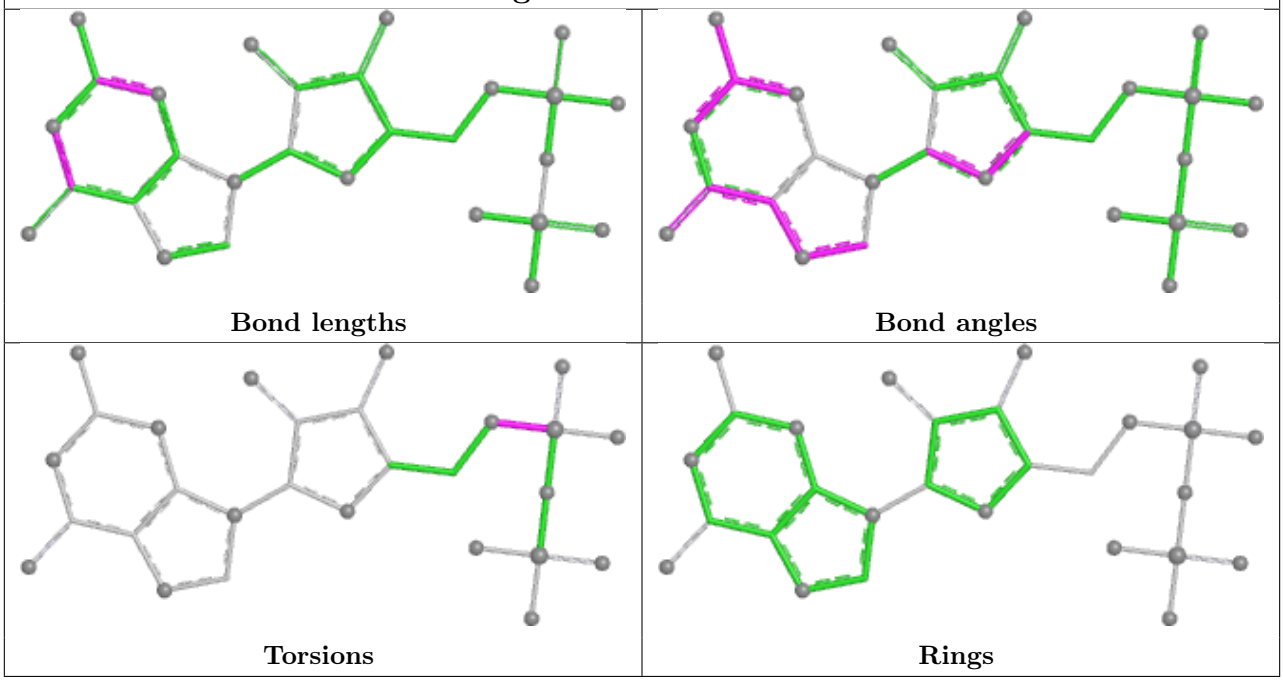

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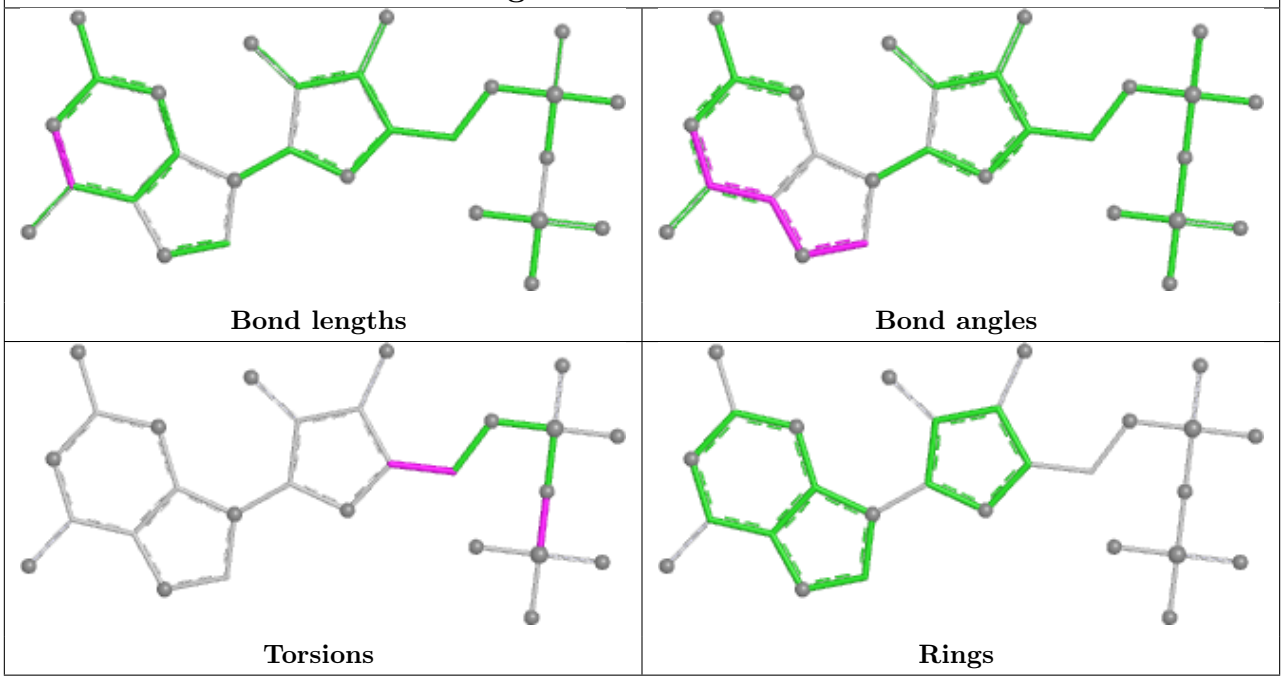

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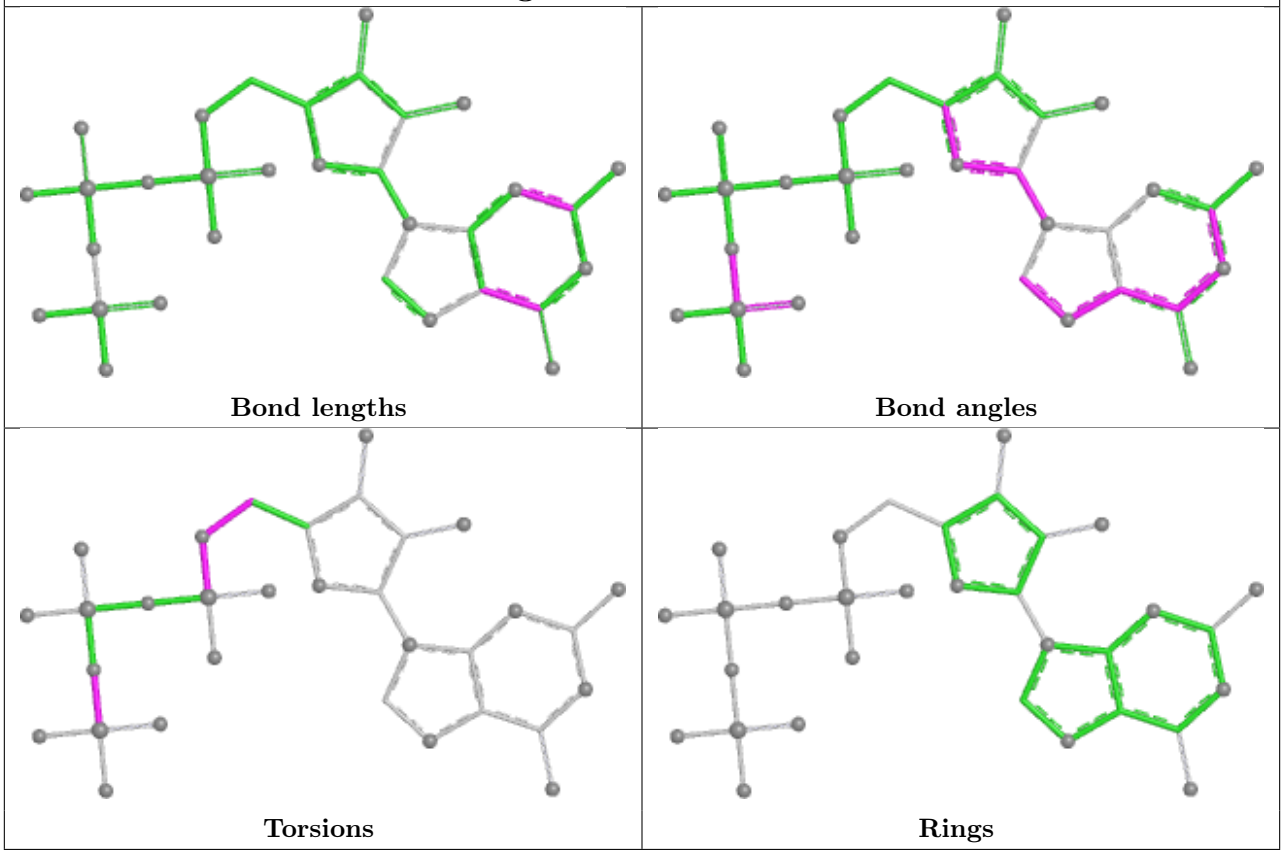

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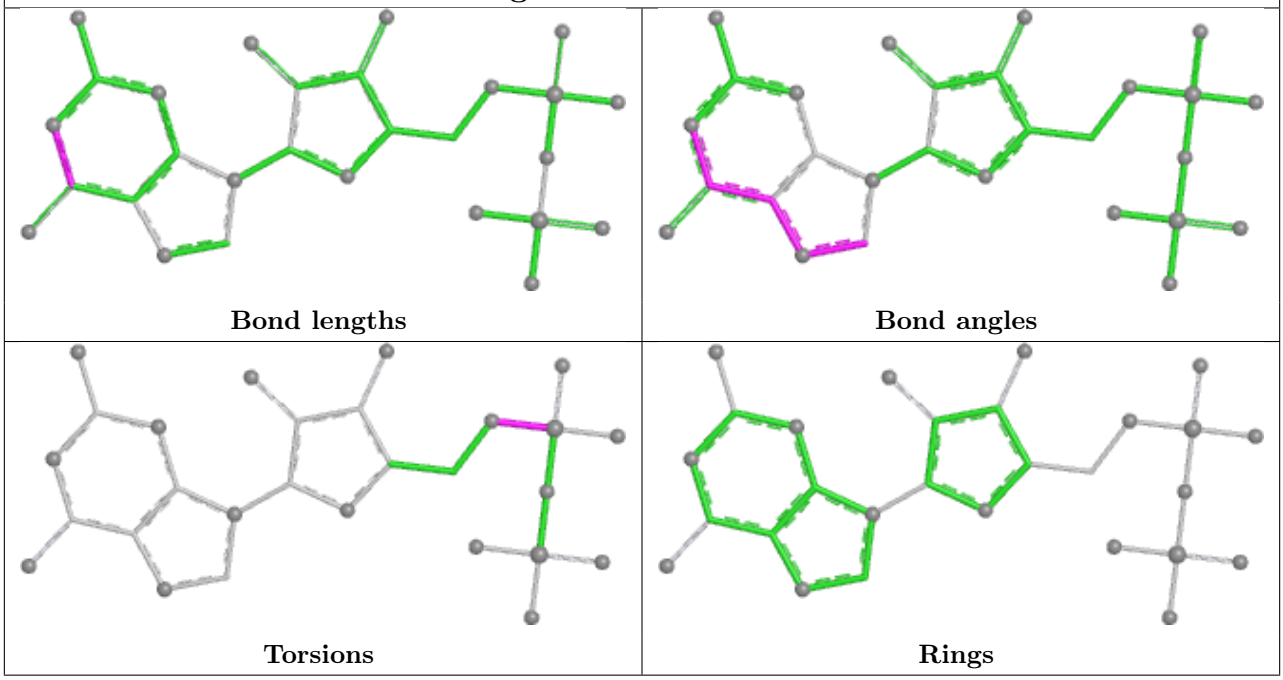

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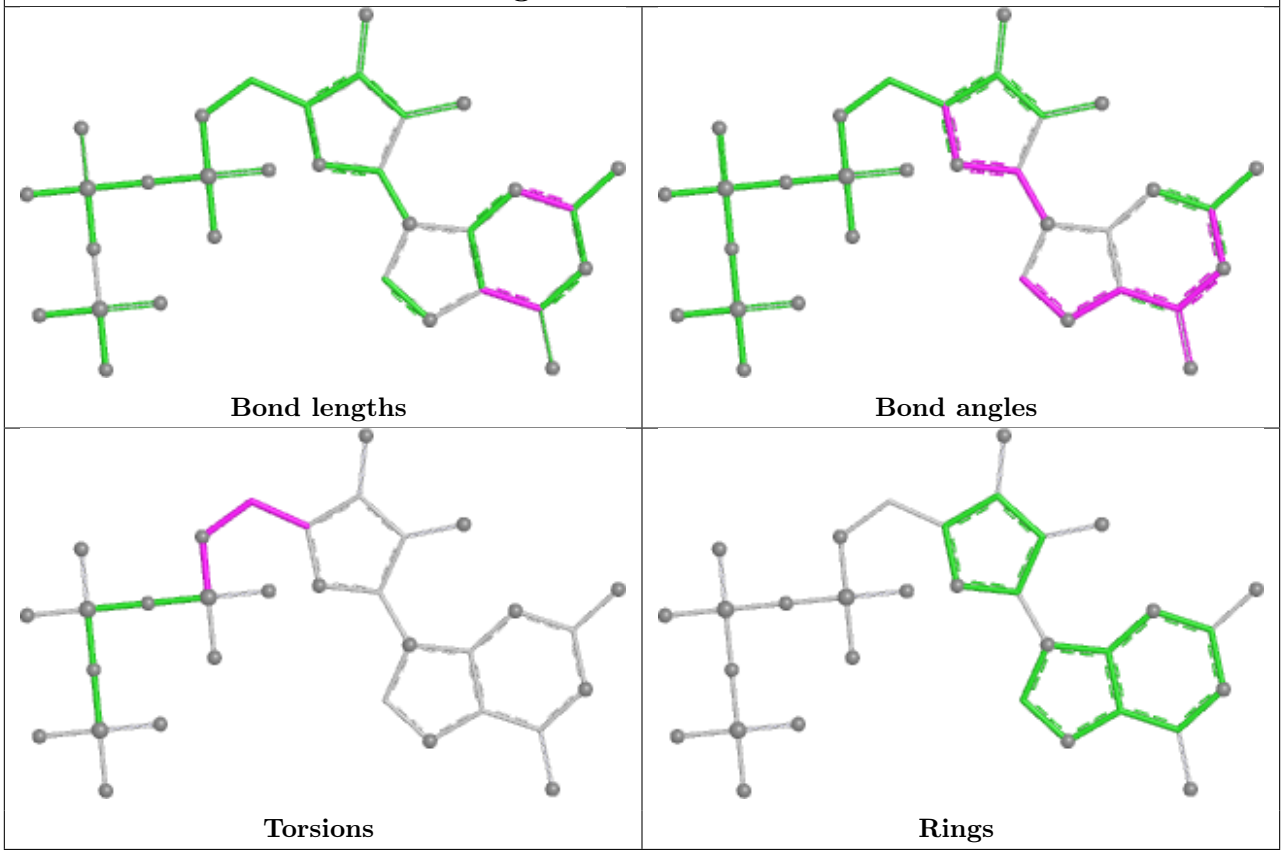

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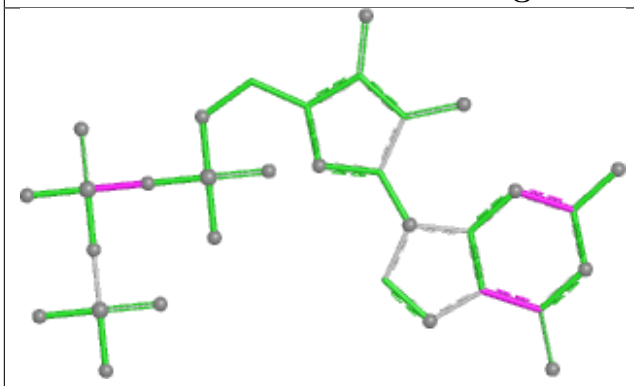
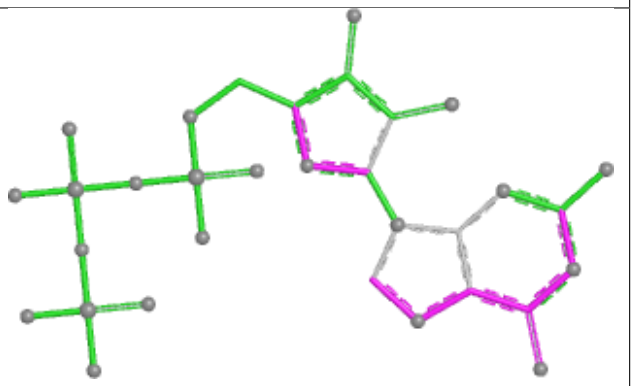
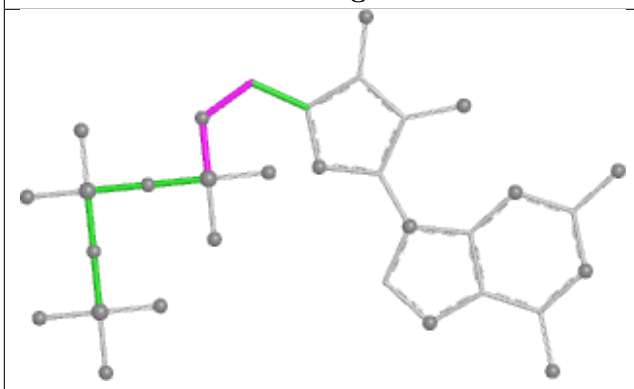


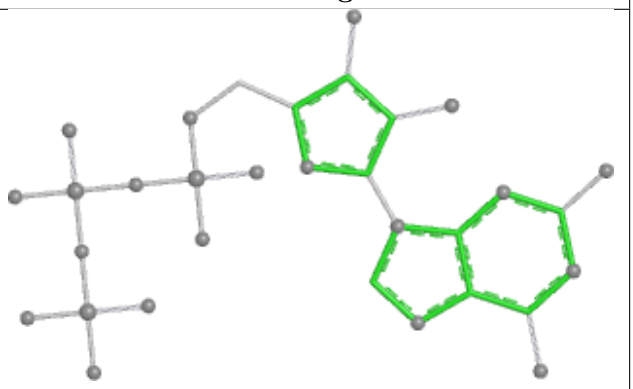
Bond lengths



Bond angles

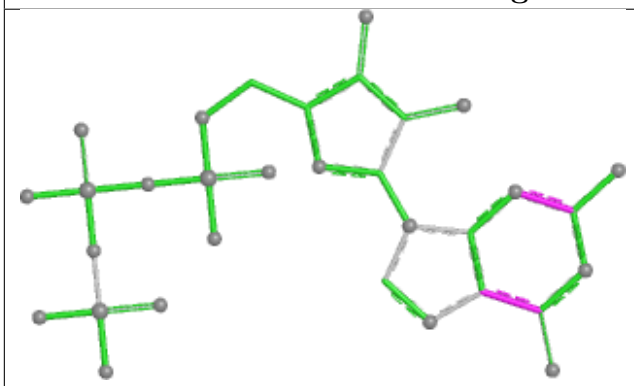


Torsions

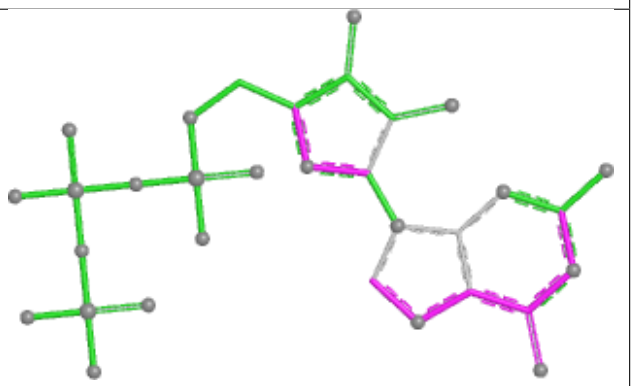


Rings

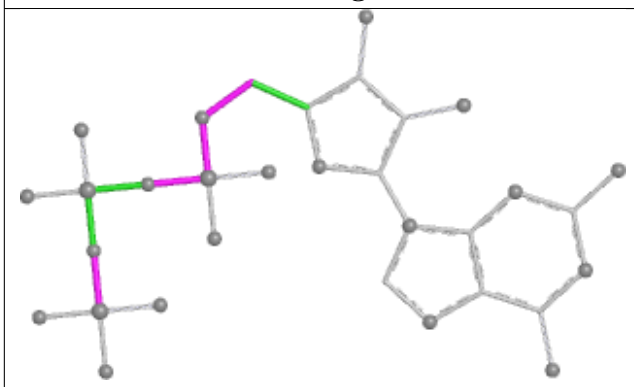
Ligand GTP KE 501



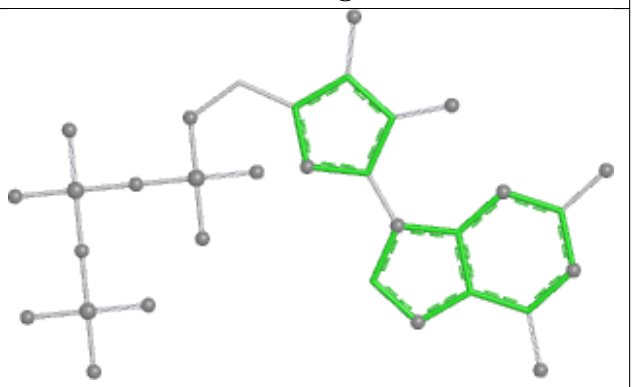
Bond lengths



Bond angles

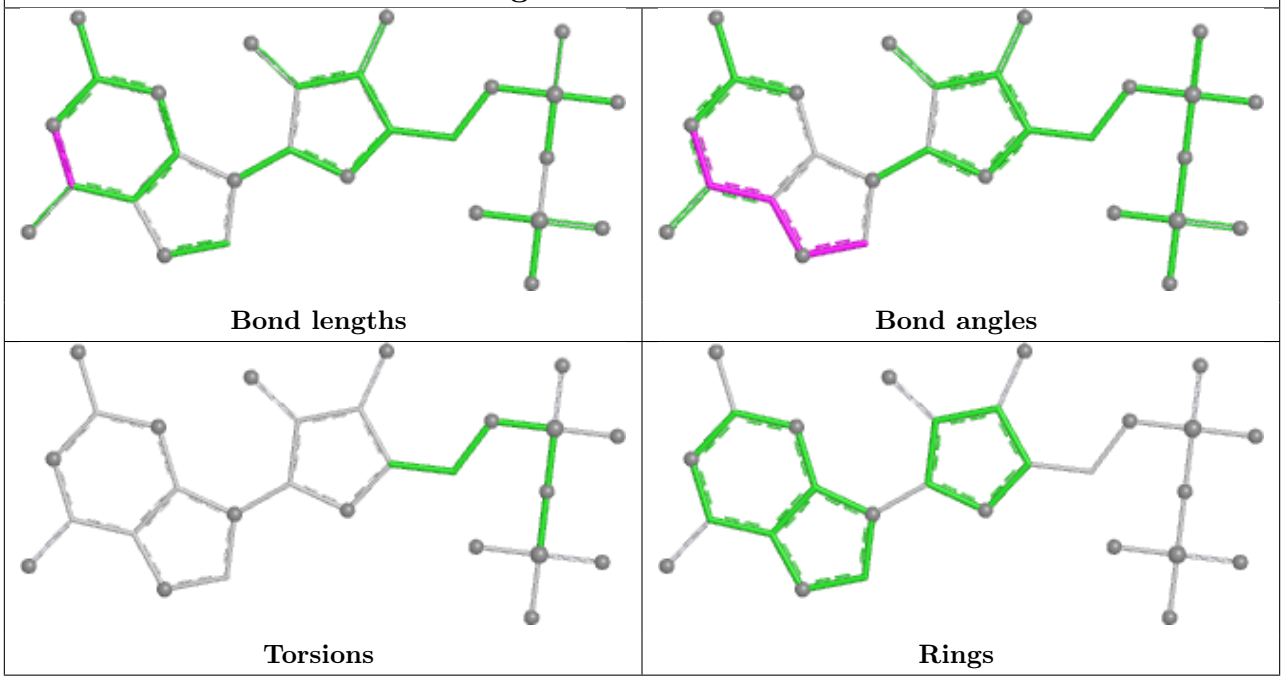


Torsions

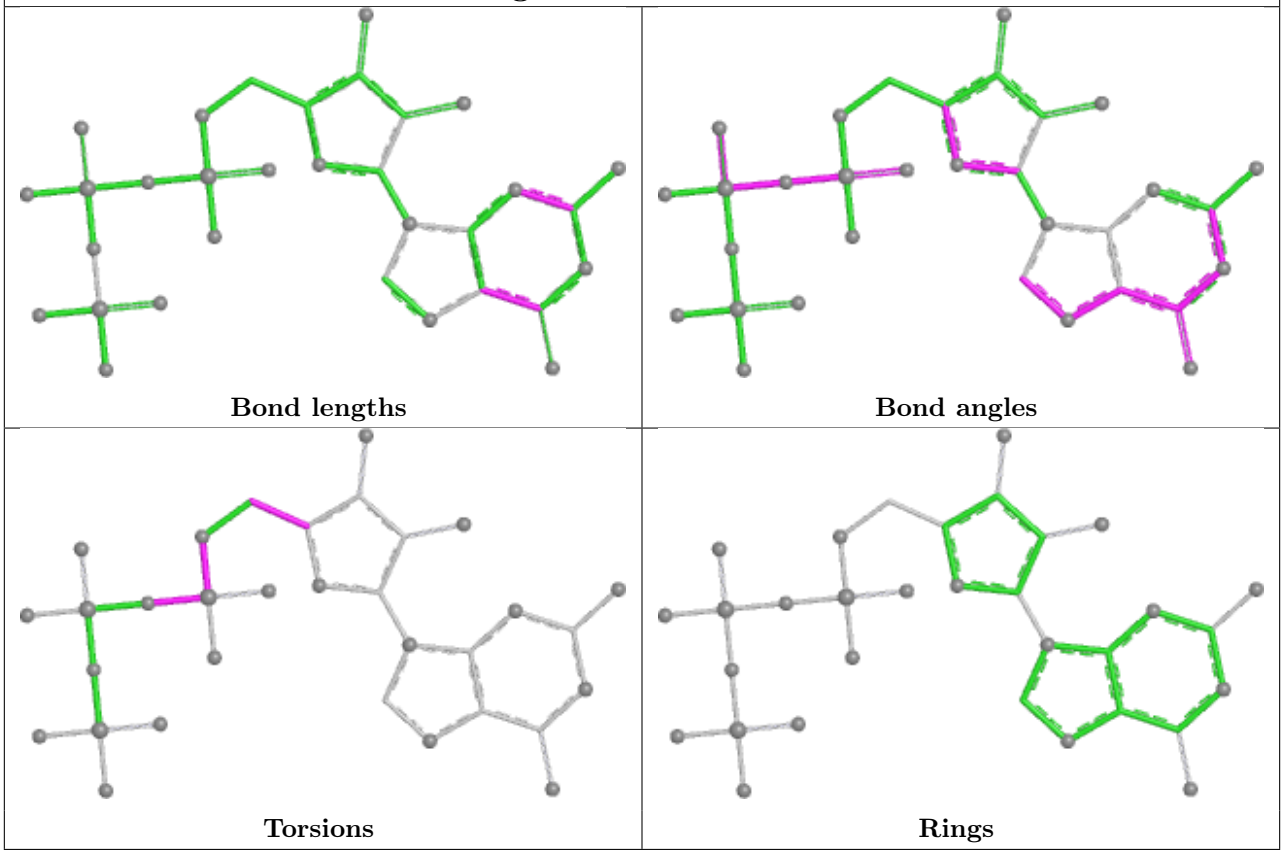


Rings

Ligand GDP RF 501



Ligand GTP RE 501



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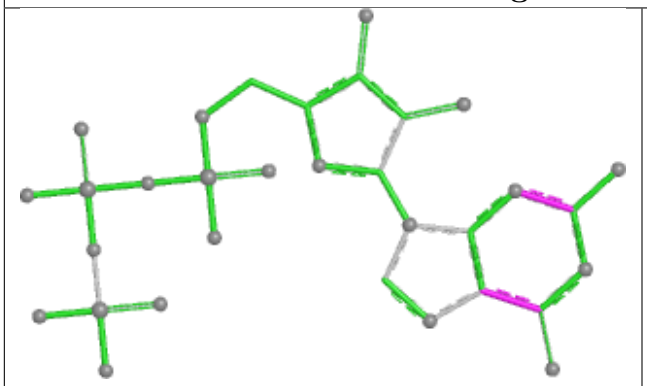

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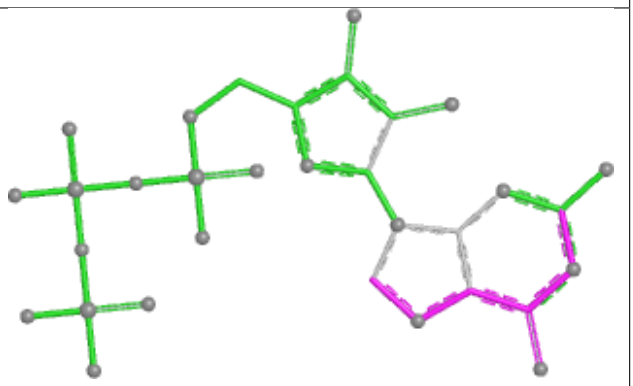

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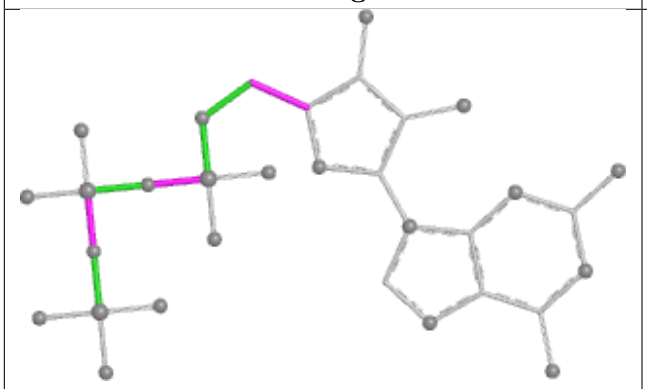

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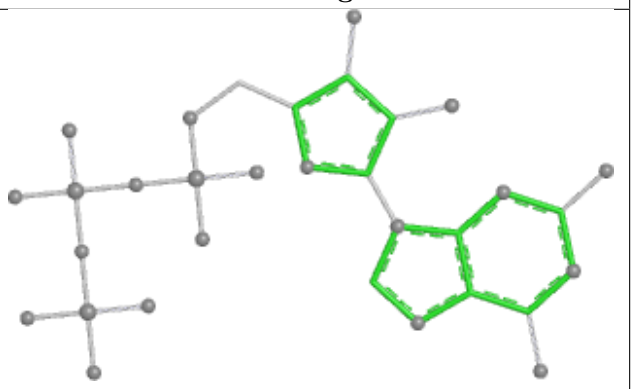
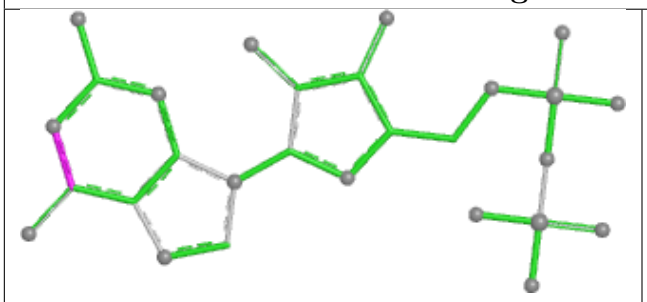


Rings

Ligand GDP AF 501



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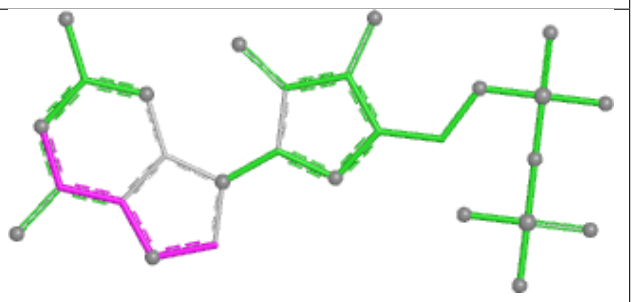

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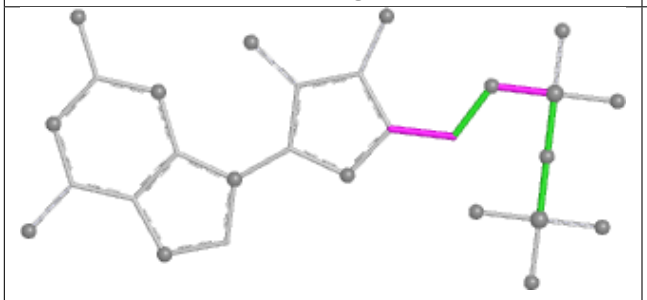

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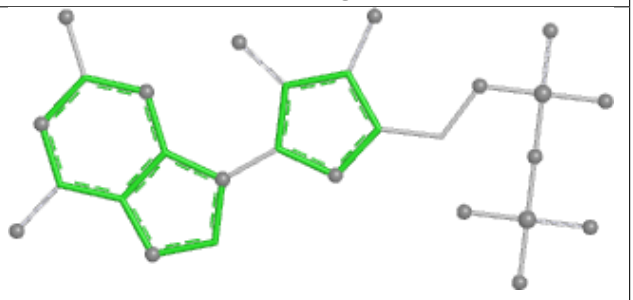
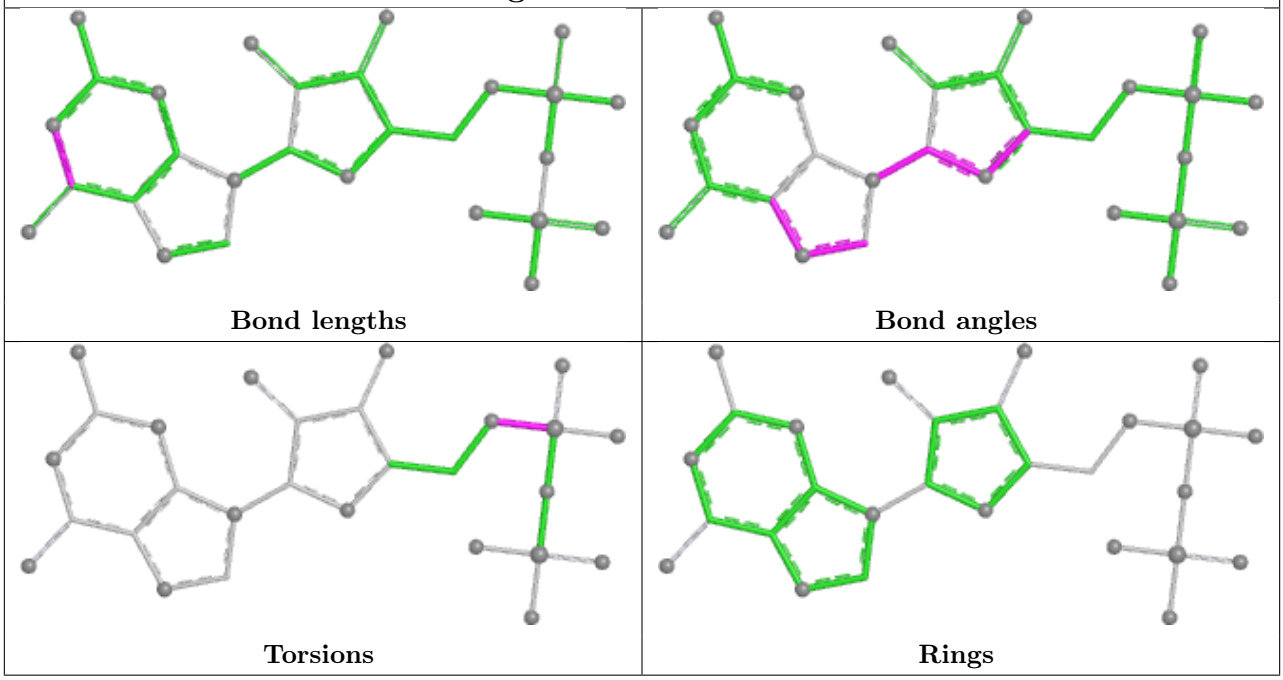
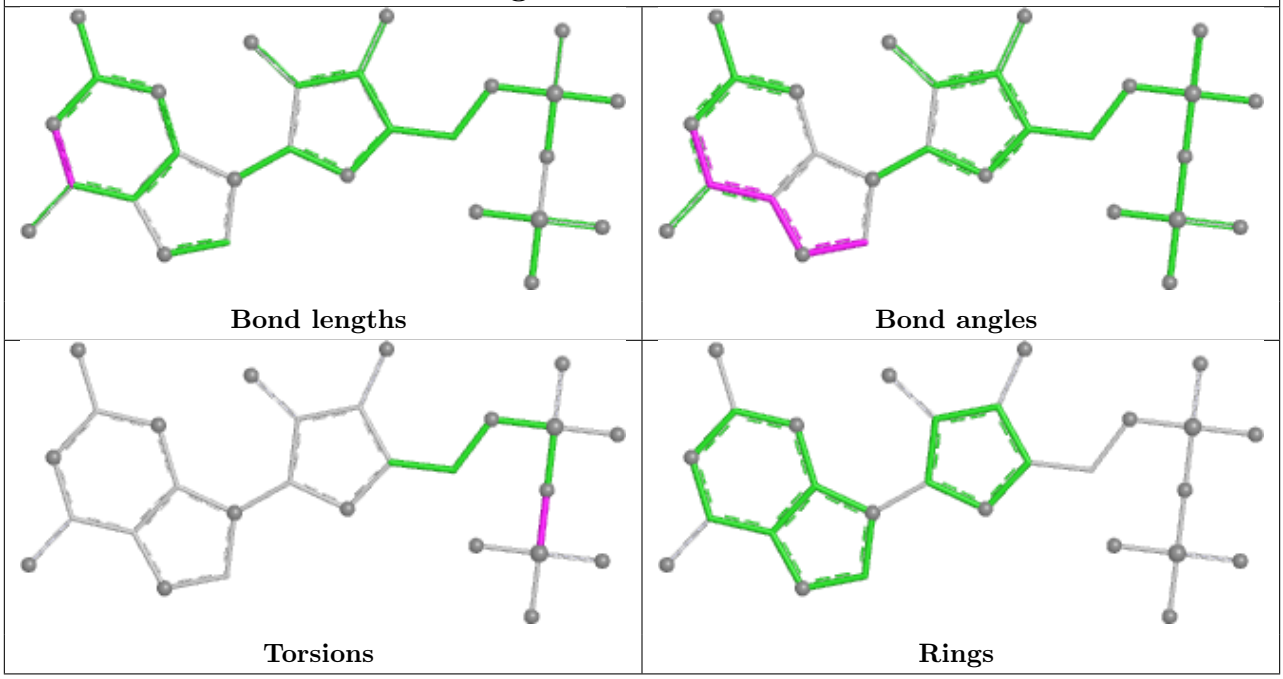


Rings

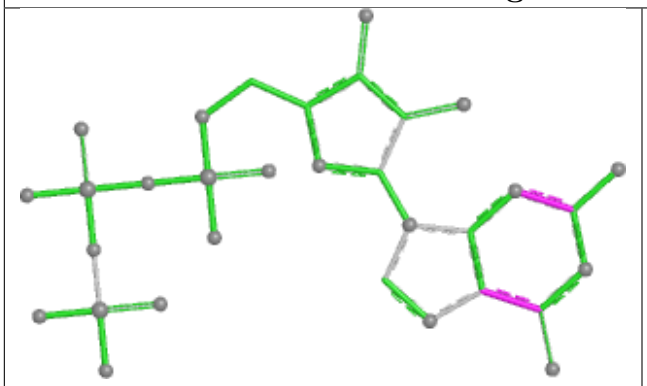
Ligand GDP DH 501



Ligand GDP KF 501



Ligand GTP WE 501



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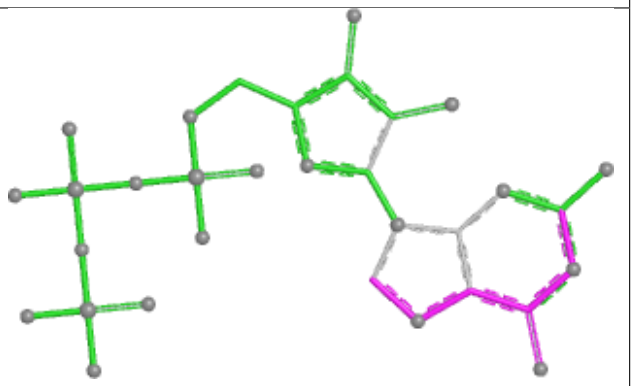
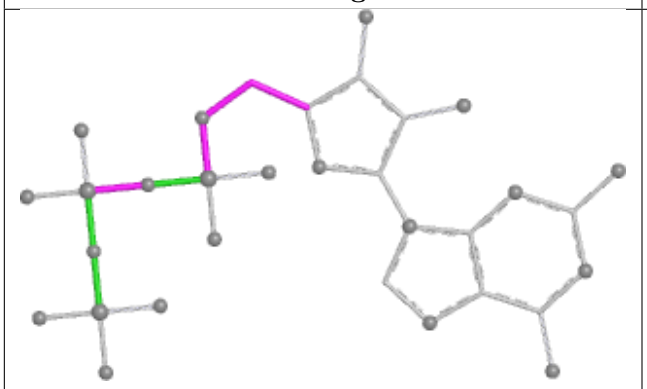


Bond angles



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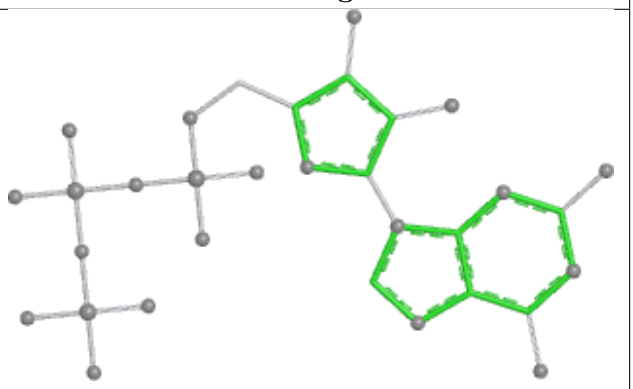
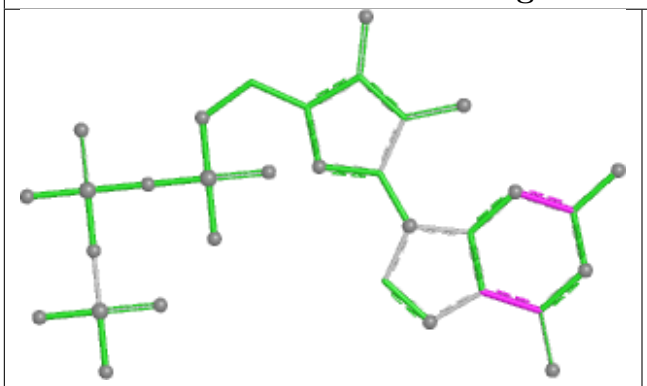


Rings

Ligand GTP QI 501



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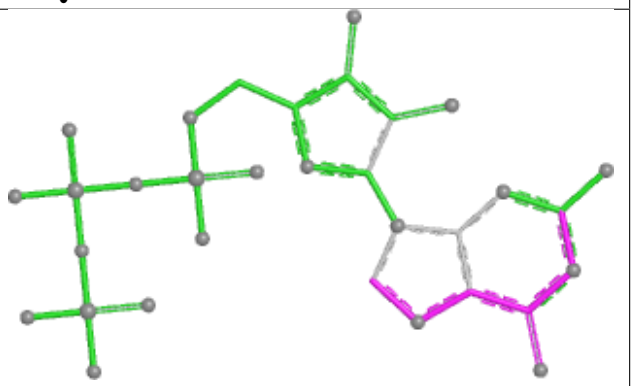

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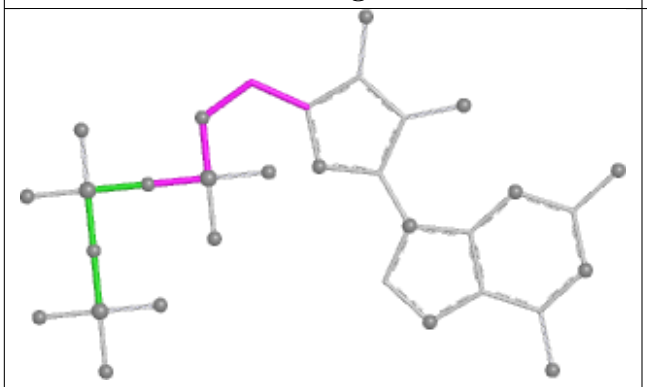

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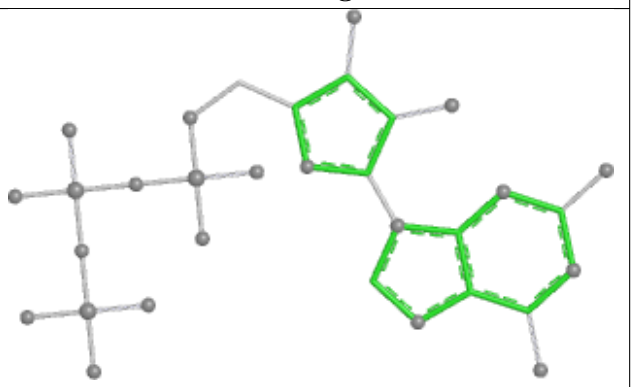
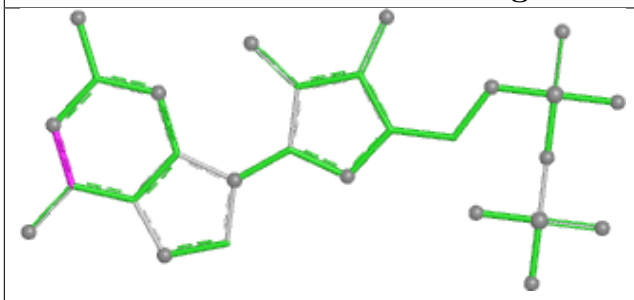


Rings

Ligand GDP VL 501



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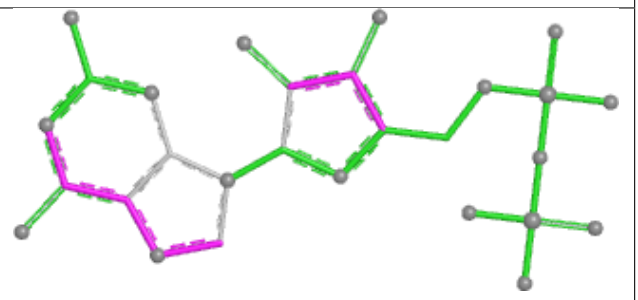

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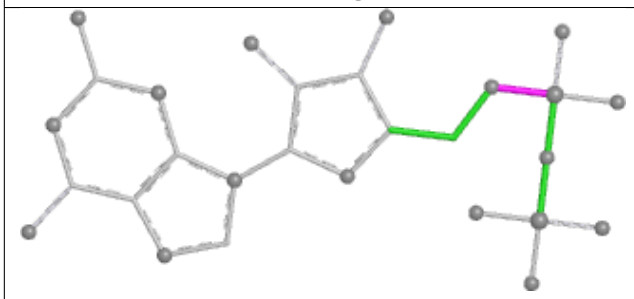

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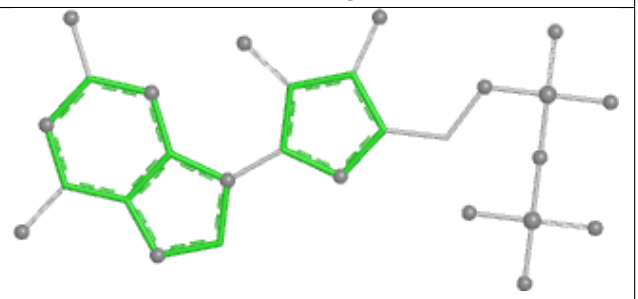
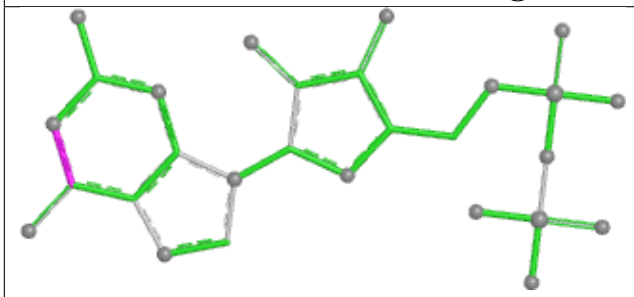


Rings

Ligand GDP MJ 501



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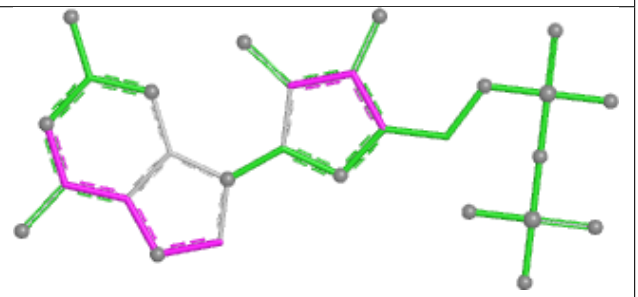

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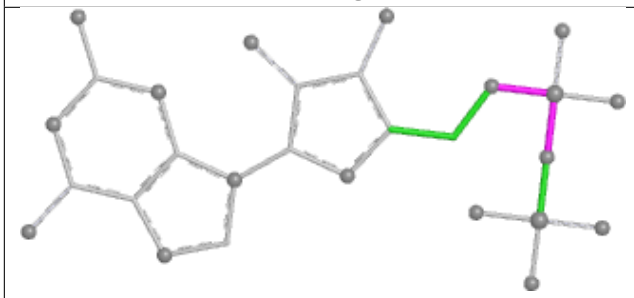

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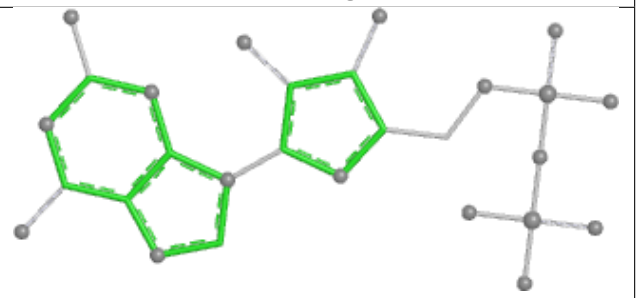
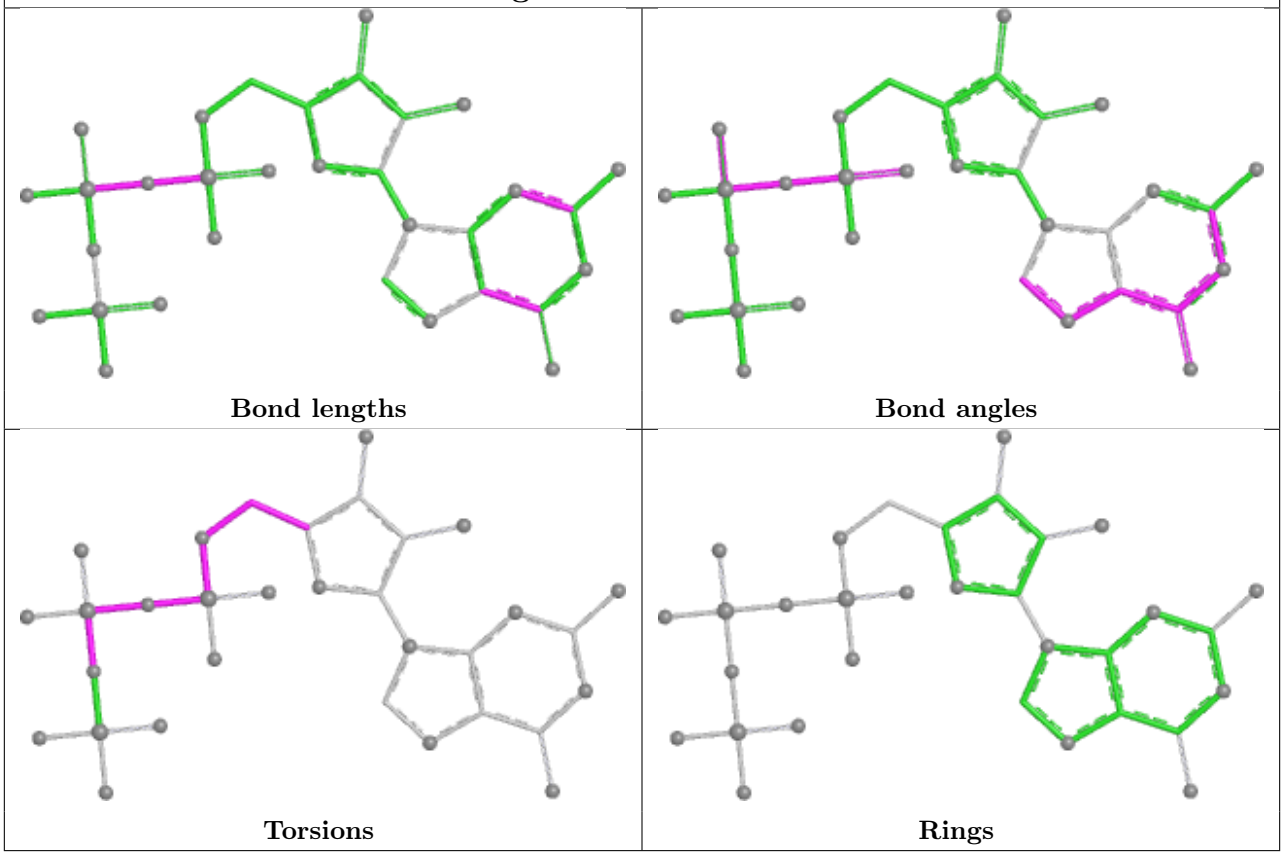
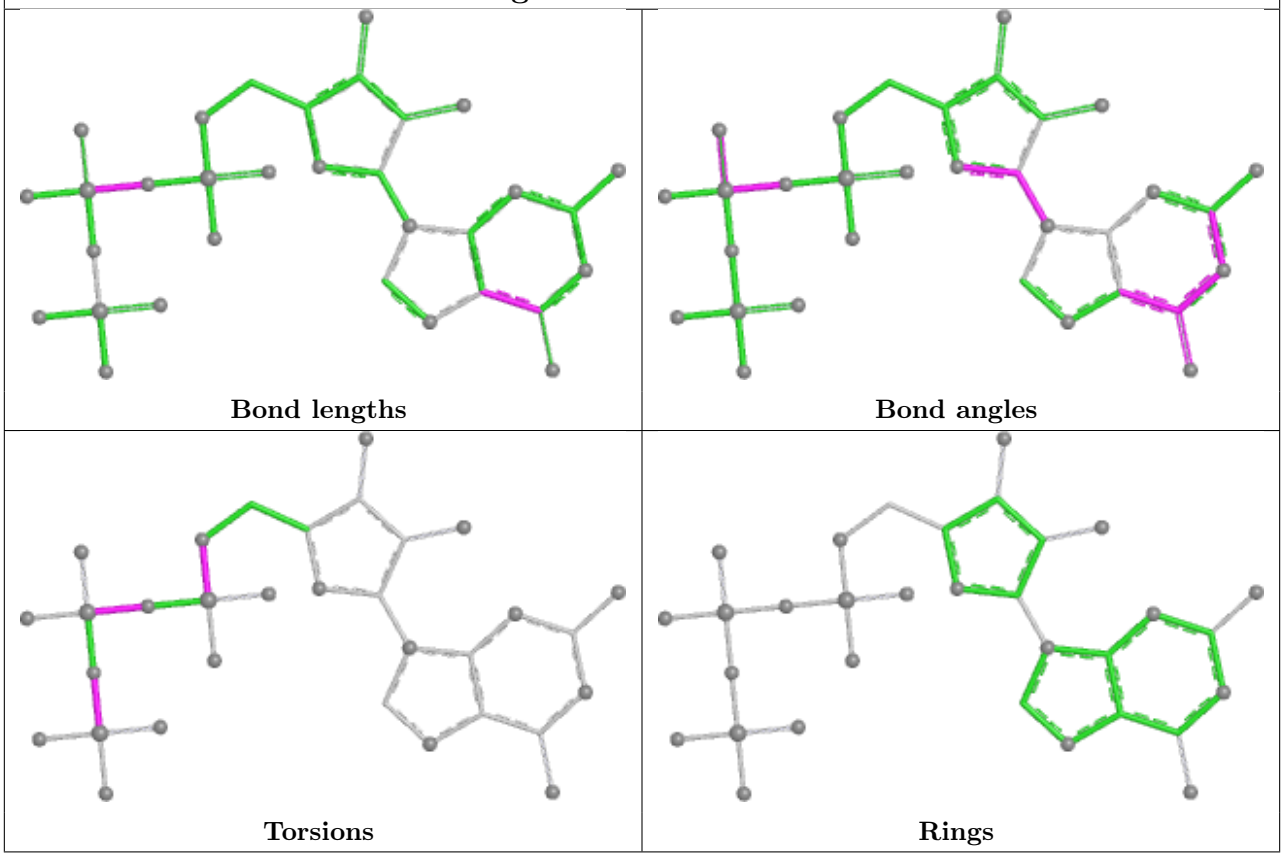


Rings

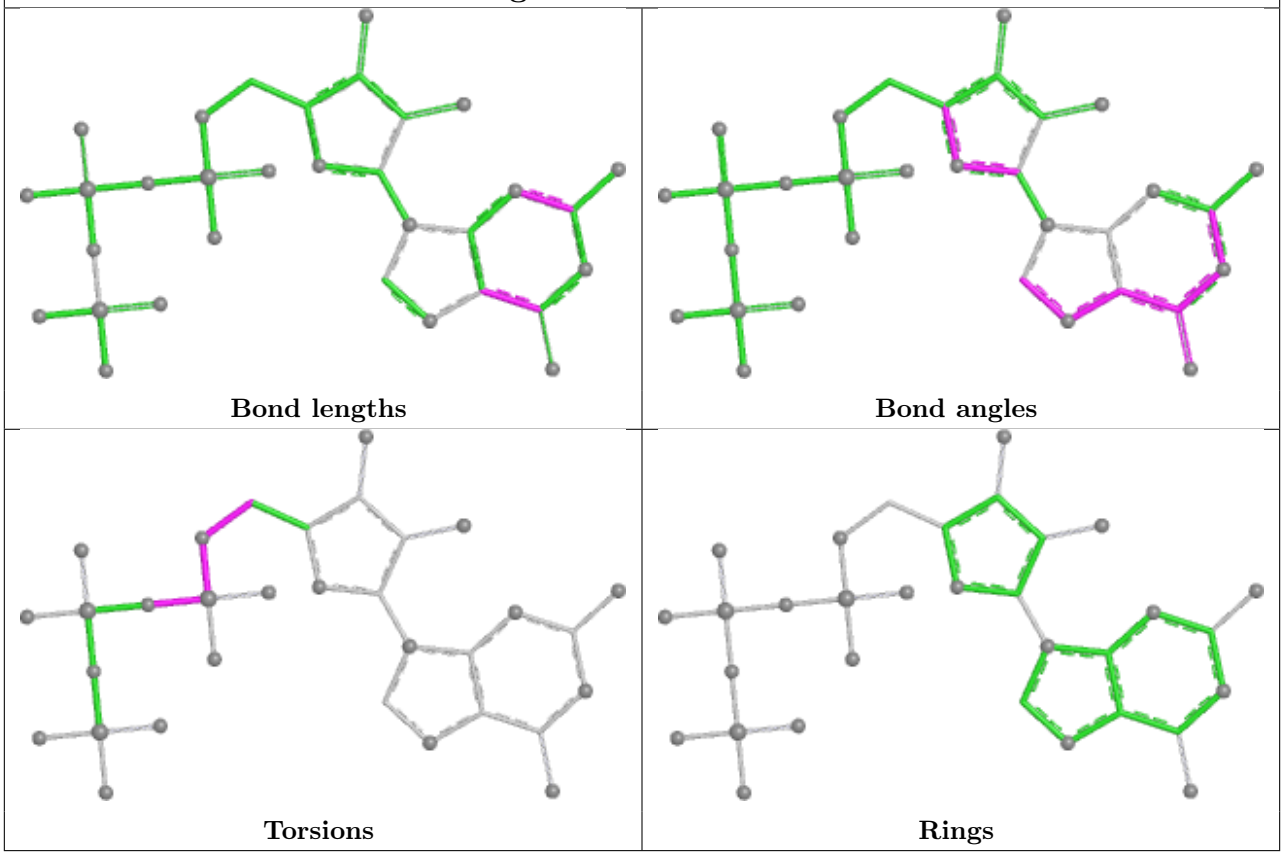
Ligand GTP LK 501



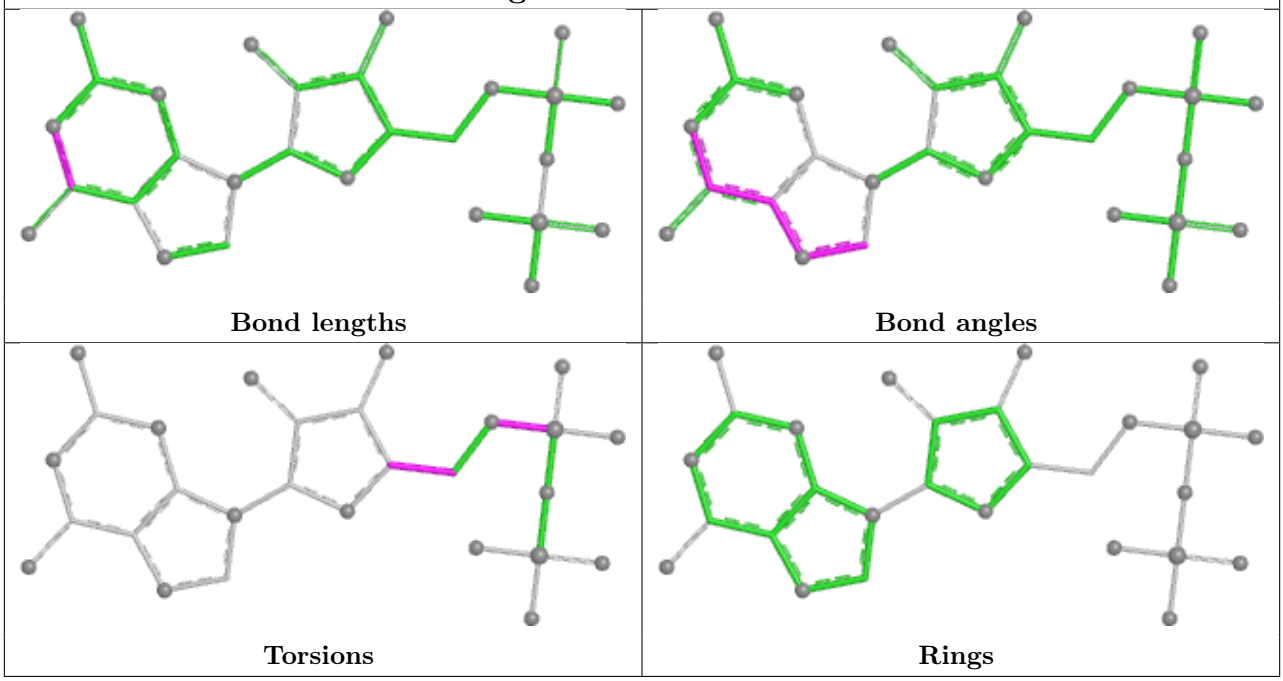
Ligand GTP GF 502



Ligand GTP HC 501



Ligand GDP NB 501



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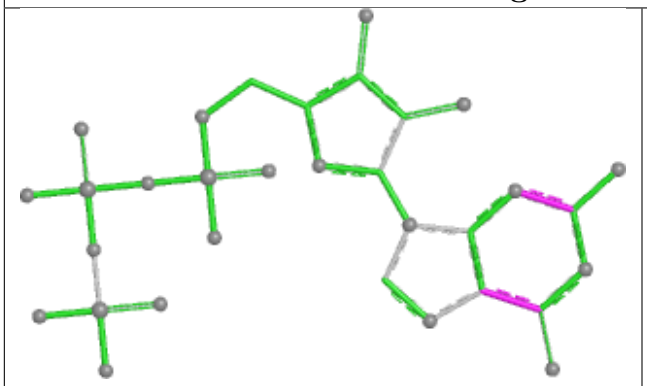
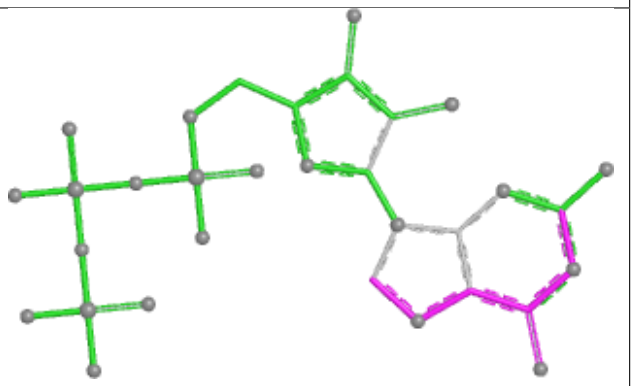
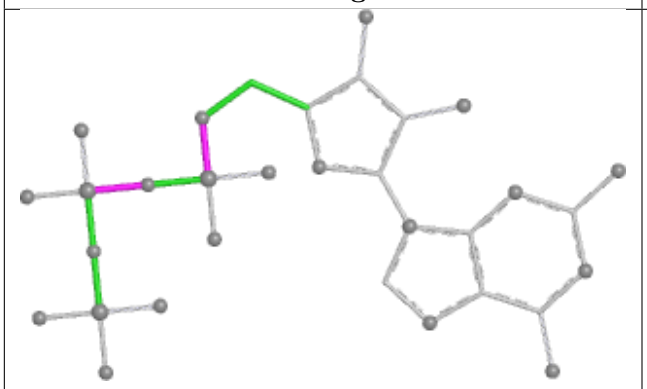


Bond lengths



Bond angles



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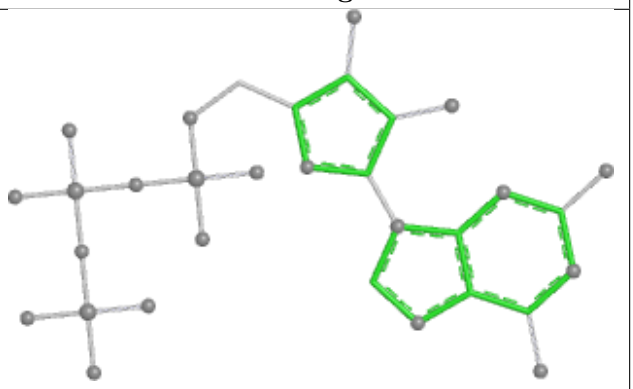
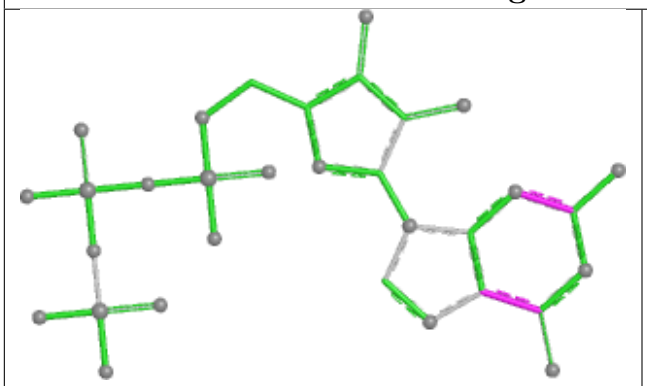


Rings

Ligand GTP DG 501



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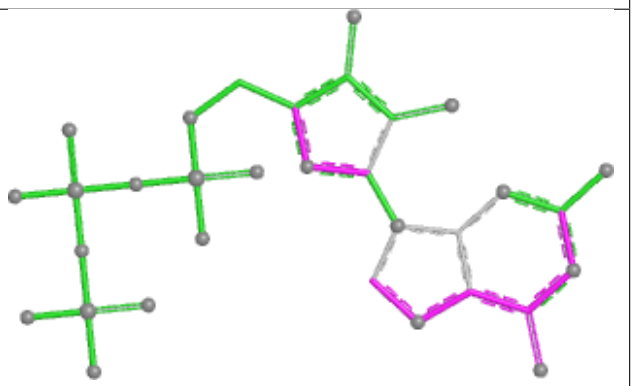
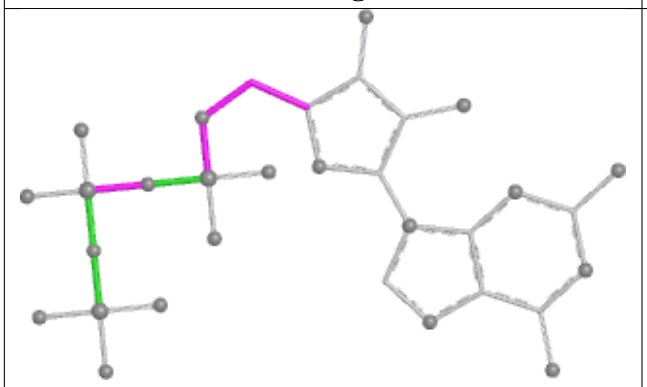


Bond angles



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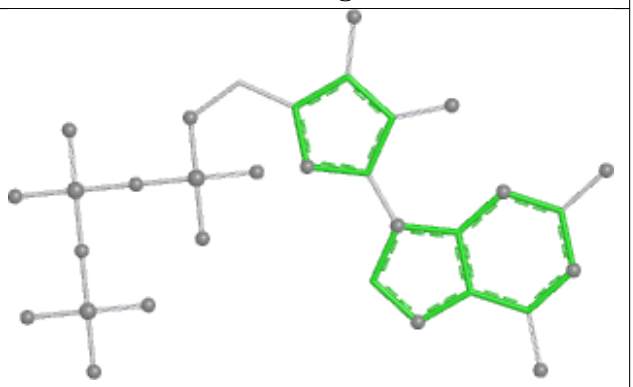

Rings

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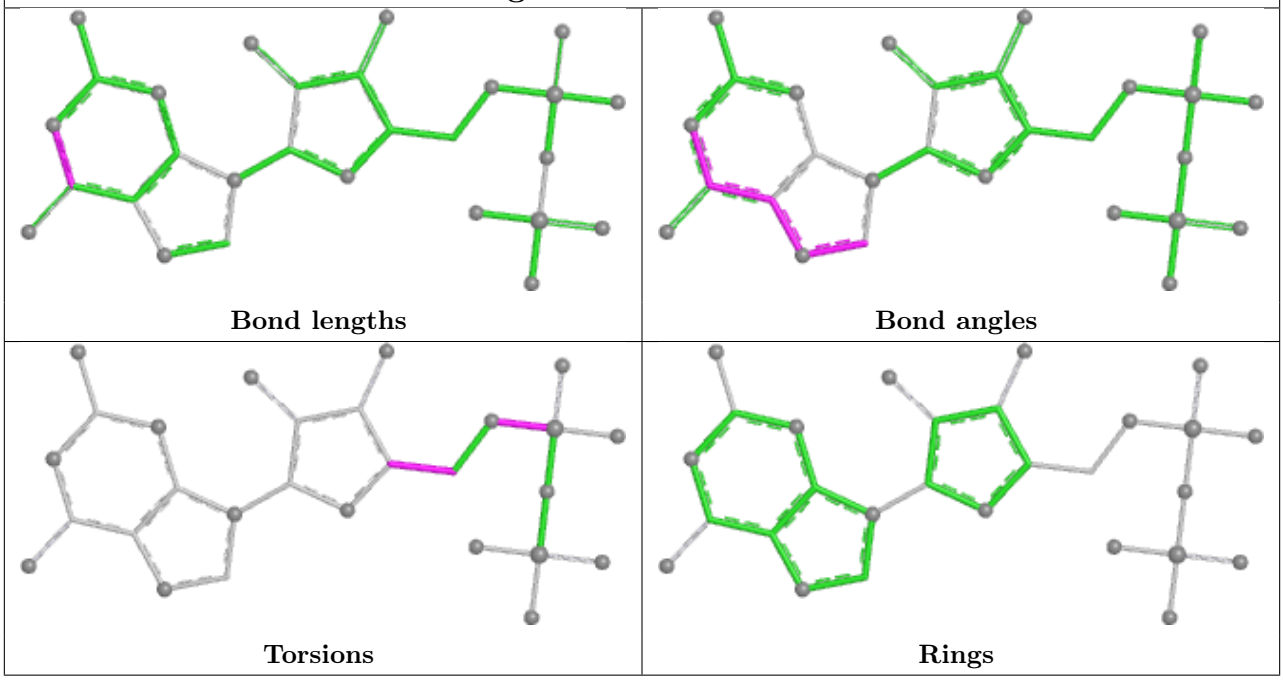

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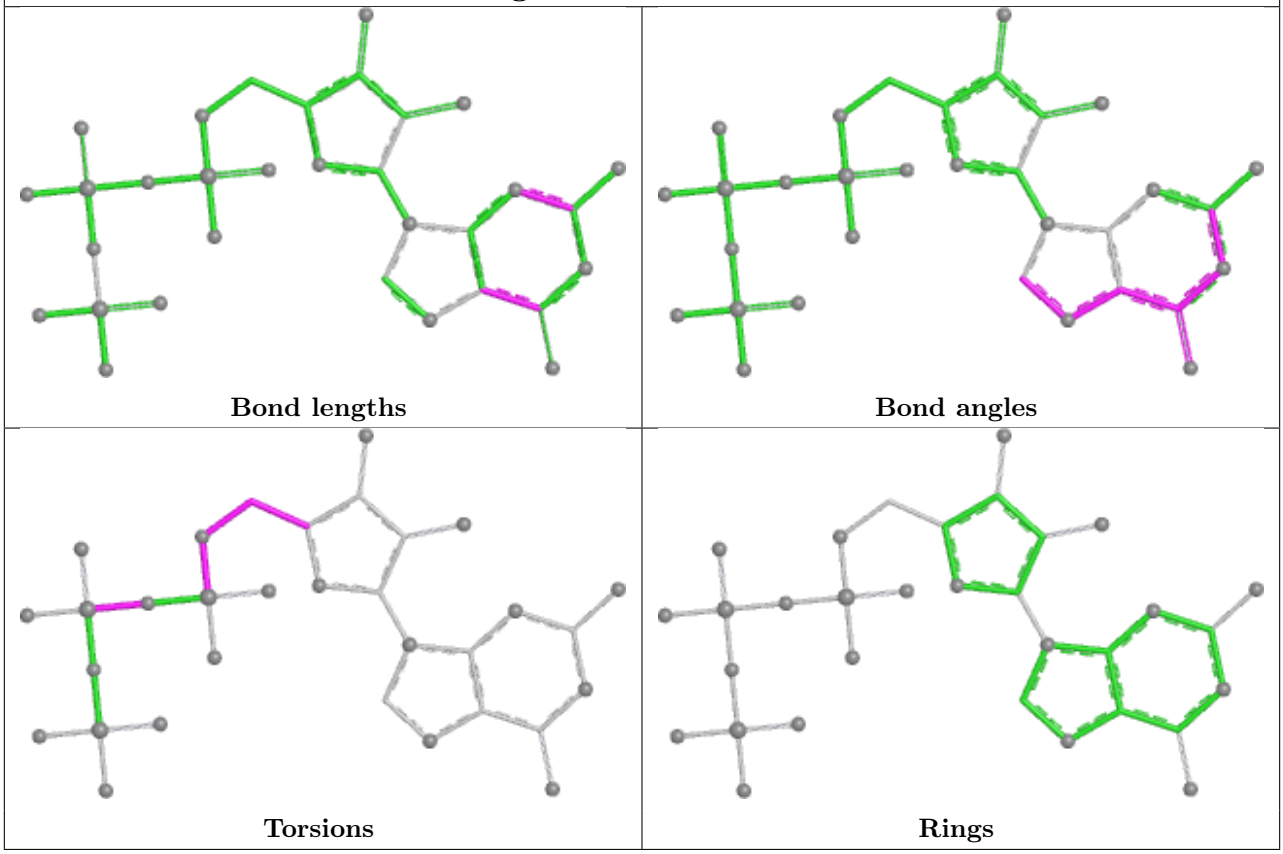

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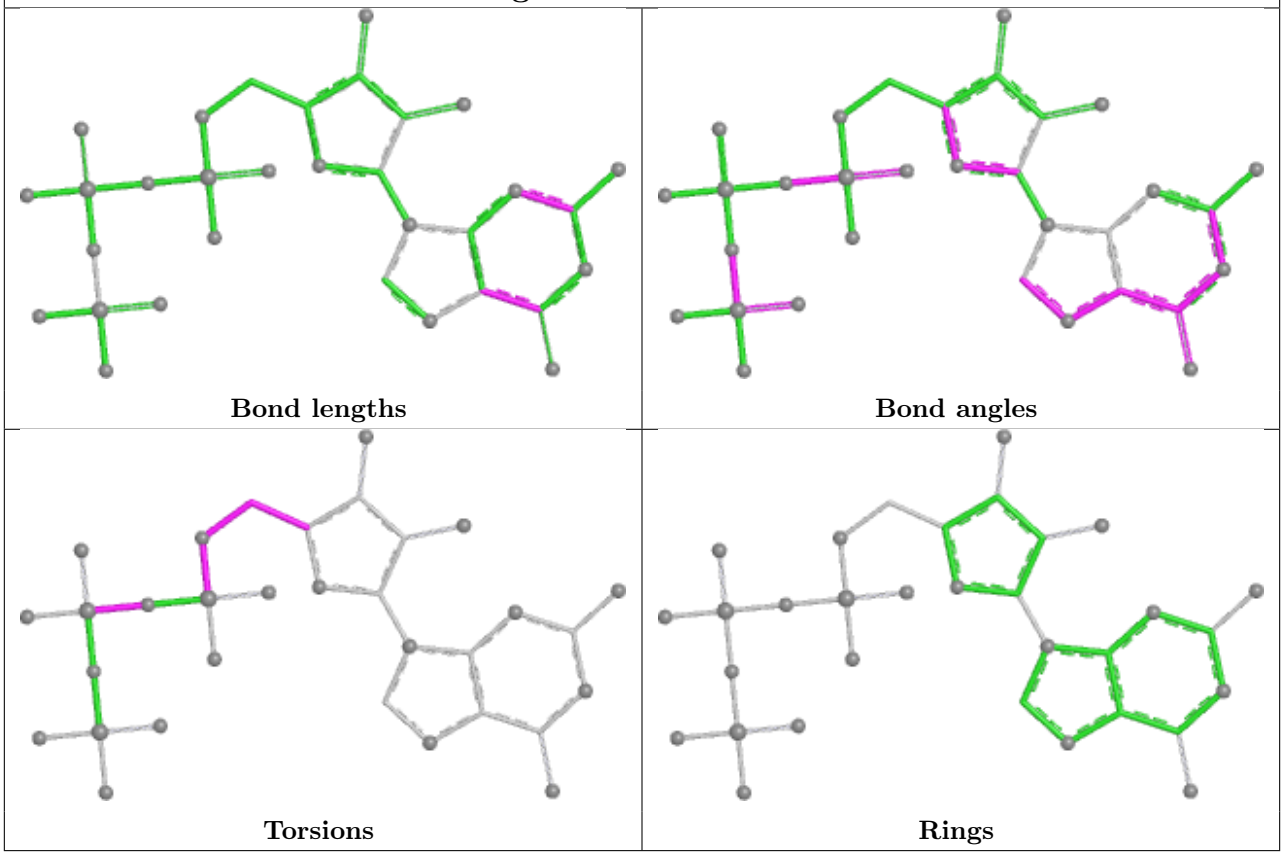

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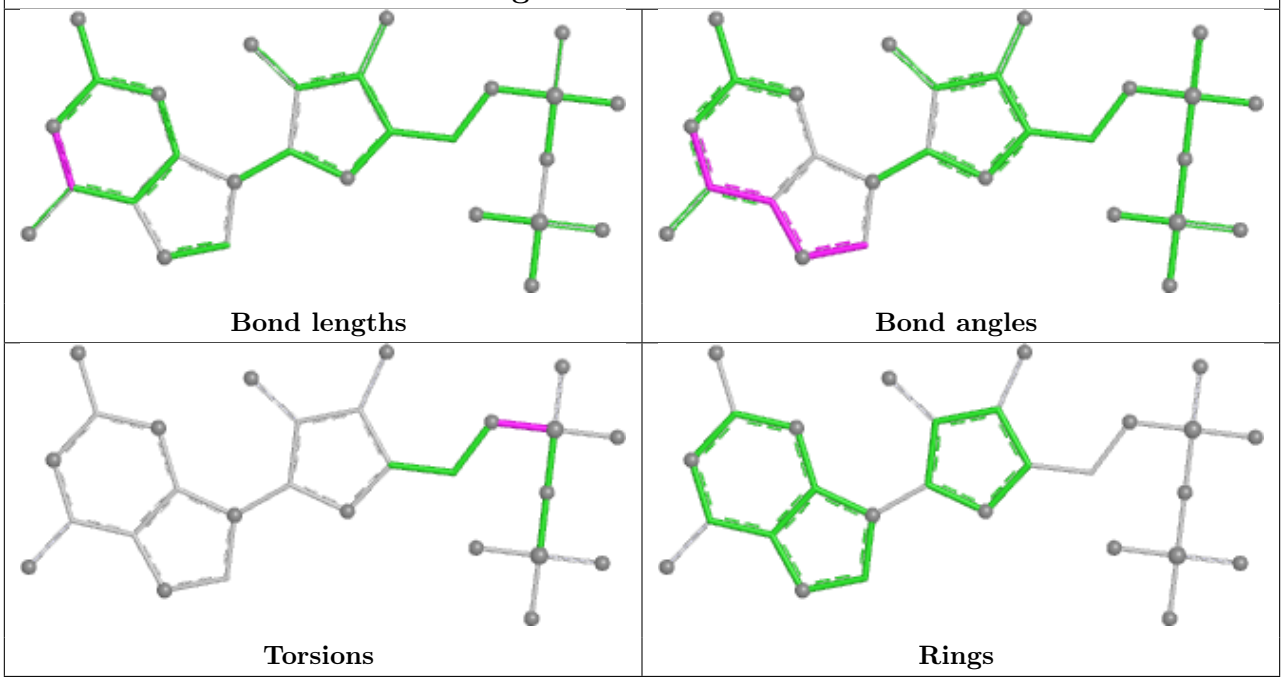

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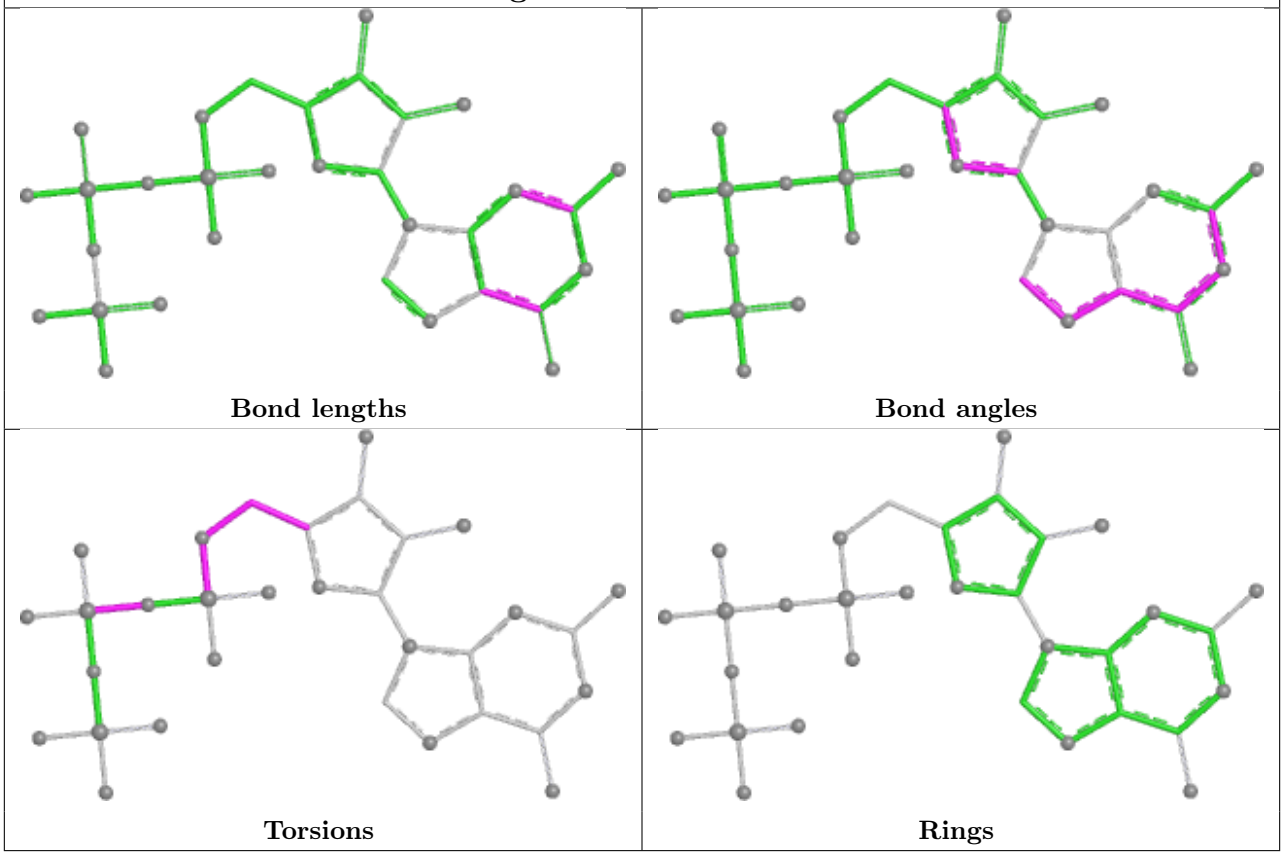

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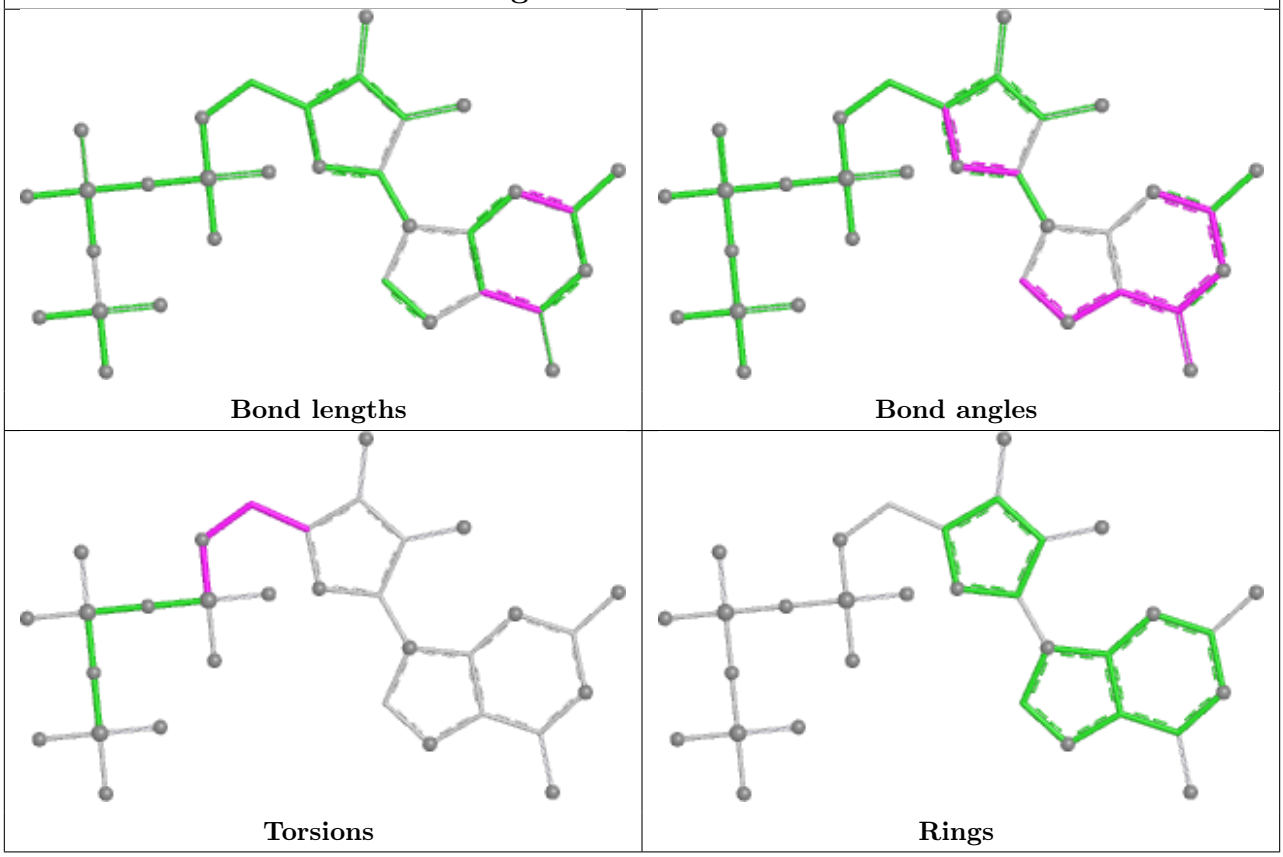

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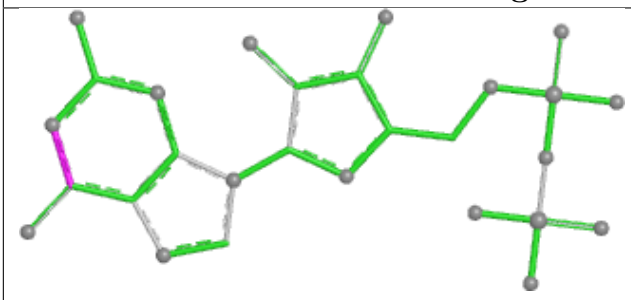
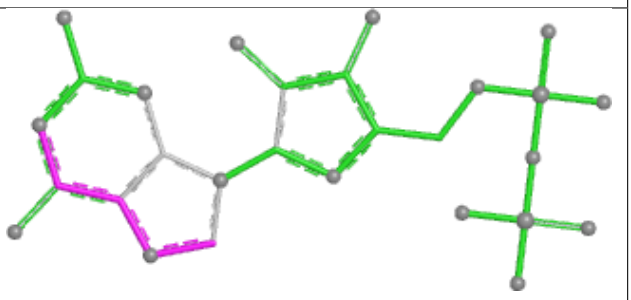
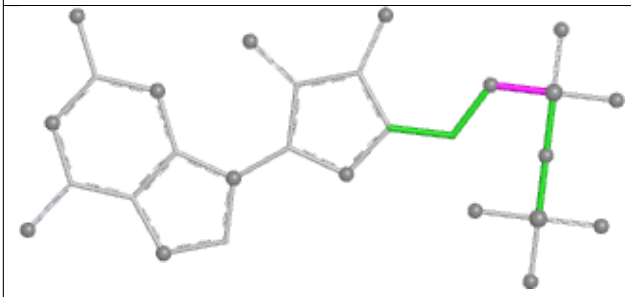
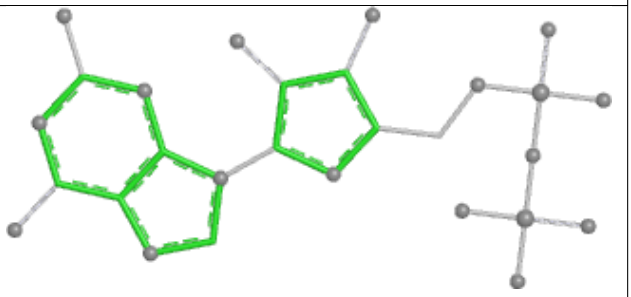
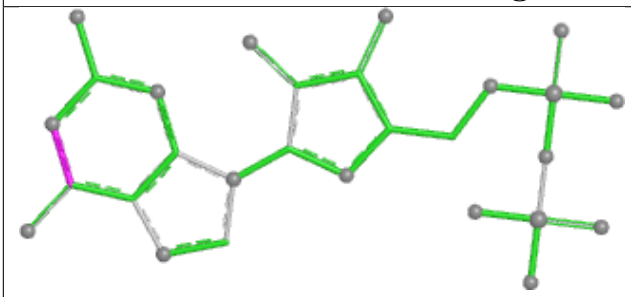
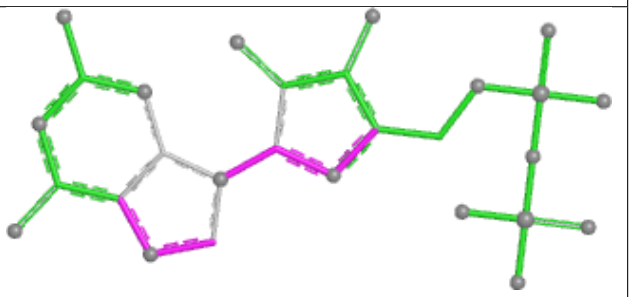
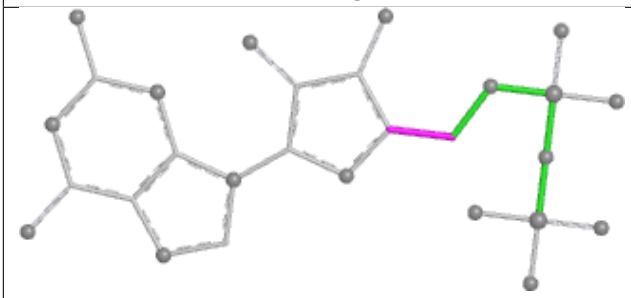
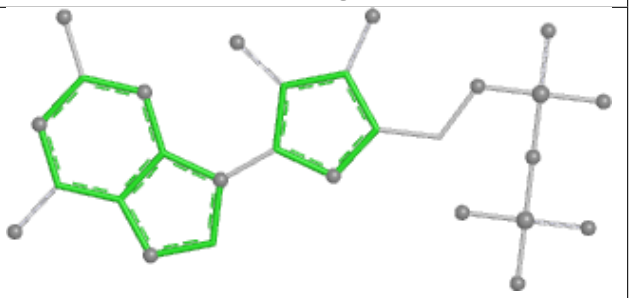
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP JH 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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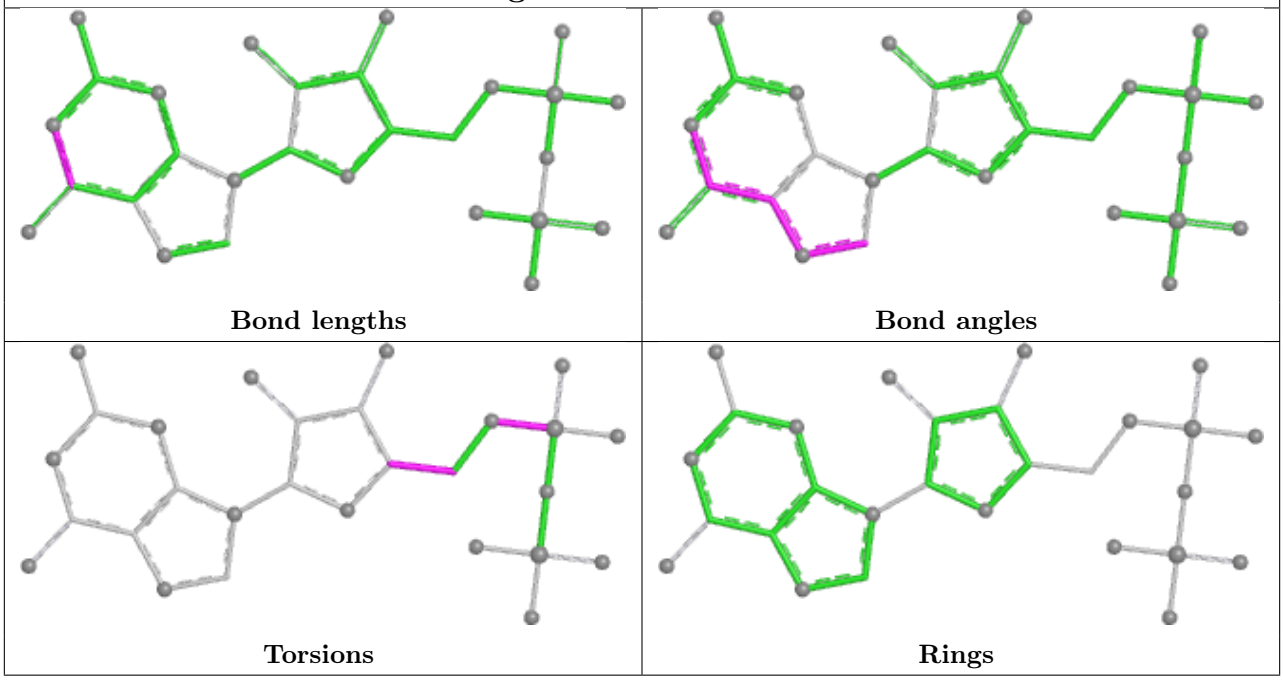

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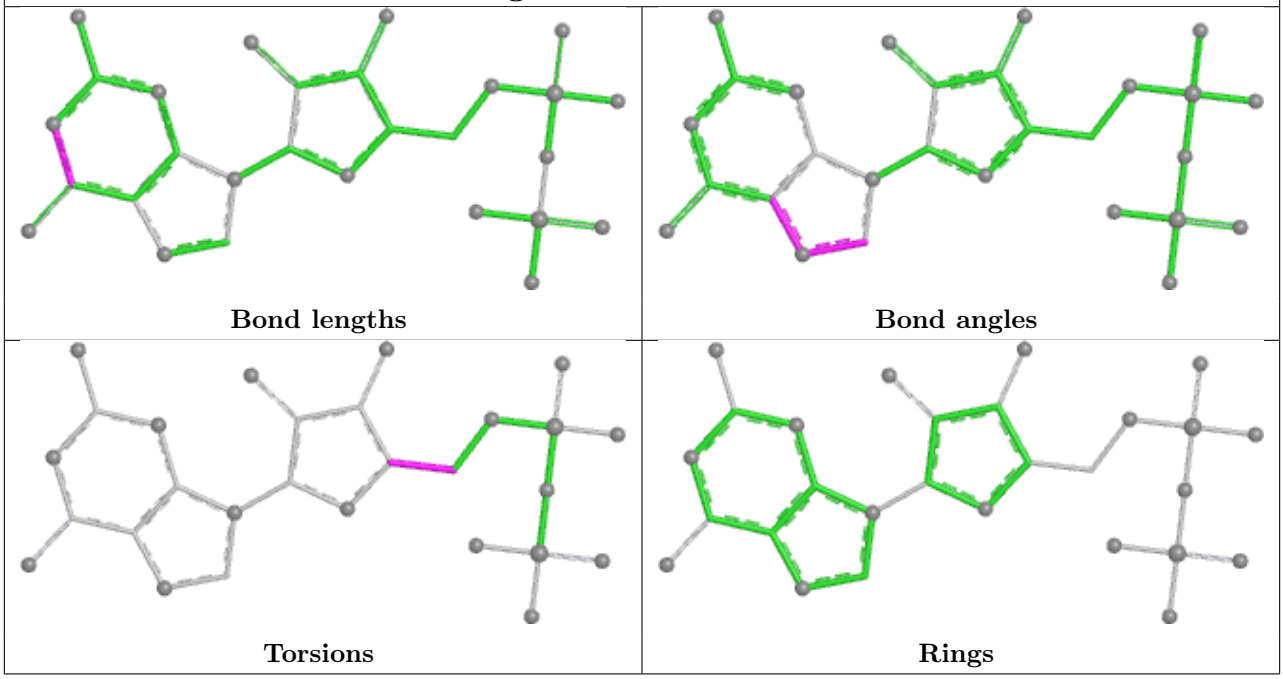

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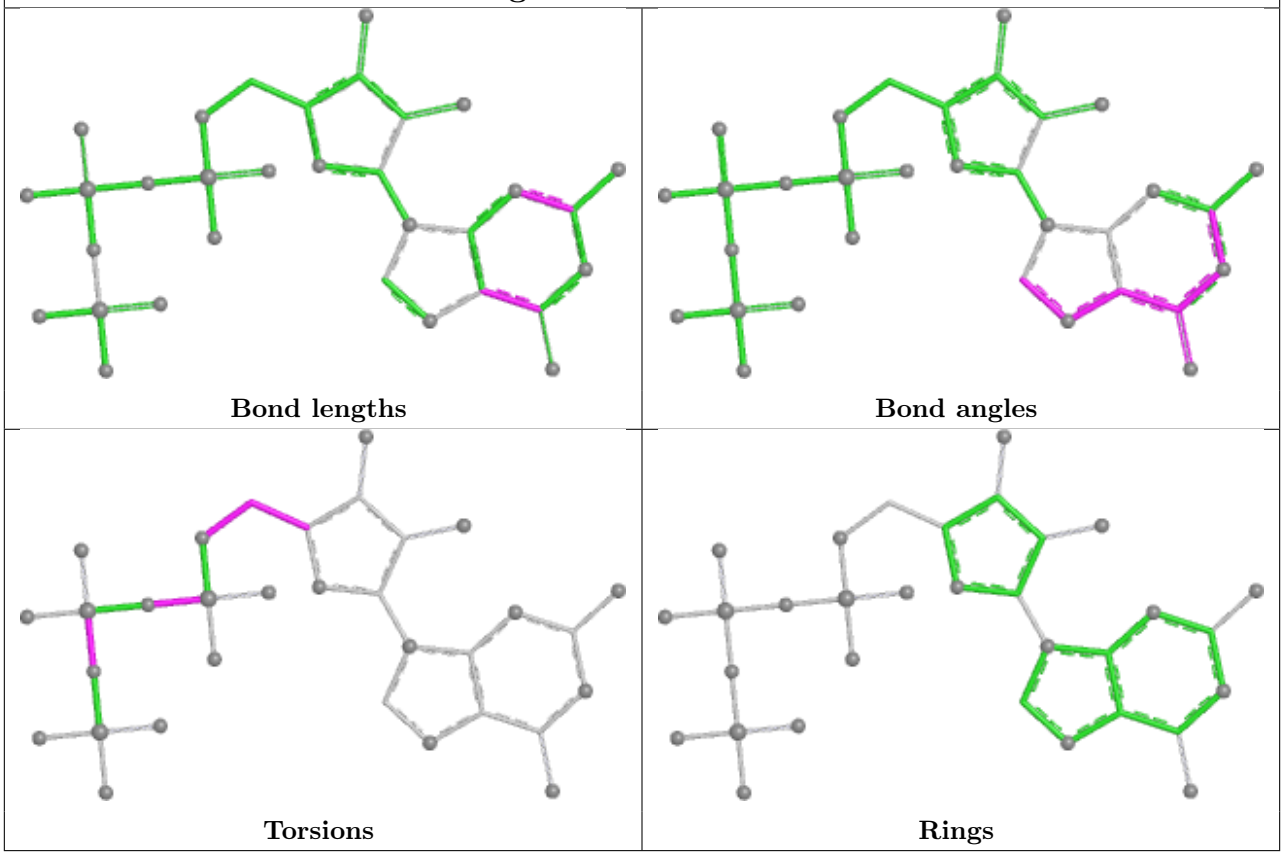

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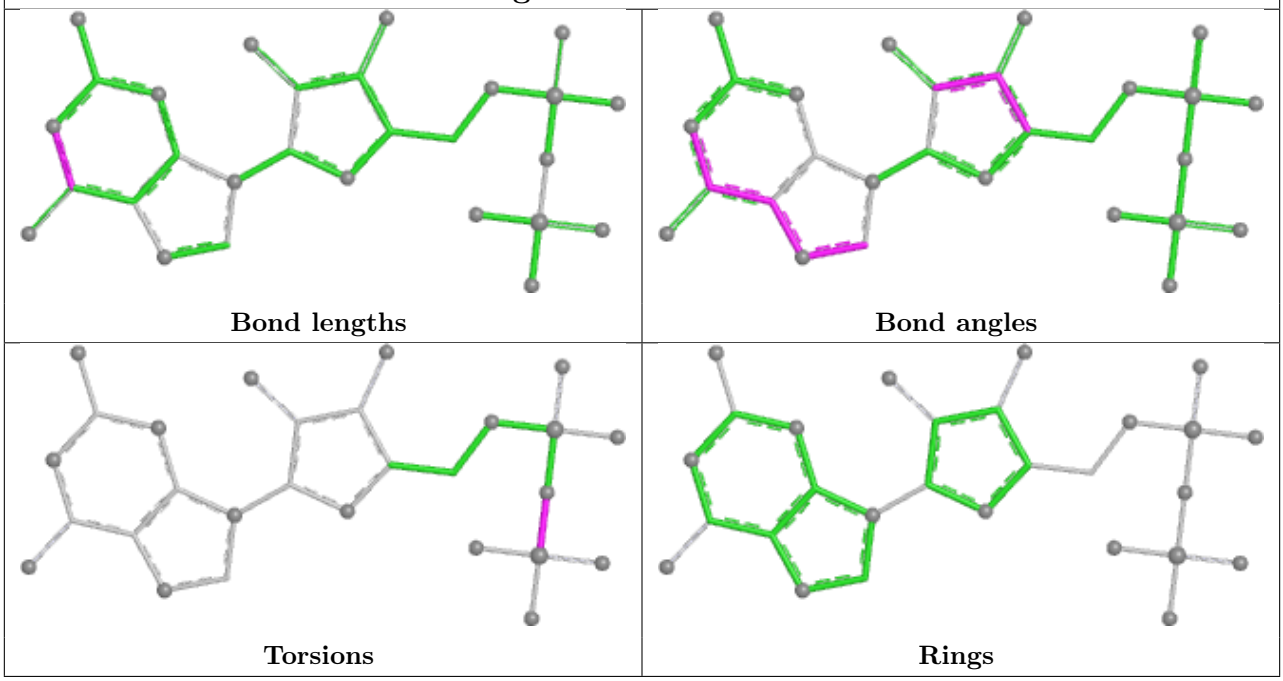

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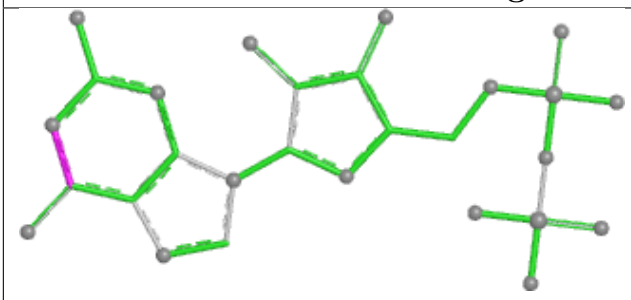

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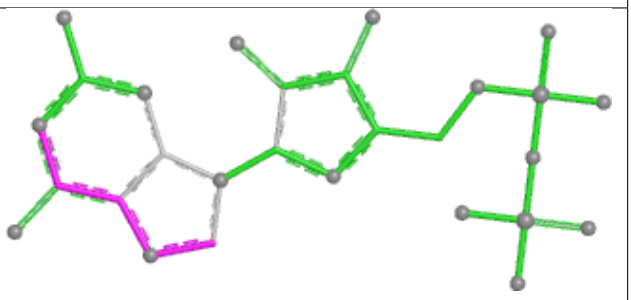
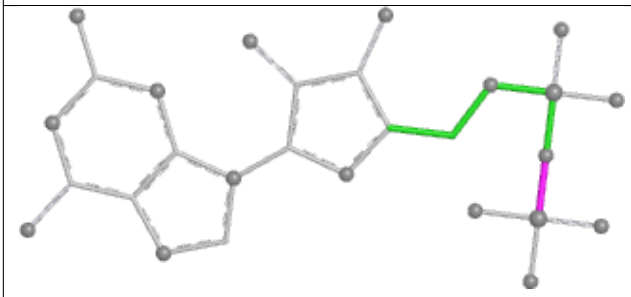


Bond angles



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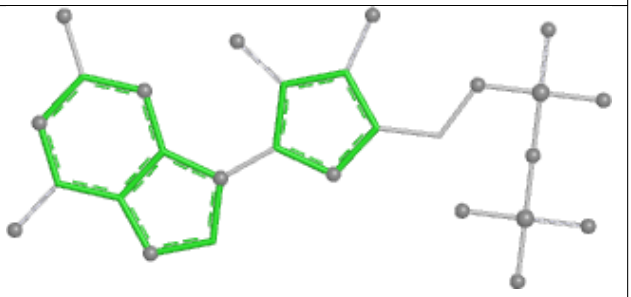
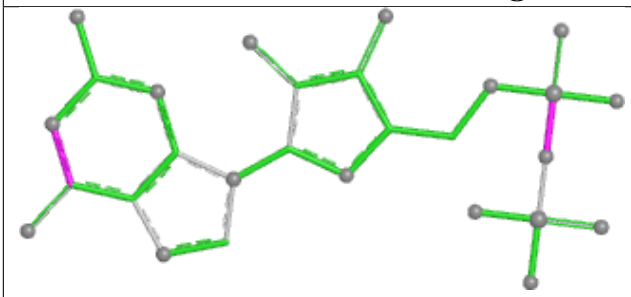


Rings

Ligand GDP TD 501



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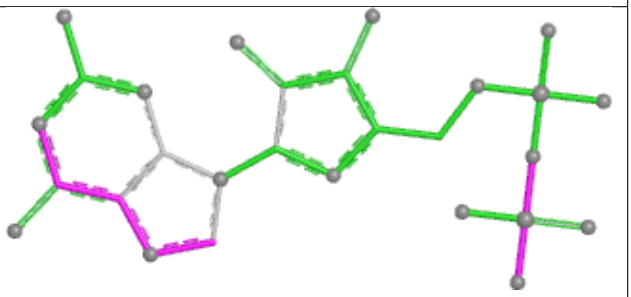

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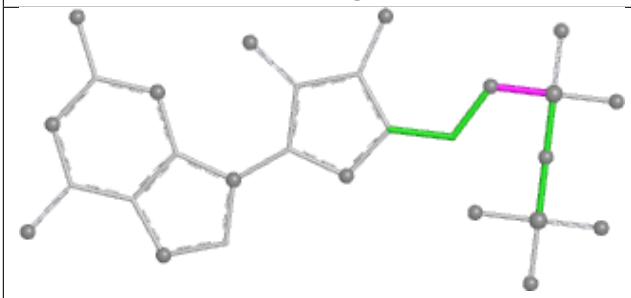

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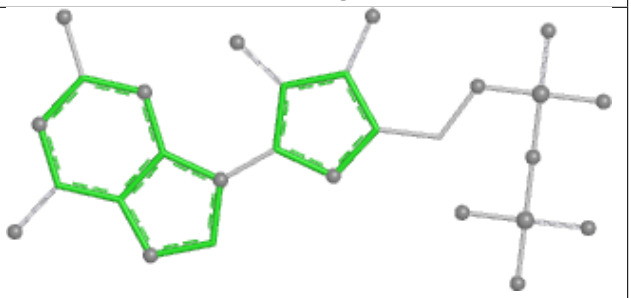

Rings

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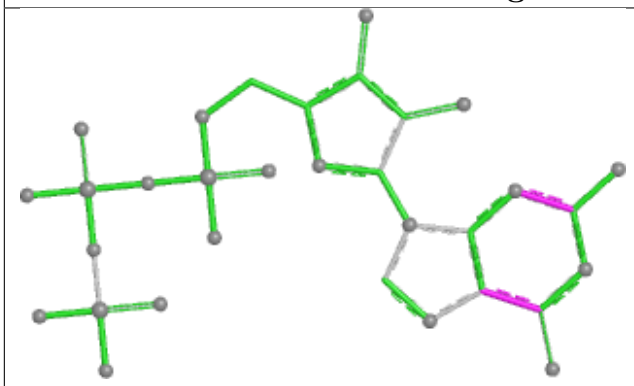

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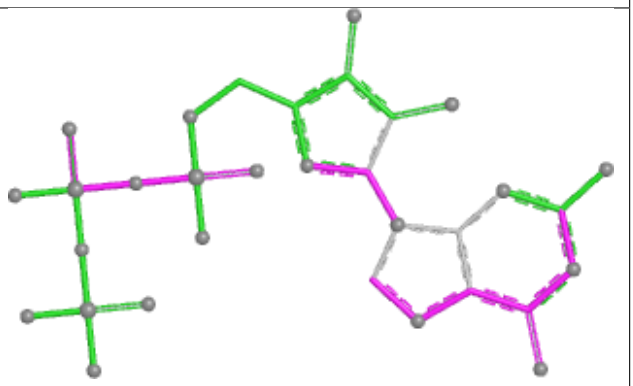

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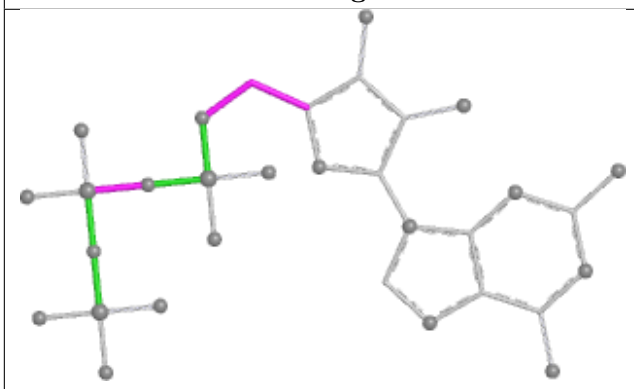

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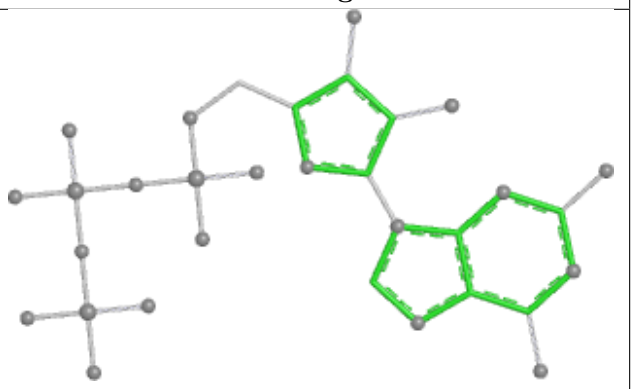

Rings

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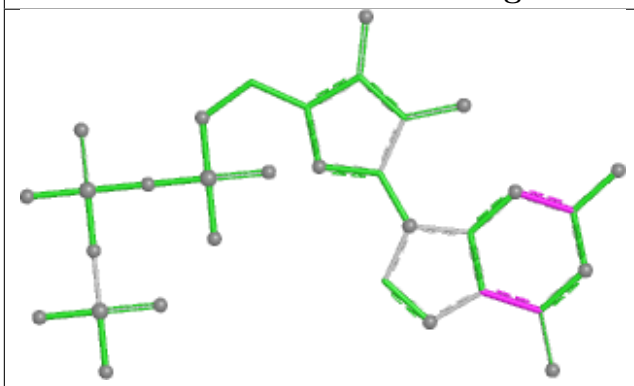

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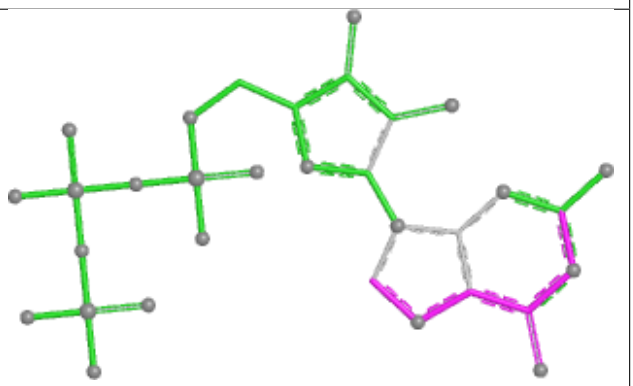

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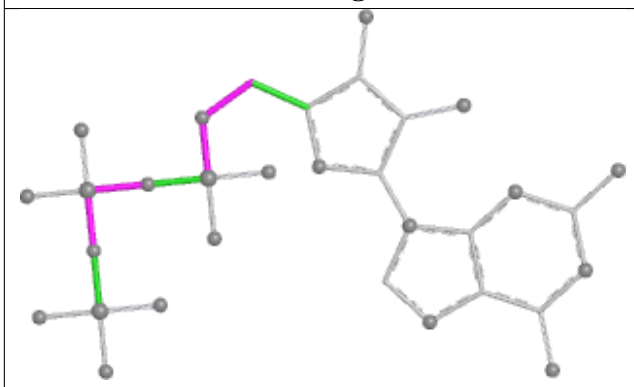

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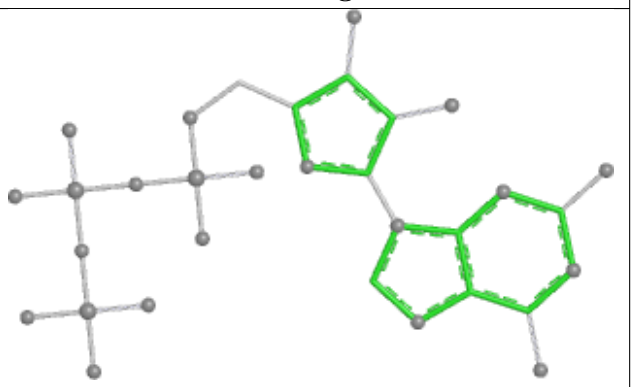

Rings

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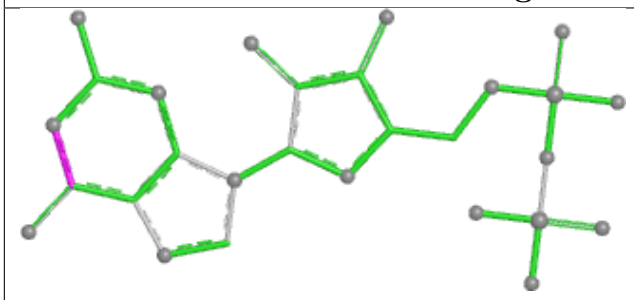

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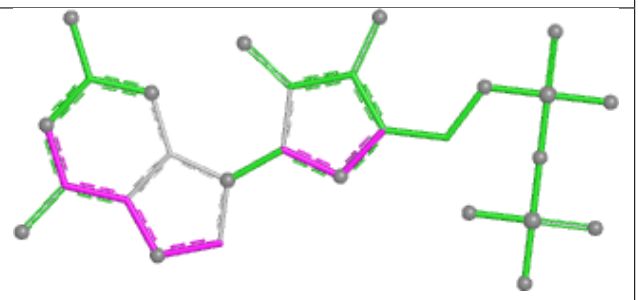

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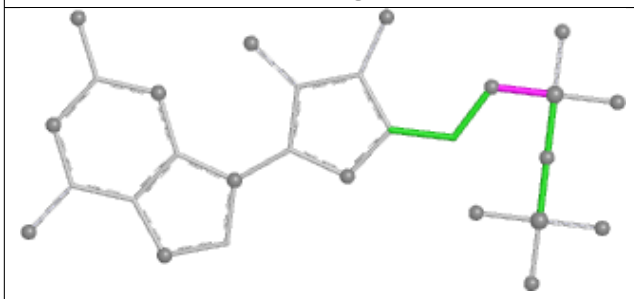

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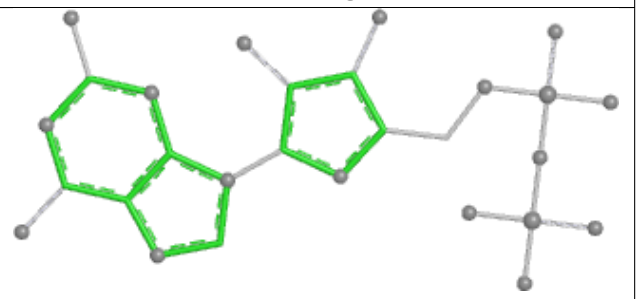

Rings

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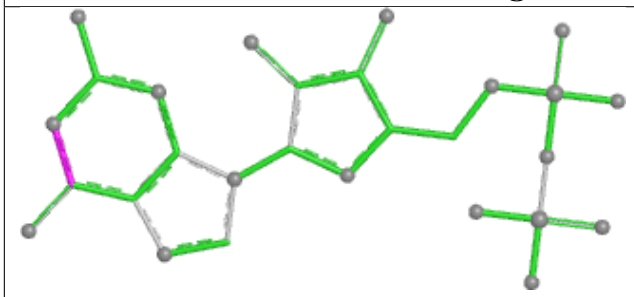

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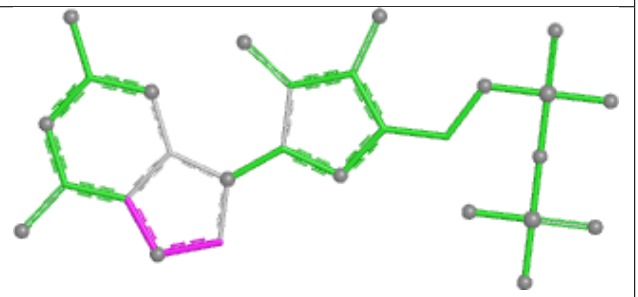

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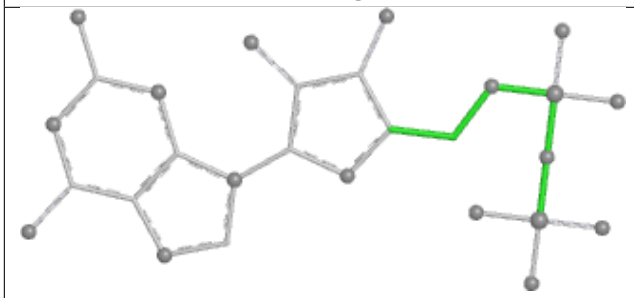

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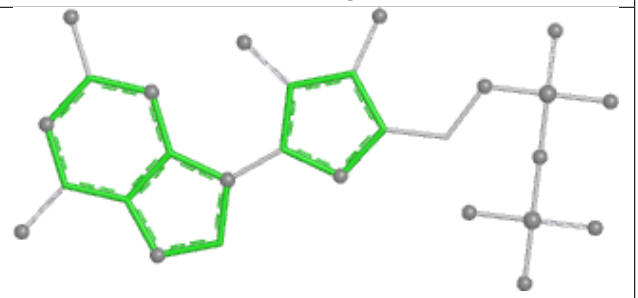

Rings

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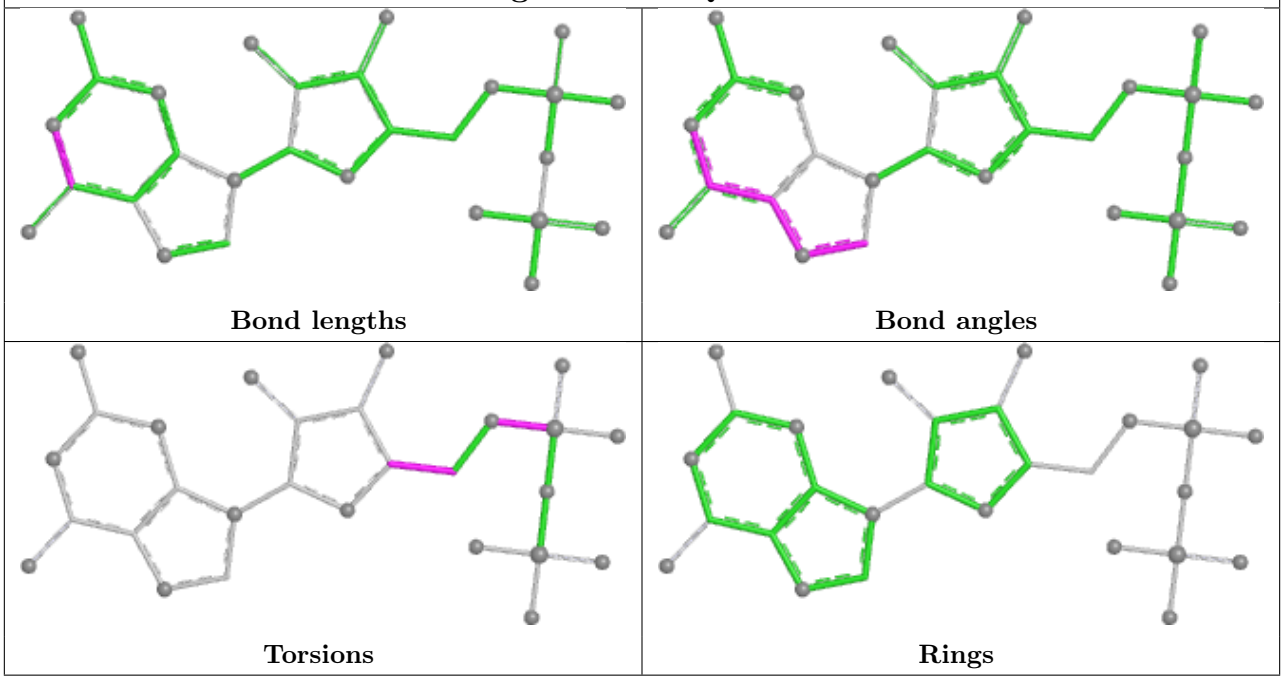

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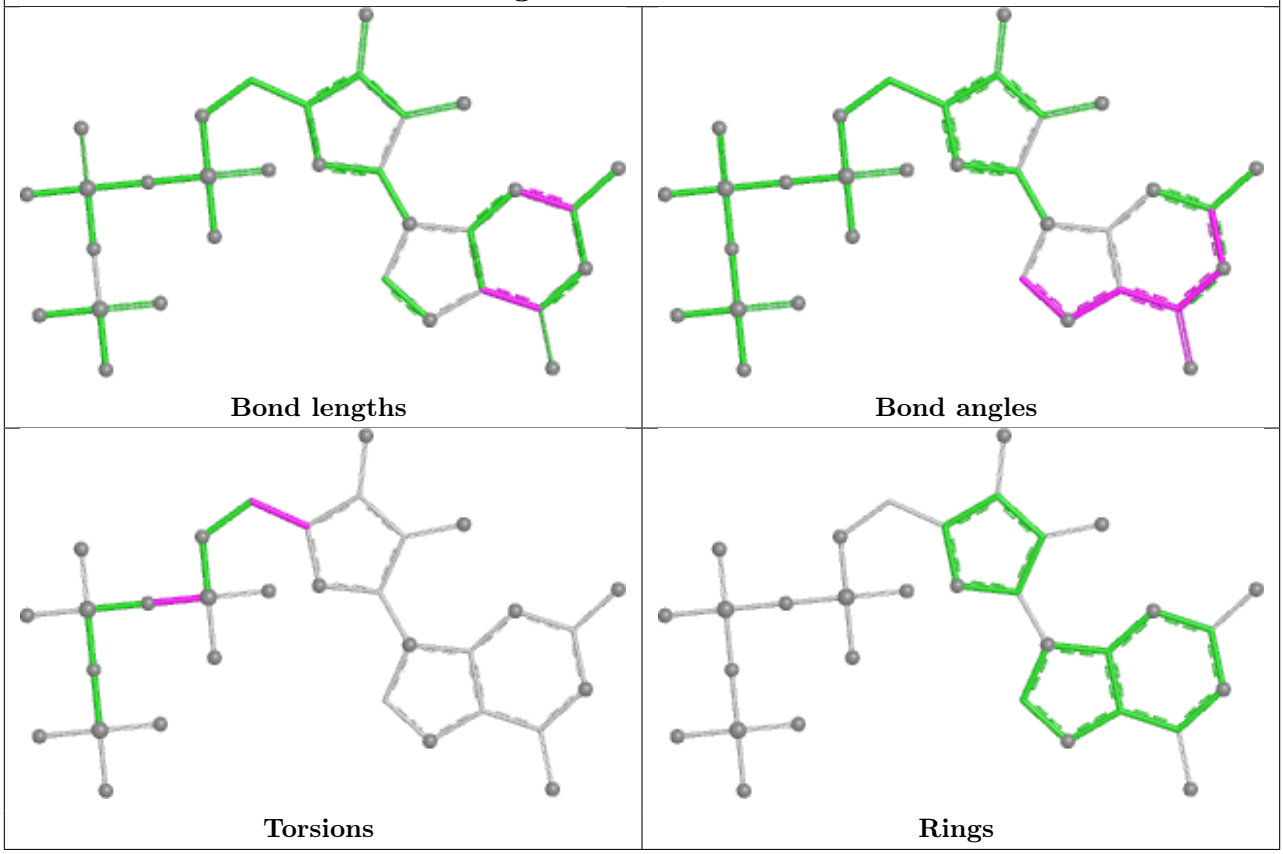

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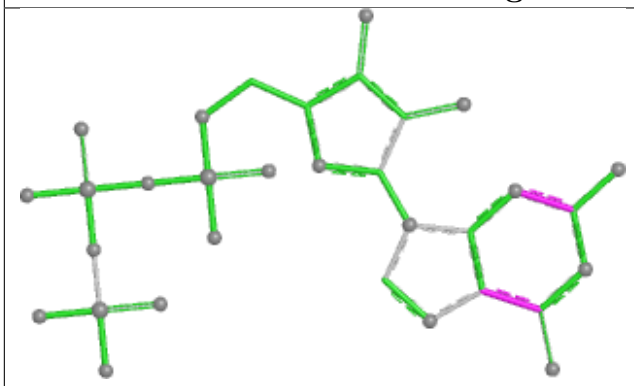

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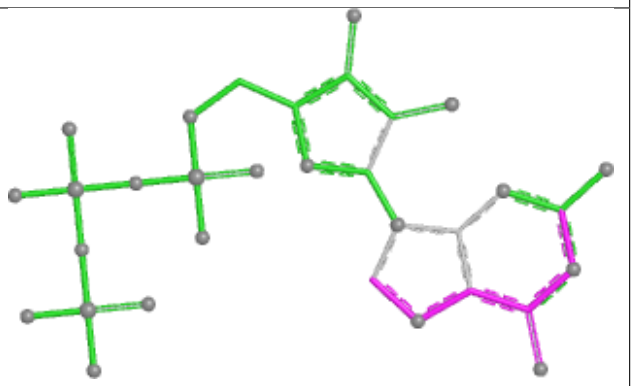

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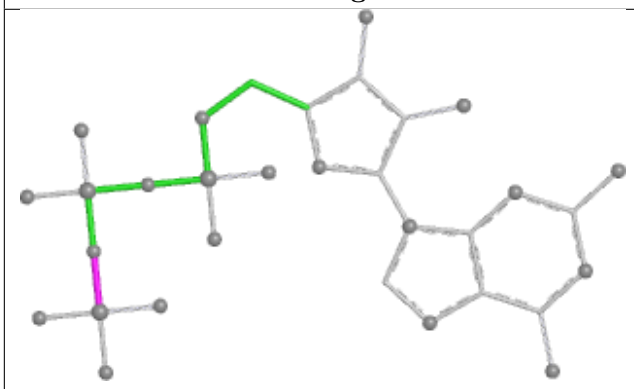

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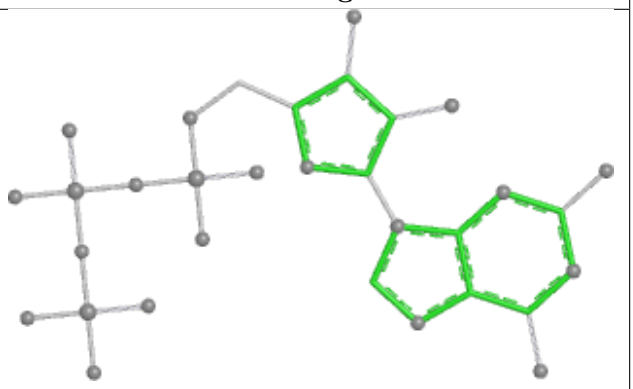

Rings

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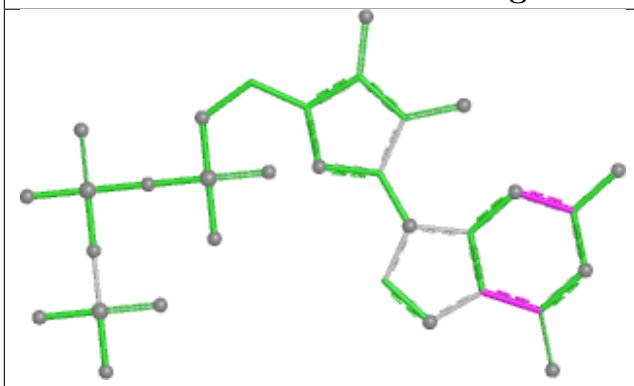

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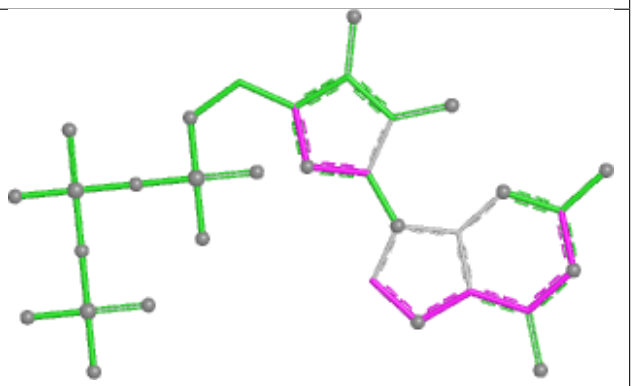

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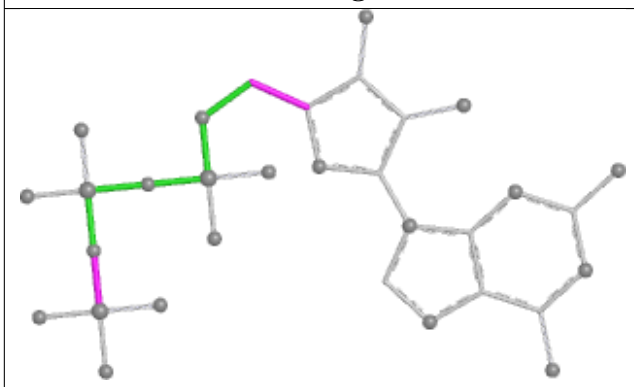

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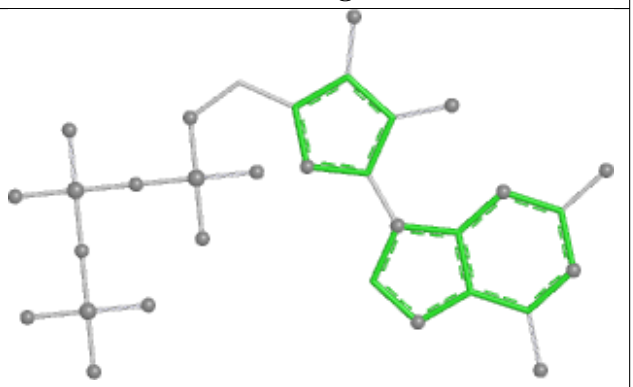

Rings

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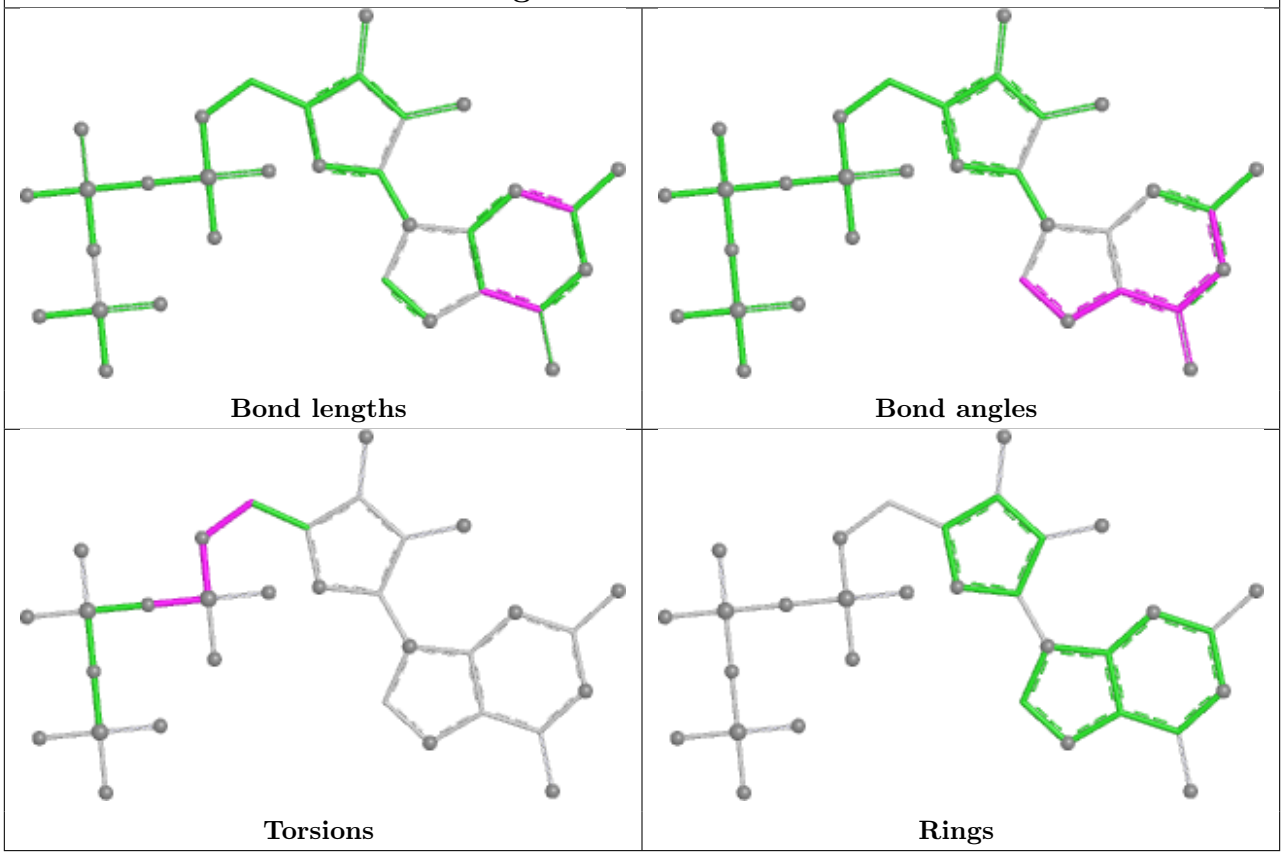

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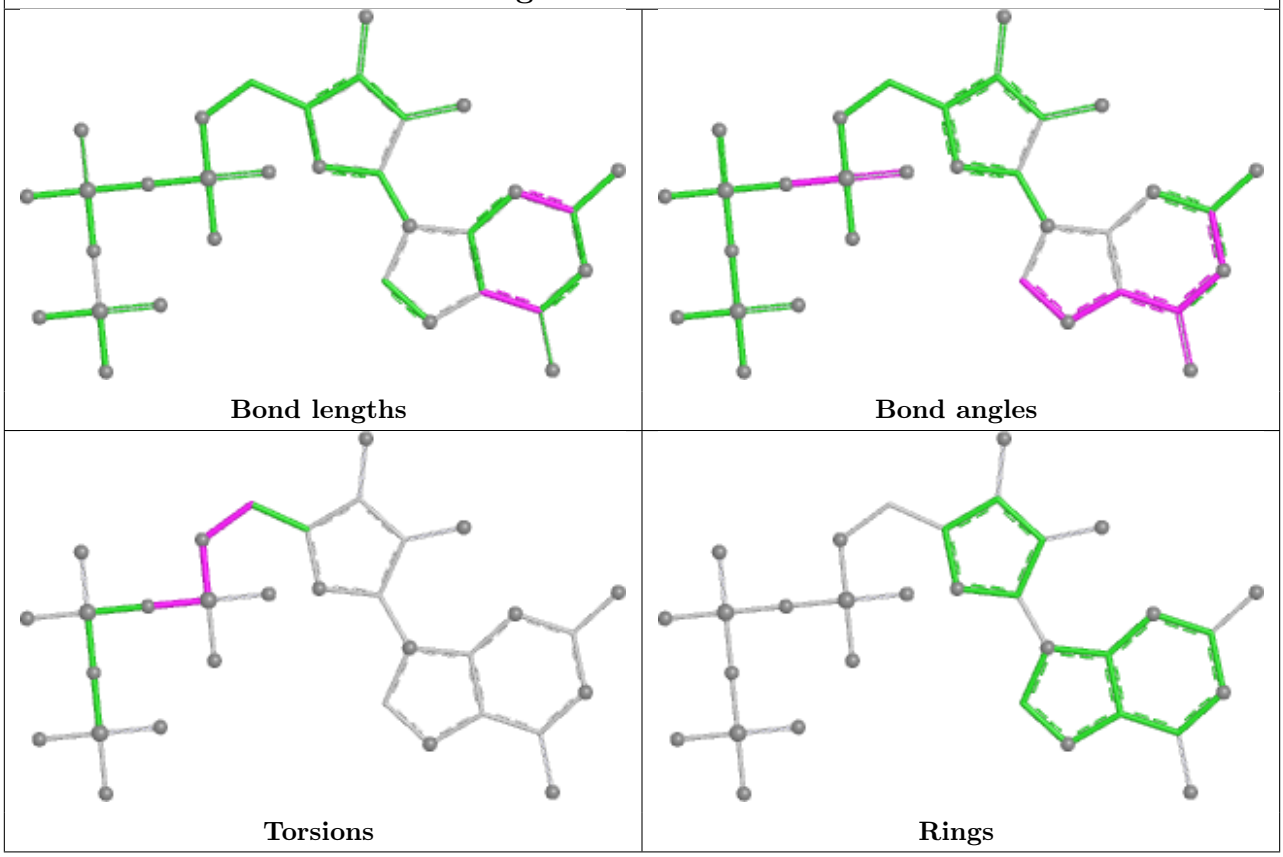

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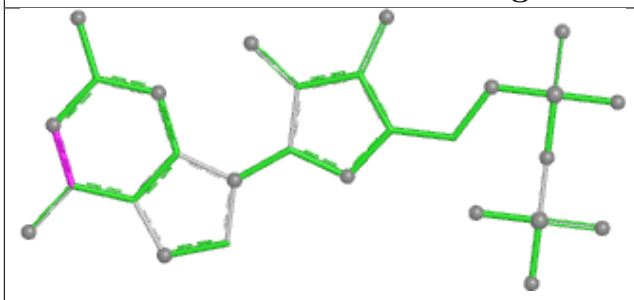

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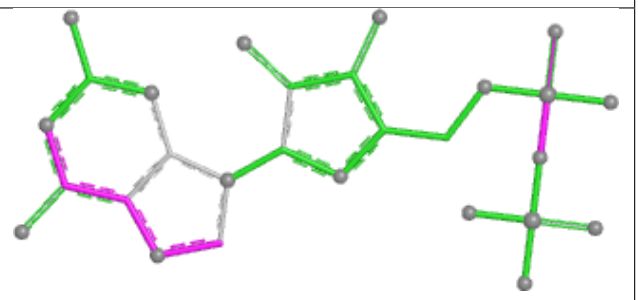

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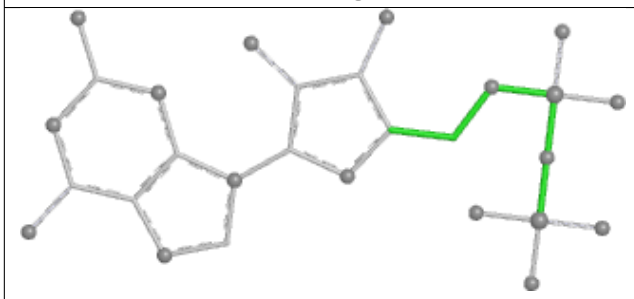

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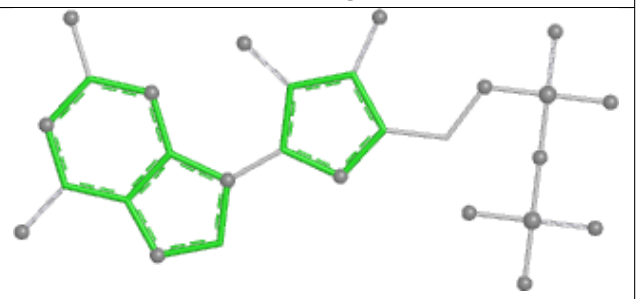

Rings

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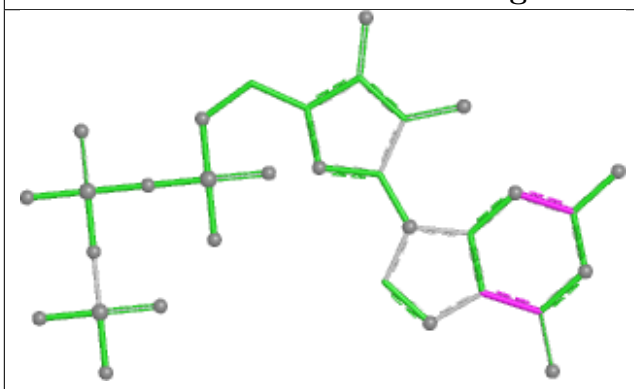

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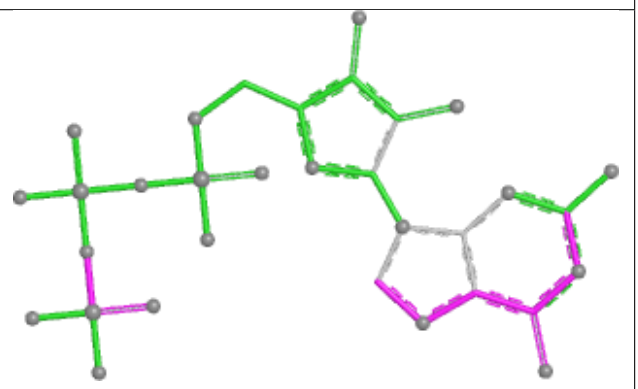

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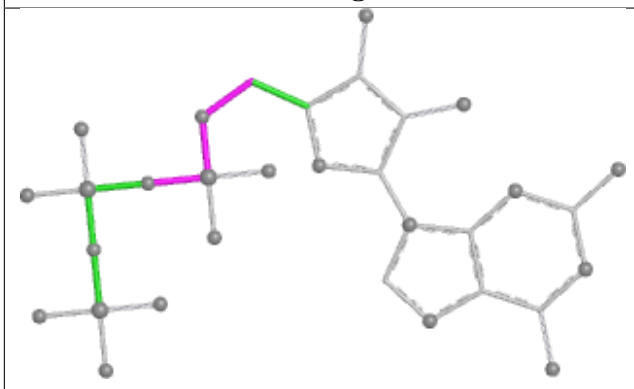

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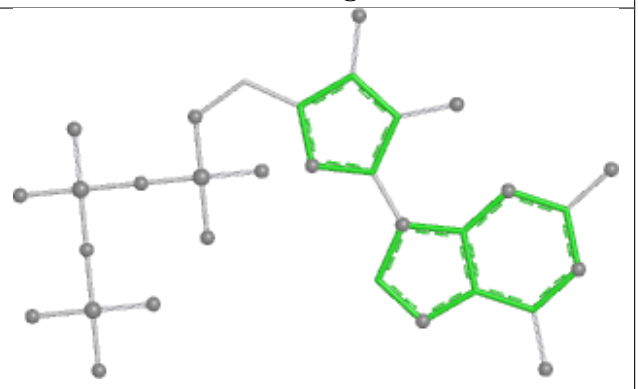

Rings

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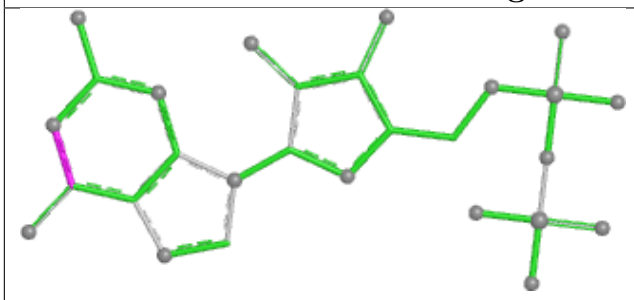
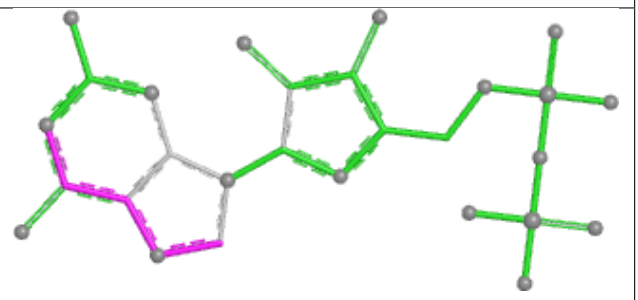
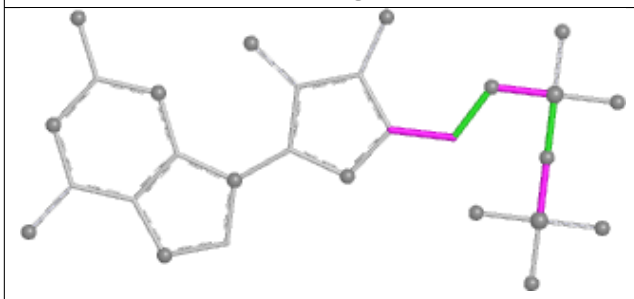


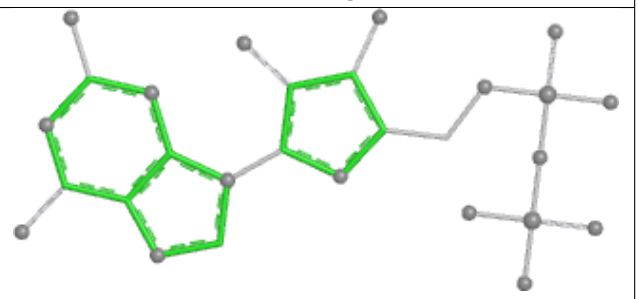
Bond lengths



Bond angles

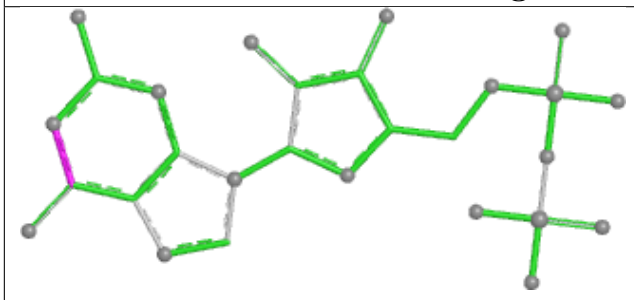


Torsions



Rings

Ligand GDP FH 501



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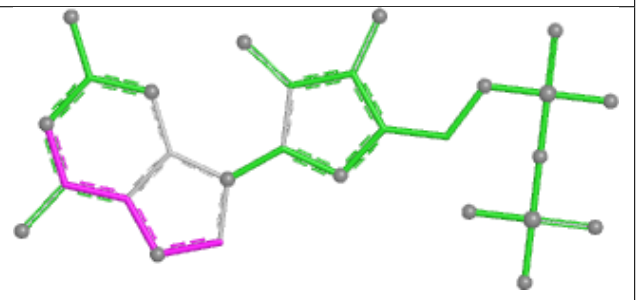

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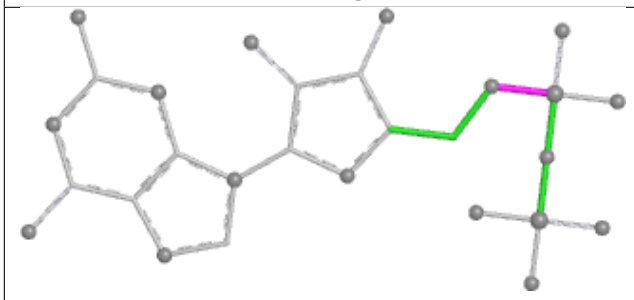

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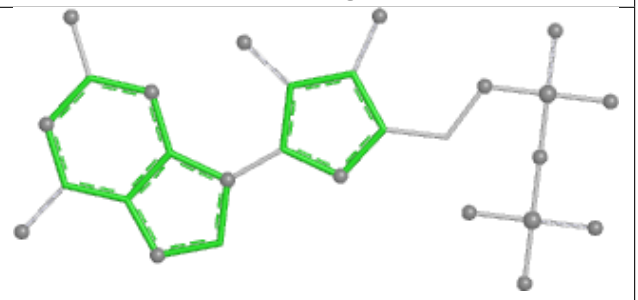
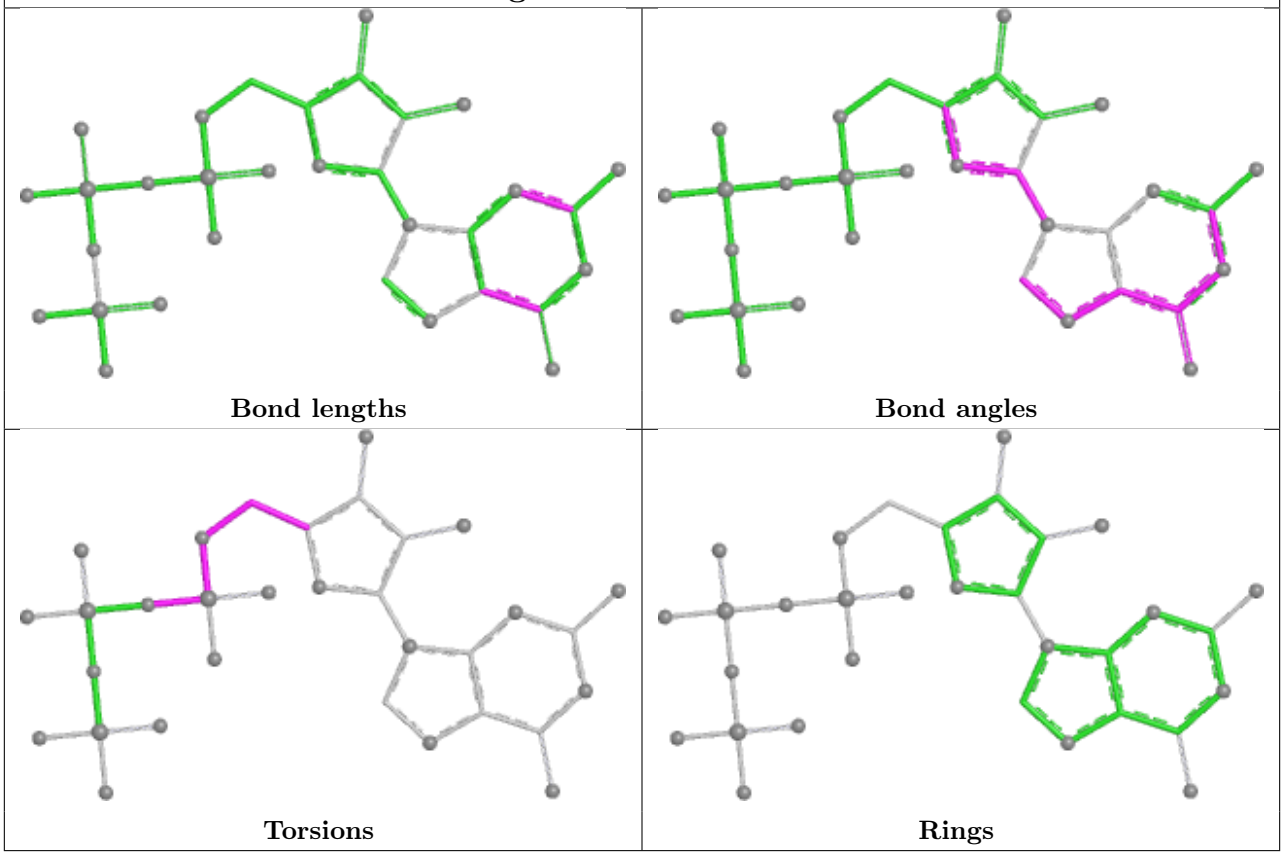


Rings

Ligand GTP HK 501



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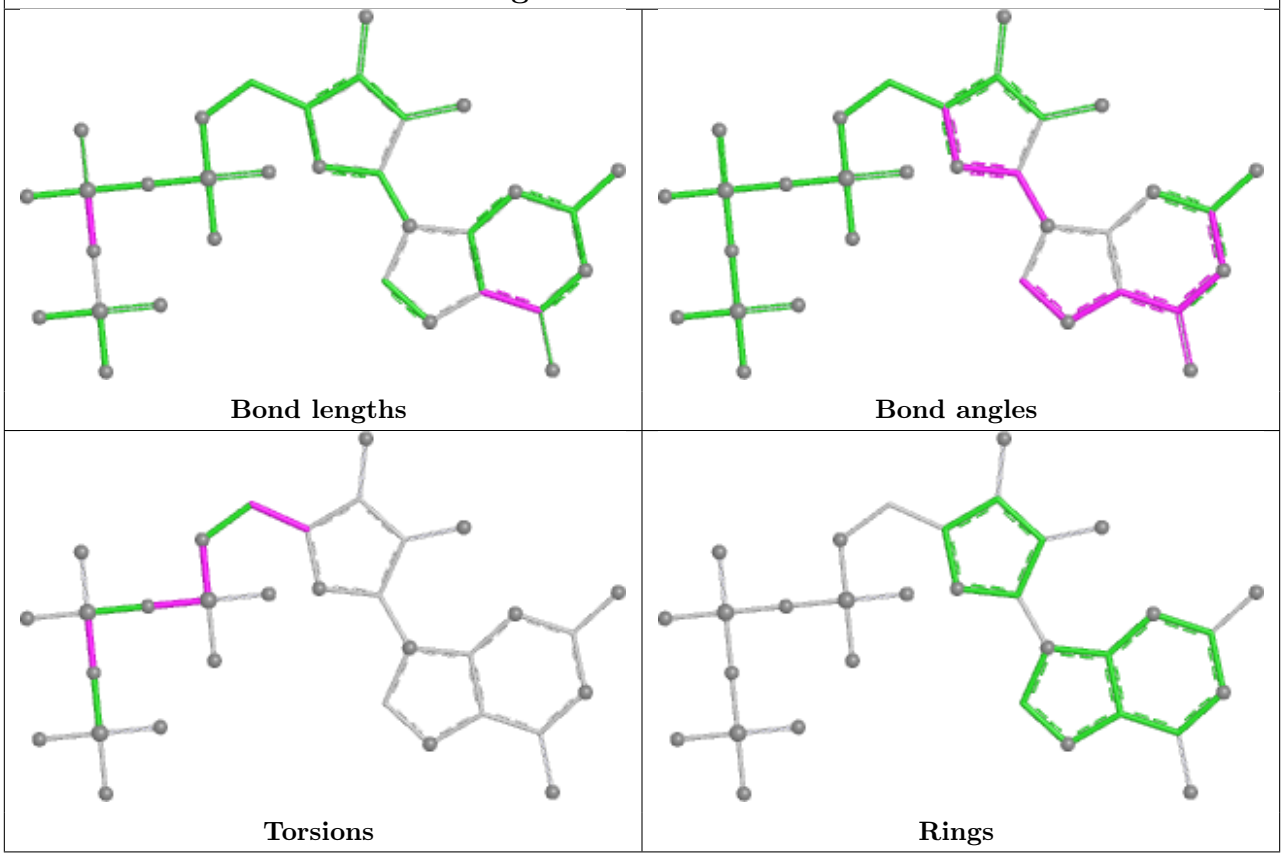

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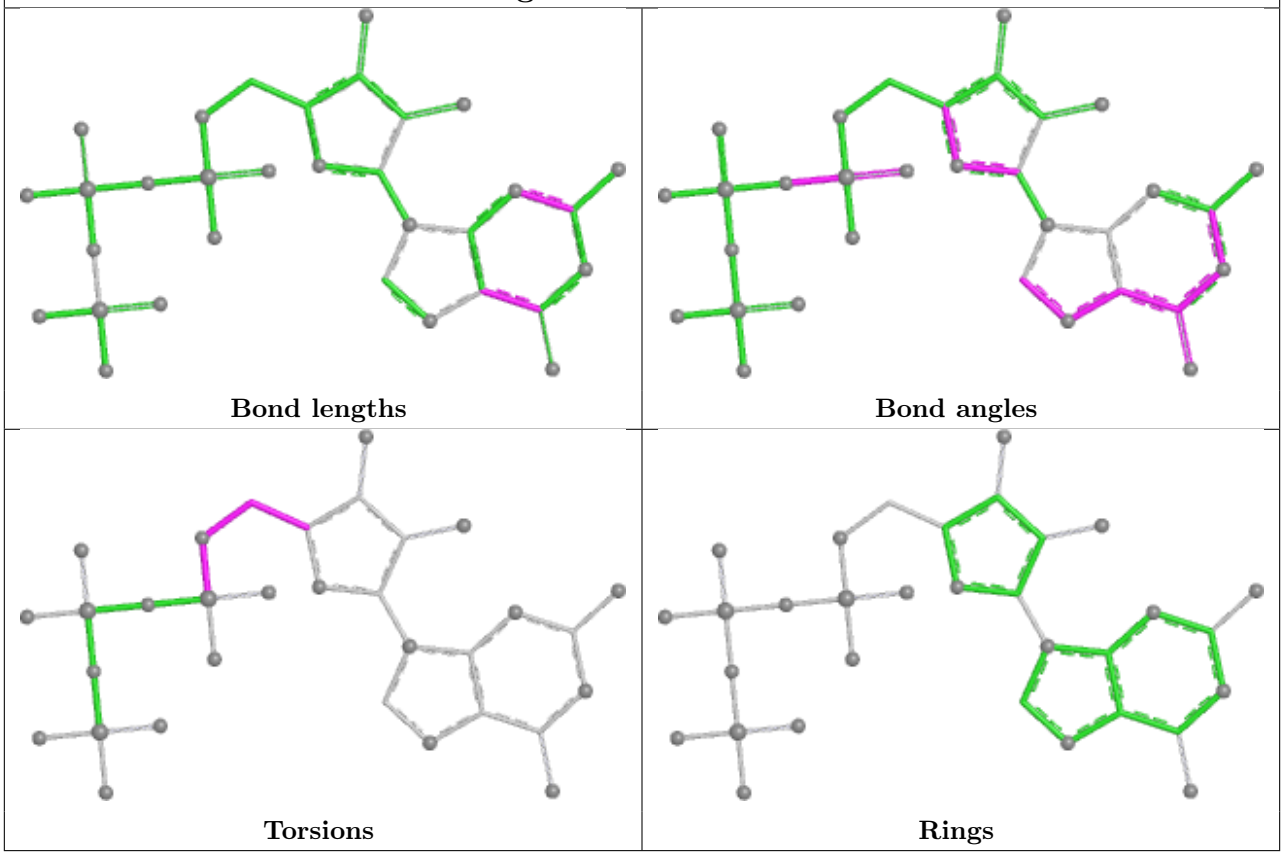
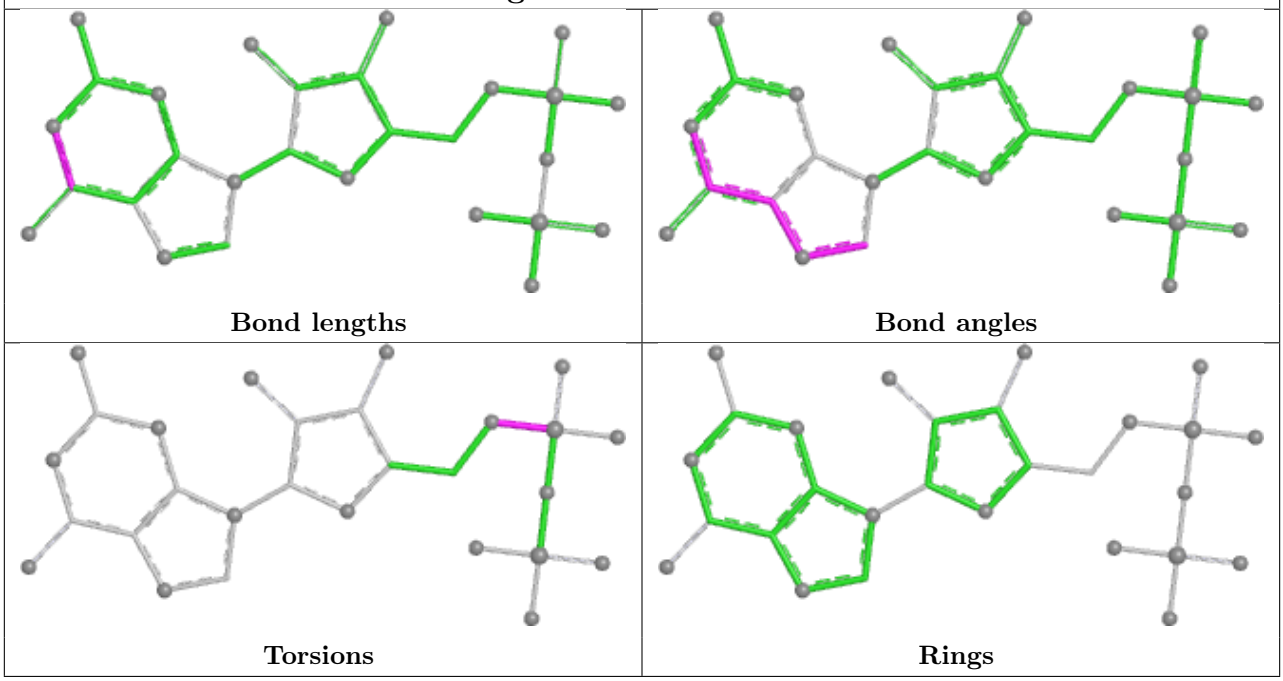


Ligand GDP NH 501



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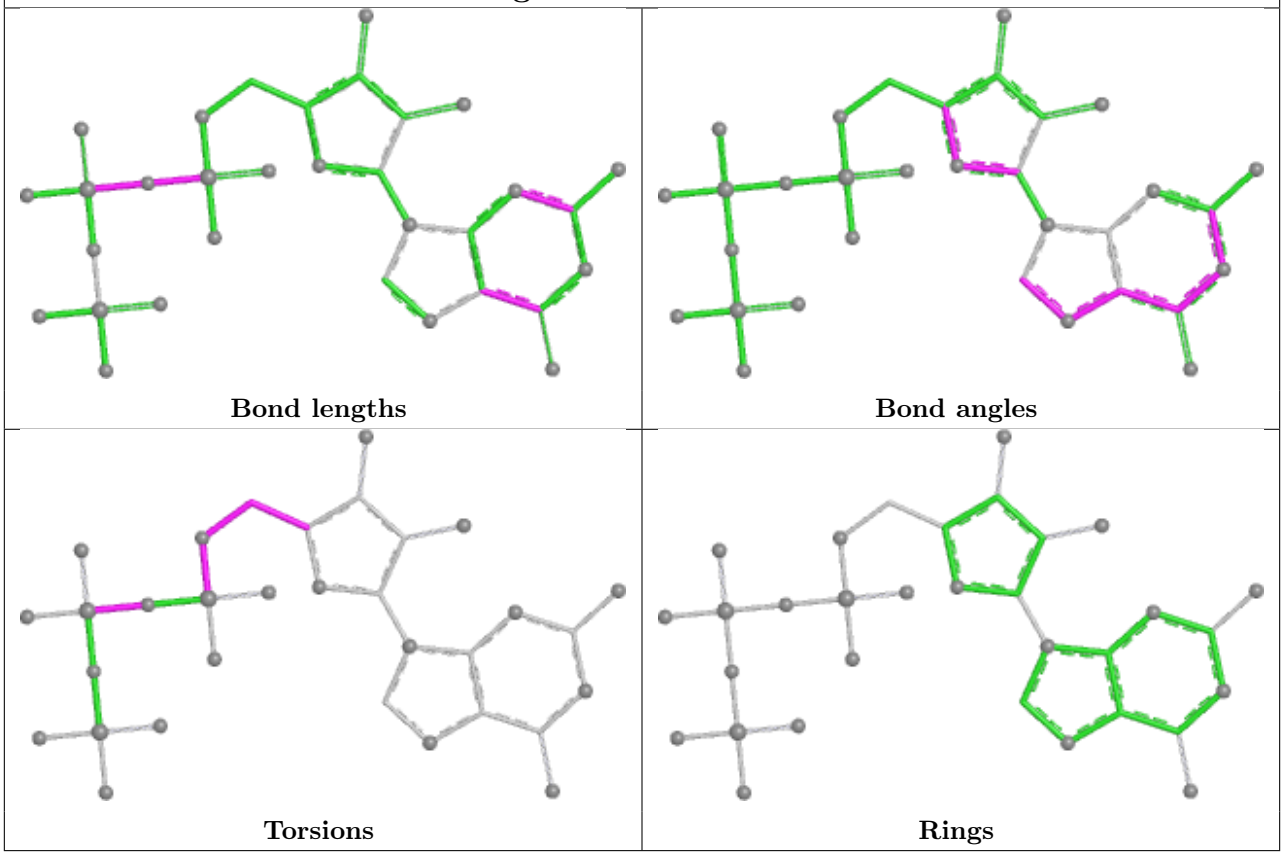

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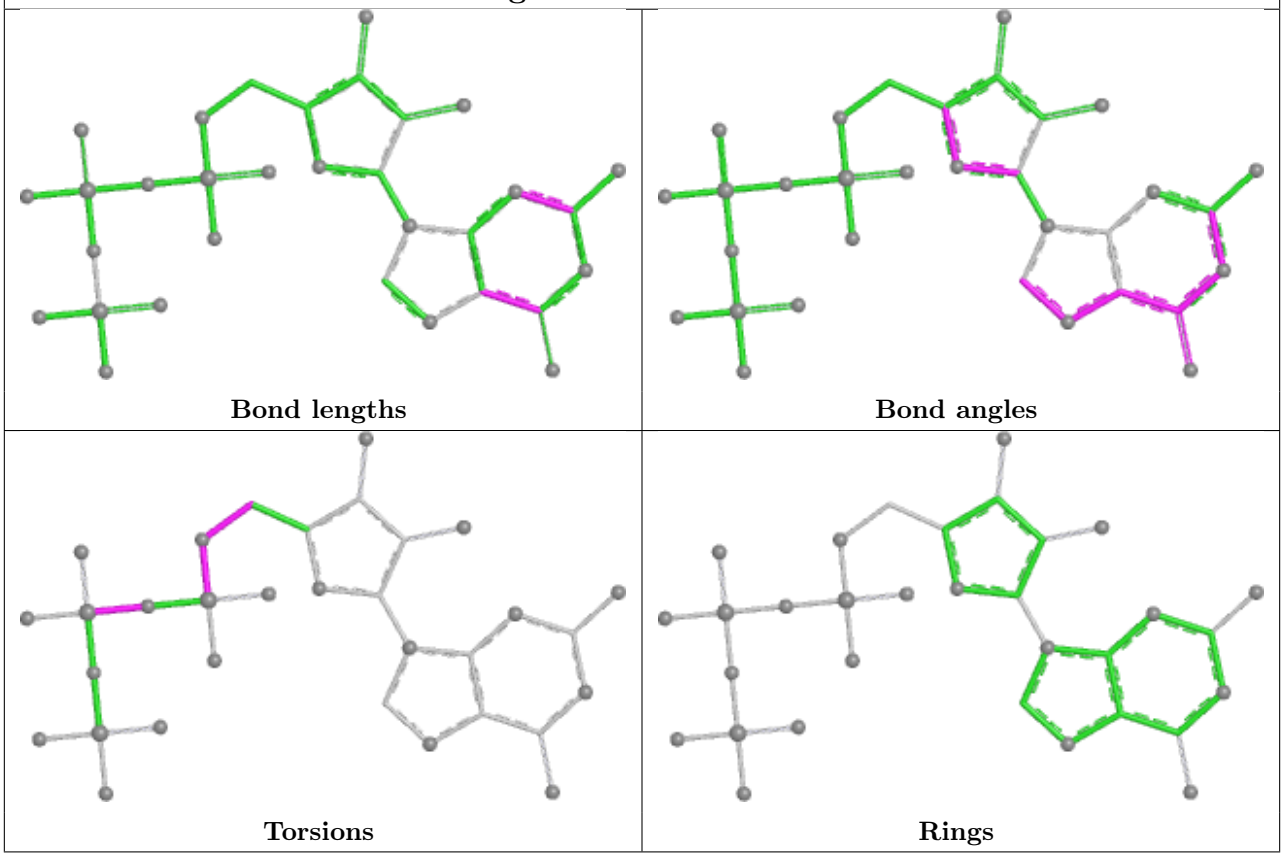

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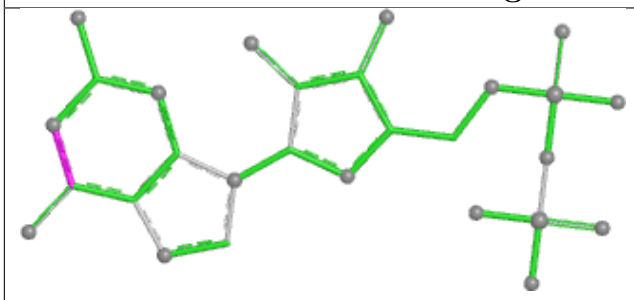

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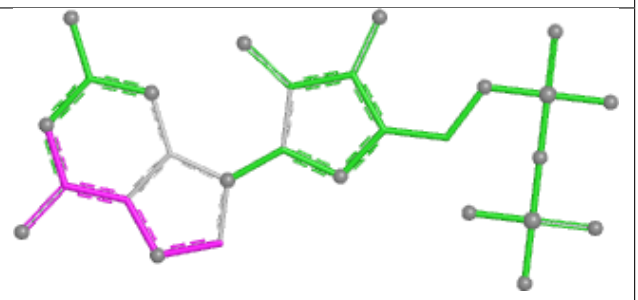
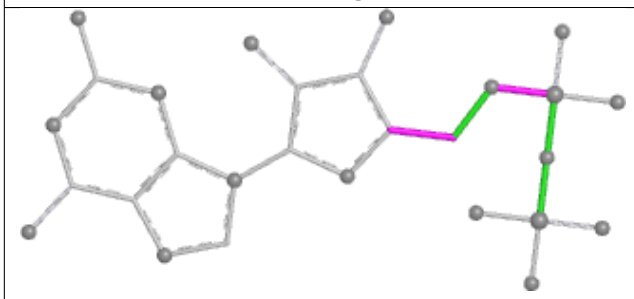
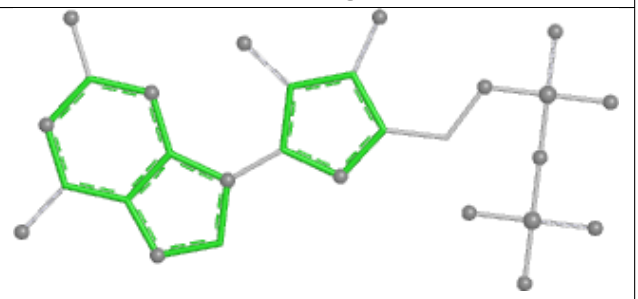


Bond angles

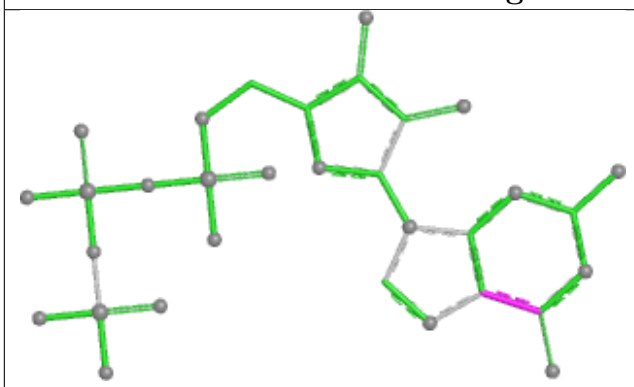


Torsions



Rings

Ligand GTP UM 501



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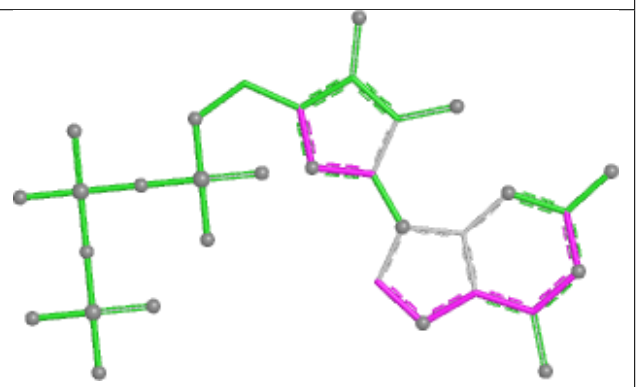

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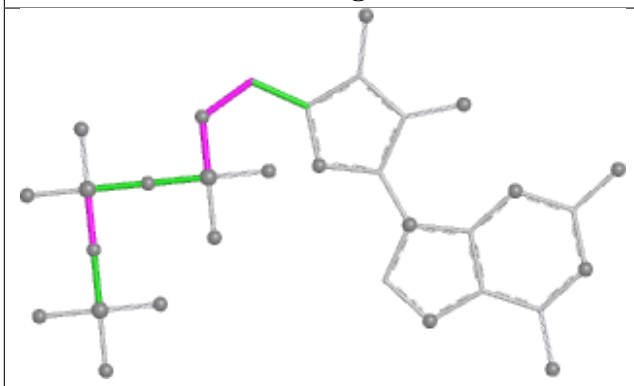

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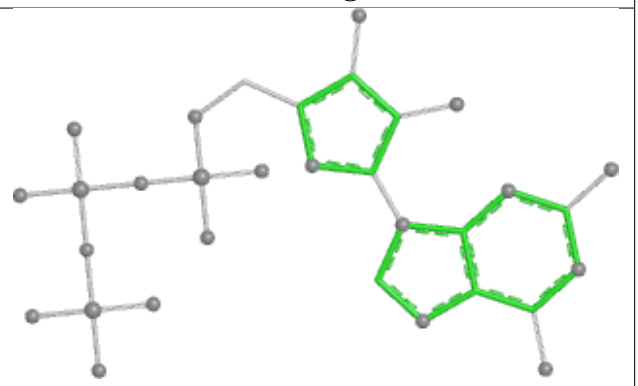

Rings

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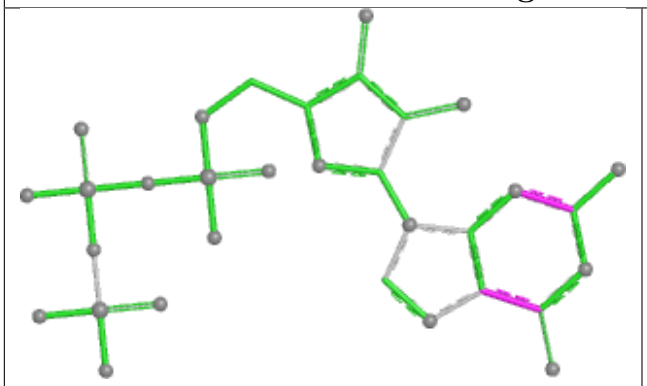

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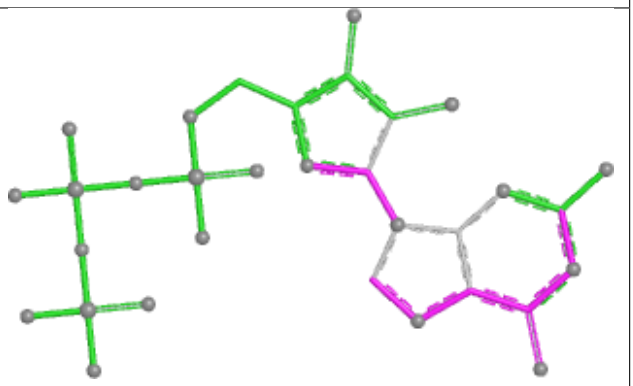

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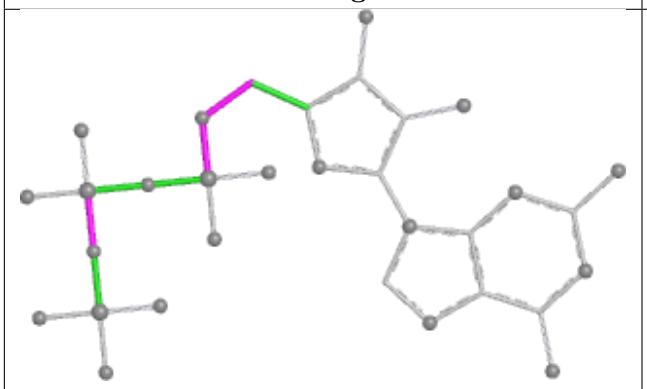

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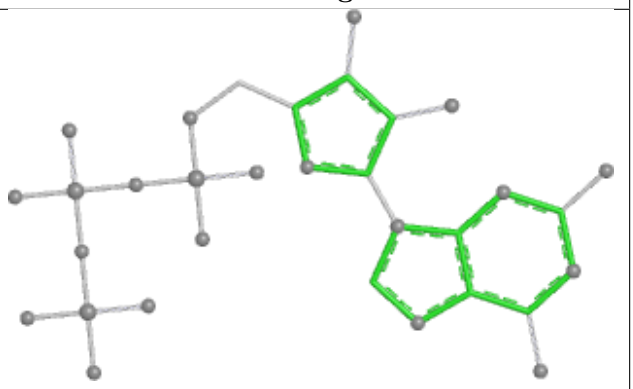
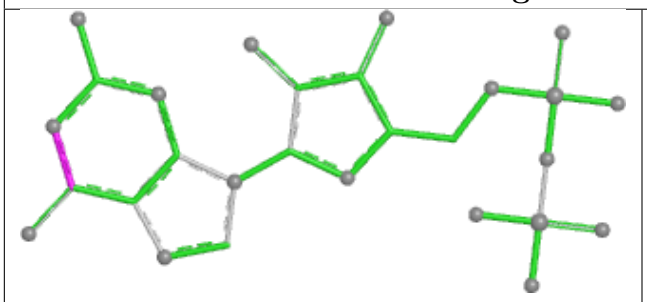


Rings

Ligand GDP EF 501



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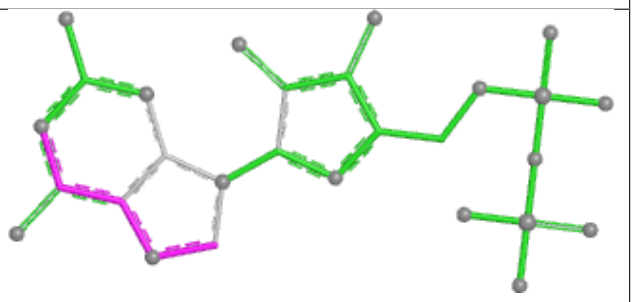

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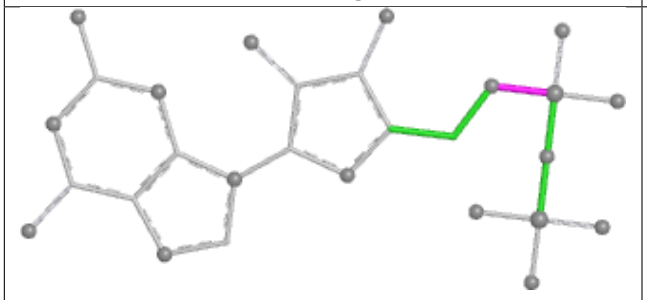

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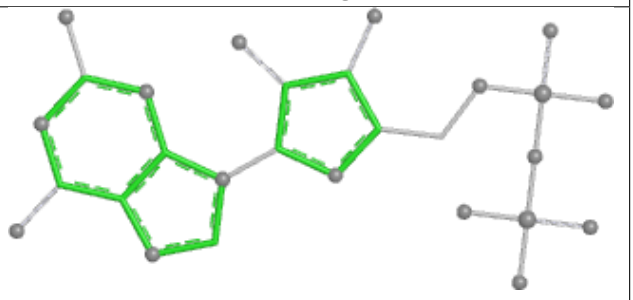

Rings

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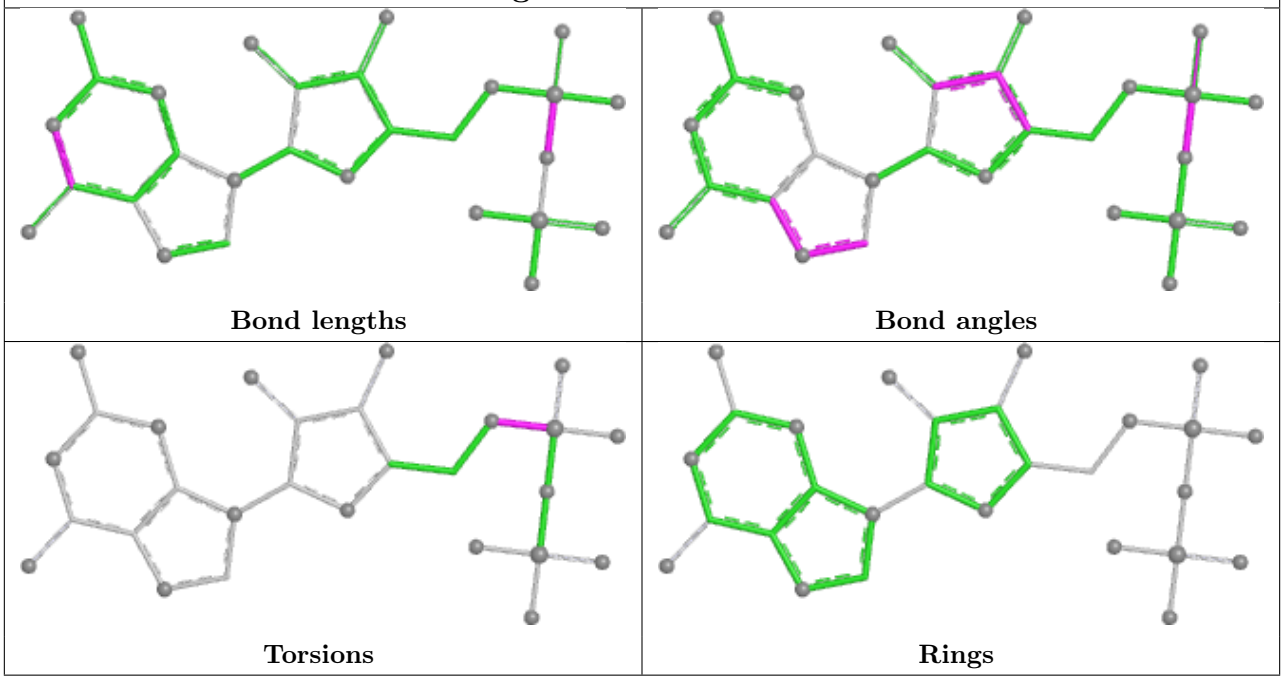

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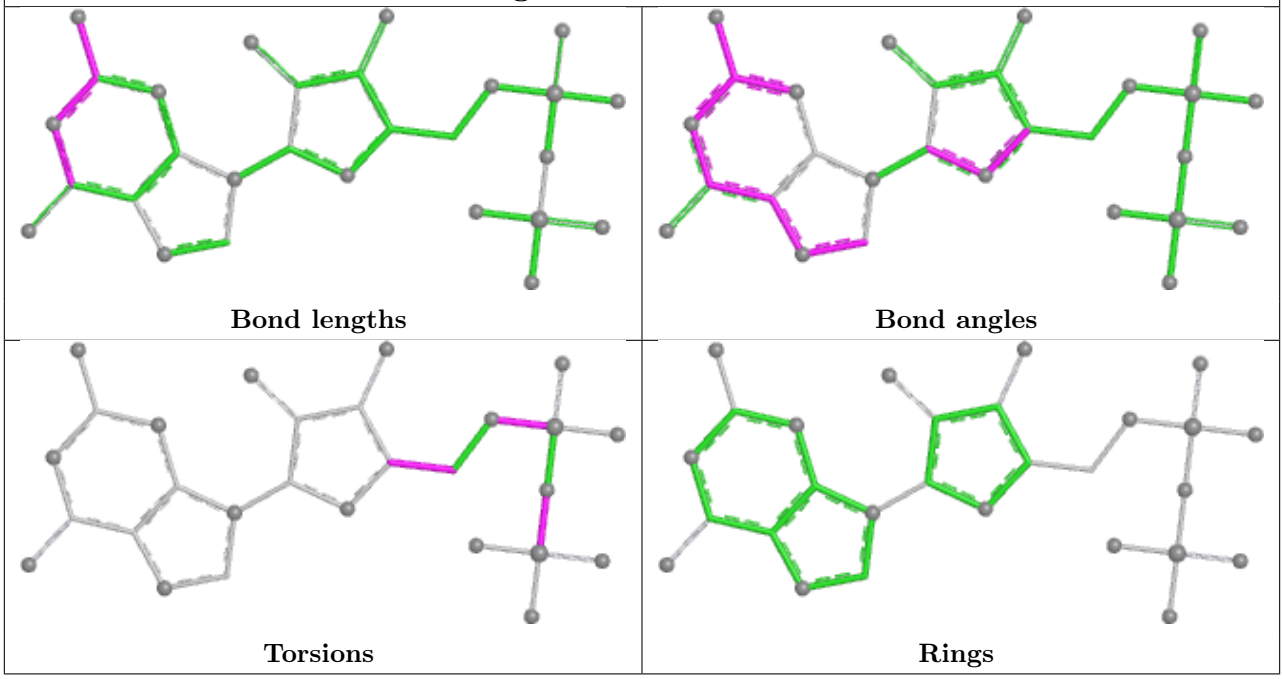

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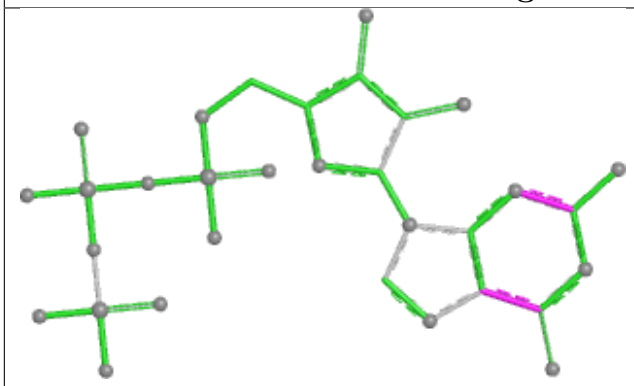

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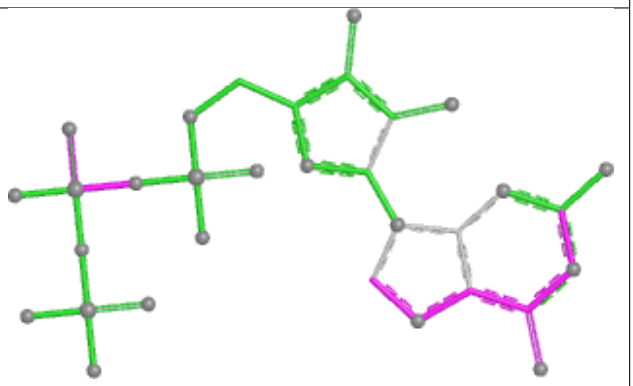

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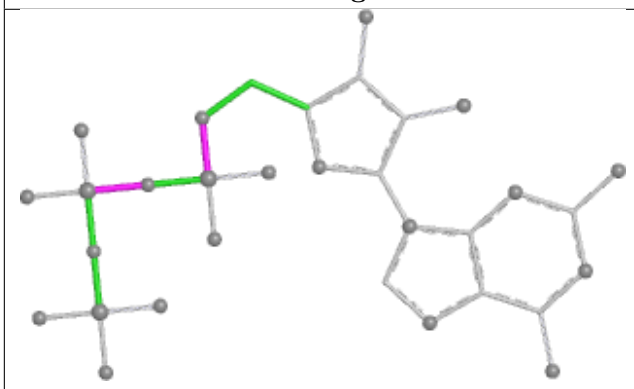

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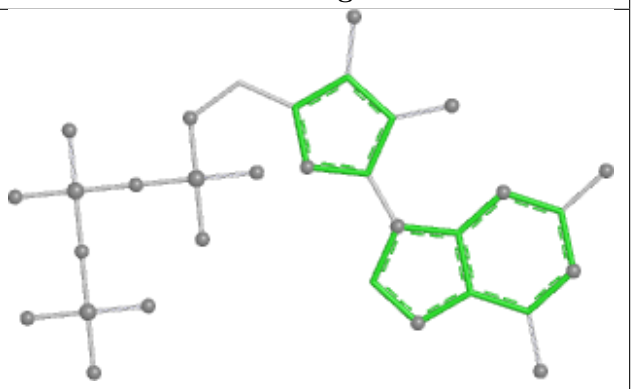

Rings

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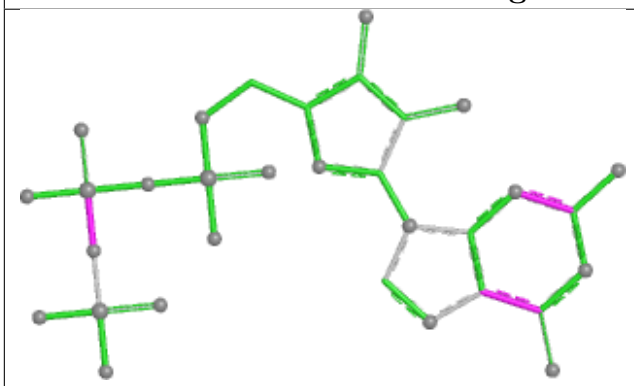

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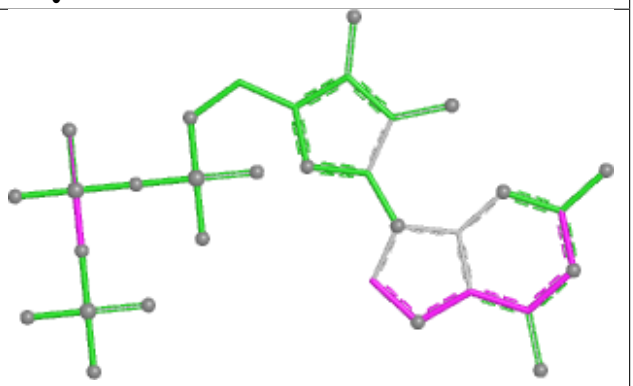

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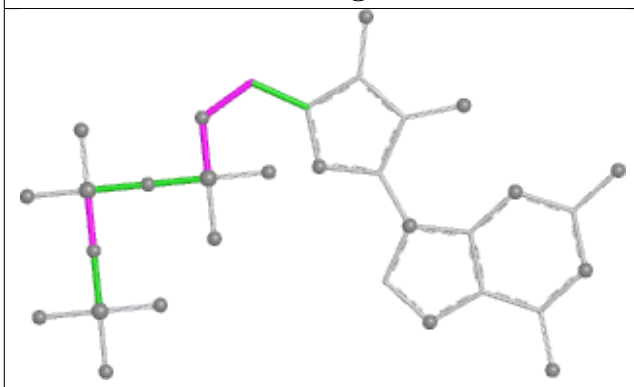

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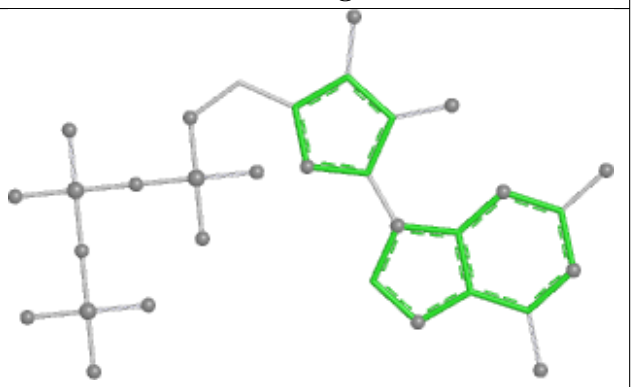

Rings

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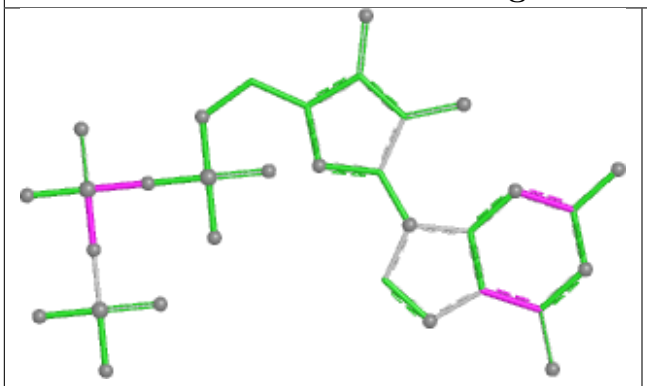

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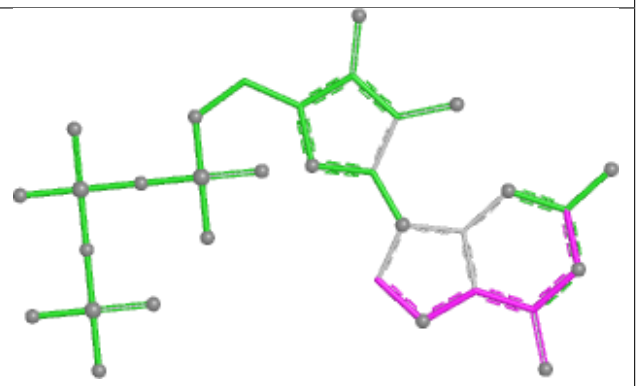

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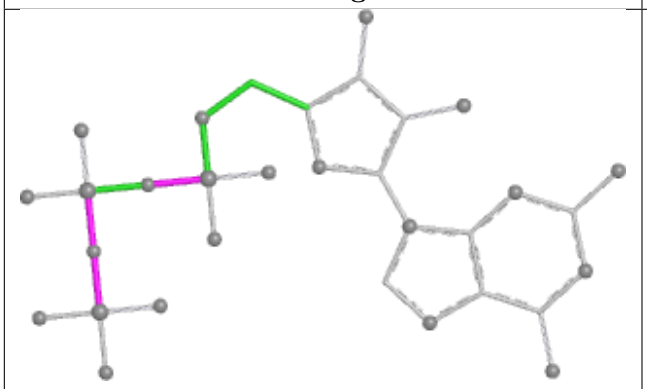

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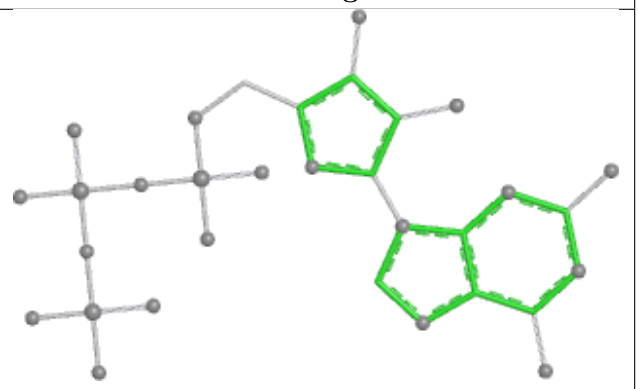
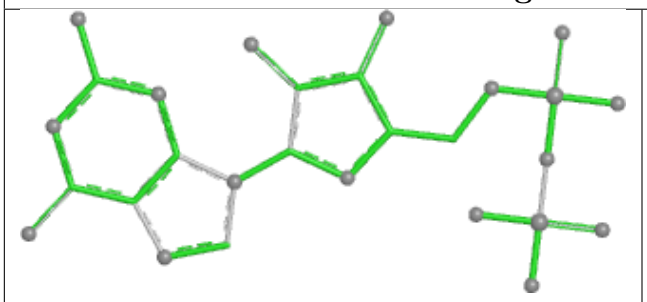


Rings

Ligand GDP IN 501



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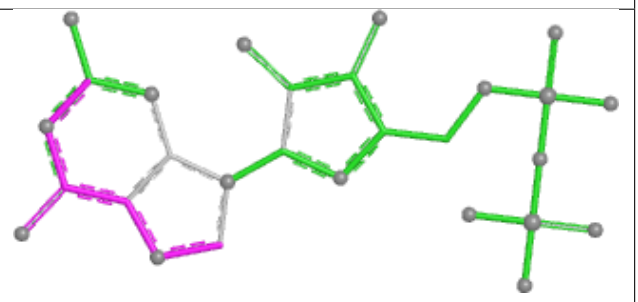

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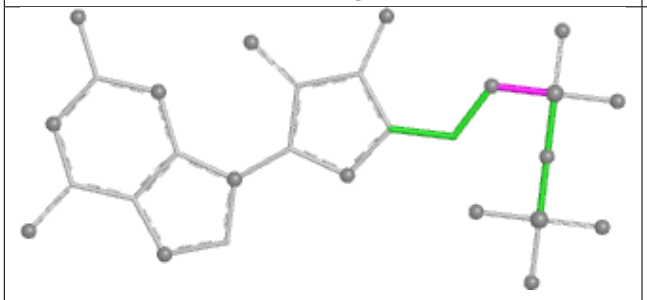

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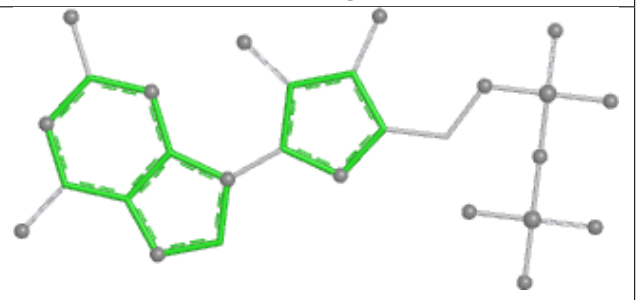
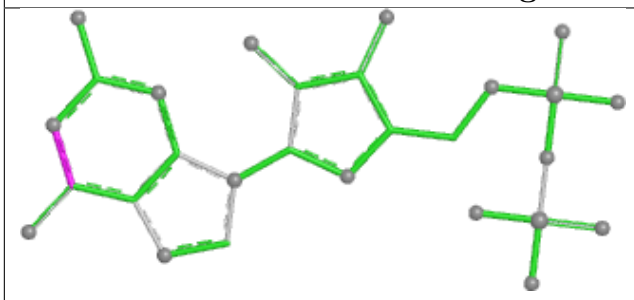


Rings

Ligand GDP IJ 501



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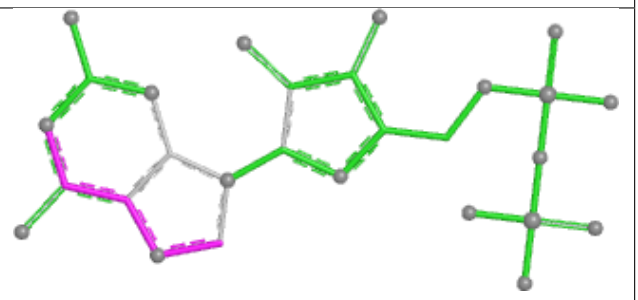

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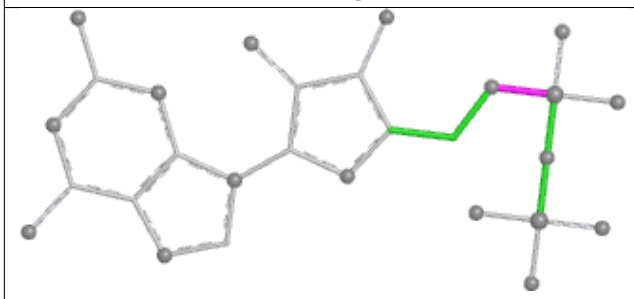

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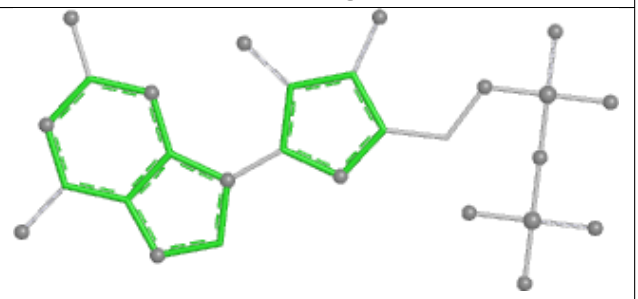
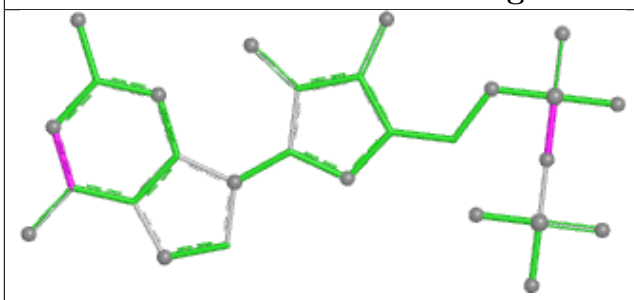


Rings

Ligand GDP MF 501



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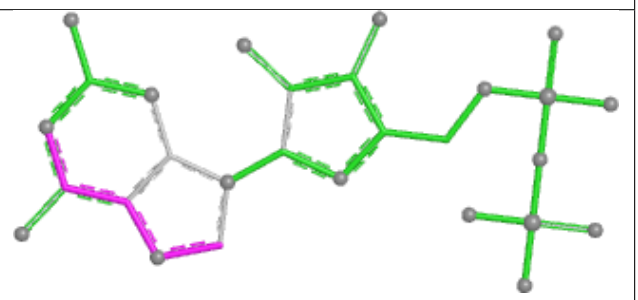

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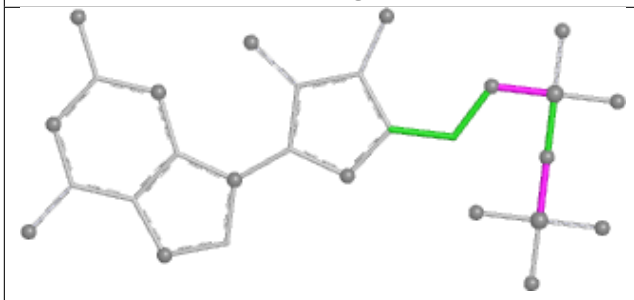
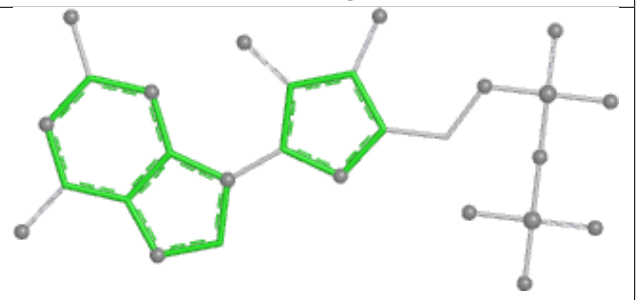
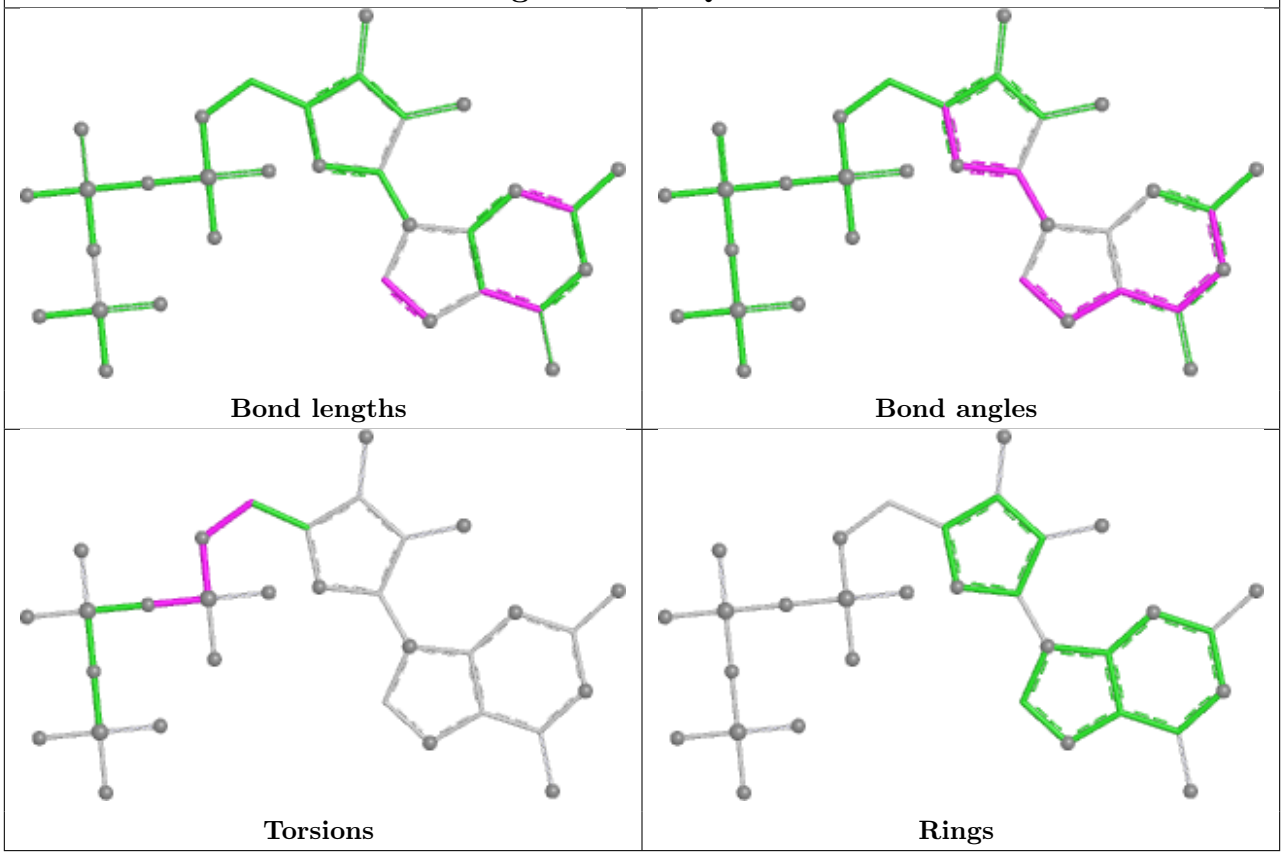


Torsions



Rings

Ligand GTP QE 501



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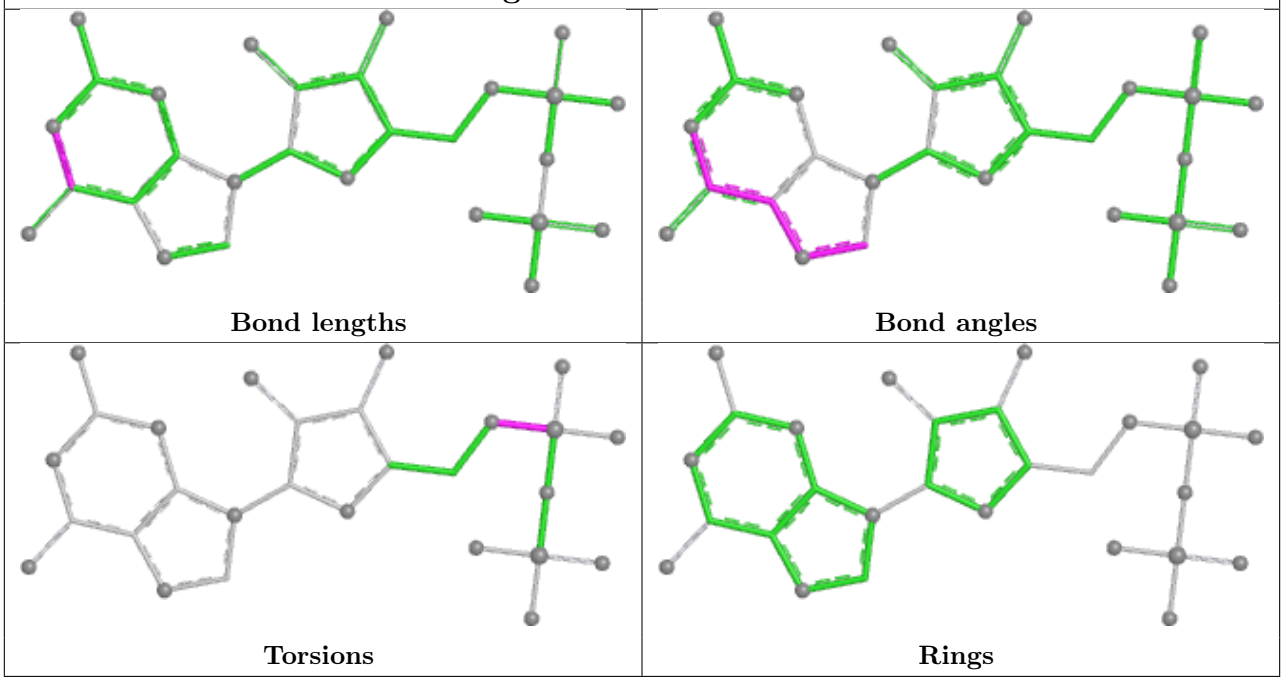
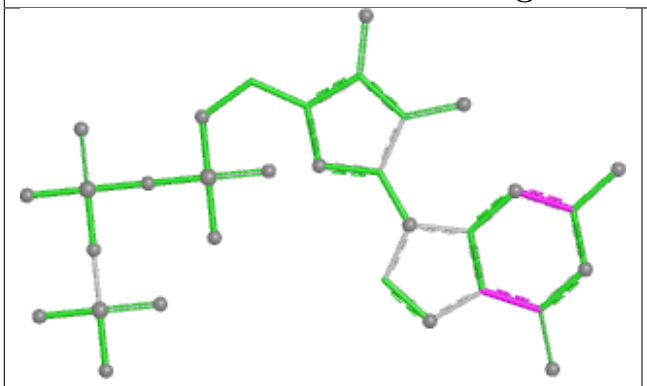


Ligand GTP IG 501



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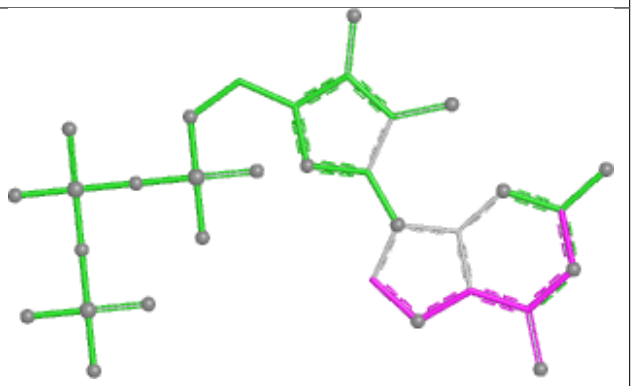

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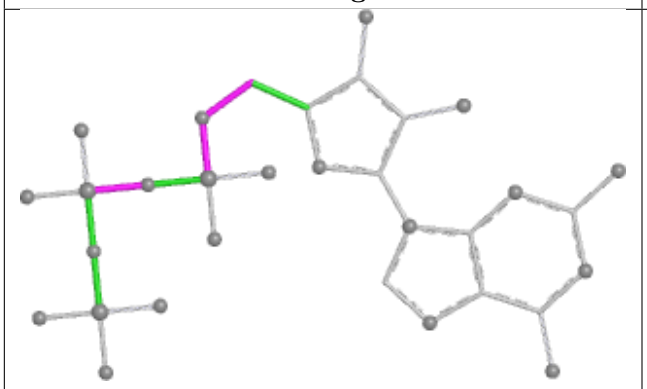

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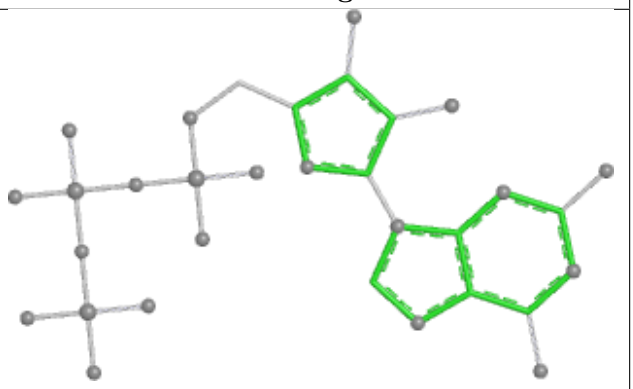
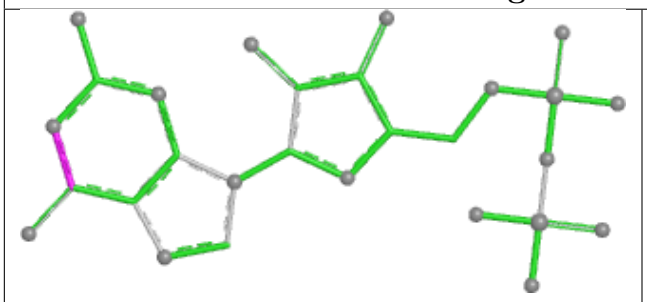


Rings

Ligand GDP DD 501



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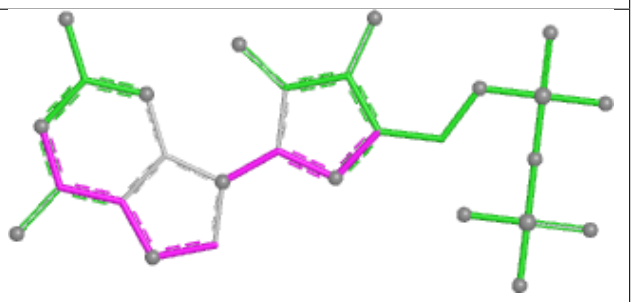

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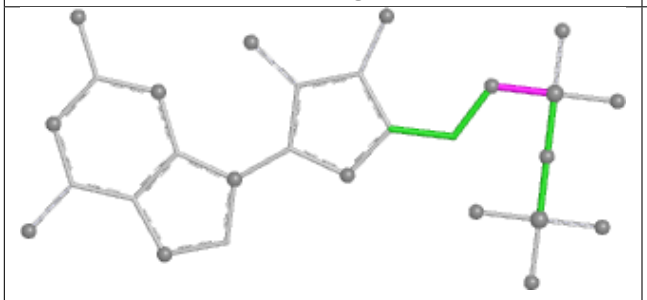

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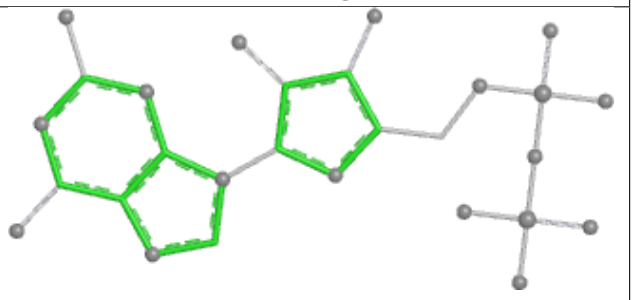

Rings

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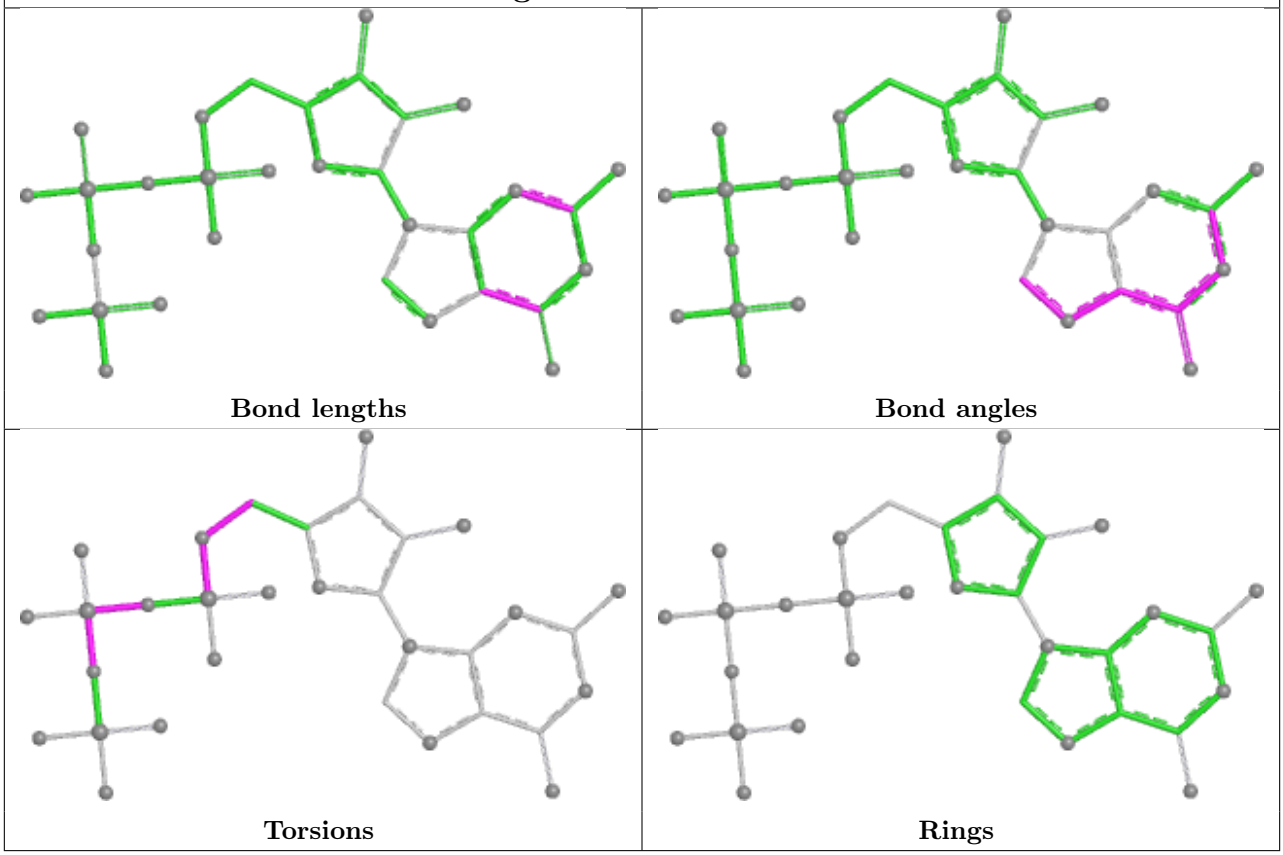

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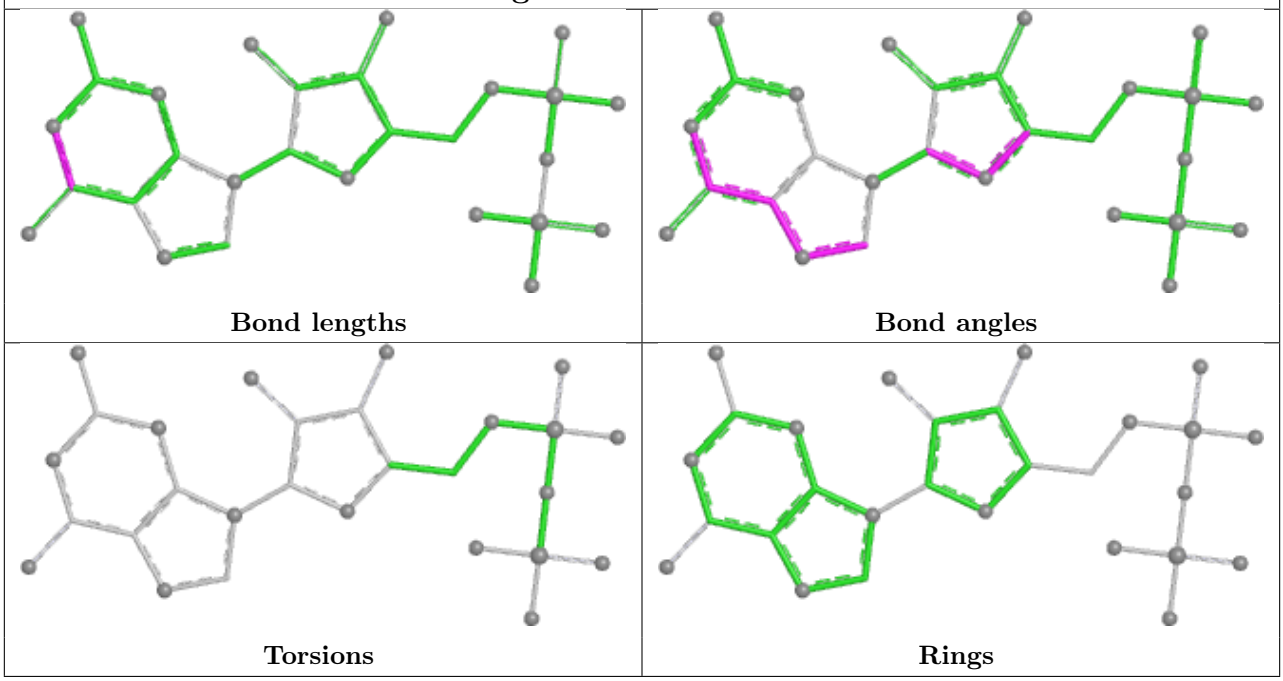

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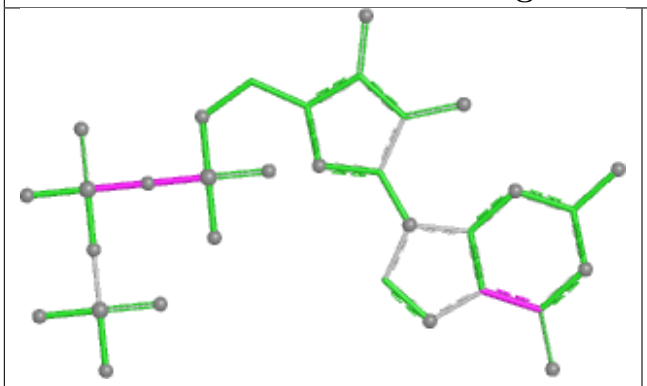

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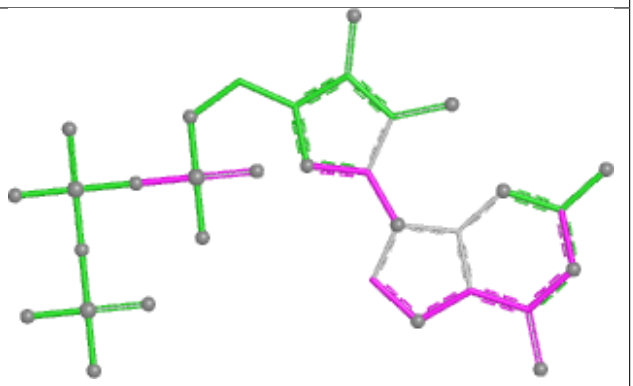

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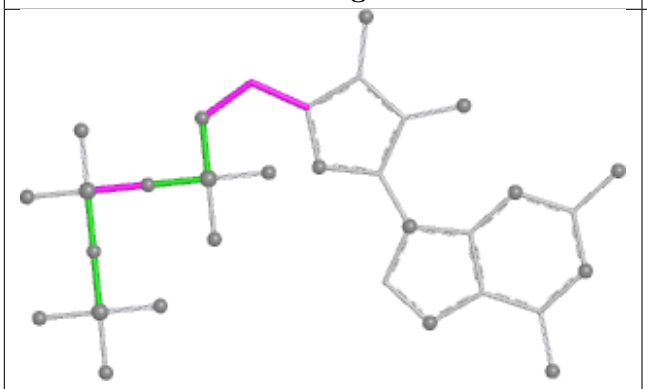

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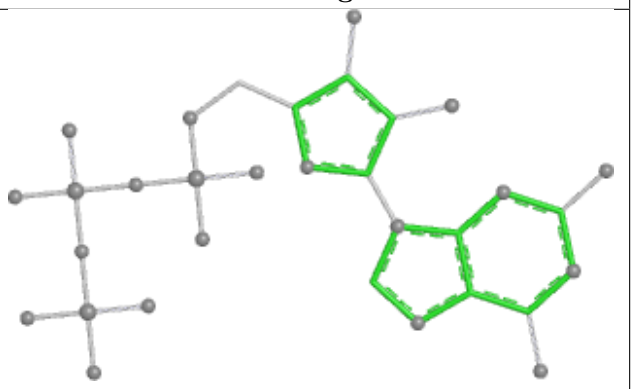
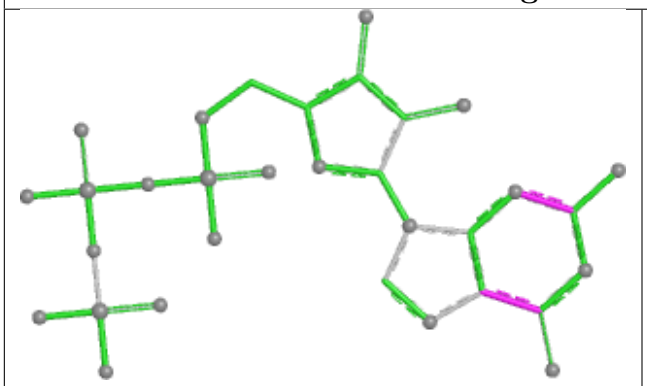


Rings

Ligand GTP JI 501



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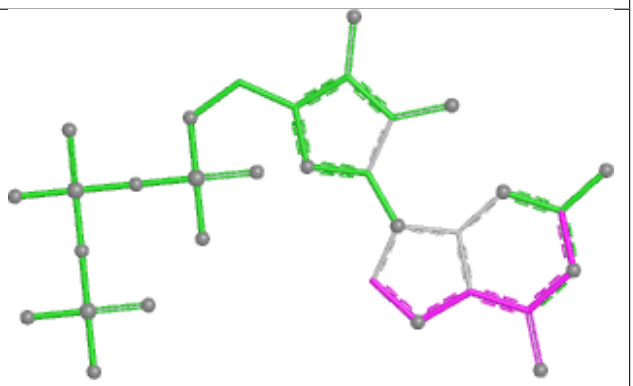

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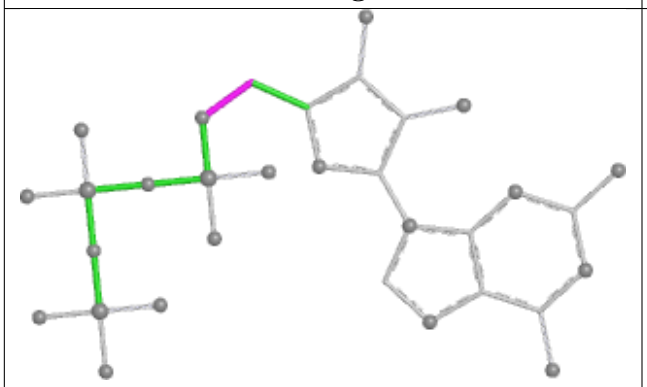

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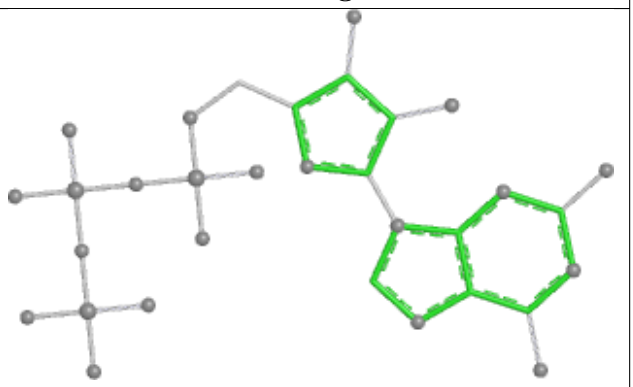
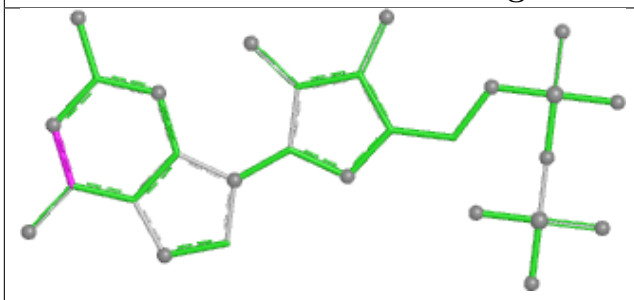


Rings

Ligand GDP VH 501



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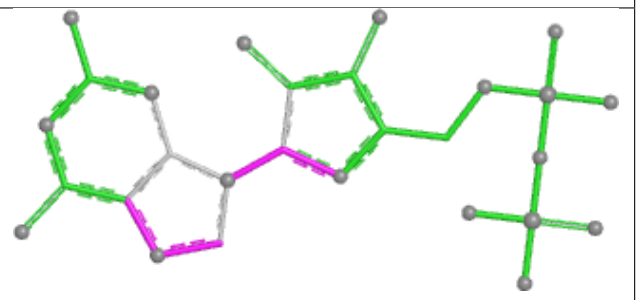

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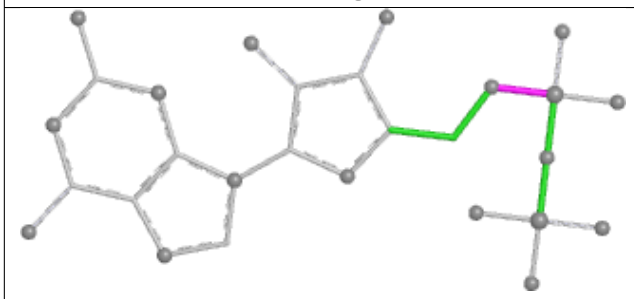

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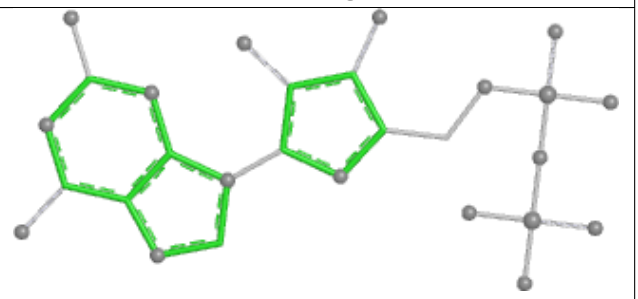

Rings

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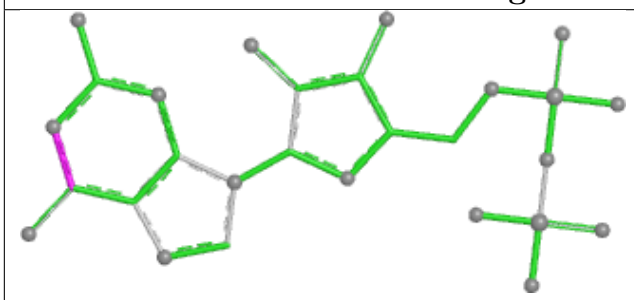

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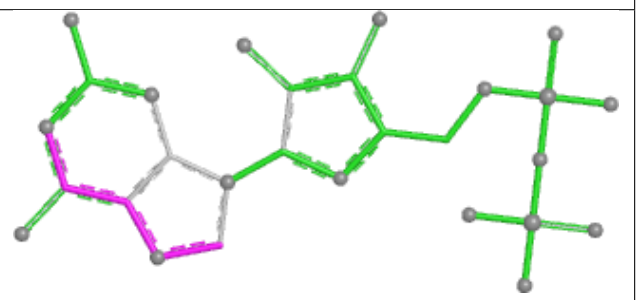

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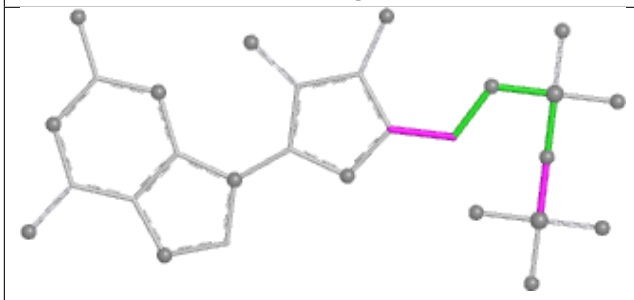

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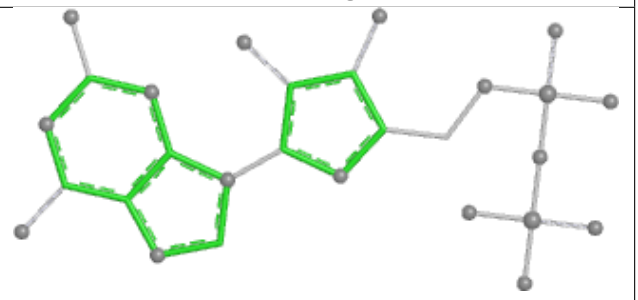
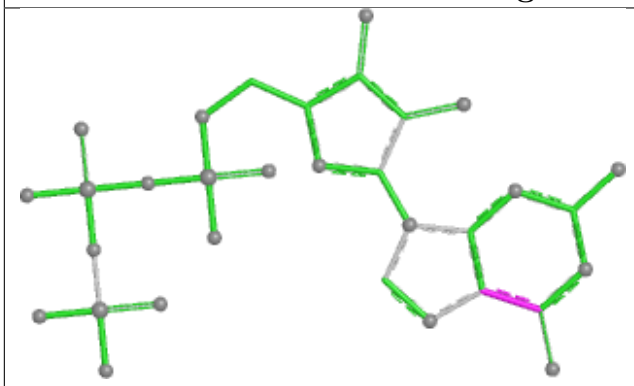


Rings

Ligand GTP IC 501



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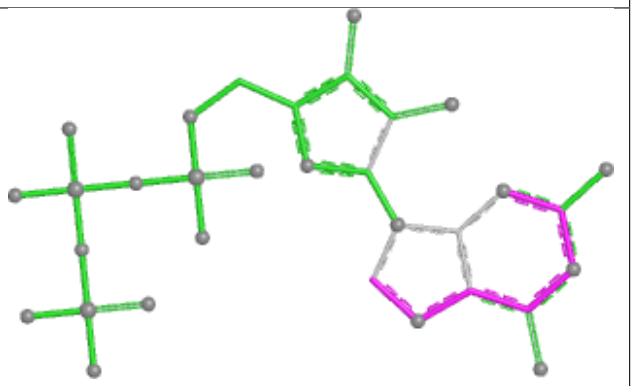

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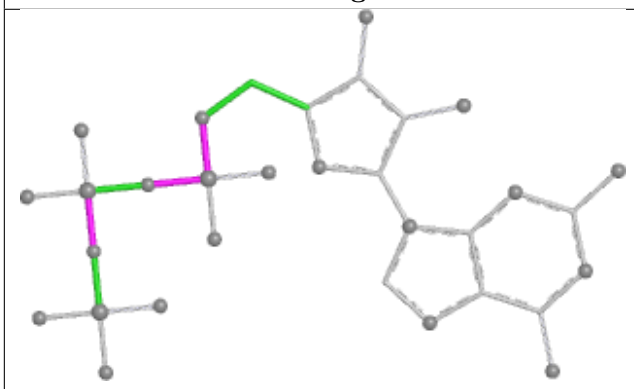

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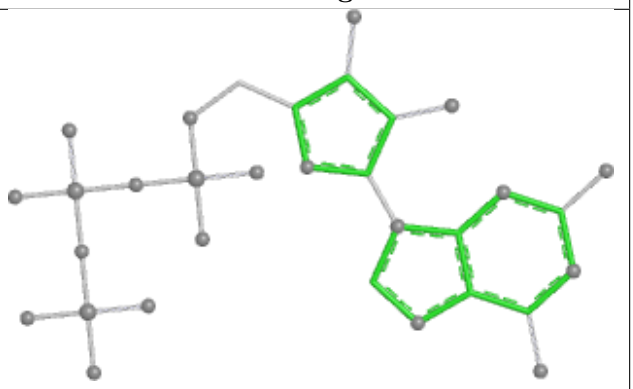
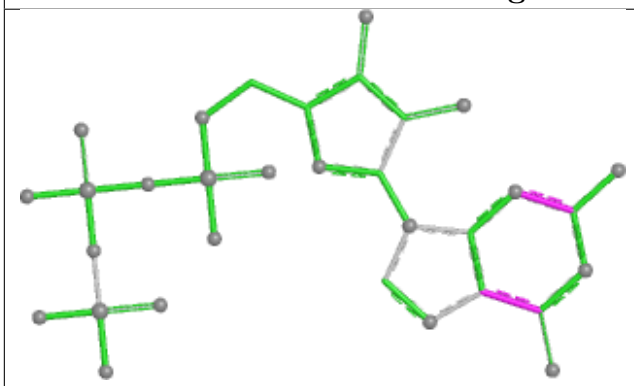


Rings

Ligand GTP ME 501



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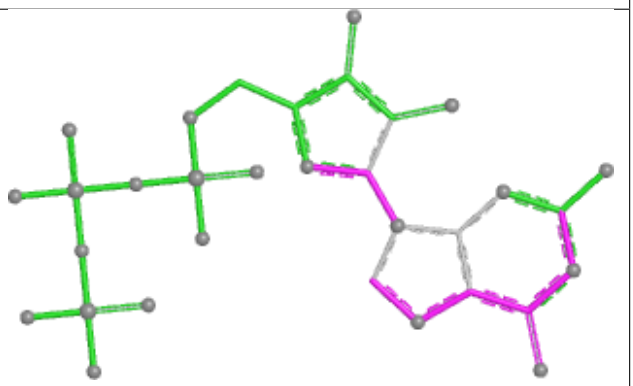

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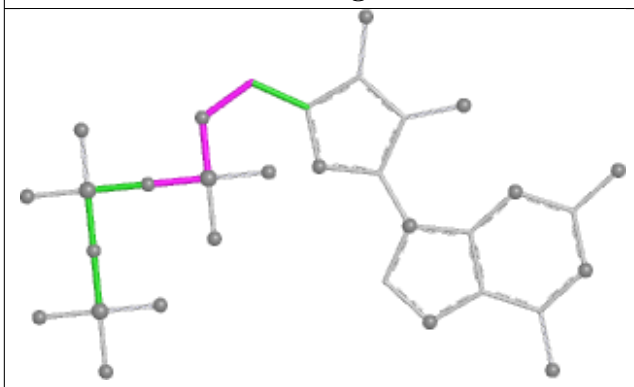

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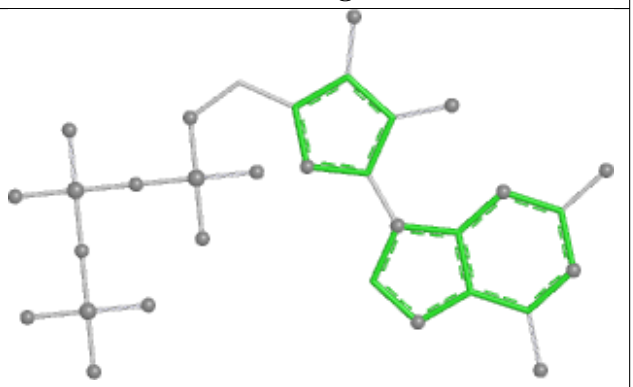
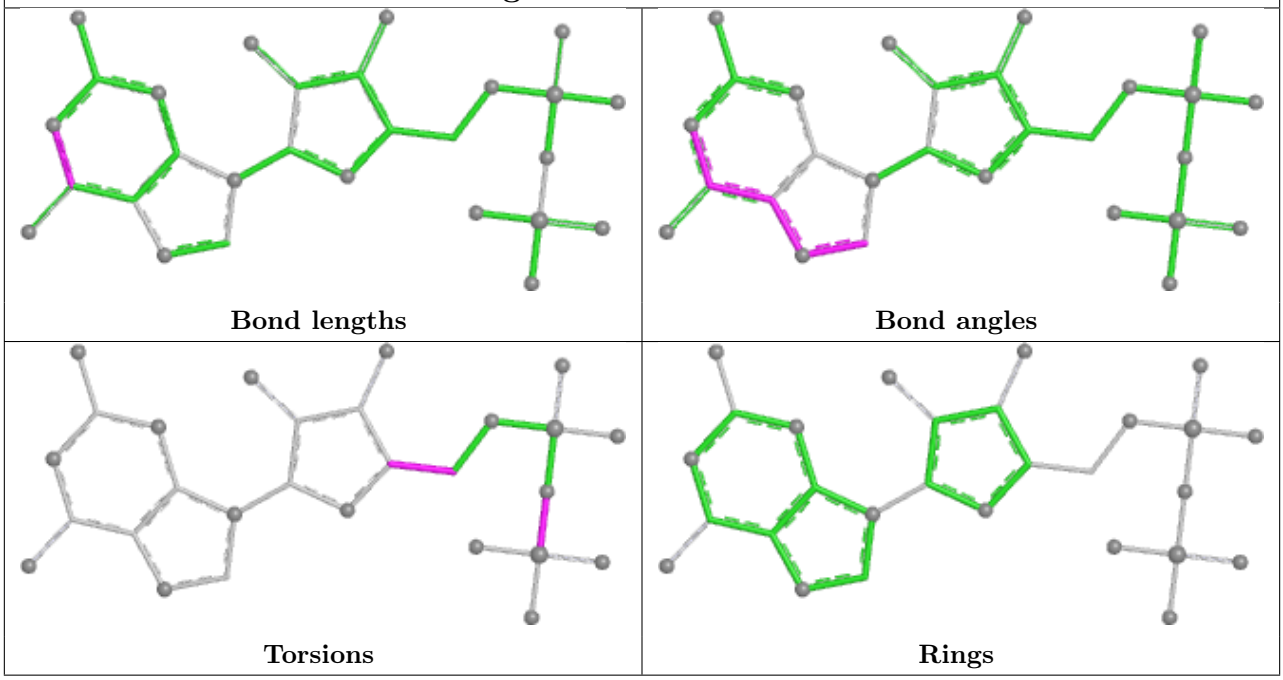


Rings

Ligand GDP WH 501



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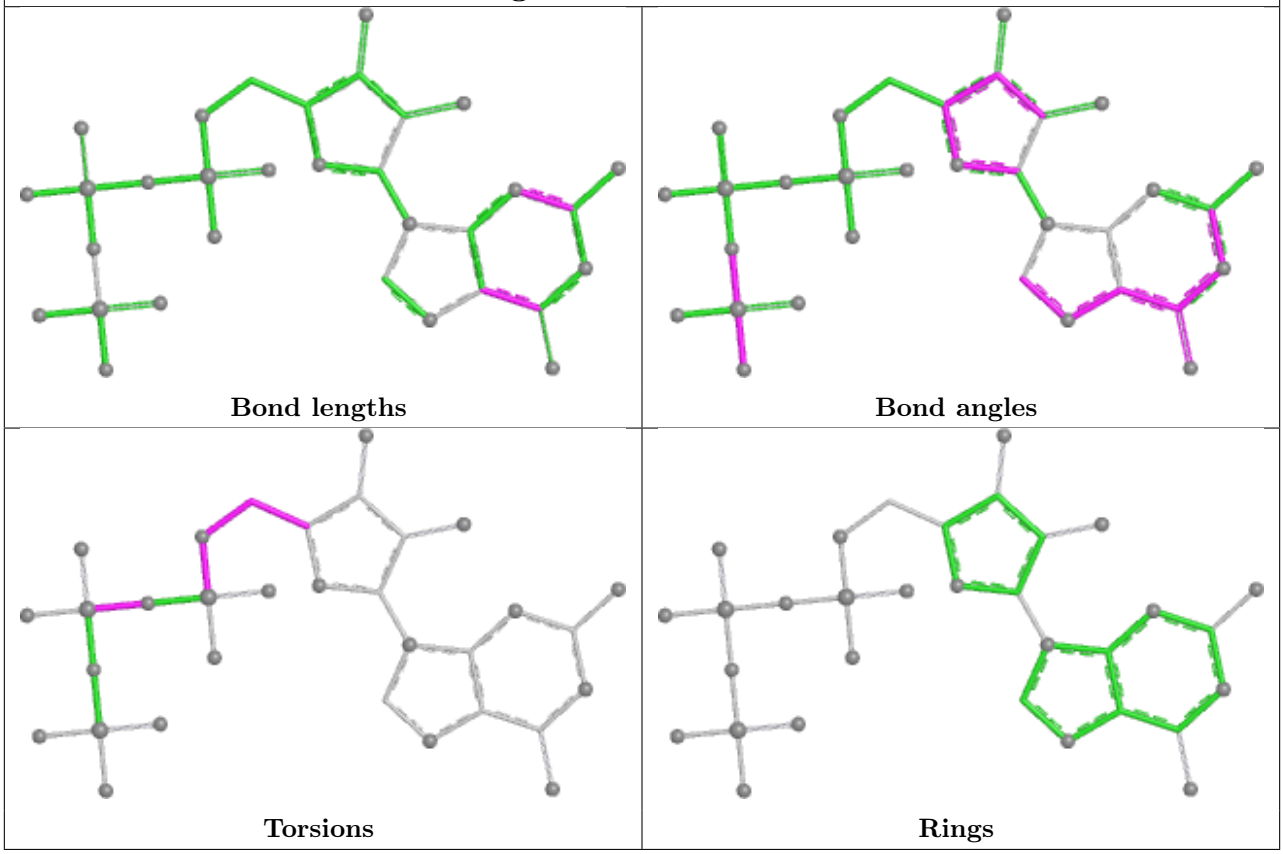

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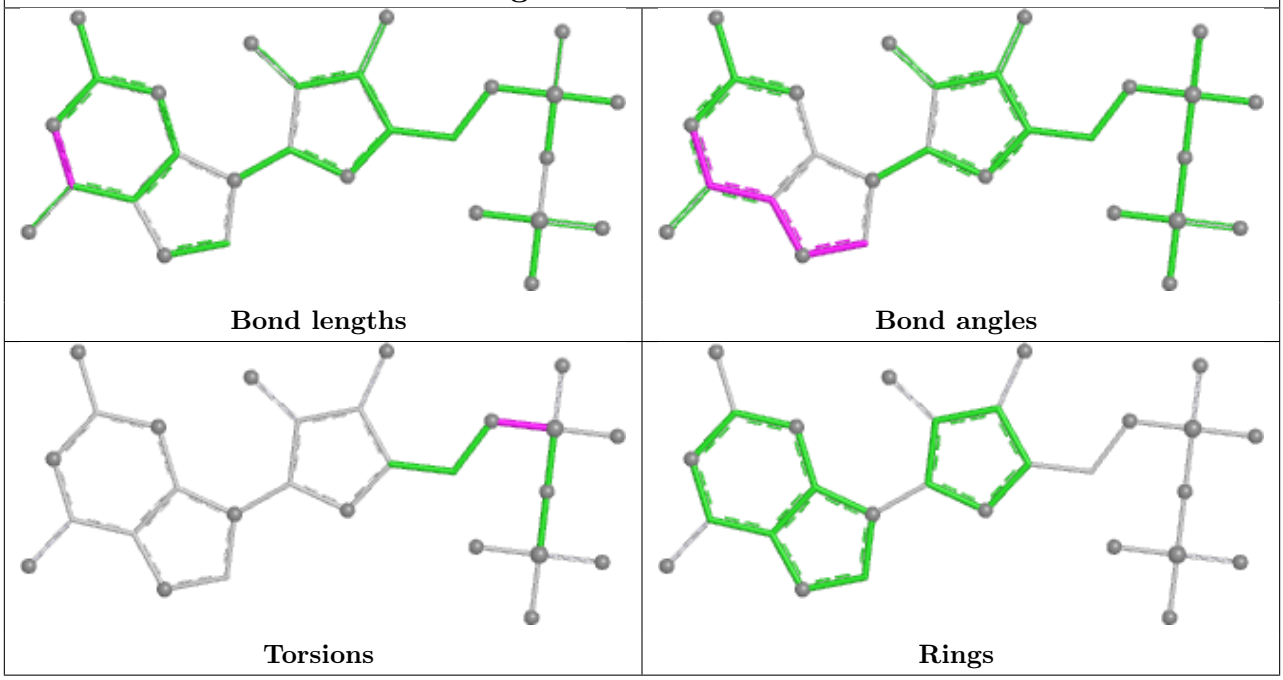

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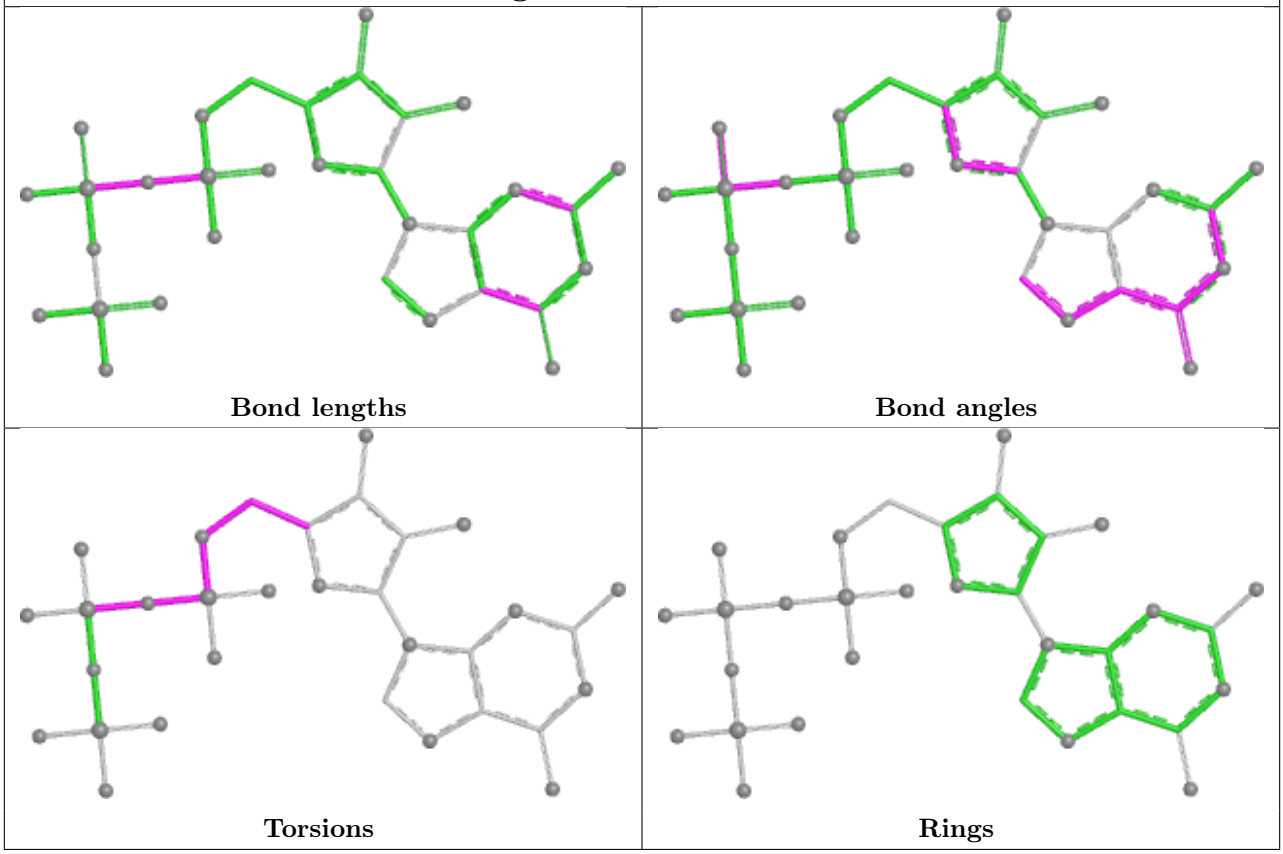

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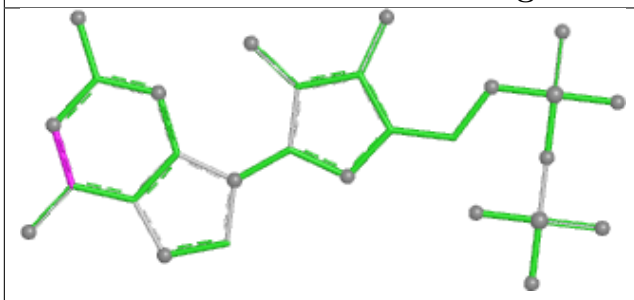

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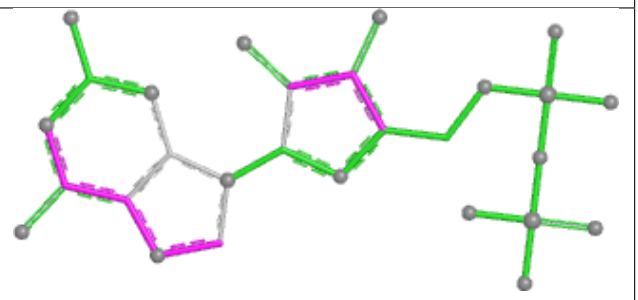
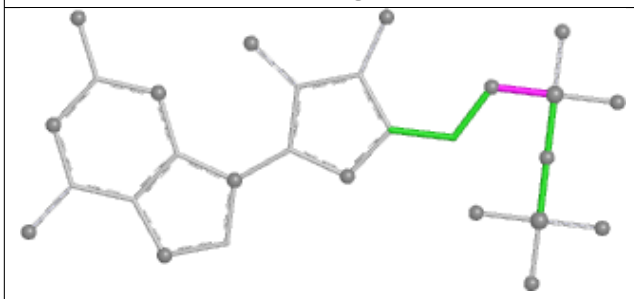
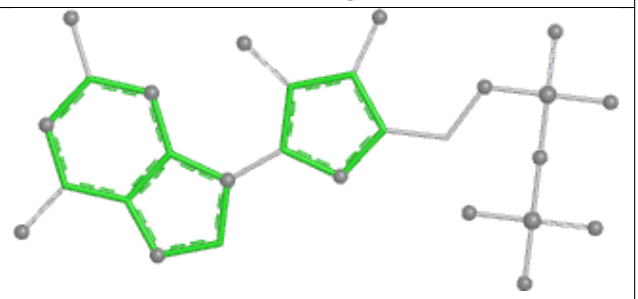


Bond angles



Torsions



Rings

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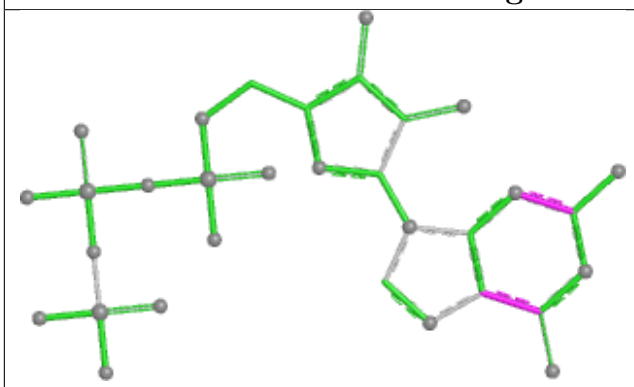

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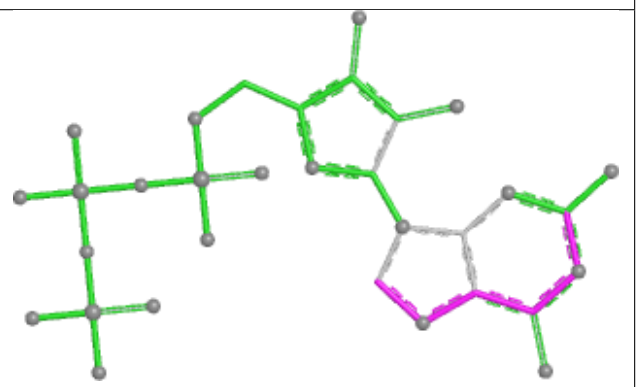

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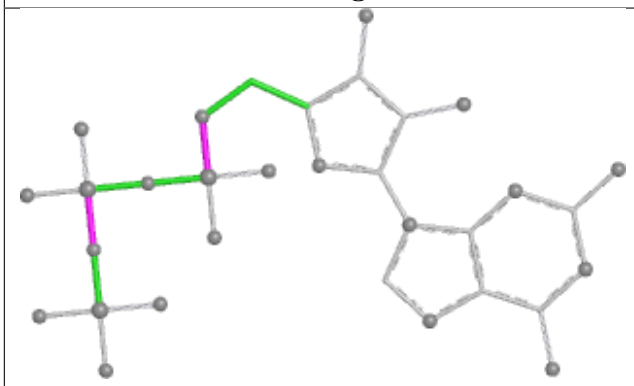

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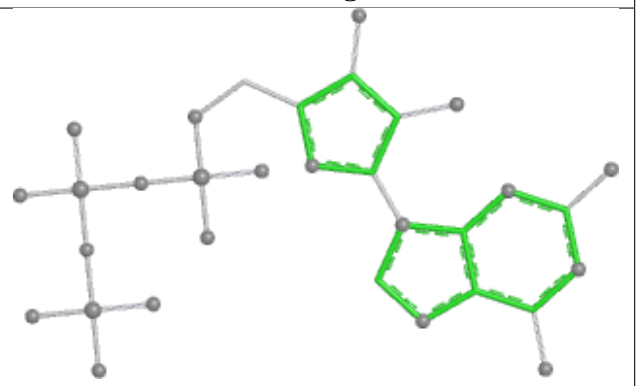
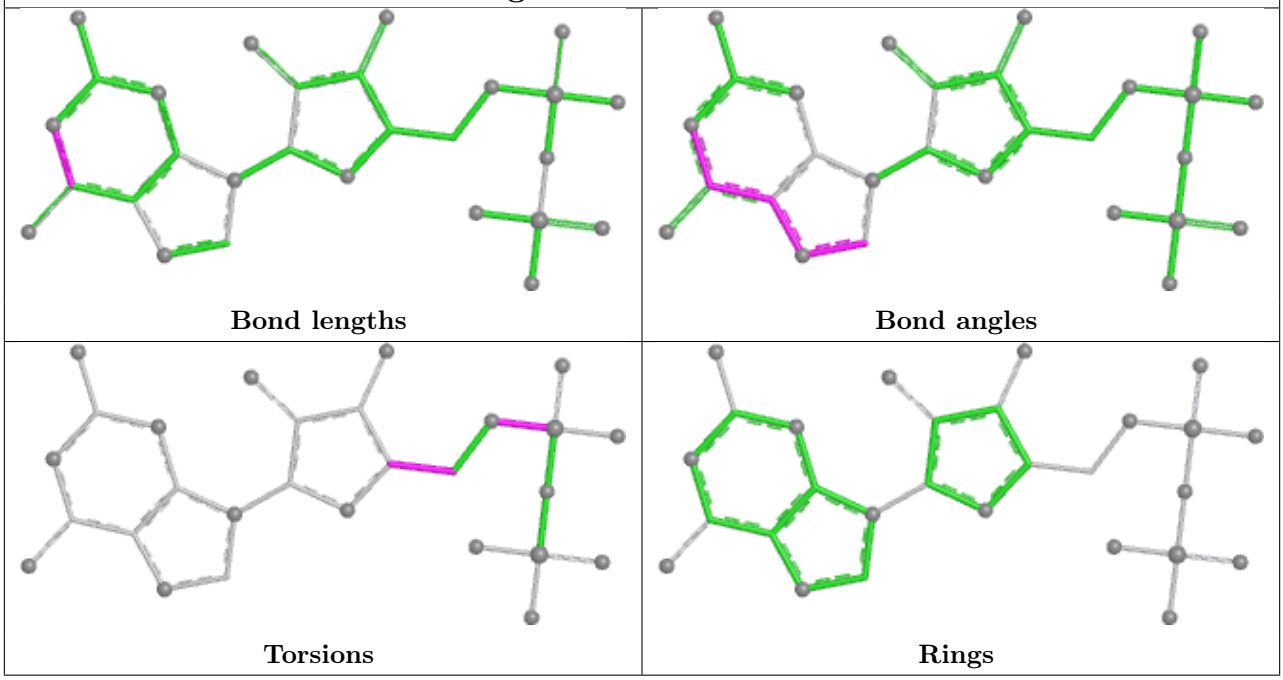


Rings

Ligand GDP WJ 501



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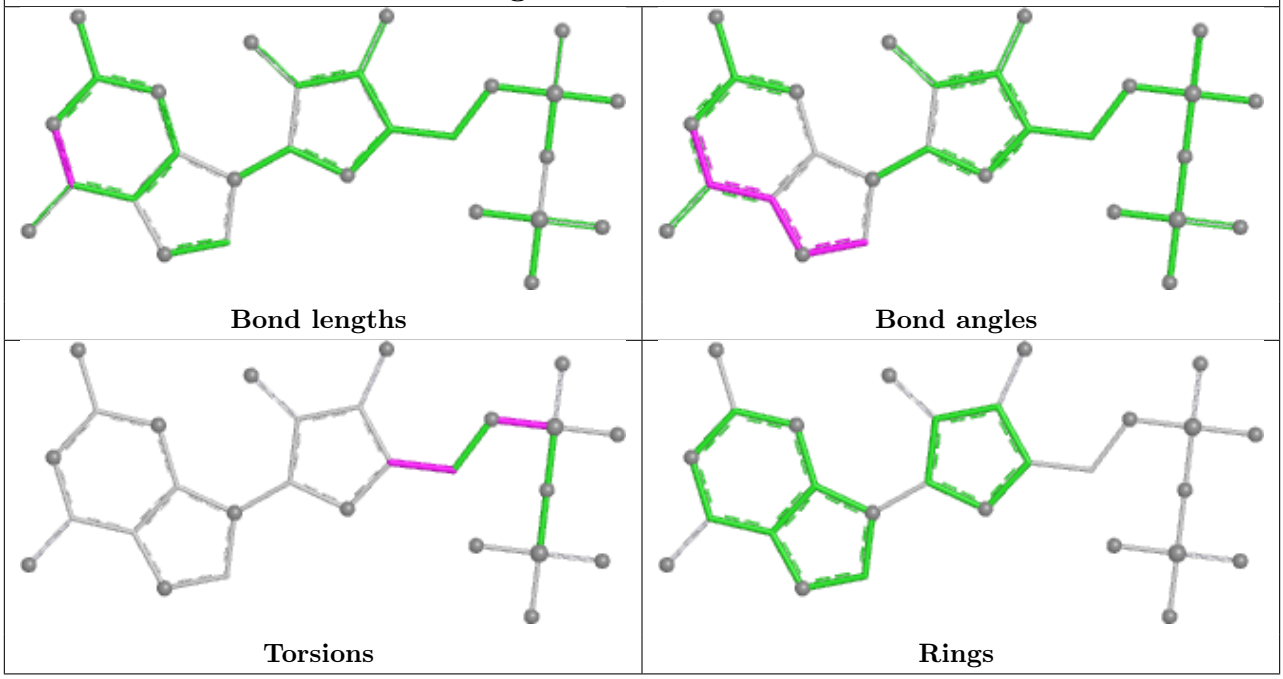
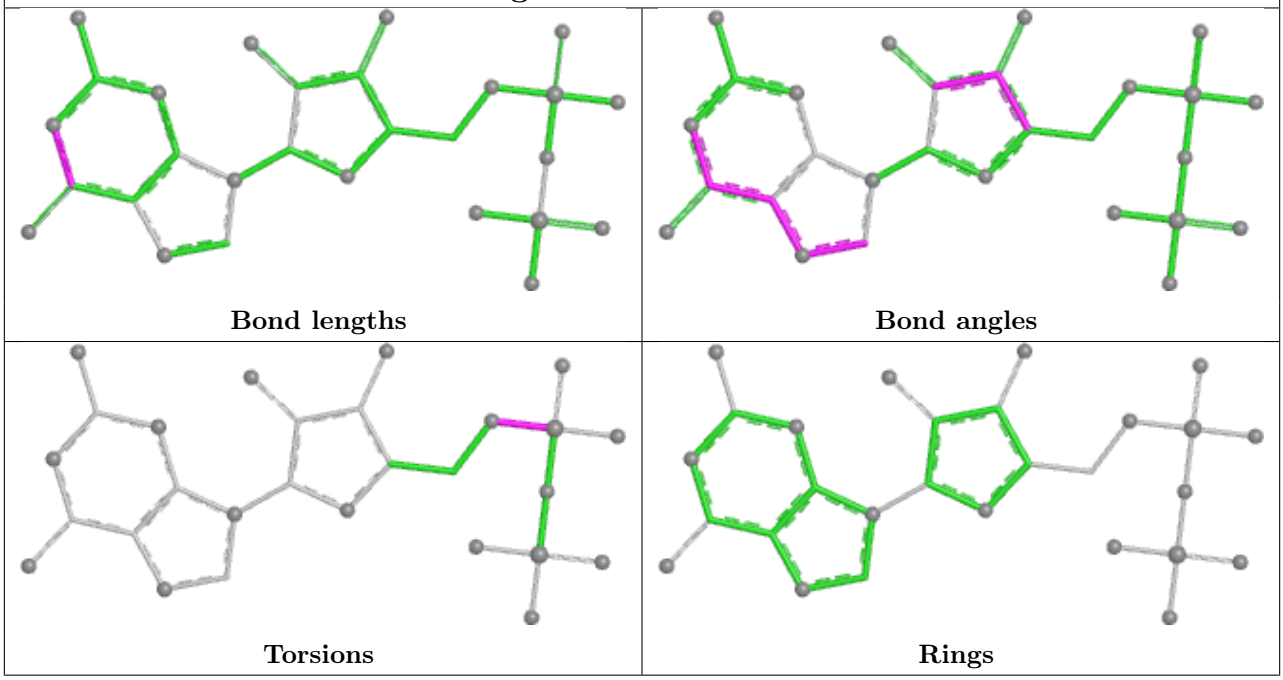


Ligand GDP VF 501



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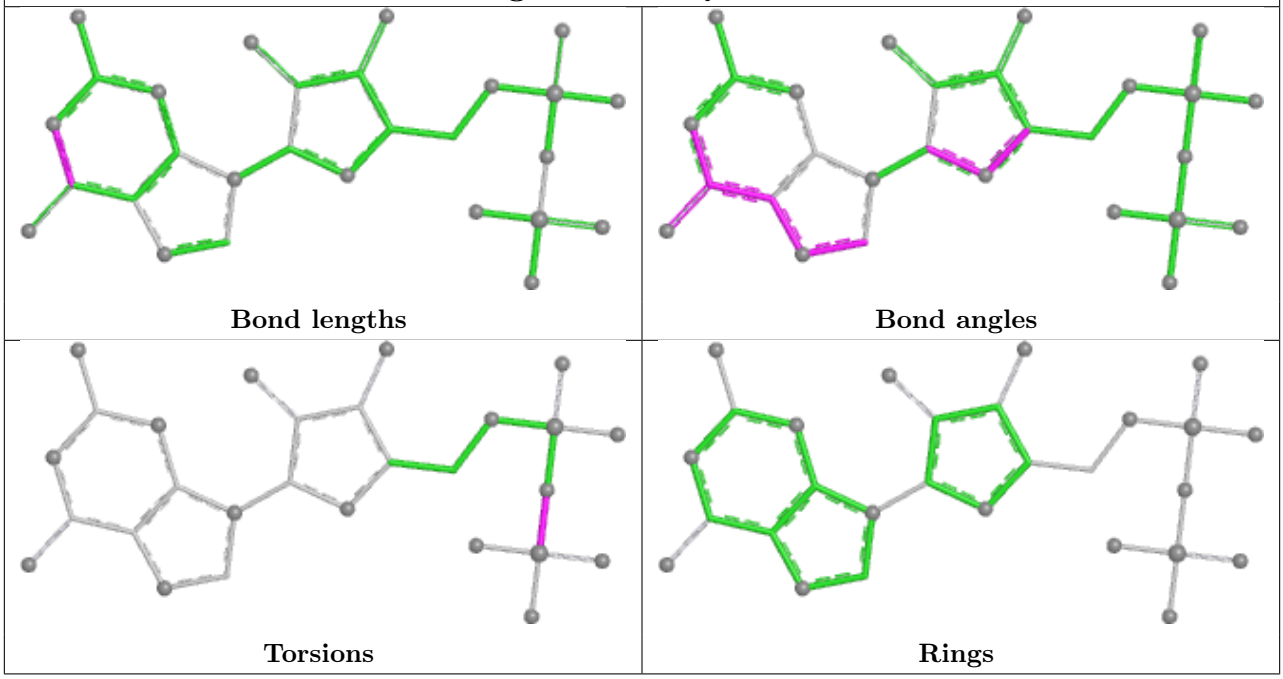

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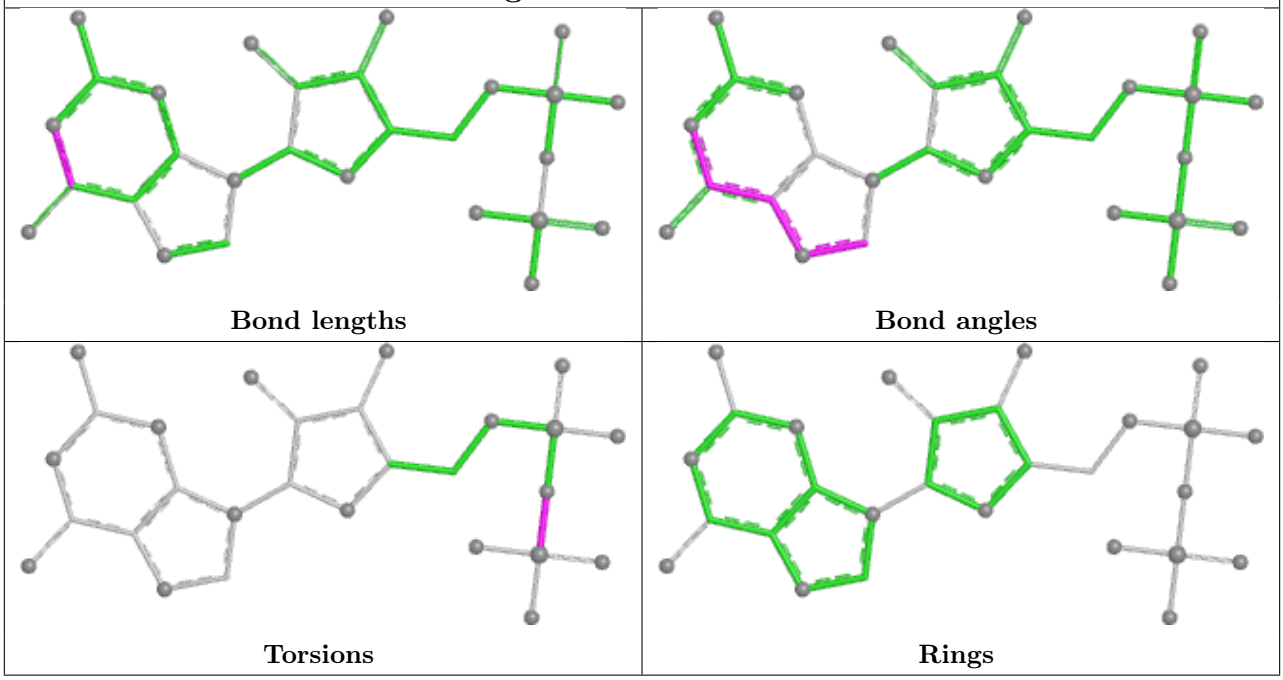
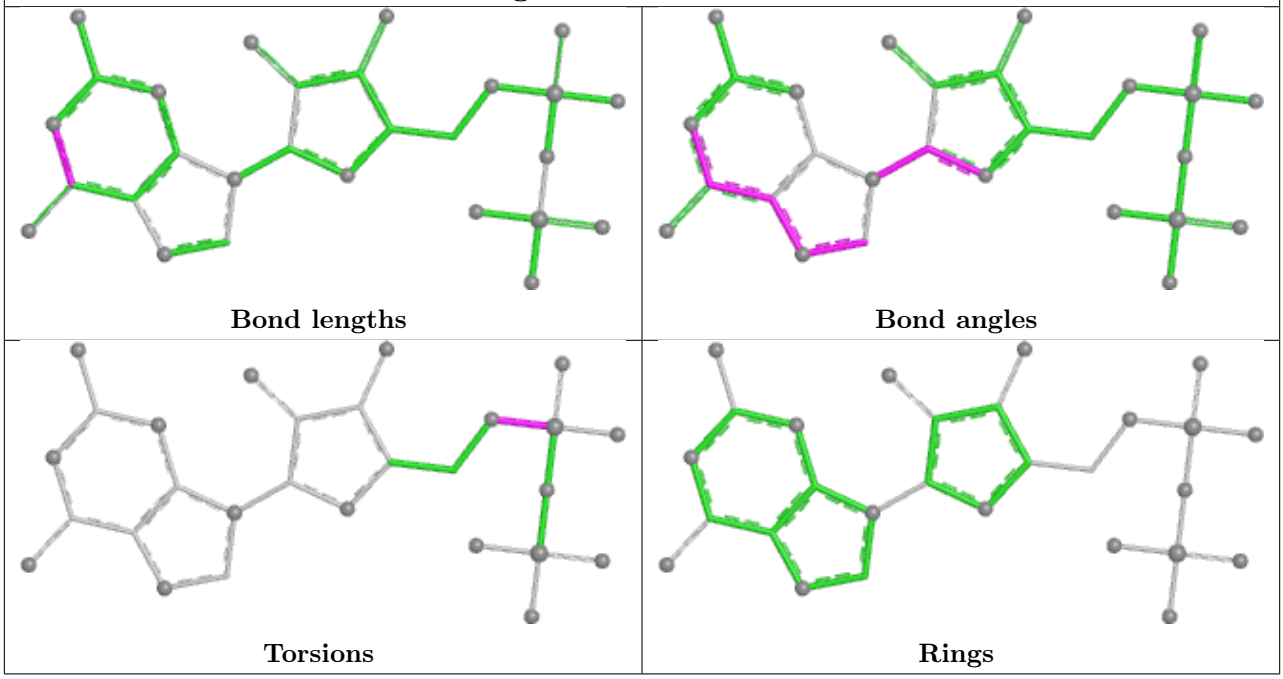


Ligand GDP PF 501



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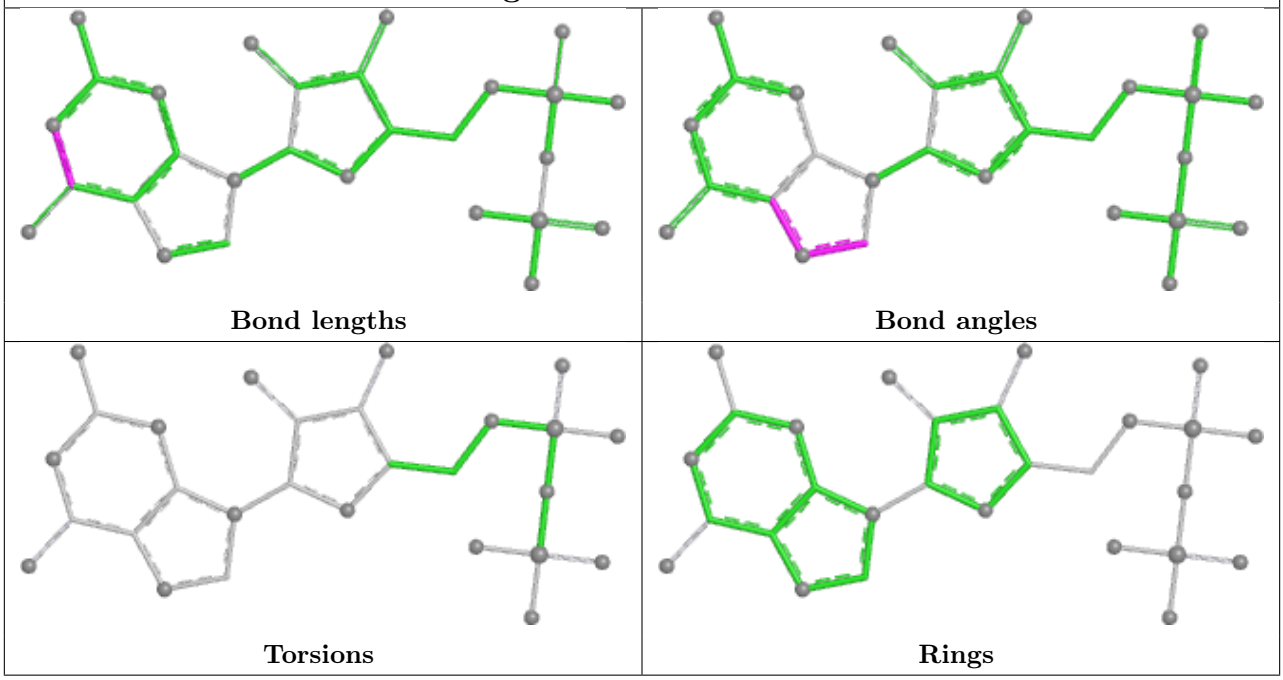

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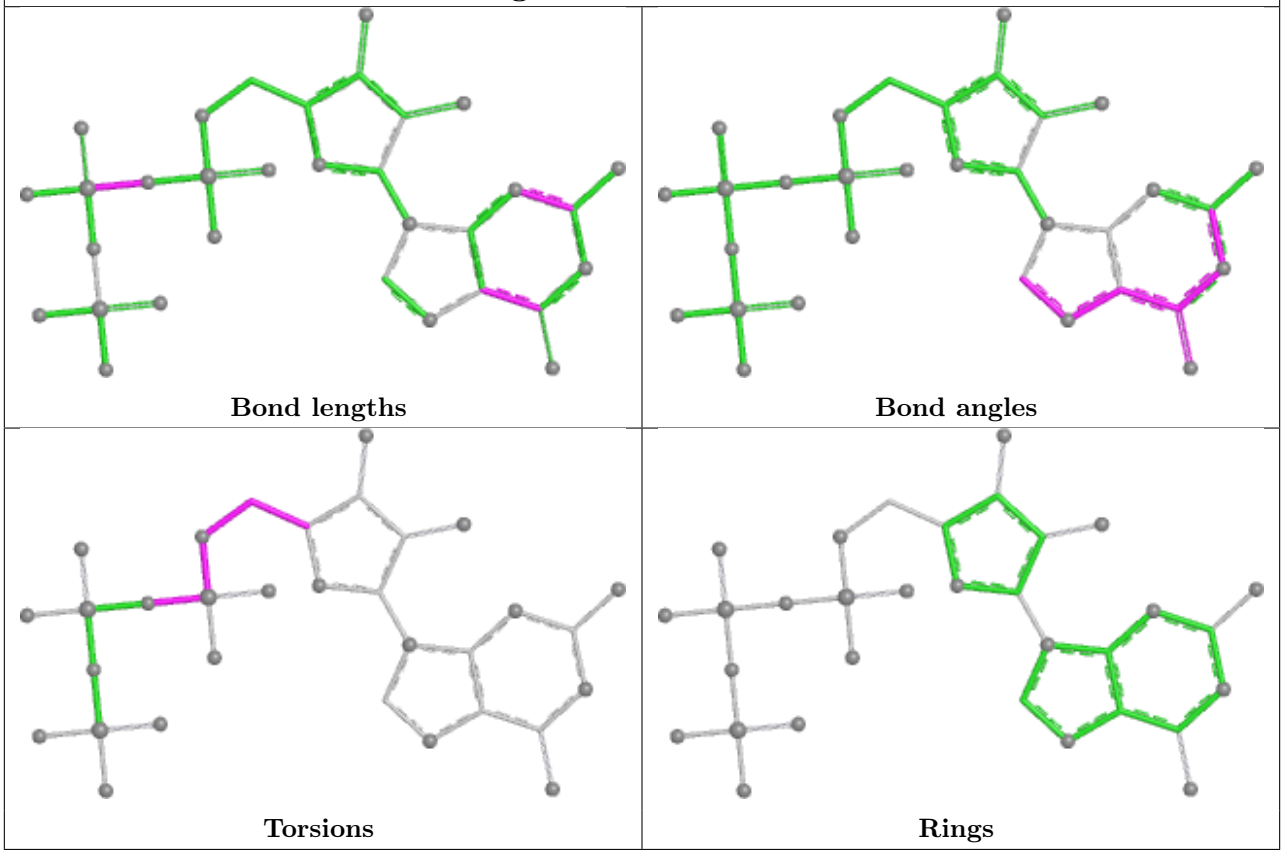

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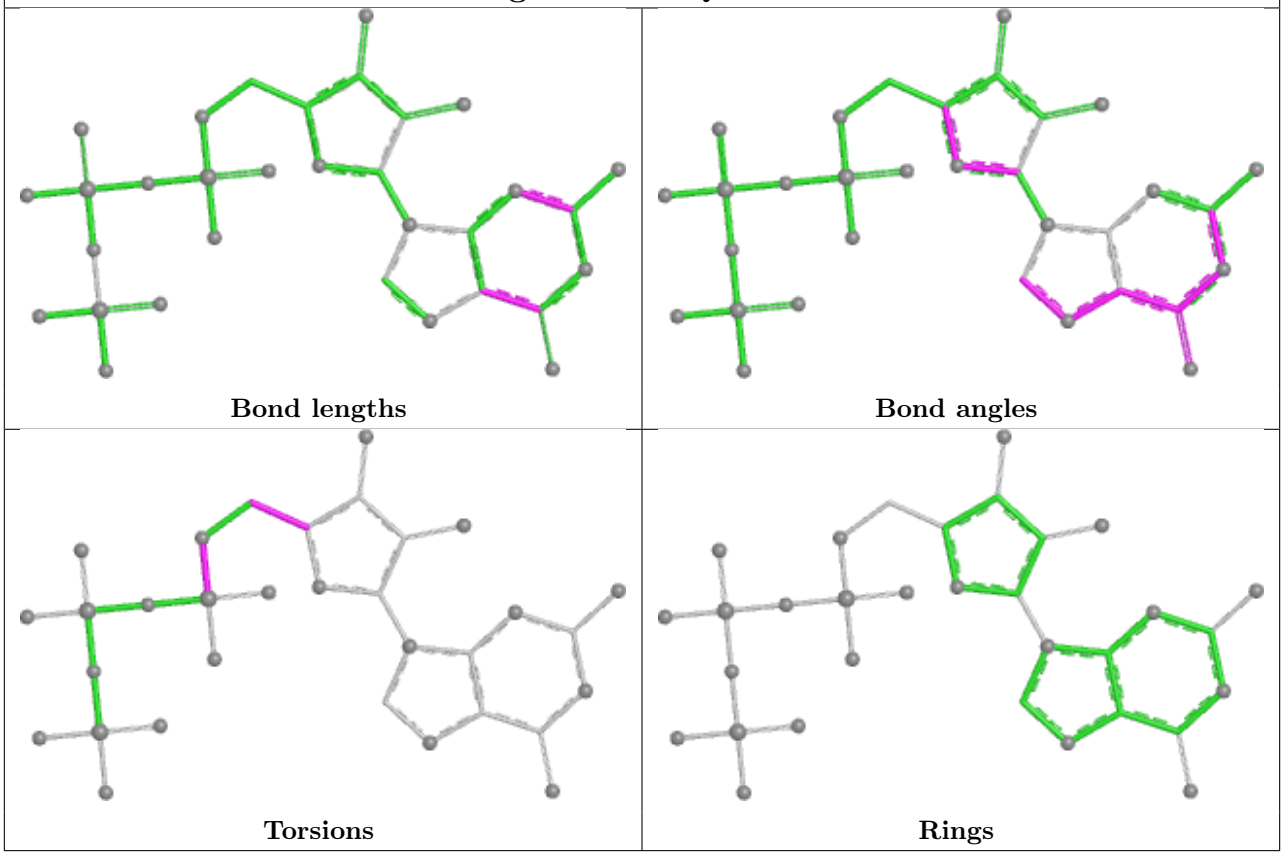

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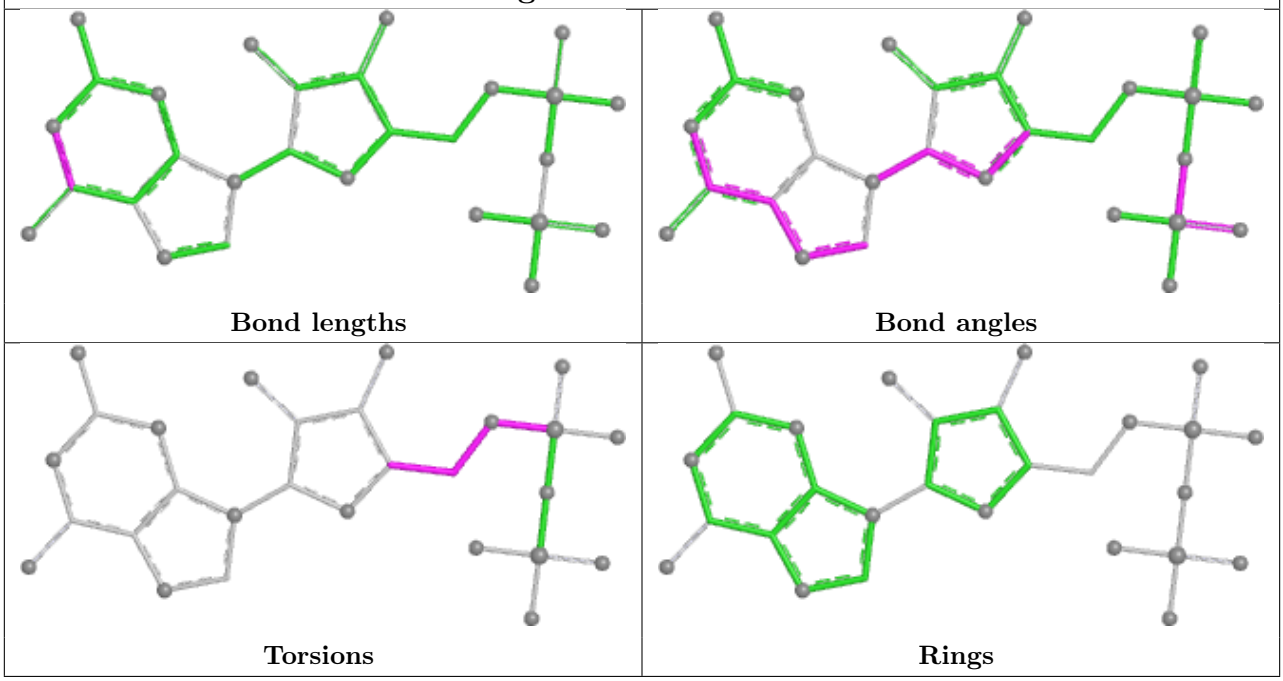

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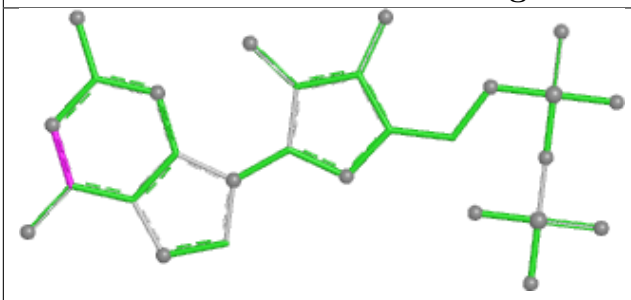
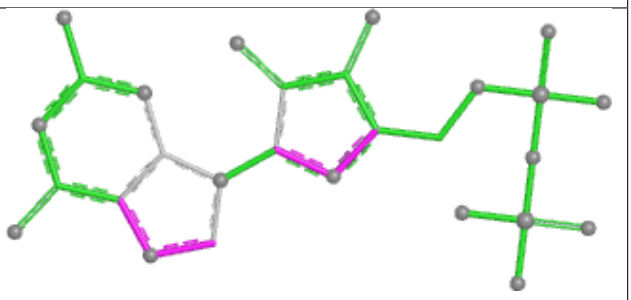
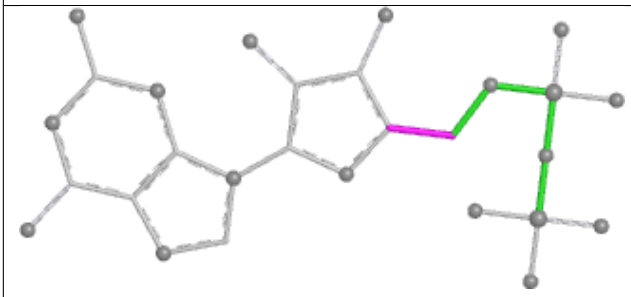


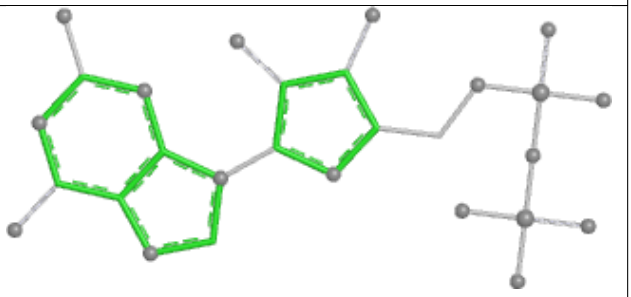
Bond lengths



Bond angles

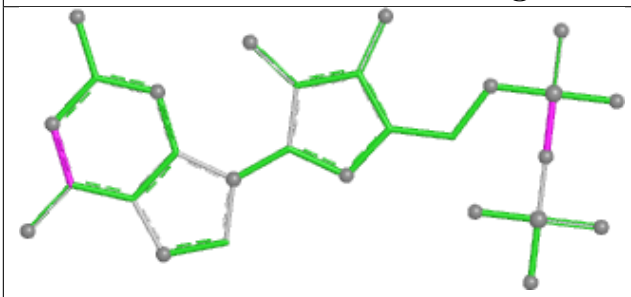


Torsions



Rings

Ligand GDP BL 501



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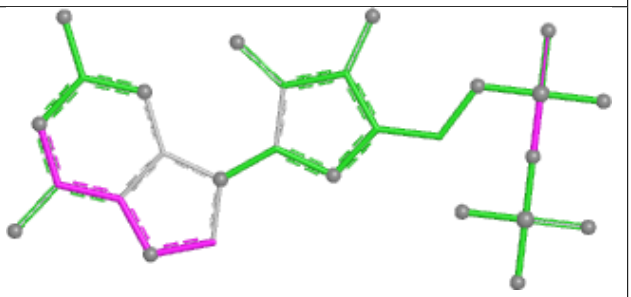
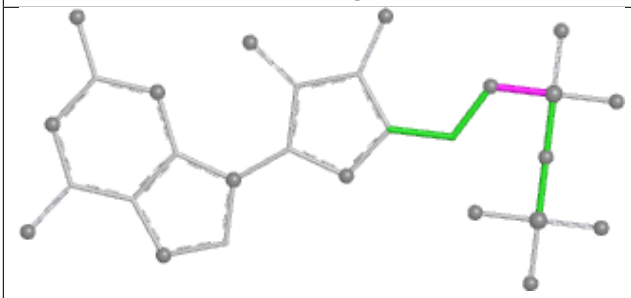
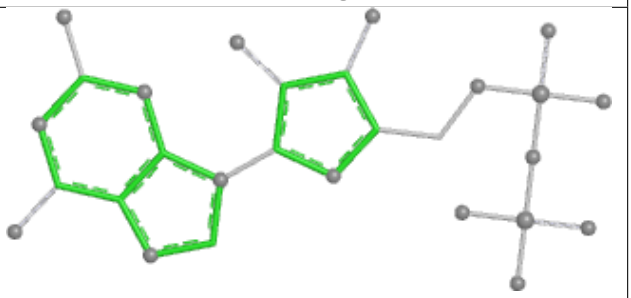


Bond angles



Torsions



Rings

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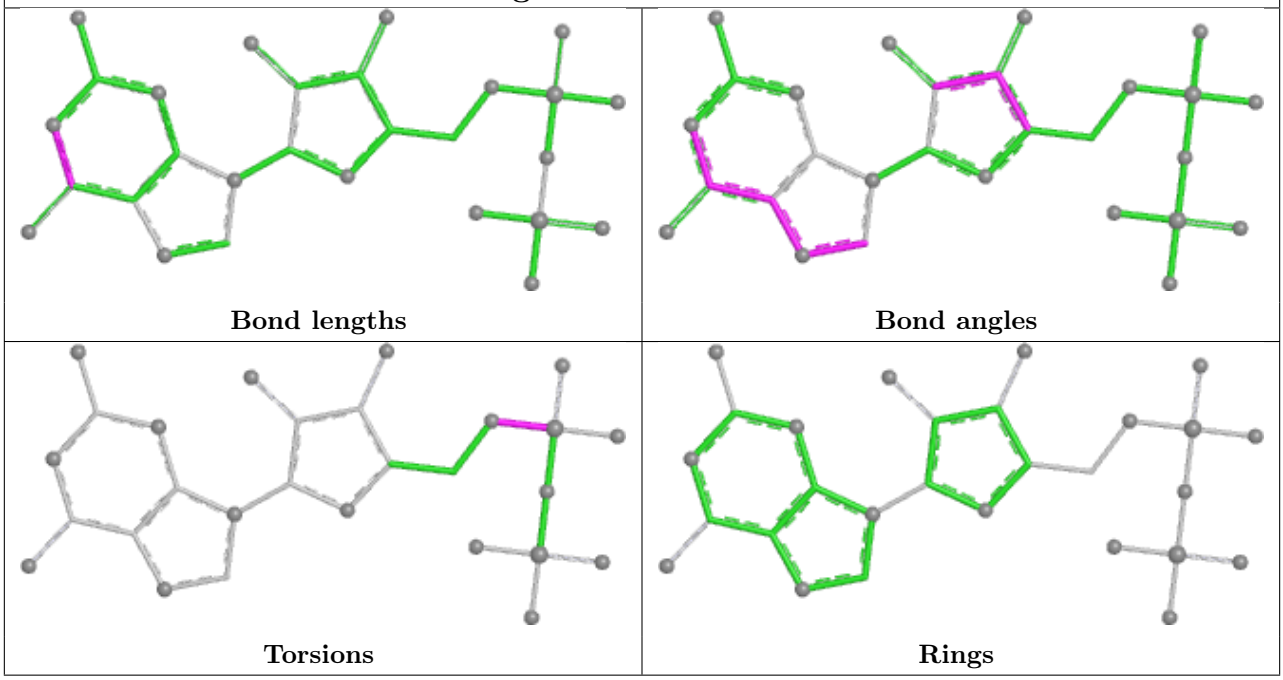

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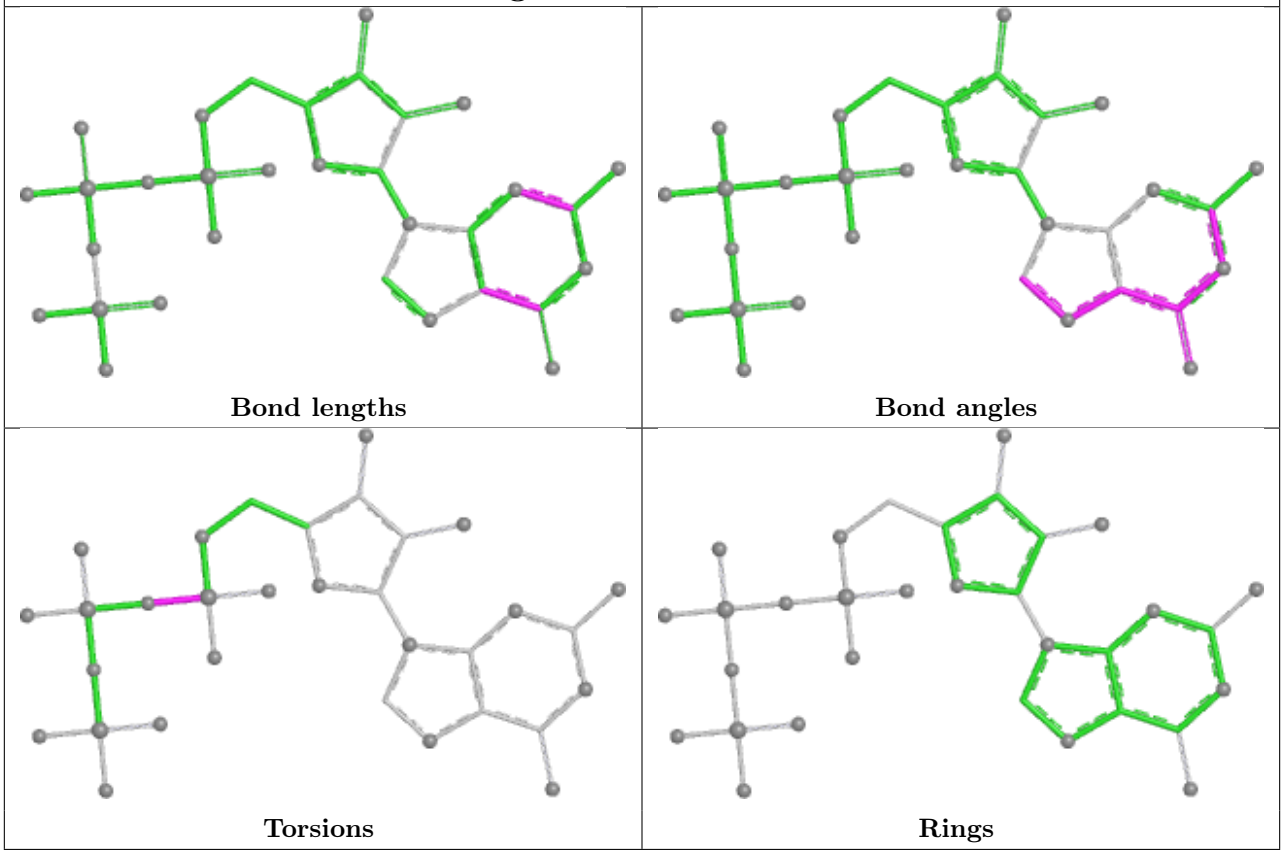

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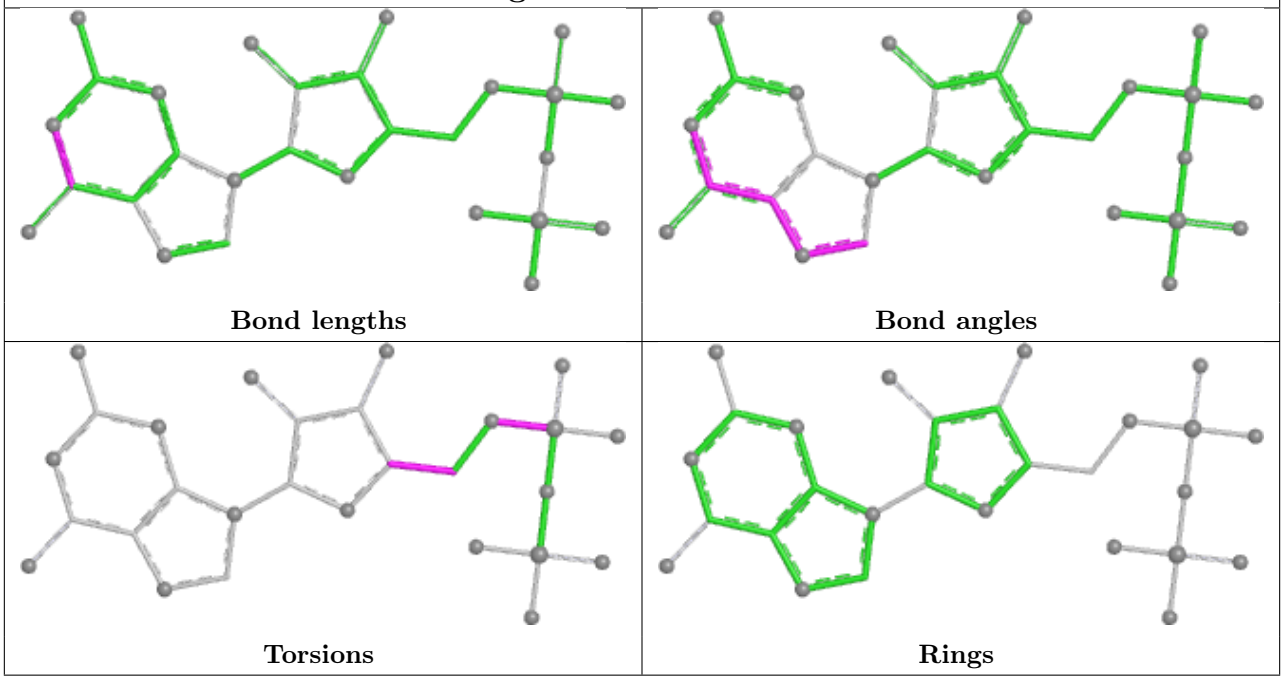

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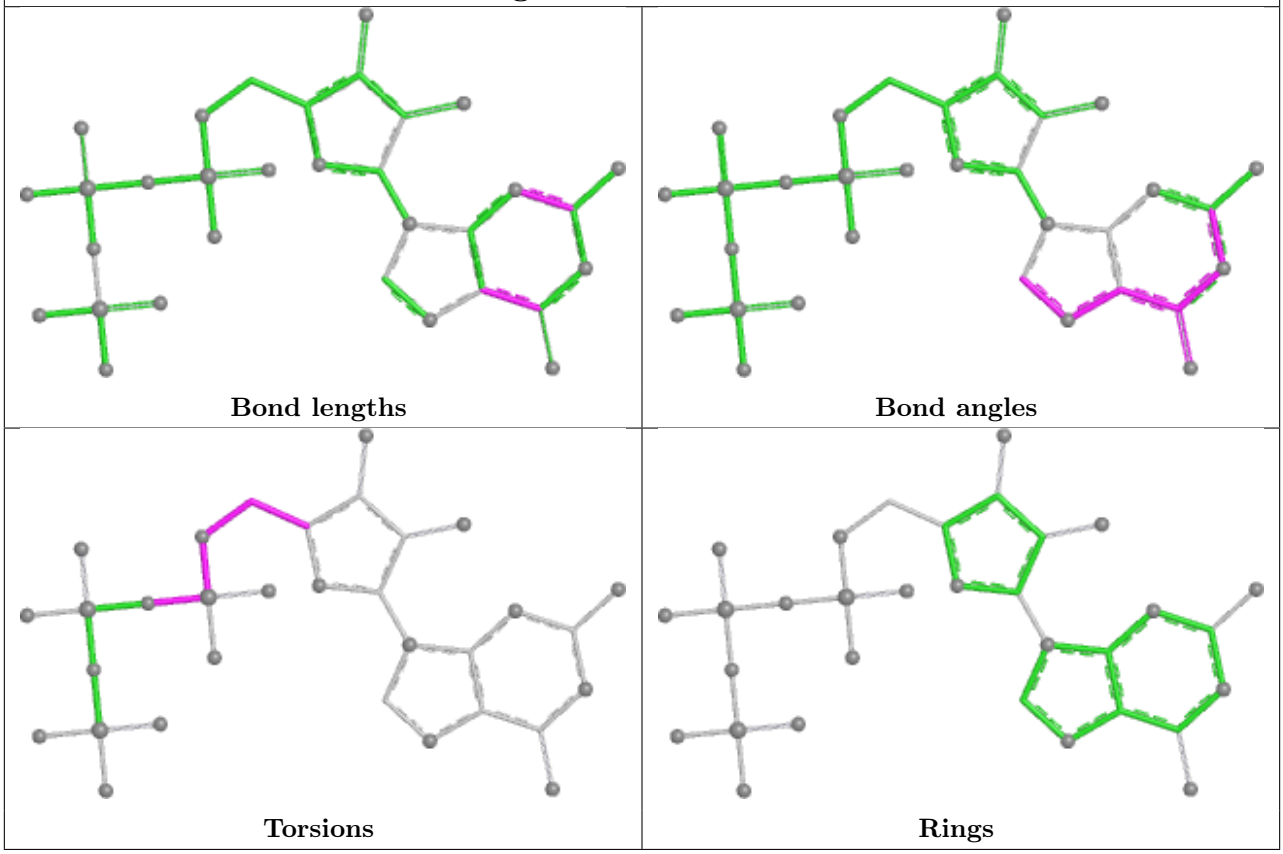

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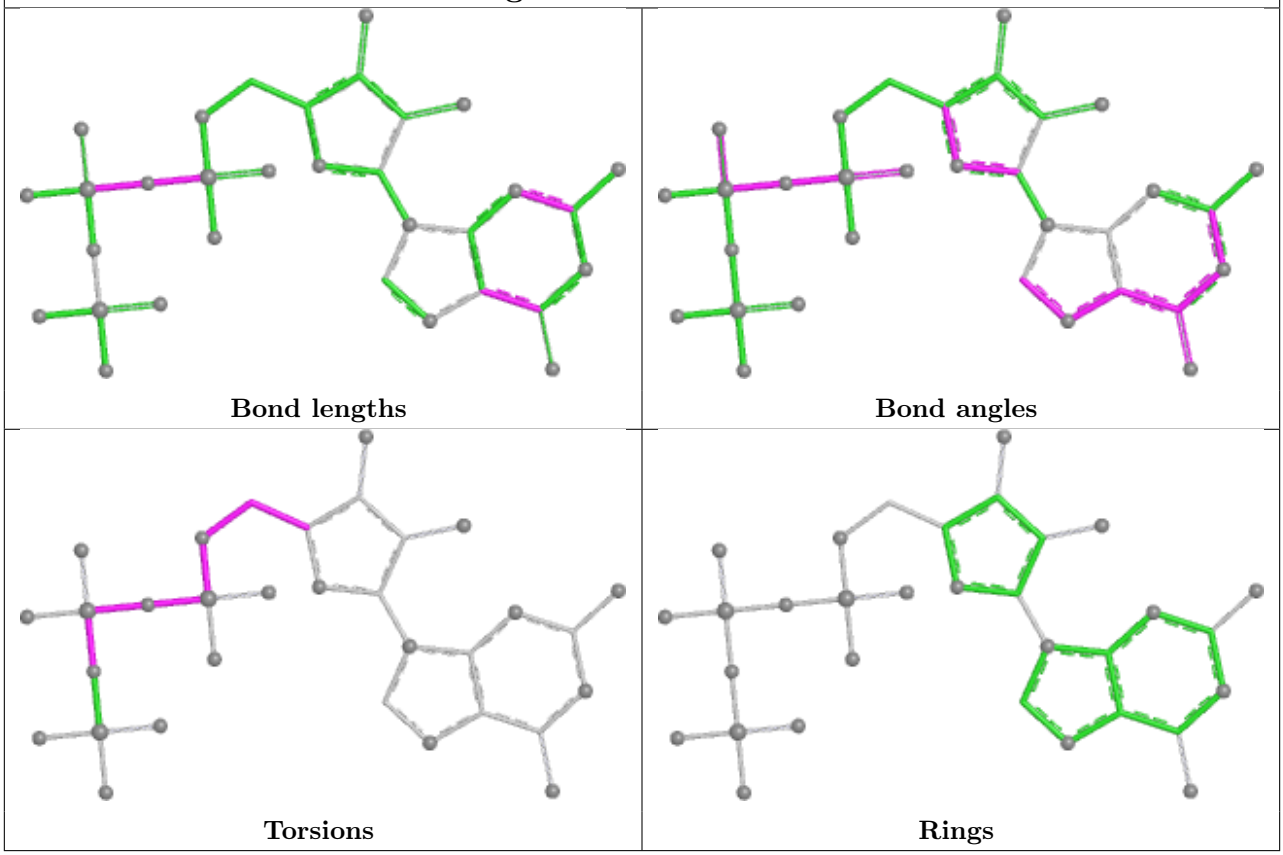

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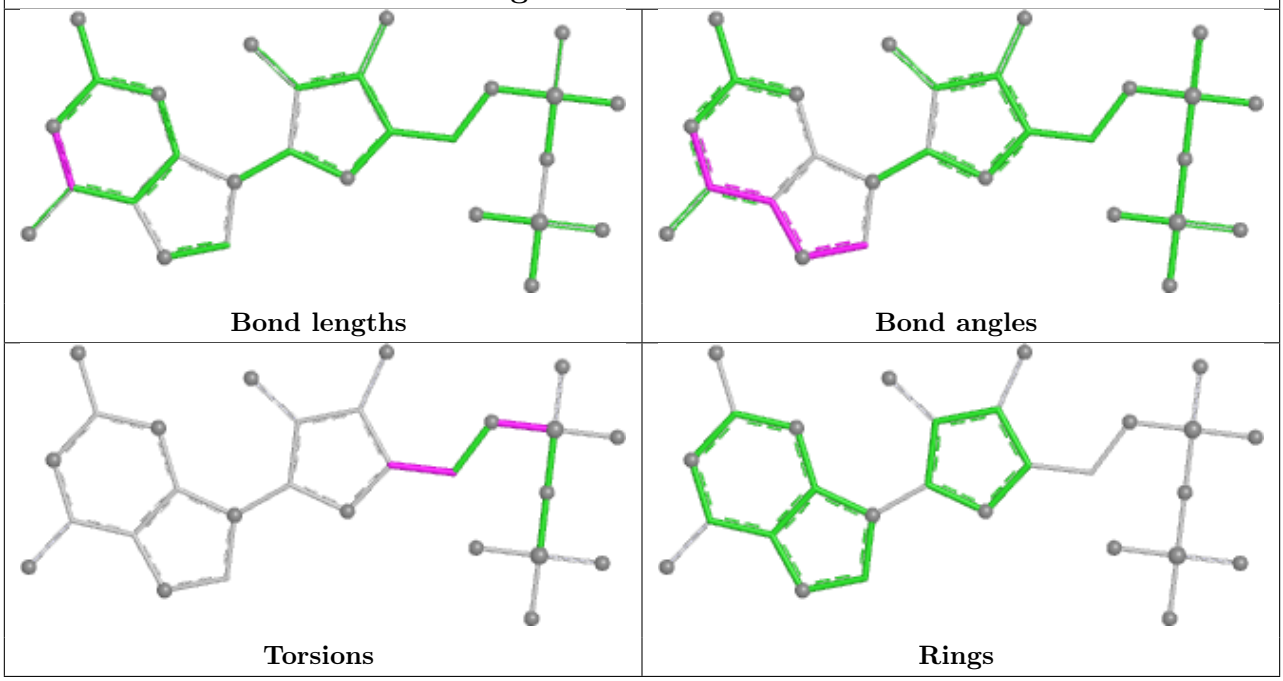

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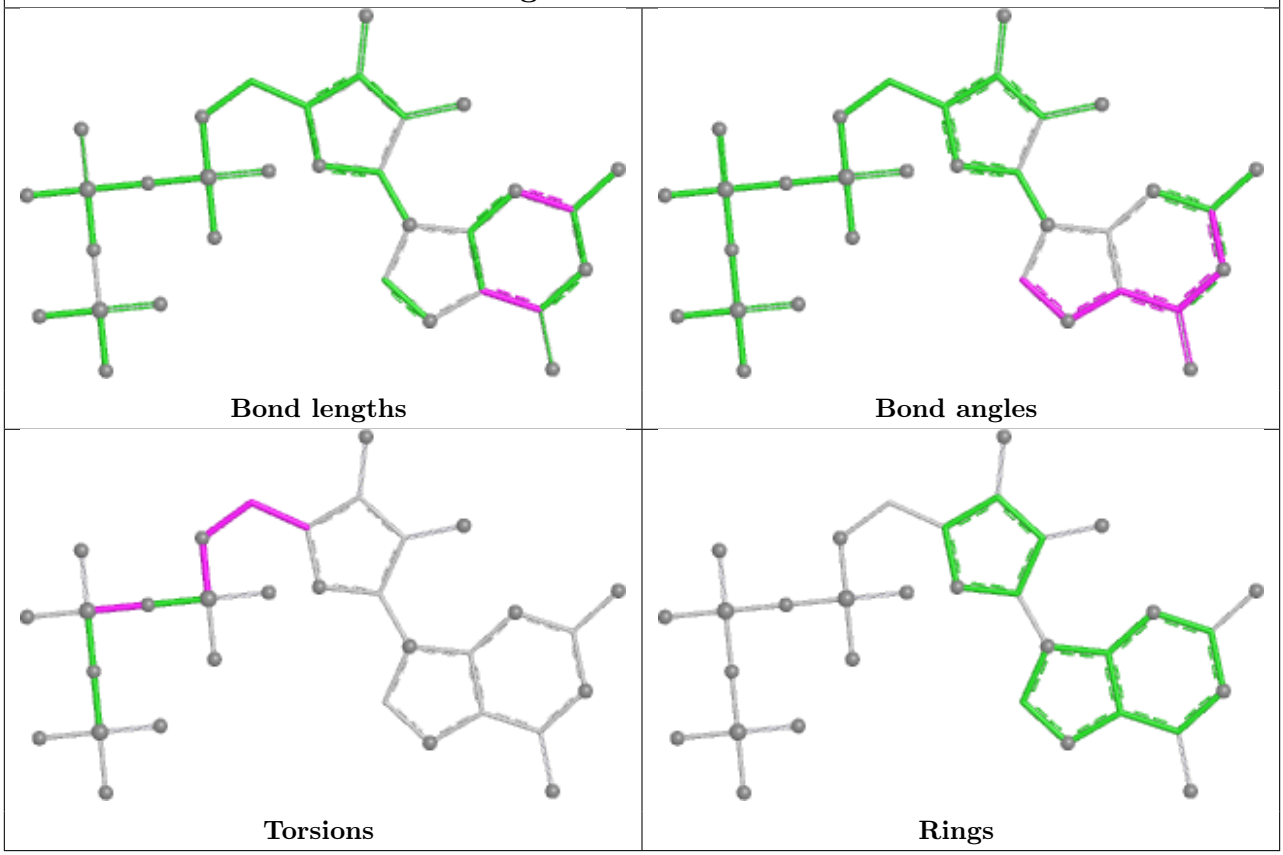

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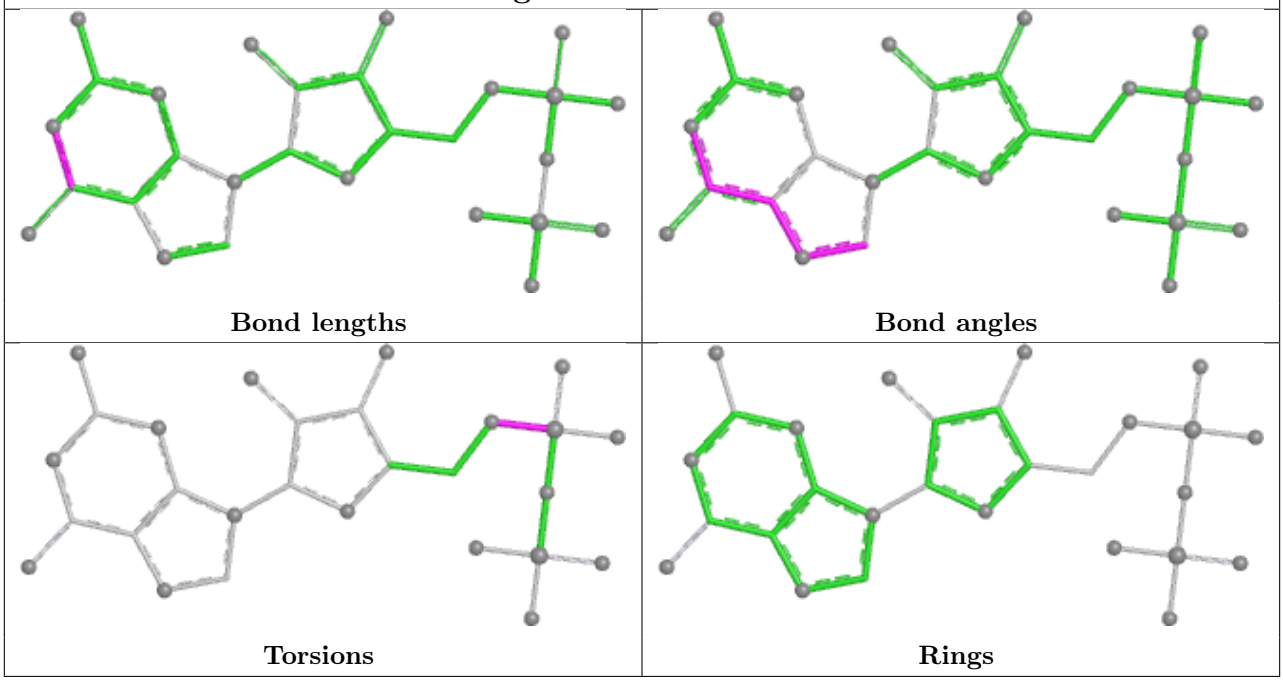

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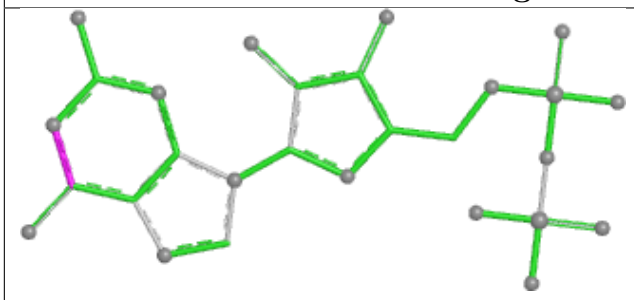
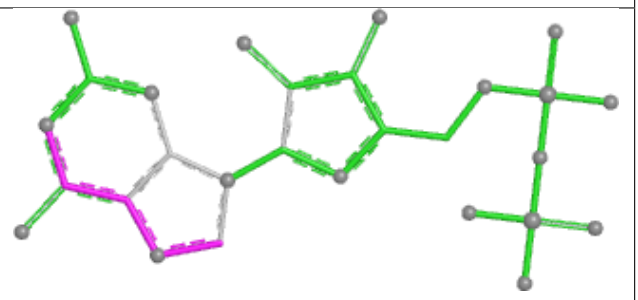
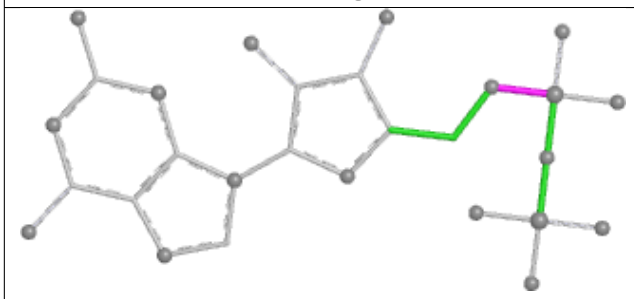


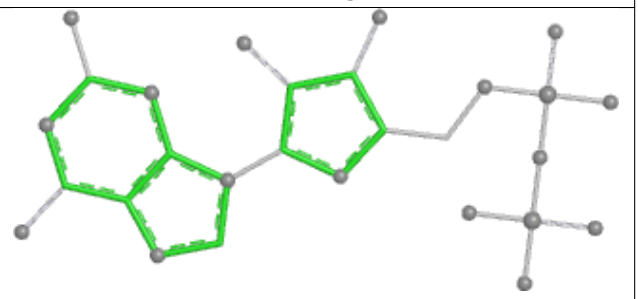
Bond lengths



Bond angles

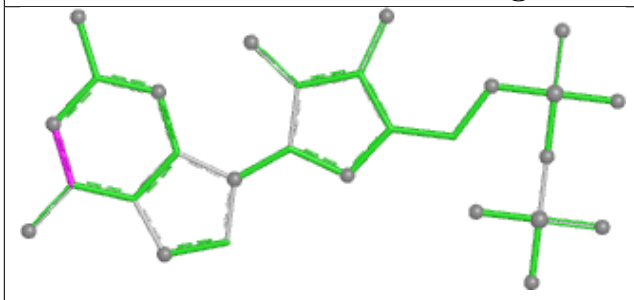


Torsions



Rings

Ligand GDP GF 501



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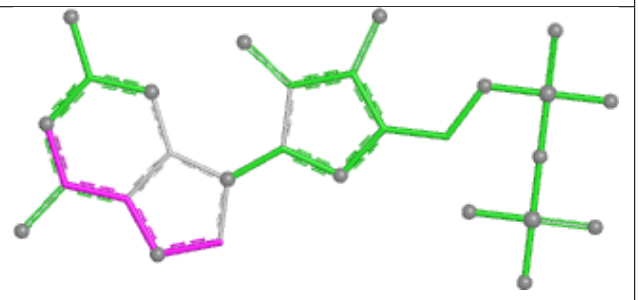

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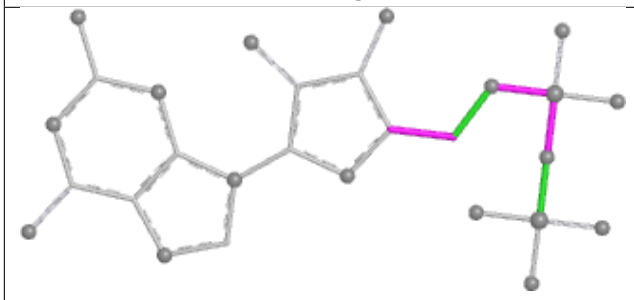

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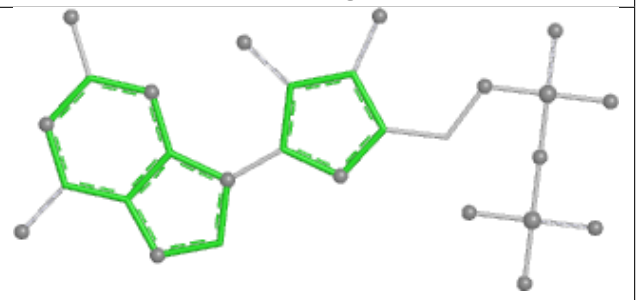

Rings

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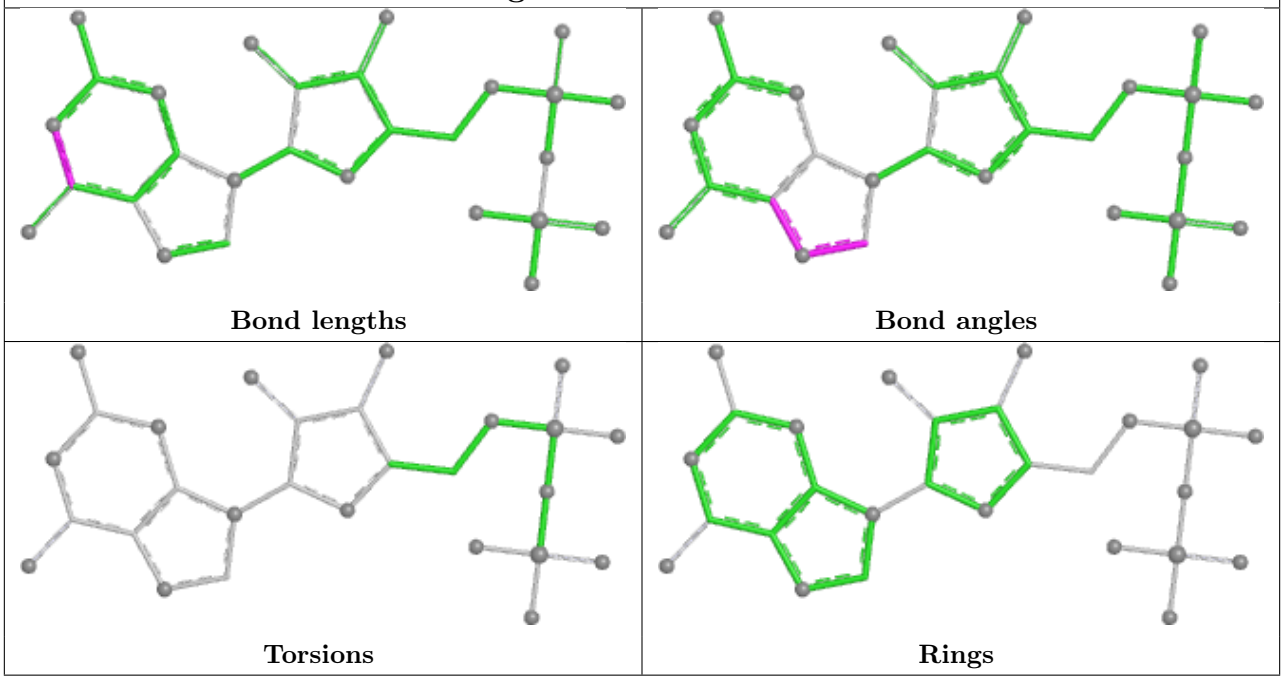

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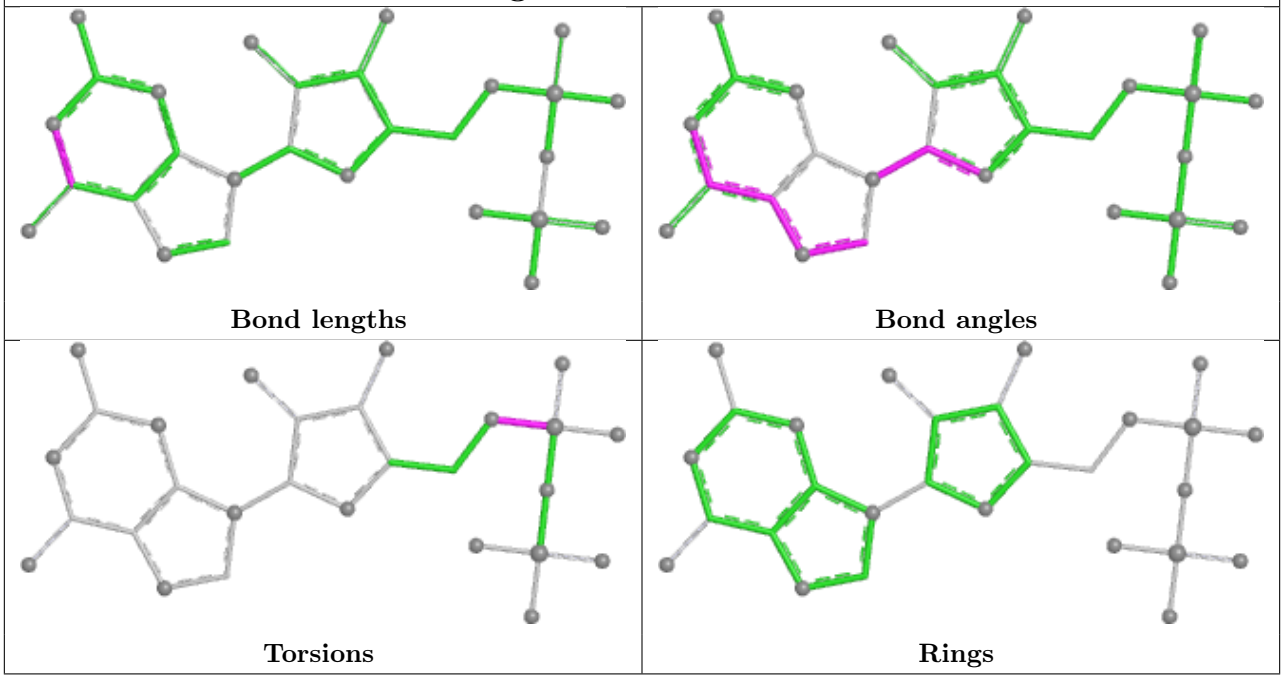

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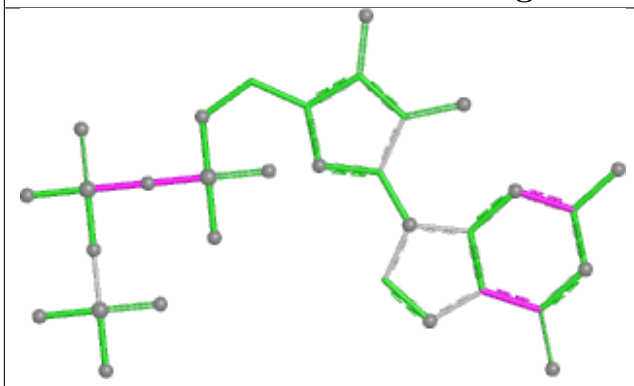

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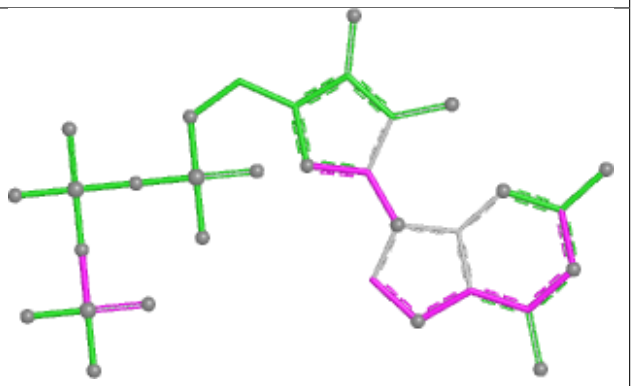
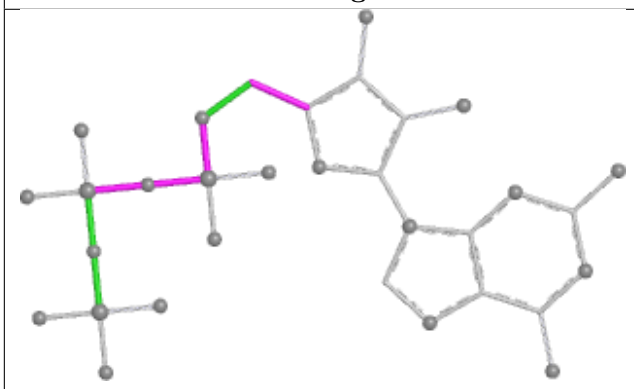


Bond angles



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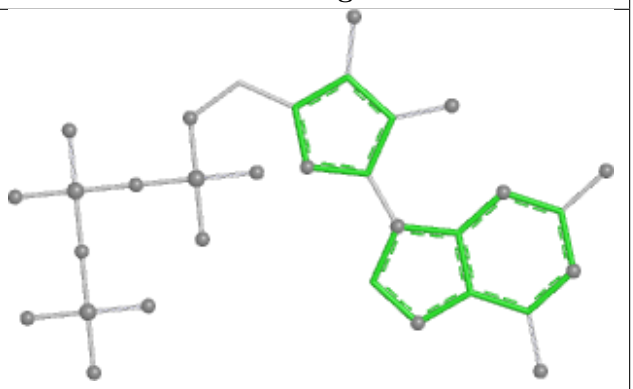

Rings

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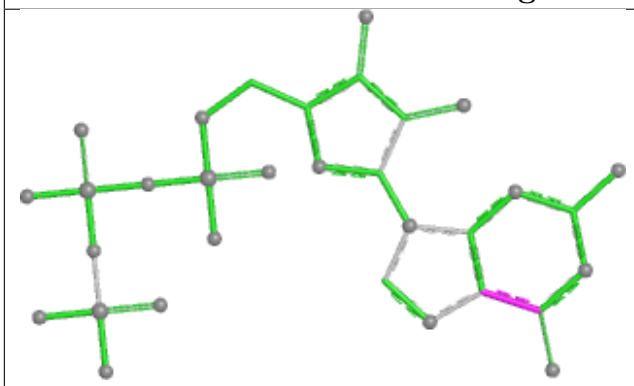

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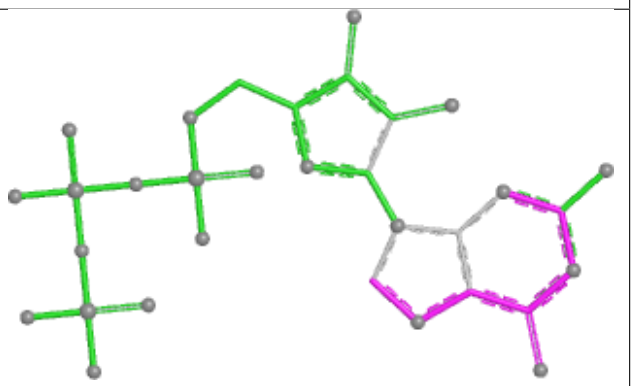

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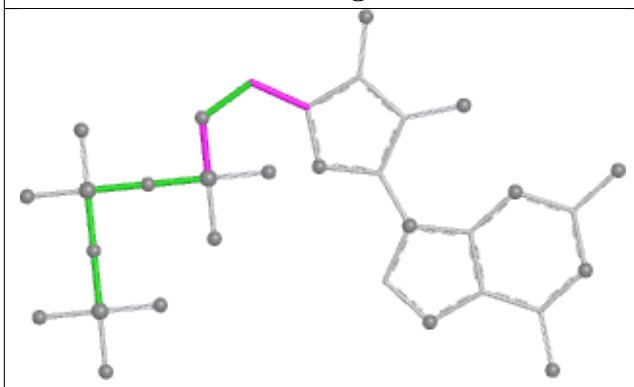

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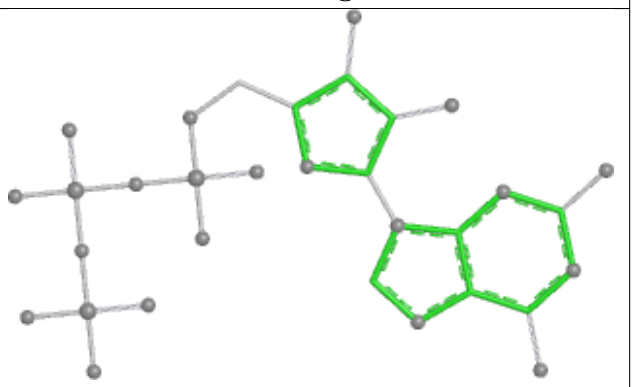

Rings

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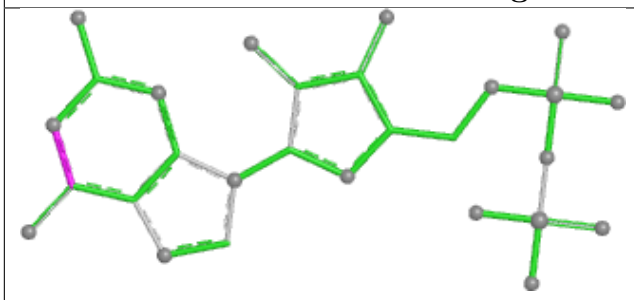

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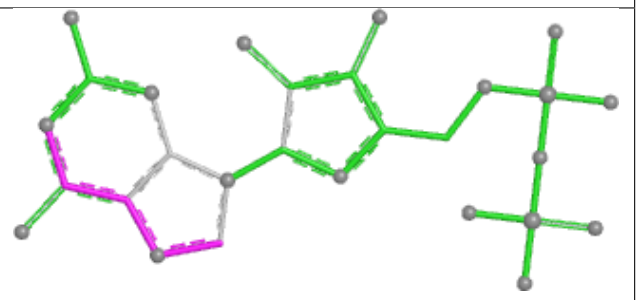

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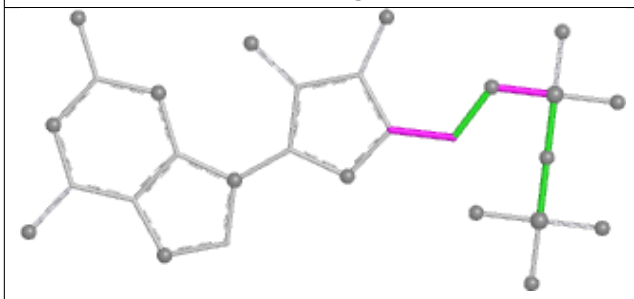

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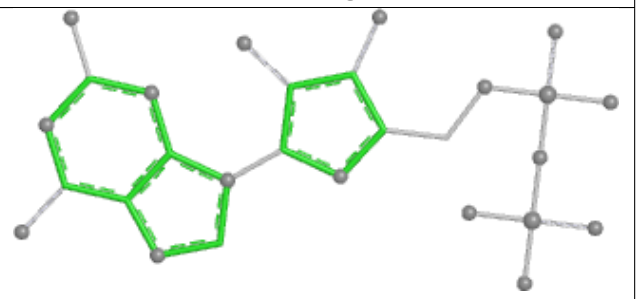
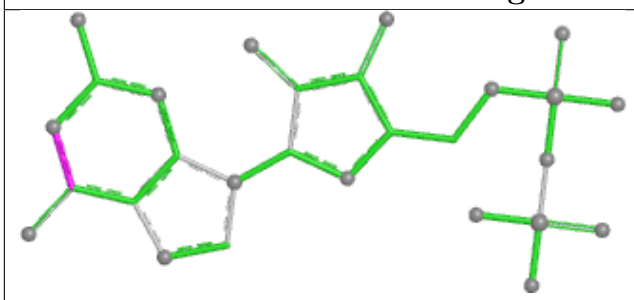


Rings

Ligand GDP ML 501



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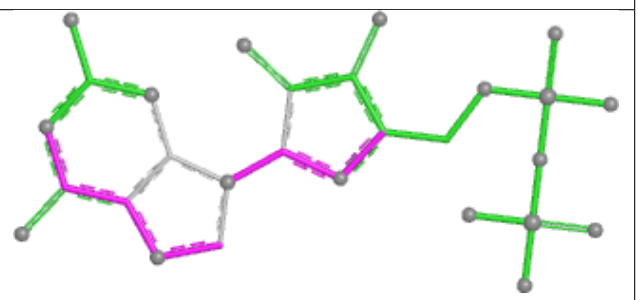
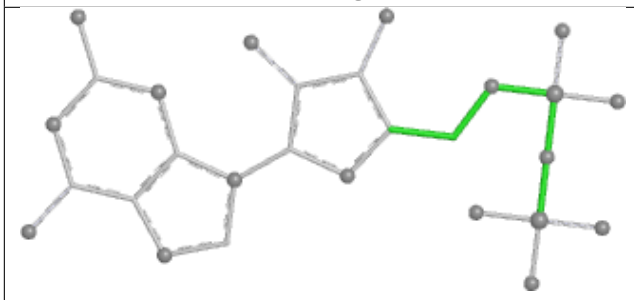
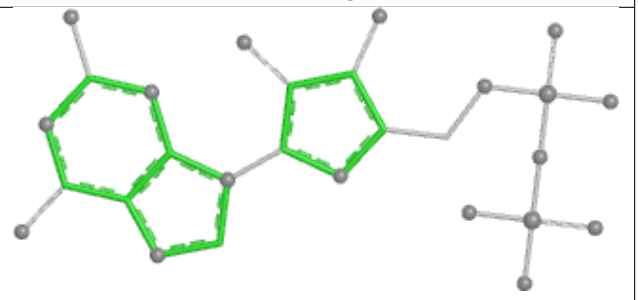


Bond angles

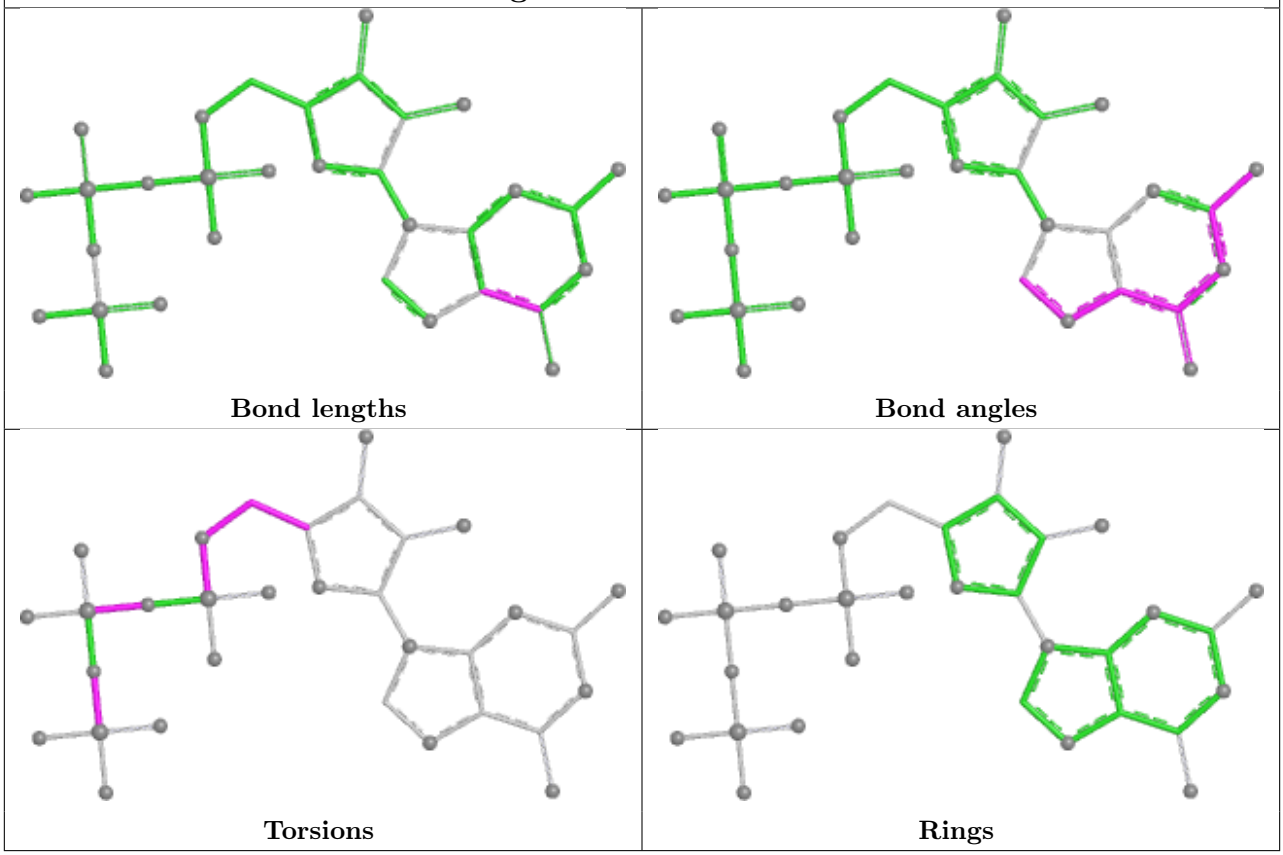


Torsions

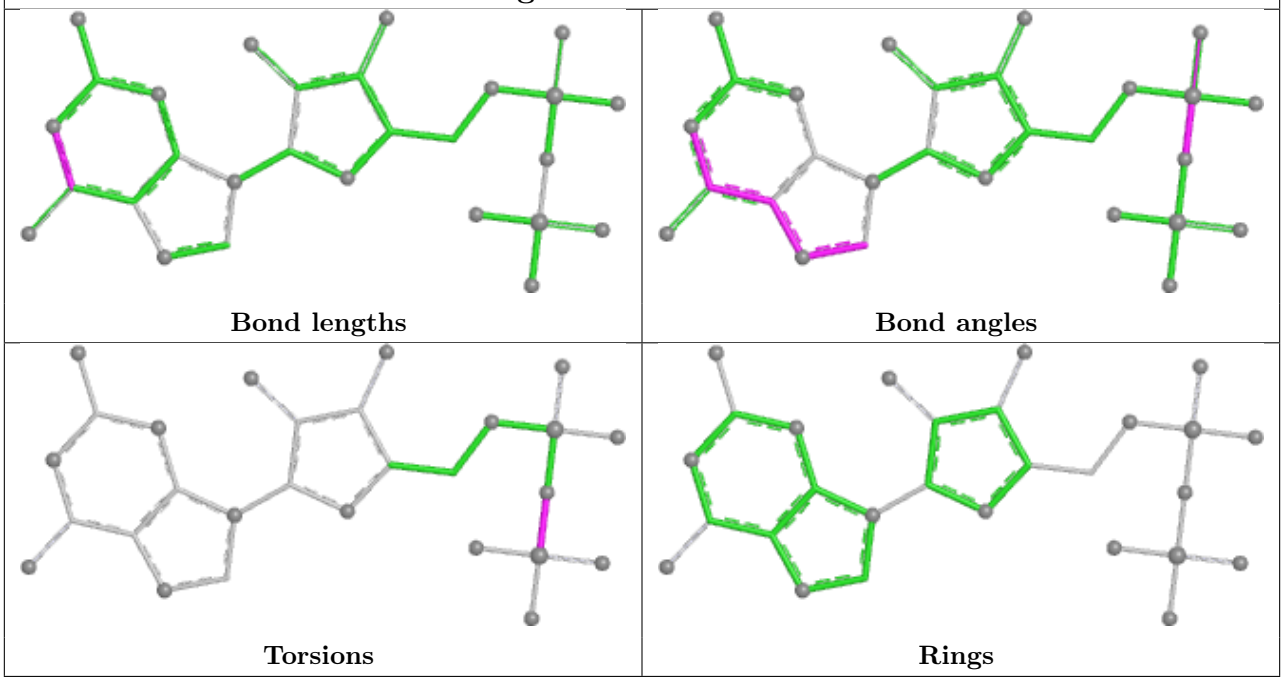


Rings

Ligand GTP DC 501



Ligand GDP IF 501



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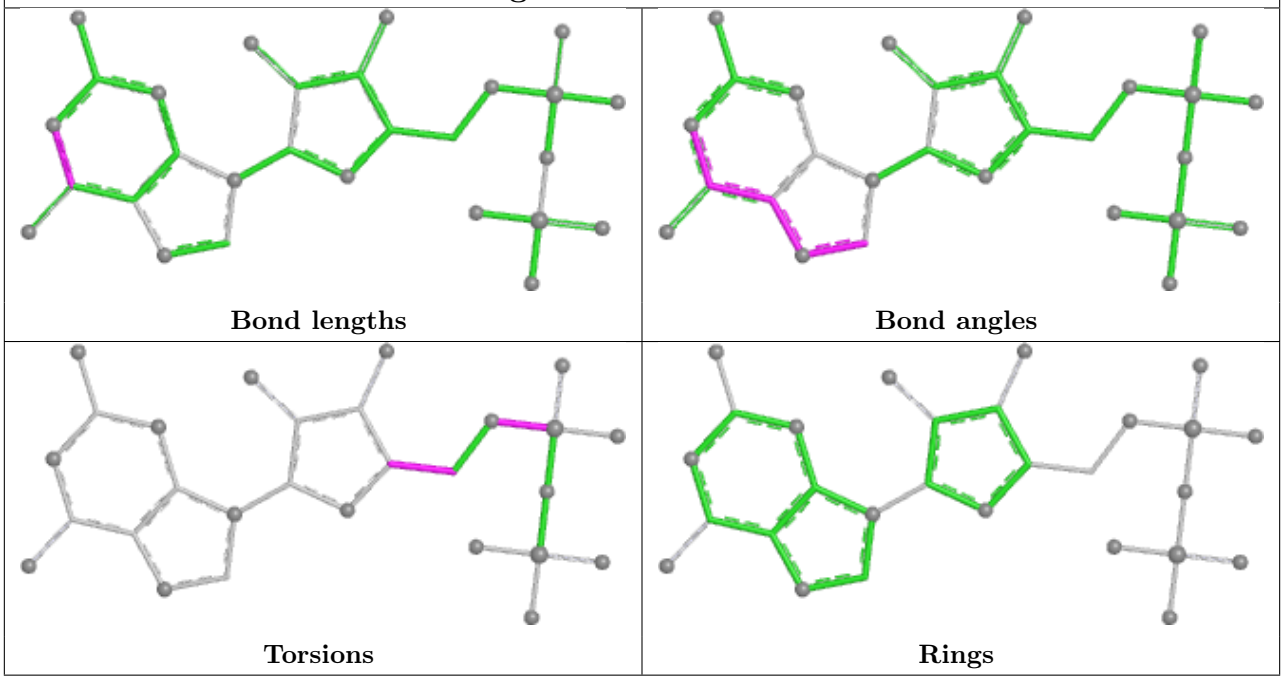
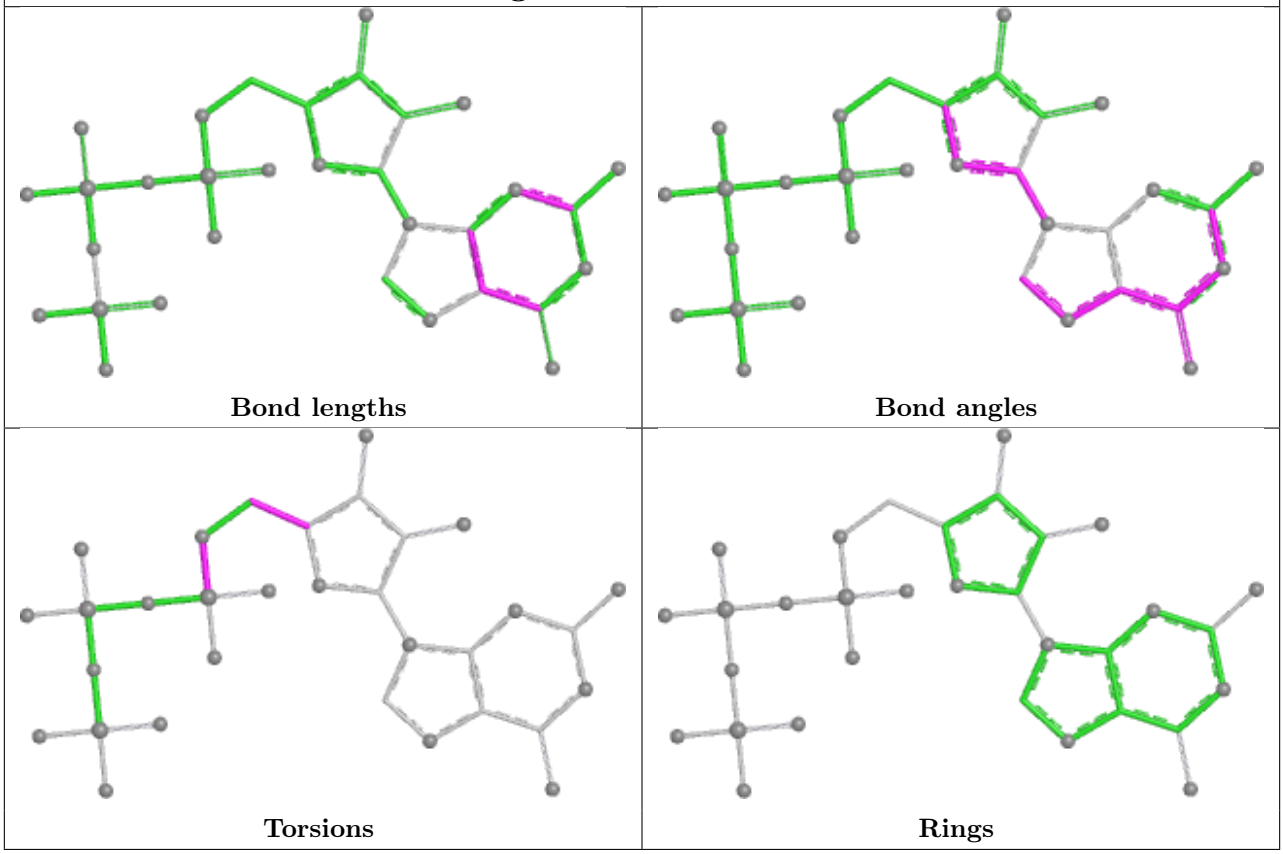


Ligand GTP GC 501



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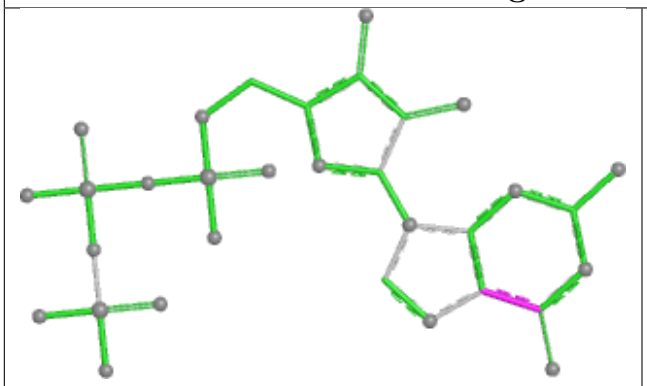
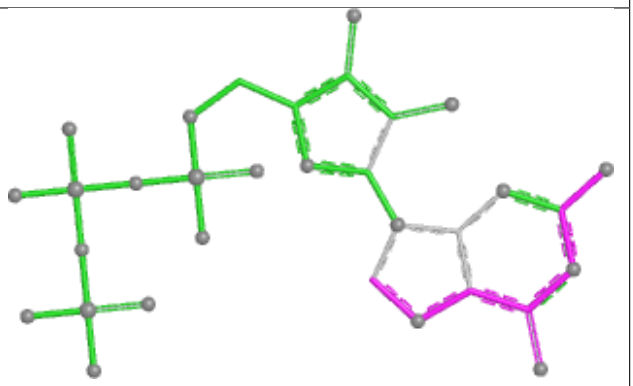
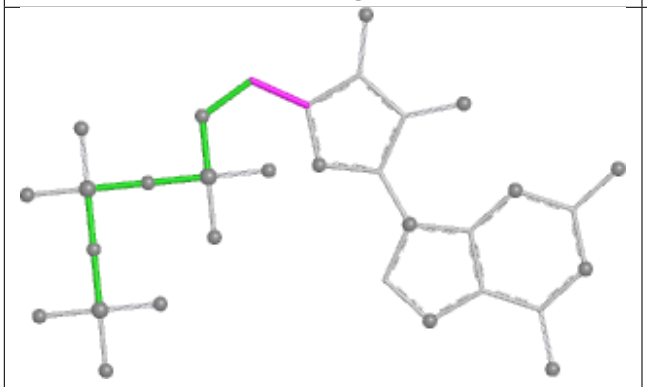


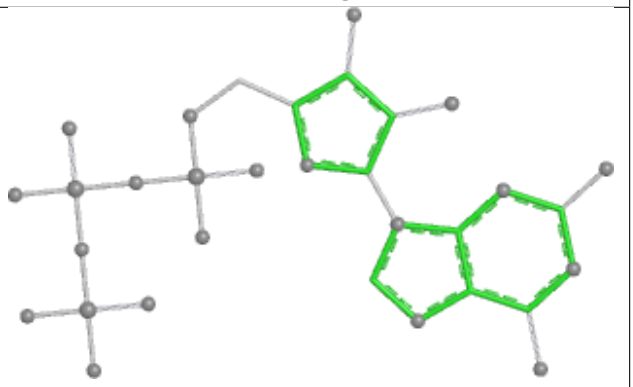
Bond lengths



Bond angles

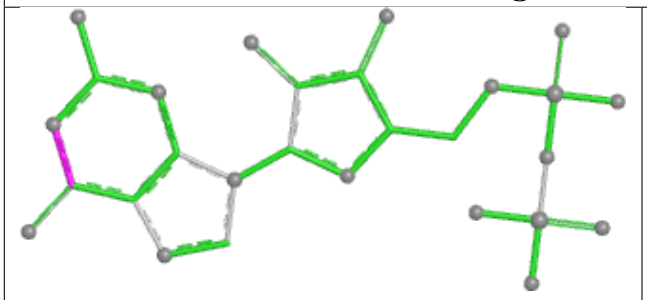


Torsions



Rings

Ligand GDP DL 501



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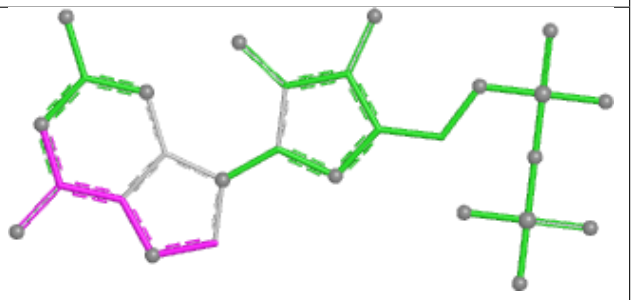
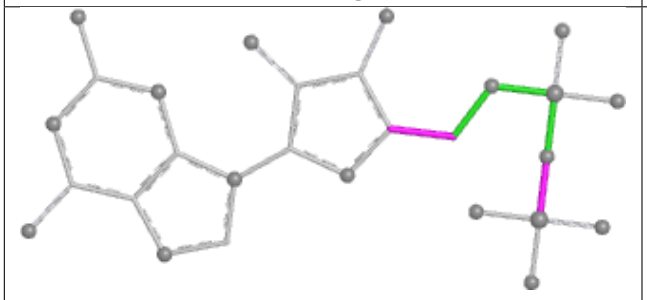


Bond angles



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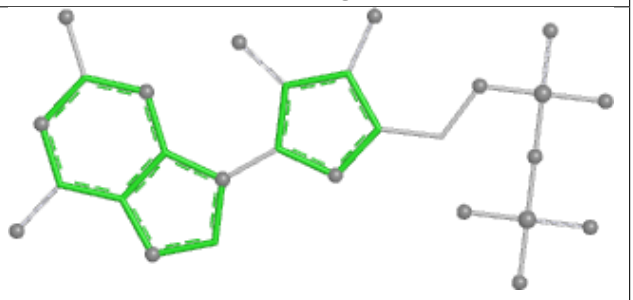
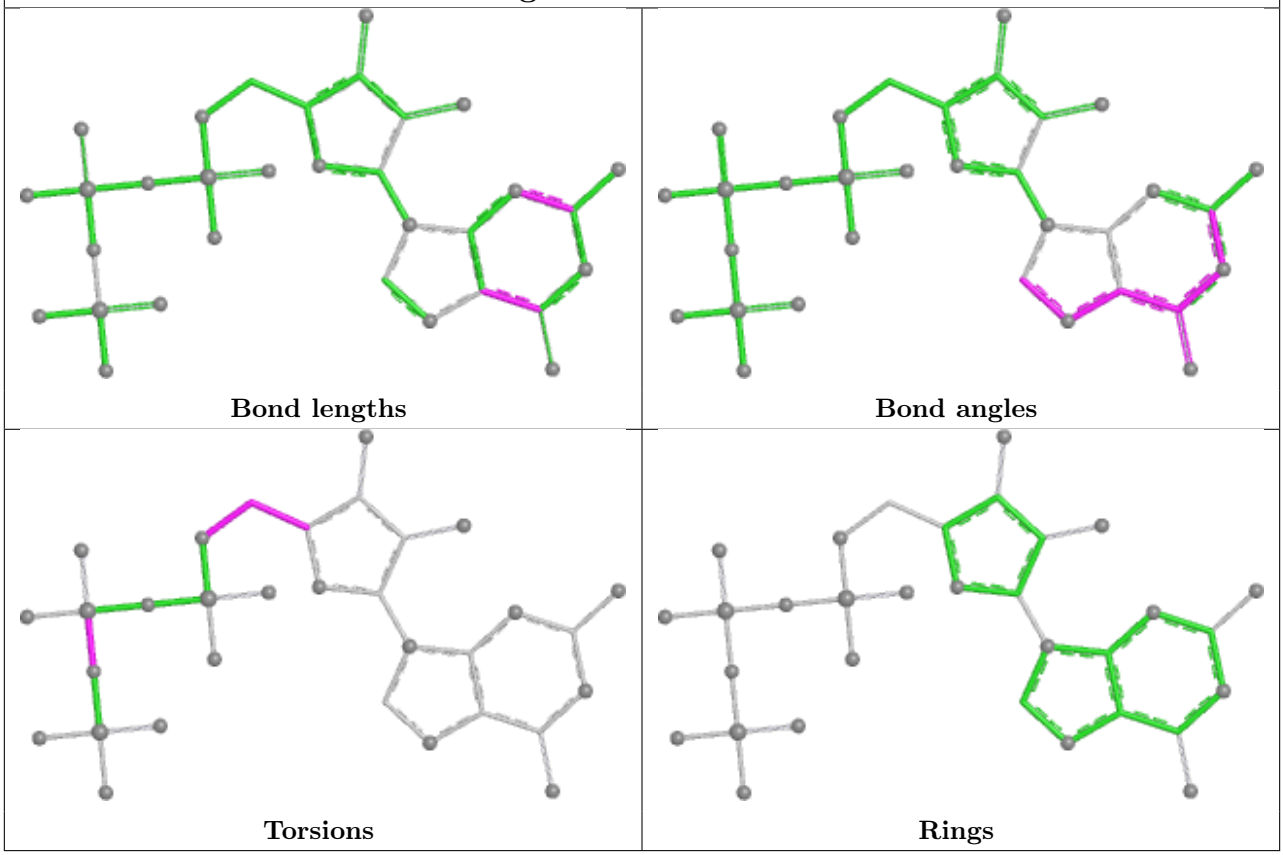


Rings

Ligand GTP LI 501



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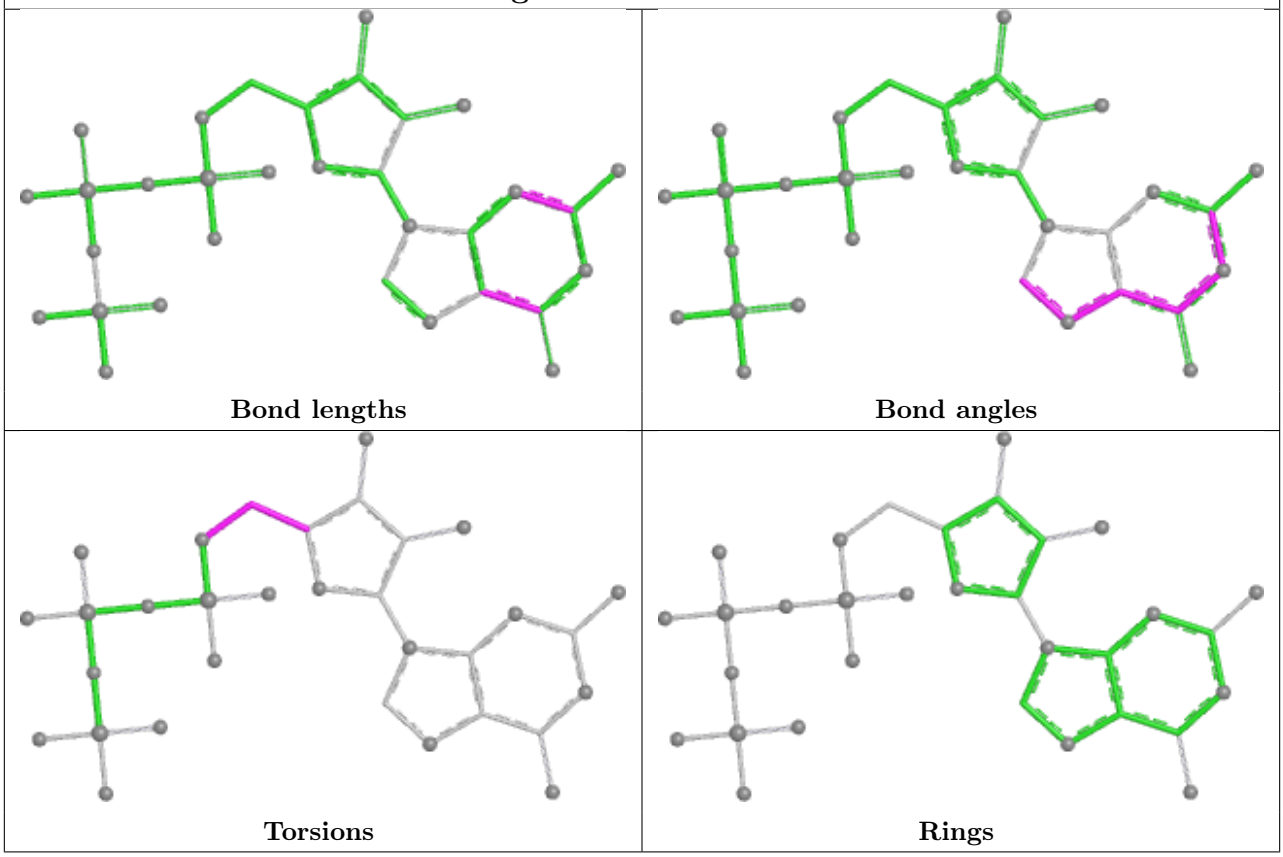
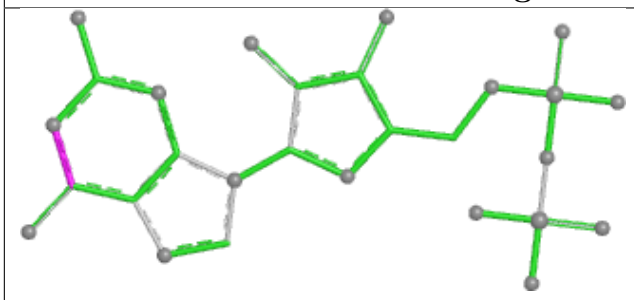


Ligand GDP LL 501



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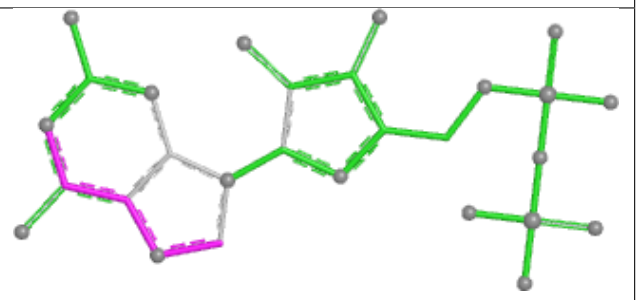

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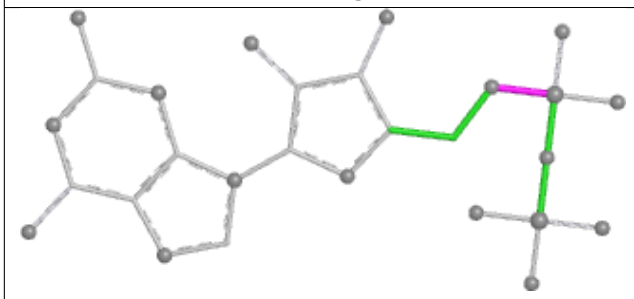

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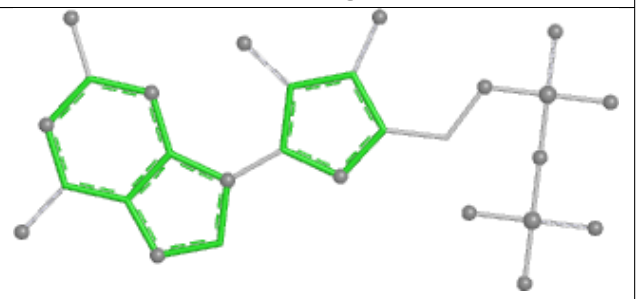
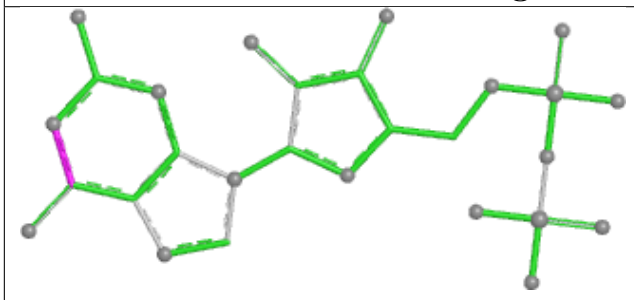


Rings

Ligand GDP TF 501



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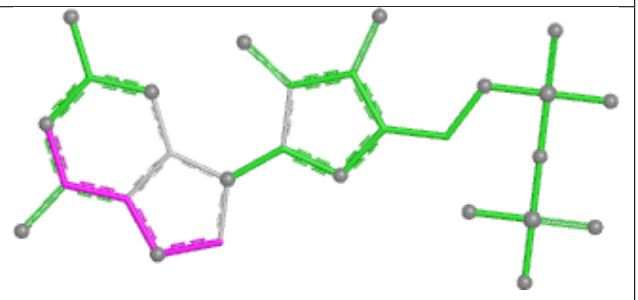

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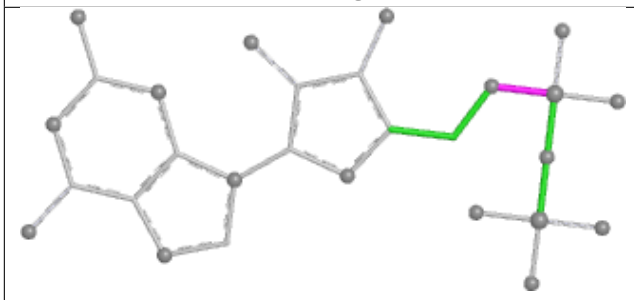

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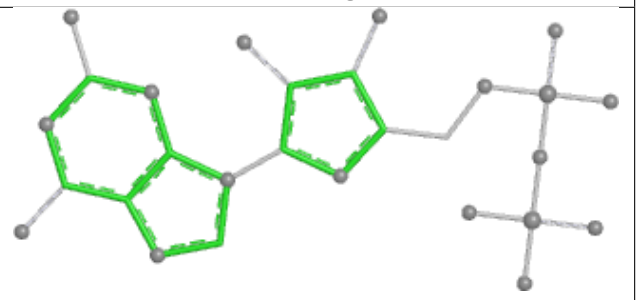
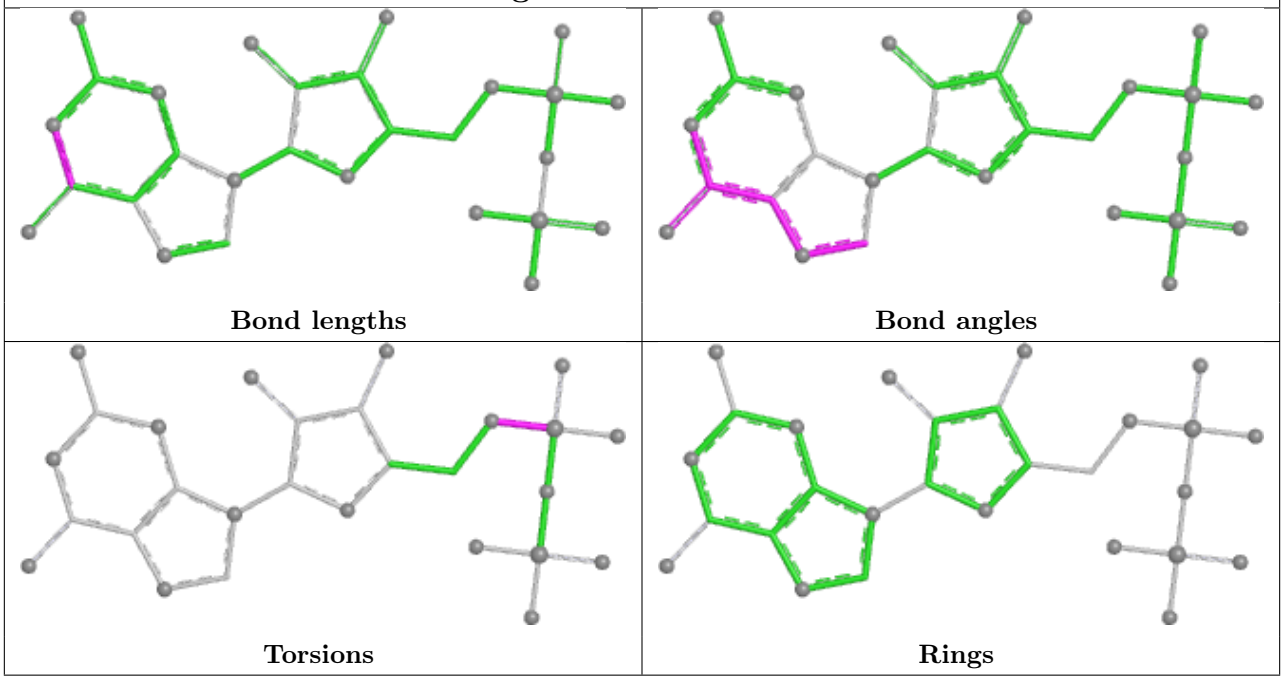


Rings

Ligand GDP TL 501



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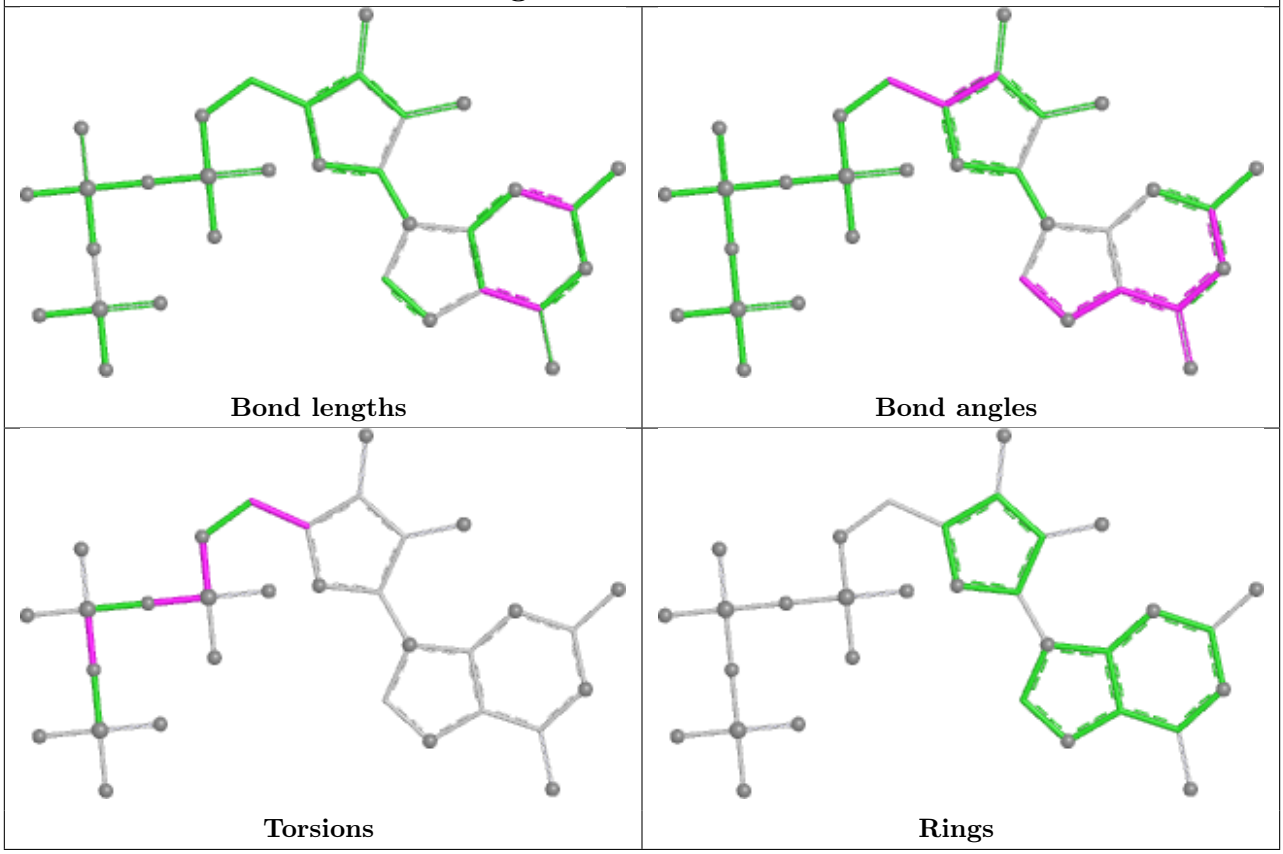
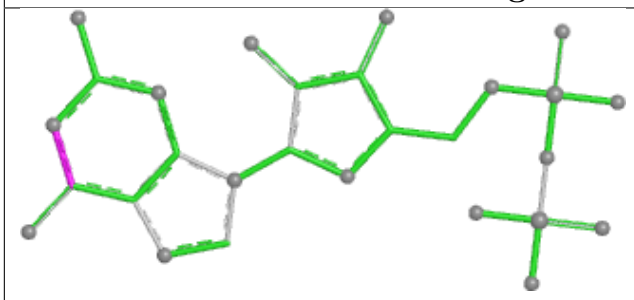


Ligand GDP QD 501



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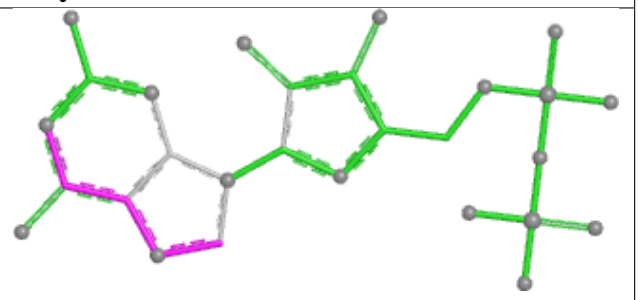

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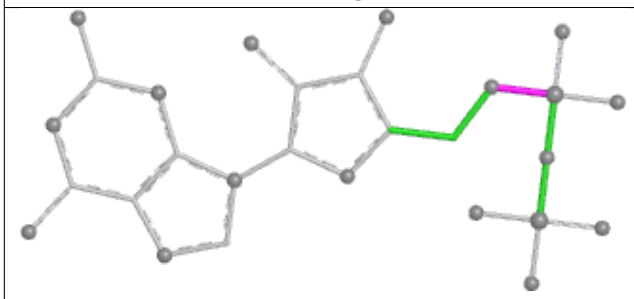

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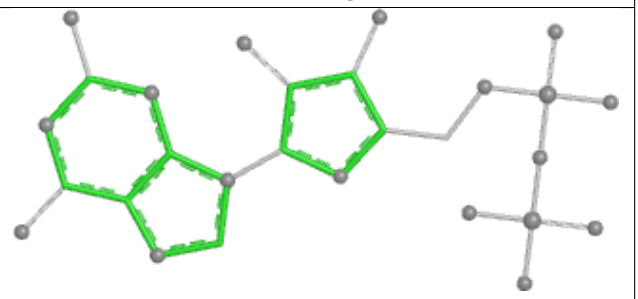
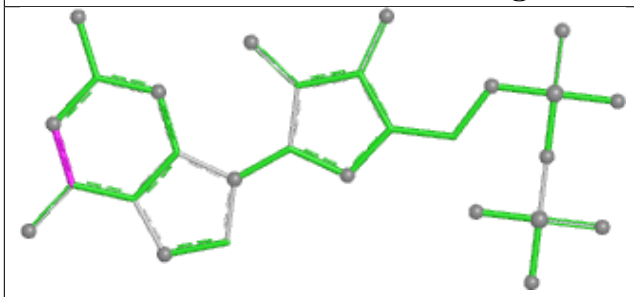


Rings

Ligand GDP QF 501



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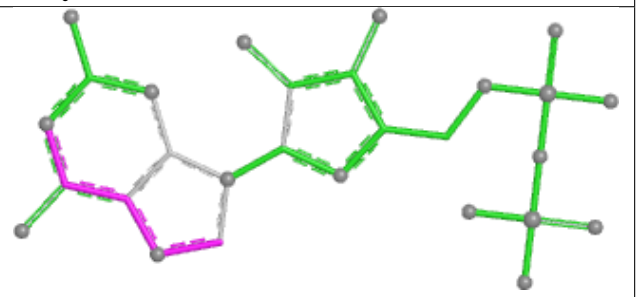

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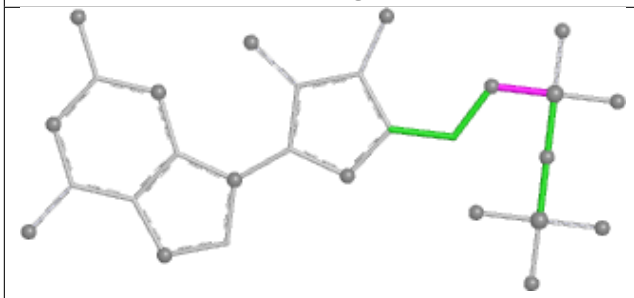

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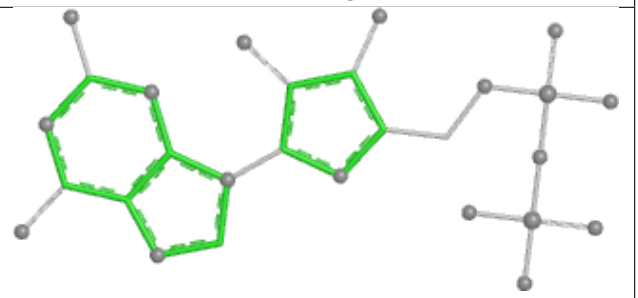
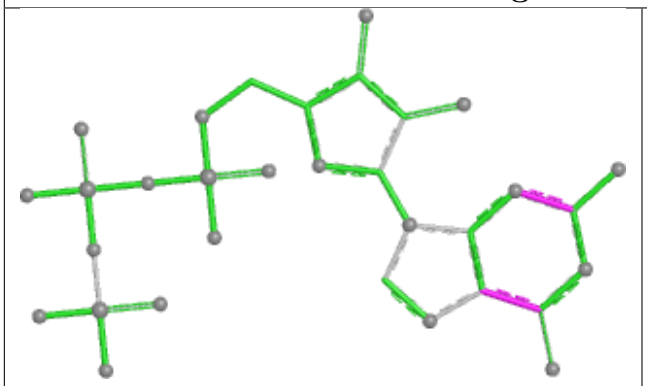


Rings

Ligand GTP OE 501



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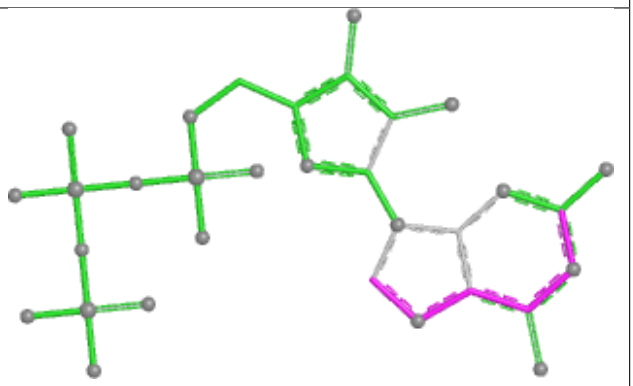

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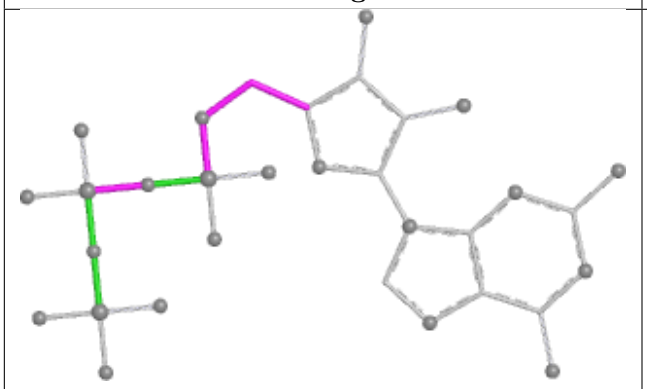

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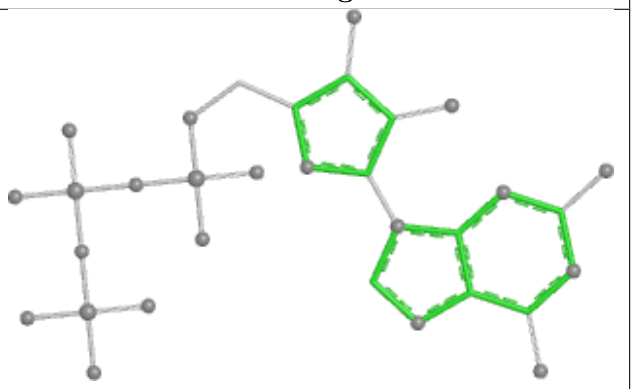
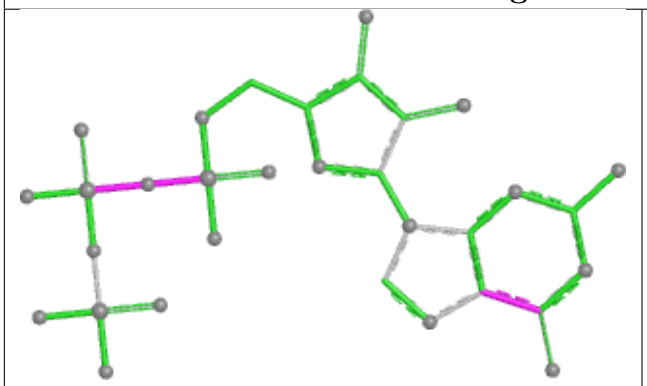


Rings

Ligand GTP UC 501



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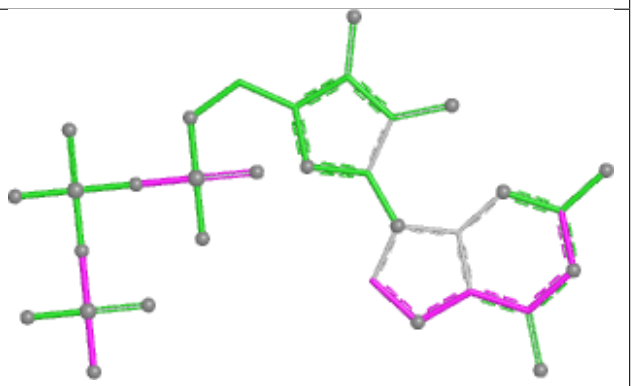

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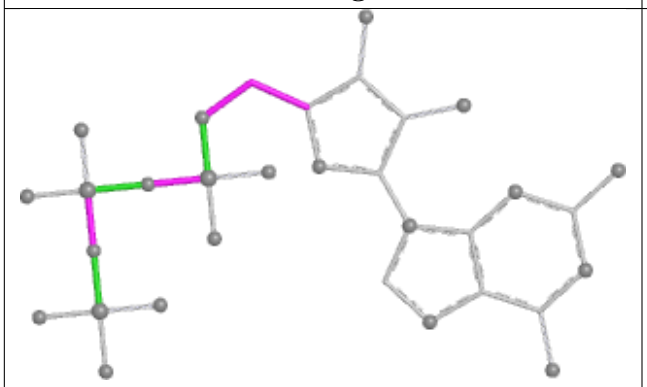

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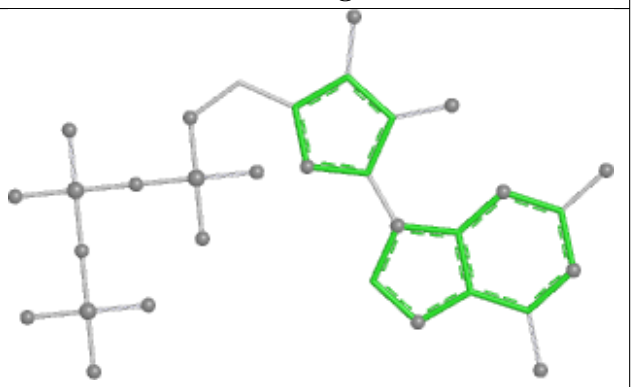
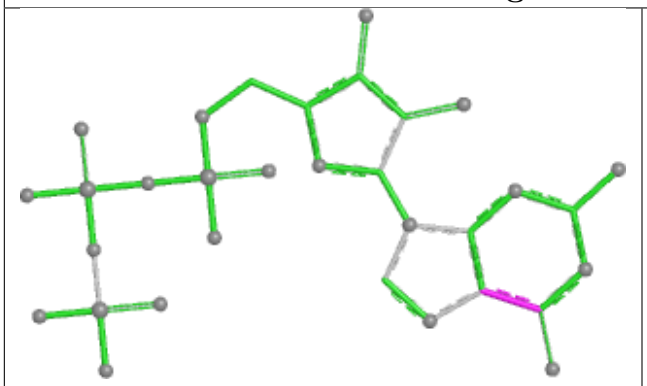


Rings

Ligand GTP CM 501



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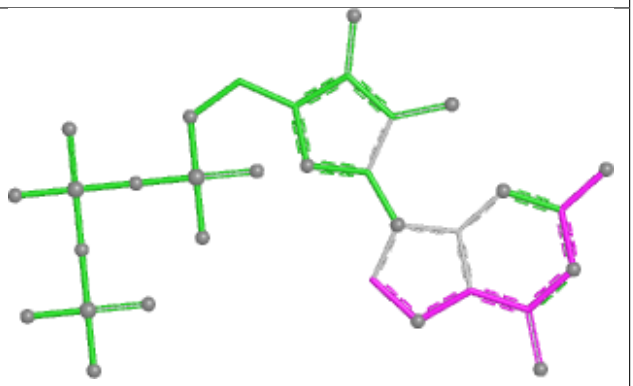

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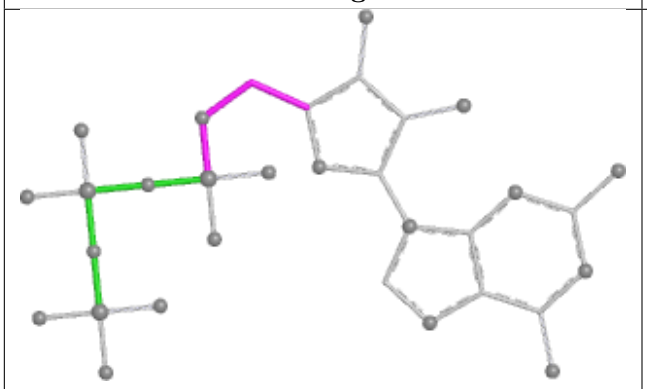

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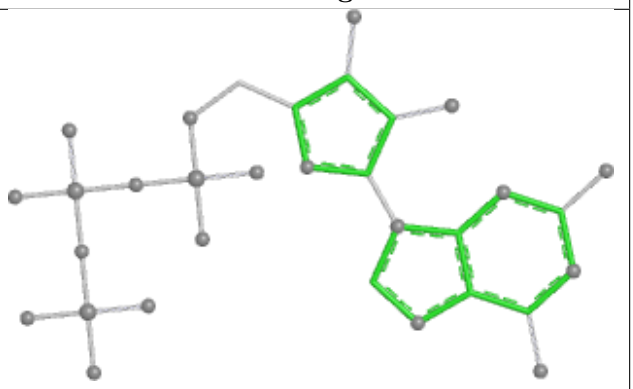
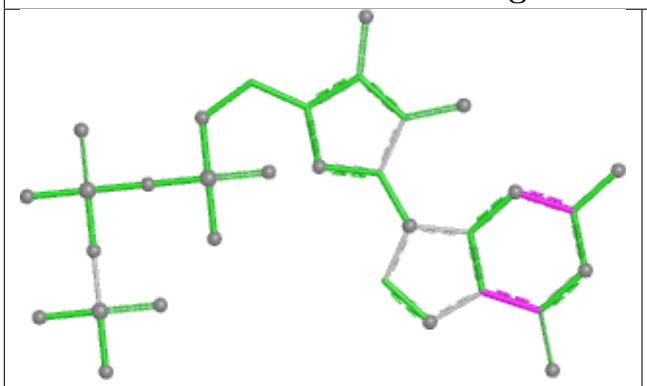


Rings

Ligand GTP NA 501



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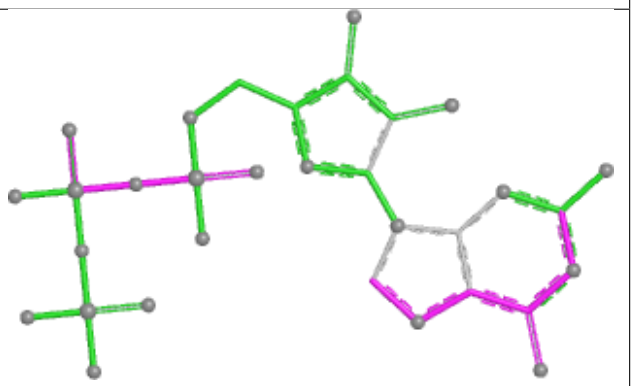

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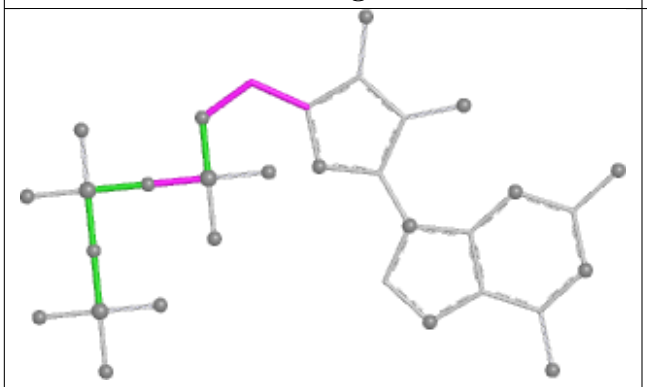

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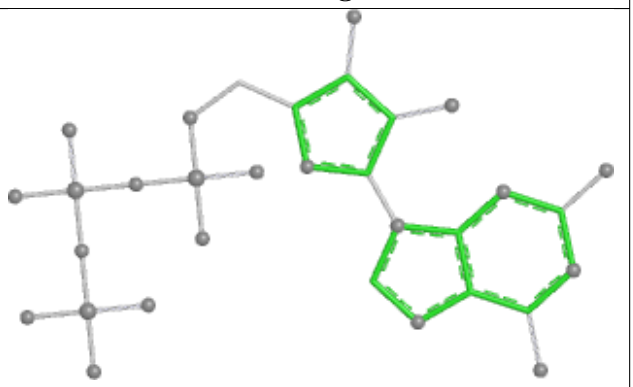

Rings

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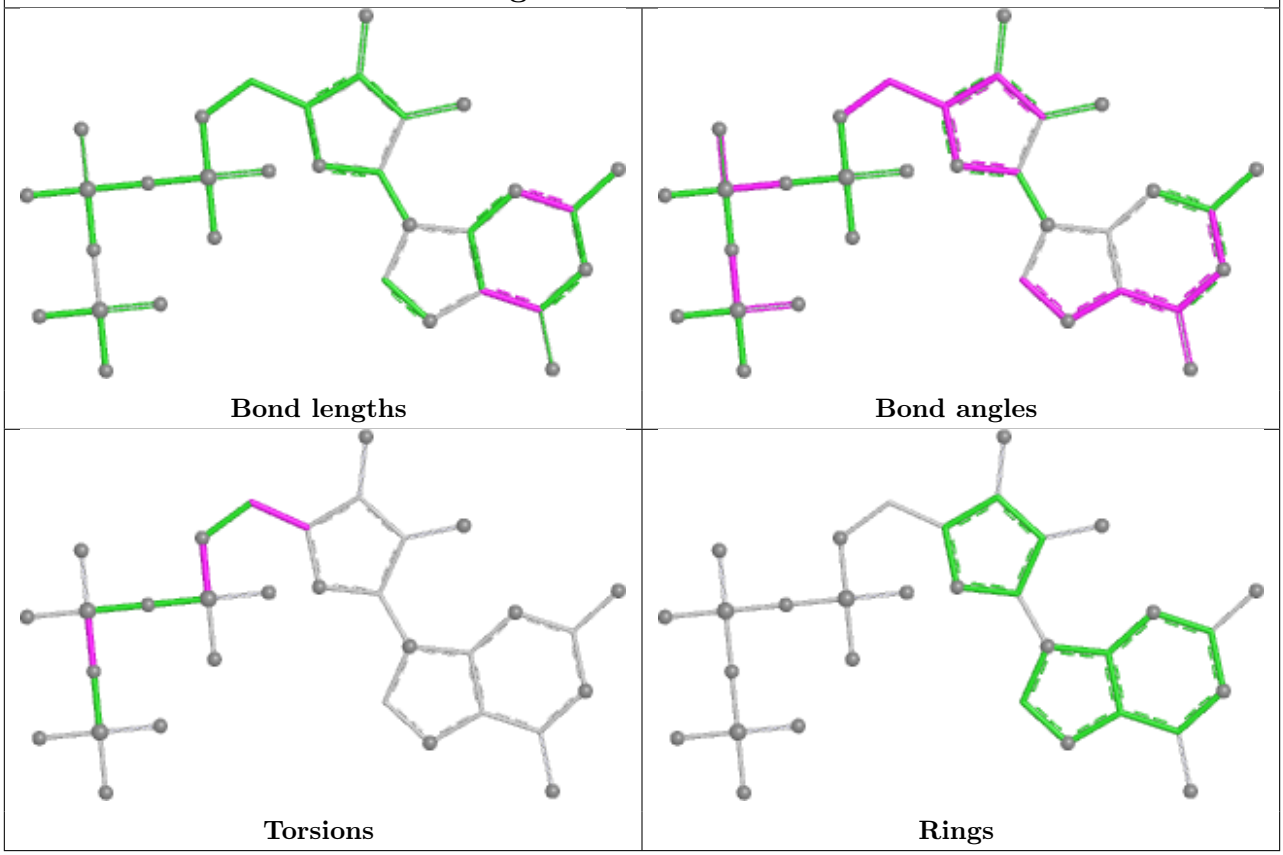

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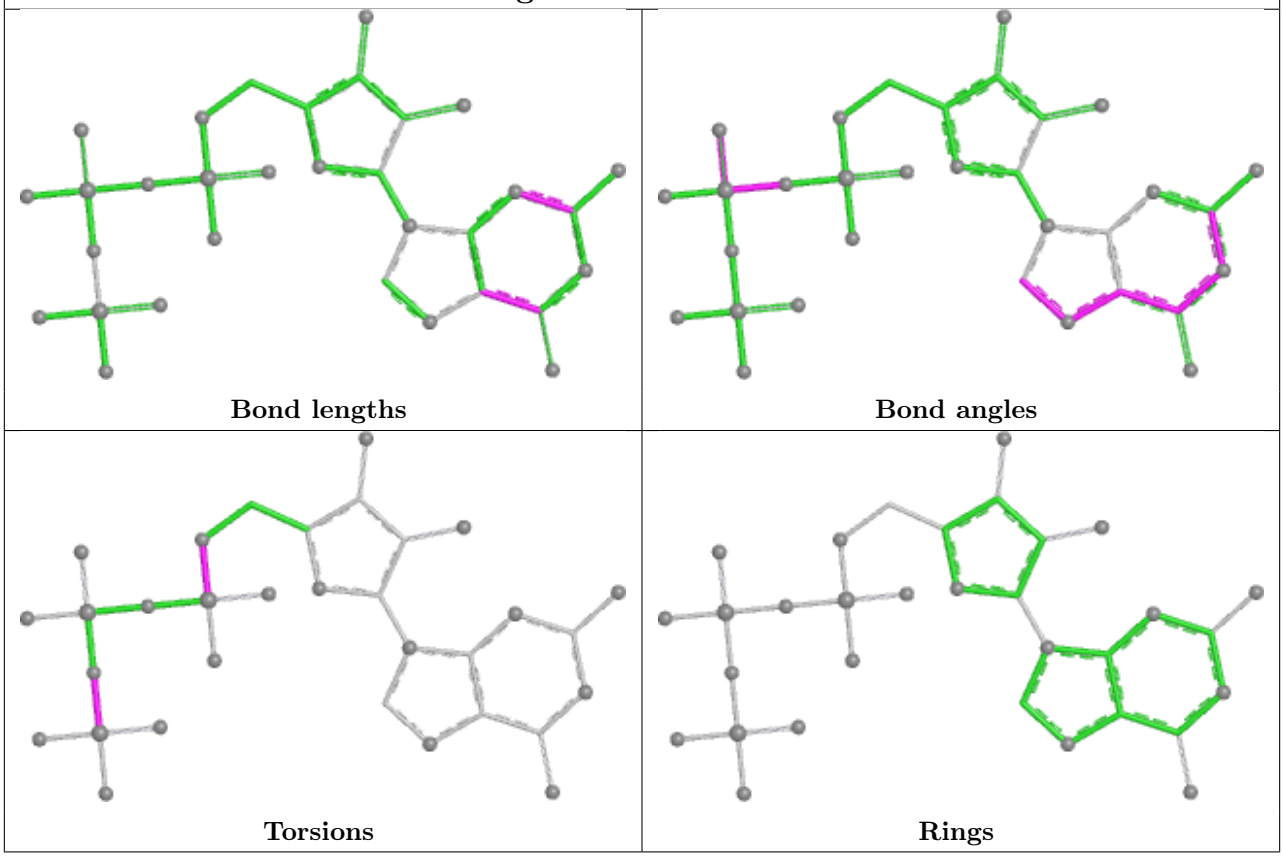

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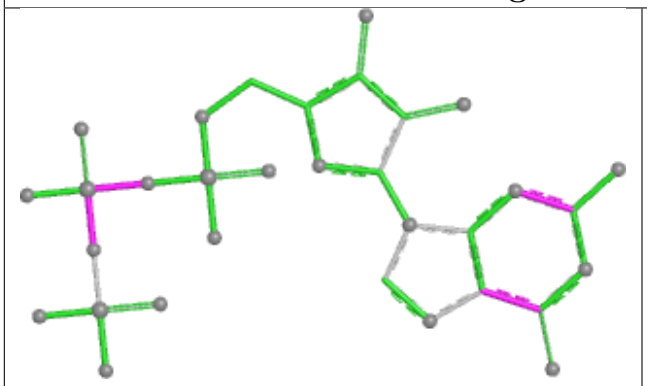

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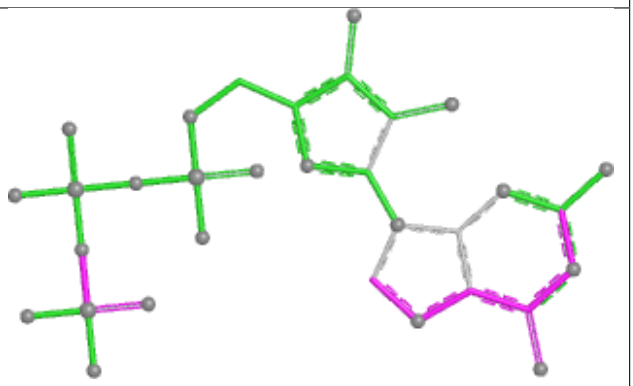
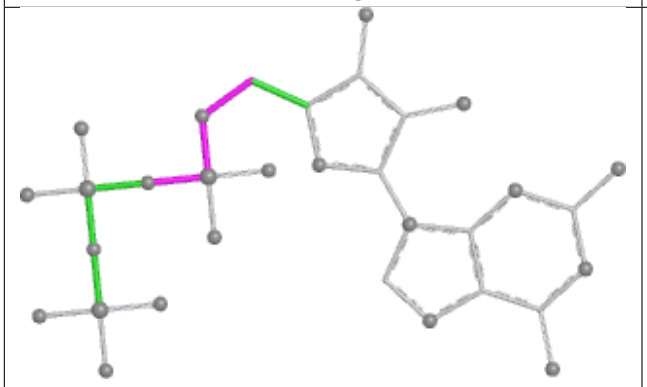


Bond angles



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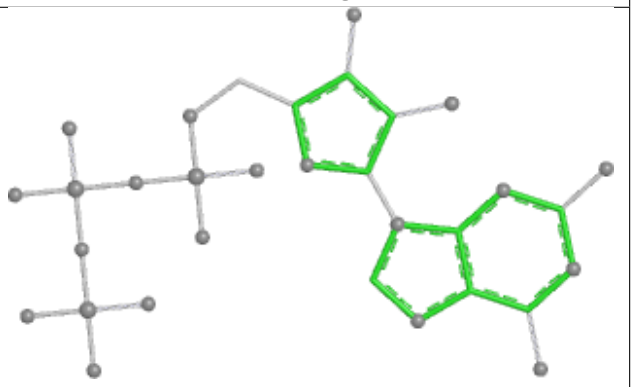

Rings

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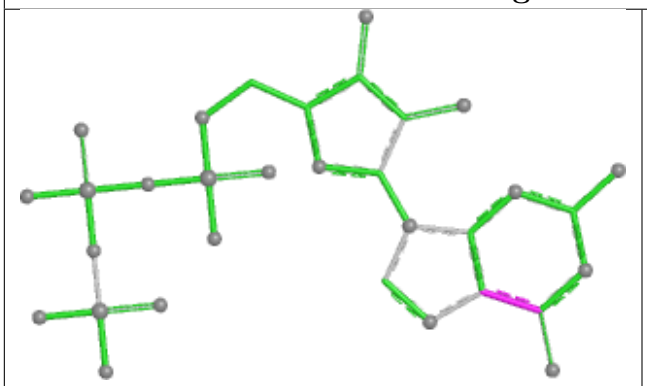

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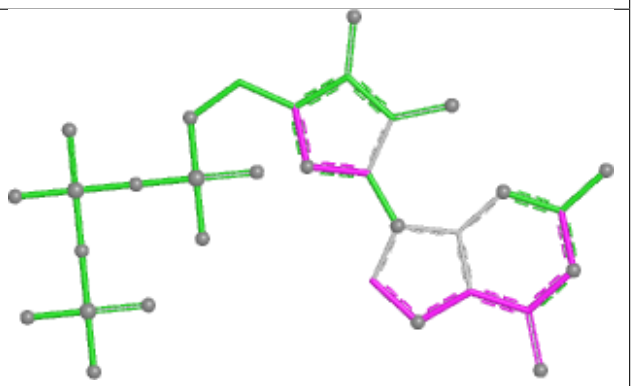

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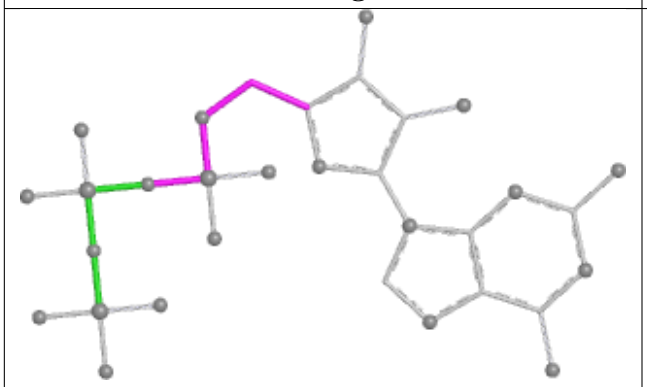

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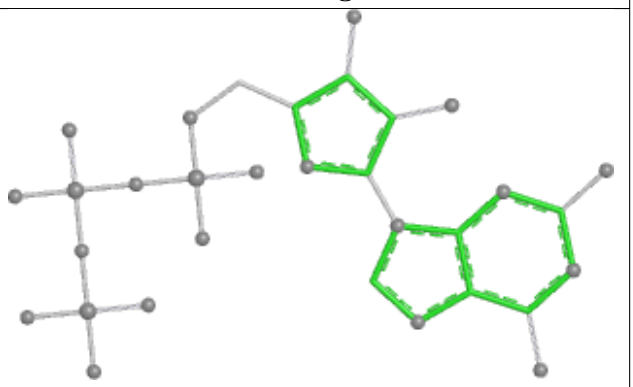

Rings

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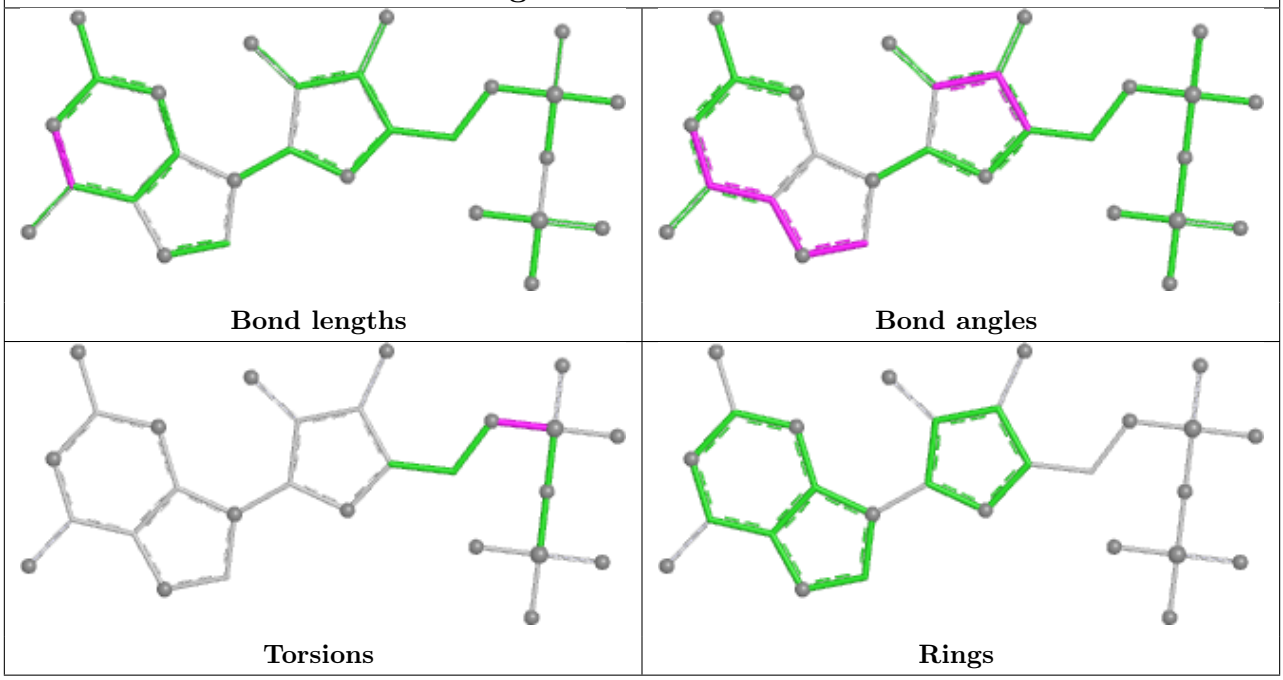

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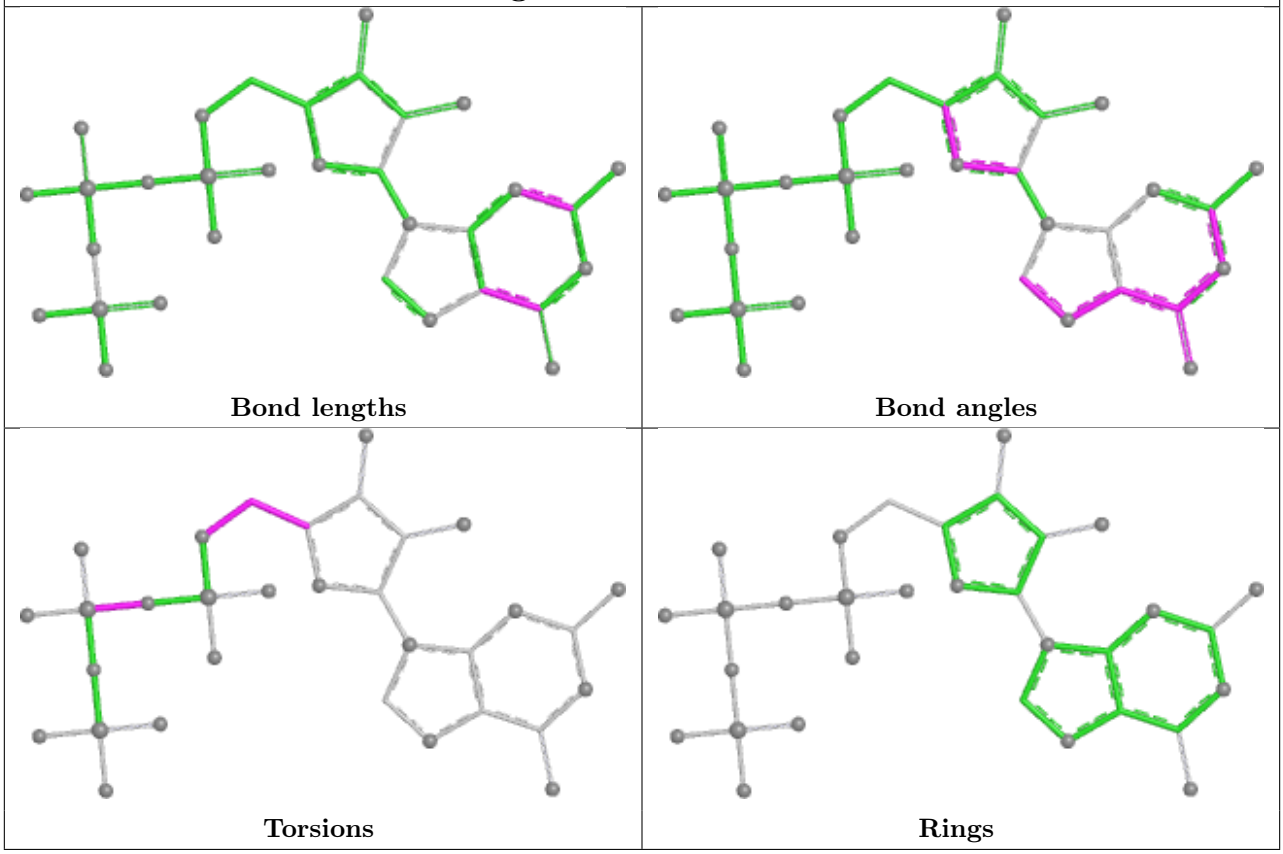

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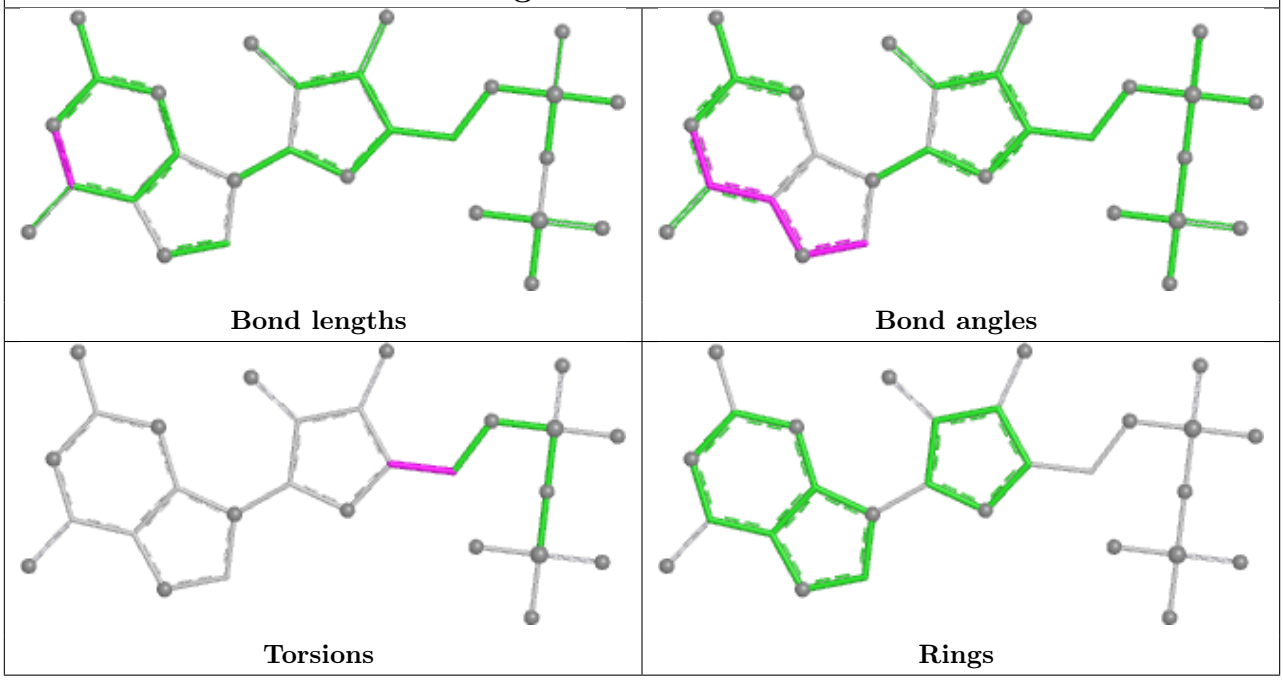
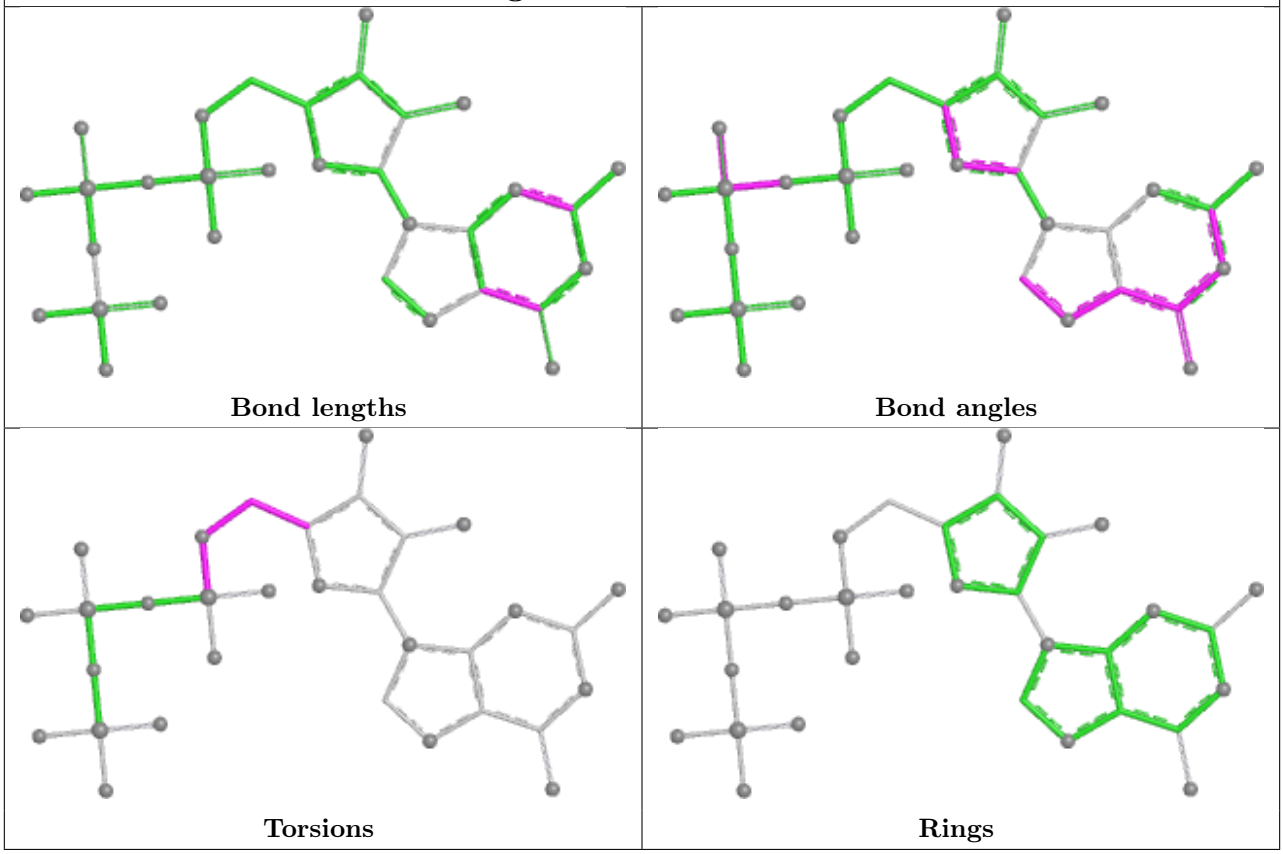
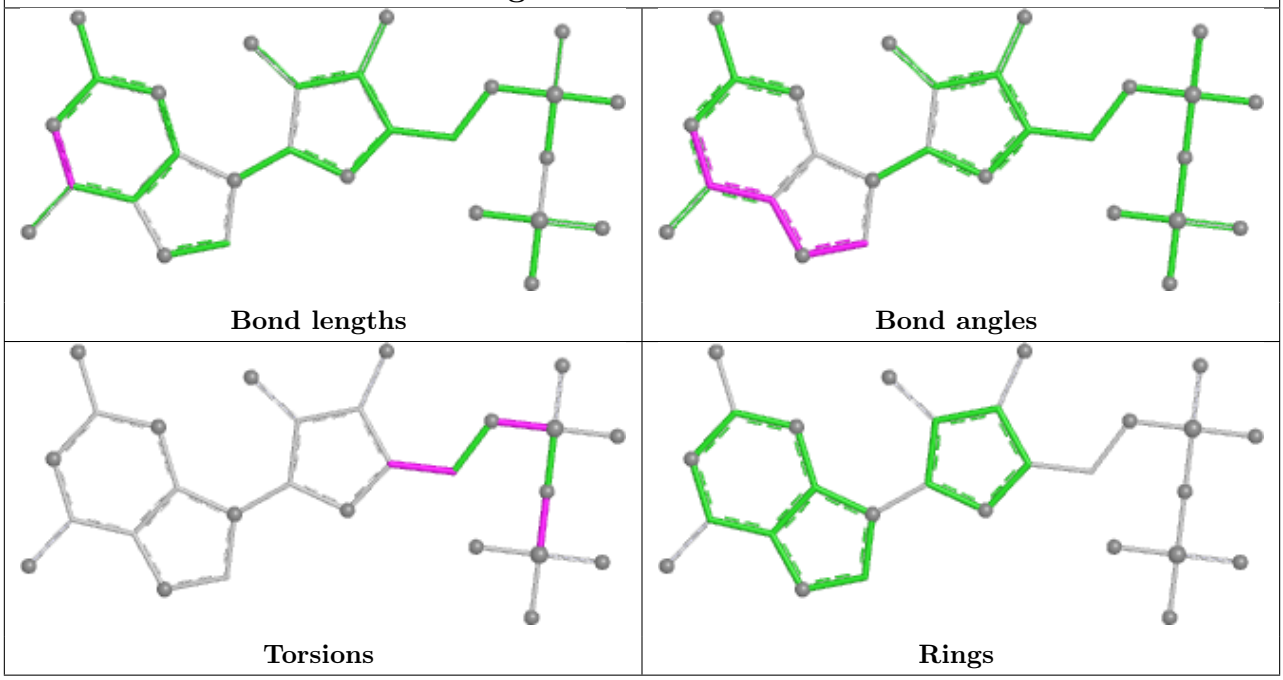


Ligand GTP MC 501



Ligand GDP AD 501



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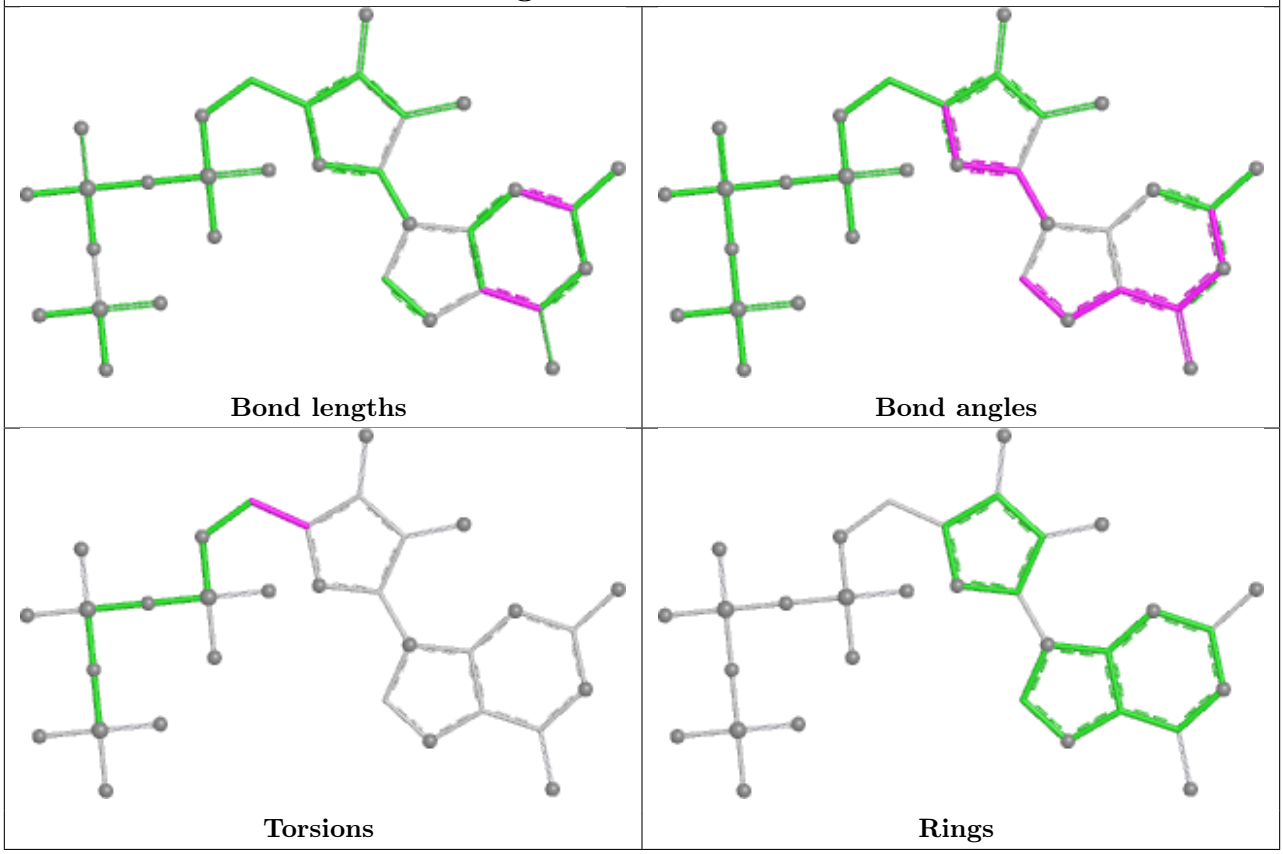

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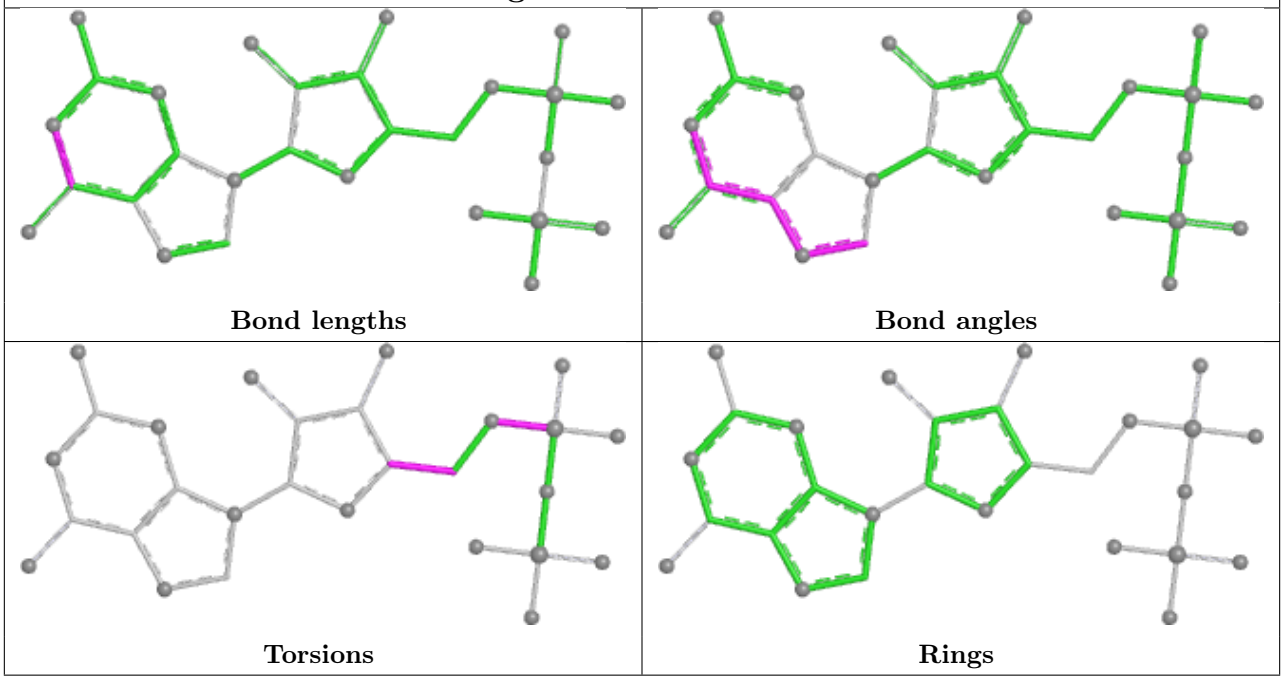

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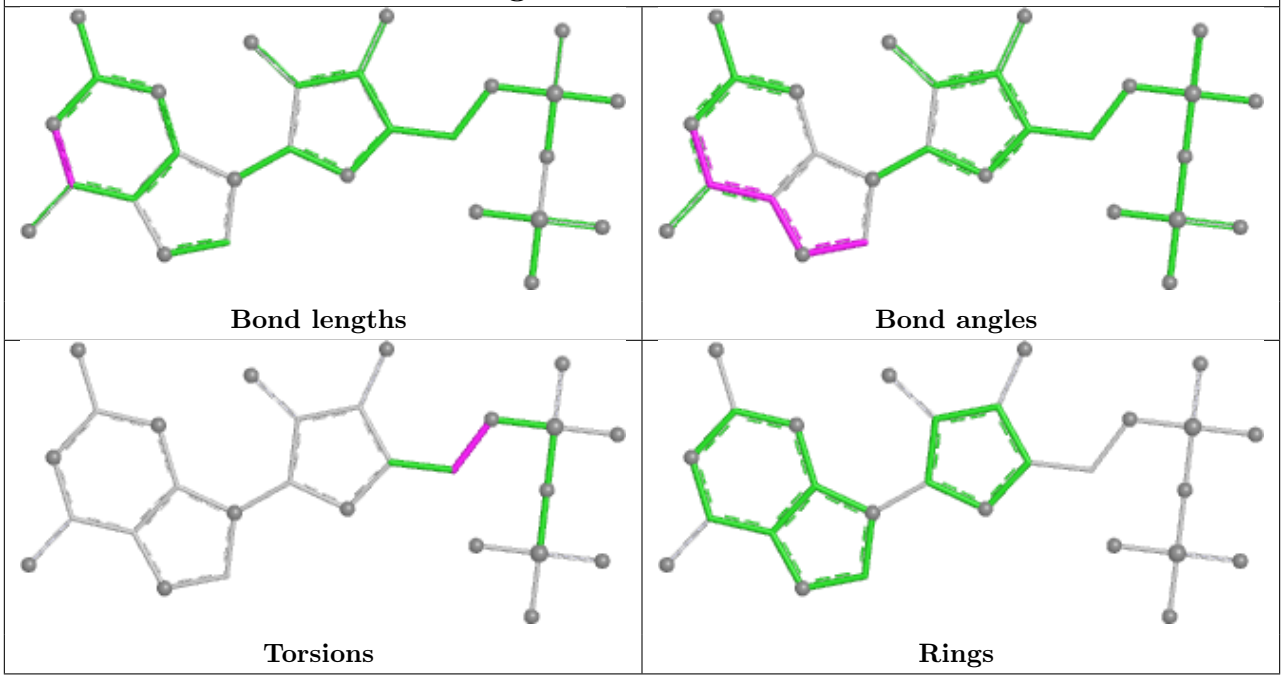

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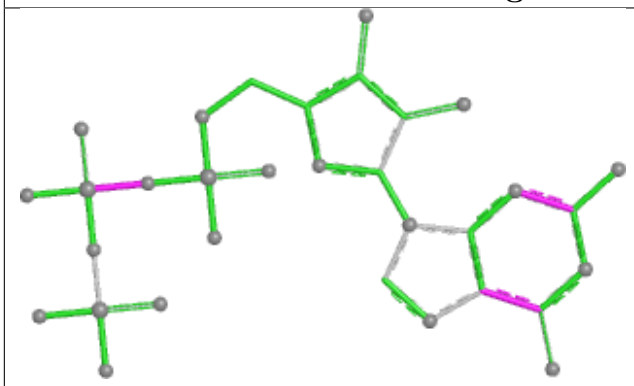
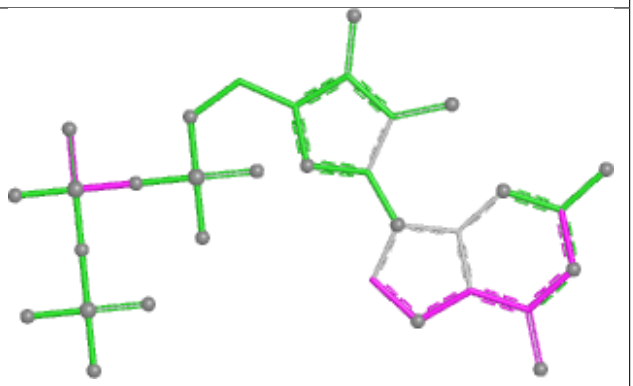
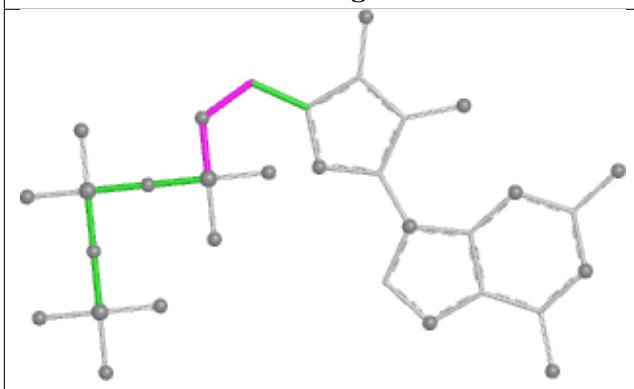


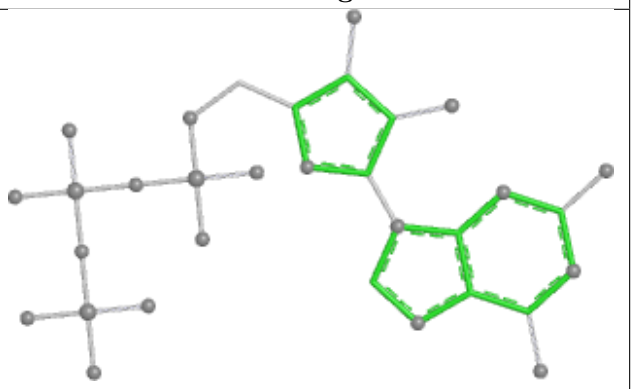
Bond lengths



Bond angles

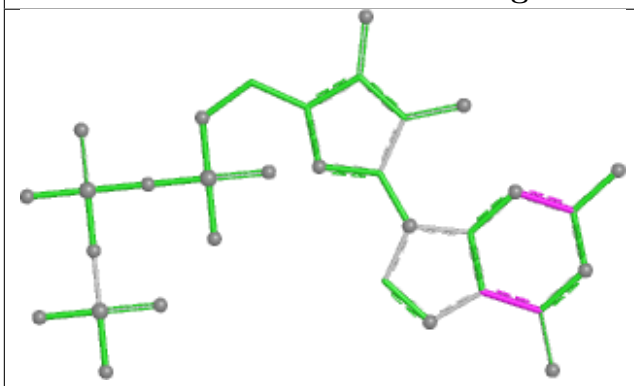


Torsions



Rings

Ligand GTP HE 501



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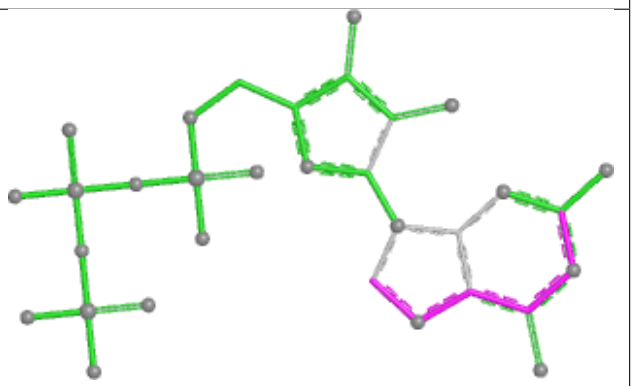

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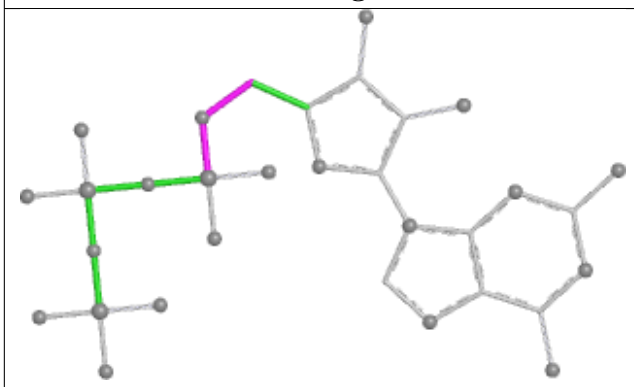

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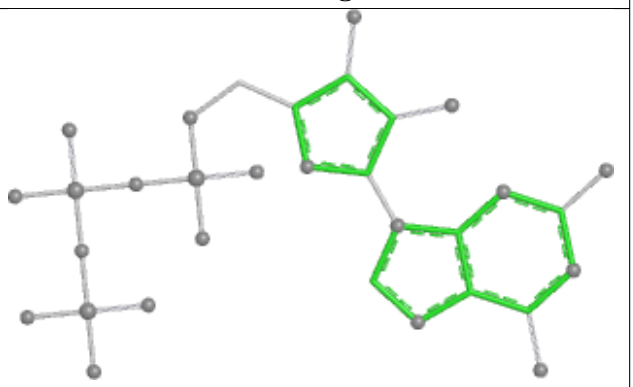

Rings

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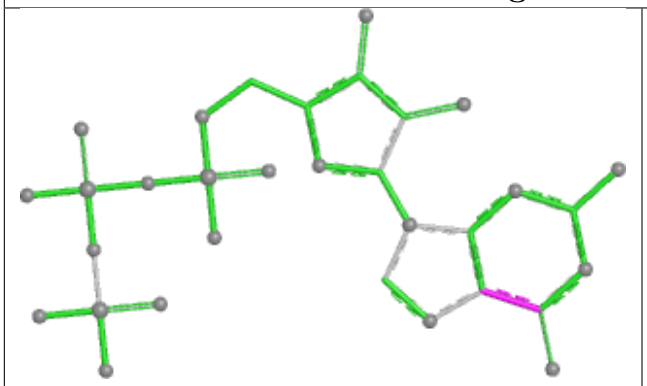

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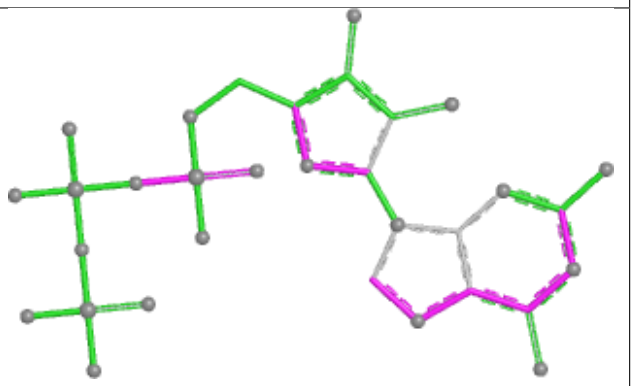
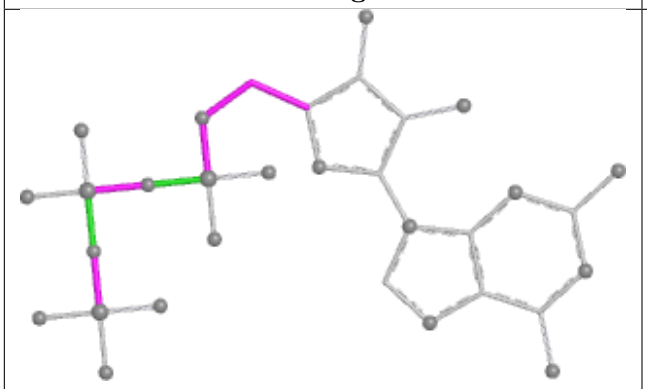


Bond angles



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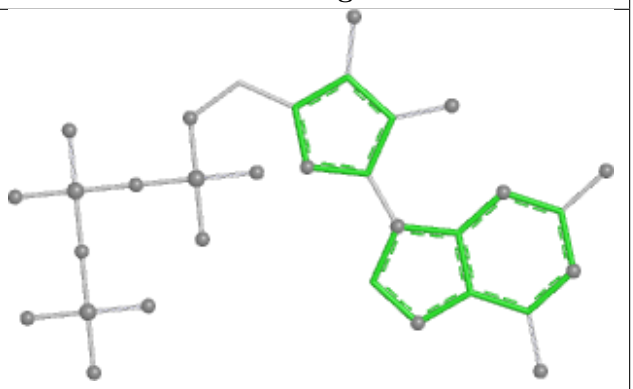

Rings

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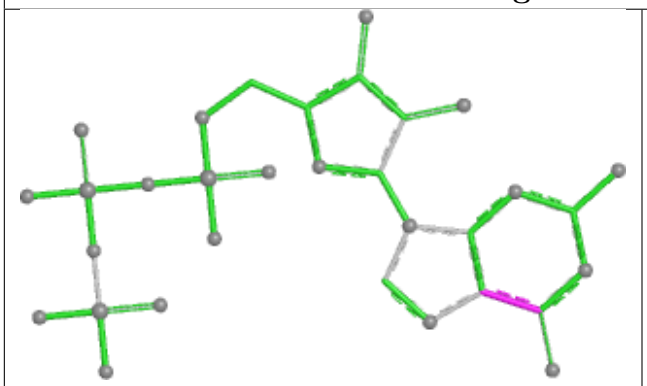

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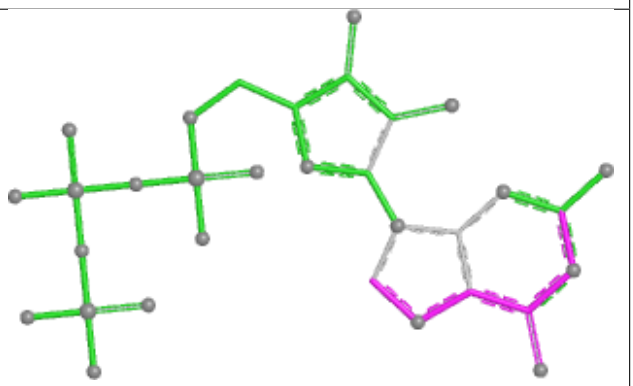
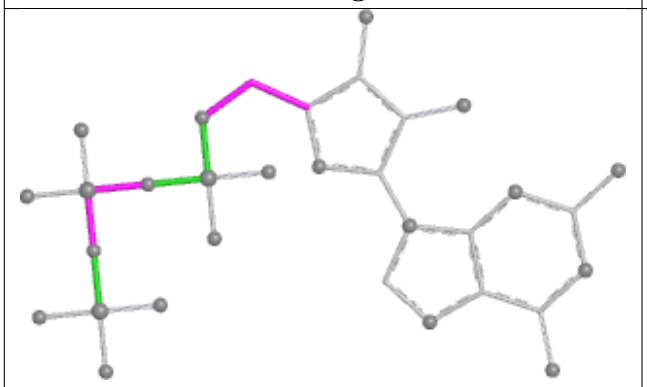


Bond angles



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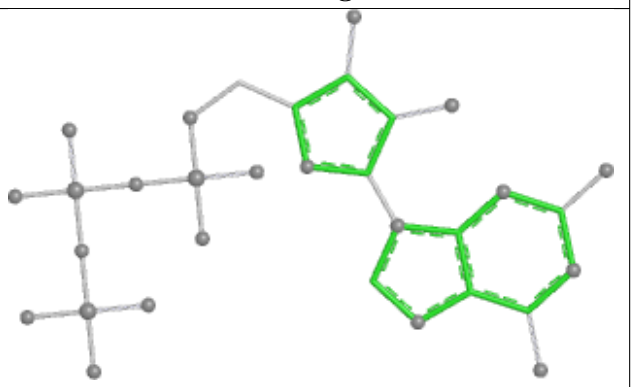
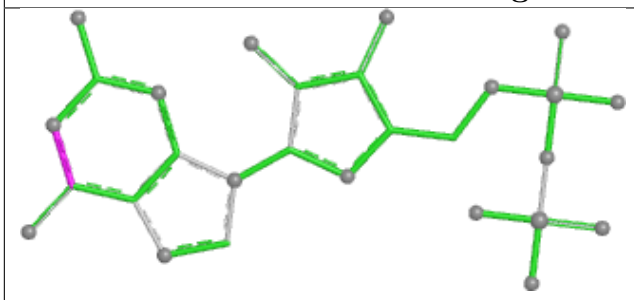


Rings

Ligand GDP RL 501



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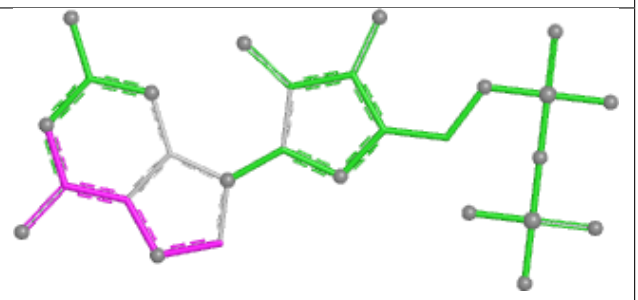

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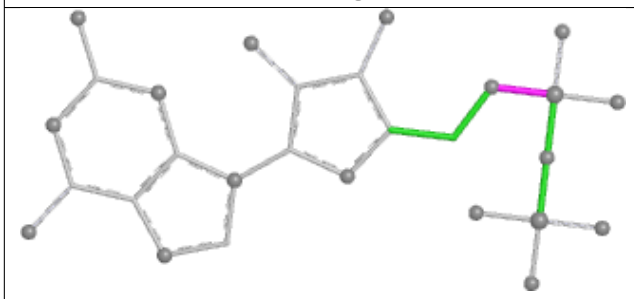

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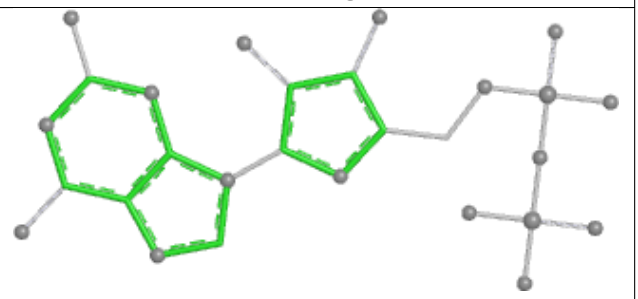

Rings

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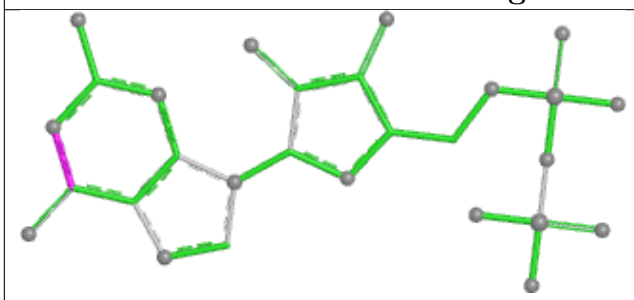

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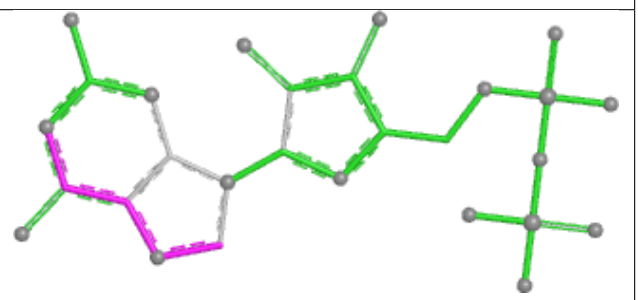

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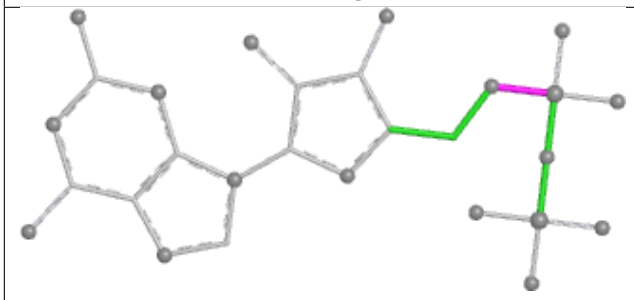

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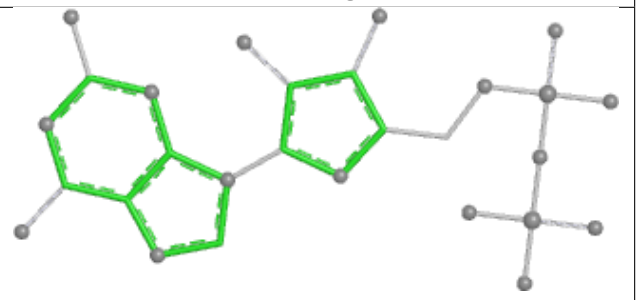

Rings

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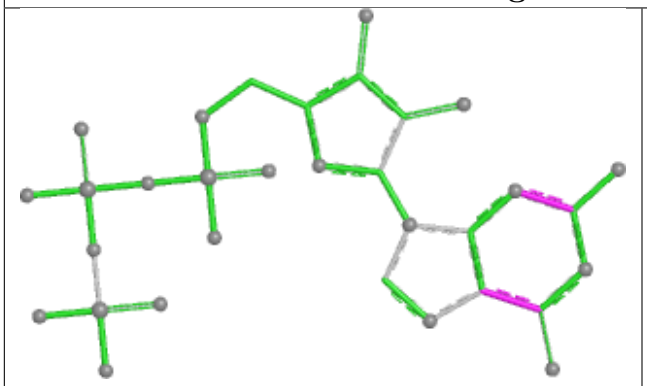

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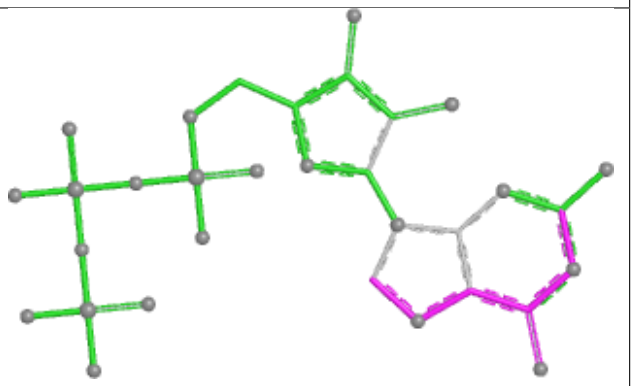

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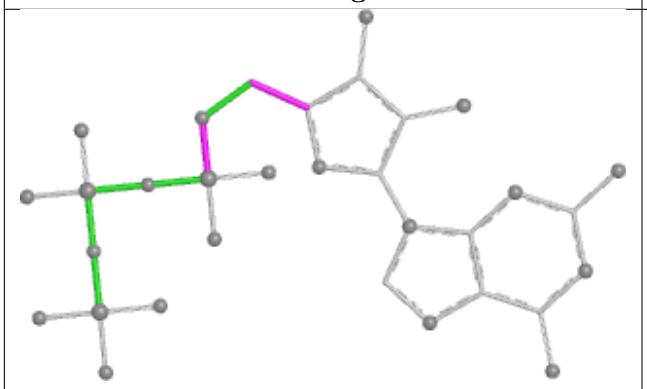

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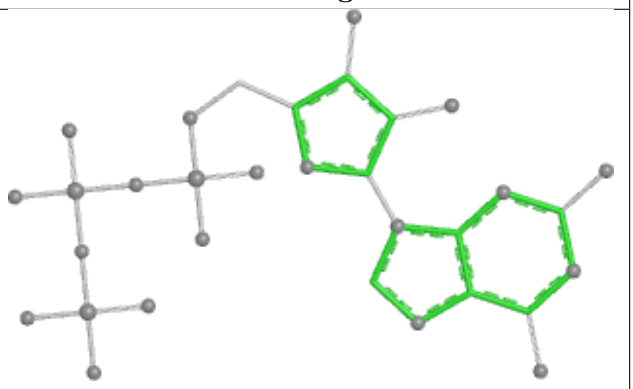

Rings

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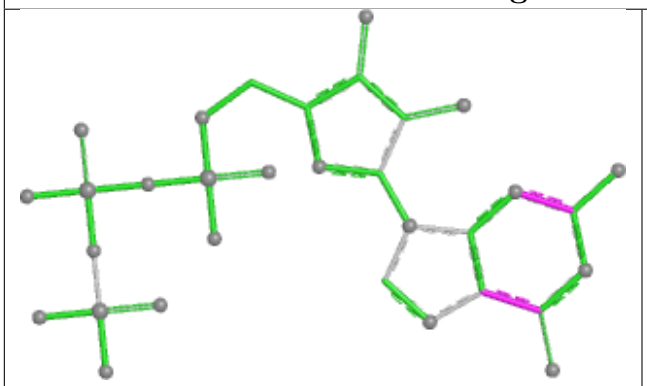

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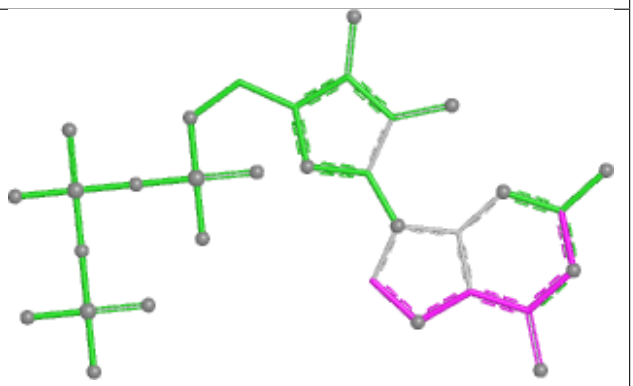

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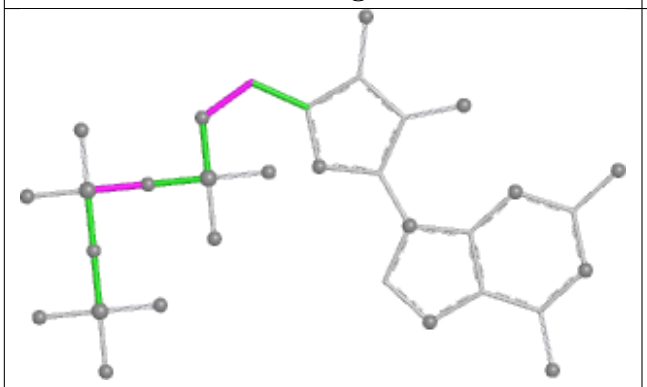

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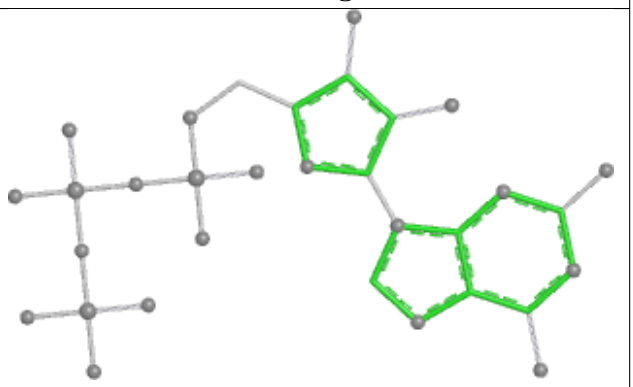
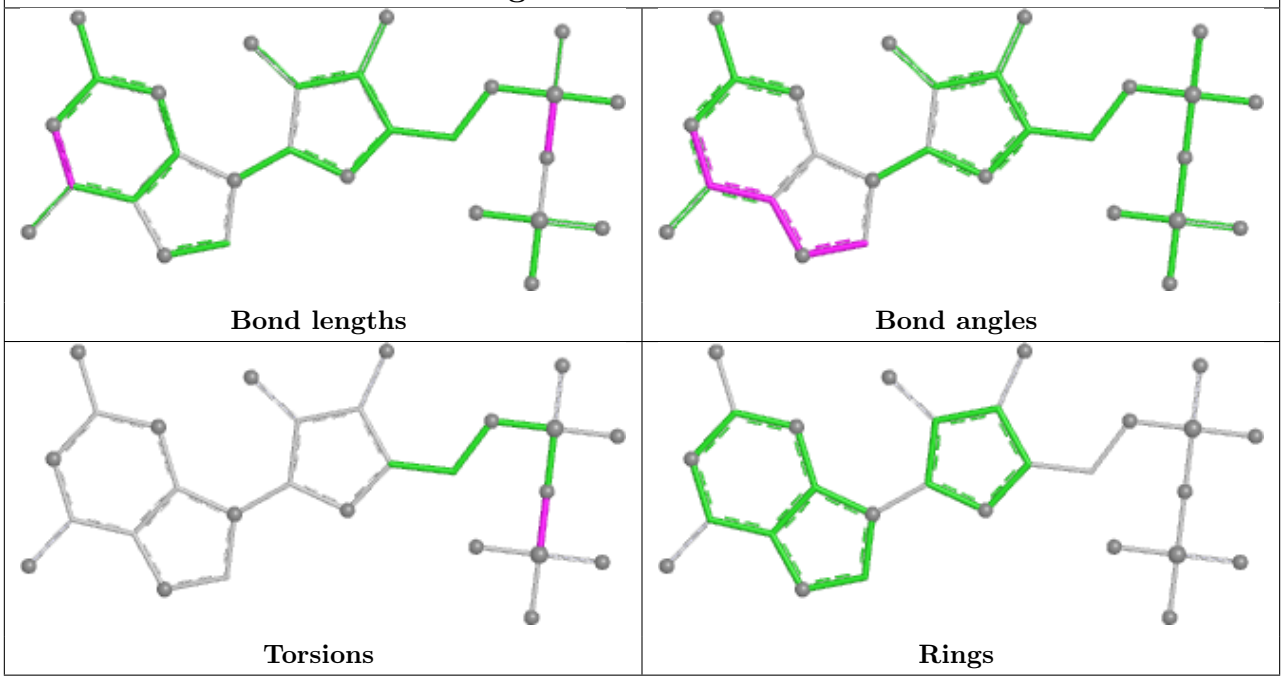
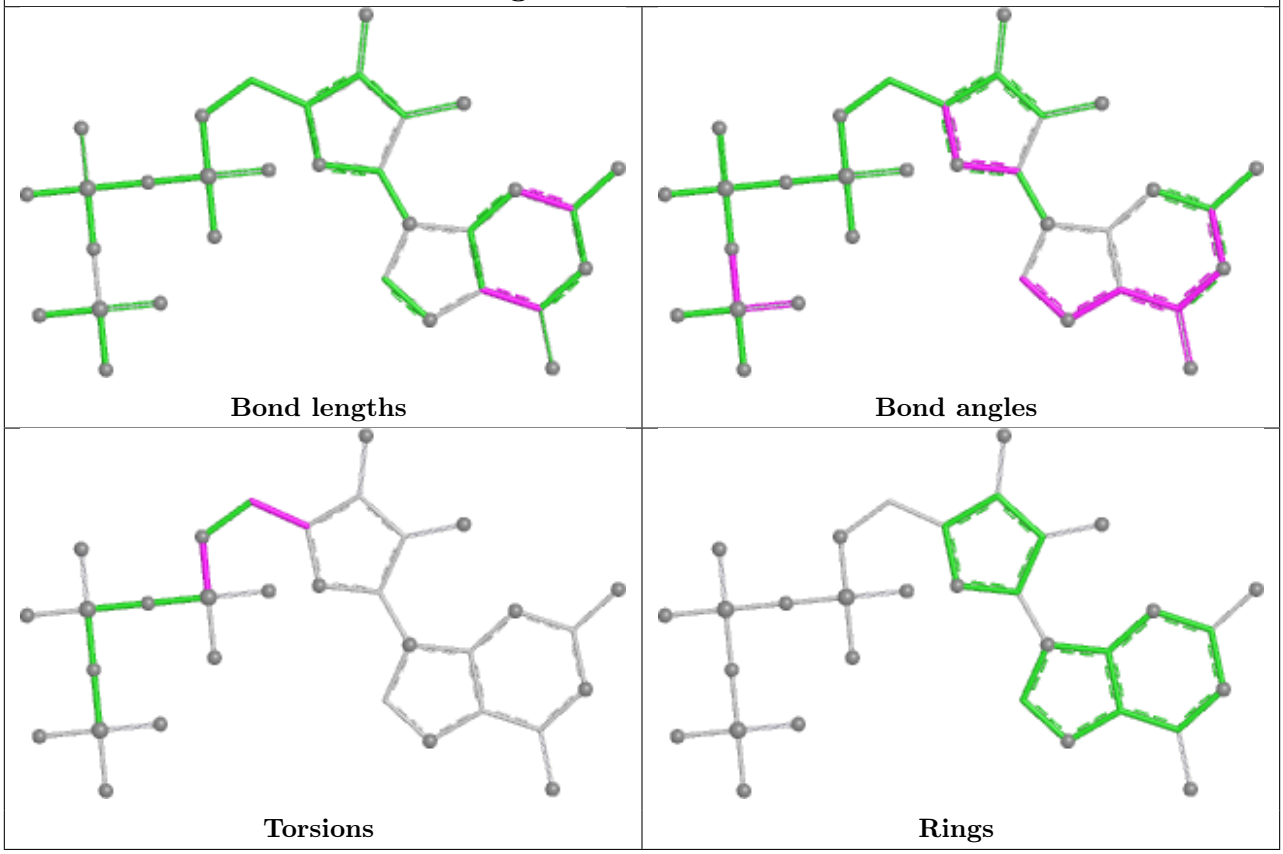


Rings

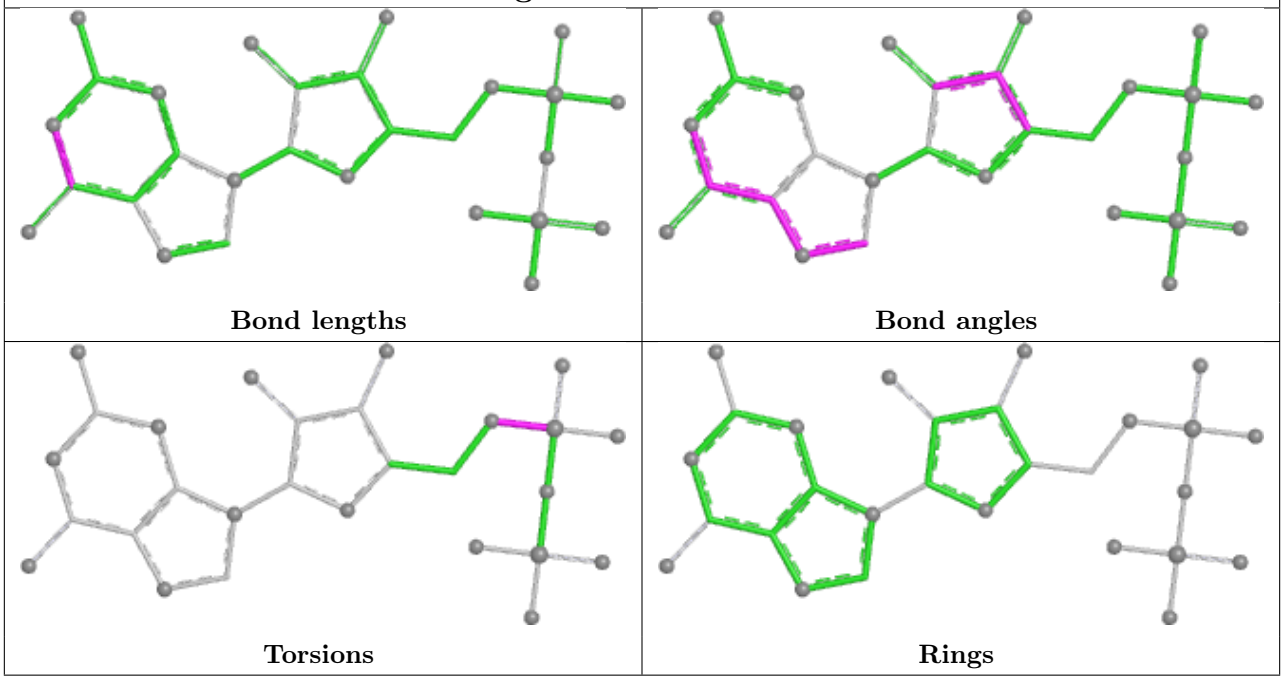
Ligand GDP OD 501



Ligand GTP CK 501



Ligand GDP ID 501



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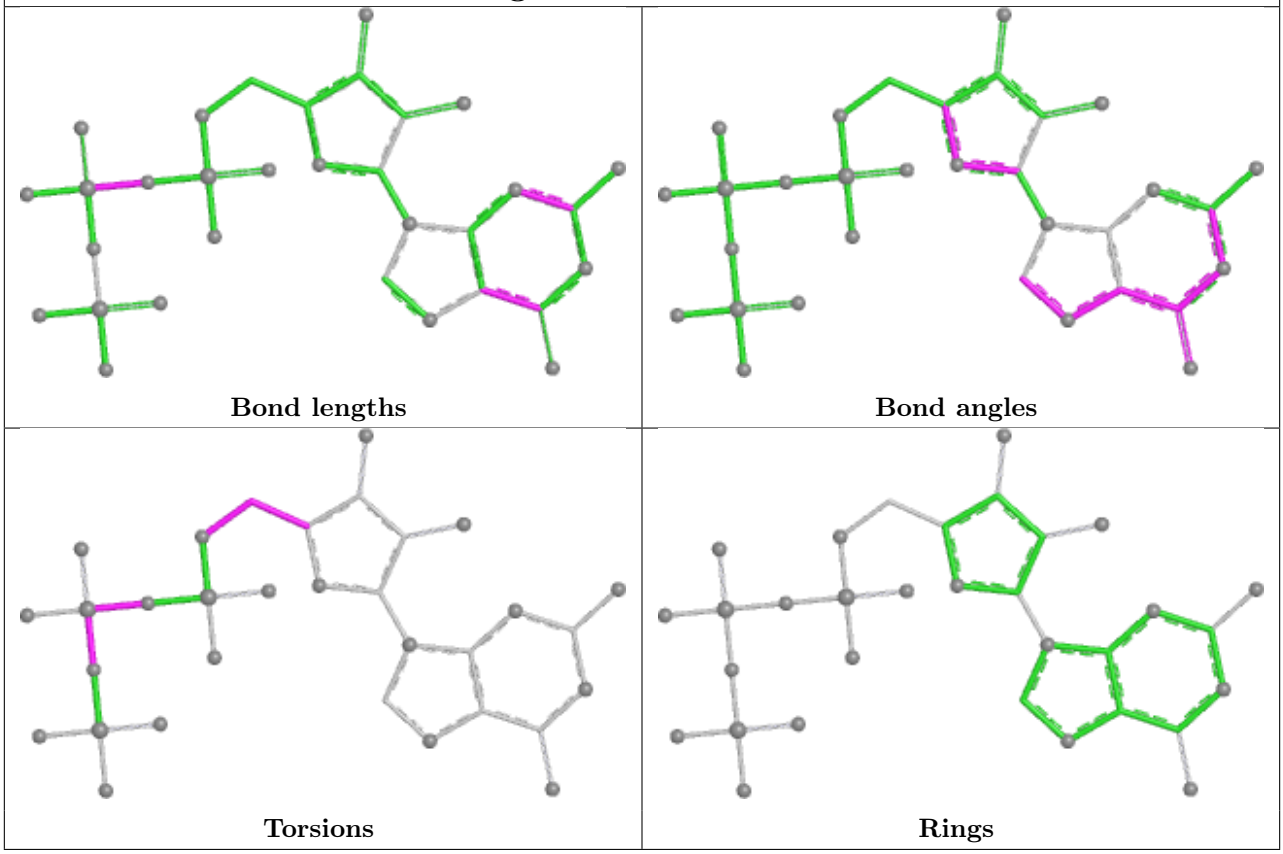
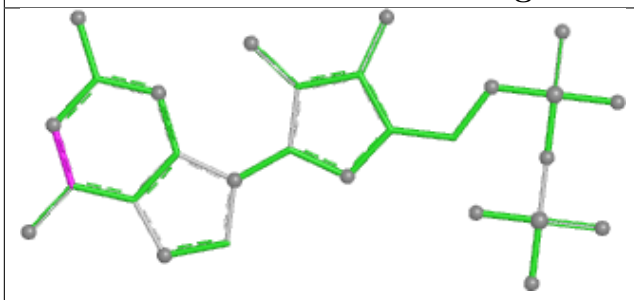
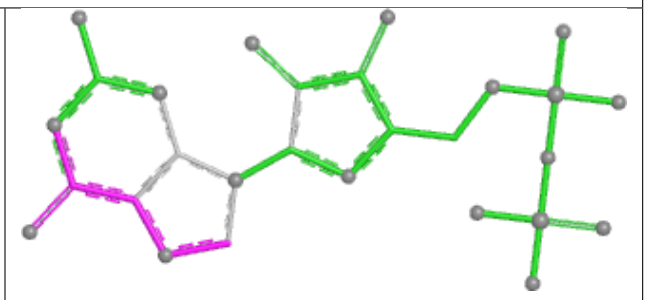


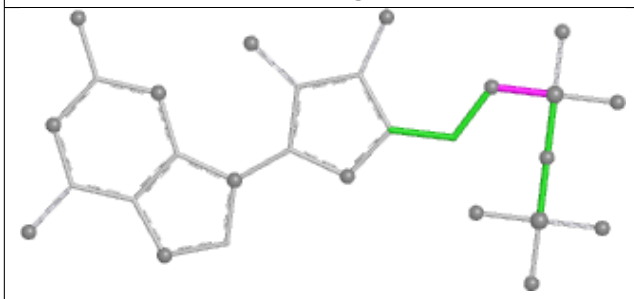
Ligand GDP SL 501



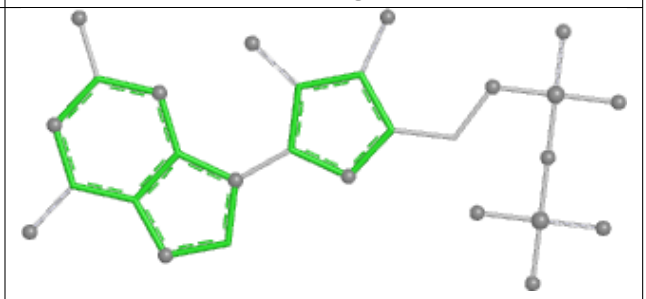
Bond lengths



Bond angles

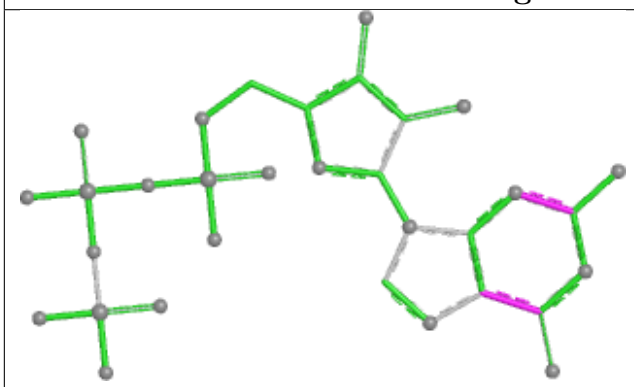


Torsions



Rings

Ligand GTP FF 502



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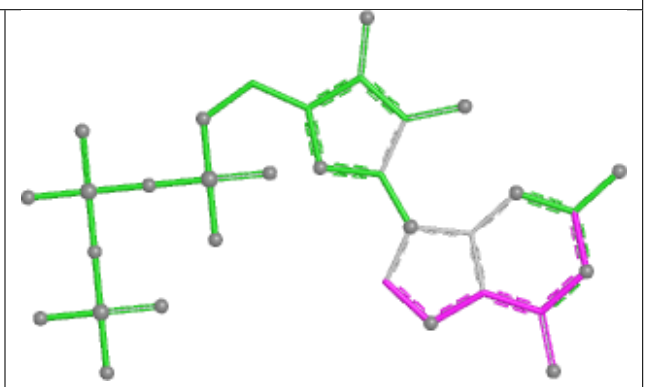

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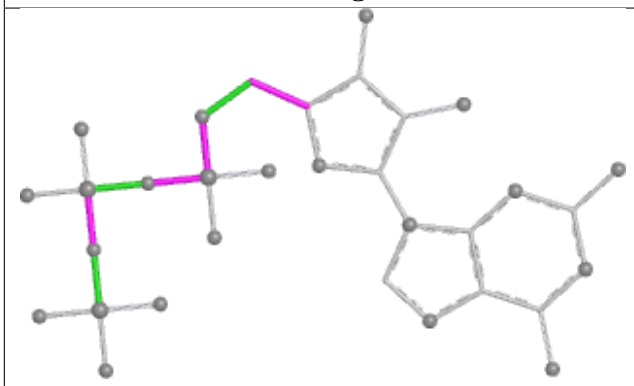

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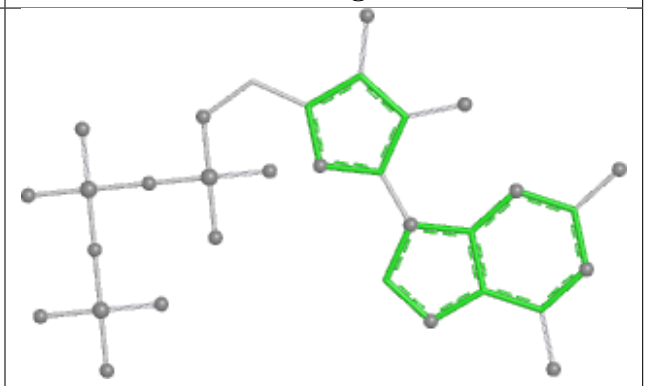

Rings

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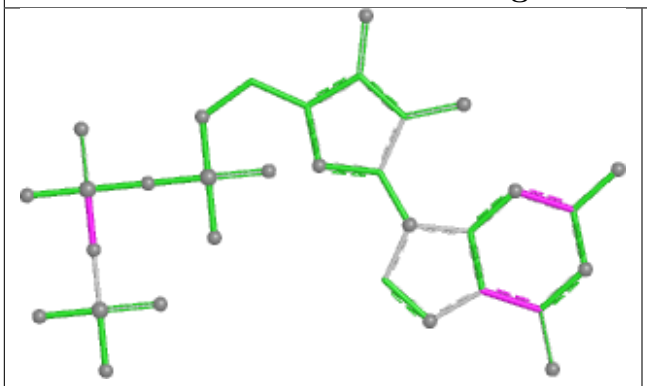

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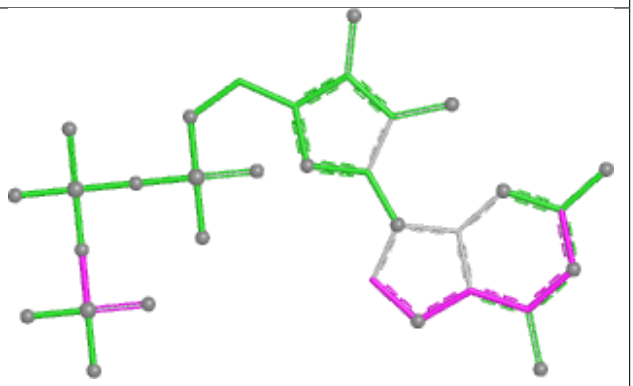
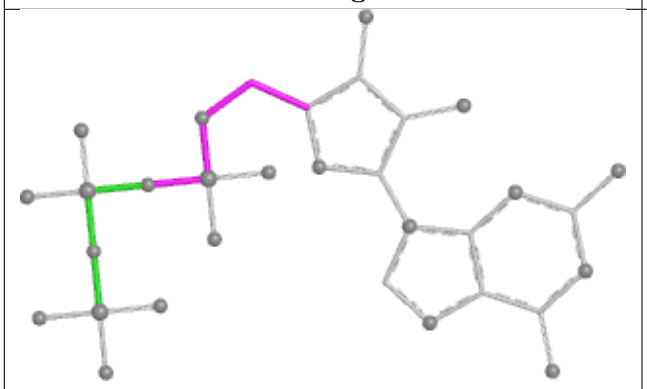


Bond angles



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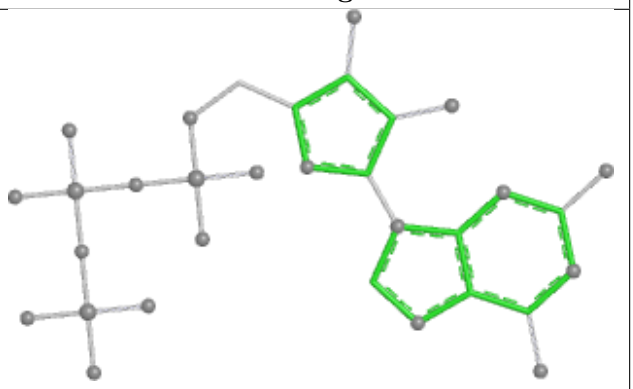
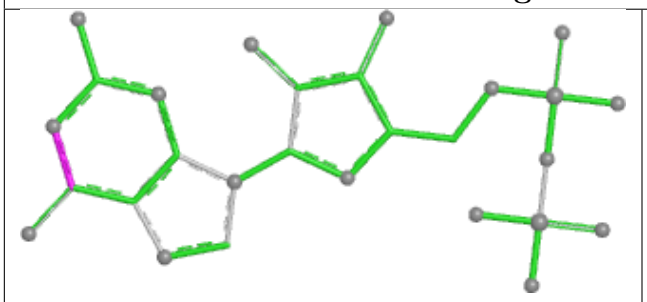
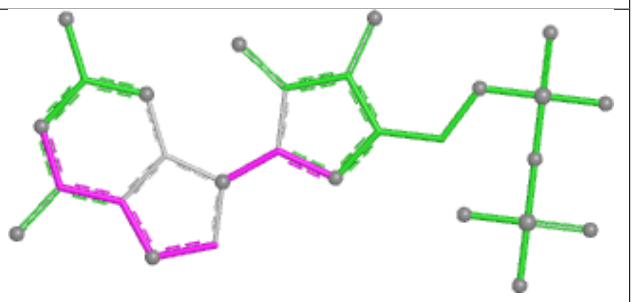


Rings

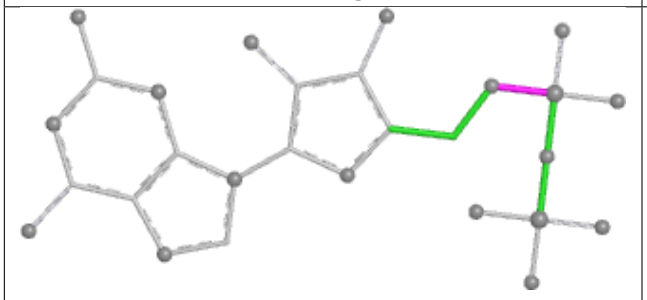
Ligand GDP PJ 501



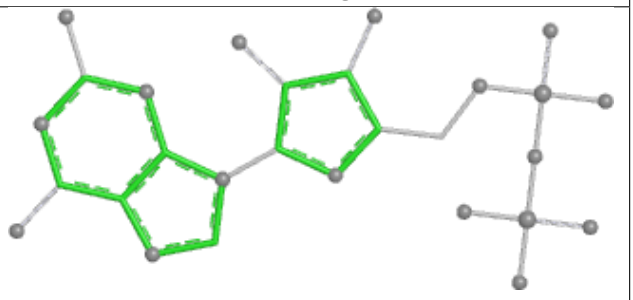
Bond lengths



Bond angles

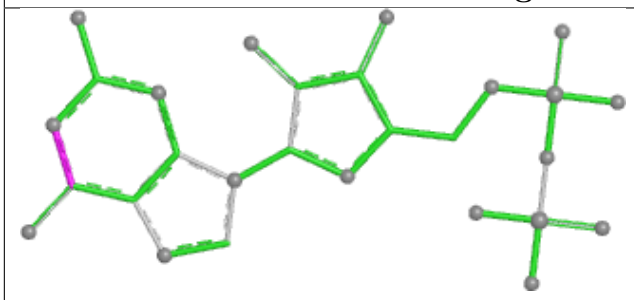


Torsions

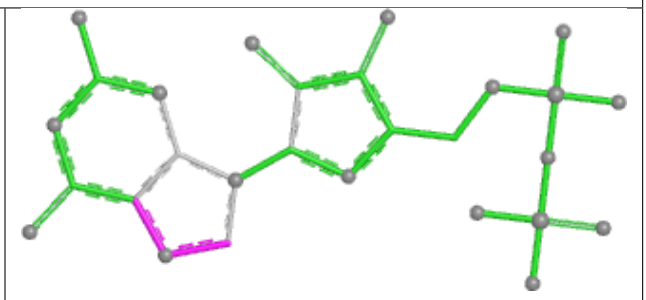


Rings

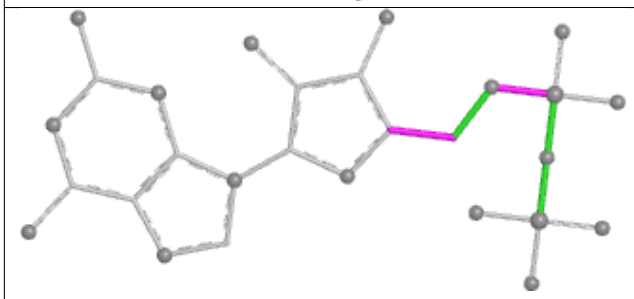
Ligand GDP FJ 501



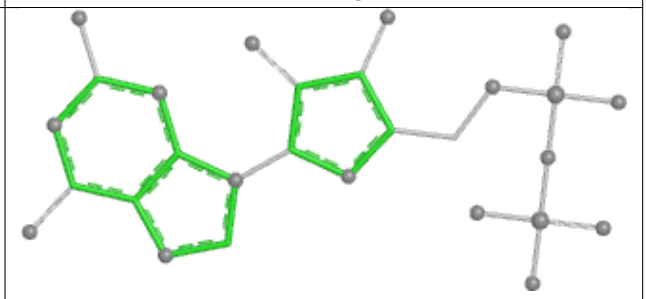
Bond lengths



Bond angles

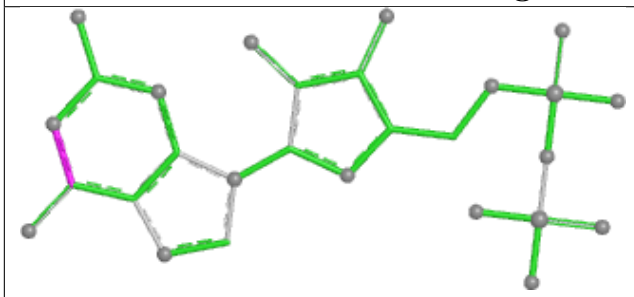


Torsions

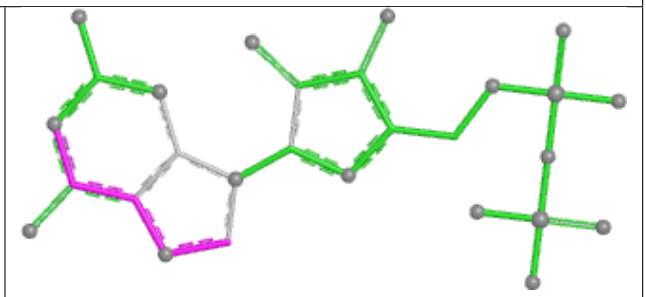


Rings

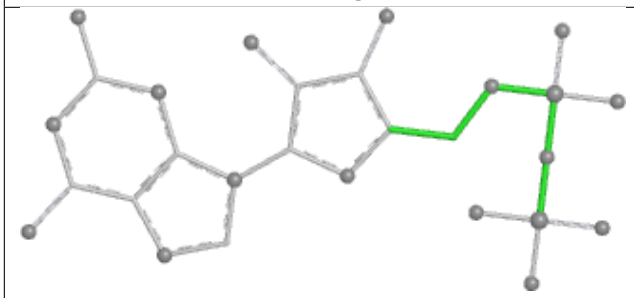
Ligand GDP TJ 501



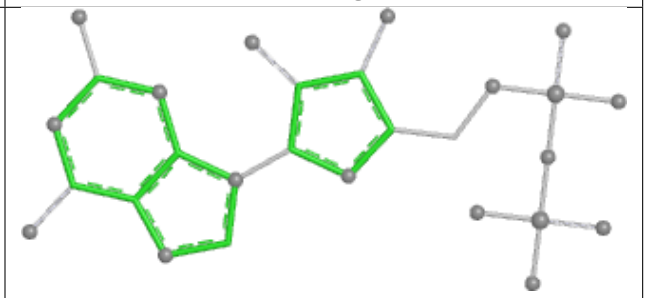
Bond lengths



Bond angles

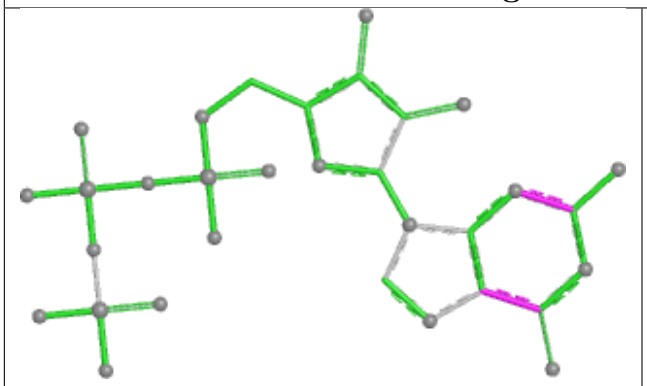


Torsions



Rings

Ligand GTP MM 501



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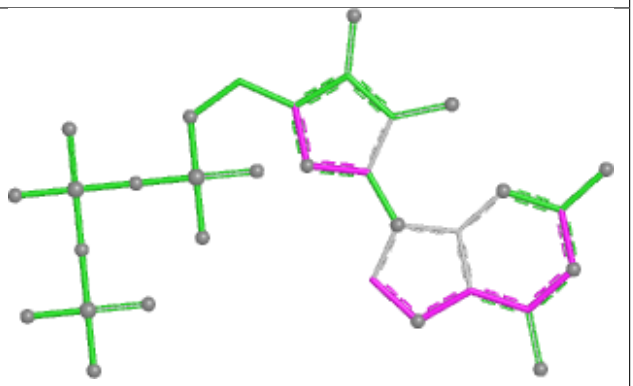
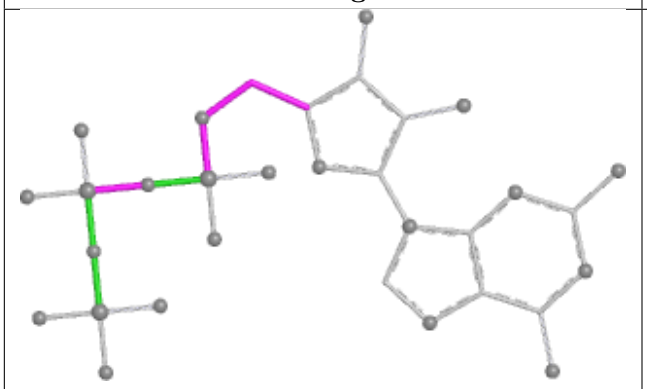
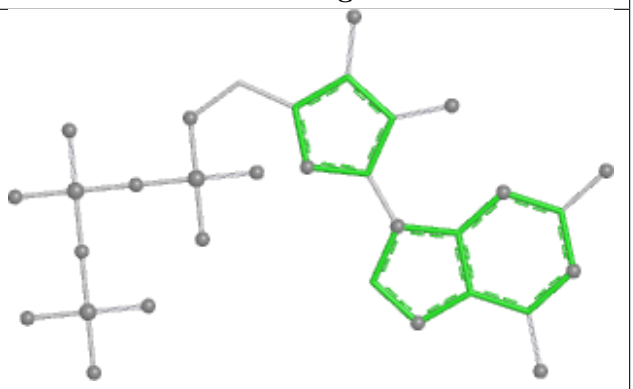


Bond angles

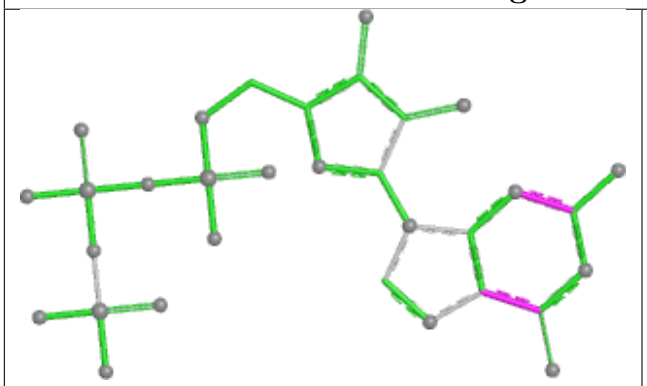


Torsions

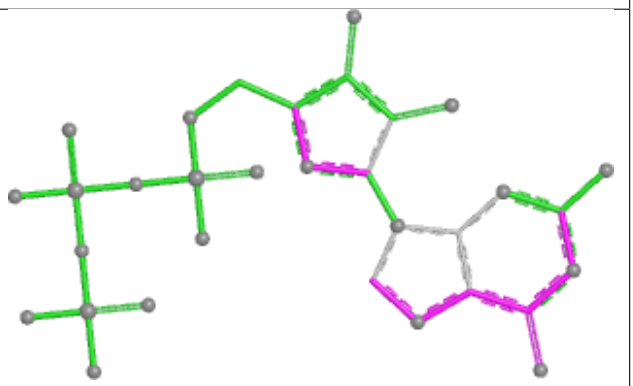


Rings

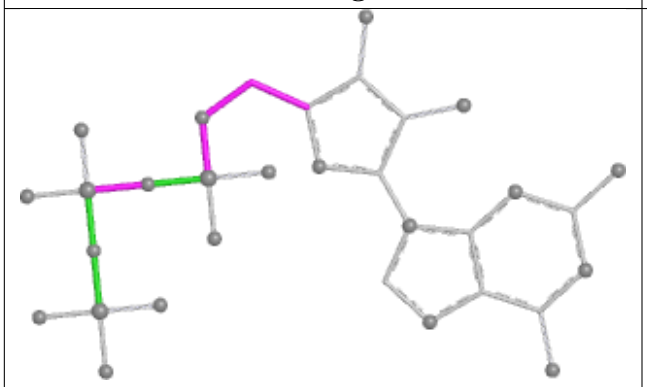
Ligand GTP BG 501



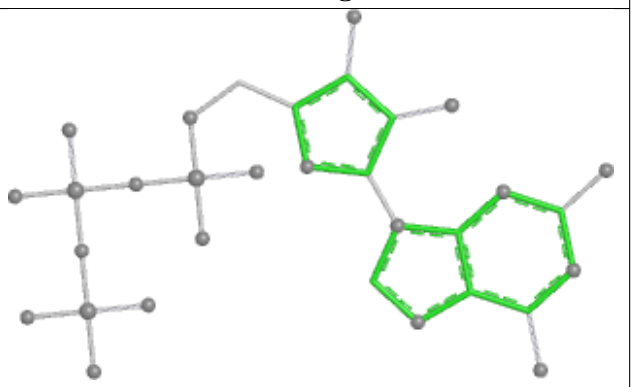
Bond lengths



Bond angles

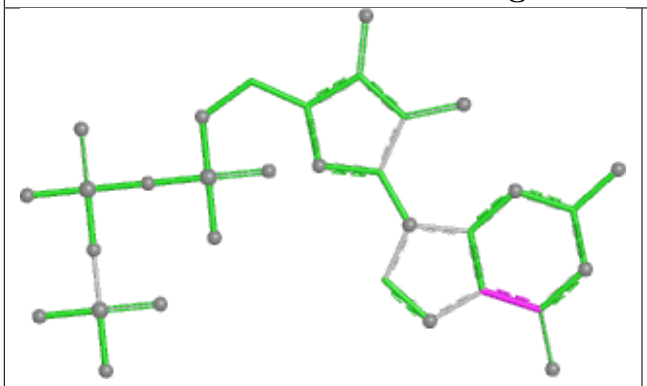


Torsions

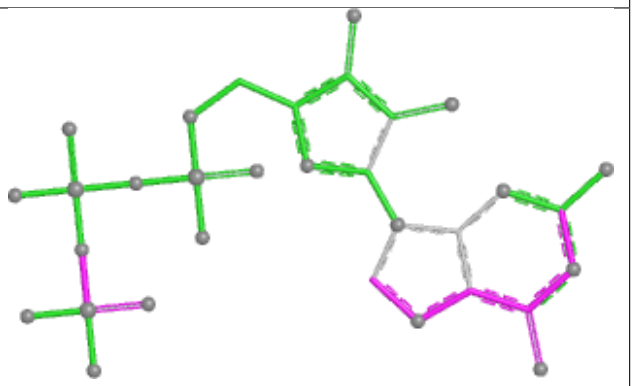


Rings

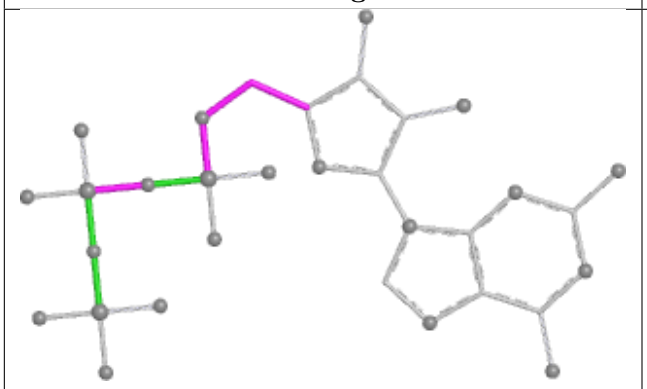
Ligand GTP NG 501



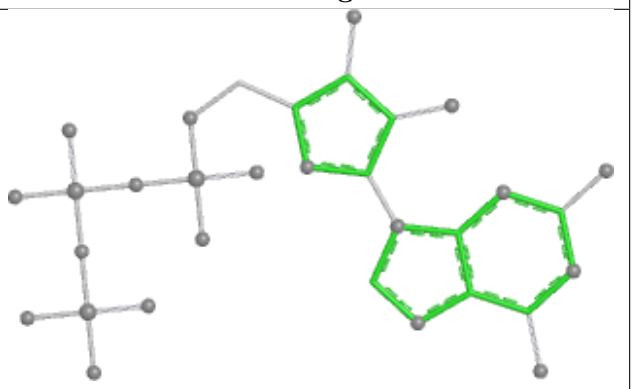
Bond lengths



Bond angles

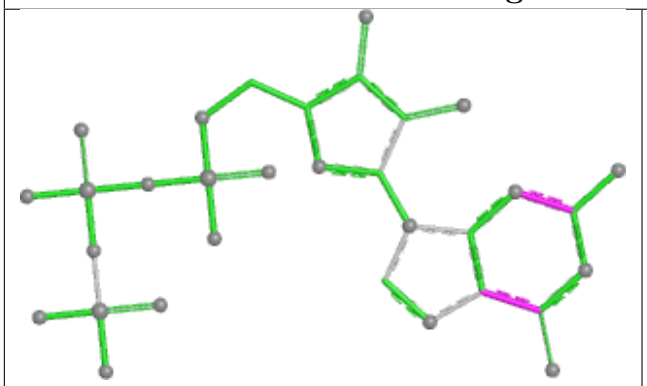


Torsions

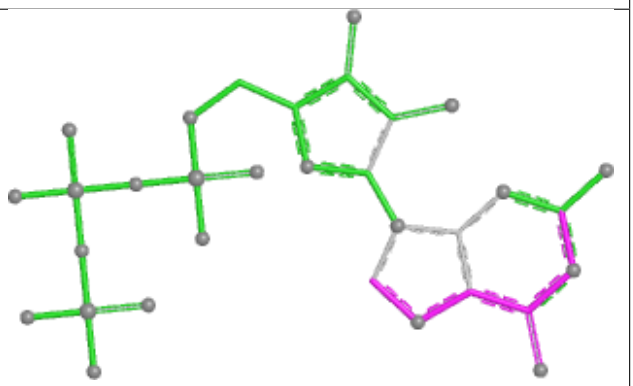


Rings

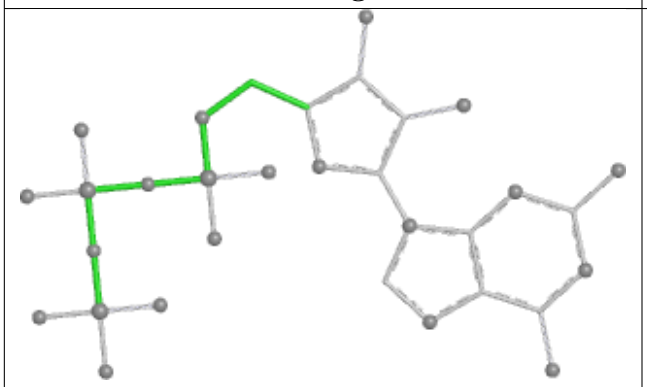
Ligand GTP WC 501



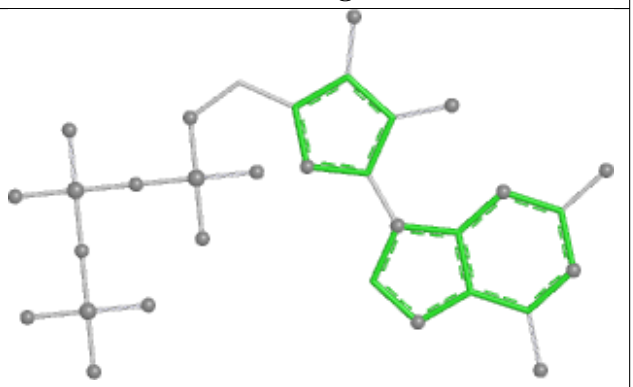
Bond lengths



Bond angles

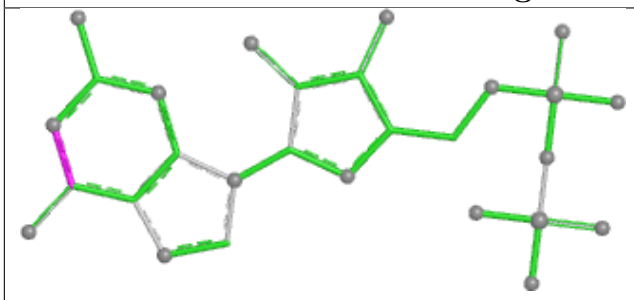


Torsions

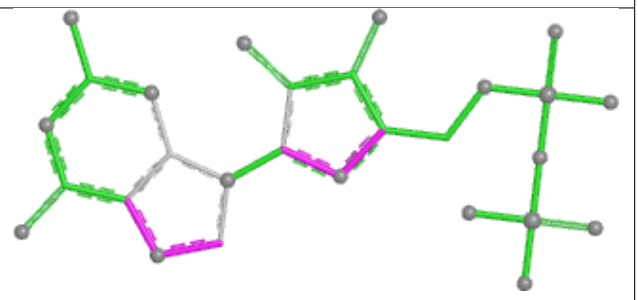


Rings

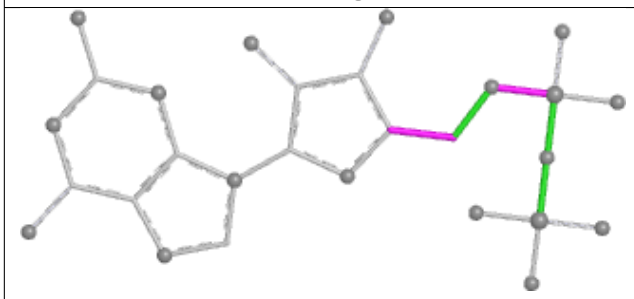
Ligand GDP EJ 501



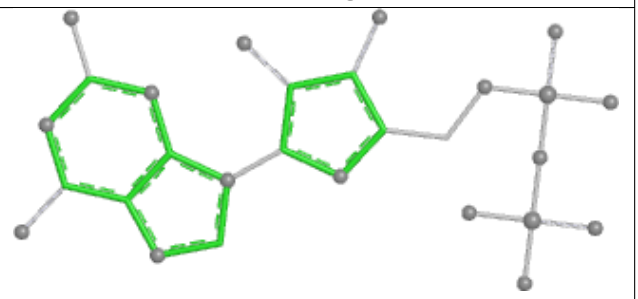
Bond lengths



Bond angles

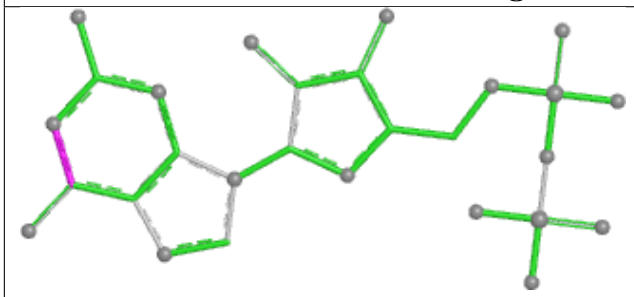


Torsions

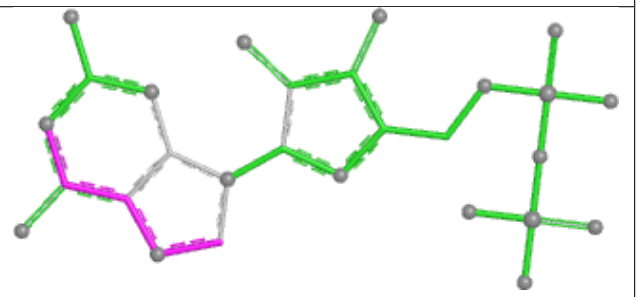


Rings

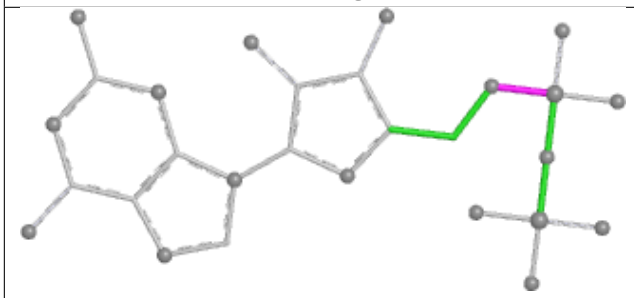
Ligand GDP UH 501



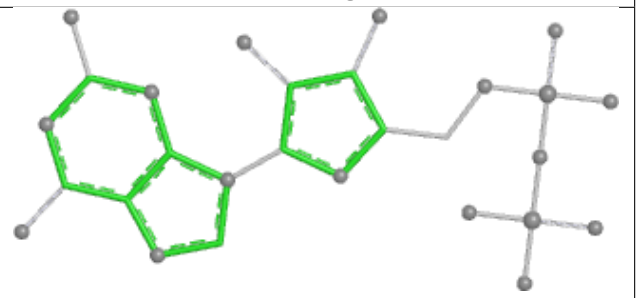
Bond lengths



Bond angles

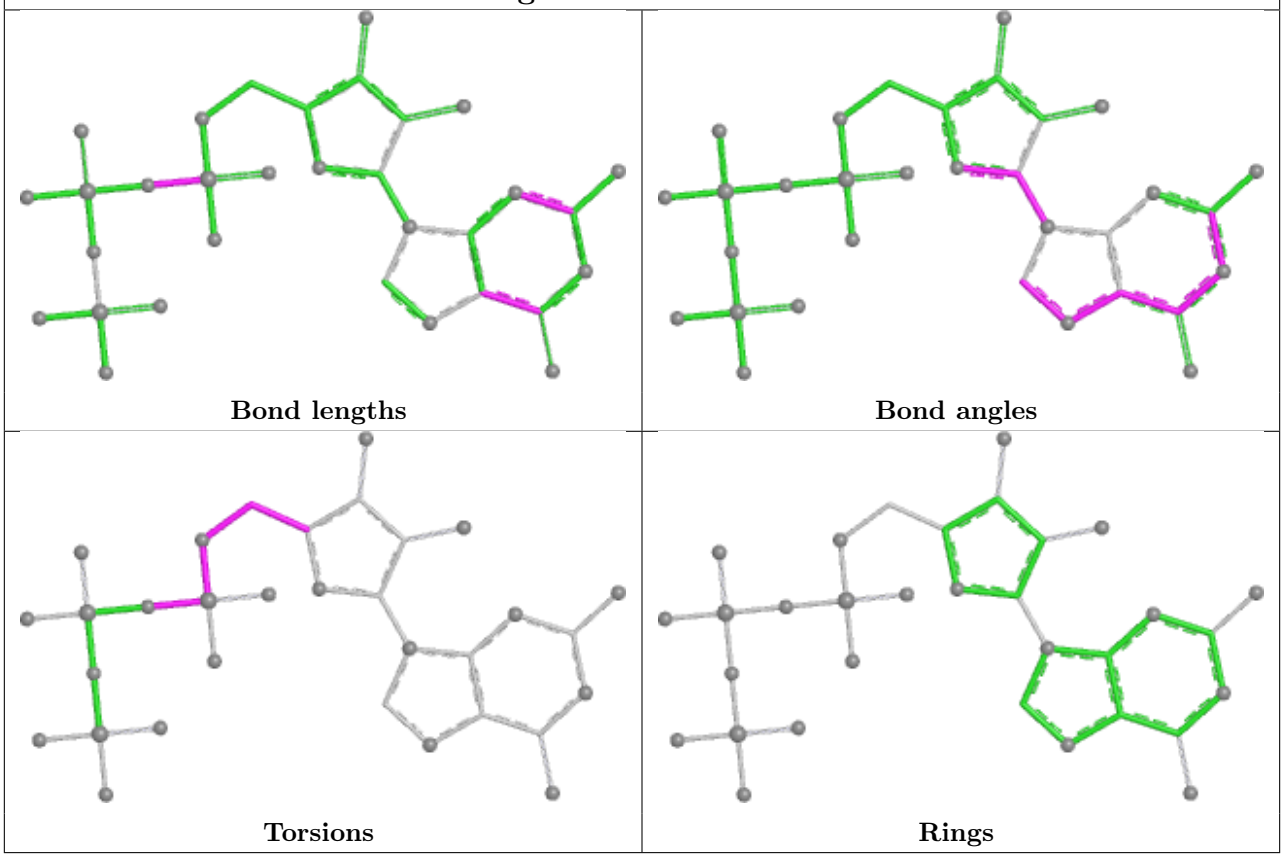


Torsions



Rings

Ligand GTP TI 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

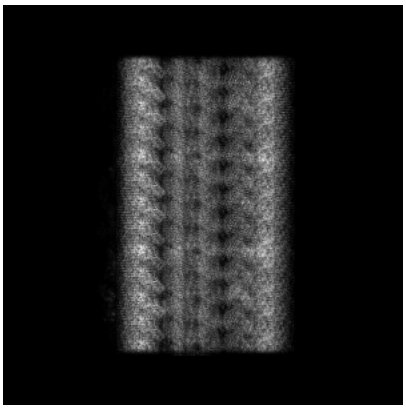
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-45801. These allow visual inspection of the internal detail of the map and identification of artifacts.

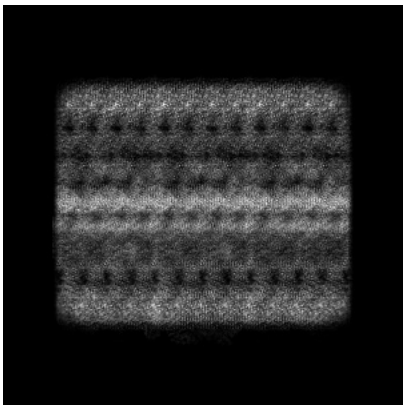
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

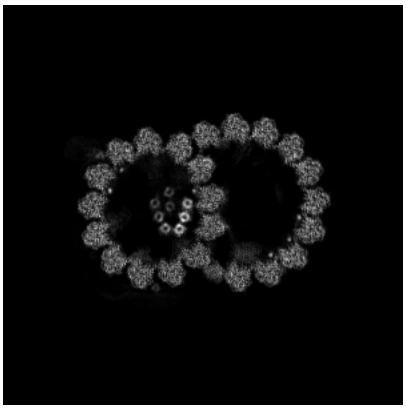
6.1.1 Primary map



X

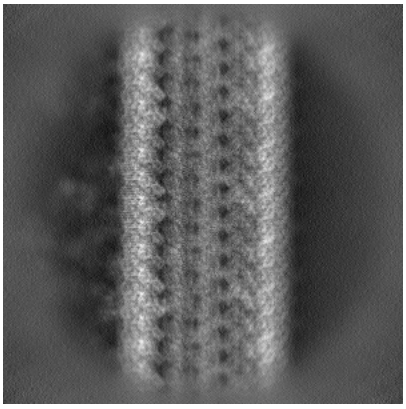


Y

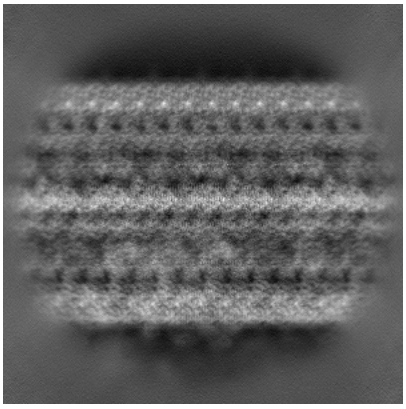


Z

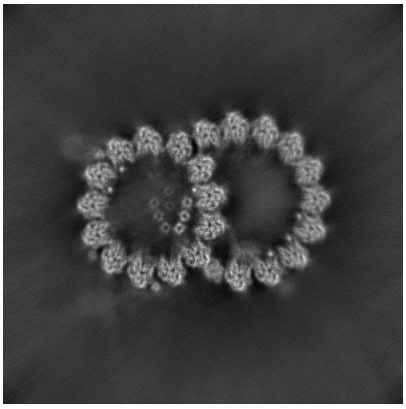
6.1.2 Raw map



X



Y

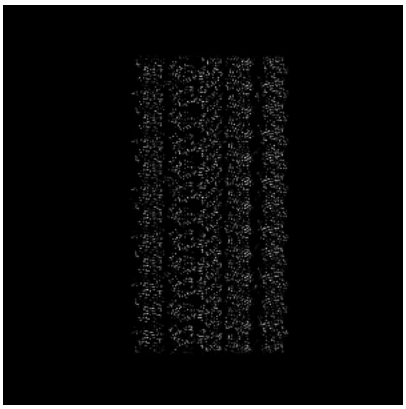


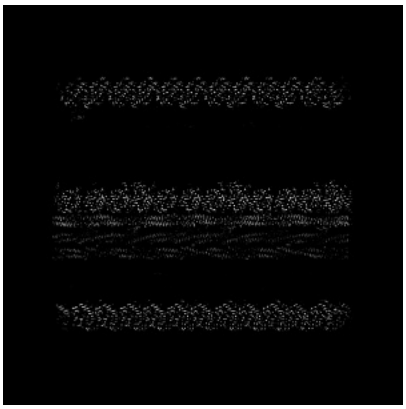
Z

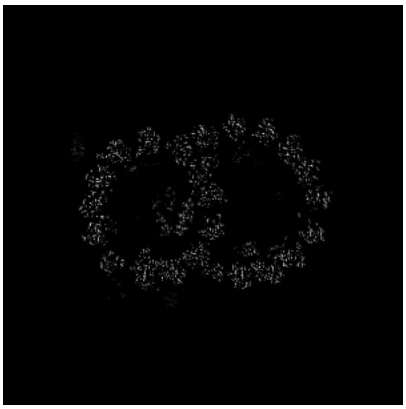
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

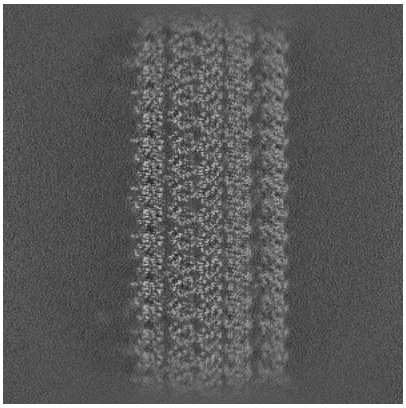
6.2.1 Primary map

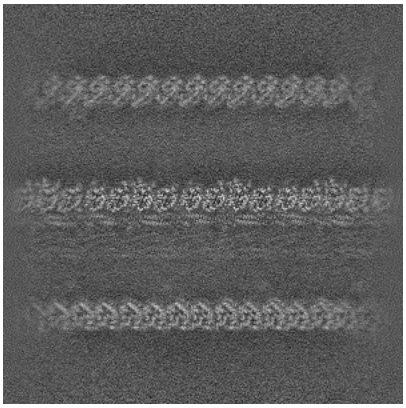

X Index: 256

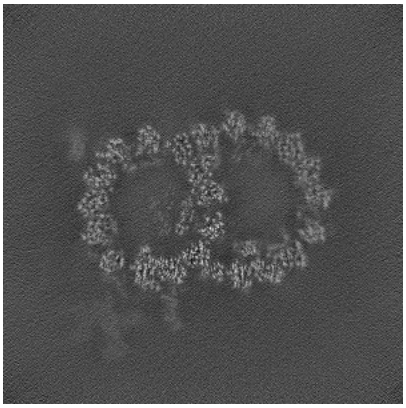

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

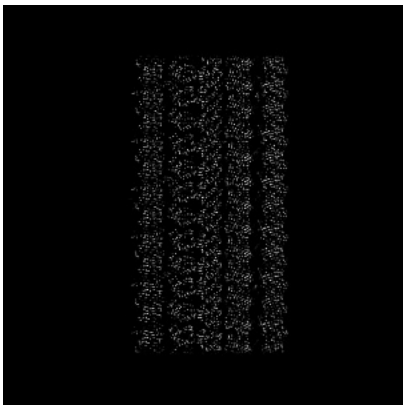

Y Index: 256


Z Index: 256

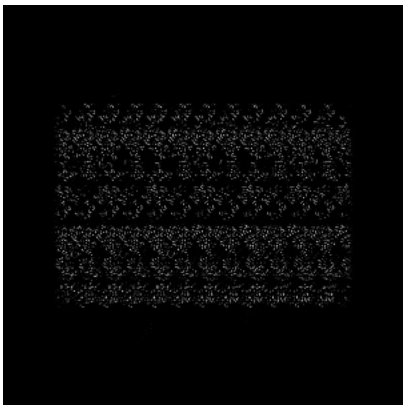
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

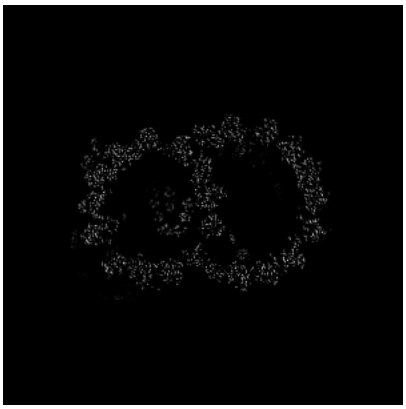
6.3.1 Primary map



X Index: 256

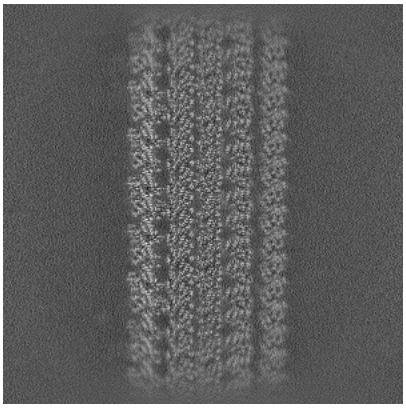


Y Index: 176

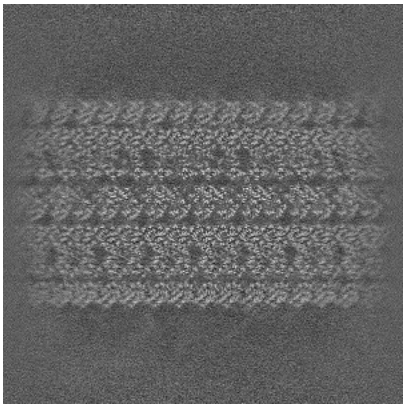


Z Index: 199

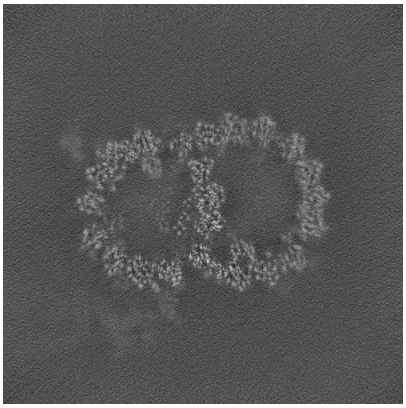
6.3.2 Raw map



X Index: 261



Y Index: 177

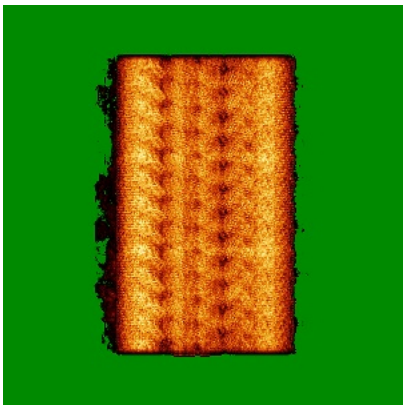


Z Index: 266

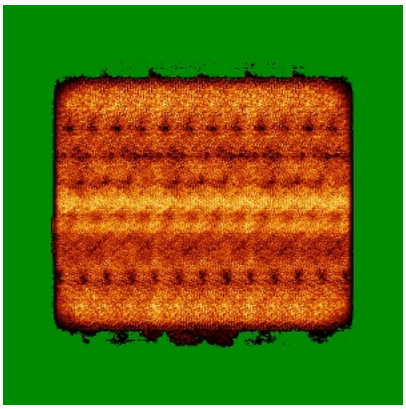
The images above show the largest variance slices of the map in three orthogonal directions.

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

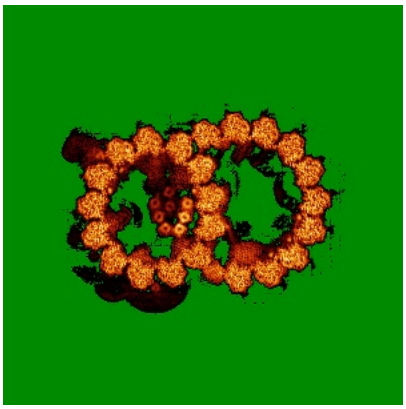
6.4.1 Primary map



X

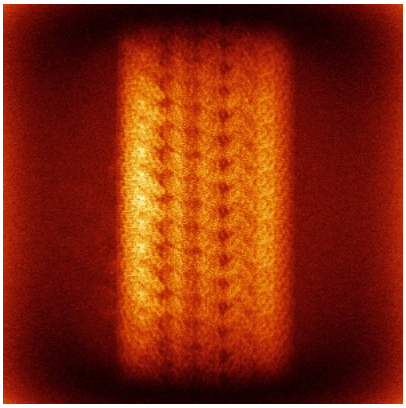


Y

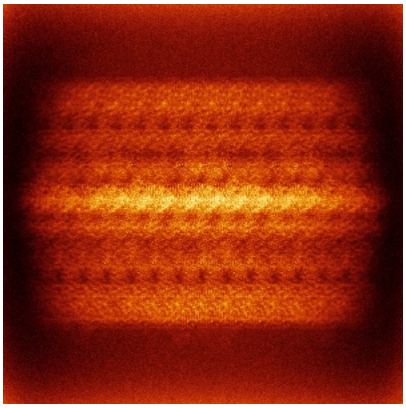


Z

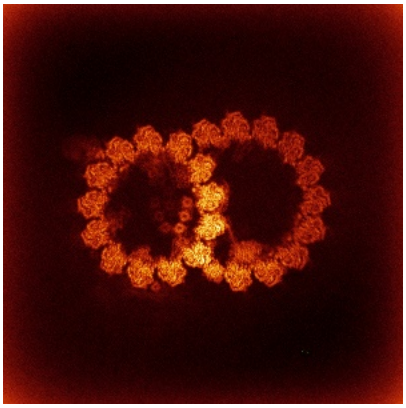
6.4.2 Raw map



X



Y

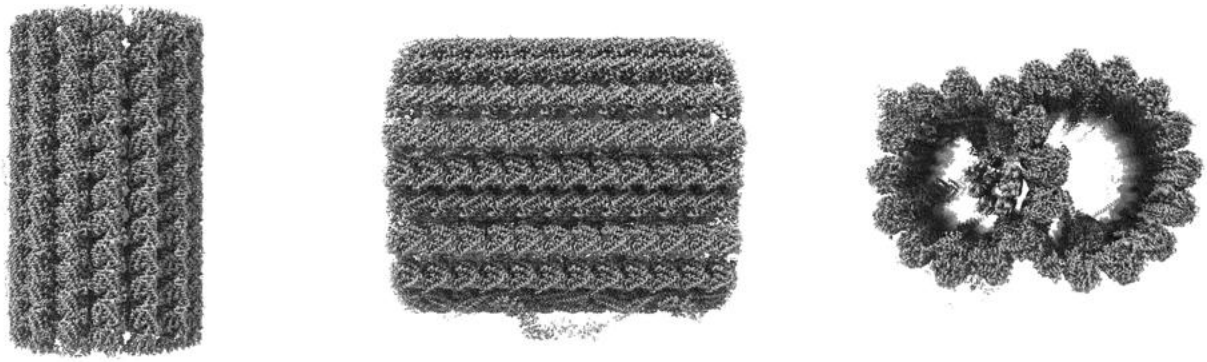


Z

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)

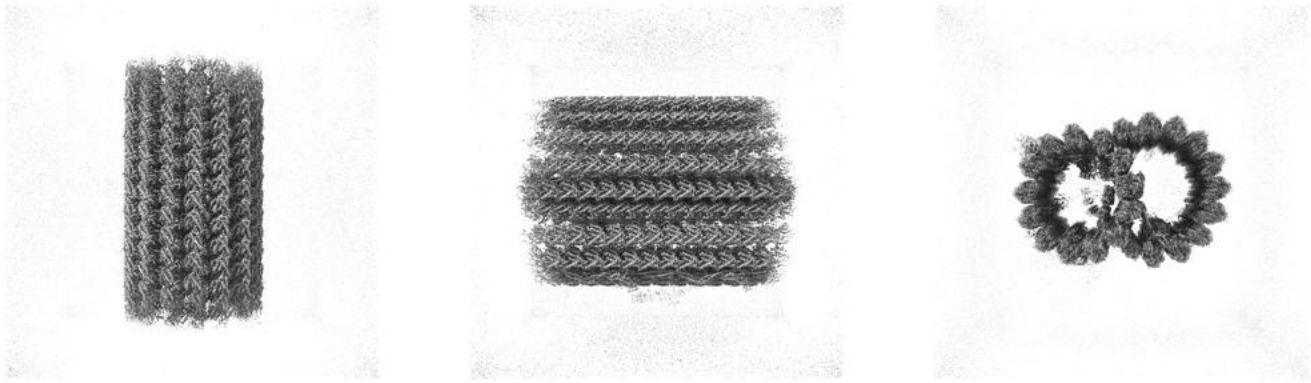
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

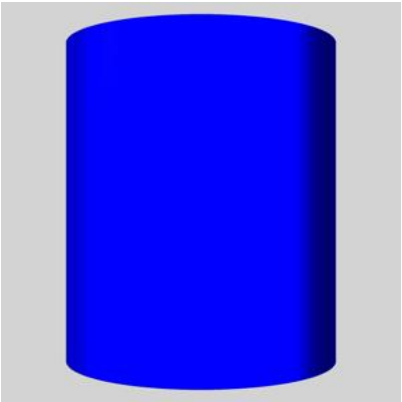
6.6 Mask visualisation (i)

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

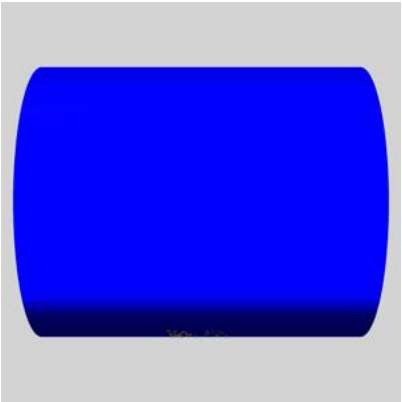
A mask typically either:

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

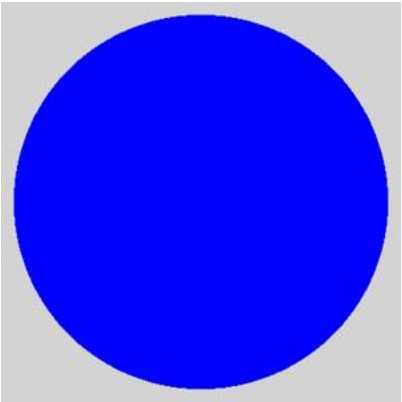
6.6.1 emd_45801_msk_1.map (i)



X



Y

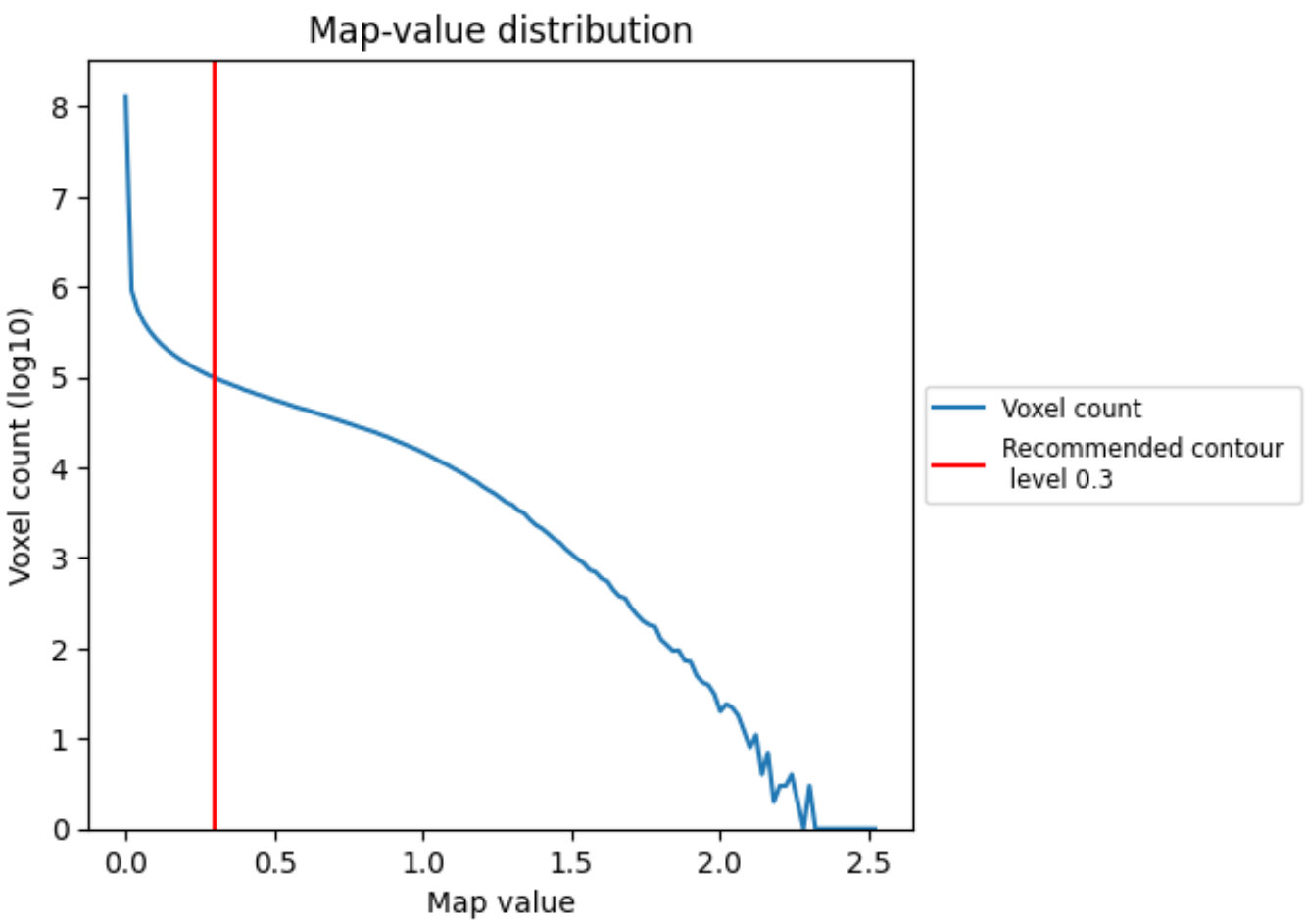


Z

7 Map analysis (i)

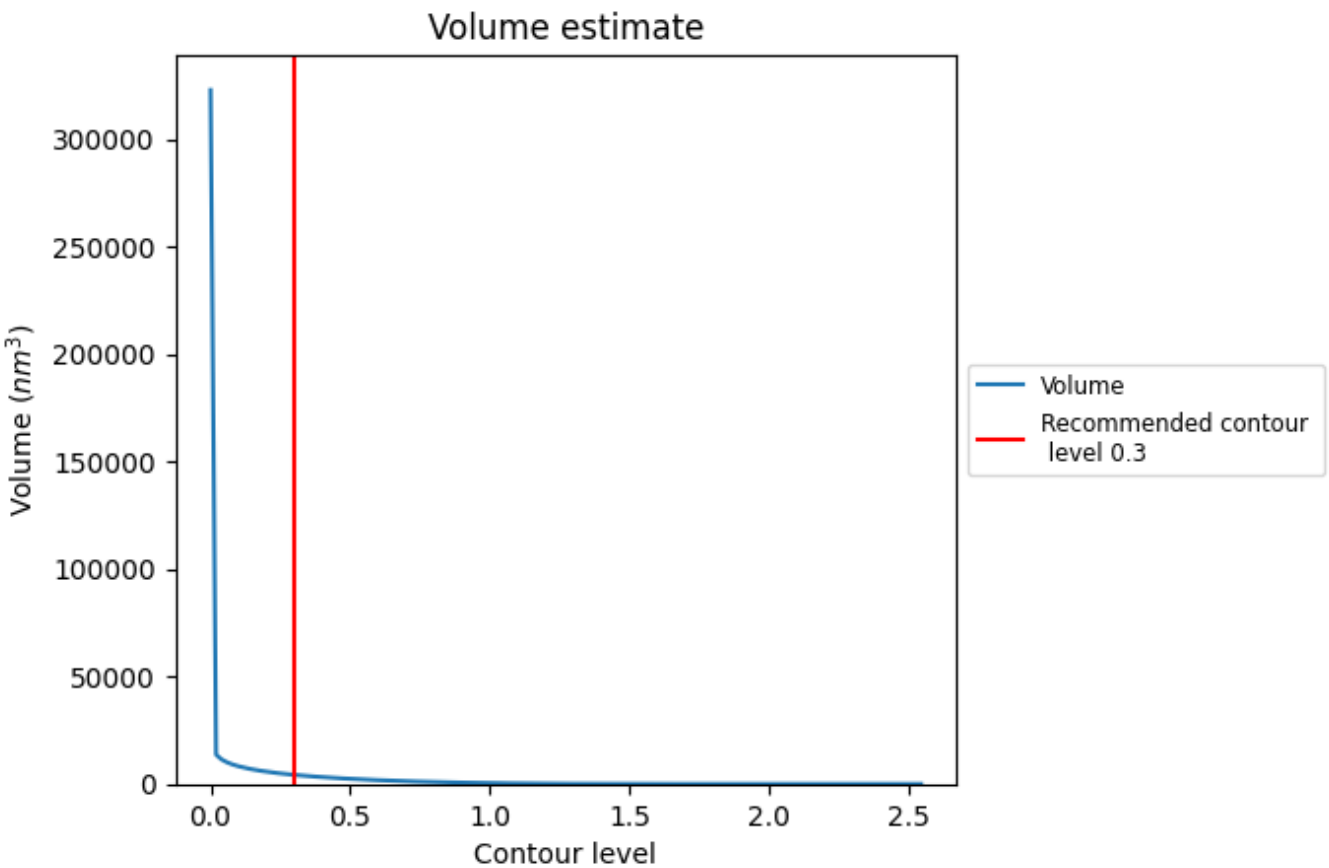
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

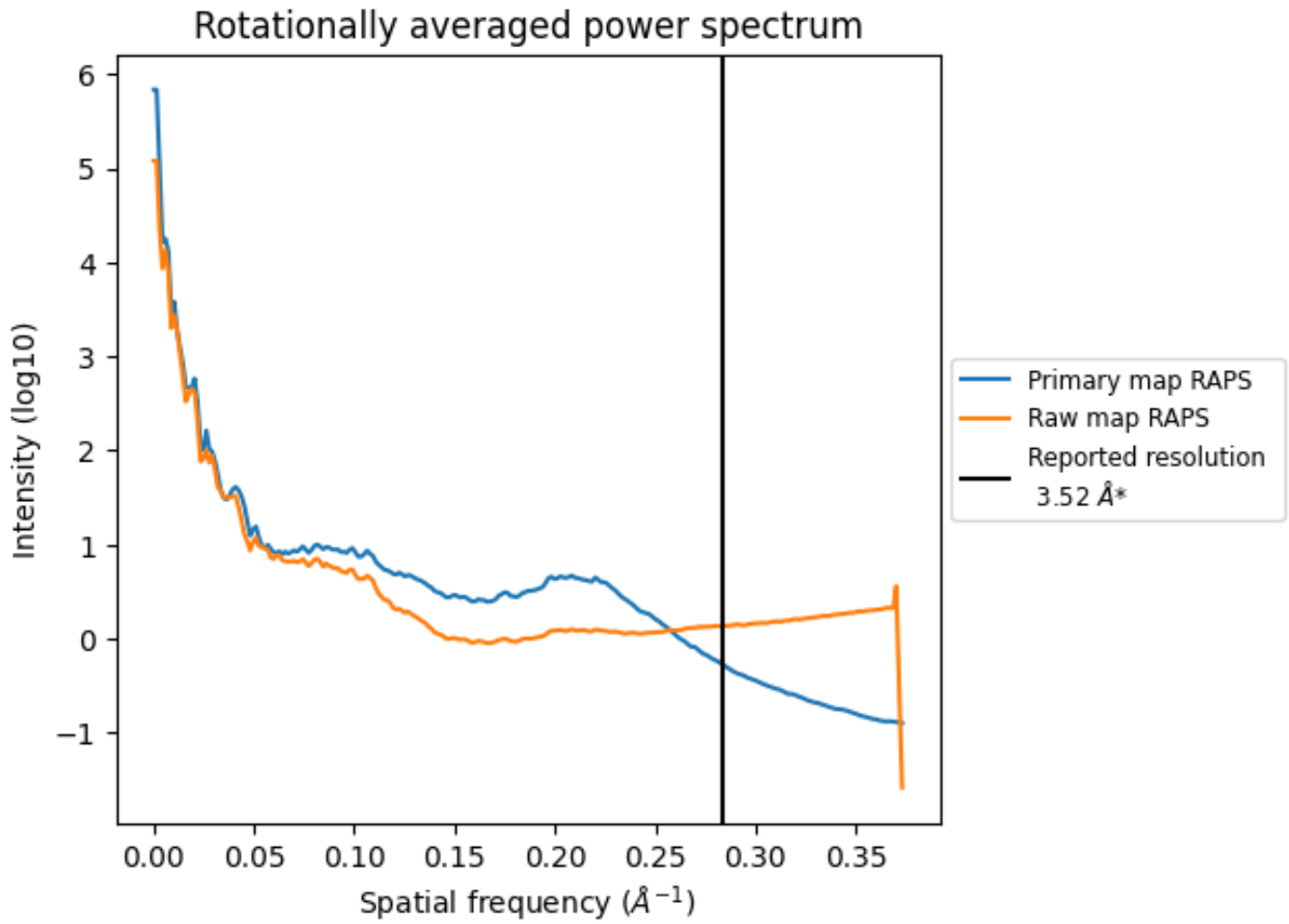
7.2 Volume estimate (i)



The volume at the recommended contour level is 4225 nm^3; this corresponds to an approximate mass of 3816 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)

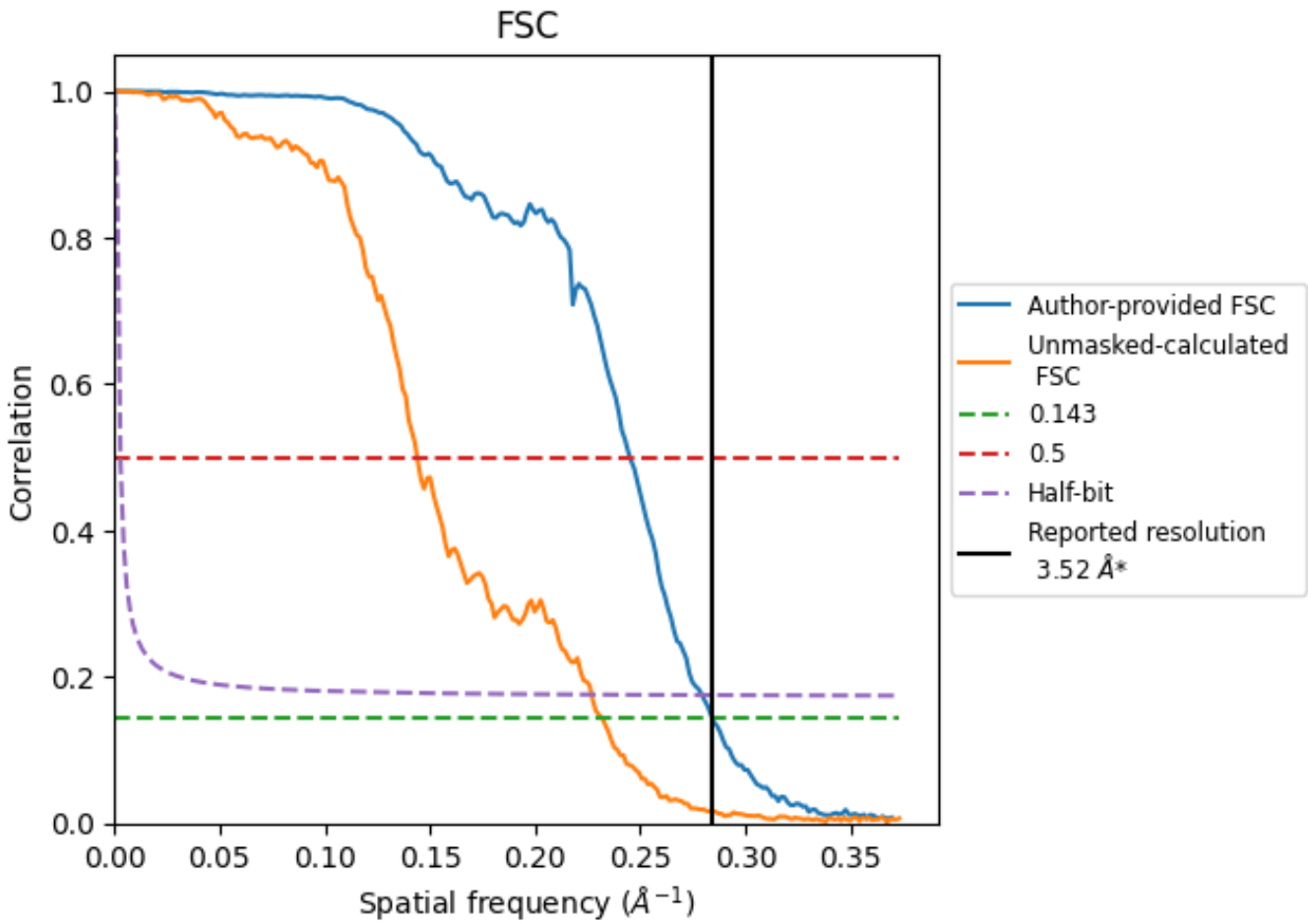


*Reported resolution corresponds to spatial frequency of 0.284 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.284 Å^{-1}

8.2 Resolution estimates (i)

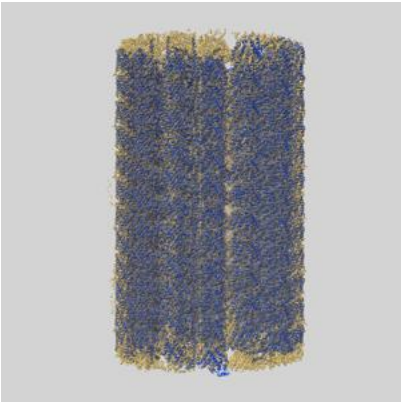
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	3.52	4.08	3.58
Unmasked-calculated*	4.31	6.95	4.41

*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 4.31 differs from the reported value 3.52 by more than 10 %

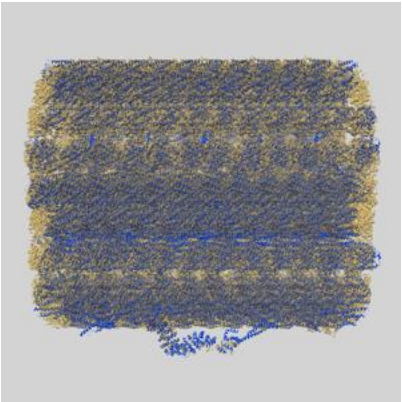
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-45801 and PDB model 9CPB. Per-residue inclusion information can be found in section 3 on page 61.

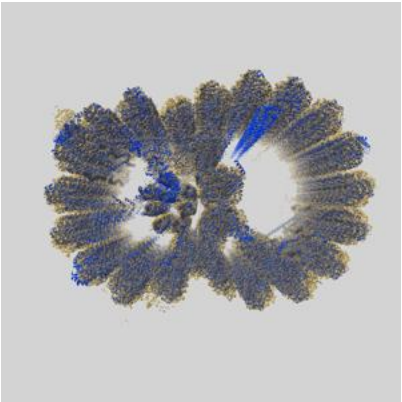
9.1 Map-model overlay (i)



X



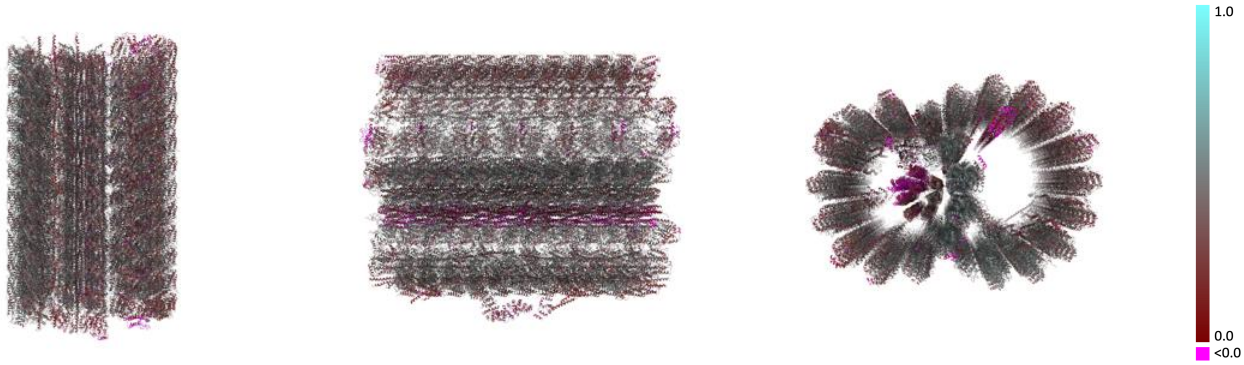
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

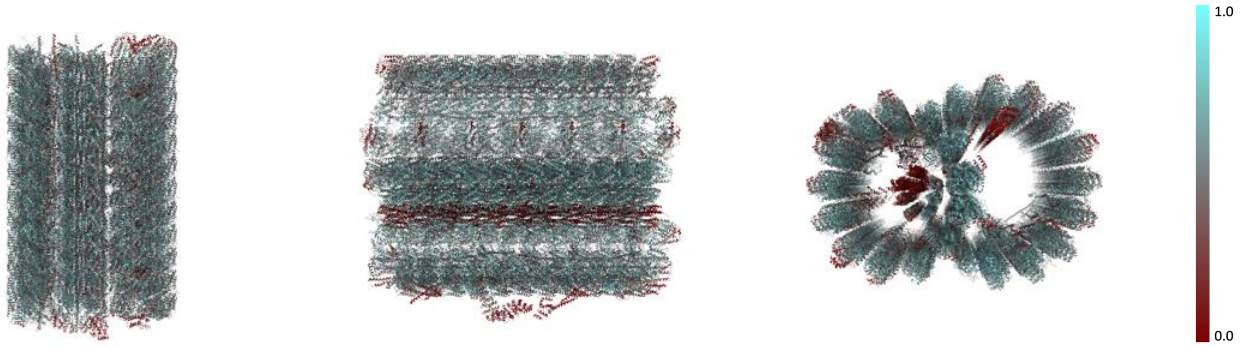
9.2 Q-score mapped to coordinate model (i)



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.

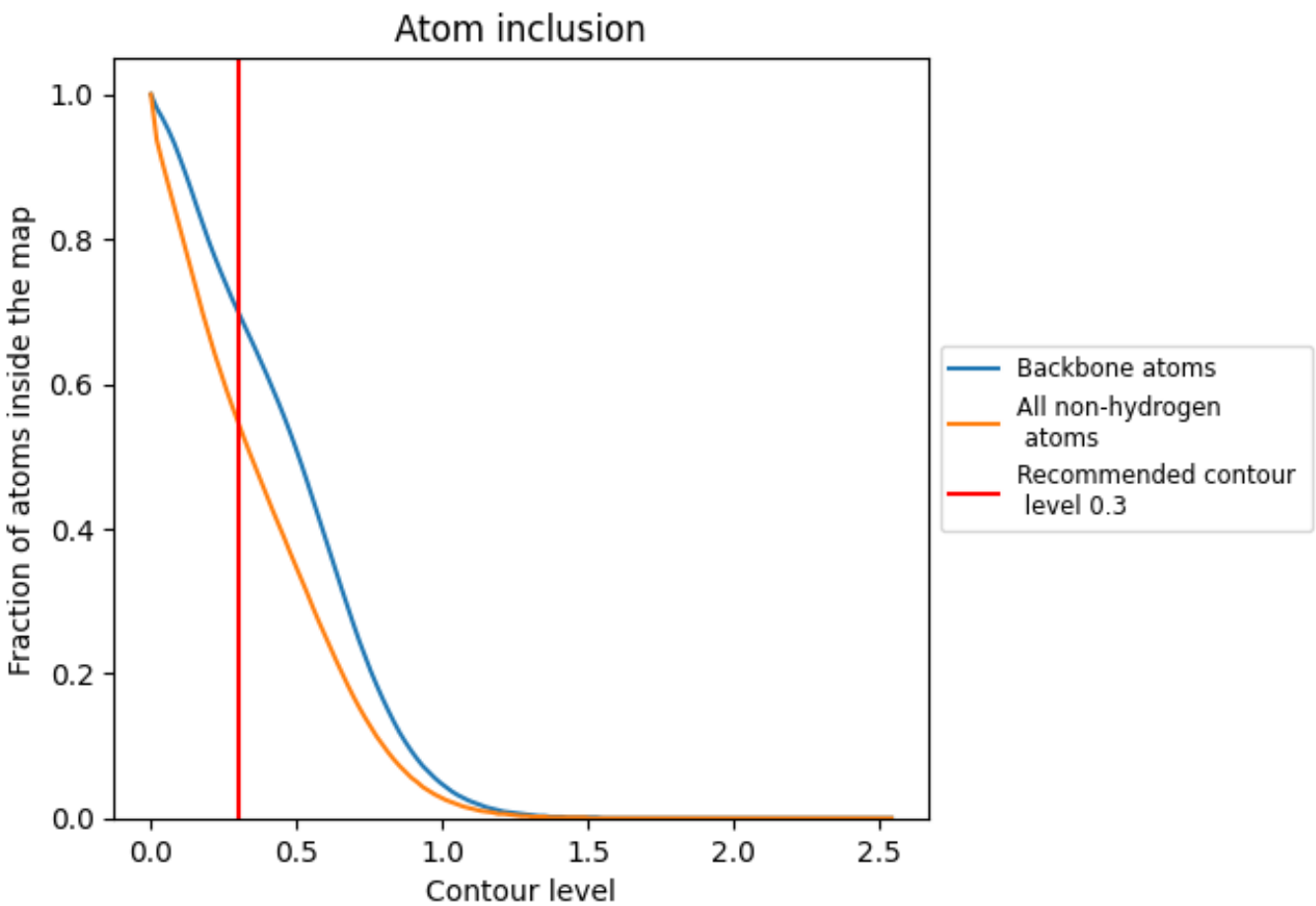
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5460	0.3920
1A	0.2040	0.2830
1D	0.2740	0.2720
1E	0.3550	0.3350
1F	0.2100	0.2710
1H	0.5480	0.3650
1I	0.4580	0.3370
1K	0.3820	0.2800
1L	0.3540	0.2590
1N	0.6230	0.4340
1O	0.6220	0.4400
1P	0.6200	0.4770
1R	0.4690	0.3600
1T	0.5810	0.4230
1U	0.5540	0.4450
1W	0.5540	0.4510
1X	0.6030	0.4470
1Y	0.6210	0.4540
1Z	0.6040	0.4540
2A	0.5920	0.4340
2B	0.6040	0.4330
2D	0.2690	0.2750
2E	0.0250	0.0980
2F	0.5530	0.4210
2G	0.4940	0.3720
2H	0.4890	0.3390
2J	0.3500	0.3190
2K	0.3870	0.3070
2L	0.3080	0.2520
2M	0.3770	0.2950
2O	0.5800	0.4570
2P	0.5590	0.4490
2Q	0.5720	0.4490
2S	0.4100	0.3040
2T	0.4100	0.2870

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Chain	Atom inclusion	Q-score
2V	0.1390	-0.0150
2W	0.3370	0.2550
2X	0.3520	0.2760
2Y	0.3690	0.2800
3A	0.4000	0.3830
3C	0.4600	0.3360
3D	0.5340	0.4000
3F	0.0420	0.2660
3H	0.3180	0.3930
3J	0.5180	0.4190
3K	0.4680	0.4010
3L	0.4650	0.3680
3N	0.3920	0.3480
3O	0.4250	0.3650
3P	0.3700	0.3330
3Q	0.2450	0.2160
3S	0.5410	0.4300
3T	0.4850	0.3910
3U	0.4690	0.3780
3V	0.4470	0.3350
3X	0.0820	0.2370
3Y	0.4360	0.4040
3Z	0.3760	0.3380
4A	0.1380	0.2790
4B	0.3080	0.2200
4C	0.0020	0.1020
4D	0.4980	0.3650
4F	0.4550	0.3510
4G	0.3710	0.3260
4I	0.3360	0.2280
4J	0.4140	0.3060
4K	0.3390	0.3180
4L	0.3770	0.3370
4M	0.2750	0.2790
4O	0.5780	0.4440
4P	0.5660	0.4490
4Q	0.5820	0.4590
4R	0.5250	0.4620
4S	0.5690	0.4270
4T	0.3050	0.3740
4V	0.2690	0.2540
4W	0.5160	0.3540

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Chain	Atom inclusion	Q-score
4Y	0.3370	0.3590
5A	0.4910	0.3610
5B	0.5000	0.3280
5D	0.0520	-0.0100
5E	0.2100	0.2210
5F	0.0620	0.1350
5G	0.1220	0.1700
5H	0.0360	0.1140
5I	0.0320	-0.0550
5J	0.0310	0.0560
5L	0.6150	0.3740
5M	0.5970	0.3530
5N	0.6160	0.3620
5O	0.6040	0.3500
5Q	0.5450	0.3690
5R	0.6430	0.3940
5S	0.6420	0.3740
5T	0.6410	0.3650
5V	0.1370	0.0700
5W	0.1440	0.0860
5X	0.1630	0.0950
5Y	0.1310	0.0650
6A	0.2820	0.2230
6B	0.3180	0.2350
6C	0.3330	0.2370
6D	0.3040	0.2120
6E	0.0130	0.0920
6F	0.0340	0.0620
6G	0.0650	0.0790
6H	0.0390	0.0820
6I	0.0200	0.1010
6J	0.0090	0.0610
6K	0.0290	0.0970
6L	0.0500	0.1060
6M	0.0410	0.1000
6N	0.0390	0.1450
6P	0.4010	0.2870
6Q	0.5080	0.2980
6R	0.5000	0.3070
6S	0.4950	0.2900
6T	0.0350	-0.0600
6U	0.0700	-0.0260

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Chain	Atom inclusion	Q-score
6V	0.0620	-0.0320
6W	0.0520	-0.0170
6Y	0.4020	0.3500
6Z	0.4620	0.3810
7C	0.3440	0.2210
7D	0.4260	0.2720
7E	0.2640	0.2970
7F	0.3700	0.3690
7H	0.2210	0.2830
7I	0.2790	0.3550
7K	0.4600	0.3700
7L	0.3100	0.3060
7N	0.0510	0.2710
AB	0.5700	0.4050
AC	0.6350	0.4920
AD	0.6190	0.4800
AE	0.6340	0.4870
AF	0.6370	0.4890
AG	0.6320	0.4980
AH	0.6310	0.5090
AI	0.6310	0.5080
AJ	0.6310	0.4870
AK	0.6400	0.5070
AL	0.6180	0.4780
BB	0.5860	0.4230
BC	0.5780	0.4410
BD	0.6070	0.4760
BE	0.6200	0.4480
BF	0.6000	0.4520
BG	0.6220	0.4610
BH	0.6070	0.4630
BI	0.6350	0.4850
BJ	0.5630	0.3930
BK	0.6130	0.4550
BL	0.6010	0.4380
CB	0.5450	0.3650
CC	0.5940	0.4470
CD	0.5890	0.4580
CE	0.5820	0.4060
CF	0.6000	0.4560
CG	0.5930	0.4600
CH	0.5890	0.4460

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Chain	Atom inclusion	Q-score
CI	0.6020	0.4170
CJ	0.5980	0.4590
CK	0.5940	0.4520
CL	0.5860	0.4340
CM	0.5100	0.3960
DB	0.4320	0.3090
DC	0.5410	0.3610
DD	0.5570	0.3830
DE	0.5670	0.3890
DF	0.5790	0.3890
DG	0.5780	0.4020
DH	0.5800	0.4140
DI	0.5720	0.3900
DJ	0.6020	0.4180
DK	0.5900	0.4240
DL	0.5820	0.3930
DM	0.5110	0.3440
EC	0.5670	0.3550
ED	0.6280	0.4390
EE	0.6350	0.4520
EF	0.6260	0.4120
EG	0.6360	0.4370
EH	0.5960	0.3960
EI	0.6240	0.4170
EJ	0.6070	0.3850
EK	0.6110	0.4260
EL	0.6030	0.3990
EM	0.5730	0.4010
FC	0.5500	0.4020
FD	0.6120	0.4360
FE	0.5840	0.3870
FF	0.5990	0.3850
FG	0.5760	0.3780
FH	0.5530	0.3520
FI	0.5670	0.3660
FJ	0.5830	0.3680
FK	0.5990	0.4230
FL	0.5940	0.4330
FM	0.5160	0.3240
GC	0.5030	0.3490
GD	0.5990	0.4260
GE	0.5940	0.4020

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Chain	Atom inclusion	Q-score
GF	0.5980	0.3900
GG	0.5950	0.4110
GH	0.5920	0.4030
GI	0.5950	0.4030
GJ	0.6400	0.4570
GK	0.5790	0.3990
GL	0.5890	0.3900
GM	0.5880	0.4340
HB	0.5470	0.4140
HC	0.5640	0.4120
HD	0.6130	0.4560
HE	0.6020	0.4030
HF	0.5920	0.4070
HG	0.6210	0.4610
HH	0.6030	0.4040
HI	0.6230	0.4700
HJ	0.6300	0.4650
HK	0.5910	0.4040
HL	0.6130	0.4590
HM	0.6100	0.4650
IC	0.4960	0.3630
ID	0.5900	0.4230
IE	0.5980	0.4560
IF	0.5910	0.4320
IG	0.6060	0.4190
IH	0.6060	0.4290
II	0.6070	0.4400
IJ	0.5980	0.4180
IK	0.5890	0.3910
IL	0.5900	0.4210
IM	0.5900	0.4270
IN	0.5940	0.4370
JC	0.5970	0.3990
JD	0.6240	0.4250
JE	0.6160	0.4260
JF	0.6330	0.4350
JG	0.6290	0.4430
JH	0.5840	0.3880
JI	0.6010	0.4120
JJ	0.6350	0.4320
JK	0.6120	0.4630
JL	0.6090	0.4530

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Chain	Atom inclusion	Q-score
JM	0.6200	0.4530
KC	0.6470	0.4860
KD	0.6560	0.4770
KE	0.6630	0.5030
KF	0.6560	0.4950
KG	0.6820	0.5090
KH	0.6590	0.5010
KI	0.6710	0.5110
KJ	0.6600	0.5020
KK	0.6740	0.4970
KL	0.6710	0.5120
KM	0.6560	0.5100
KN	0.6520	0.4720
LC	0.6600	0.4890
LD	0.6610	0.5140
LE	0.6550	0.5040
LF	0.6650	0.5060
LG	0.6770	0.5200
LH	0.6640	0.5070
LI	0.6520	0.4980
LJ	0.6770	0.5080
LK	0.6680	0.5110
LL	0.6570	0.5070
LM	0.6570	0.4930
LN	0.6240	0.4670
MC	0.6420	0.4420
MD	0.6520	0.4940
ME	0.6580	0.4610
MF	0.6540	0.4700
MG	0.6500	0.4750
MH	0.6400	0.4680
MI	0.6500	0.4610
MJ	0.6530	0.4490
MK	0.5810	0.3820
ML	0.6180	0.4290
MM	0.6300	0.4280
MN	0.4990	0.3940
NA	0.5850	0.4170
NB	0.5880	0.4270
NC	0.6010	0.4600
ND	0.6070	0.4340
NE	0.5810	0.4280

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Chain	Atom inclusion	Q-score
NF	0.5930	0.4390
NG	0.5920	0.4340
NH	0.6030	0.4250
NI	0.5850	0.4310
NJ	0.5780	0.4160
NK	0.5920	0.4240
NL	0.5160	0.3490
OA	0.5470	0.3810
OB	0.5900	0.4270
OC	0.5890	0.4240
OD	0.5710	0.3930
OE	0.5850	0.4070
OF	0.5720	0.4060
OG	0.5790	0.4250
OH	0.5880	0.4070
OI	0.5980	0.4170
OJ	0.5710	0.4120
OK	0.5730	0.4060
OL	0.5520	0.3660
PA	0.4730	0.3190
PB	0.5660	0.3680
PC	0.5570	0.3660
PD	0.5720	0.3760
PE	0.5980	0.3810
PF	0.5710	0.3790
PG	0.6050	0.4290
PH	0.5920	0.4070
PI	0.6180	0.4180
PJ	0.5900	0.4140
PK	0.5620	0.3790
PL	0.5300	0.3260
QB	0.4960	0.3060
QC	0.5190	0.3250
QD	0.5360	0.3380
QE	0.5570	0.3270
QF	0.5300	0.3290
QG	0.5240	0.3330
QH	0.5330	0.3380
QI	0.5760	0.3530
QJ	0.5500	0.3540
QK	0.5290	0.3560
QL	0.4900	0.3010

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Chain	Atom inclusion	Q-score
RB	0.4370	0.2990
RC	0.5110	0.3280
RD	0.5640	0.3630
RE	0.5770	0.3420
RF	0.5690	0.3590
RG	0.5390	0.3510
RH	0.5480	0.3450
RI	0.5740	0.3480
RJ	0.5730	0.3710
RK	0.5380	0.3490
RL	0.4980	0.3130
SC	0.5320	0.3420
SD	0.5630	0.3710
SE	0.5790	0.3810
SF	0.5670	0.3680
SG	0.5580	0.3760
SH	0.5470	0.3600
SI	0.6040	0.3840
SJ	0.5610	0.3610
SK	0.5590	0.3610
SL	0.5360	0.3540
SM	0.3420	0.2680
TC	0.5040	0.3190
TD	0.5780	0.3830
TE	0.5620	0.3820
TF	0.5940	0.3710
TG	0.5440	0.3610
TH	0.5600	0.3740
TI	0.5710	0.3790
TJ	0.5910	0.3880
TK	0.5900	0.4080
TL	0.5680	0.3900
TM	0.4470	0.2940
UC	0.5560	0.3890
UD	0.5870	0.4120
UE	0.5780	0.3990
UF	0.6050	0.4050
UG	0.6000	0.4160
UH	0.5900	0.4140
UI	0.5850	0.3980
UJ	0.6150	0.4180
UK	0.5930	0.4170

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Chain	Atom inclusion	Q-score
UL	0.5880	0.4190
UM	0.5600	0.3950
VC	0.5880	0.4470
VD	0.5930	0.4580
VE	0.6060	0.4660
VF	0.6180	0.4600
VG	0.5950	0.4540
VH	0.6110	0.4630
VI	0.6100	0.4620
VJ	0.6150	0.4410
VK	0.5840	0.4470
VL	0.5990	0.4640
VM	0.5910	0.4510
WC	0.6050	0.4720
WD	0.6300	0.4840
WE	0.6230	0.4850
WF	0.6320	0.4720
WG	0.6190	0.4750
WH	0.6310	0.4790
WI	0.6330	0.4820
WJ	0.6290	0.4780
WK	0.6170	0.4750
WL	0.6350	0.4870
WM	0.6230	0.4750
WN	0.5790	0.4420