wwPDB EM Validation Summary Report (i)

Dec 27, 2024 – 12:44 AM EST

PDB ID	:	6U42
EMDB ID	:	EMD-20631
Title	:	Natively decorated ciliary doublet microtubule
Authors	:	Ma, M.; Stoyanova, M.; Rademacher, G.; Dutcher, S.K.; Brown, A.; Zhang, R.
Deposited on	:	2019-08-22
Resolution	:	3.40 Å(reported)

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

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

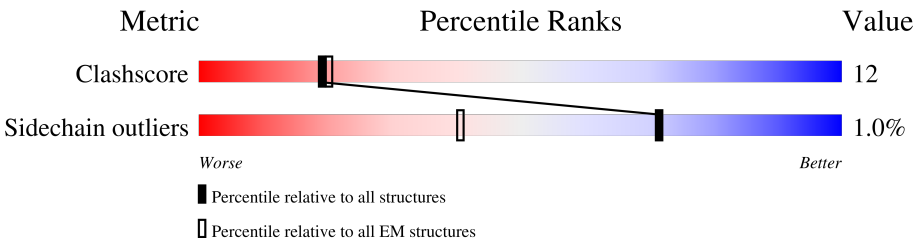
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
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	0A	443	• 63% 33% •
1	0C	443	19% 64% 32% •
1	0E	443	17% 57% 39% •
1	0G	443	5% 63% 33% •
1	0I	443	5% 63% 33% •
1	0K	443	• 62% 34% •
1	0M	443	• 62% 34% •
1	0O	443	6% 61% 35% •
1	0Q	443	• 64% 33% •

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Mol	Chain	Length	Quality of chain
1	0S	443	49% 62% 34%
1	0U	443	15% 61% 35%
1	0W	443	6% 63% 33%
1	0Y	443	7% 65% 31%
1	1	443	29% 69%
1	1A	443	5% 70% 26%
1	1C	443	5% 65% 31%
1	1E	443	7% 60% 36%
1	1G	443	8% 65% 31%
1	1K	443	64% 32%
1	1M	443	66% 30%
1	1O	443	68% 28%
1	1Q	443	66% 30%
1	1S	443	69% 28%
1	1U	443	65% 31%
1	1W	443	65% 31%
1	2A	443	67% 28%
1	2C	443	67% 29%
1	2E	443	66% 30%
1	2G	443	71% 25%
1	2I	443	68% 28%
1	2K	443	73% 23%
1	2M	443	64% 32%
1	2Q	443	67% 29%
1	2S	443	71% 25%

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Mol	Chain	Length	Quality of chain
1	2U	443	68% 28%
1	2W	443	73% 23%
1	2Y	443	67% 28%
1	3	443	95%
1	3A	443	66% 30%
1	3C	443	61% 34%
1	3G	443	70% 26%
1	3I	443	70% 26%
1	3K	443	66% 30%
1	3M	443	71% 25%
1	3O	443	69% 27%
1	3Q	443	67% 30%
1	3S	443	59% 37%
1	5	443	93% 5%
1	7	443	95%
1	9	443	94%
1	A1	443	95%
1	A3	443	92% 6%
1	A5	443	96%
1	A7	443	95%
1	A9	443	94%
1	B1	443	94%
1	B3	443	94%
1	B5	443	94%
1	B8	443	93%

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Mol	Chain	Length	Quality of chain
1	C0	443	95%
1	C2	443	95%
1	C4	443	95%
1	C6	443	95%
1	C8	443	95%
1	D0	443	95%
1	D2	443	95%
1	D4	443	93%
1	D6	443	94%
1	D8	443	23% 95%
1	E0	443	94%
1	E2	443	94%
1	E4	443	95%
1	E6	443	94%
1	E8	443	94%
1	F0	443	95%
1	F2	443	94%
1	F6	443	94%
1	F8	443	94%
1	G0	443	93%
1	G2	443	65% 31%
1	G4	443	67% 29%
1	G6	443	63% 33%
1	G8	443	63% 33%
1	H2	443	65% 31%

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Mol	Chain	Length	Quality of chain
1	H4	443	67% 29%
1	H6	443	69% 27%
1	H8	443	74% 21%
1	I0	443	72% 24%
1	I2	443	69% 27%
1	I4	443	64% 32%
1	I8	443	66% 30%
1	J0	443	69% 27%
1	J2	443	73% 23%
1	J4	443	70% 26%
1	J6	443	71% 25%
1	J8	443	74% 22%
1	K0	443	74% 22%
1	K4	443	70% 26%
1	K6	443	73% 23%
1	K8	443	71% 25%
1	L0	443	72% 24%
1	L2	443	70% 26%
1	L4	443	70% 26%
1	L6	443	68% 28%
1	M0	443	69% 27%
1	M2	443	72% 24%
1	M4	443	72% 24%
1	M6	443	69% 27%
1	M8	443	72% 24%

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Mol	Chain	Length	Quality of chain
1	N0	443	71% 25%
1	N2	443	70% 27%
1	N6	443	73% 23%
1	N8	443	72% 24%
1	O0	443	75% 21%
1	O2	443	72% 24%
1	O4	443	69% 27%
1	O6	443	75% 21%
1	O8	443	75% 21%
1	P4	443	65% 31%
1	P6	443	71% 25%
1	P8	443	70% 26%
1	Q0	443	74% 23%
1	Q2	443	70% 27%
1	Q4	443	70% 26%
1	Q6	443	70% 26%
1	Q8	443	37% 61% 33% 5%
1	R0	443	72% 26%
1	R2	443	71% 25%
1	R4	443	67% 29%
1	R6	443	69% 27%
1	R8	443	70% 27%
1	S0	443	69% 26%
1	S2	443	70% 27%
1	S4	443	14% 60% 36%

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Mol	Chain	Length	Quality of chain
1	S6	443	68% 28%
1	S8	443	67% 29%
1	T0	443	69% 28%
1	T2	443	65% 31%
1	T4	443	68% 28%
1	T6	443	59% 37%
1	T8	443	68% 28%
1	U2	443	68% 28%
1	U4	443	69% 27%
1	U6	443	5% 66% 30%
1	U8	443	69% 28%
1	V0	443	73% 23%
1	V2	443	68% 28%
1	V4	443	74% 22%
1	V6	443	31% 57% 39%
1	V8	443	67% 29%
1	W0	443	68% 28%
1	W2	443	71% 25%
1	W4	443	66% 30%
1	W6	443	69% 27%
1	W8	443	70% 26%
1	X0	443	68% 28%
1	X2	443	21% 61% 35%
1	X4	443	63% 33%
1	X6	443	66% 30%

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Mol	Chain	Length	Quality of chain
1	X8	443	70% 26%
1	Y0	443	66% 30%
1	Y2	443	71% 25%
1	Y4	443	70% 27%
1	Y6	443	73% 23%
1	Y8	443	24% 59% 37%
1	Z0	443	6% 59% 37%
1	Z2	443	9% 59% 37%
1	Z4	443	61% 35%
1	Z6	443	61% 35%
1	Z8	443	6% 56% 40%
2	0B	451	62% 33% 5%
2	0F	451	59% 35% 5%
2	0H	451	61% 33% 5%
2	0J	451	6% 60% 35% 5%
2	0L	451	59% 36% 5%
2	0N	451	6% 57% 37% 5%
2	0P	451	65% 30% 5%
2	0R	451	5% 59% 36% 5%
2	0V	451	8% 59% 35% 5%
2	0X	451	7% 61% 33% 5%
2	0Z	451	64% 30% 5%
2	1B	451	5% 65% 29% 5%
2	1D	451	7% 62% 32% 5%
2	1F	451	6% 58% 36% 5%

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Mol	Chain	Length	Quality of chain
2	1H	451	16% 59% 35% 5%
2	1L	451	66% 29% 5%
2	1N	451	64% 30% 5%
2	1P	451	68% 26% 5%
2	1R	451	63% 30% 5%
2	1T	451	65% 29% 5%
2	1V	451	63% 31% 5%
2	1X	451	16% 60% 34% 5%
2	1Z	451	24% 65% 29% 5%
2	2	451	94%
2	2B	451	69% 26% 5%
2	2D	451	70% 24% 5%
2	2F	451	67% 28% 5%
2	2H	451	67% 27% 5%
2	2J	451	68% 26% 5%
2	2L	451	69% 26% 5%
2	2N	451	13% 61% 33% 5%
2	2P	451	64% 30% 5%
2	2R	451	70% 25% 5%
2	2T	451	67% 27% 5%
2	2V	451	69% 25% 5%
2	2X	451	67% 30%
2	2Z	451	64% 30% 5%
2	3B	451	63% 33%
2	3D	451	10% 62% 33% 5%

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Mol	Chain	Length	Quality of chain
2	3F	451	67% 28% 5%
2	3H	451	67% 27% 5%
2	3J	451	70% 25% 5%
2	3L	451	71% 24% 5%
2	3N	451	69% 25% 5%
2	3P	451	67% 28% 5%
2	3R	451	63% 34%
2	3T	451	16% 58% 36% 5%
2	4	451	93%
2	6	451	95%
2	8	451	91% 5%
2	A0	451	95%
2	A2	451	91% 5%
2	A4	451	93%
2	A8	451	93% 5%
2	B0	451	93% 5%
2	B2	451	93% 5%
2	B4	451	93% 5%
2	B7	451	92% 5%
2	B9	451	93% 5%
2	C1	451	93% 5%
2	C5	451	94%
2	C7	451	95%
2	C9	451	93% 5%
2	D1	451	93% 5%

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Mol	Chain	Length	Quality of chain
2	D3	451	94% • 5%
2	D5	451	93% • 5%
2	D7	451	94% • 5%
2	E1	451	93% • 5%
2	E3	451	93% • 5%
2	E5	451	92% • 5%
2	E7	451	92% • 5%
2	E9	451	92% • 5%
2	F1	451	92% • 5%
2	F3	451	8% 92% • 5%
2	F5	451	51% 92% • 5%
2	F7	451	92% • 5%
2	F9	451	94% • •
2	G1	451	76% 20% • •
2	G3	451	65% 31% • •
2	G5	451	66% 29% 5%
2	G7	451	61% 33% 5%
2	G9	451	20% 56% 39% 5%
2	H1	451	29% 62% 33% 5%
2	H3	451	65% 29% 5%
2	H5	451	68% 27% 5%
2	H7	451	69% 25% 5%
2	H9	451	68% 27% 5%
2	I1	451	66% 28% 5%
2	I3	451	67% 27% 5%

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Mol	Chain	Length	Quality of chain
2	I5	451	33% 59% 35% 5%
2	I7	451	8% 68% 27% 5%
2	I9	451	63% 31% • 5%
2	J1	451	• 63% 32% 5%
2	J3	451	68% 27% 5%
2	J5	451	• 68% 29% •
2	J7	451	• 65% 29% • 5%
2	J9	451	• 64% 33% •
2	K1	451	41% 62% 32% 5%
2	K3	451	• 65% 29% 5%
2	K5	451	70% 24% 5%
2	K7	451	• 70% 25% 5%
2	K9	451	71% 24% 5%
2	L1	451	• 72% 22% 5%
2	L3	451	67% 27% • 5%
2	L5	451	• 67% 28% 5%
2	L7	451	40% 59% 35% 5%
2	L9	451	70% 25% 5%
2	M1	451	• 71% 24% 5%
2	M3	451	• 67% 29% • •
2	M5	451	69% 26% 5%
2	M7	451	• 71% 25% •
2	M9	451	• 67% 30% •
2	N1	451	• 68% 27% 5%
2	N3	451	42% 61% 33% 5%

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Mol	Chain	Length	Quality of chain
2	N5	451	66% 28% 5%
2	N7	451	64% 30% 5%
2	N9	451	65% 30% 5%
2	O1	451	70% 24% 5%
2	O3	451	65% 30% 5%
2	O5	451	65% 29% 5%
2	O7	451	67% 28%
2	O9	451	71% 24% 5%
2	P3	451	70% 25% 5%
2	P5	451	69% 27%
2	P7	451	71% 24% 5%
2	P9	451	69% 28%
2	Q1	451	72% 23% 5%
2	Q3	451	69% 26% 5%
2	Q5	451	69% 26% 5%
2	Q9	451	64% 31% 5%
2	R1	451	65% 29% 5%
2	R3	451	68% 27% 5%
2	R5	451	69% 27%
2	R7	451	70% 24% 5%
2	R9	451	68% 29%
2	S1	451	68% 26% 5%
2	S5	451	69% 25% 5%
2	S7	451	66% 30%
2	S9	451	65% 29% 5%

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Mol	Chain	Length	Quality of chain
2	T1	451	65% 29% 5%
2	T3	451	70% 23% • 5%
2	T5	451	66% 29% 5%
2	T7	451	68% 26% 5%
2	U1	451	70% 25% 5%
2	U3	451	71% 24% 5%
2	U5	451	68% 27% 5%
2	U7	451	69% 25% 5%
2	U9	451	65% 29% 5%
2	V1	451	65% 29% 5%
2	V3	451	65% 29% • 5%
2	V7	451	64% 31% 5%
2	V9	451	69% 26% 5%
2	W1	451	69% 25% 5%
2	W3	451	71% 24% 5%
2	W5	451	73% 22% 5%
2	W7	451	63% 32% 5%
2	W9	451	61% 32% • 5%
2	X3	451	58% 37% 5%
2	X5	451	62% 32% 5%
2	X7	451	64% 30% 5%
2	X9	451	67% 27% • 5%
2	Y1	451	66% 29% 5%
2	Y3	451	65% 29% 5%
2	Y5	451	66% 28% 5%

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Mol	Chain	Length	Quality of chain
2	Y9	451	9% 58% 36% 5%
2	Z1	451	10% 64% 31% 5%
2	Z3	451	8% 60% 35% 5%
2	Z5	451	6% 59% 35% 5%
2	Z7	451	7% 61% 33% 5%
2	Z9	451	5% 64% 30% 5%
3	3V	307	7% 66% 27%
3	3X	307	40% 64% 29%
3	3Z	307	7% 65% 29%
3	4B	307	18% 66% 27%
3	4D	307	6% 65% 28%
3	4F	307	16% 64% 29%
3	4H	307	8% 64% 29%
3	4J	307	26% 46% 21% 34%
4	3W	190	59% 35%
4	3Y	190	61% 34%
4	4A	190	61% 34%
4	4C	190	59% 35%
4	4E	190	62% 33%
4	4G	190	61% 34%
4	4I	190	61% 34%
5	4L	482	5% 34% 16% 51%
5	4M	482	47% 18% 34%
6	4N	505	7% 90%
6	4O	505	17% 67% 28% 5%

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Mol	Chain	Length	Quality of chain
6	4P	505	30% 8% 62%
7	4Q	367	15% 83%
7	4R	367	74% 25%
7	4S	367	9% 88%
7	4T	367	42% 11% 47%
7	4U	367	59% 18% 23%
8	4V	475	13% 83%
8	4W	475	28% 51% 23% 26%
8	4X	475	9% 88%
9	4Y	462	18% 9% 73%
9	4Z	462	23% 55% 29% 16%
10	5A	501	10% 31% 15% 54%
10	5B	501	12% 33% 17% 50%
10	5C	501	11% 51% 23% 26%
10	5D	501	14% 7% 79%
11	5E	274	43% 69% 24% 6%
12	5F	391	5% 70% 26%
12	5G	391	24% 12% 64%
12	7B	391	17% 8% 75%
13	5H	137	61% 30% 8%
13	5I	137	57% 34% 7%
13	5J	137	60% 31% 8%
13	5K	137	58% 33% 8%
14	5L	633	50% 44% 5%
14	5M	633	51% 43%

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Mol	Chain	Length	Quality of chain
14	5N	633	51% 43% 5%
15	5O	380	8% 45% 46% 8%
15	5P	380	57% 40%
16	5Q	197	6% 63% 32%
17	5R	240	7% 91%
17	5S	240	15% 50% 29% 5% 17%
17	5T	240	14% 51% 25% 6% 18%
17	5U	240	18% 50% 28% 17%
17	5V	240	7% 32% 13% 55%
18	5X	230	52% 37% 8%
18	5Y	230	5% 53% 36% 7%
18	5Z	230	21% 53% 37% 6%
18	6A	230	7% 54% 35% 7%
18	6B	230	31% 53% 37% 6%
18	6C	230	20% 54% 36% 7%
18	6D	230	12% 54% 36% 7%
19	6E	268	62% 33% 5%
20	6F	403	70% 28%
21	6G	214	17% 68% 18% 14%
21	6H	214	23% 60% 30% 10%
22	6I	352	11% 68% 26% 7%
22	6J	352	12% 70% 23% 7%
22	6K	352	14% 70% 23% 7%
22	6L	352	14% 66% 28% 7%
22	6M	352	15% 68% 25% 7%

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Mol	Chain	Length	Quality of chain
22	6N	352	20% 67% 26% 7%
22	6O	352	16% 68% 25% 7%
22	6P	352	28% 55% 28% • 16%
23	6Q	87	7% 61% 29% 8% •
23	6R	87	• 63% 26% 8% •
23	6S	87	14% 68% 24% 6% •
24	6T	635	7% 57% 31% 11%
24	6U	635	9% 57% 32% • 10%
24	6V	635	9% 57% 31% 12%
24	6W	635	7% 62% 26% • 11%
24	6X	635	8% 55% 33% • 10%
24	6Y	635	10% 56% 32% • 11%
24	6Z	635	8% 57% 31% 11%
24	7A	635	• 20% 10% 70%
25	7C	111	14% 65% 23% 12%
26	7D	146	• 53% 33% 5% 10%
26	7E	146	• 52% 34% 5% 10%
26	7F	146	21% 47% 37% 6% 10%
27	7G	235	9% 63% 32% 5%
28	7H	471	• 19% 9% • 71%
28	7X	471	• 18% 9% • 71%
29	7I	483	6% 34% 13% 53%
29	7J	483	• 54% 21% 25%
30	7K	458	8% 64% 28% 8%
30	7L	458	• 30% 9% 62%

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Mol	Chain	Length	Quality of chain
31	7M	139	6% 36% 24% • 39%
31	7N	139	22% 57% 33% • 9%
32	7O	238	• 17% 8% 75%
32	7P	238	7% 60% 17% 24%
33	7Q	189	6% 24% 14% 62%
34	7R	749	9% 19% 7% 74%
34	7S	749	5% 16% 5% 79%
35	7T	552	13% 28% 10% 61%
35	7U	552	9% 25% 7% 67%
36	7V	184	20% 26% 18% • 52%
36	7W	184	31% 24% 20% • 52%
37	7Y	312	26% 46% 32% • 21%
38	7Z	242	• 7% 10% 84%
38	8A	242	16% 45% 39% • 14%
38	8B	242	19% 44% 41% • 12%
38	8C	242	9% 46% 39% • 12%
38	8D	242	17% 34% 28% • 35%

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 1358547 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 Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	138	1120	701	192	214	13	0	0
			Total	C	N	O	S		
1	3	433	3397	2131	581	655	30	0	0
			Total	C	N	O	S		
1	5	436	3421	2147	584	660	30	0	0
			Total	C	N	O	S		
1	7	437	3430	2152	585	663	30	0	0
			Total	C	N	O	S		
1	9	436	3421	2147	584	660	30	0	0
			Total	C	N	O	S		
1	A1	432	3388	2126	580	652	30	0	0
			Total	C	N	O	S		
1	A3	435	3410	2138	583	659	30	0	0
			Total	C	N	O	S		
1	A5	430	3370	2116	578	646	30	0	0
			Total	C	N	O	S		
1	A7	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	A9	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	B1	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	B3	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	B5	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	B8	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	C0	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	C2	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	C4	426	3346	2103	574	639	30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	C8	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	D0	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	D2	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	D4	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	D6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	D8	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	E0	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	E2	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	E4	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	E6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	E8	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	F0	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	F2	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	F6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	F8	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	G0	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	G2	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	G4	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	G6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	G8	426	3346	2103	574	639	30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H2	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	H4	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	H6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	H8	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	I0	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	I2	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	I4	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	I8	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	J0	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	J2	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	J4	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	J6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	J8	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	K0	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	K4	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	K6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	K8	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	L0	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	L2	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	L4	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	L6	426	3346	2103	574	639	30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	M0	426	3346	2103	574	639	30	0	0
1	M2	426	3346	2103	574	639	30	0	0
1	M4	426	3346	2103	574	639	30	0	0
1	M6	426	3346	2103	574	639	30	0	0
1	M8	426	3346	2103	574	639	30	0	0
1	N0	426	3346	2103	574	639	30	0	0
1	N2	426	3346	2103	574	639	30	0	0
1	N6	426	3346	2103	574	639	30	0	0
1	N8	426	3346	2103	574	639	30	0	0
1	O0	426	3346	2103	574	639	30	0	0
1	O2	426	3346	2103	574	639	30	0	0
1	O4	426	3346	2103	574	639	30	0	0
1	O6	426	3346	2103	574	639	30	0	0
1	O8	426	3346	2103	574	639	30	0	0
1	P4	426	3346	2103	574	639	30	0	0
1	P6	426	3346	2103	574	639	30	0	0
1	P8	426	3346	2103	574	639	30	0	0
1	Q0	426	3346	2103	574	639	30	0	0
1	Q2	426	3346	2103	574	639	30	0	0
1	Q4	426	3346	2103	574	639	30	0	0
1	Q6	426	3346	2103	574	639	30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Q8	420	3293	2070	563	631	29	0	0
			Total	C	N	O	S		
1	R0	434	3401	2133	582	656	30	0	0
			Total	C	N	O	S		
1	R2	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	R4	430	3370	2116	578	646	30	0	0
			Total	C	N	O	S		
1	R6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	R8	431	3379	2121	579	649	30	0	0
			Total	C	N	O	S		
1	S0	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	S2	431	3379	2121	579	649	30	0	0
			Total	C	N	O	S		
1	S4	427	3354	2107	575	642	30	0	0
			Total	C	N	O	S		
1	S6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	S8	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	T0	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	T2	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	T4	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	T6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	T8	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	U2	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	U4	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	U6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	U8	430	3370	2116	578	646	30	0	0
			Total	C	N	O	S		
1	V0	426	3346	2103	574	639	30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	V2	426	3346	2103	574	639	30	0	0
1	V4	426	3346	2103	574	639	30	0	0
1	V6	426	3346	2103	574	639	30	0	0
1	V8	426	3346	2103	574	639	30	0	0
1	W0	426	3346	2103	574	639	30	0	0
1	W2	426	3346	2103	574	639	30	0	0
1	W4	426	3346	2103	574	639	30	0	0
1	W6	426	3346	2103	574	639	30	0	0
1	W8	426	3346	2103	574	639	30	0	0
1	X0	426	3346	2103	574	639	30	0	0
1	X2	426	3346	2103	574	639	30	0	0
1	X4	426	3346	2103	574	639	30	0	0
1	X6	426	3346	2103	574	639	30	0	0
1	X8	426	3346	2103	574	639	30	0	0
1	Y0	426	3346	2103	574	639	30	0	0
1	Y2	426	3346	2103	574	639	30	0	0
1	Y4	426	3346	2103	574	639	30	0	0
1	Y6	426	3346	2103	574	639	30	0	0
1	Y8	426	3346	2103	574	639	30	0	0
1	Z0	426	3346	2103	574	639	30	0	0
1	Z2	426	3346	2103	574	639	30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Z4	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	Z6	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	Z8	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0A	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0C	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0E	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0G	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0I	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0K	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0M	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0O	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0Q	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0S	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0U	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0W	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	0Y	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	1A	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	1C	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	1E	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	1G	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	1K	426	3346	2103	574	639	30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1M	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	1O	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	1Q	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	1S	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	1U	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	1W	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	2A	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	2C	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	2E	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	2G	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	2I	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	2K	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	2M	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	2Q	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	2S	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	2U	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	2W	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	2Y	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	3A	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	3C	426	3346	2103	574	639	30	0	0
			Total	C	N	O	S		
1	3G	426	3346	2103	574	639	30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	3I	426	3346	2103	574	639	30	0	0
1	3K	426	3346	2103	574	639	30	0	0
1	3M	426	3346	2103	574	639	30	0	0
1	3O	426	3346	2103	574	639	30	0	0
1	3Q	426	3346	2103	574	639	30	0	0
1	3S	426	3346	2103	574	639	30	0	0

- Molecule 2 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	436	3376	2136	575	644	21	0	0
2	4	436	3376	2136	575	644	21	0	0
2	6	436	3376	2136	575	644	21	0	0
2	8	436	3376	2136	575	644	21	0	0
2	A0	436	3376	2136	575	644	21	0	0
2	A2	436	3376	2136	575	644	21	0	0
2	A4	436	3376	2136	575	644	21	0	0
2	A8	427	3318	2103	565	629	21	0	0
2	B0	427	3318	2103	565	629	21	0	0
2	B2	427	3318	2103	565	629	21	0	0
2	B4	427	3318	2103	565	629	21	0	0
2	B7	427	3318	2103	565	629	21	0	0
2	B9	427	3318	2103	565	629	21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	C5	436	3376	2136	575	644	21	0	0
			Total	C	N	O	S		
2	C7	436	3376	2136	575	644	21	0	0
			Total	C	N	O	S		
2	C9	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	D1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	D3	428	3324	2106	566	631	21	0	0
			Total	C	N	O	S		
2	D5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	D7	428	3324	2106	566	631	21	0	0
			Total	C	N	O	S		
2	E1	428	3324	2106	566	631	21	0	0
			Total	C	N	O	S		
2	E3	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	E5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	E7	428	3324	2106	566	631	21	0	0
			Total	C	N	O	S		
2	E9	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	F1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	F3	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	F5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	F7	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	F9	436	3376	2136	575	644	21	0	0
			Total	C	N	O	S		
2	G1	436	3376	2136	575	644	21	0	0
			Total	C	N	O	S		
2	G3	436	3376	2136	575	644	21	0	0
			Total	C	N	O	S		
2	G5	427	3318	2103	565	629	21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G7	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	G9	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	H1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	H3	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	H5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	H7	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	H9	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	I1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	I3	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	I5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	I7	429	3332	2110	567	634	21	0	0
			Total	C	N	O	S		
2	I9	428	3324	2106	566	631	21	0	0
			Total	C	N	O	S		
2	J1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	J3	428	3326	2107	566	632	21	0	0
			Total	C	N	O	S		
2	J5	437	3385	2141	576	647	21	0	0
			Total	C	N	O	S		
2	J7	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	J9	437	3385	2141	576	647	21	0	0
			Total	C	N	O	S		
2	K1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	K3	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	K5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	K7	427	3318	2103	565	629	21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	K9	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	L1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	L3	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	L5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	L7	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	L9	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	M1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	M3	436	3376	2136	575	644	21	0	0
			Total	C	N	O	S		
2	M5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	M7	436	3376	2136	575	644	21	0	0
			Total	C	N	O	S		
2	M9	437	3385	2141	576	647	21	0	0
			Total	C	N	O	S		
2	N1	428	3324	2106	566	631	21	0	0
			Total	C	N	O	S		
2	N3	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	N5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	N7	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	N9	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	O1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	O3	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	O5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	O7	431	3340	2114	569	636	21	0	0
			Total	C	N	O	S		
2	O9	427	3318	2103	565	629	21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P3	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	P5	436	3376	2136	575	644	21	0	0
			Total	C	N	O	S		
2	P7	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	P9	436	3376	2136	575	644	21	0	0
			Total	C	N	O	S		
2	Q1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	Q3	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	Q5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	Q9	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	R1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	R3	428	3327	2108	566	632	21	0	0
			Total	C	N	O	S		
2	R5	436	3376	2136	575	644	21	0	0
			Total	C	N	O	S		
2	R7	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	R9	436	3376	2136	575	644	21	0	0
			Total	C	N	O	S		
2	S1	429	3333	2111	567	634	21	0	0
			Total	C	N	O	S		
2	S5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	S7	436	3376	2136	575	644	21	0	0
			Total	C	N	O	S		
2	S9	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	T1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	T3	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	T5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	T7	427	3318	2103	565	629	21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	U1	427	3318	2103	565	629	21	0	0
2	U3	427	3318	2103	565	629	21	0	0
2	U5	427	3318	2103	565	629	21	0	0
2	U7	427	3318	2103	565	629	21	0	0
2	U9	427	3318	2103	565	629	21	0	0
2	V1	427	3318	2103	565	629	21	0	0
2	V3	427	3318	2103	565	629	21	0	0
2	V7	427	3318	2103	565	629	21	0	0
2	V9	427	3318	2103	565	629	21	0	0
2	W1	427	3318	2103	565	629	21	0	0
2	W3	427	3318	2103	565	629	21	0	0
2	W5	427	3318	2103	565	629	21	0	0
2	W7	427	3318	2103	565	629	21	0	0
2	W9	427	3318	2103	565	629	21	0	0
2	X3	427	3318	2103	565	629	21	0	0
2	X5	427	3318	2103	565	629	21	0	0
2	X7	427	3318	2103	565	629	21	0	0
2	X9	427	3318	2103	565	629	21	0	0
2	Y1	427	3318	2103	565	629	21	0	0
2	Y3	427	3318	2103	565	629	21	0	0
2	Y5	427	3318	2103	565	629	21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Y9	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	Z1	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	Z3	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	Z5	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	Z7	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	Z9	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	0B	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	0F	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	0H	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	0J	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	0L	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	0N	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	0P	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	0R	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	0V	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	0X	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	0Z	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	1B	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	1D	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	1F	427	3318	2103	565	629	21	0	0
			Total	C	N	O	S		
2	1H	427	3318	2103	565	629	21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1L	427	3318	2103	565	629	21	0	0
2	1N	427	3318	2103	565	629	21	0	0
2	1P	427	3318	2103	565	629	21	0	0
2	1R	427	3318	2103	565	629	21	0	0
2	1T	427	3318	2103	565	629	21	0	0
2	1V	427	3318	2103	565	629	21	0	0
2	1X	427	3318	2103	565	629	21	0	0
2	1Z	427	3318	2103	565	629	21	0	0
2	2B	427	3318	2103	565	629	21	0	0
2	2D	427	3318	2103	565	629	21	0	0
2	2F	427	3318	2103	565	629	21	0	0
2	2H	427	3318	2103	565	629	21	0	0
2	2J	427	3318	2103	565	629	21	0	0
2	2L	427	3318	2103	565	629	21	0	0
2	2N	427	3318	2103	565	629	21	0	0
2	2P	427	3318	2103	565	629	21	0	0
2	2R	427	3318	2103	565	629	21	0	0
2	2T	427	3318	2103	565	629	21	0	0
2	2V	427	3318	2103	565	629	21	0	0
2	2X	437	3385	2141	576	647	21	0	0
2	2Z	427	3318	2103	565	629	21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3B	437	3383	2140	576	646	21	0	0
2	3D	427	3318	2103	565	629	21	0	0
2	3F	427	3318	2103	565	629	21	0	0
2	3H	427	3318	2103	565	629	21	0	0
2	3J	427	3318	2103	565	629	21	0	0
2	3L	427	3318	2103	565	629	21	0	0
2	3N	427	3318	2103	565	629	21	0	0
2	3P	427	3318	2103	565	629	21	0	0
2	3R	437	3385	2141	576	647	21	0	0
2	3T	427	3318	2103	565	629	21	0	0

- Molecule 3 is a protein called PACRG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3V	297	2329	1491	401	428	9	0	0
3	3X	297	2329	1491	401	428	9	0	0
3	3Z	297	2329	1491	401	428	9	0	0
3	4B	297	2329	1491	401	428	9	0	0
3	4D	297	2329	1491	401	428	9	0	0
3	4F	297	2329	1491	401	428	9	0	0
3	4H	297	2329	1491	401	428	9	0	0
3	4J	204	1643	1060	281	296	6	0	0

- Molecule 4 is a protein called FAP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3W	184	1515	971	264	273	7	0	0
4	3Y	184	1515	971	264	273	7	0	0
4	4A	184	1515	971	264	273	7	0	0
4	4C	184	1515	971	264	273	7	0	0
4	4E	184	1515	971	264	273	7	0	0
4	4G	184	1515	971	264	273	7	0	0
4	4I	184	1515	971	264	273	7	0	0

- Molecule 5 is a protein called FAP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4L	238	1921	1164	366	381	10	0	0
5	4M	316	2622	1589	514	503	16	0	0

- Molecule 6 is a protein called FAP127.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	4N	52	422	260	76	85	1	0	0
6	4O	478	3995	2407	778	791	19	0	0
6	4P	194	1588	956	313	315	4	0	0

- Molecule 7 is a protein called RIB43a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	4Q	63	525	324	101	98	2	0	0
7	4R	366	2982	1819	561	589	13	0	0
7	4S	45	Total	C	N	O		0	0
			371	228	71	72			

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	4T	194	1574	961	295	307	11	0	0
7	4U	283	2285	1392	423	461	9	0	0

- Molecule 8 is a protein called FAP112.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	4V	83	653	396	129	124	4	0	0
8	4W	353	2750	1649	552	538	11	0	0
8	4X	59	462	284	85	90	3	0	0

- Molecule 9 is a protein called FAP210.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	4Y	126	1004	625	187	189	3	0	0
9	4Z	389	3158	1908	627	615	8	0	0

- Molecule 10 is a protein called FAP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	5A	228	1902	1154	367	372	9	0	0
10	5B	249	2074	1257	391	410	16	0	0
10	5C	370	3103	1881	597	604	21	0	0
10	5D	106	901	542	176	174	9	0	0

- Molecule 11 is a protein called RIB30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	5E	258	1981	1245	352	380	4	0	0

- Molecule 12 is a protein called FAP363.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	5F	381	3020	1921	520	569	10	0	0
12	5G	141	1123	711	203	206	3	0	0
12	7B	97	753	476	125	148	4	0	0

- Molecule 13 is a protein called FAP126.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	5H	135	1069	674	190	202	3	0	0
13	5I	135	1069	674	190	202	3	0	0
13	5J	135	1069	674	190	202	3	0	0
13	5K	135	1069	674	190	202	3	0	0

- Molecule 14 is a protein called FAP52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	5L	626	4757	2992	827	912	26	0	0
14	5M	626	4757	2992	827	912	26	0	0
14	5N	626	4757	2992	827	912	26	0	0

- Molecule 15 is a protein called FAP67.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	5O	376	2927	1862	503	547	15	0	0
15	5P	376	2927	1862	503	547	15	0	0

- Molecule 16 is a protein called FAP85.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	5Q	191	1523	961	267	293	2	0	0

- Molecule 17 is a protein called FAP106.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	5R	22	162	100	33	28	1	0	0
17	5S	199	1572	989	291	288	4	0	0
17	5T	198	1563	984	290	285	4	0	0
17	5U	199	1572	989	291	288	4	0	0
17	5V	109	879	551	164	162	2	0	0

- Molecule 18 is a protein called FAP115.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	5X	221	1793	1153	302	330	8	0	0
18	5Y	221	1793	1153	302	330	8	0	0
18	5Z	221	1793	1153	302	330	8	0	0
18	6A	221	1793	1153	302	330	8	0	0
18	6B	221	1793	1153	302	330	8	0	0
18	6C	221	1793	1153	302	330	8	0	0
18	6D	221	1793	1153	302	330	8	0	0

- Molecule 19 is a protein called FAP143.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	6E	255	1952	1208	345	390	9	0	0

- Molecule 20 is a protein called FAP161.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	6F	394	2950	1852	518	566	14	0	0

- Molecule 21 is a protein called FAP166.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	6G	183	1420	891	251	269	9	0	0
21	6H	193	1493	937	265	282	9	0	0

- Molecule 22 is a protein called FAP252.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	6I	329	2617	1660	442	501	14	0	0
22	6J	329	2617	1660	442	501	14	0	0
22	6K	329	2617	1660	442	501	14	0	0
22	6L	329	2617	1660	442	501	14	0	0
22	6M	329	2617	1660	442	501	14	0	0
22	6N	329	2617	1660	442	501	14	0	0
22	6O	329	2617	1660	442	501	14	0	0
22	6P	297	2366	1499	399	454	14	0	0

- Molecule 23 is a protein called FAP276.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	6Q	85	694	434	130	127	3	0	0
23	6R	85	694	434	130	127	3	0	0
23	6S	85	694	434	130	127	3	0	0

- Molecule 24 is a protein called RIB72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	6T	564	4590	2928	792	854	16	0	0
24	6U	569	4623	2949	798	860	16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	6V	561	4569	2915	789	849	16	0	0
24	6W	566	4606	2938	795	857	16	0	0
24	6X	569	4631	2954	799	862	16	0	0
24	6Y	562	4579	2923	791	849	16	0	0
24	6Z	563	4585	2925	791	853	16	0	0
24	7A	189	1518	962	267	284	5	0	0

- Molecule 25 is a protein called FAP141.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	7C	98	794	486	157	149	2	0	0

- Molecule 26 is a protein called FAP222.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	7D	132	1016	637	183	189	7	0	0
26	7E	132	1016	637	183	189	7	0	0
26	7F	132	1016	637	183	189	7	0	0

- Molecule 27 is a protein called FAP95.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	7G	224	1728	1083	305	336	4	0	0

- Molecule 28 is a protein called FAP182.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	7H	138	1046	651	194	196	5	0	0
28	7X	138	1046	651	194	196	5	0	0

- Molecule 29 is a protein called FAP129.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	7I	228	1716	1065	311	334	6	0	0
29	7J	362	2741	1691	505	535	10	0	0

- Molecule 30 is a protein called FAP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	7K	423	3276	2026	620	625	5	0	0
30	7L	176	1333	819	254	257	3	0	0

- Molecule 31 is a protein called FAP273.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	7M	85	662	411	123	125	3	0	0
31	7N	126	977	607	179	186	5	0	0

- Molecule 32 is a protein called FAP107.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O			
32	7O	59	443	270	81	92		0	0
32	7P	182	1398	865	257	273	3	0	0

- Molecule 33 is a protein called RIB21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	7Q	71	567	352	98	117	0	0

- Molecule 34 is a protein called DC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	7R	195	1619	988	308	317	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	7S	160	1347	818	260	263	6	0	0

- Molecule 35 is a protein called DC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	7T	213	1738	1068	326	335	9	0	0
			Total	C	N	O	S		
35	7U	181	1476	904	278	285	9	0	0

- Molecule 36 is a protein called DC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	7V	89	735	457	123	150	5	0	0
			Total	C	N	O	S		
36	7W	89	735	457	123	150	5	0	0

- Molecule 37 is a protein called FAP68.

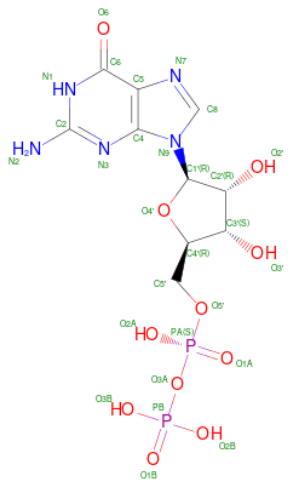
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	7Y	247	1971	1221	372	370	8	0	0

- Molecule 38 is a protein called FAP90.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	7Z	39	298	184	50	62	2	0	0
			Total	C	N	O	S		
38	8A	207	1691	1058	305	322	6	0	0
			Total	C	N	O	S		
38	8B	213	1728	1078	311	332	7	0	0
			Total	C	N	O	S		
38	8C	213	1728	1078	311	332	7	0	0
			Total	C	N	O	S		
38	8D	157	1311	820	236	250	5	0	0

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

GDP



Mol	Chain	Residues	Atoms					AltConf
39	2	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	3	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	5	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	7	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	9	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	A9	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	B1	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	B3	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	B8	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	C0	1	28	10	5	11	2	0
39	C2	1	28	10	5	11	2	0
39	C4	1	28	10	5	11	2	0
39	C6	1	28	10	5	11	2	0
39	C8	1	28	10	5	11	2	0
39	D0	1	28	10	5	11	2	0
39	D2	1	28	10	5	11	2	0
39	D4	1	28	10	5	11	2	0
39	D6	1	28	10	5	11	2	0
39	D8	1	28	10	5	11	2	0
39	E0	1	28	10	5	11	2	0
39	E2	1	28	10	5	11	2	0
39	E4	1	28	10	5	11	2	0
39	E6	1	28	10	5	11	2	0
39	E8	1	28	10	5	11	2	0
39	F0	1	28	10	5	11	2	0
39	F2	1	28	10	5	11	2	0
39	F6	1	28	10	5	11	2	0
39	F8	1	28	10	5	11	2	0
39	G0	1	28	10	5	11	2	0
39	G2	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	G4	1	28	10	5	11	2	0
39	G6	1	28	10	5	11	2	0
39	G8	1	28	10	5	11	2	0
39	H2	1	28	10	5	11	2	0
39	H4	1	28	10	5	11	2	0
39	H6	1	28	10	5	11	2	0
39	H8	1	28	10	5	11	2	0
39	I0	1	28	10	5	11	2	0
39	I2	1	28	10	5	11	2	0
39	I4	1	28	10	5	11	2	0
39	I8	1	28	10	5	11	2	0
39	J0	1	28	10	5	11	2	0
39	J2	1	28	10	5	11	2	0
39	J4	1	28	10	5	11	2	0
39	J6	1	28	10	5	11	2	0
39	J8	1	28	10	5	11	2	0
39	K0	1	28	10	5	11	2	0
39	K4	1	28	10	5	11	2	0
39	K6	1	28	10	5	11	2	0
39	K8	1	28	10	5	11	2	0
39	L0	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	L2	1	28	10	5	11	2	0
39	L4	1	28	10	5	11	2	0
39	L6	1	28	10	5	11	2	0
39	M0	1	28	10	5	11	2	0
39	M2	1	28	10	5	11	2	0
39	M4	1	28	10	5	11	2	0
39	M6	1	28	10	5	11	2	0
39	M8	1	28	10	5	11	2	0
39	N0	1	28	10	5	11	2	0
39	N2	1	28	10	5	11	2	0
39	N6	1	28	10	5	11	2	0
39	N8	1	28	10	5	11	2	0
39	O0	1	28	10	5	11	2	0
39	O2	1	28	10	5	11	2	0
39	O4	1	28	10	5	11	2	0
39	O6	1	28	10	5	11	2	0
39	O8	1	28	10	5	11	2	0
39	P4	1	28	10	5	11	2	0
39	P6	1	28	10	5	11	2	0
39	P8	1	28	10	5	11	2	0
39	Q0	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	Q2	1	28	10	5	11	2	0
39	Q4	1	28	10	5	11	2	0
39	Q6	1	28	10	5	11	2	0
39	Q8	1	28	10	5	11	2	0
39	R0	1	28	10	5	11	2	0
39	R2	1	28	10	5	11	2	0
39	R4	1	28	10	5	11	2	0
39	R6	1	28	10	5	11	2	0
39	R8	1	28	10	5	11	2	0
39	S0	1	28	10	5	11	2	0
39	S2	1	28	10	5	11	2	0
39	S4	1	28	10	5	11	2	0
39	S6	1	28	10	5	11	2	0
39	S8	1	28	10	5	11	2	0
39	T0	1	28	10	5	11	2	0
39	T2	1	28	10	5	11	2	0
39	T4	1	28	10	5	11	2	0
39	T6	1	28	10	5	11	2	0
39	T8	1	28	10	5	11	2	0
39	U2	1	28	10	5	11	2	0
39	U4	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	U6	1	28	10	5	11	2	0
39	U8	1	28	10	5	11	2	0
39	V0	1	28	10	5	11	2	0
39	V2	1	28	10	5	11	2	0
39	V4	1	28	10	5	11	2	0
39	V6	1	28	10	5	11	2	0
39	V8	1	28	10	5	11	2	0
39	W0	1	28	10	5	11	2	0
39	W2	1	28	10	5	11	2	0
39	W4	1	28	10	5	11	2	0
39	W6	1	28	10	5	11	2	0
39	W8	1	28	10	5	11	2	0
39	X0	1	28	10	5	11	2	0
39	X2	1	28	10	5	11	2	0
39	X4	1	28	10	5	11	2	0
39	X6	1	28	10	5	11	2	0
39	X8	1	28	10	5	11	2	0
39	Y0	1	28	10	5	11	2	0
39	Y2	1	28	10	5	11	2	0
39	Y4	1	28	10	5	11	2	0
39	Y6	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	Y8	1	28	10	5	11	2	0
39	Z0	1	28	10	5	11	2	0
39	Z2	1	28	10	5	11	2	0
39	Z4	1	28	10	5	11	2	0
39	Z6	1	28	10	5	11	2	0
39	Z8	1	28	10	5	11	2	0
39	0A	1	28	10	5	11	2	0
39	0C	1	28	10	5	11	2	0
39	0E	1	28	10	5	11	2	0
39	0G	1	28	10	5	11	2	0
39	0I	1	28	10	5	11	2	0
39	0K	1	28	10	5	11	2	0
39	0M	1	28	10	5	11	2	0
39	0O	1	28	10	5	11	2	0
39	0Q	1	28	10	5	11	2	0
39	0S	1	28	10	5	11	2	0
39	0U	1	28	10	5	11	2	0
39	0W	1	28	10	5	11	2	0
39	0Y	1	28	10	5	11	2	0
39	1A	1	28	10	5	11	2	0
39	1C	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	1E	1	28	10	5	11	2	0
39	1G	1	28	10	5	11	2	0
39	1K	1	28	10	5	11	2	0
39	1M	1	28	10	5	11	2	0
39	1O	1	28	10	5	11	2	0
39	1Q	1	28	10	5	11	2	0
39	1S	1	28	10	5	11	2	0
39	1U	1	28	10	5	11	2	0
39	1W	1	28	10	5	11	2	0
39	2A	1	28	10	5	11	2	0
39	2C	1	28	10	5	11	2	0
39	2E	1	28	10	5	11	2	0
39	2G	1	28	10	5	11	2	0
39	2I	1	28	10	5	11	2	0
39	2K	1	28	10	5	11	2	0
39	2M	1	28	10	5	11	2	0
39	2Q	1	28	10	5	11	2	0
39	2S	1	28	10	5	11	2	0
39	2U	1	28	10	5	11	2	0
39	2W	1	28	10	5	11	2	0
39	2Y	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	3A	1	28	10	5	11	2	0
39	3C	1	28	10	5	11	2	0
39	3G	1	28	10	5	11	2	0
39	3I	1	28	10	5	11	2	0
39	3K	1	28	10	5	11	2	0
39	3M	1	28	10	5	11	2	0
39	3O	1	28	10	5	11	2	0
39	3Q	1	28	10	5	11	2	0
39	3S	1	28	10	5	11	2	0

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
40	2	1	1	1	0
40	4	1	1	1	0
40	6	1	1	1	0
40	8	1	1	1	0
40	A0	1	1	1	0
40	A2	1	1	1	0
40	A4	1	1	1	0
40	A8	1	1	1	0
40	B0	1	1	1	0
40	B2	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
40	B4	1	1	1	0
40	B7	1	1	1	0
40	B9	1	1	1	0
40	C1	1	1	1	0
40	C5	1	1	1	0
40	C7	1	1	1	0
40	C9	1	1	1	0
40	D1	1	1	1	0
40	D3	1	1	1	0
40	D5	1	1	1	0
40	D7	1	1	1	0
40	E1	1	1	1	0
40	E3	1	1	1	0
40	E5	1	1	1	0
40	E7	1	1	1	0
40	E9	1	1	1	0
40	F1	1	1	1	0
40	F3	1	1	1	0
40	F5	1	1	1	0
40	F7	1	1	1	0
40	F9	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
40	G1	1	1	1	0
40	G3	1	1	1	0
40	G5	1	1	1	0
40	G7	1	1	1	0
40	G9	1	1	1	0
40	H2	1	1	1	0
40	H3	1	1	1	0
40	H5	1	1	1	0
40	H8	1	1	1	0
40	H9	1	1	1	0
40	I1	1	1	1	0
40	I3	1	1	1	0
40	I5	1	1	1	0
40	I7	1	1	1	0
40	I9	1	1	1	0
40	J1	1	1	1	0
40	J4	1	1	1	0
40	J5	1	1	1	0
40	J7	1	1	1	0
40	J9	1	1	1	0
40	K1	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
40	K3	1	1	1	0
40	K5	1	1	1	0
40	K7	1	1	1	0
40	K9	1	1	1	0
40	L1	1	1	1	0
40	L3	1	1	1	0
40	L5	1	1	1	0
40	L7	1	1	1	0
40	L9	1	1	1	0
40	M1	1	1	1	0
40	M3	1	1	1	0
40	M5	1	1	1	0
40	M7	1	1	1	0
40	M9	1	1	1	0
40	N1	1	1	1	0
40	N3	1	1	1	0
40	N6	1	1	1	0
40	N7	1	1	1	0
40	O0	1	1	1	0
40	O1	1	1	1	0
40	O3	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
40	O5	1	1	1	0
40	O8	1	1	1	0
40	O9	1	1	1	0
40	P4	1	1	1	0
40	P6	1	1	1	0
40	P7	1	1	1	0
40	P9	1	1	1	0
40	Q1	1	1	1	0
40	Q3	1	1	1	0
40	Q5	1	1	1	0
40	Q9	1	1	1	0
40	R1	1	1	1	0
40	R3	1	1	1	0
40	R6	1	1	1	0
40	R7	1	1	1	0
40	R9	1	1	1	0
40	S1	1	1	1	0
40	S5	1	1	1	0
40	S7	1	1	1	0
40	S9	1	1	1	0
40	T1	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
40	T3	1	1	1	0
40	T5	1	1	1	0
40	T7	1	1	1	0
40	U1	1	1	1	0
40	U3	1	1	1	0
40	U5	1	1	1	0
40	U7	1	1	1	0
40	U9	1	1	1	0
40	V2	1	1	1	0
40	V3	1	1	1	0
40	V7	1	1	1	0
40	V9	1	1	1	0
40	W2	1	1	1	0
40	W3	1	1	1	0
40	W5	1	1	1	0
40	W8	1	1	1	0
40	W9	1	1	1	0
40	X3	1	1	1	0
40	X5	1	1	1	0
40	X7	1	1	1	0
40	X9	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
40	Y1	1	1	1	0
40	Y3	1	1	1	0
40	Y5	1	1	1	0
40	Y9	1	1	1	0
40	Z2	1	1	1	0
40	Z3	1	1	1	0
40	Z5	1	1	1	0
40	Z7	1	1	1	0
40	0A	1	1	1	0
40	0B	1	1	1	0
40	0F	1	1	1	0
40	0H	1	1	1	0
40	0J	1	1	1	0
40	0L	1	1	1	0
40	0N	1	1	1	0
40	0P	1	1	1	0
40	0R	1	1	1	0
40	0W	1	1	1	0
40	0X	1	1	1	0
40	1A	1	1	1	0
40	1B	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
40	1D	1	1	1	0
40	1F	1	1	1	0
40	1H	1	1	1	0
40	1L	1	1	1	0
40	1N	1	1	1	0
40	1P	1	1	1	0
40	1R	1	1	1	0
40	1T	1	1	1	0
40	1V	1	1	1	0
40	1X	1	1	1	0
40	1Z	1	1	1	0
40	2B	1	1	1	0
40	2D	1	1	1	0
40	2F	1	1	1	0
40	2H	1	1	1	0
40	2J	1	1	1	0
40	2L	1	1	1	0
40	2N	1	1	1	0
40	2P	1	1	1	0
40	2R	1	1	1	0
40	2T	1	1	1	0

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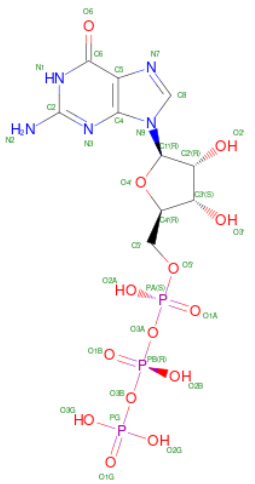
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
40	2V	1	1	1	0
40	2X	1	1	1	0
40	2Z	1	1	1	0
40	3B	1	1	1	0
40	3D	1	1	1	0
40	3F	1	1	1	0
40	3H	1	1	1	0
40	3K	1	1	1	0
40	3L	1	1	1	0
40	3N	1	1	1	0
40	3P	1	1	1	0
40	3R	1	1	1	0
40	3T	1	1	1	0

- Molecule 41 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP



Mol	Chain	Residues	Atoms					AltConf
41	3	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	4	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	7	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	8	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	A1	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	A2	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	A4	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	A9	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	B0	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	B2	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	B5	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	B7	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	C0	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	C1	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	
41	C5	1	32	10	5	14	3	0
41	C8	1	32	10	5	14	3	0
41	C9	1	32	10	5	14	3	0
41	D1	1	32	10	5	14	3	0
41	D3	1	32	10	5	14	3	0
41	D5	1	32	10	5	14	3	0
41	D7	1	32	10	5	14	3	0
41	E1	1	32	10	5	14	3	0
41	E4	1	32	10	5	14	3	0
41	E6	1	32	10	5	14	3	0
41	E8	1	32	10	5	14	3	0
41	F0	1	32	10	5	14	3	0
41	F1	1	32	10	5	14	3	0
41	F3	1	32	10	5	14	3	0
41	F5	1	32	10	5	14	3	0
41	F8	1	32	10	5	14	3	0
41	G0	1	32	10	5	14	3	0
41	G1	1	32	10	5	14	3	0
41	G4	1	32	10	5	14	3	0
41	G5	1	32	10	5	14	3	0
41	G7	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
41	G9	1	32	10	5	14	3	0
41	H2	1	32	10	5	14	3	0
41	H3	1	32	10	5	14	3	0
41	H6	1	32	10	5	14	3	0
41	H8	1	32	10	5	14	3	0
41	I0	1	32	10	5	14	3	0
41	I1	1	32	10	5	14	3	0
41	I4	1	32	10	5	14	3	0
41	I5	1	32	10	5	14	3	0
41	I8	1	32	10	5	14	3	0
41	J0	1	32	10	5	14	3	0
41	J2	1	32	10	5	14	3	0
41	J4	1	32	10	5	14	3	0
41	J6	1	32	10	5	14	3	0
41	J8	1	32	10	5	14	3	0
41	K0	1	32	10	5	14	3	0
41	K1	1	32	10	5	14	3	0
41	K4	1	32	10	5	14	3	0
41	K6	1	32	10	5	14	3	0
41	K7	1	32	10	5	14	3	0
41	K9	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
41	L2	1	32	10	5	14	3	0
41	L4	1	32	10	5	14	3	0
41	L6	1	32	10	5	14	3	0
41	L7	1	32	10	5	14	3	0
41	M0	1	32	10	5	14	3	0
41	M2	1	32	10	5	14	3	0
41	M4	1	32	10	5	14	3	0
41	M6	1	32	10	5	14	3	0
41	M7	1	32	10	5	14	3	0
41	N0	1	32	10	5	14	3	0
41	N1	1	32	10	5	14	3	0
41	N3	1	32	10	5	14	3	0
41	N6	1	32	10	5	14	3	0
41	N8	1	32	10	5	14	3	0
41	O0	1	32	10	5	14	3	0
41	O2	1	32	10	5	14	3	0
41	O4	1	32	10	5	14	3	0
41	O6	1	32	10	5	14	3	0
41	O8	1	32	10	5	14	3	0
41	O9	1	32	10	5	14	3	0
41	P4	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
41	P6	1	32	10	5	14	3	0
41	P8	1	32	10	5	14	3	0
41	P9	1	32	10	5	14	3	0
41	Q2	1	32	10	5	14	3	0
41	Q4	1	32	10	5	14	3	0
41	Q6	1	32	10	5	14	3	0
41	R0	1	32	10	5	14	3	0
41	R2	1	32	10	5	14	3	0
41	R4	1	32	10	5	14	3	0
41	R6	1	32	10	5	14	3	0
41	R8	1	32	10	5	14	3	0
41	S0	1	32	10	5	14	3	0
41	S2	1	32	10	5	14	3	0
41	S5	1	32	10	5	14	3	0
41	S8	1	32	10	5	14	3	0
41	S9	1	32	10	5	14	3	0
41	T2	1	32	10	5	14	3	0
41	T4	1	32	10	5	14	3	0
41	T6	1	32	10	5	14	3	0
41	T8	1	32	10	5	14	3	0
41	U2	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
41	U4	1	32	10	5	14	3	0
41	U6	1	32	10	5	14	3	0
41	U7	1	32	10	5	14	3	0
41	U9	1	32	10	5	14	3	0
41	V2	1	32	10	5	14	3	0
41	V3	1	32	10	5	14	3	0
41	V8	1	32	10	5	14	3	0
41	W0	1	32	10	5	14	3	0
41	W2	1	32	10	5	14	3	0
41	W4	1	32	10	5	14	3	0
41	W5	1	32	10	5	14	3	0
41	W8	1	32	10	5	14	3	0
41	X0	1	32	10	5	14	3	0
41	X4	1	32	10	5	14	3	0
41	X6	1	32	10	5	14	3	0
41	X7	1	32	10	5	14	3	0
41	Y0	1	32	10	5	14	3	0
41	Y1	1	32	10	5	14	3	0
41	Y4	1	32	10	5	14	3	0
41	Y6	1	32	10	5	14	3	0
41	Z0	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
41	Z2	1	32	10	5	14	3	0
41	Z3	1	32	10	5	14	3	0
41	Z6	1	32	10	5	14	3	0
41	Z7	1	32	10	5	14	3	0
41	0A	1	32	10	5	14	3	0
41	0C	1	32	10	5	14	3	0
41	0F	1	32	10	5	14	3	0
41	0I	1	32	10	5	14	3	0
41	0K	1	32	10	5	14	3	0
41	0M	1	32	10	5	14	3	0
41	0O	1	32	10	5	14	3	0
41	0Q	1	32	10	5	14	3	0
41	0S	1	32	10	5	14	3	0
41	0V	1	32	10	5	14	3	0
41	0Y	1	32	10	5	14	3	0
41	1A	1	32	10	5	14	3	0
41	1C	1	32	10	5	14	3	0
41	1D	1	32	10	5	14	3	0
41	1G	1	32	10	5	14	3	0
41	1H	1	32	10	5	14	3	0
41	1L	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
41	1N	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	1Q	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	1S	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	1T	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	1W	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	1X	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2A	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2C	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2E	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2G	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2I	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2K	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2L	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2N	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2Q	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2S	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2U	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2W	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	2Y	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	3A	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	3C	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
41	3D	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	3G	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	3I	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	3K	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	3M	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	3O	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	3P	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	3S	1	32	10	5	14	3	0
			Total	C	N	O	P	
41	3T	1	32	10	5	14	3	0

3 Residue-property plots (i)

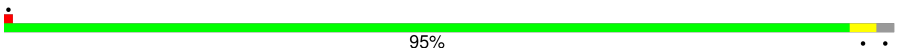
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

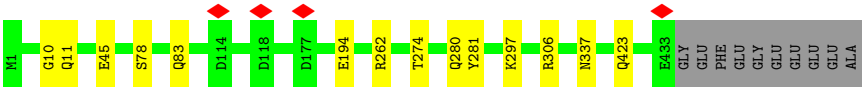
- Molecule 1: Tubulin beta

Chain 1:

- Molecule 1: Tubulin beta

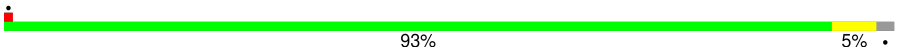
Chain 3:

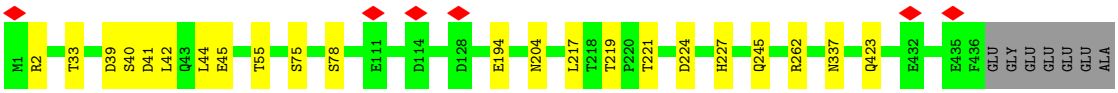




- Molecule 1: Tubulin beta

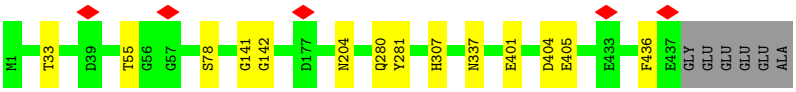
Chain 5:





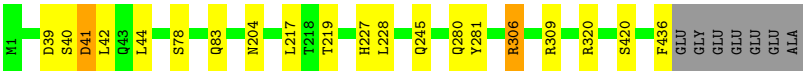
- Molecule 1: Tubulin beta

Chain 7: 95%



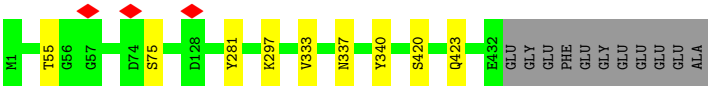
• Molecule 1: Tubulin beta

Chain 9: 94%



• Molecule 1: Tubulin beta

Chain A1: 95%

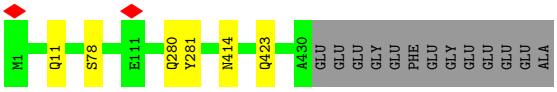


• Molecule 1: Tubulin beta

Chain A3: 92% 6%

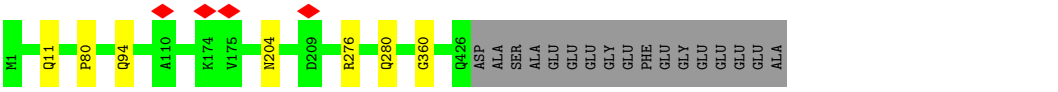
• Molecule 1: Tubulin beta

Chain A5: 96%



• Molecule 1: Tubulin beta

Chain A7: 95%

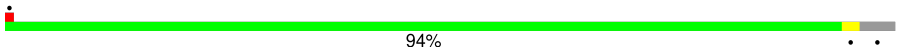


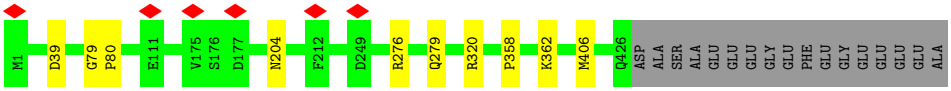
• Molecule 1: Tubulin beta

Chain A9: 94%

• Molecule 1: Tubulin beta

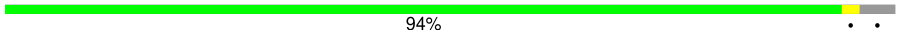
Chain B1:

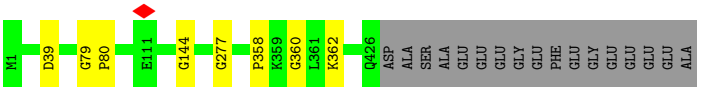




• Molecule 1: Tubulin beta

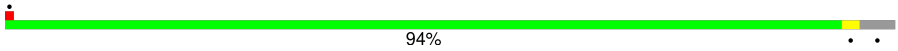
Chain B3:

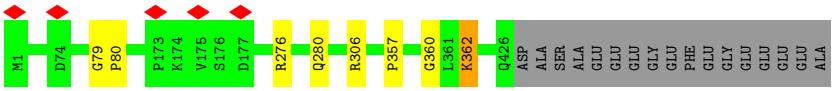




• Molecule 1: Tubulin beta

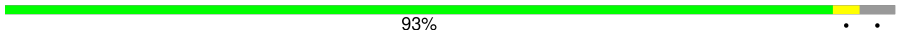
Chain B5:

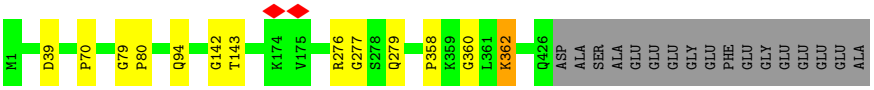




• Molecule 1: Tubulin beta

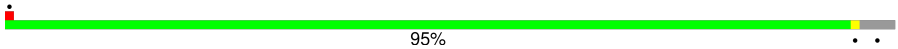
Chain B8:

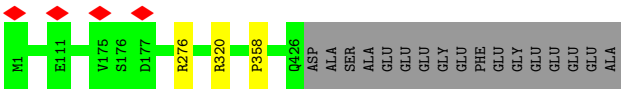




• Molecule 1: Tubulin beta

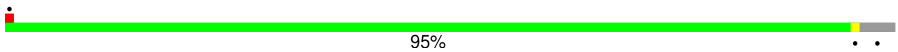
Chain C0:

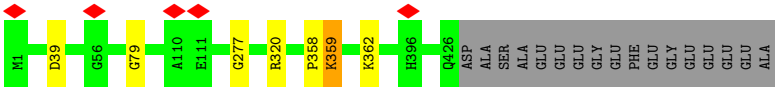




• Molecule 1: Tubulin beta

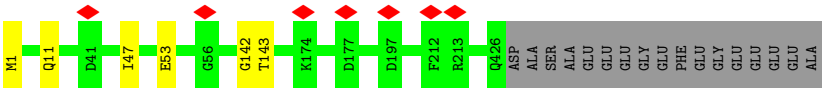
Chain C2:





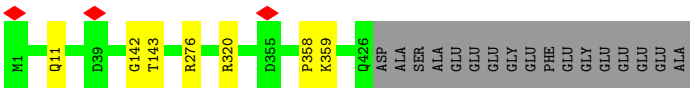
• Molecule 1: Tubulin beta

Chain C4: 95%



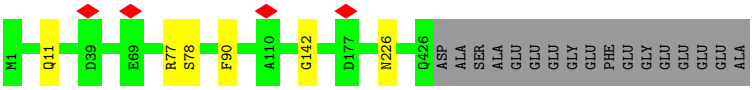
• Molecule 1: Tubulin beta

Chain C6: 95%



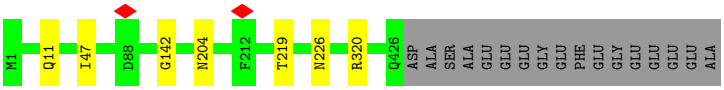
• Molecule 1: Tubulin beta

Chain C8: 95%



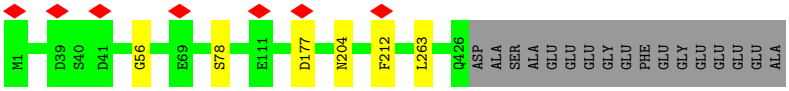
• Molecule 1: Tubulin beta

Chain D0: 95%



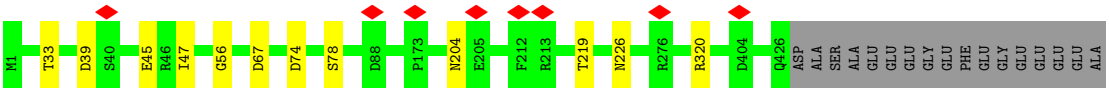
• Molecule 1: Tubulin beta

Chain D2: 95%



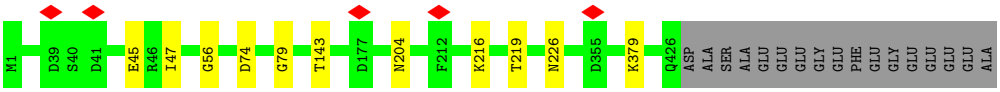
• Molecule 1: Tubulin beta

Chain D4: 93%



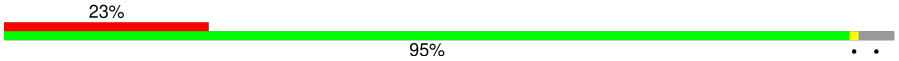
• Molecule 1: Tubulin beta

Chain D6: 94%



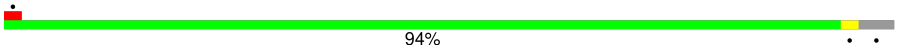
• Molecule 1: Tubulin beta

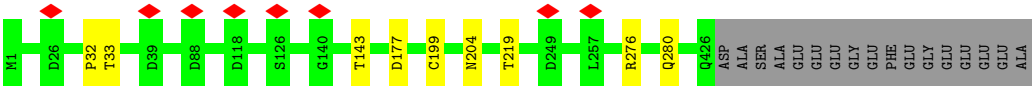
Chain D8:



• Molecule 1: Tubulin beta

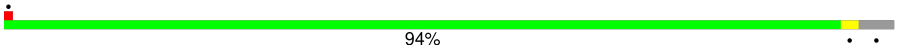
Chain E0:

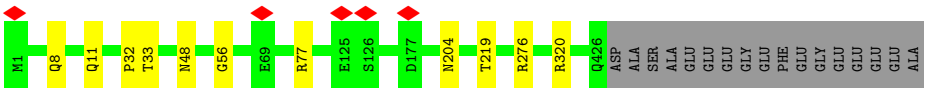




• Molecule 1: Tubulin beta

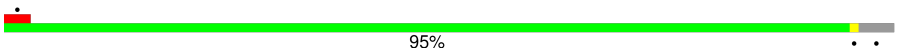
Chain E2:

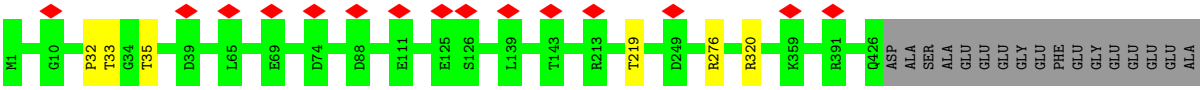




• Molecule 1: Tubulin beta

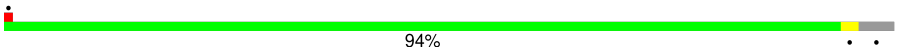
Chain E4:





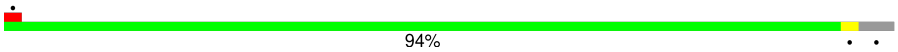
• Molecule 1: Tubulin beta

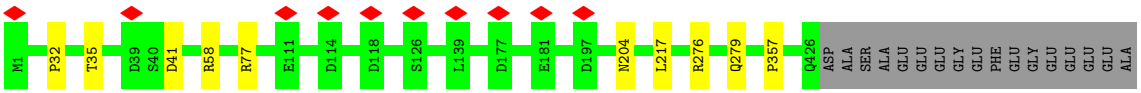
Chain E6:



• Molecule 1: Tubulin beta

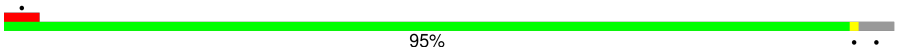
Chain E8:

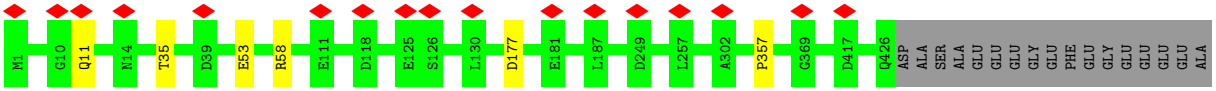




• Molecule 1: Tubulin beta

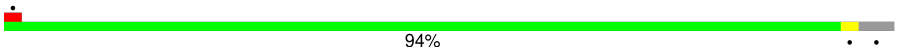
Chain F0:

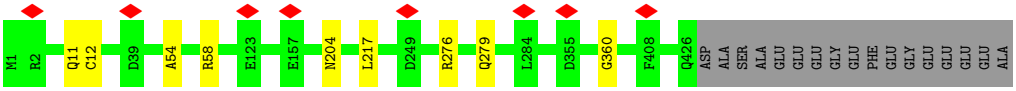




• Molecule 1: Tubulin beta

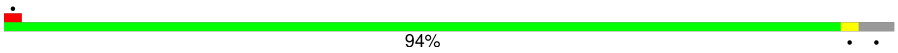
Chain F2:

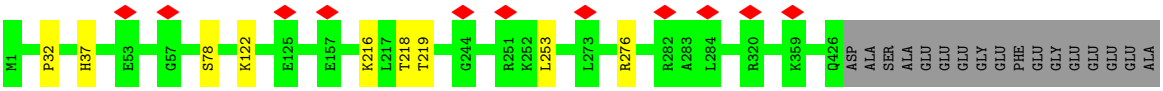




• Molecule 1: Tubulin beta

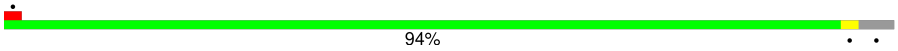
Chain F6:

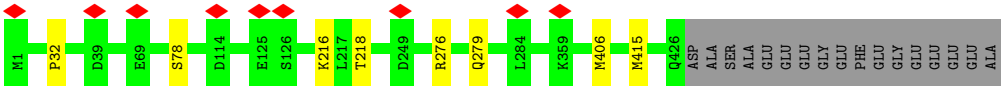




• Molecule 1: Tubulin beta

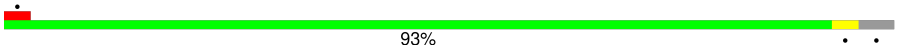
Chain F8:

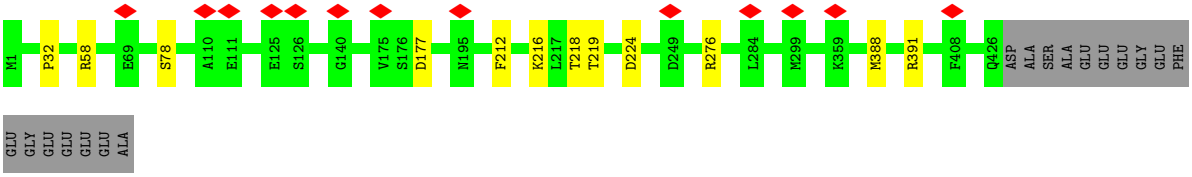




• Molecule 1: Tubulin beta

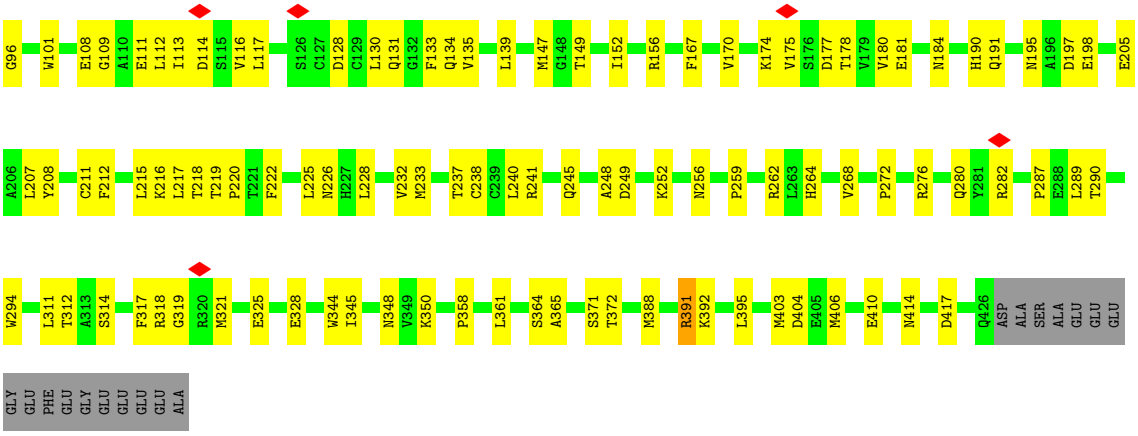
Chain G0:





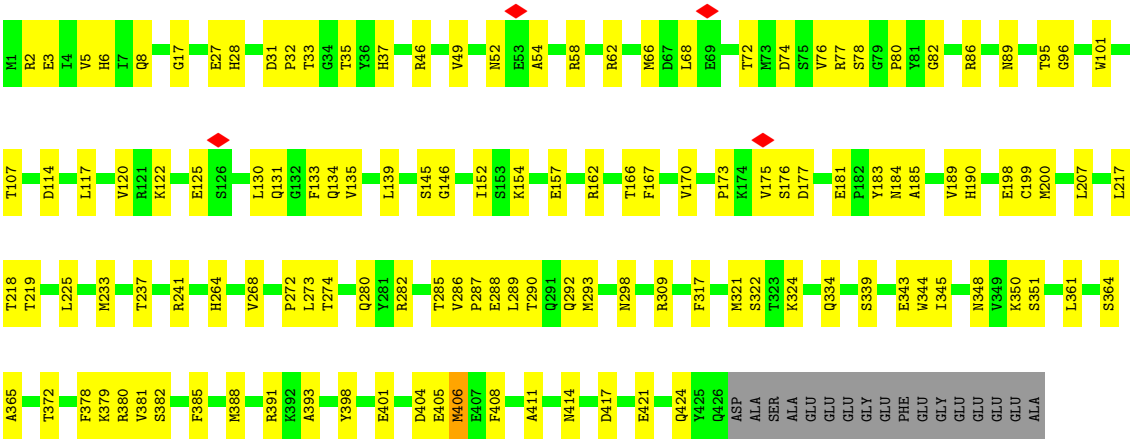
• Molecule 1: Tubulin beta

Chain G2:



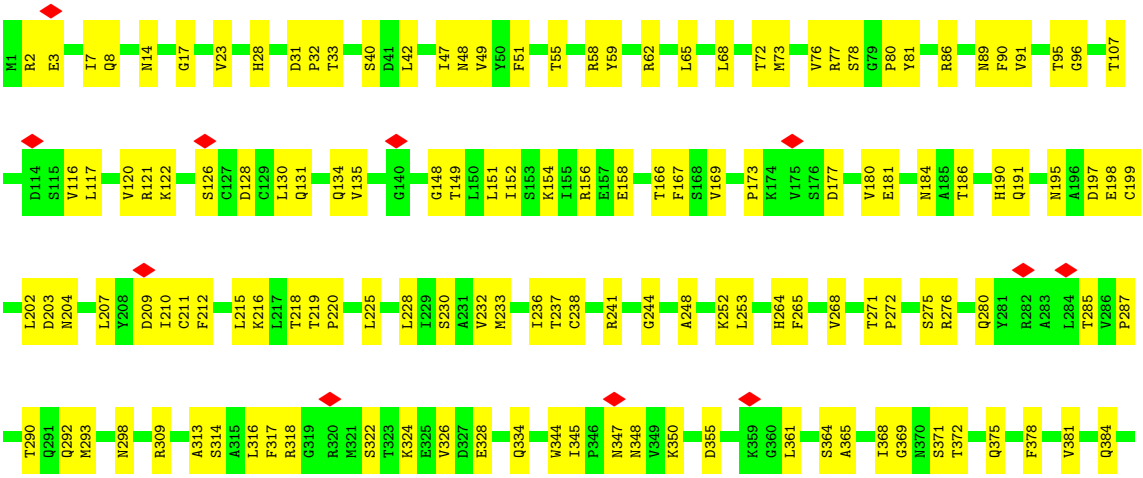
• Molecule 1: Tubulin beta

Chain G4:



• Molecule 1: Tubulin beta

Chain G6:



F389 R390 R391 K392 H396 E401 D404 E405 M406 A411 N414 D417 Q426 ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain G8:

M1 R2 E3 I7 Q8 G9 G17 D26 D31 P32 T33 G34 T35 E45 R46 V49 N52 T55 R58 P61 R62 A63 I64 L65 M66 D67 L68 P80 Y81 F85 V91 G96 N100 K103 T107 L112 I113 D114 S115 V116 L117 D118

V119 V120 R121 E125 S126 C127 D128 C129 L130 Q131 V135 C136 H137 S138 L139 G140 S145 G146 M147 L151 I152 R156 E157 E158 Y159 P160 T166 F167 S168 V169 V170 P171 S172 P173 K174 V175 S176 D177 T178 V179 V180 Y183 N184 A185 T186 H190 E194 C199 L202

L207 C211 F212 R213 T214 L215 K216 T219 P220 D224 L225 N226 H227 S230 A231 V232 M233 S234 G235 C239 L240 R241 A248 D249 K252 L253 N256 F260 P261 R262 L263 V268 P272 L273 T274 S275 Q280 Y281 R282 A283 L284 T285 V286 P287 T290

M293 M300 R309 Y310 L311 T312 A313 S314 A315 L316 F317 K324 Q334 N335 S338 I345 P346 N347 N348 V349 K350 S351 S352 K359 G360 L361 S364 A365 T366 F367 I368 G369 N370 S371 T372 R380 Q384 F385 M388 K392 L395 H396 W397 E401 D404

E405 M406 E407 E410 A411 N414 D417 Q426 ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain H2:

M1 R2 H6 I7 Q8 Q11 F20 V24 S25 D26 T33 G34 T35 Y36 H37 D41 L42 Q43 L44 E45 R46 V49 Y50 F51 N52 E53 R58 R62 M66 D67 L68 T72 V76 R77 D88 N89 F90 V91 G96 A97 K103 T107 E108

E111 L112 I113 D114 S115 V116 L117 V120 R121 K122 E125 D128 Q131 Q134 V135 L139 G140 G141 G142 T143 M147 L151 I152 S153 K154 I155 R156 T166 F167 S168 P173 K174 V175 S176 D177 T178 V179 V180 E181 N184 A185 T186 H190 Q191 L192 N195 A196

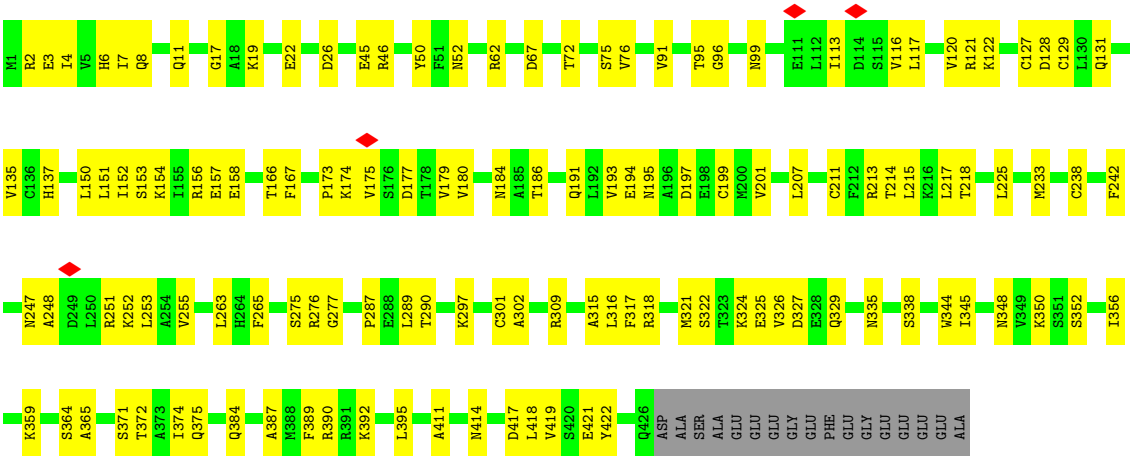
D197 E198 C199 M200 L207 Y208 D209 I210 C211 L215 T218 L225 L228 M233 L240 G244 N247 A248 D249 L250 R251 K252 L257 F265 V268 P272 R276 R282 A283 L284 T285 V286 P287 E288 L289 T290 Q291 K297 C301 A302 A303 D304

H307 G308 R309 S314 F317 M321 S322 E325 M330 Q334 N335 K336 N337 S338 S339 Y340 W344 I345 N348 V349 K359 S364 A365 T372 A373 I374 F378 K379 R380 V381 S382 T386 A387 R390 D404 E405 M406 E410 A411 N414 M415 M416 D417

L418 V419 S420 E421 Y422 Q426 ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

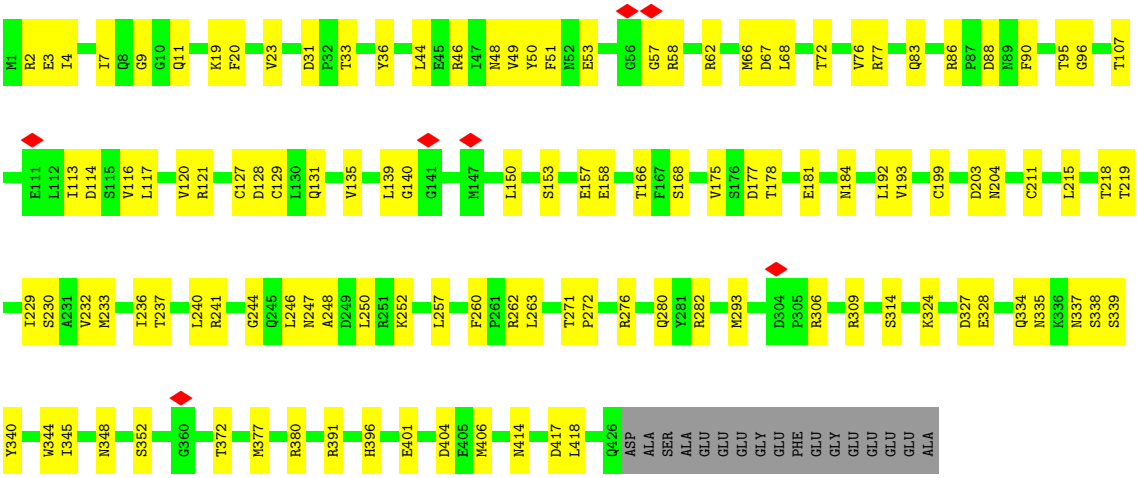
- Molecule 1: Tubulin beta

Chain H4:



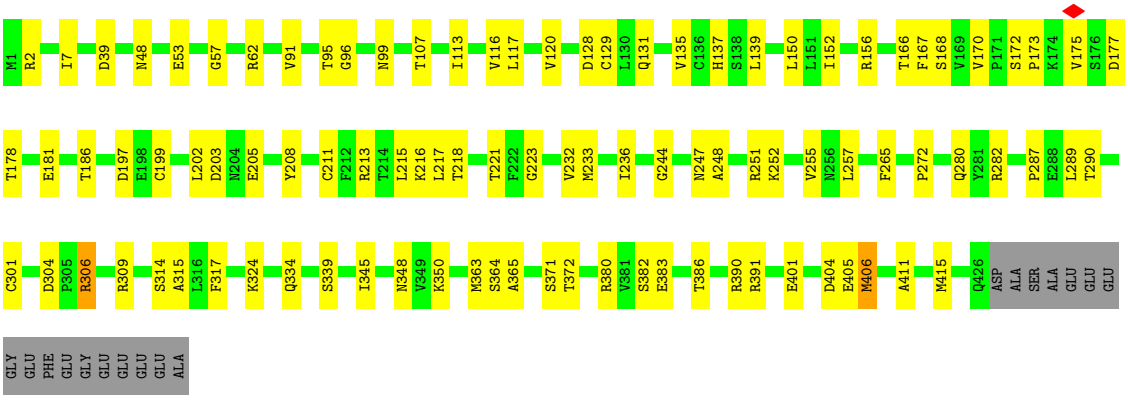
- Molecule 1: Tubulin beta

Chain H6:



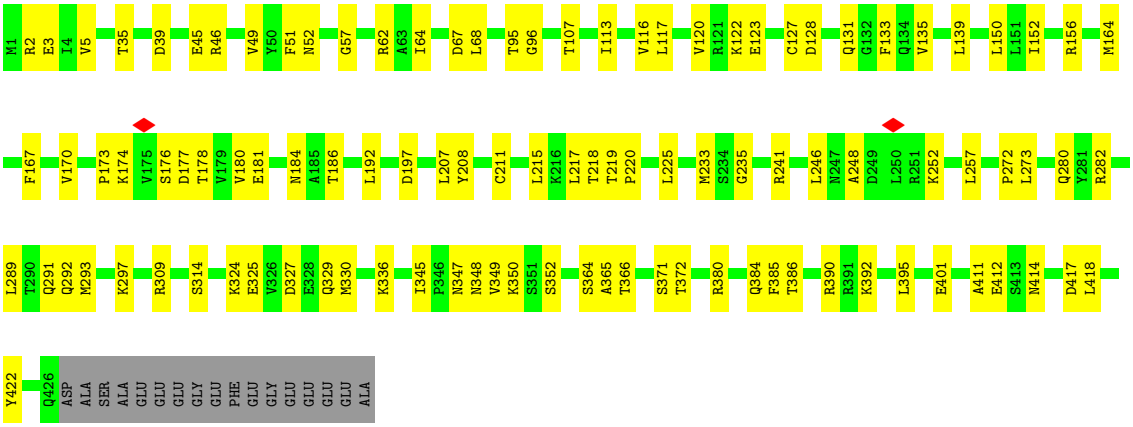
- Molecule 1: Tubulin beta

Chain H8:



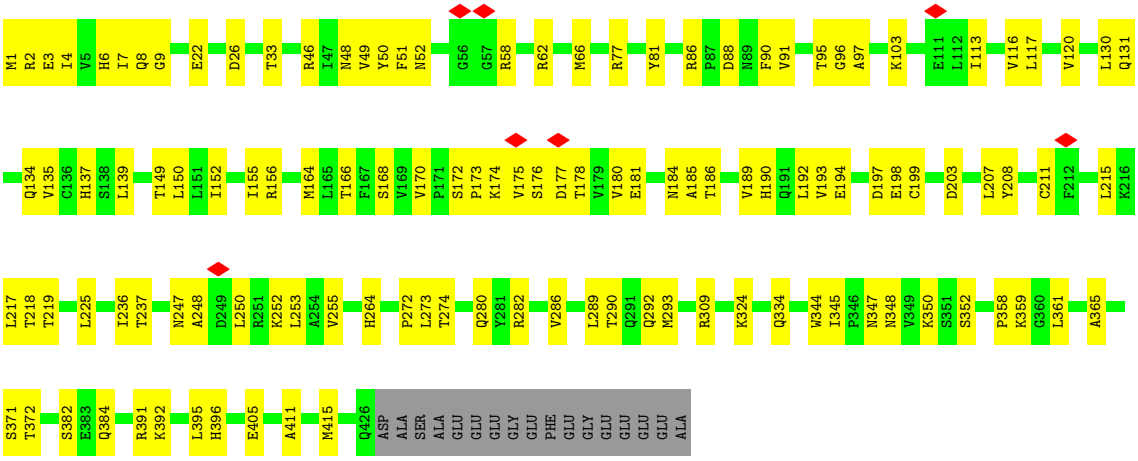
- Molecule 1: Tubulin beta

Chain I0:



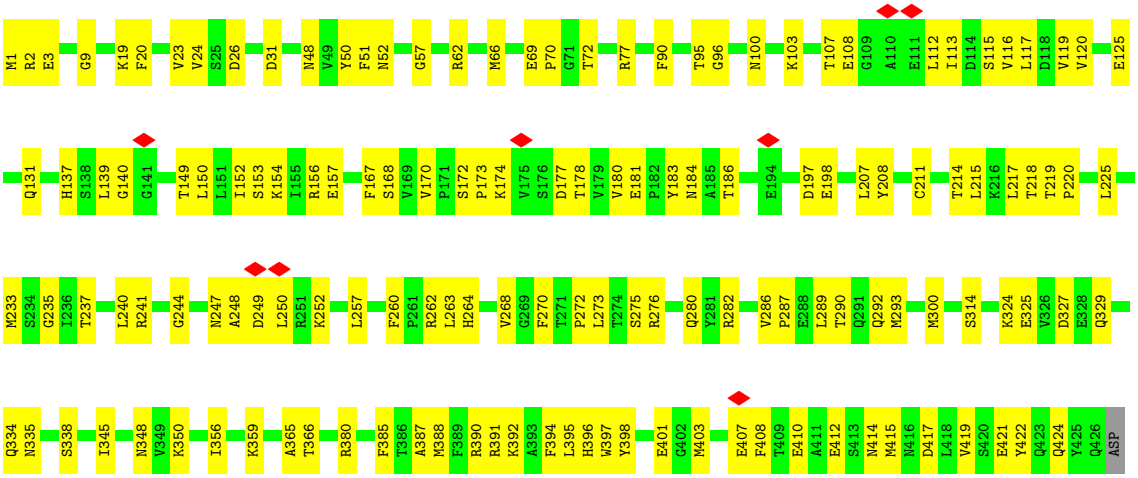
- Molecule 1: Tubulin beta

Chain I2:



- Molecule 1: Tubulin beta

Chain I4:



ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain I8:

M1 R2 E3 I7 G17 A18 K19 F20 W21 E22 V23 V24 D39 S40 D41 E45 R46 I47 N48 V49 Y50 F51 R58 R62 L68 E69 P70 D74 R77 Q83 V91 F92 T95 G96 A97 K103 T107 I113 D114 S115 V116 L117 D118 V119 V120

C127 D128 C129 L130 Q131 V135 C136 H137 S138 L139 G140 S145 G146 M147 L150 L151 I152 S153 K154 E157 M164 L165 T166 V170 P171 S172 V175 S176 D177 T178 V179 N184 A185 S188 V189 L192 D203 L207 Y208 D209 I210 C211 L215 K216 L217

P220 L225 I236 T237 L240 R241 L246 W247 A248 D249 K252 F260 L263 V268 T271 P272 L273 T274 S275 R276 Q279 T285 E288 Q291 Q292 M293 M300 C301 A302 A303 R309 F317 M321 S322 T323 K324 Q334 F341 I345 P346

N347 N348 Y349 K350 S351 S352 D355 I356 K359 G360 S364 A365 T372 A373 I374 Q375 E376 K379 F389 R390 R391 K392 H396 W397 Y398 T399 G400 E401 G402 M403 D404 E405 M406 N414 D417 L418 V419 S420 E421 Q424 Y425 Q426 ASP ALA SER ALA GLU GLU GLU GLY

GLU PHE GLU GLY GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain J0:

M1 R2 E3 I4 I7 W21 S25 I30 D39 S40 Q43 V49 Y50 F51 N52 G56 G57 R58 Y59 V60 P61 R62 A63 E69 P70 R77 I84 F85 R86 P87 D88 N89 F90 V91 F92 T95 G96 N100 K103 T107 E111 L112 I113 D114

S115 V116 K122 E125 S126 C129 L130 Q131 V135 C136 H137 S138 L139 G140 I152 S153 E157 M164 L165 T166 V170 P173 K174 V175 S176 D177 T178 V179 V180 N184 Q191 L192 V193 E194 C199 L207 C211 L215 K216 L217 T218 T219 P220 T221 F222

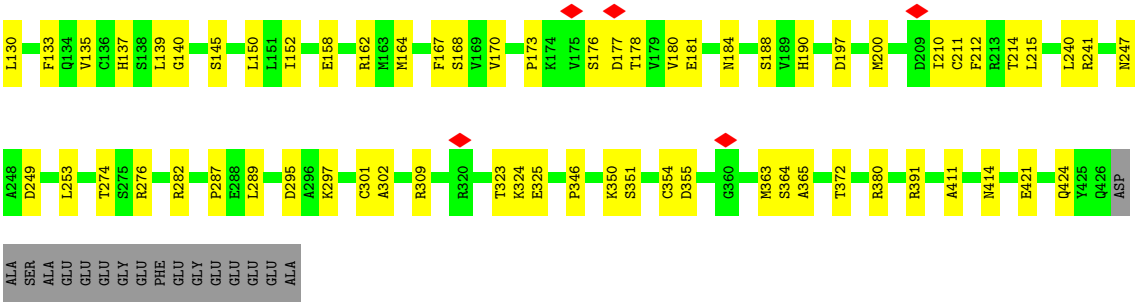
L225 V232 R241 A248 D249 L250 R251 K252 F260 L263 H264 F265 F270 T271 P272 R282 V286 L289 T290 Q291 Q292 M293 R309 F317 R320 M321 K324 Q334 S339 W344 I345 P346 N347 N348 Y349 K350 S351 A365 S371 T372

Q375 E376 M377 R380 V381 S382 T386 R390 E401 D404 E405 M406 M415 N416 D417 L418 V419 S420 Q426 ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

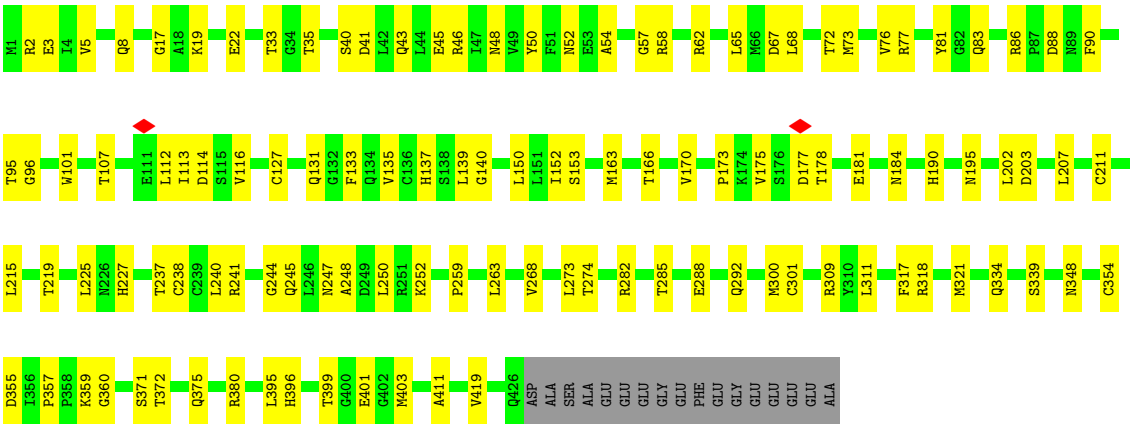
Chain J2:

M1 R2 V5 H6 I7 G10 Q11 D41 L44 E45 R46 V49 N52 V60 P61 R62 D67 L68 E69 P70 G71 D74 R77 I84 F85 R86 P87 D88 F92 A97 G98 N99 N100 K103 E111 L112 I113 D114 S115 V116 R121 K122 E123



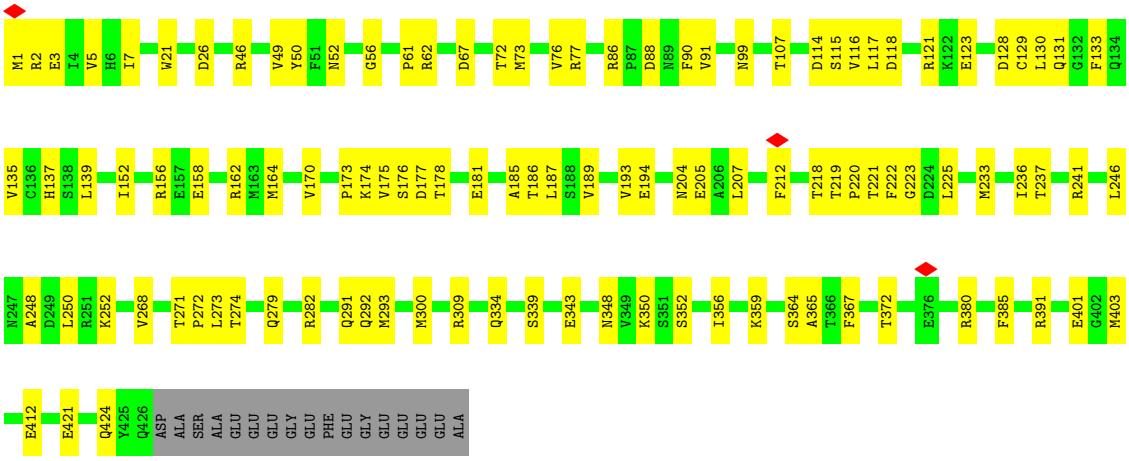
• Molecule 1: Tubulin beta

Chain J4:



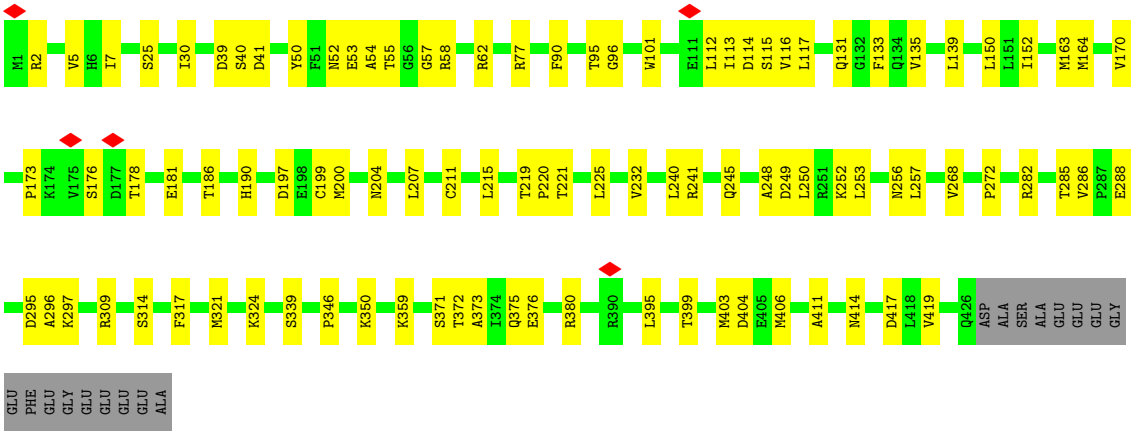
• Molecule 1: Tubulin beta

Chain J6:



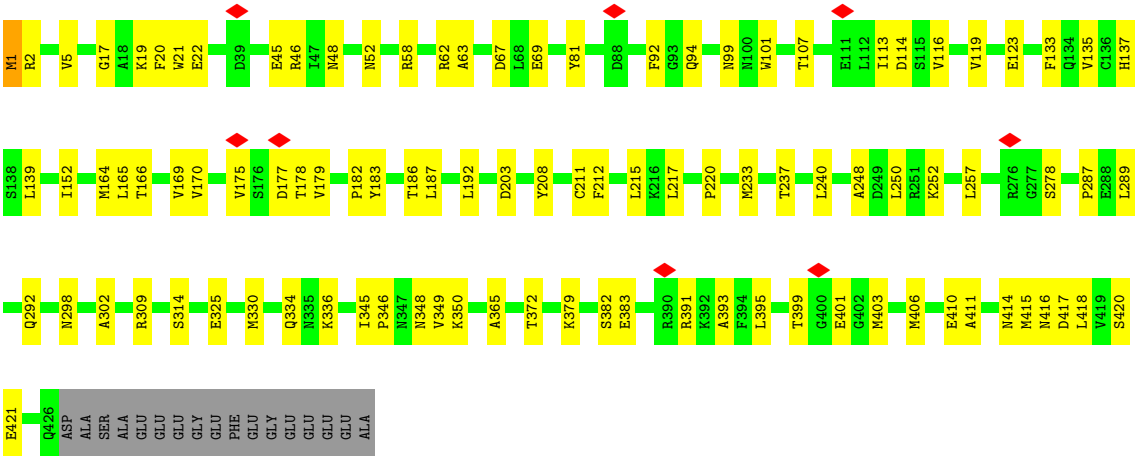
• Molecule 1: Tubulin beta

Chain J8:



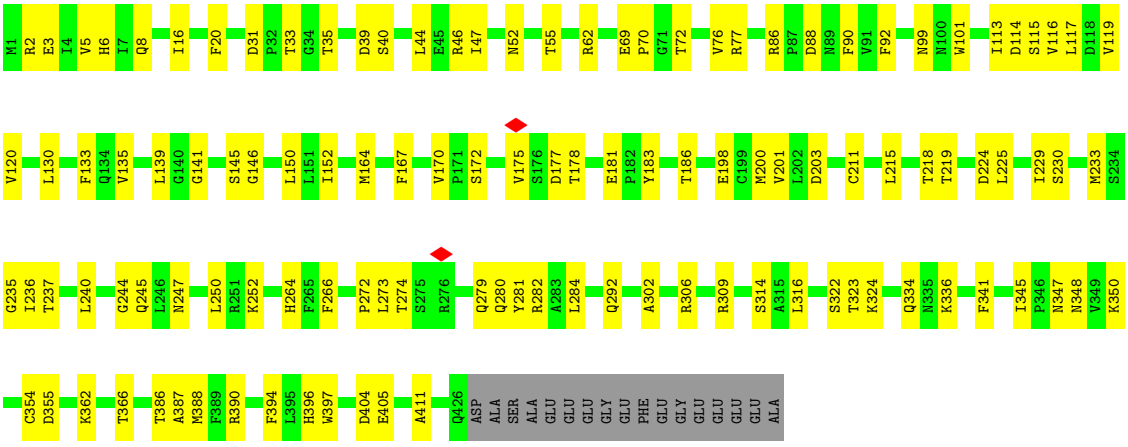
• Molecule 1: Tubulin beta

Chain K0:



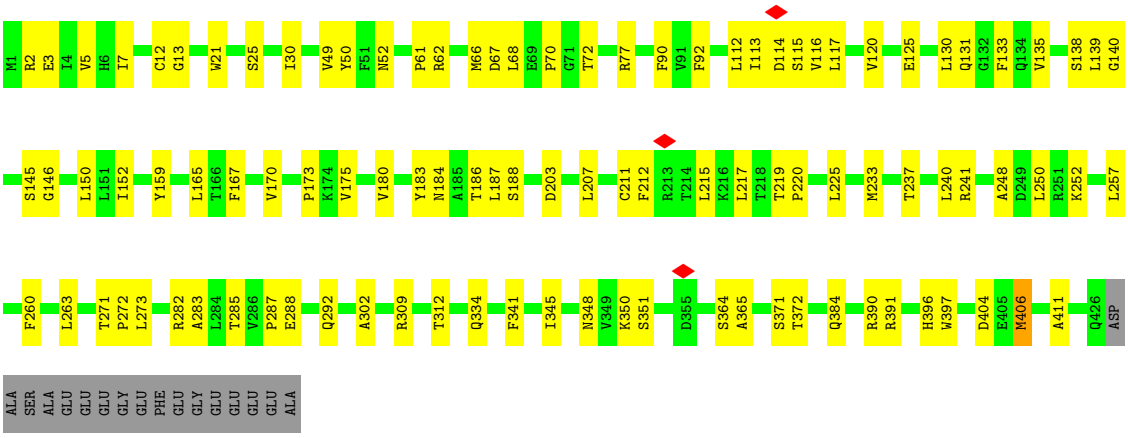
• Molecule 1: Tubulin beta

Chain K4:



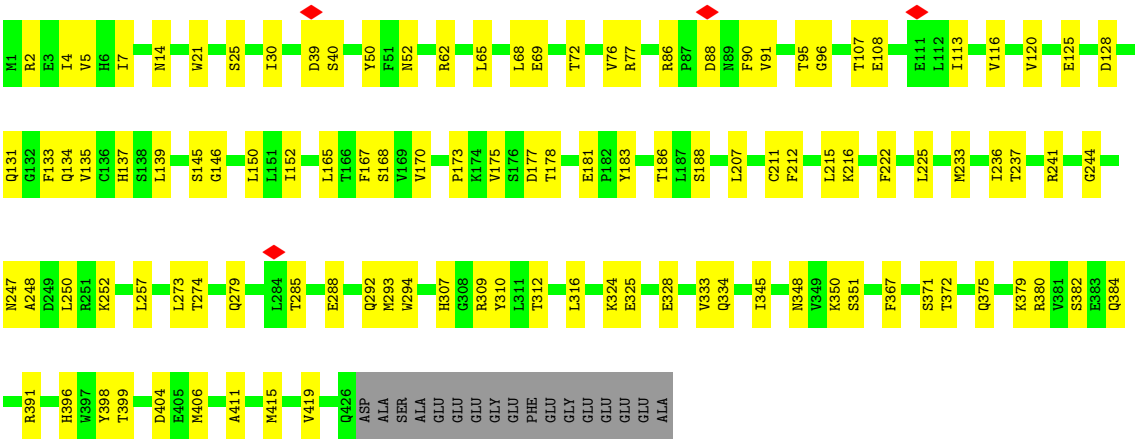
• Molecule 1: Tubulin beta

Chain K6:



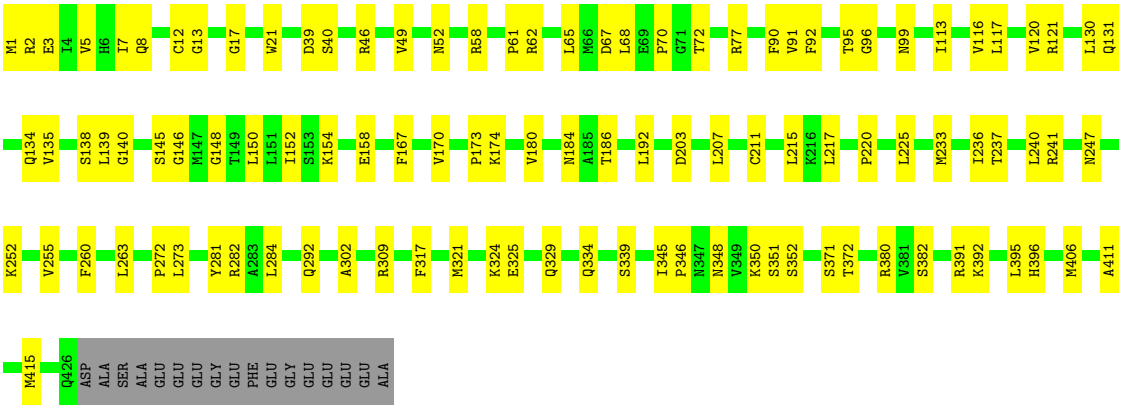
- Molecule 1: Tubulin beta

Chain K8:



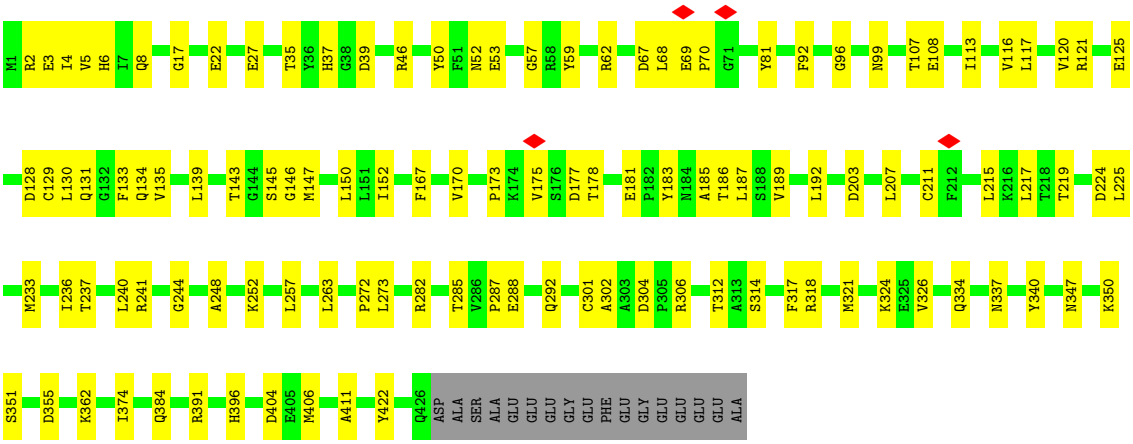
- Molecule 1: Tubulin beta

Chain L0:



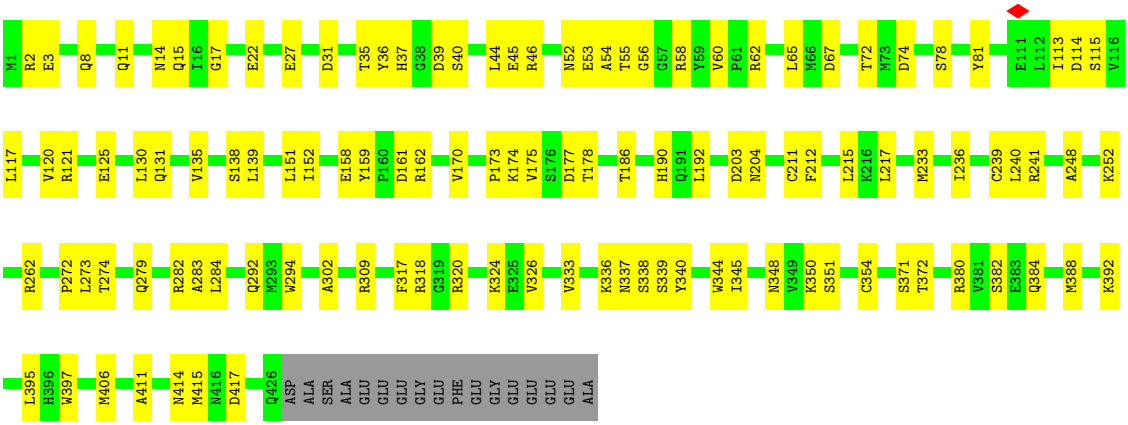
- Molecule 1: Tubulin beta

Chain L2:



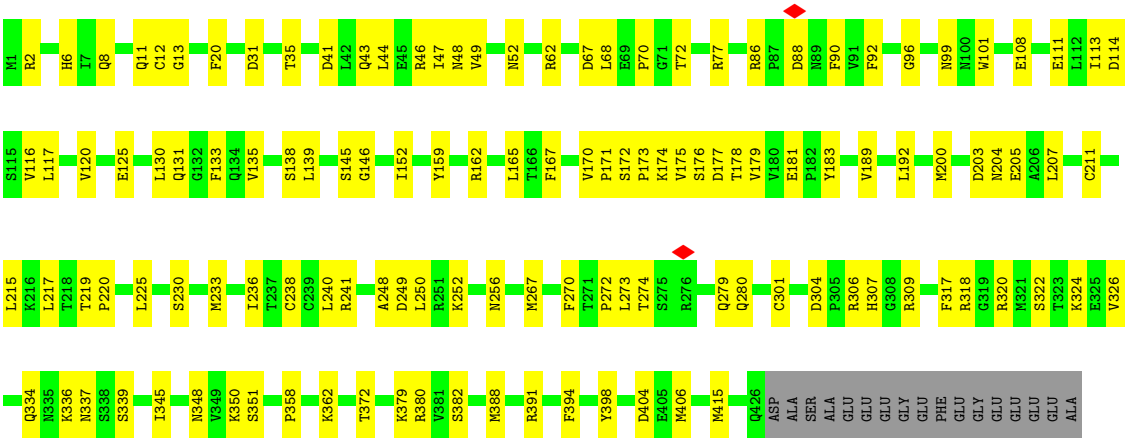
• Molecule 1: Tubulin beta

Chain L4:



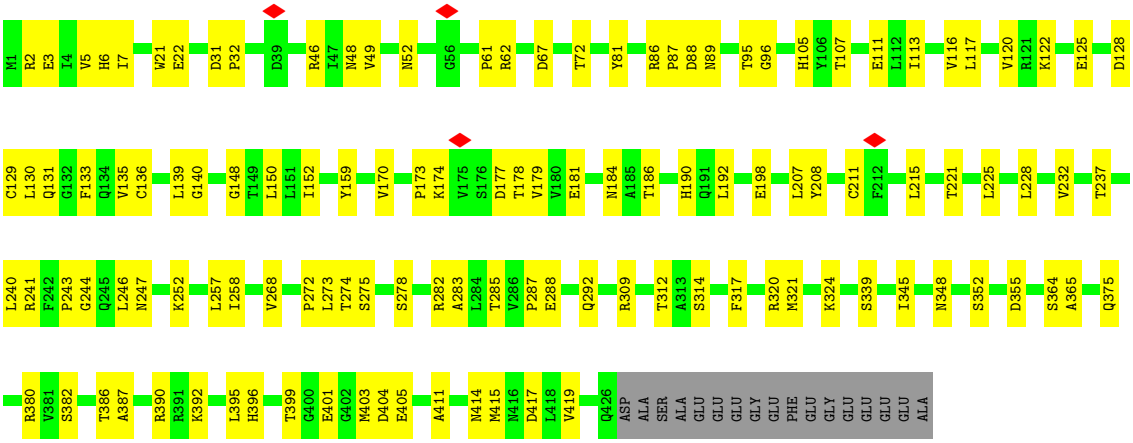
• Molecule 1: Tubulin beta

Chain L6:



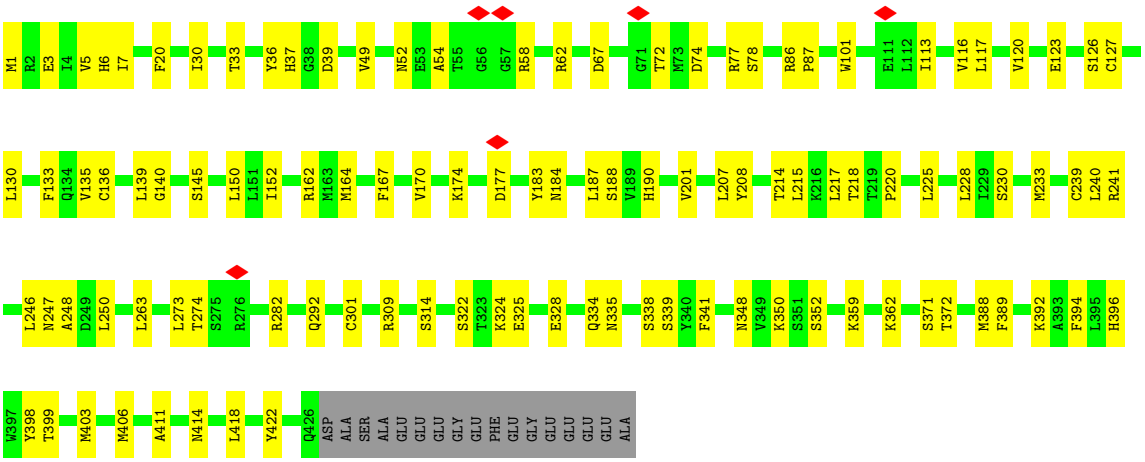
- Molecule 1: Tubulin beta

Chain M0:



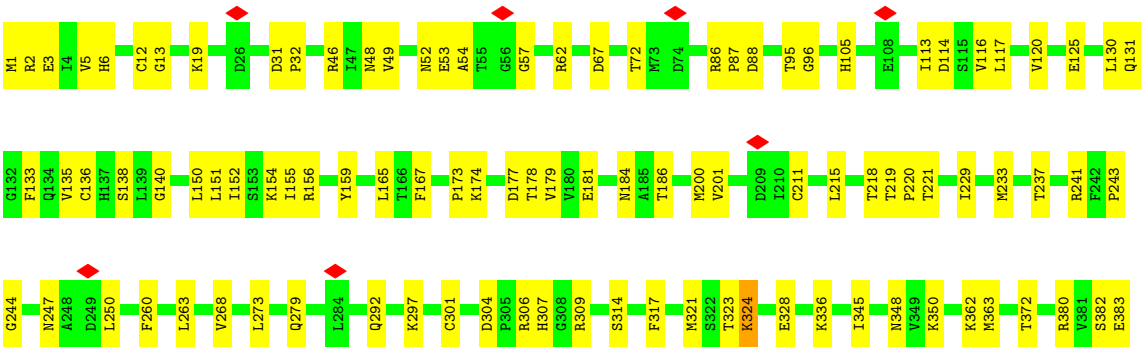
- Molecule 1: Tubulin beta

Chain M2:



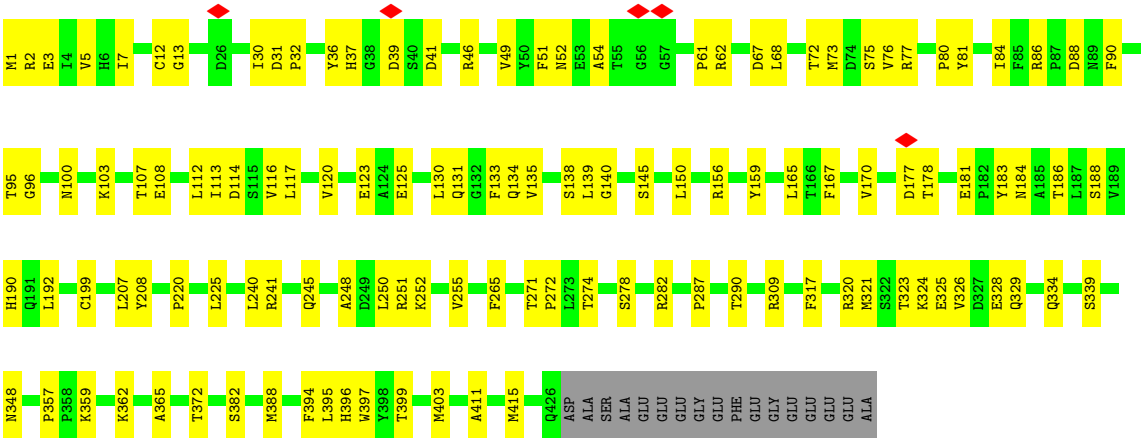
- Molecule 1: Tubulin beta

Chain M4:



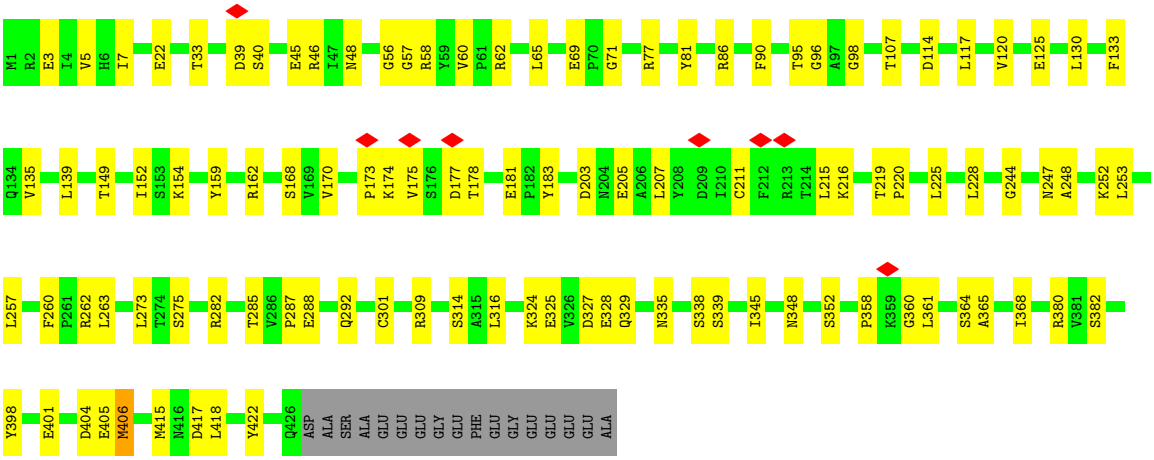
• Molecule 1: Tubulin beta

Chain M6:



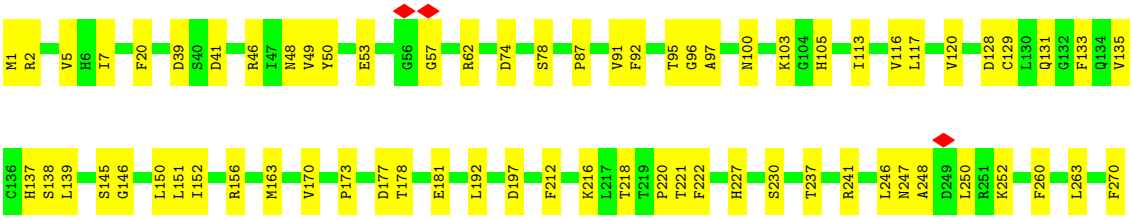
• Molecule 1: Tubulin beta

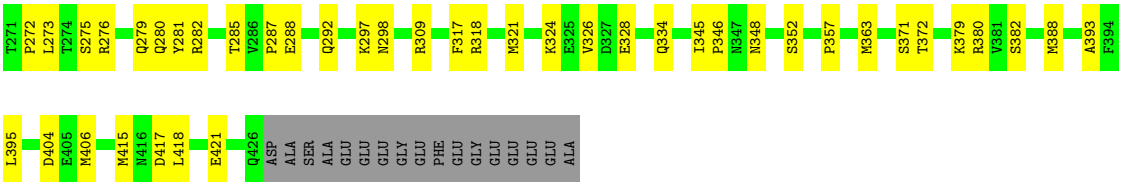
Chain M8:



• Molecule 1: Tubulin beta

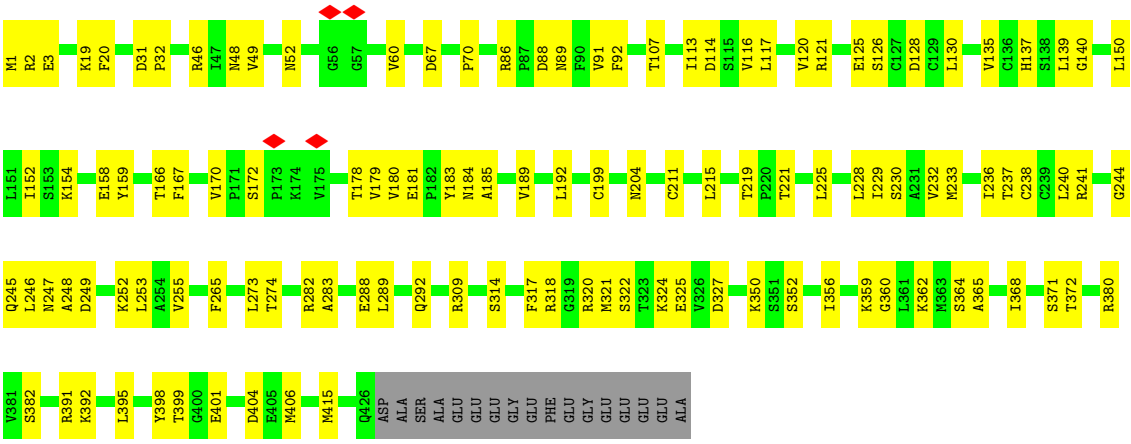
Chain N0:





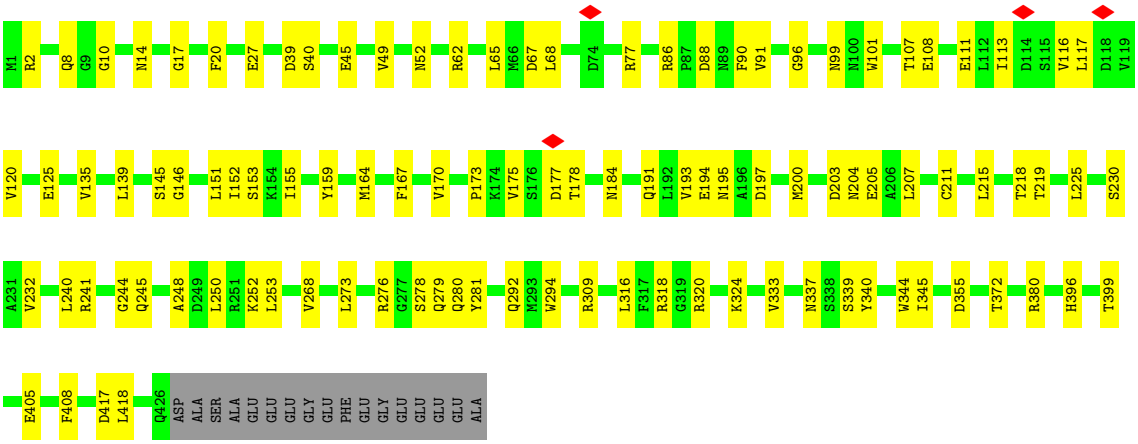
• Molecule 1: Tubulin beta

Chain N2:



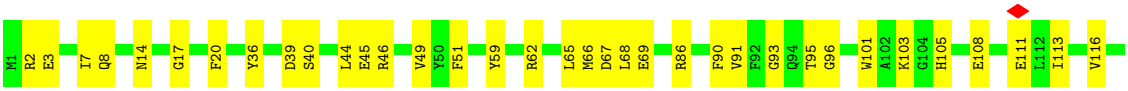
• Molecule 1: Tubulin beta

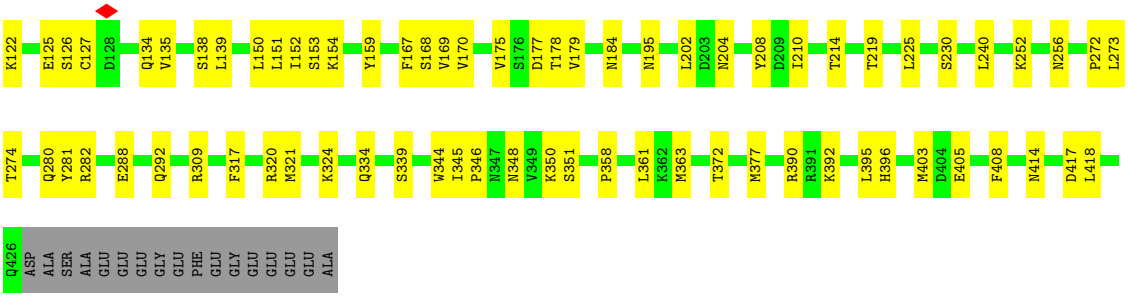
Chain N6:



• Molecule 1: Tubulin beta

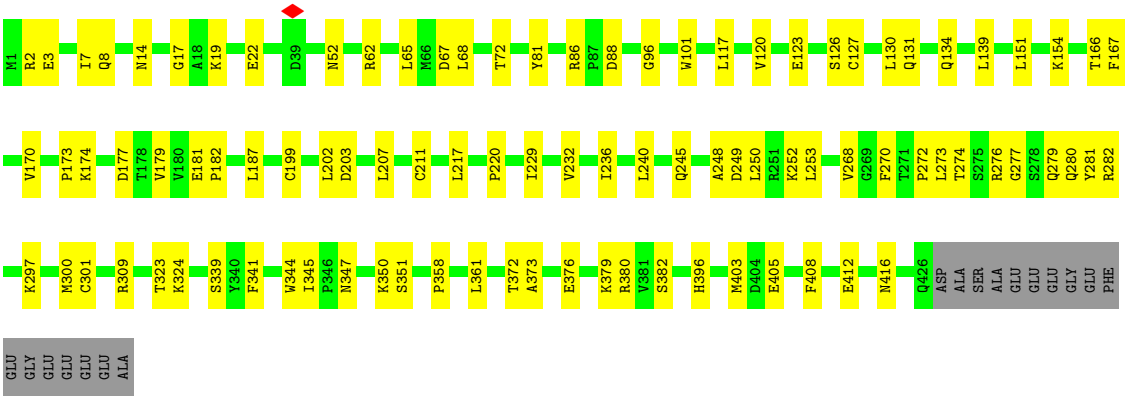
Chain N8:





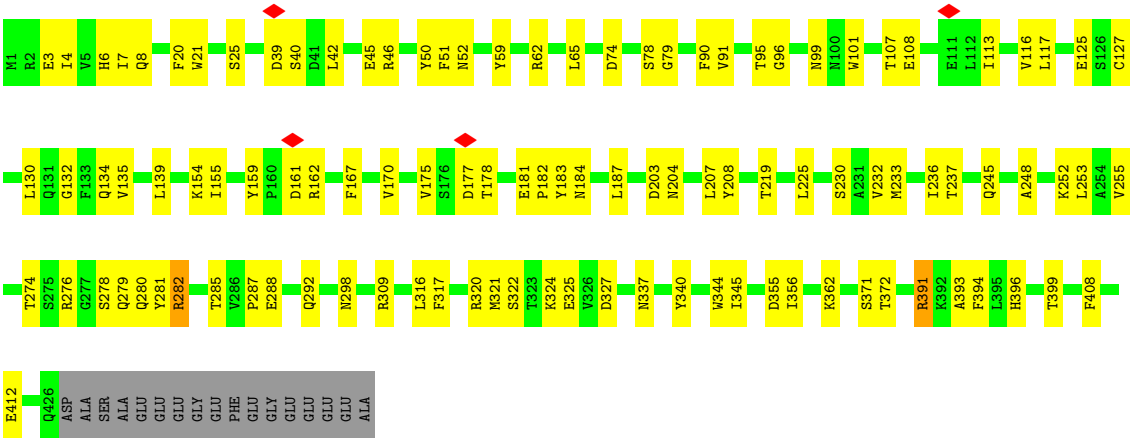
• Molecule 1: Tubulin beta

Chain O0:



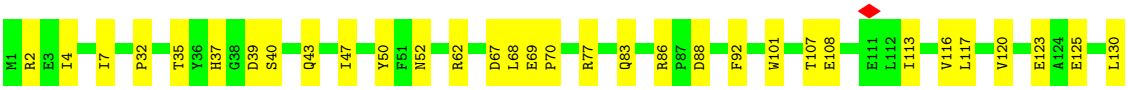
• Molecule 1: Tubulin beta

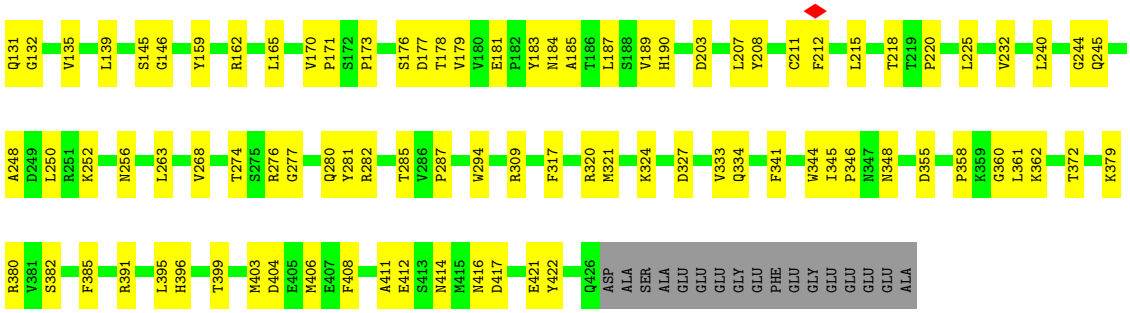
Chain O2:



• Molecule 1: Tubulin beta

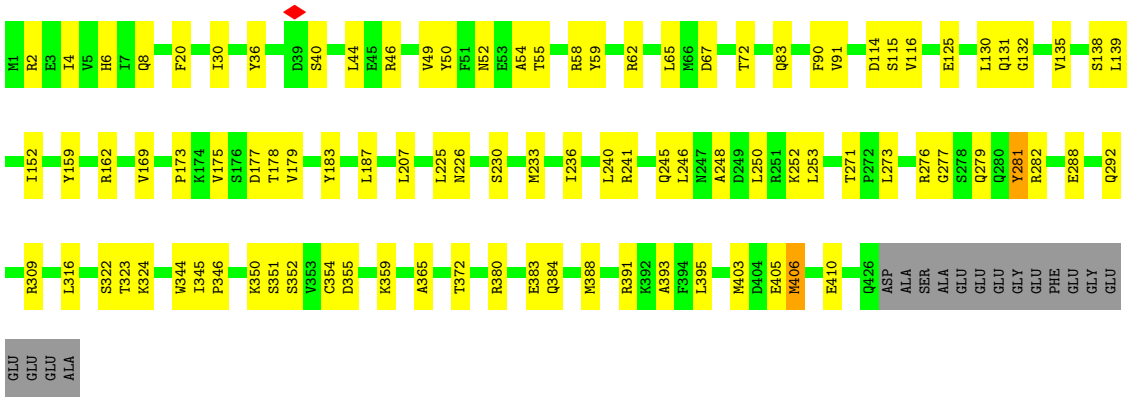
Chain O4:





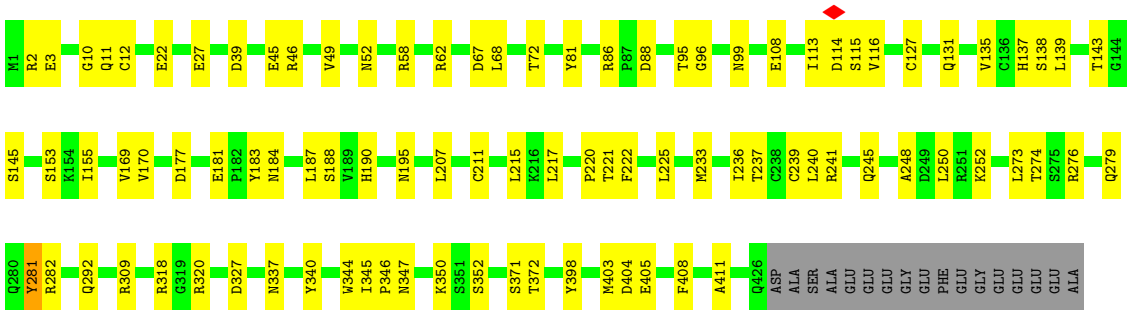
- Molecule 1: Tubulin beta

Chain O6:



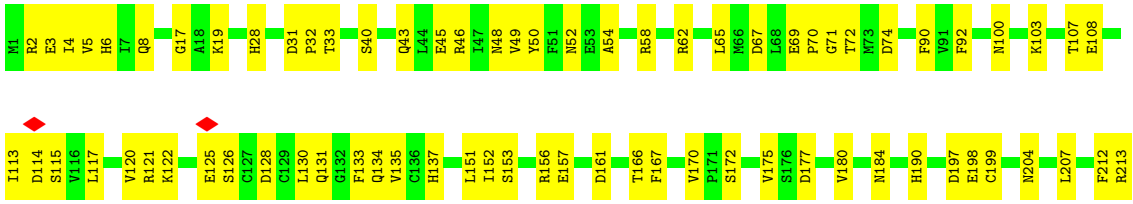
- Molecule 1: Tubulin beta

Chain O8:



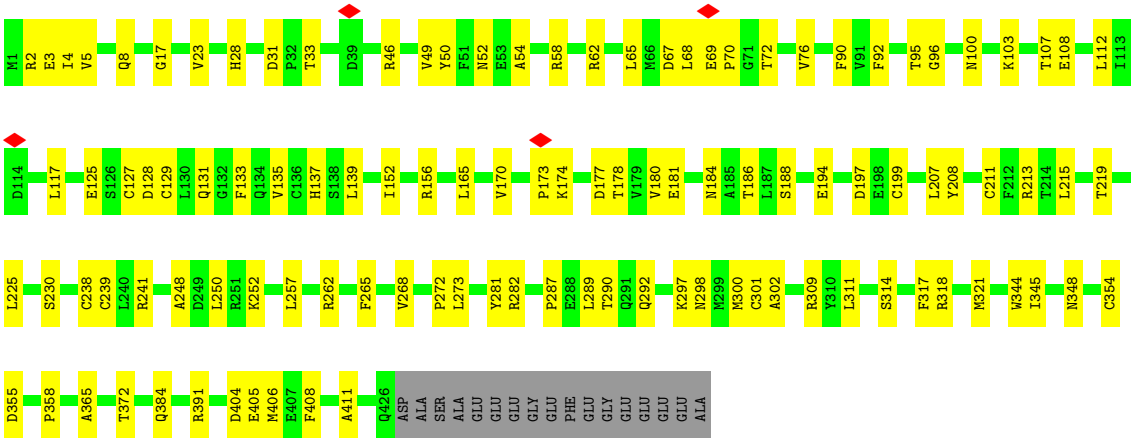
- Molecule 1: Tubulin beta

Chain P4:



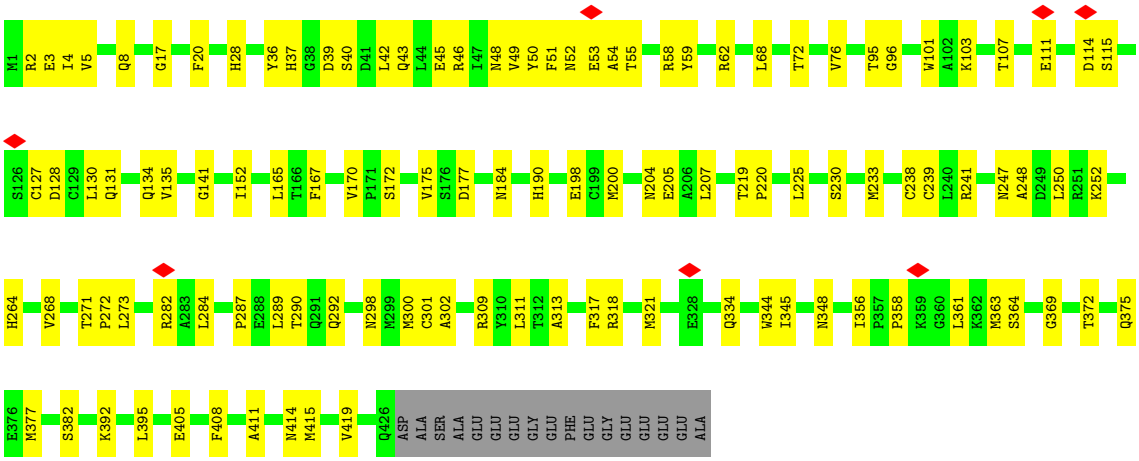
• Molecule 1: Tubulin beta

Chain P6:



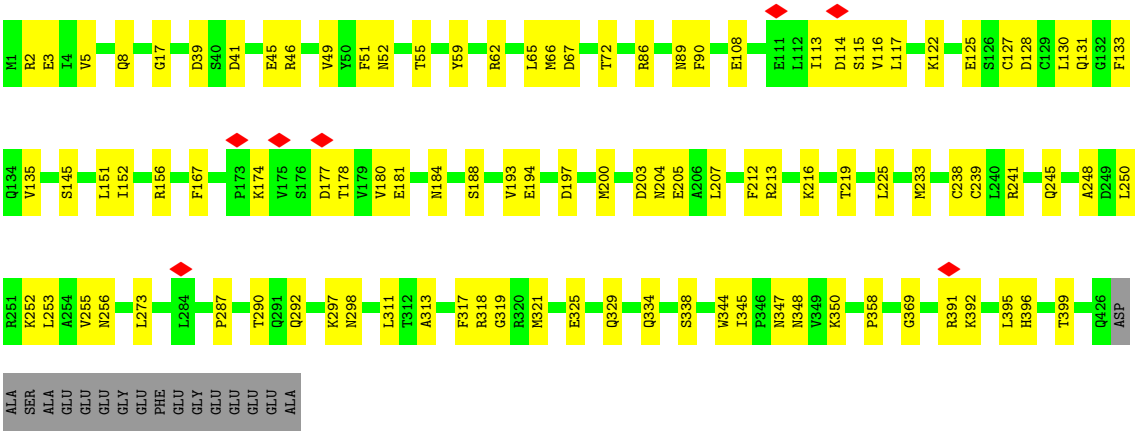
• Molecule 1: Tubulin beta

Chain P8:



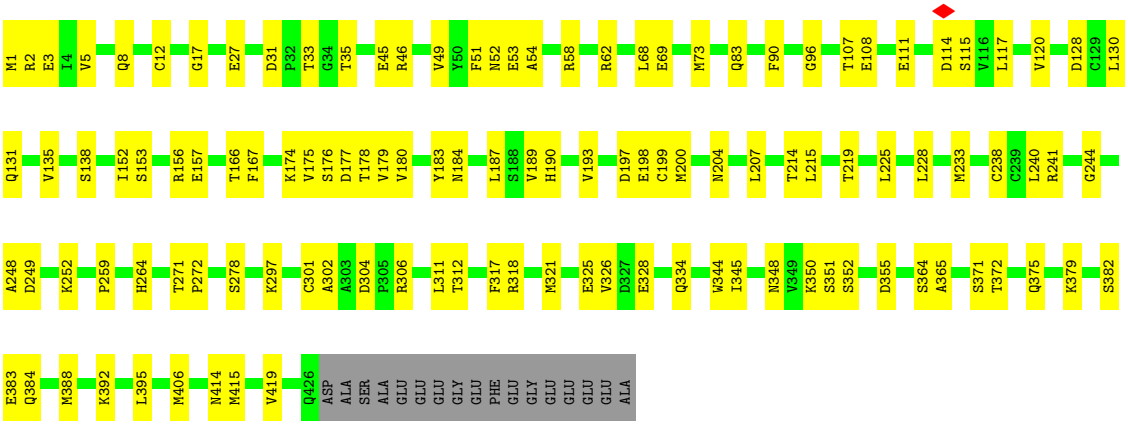
• Molecule 1: Tubulin beta

Chain Q0:



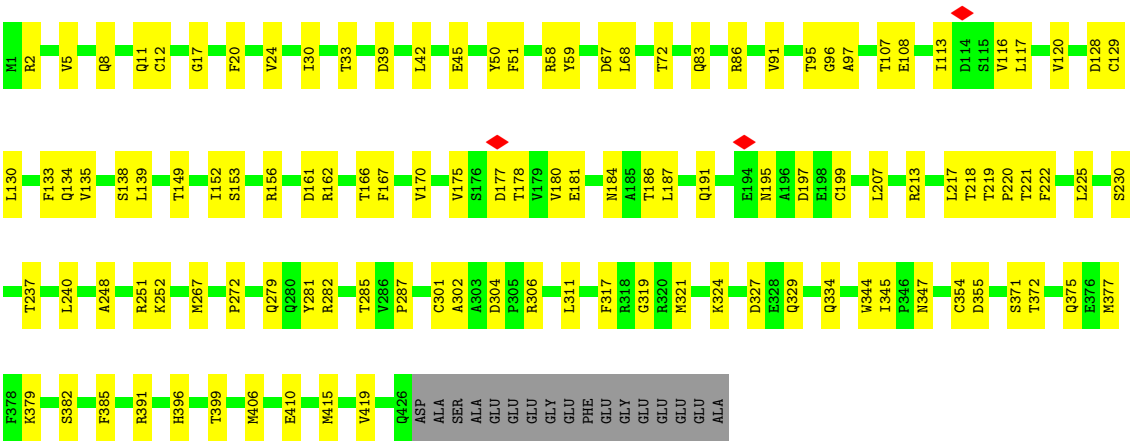
- Molecule 1: Tubulin beta

Chain Q2:



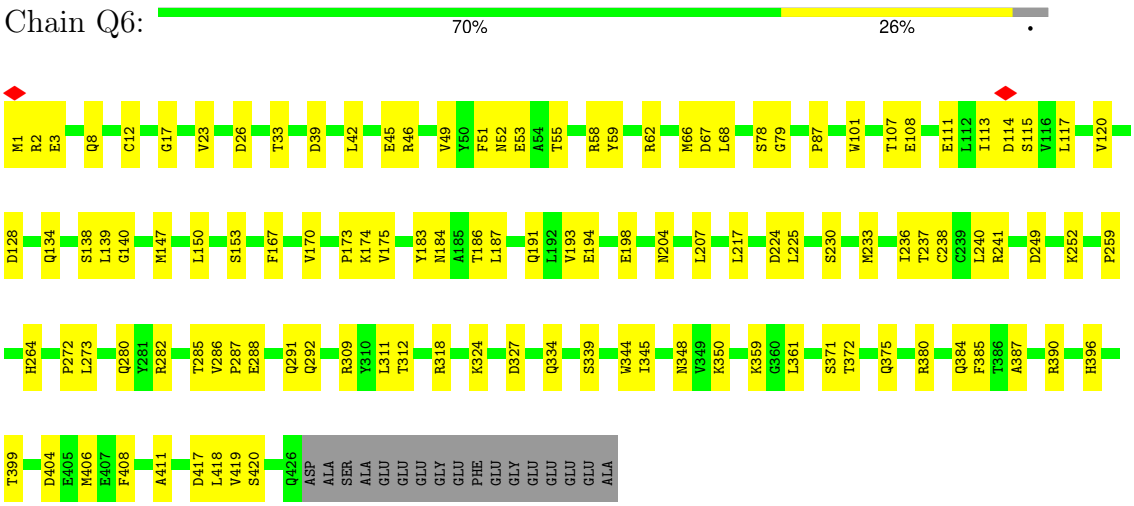
- Molecule 1: Tubulin beta

Chain Q4:



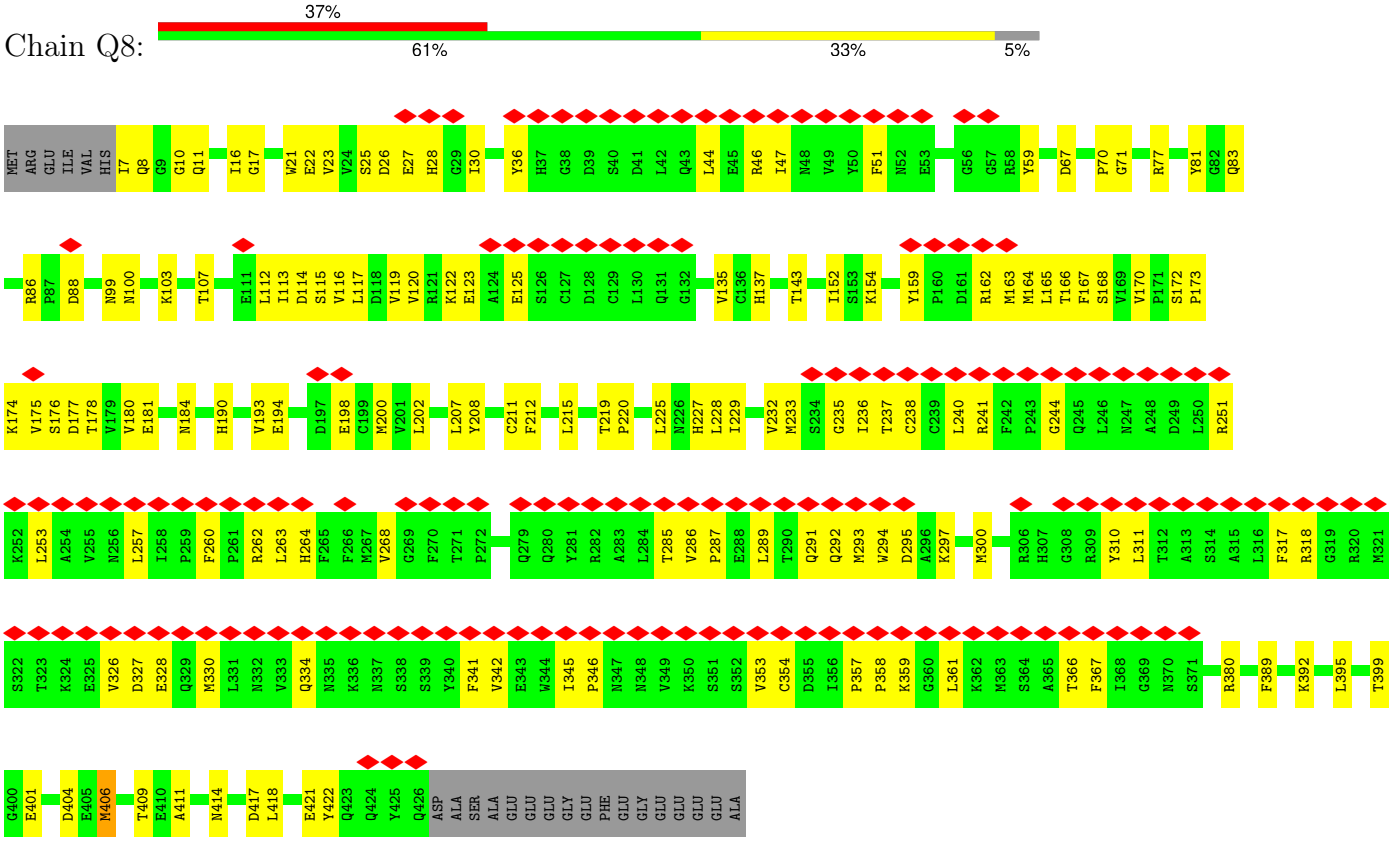
- Molecule 1: Tubulin beta

Chain Q6:



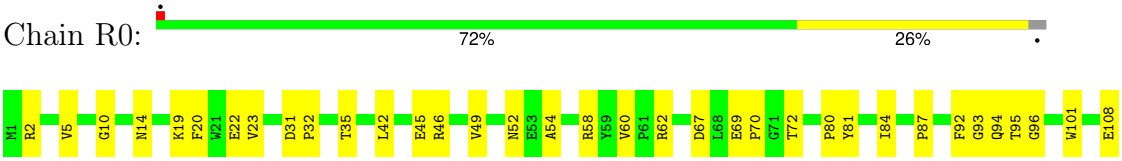
- Molecule 1: Tubulin beta

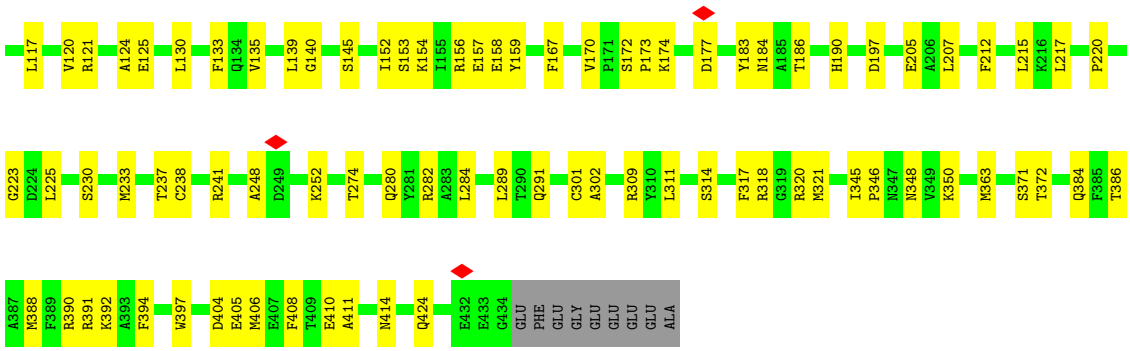
Chain Q8:



- Molecule 1: Tubulin beta

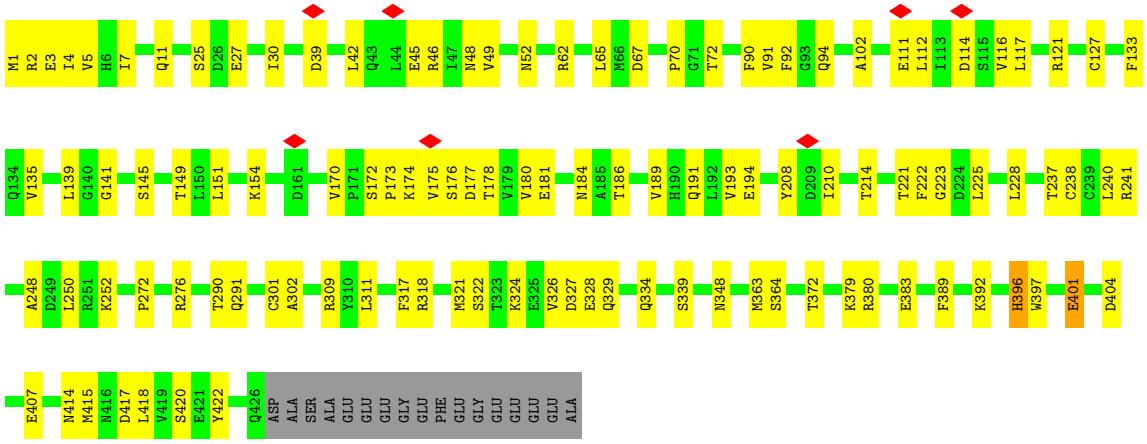
Chain R0:





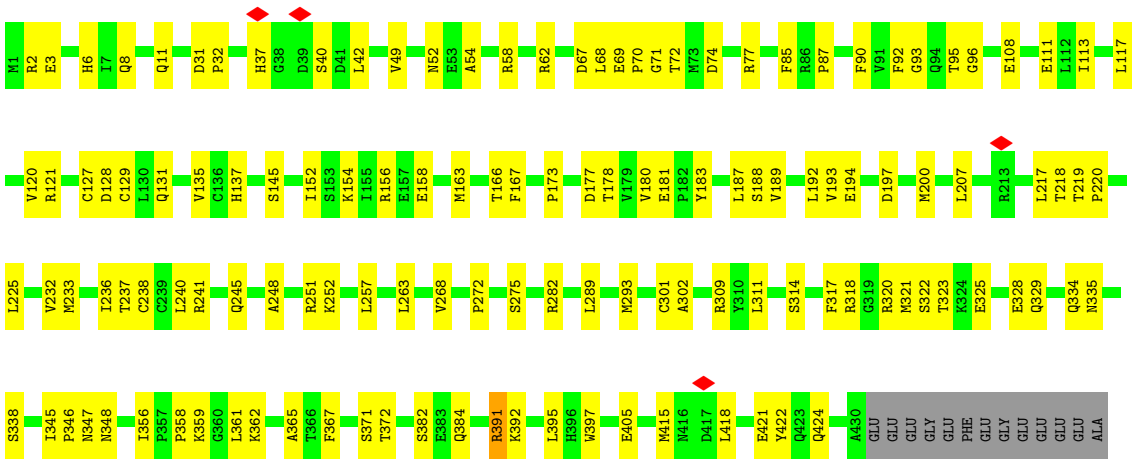
- Molecule 1: Tubulin beta

Chain R2:



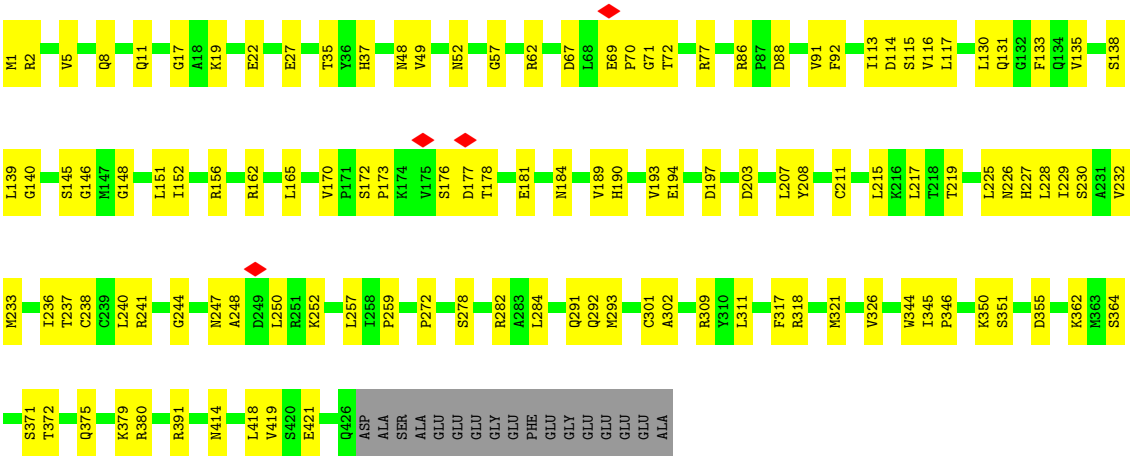
- Molecule 1: Tubulin beta

Chain R4:



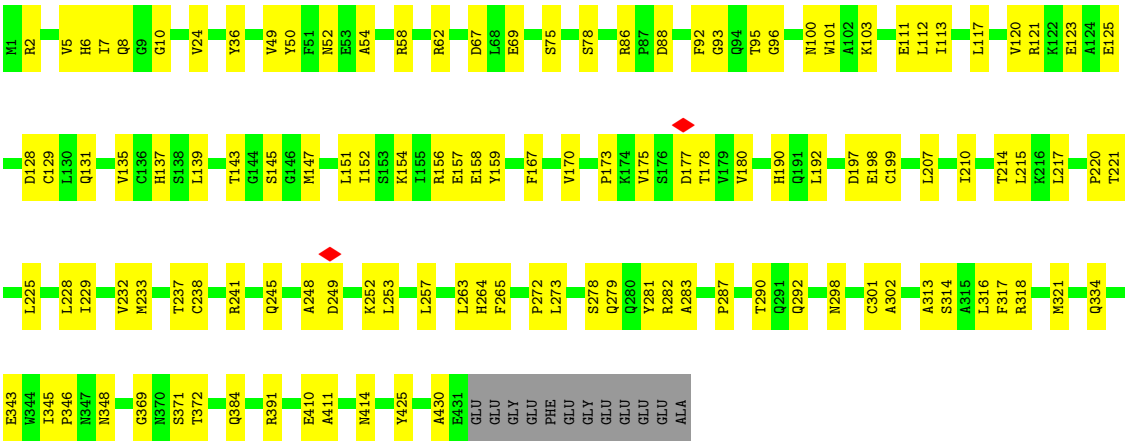
- Molecule 1: Tubulin beta

Chain R6:



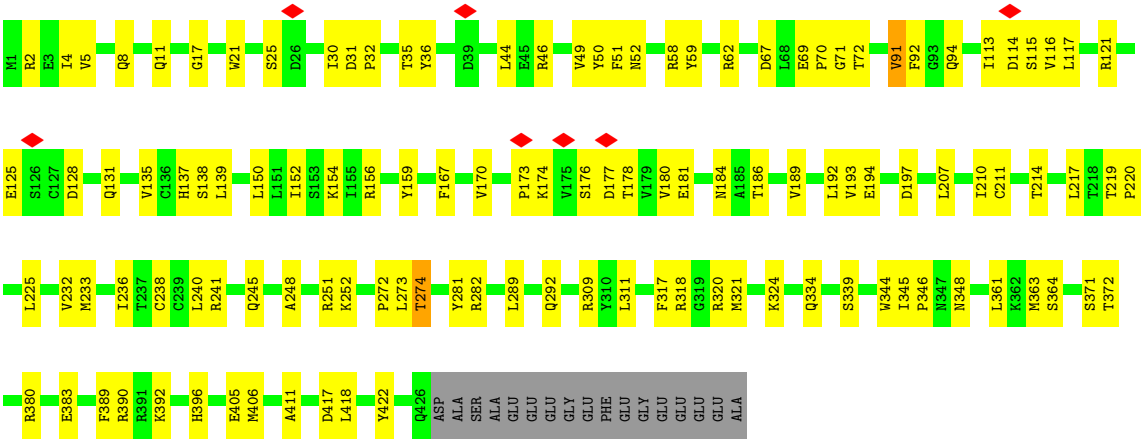
- Molecule 1: Tubulin beta

Chain R8:



- Molecule 1: Tubulin beta

Chain S0:



- Molecule 1: Tubulin beta

Chain S2: 70% 27% •

M1 R2 Q8 Q11 Q15 I16 G17 A18 K19 H28 D31 P32 T33 H37 E45 R46 V49 Y50 F51 N52 E53 A54 R58 Y59 R62 E69 P80 Q83 N89 Q94 T95 G96 N100 K103 E108 I113 V116 L117 D118 V119

V120 R121 K122 E123 A124 E125 Q131 Q134 V135 L139 I152 S153 R156 E157 E158 Y159 M164 F167 V170 P173 K174 V175 E181 P182 Y183 V189 H190 Q191 L192 V193 E194 D197 L207 T219 F222 L225 V232 M233 I236 T237 C238 C239

L240 R241 A248 K252 L253 L263 V268 L273 T274 Q280 Y281 R282 A283 L284 T285 V286 Q292 M300 R309 Y310 L311 S314 A315 L316 F317 R318 G319 R320 M321 E328 Q329 N332 I345 N348 V349 K350 K359 K362 M363 T372 M377 F378

K379 R380 E383 Q384 F385 T386 A387 R390 L395 E405 F408 T409 E410 N414 Q424 Y425 E431 GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

• Molecule 1: Tubulin beta

Chain S4: 14% 60% 36% •

M1 R2 E3 I4 V5 H6 I7 Q11 W21 D26 E27 S40 D41 L42 E45 R46 V49 Y50 F51 N52 P61 R62 D67 G71 T72 M73 D74 R77 R86 P87 D88 V91 N100 K103 T107 L112 I113 V116 V120 E125

D128 C129 L130 Q131 G132 F133 Q134 V135 L139 M147 L150 L151 I152 M163 M164 F167 V170 P171 S172 P173 K174 V175 S176 D177 T178 V179 V180 E181 P182 Y183 N184 A185 T186 L187 S188 V189 L192 V193 E194 N195 A196 D197 E198 V201 L202 D203 N204 E205 I210 C211 F212

R213 T214 L215 K216 T219 P220 T221 F222 G223 D224 L225 N226 H227 L228 V232 M233 T237 C238 C239 L240 R241 F242 P243 G244 Q245 L246 N247 A248 D249 L250 R251 K252 V255 N256 L257 I258 P259 F260 L263 M267 V268 T271 P272 L273 T274 S275 Q280 Y281 R282 A283 L284 T285

V286 P287 E288 L289 T290 Q291 Q292 M293 K297 C301 A302 A303 R309 Y310 L311 T312 A313 S314 F317 R318 G319 R320 M321 S322 T323 K324 E325 V326 D327 E328 Q329 M330 L331 N332 V333 Q334 N335 K336 N337 S338 S339 V342 E343 W344 I345 P346 M347 N348 V349 K350 S351 S352 V353 C354 D355

I356 K359 K362 M363 S364 A365 I368 S371 T372 A373 I374 Q375 E376 R380 F385 R391 K392 H396 T399 G400 E401 D404 E405 M406 E407 F408 T409 N414 Y422 D427 ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

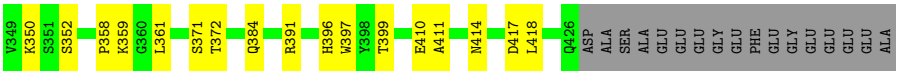
• Molecule 1: Tubulin beta

Chain S6: 68% 28% •

M1 R2 E3 I4 V5 Q8 G17 F20 D39 S40 E45 V49 Y50 F51 N52 R58 Y59 V60 P61 R62 L65 M66 D67 L68 E69 T72 Q83 R86 F90 V91 F92 G96 N100 W101 A102 K103 T107 E108 I113 D114 S115 V116 L117

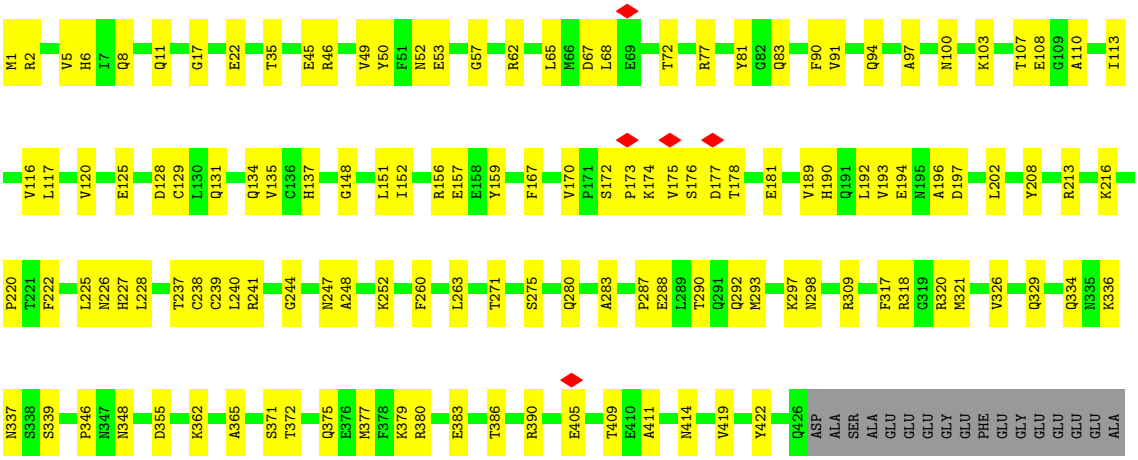
R121 K122 E125 D128 C129 L130 Q131 G132 V135 S138 L139 T149 L150 L151 I152 S153 K154 I155 R156 R162 M163 M164 F167 V170 P173 T178 E181 T186 L187 H190 Q191 L192 D197 E198 L207 Y208 D209 R213 L225 M226 H227 S230

M233 L240 R241 G244 Q245 L246 N247 A248 D249 L250 R251 K252 L257 I258 P259 L263 S275 R276 Q279 Q280 Y281 P287 E288 L289 Q292 D295 A296 K297 N298 R309 S314 R320 E325 V326 D327 E328 Q329 Q334 E343 W344 I345 P346 N347 N348



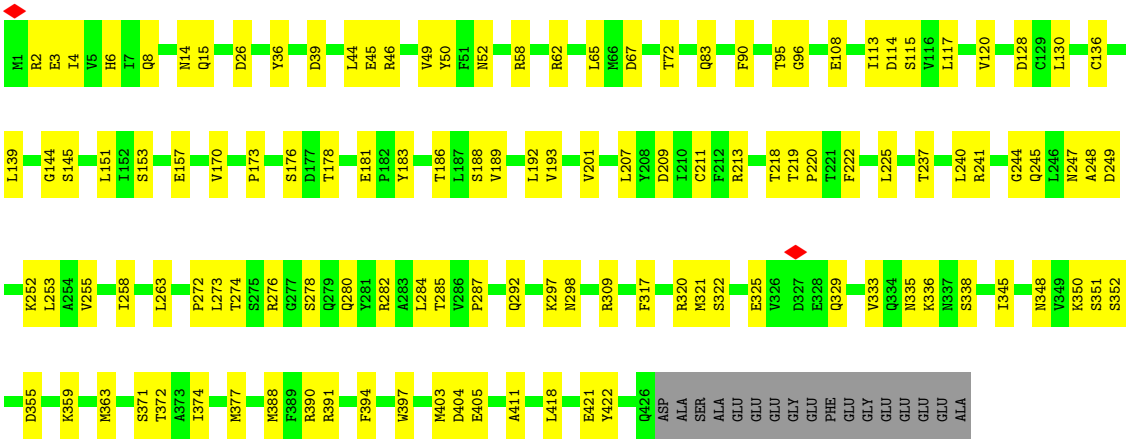
• Molecule 1: Tubulin beta

Chain S8:



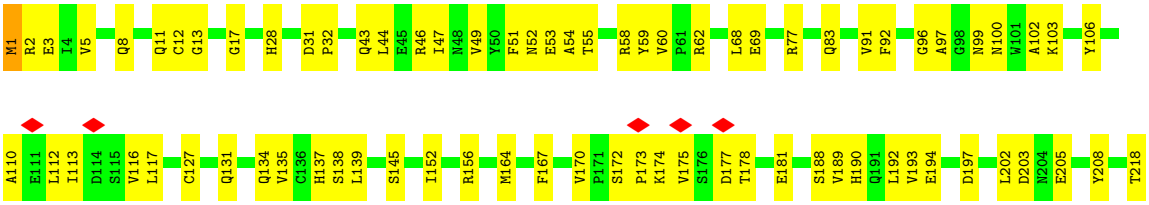
• Molecule 1: Tubulin beta

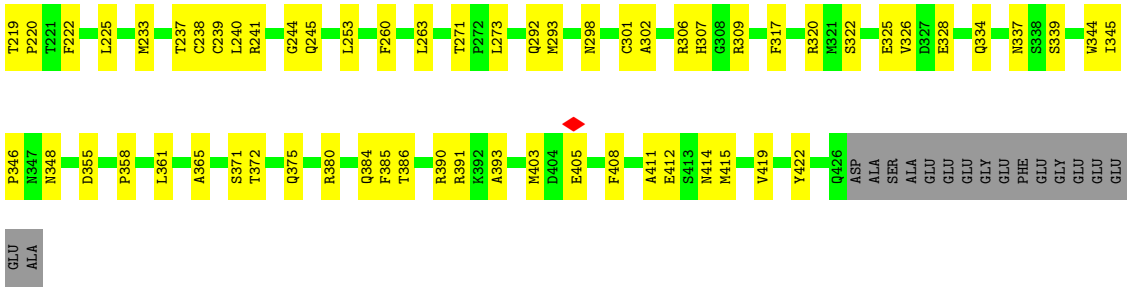
Chain T0:



• Molecule 1: Tubulin beta

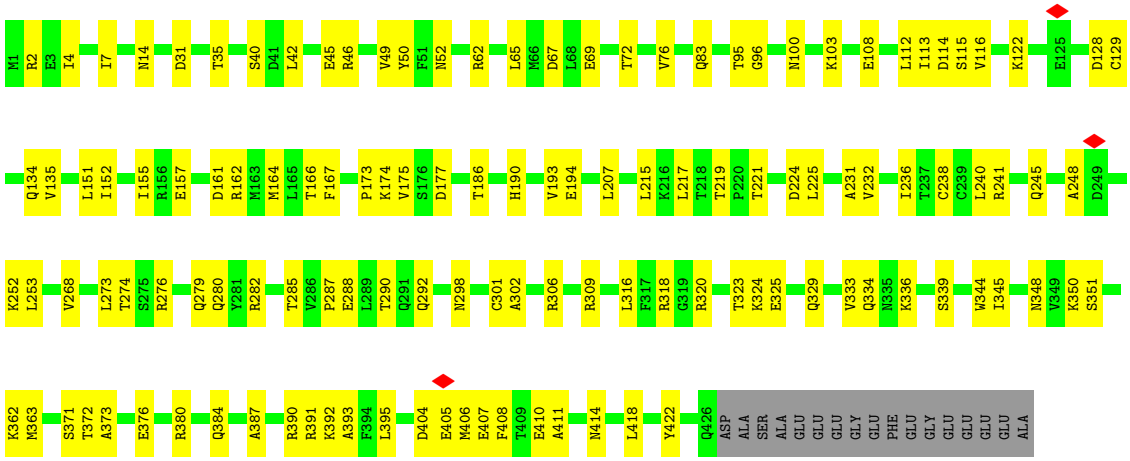
Chain T2:





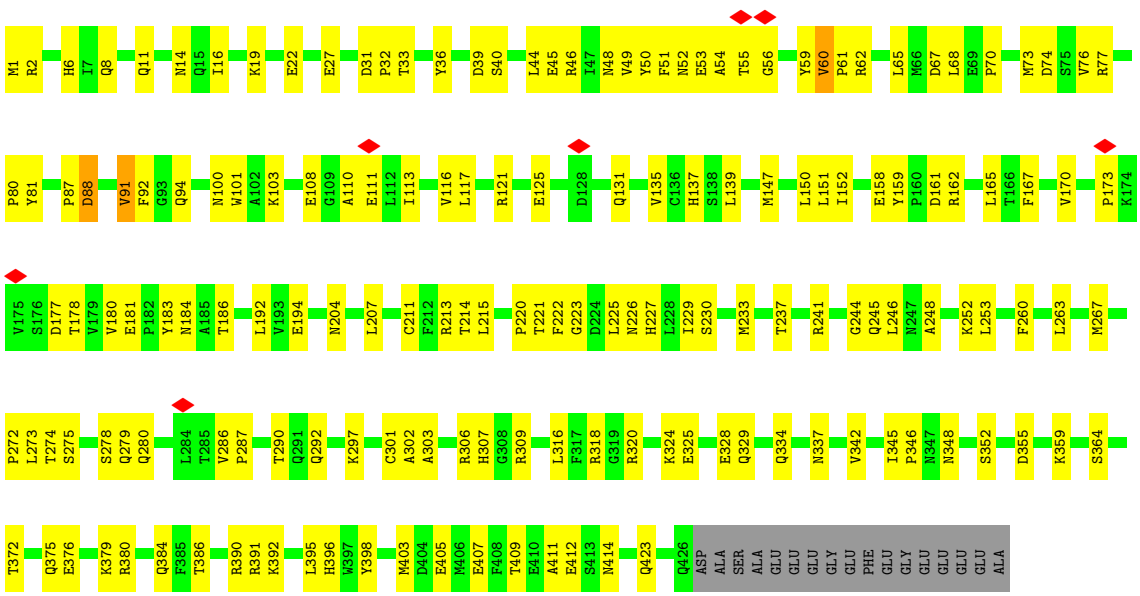
• Molecule 1: Tubulin beta

Chain T4:



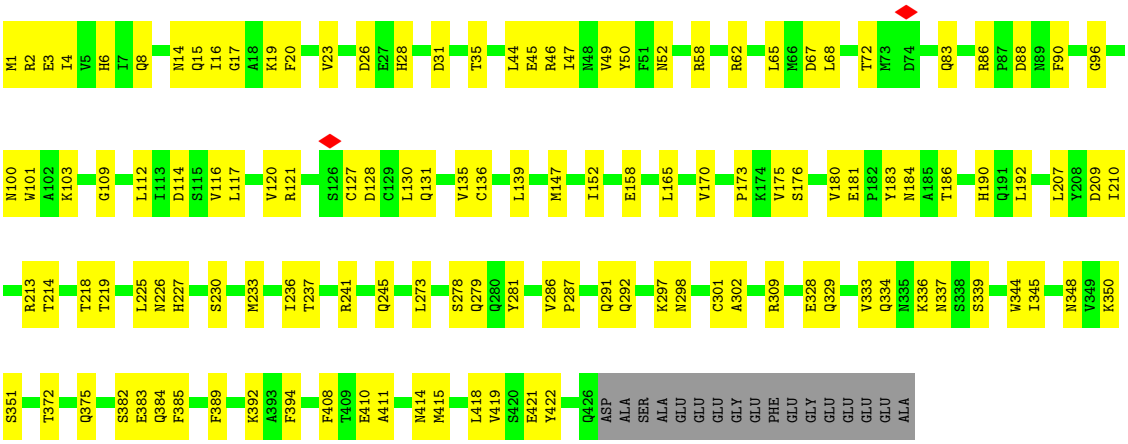
• Molecule 1: Tubulin beta

Chain T6:



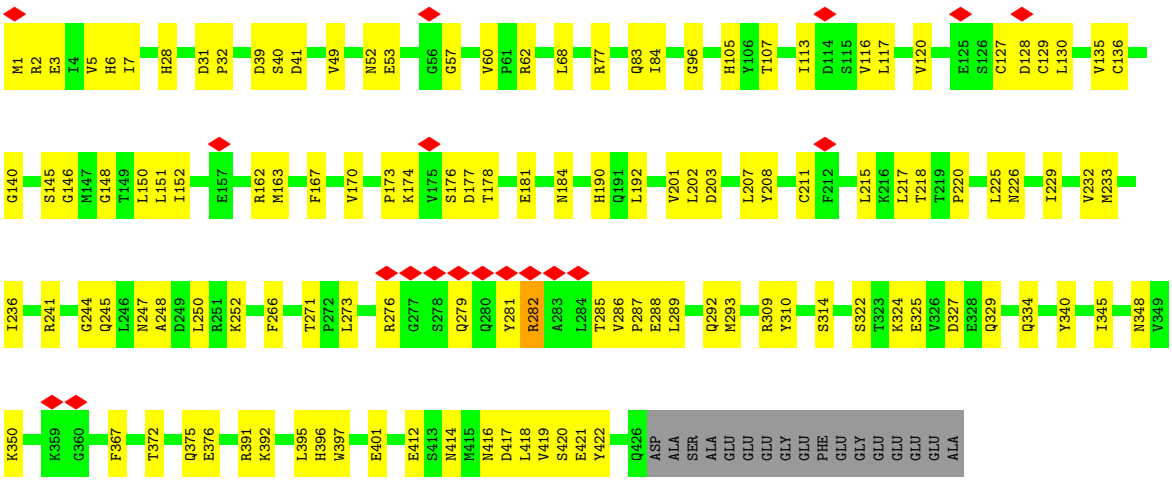
• Molecule 1: Tubulin beta

Chain T8:



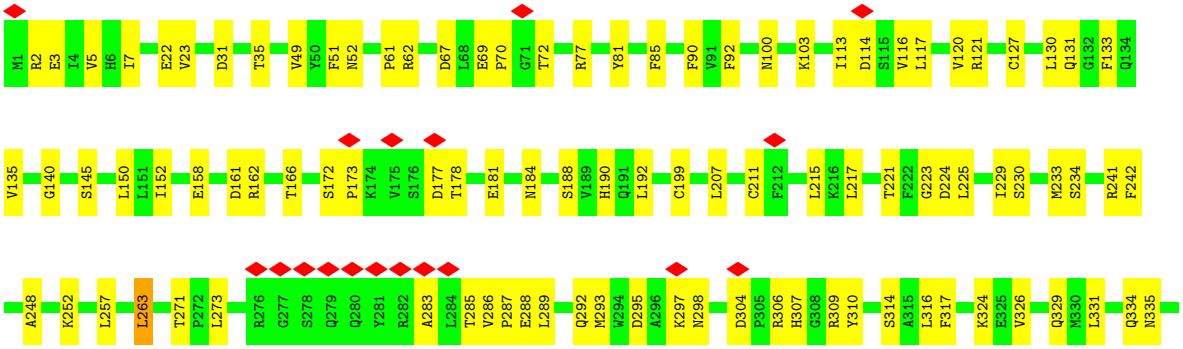
- Molecule 1: Tubulin beta

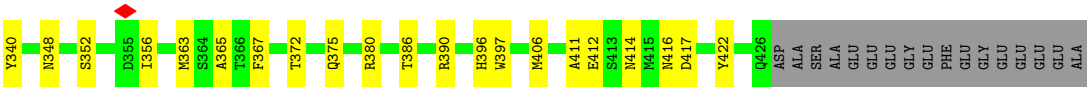
Chain U2:



- Molecule 1: Tubulin beta

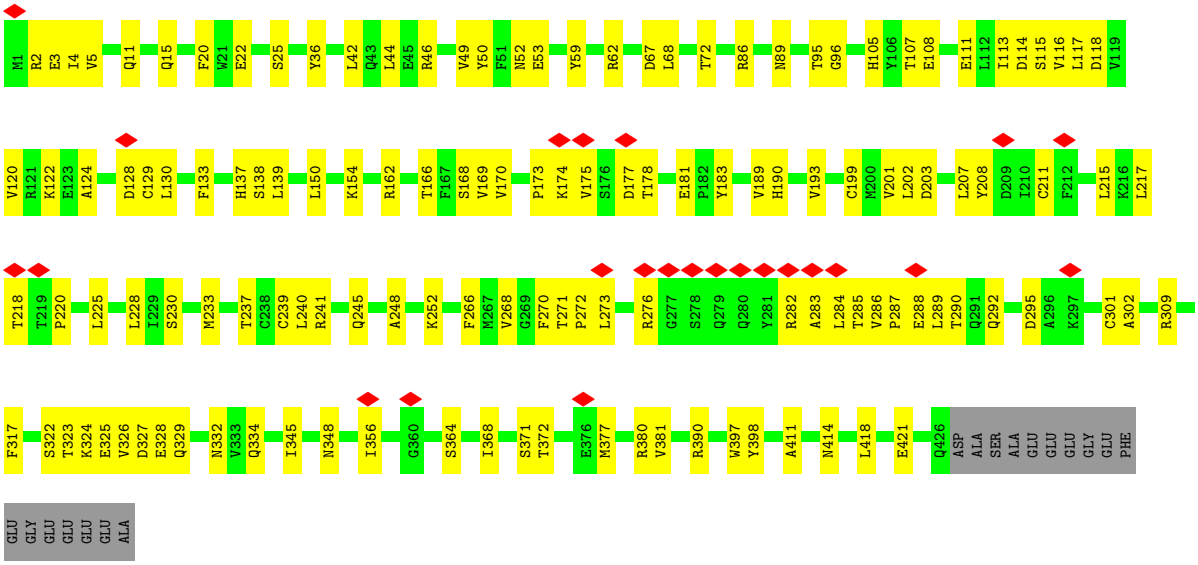
Chain U4:





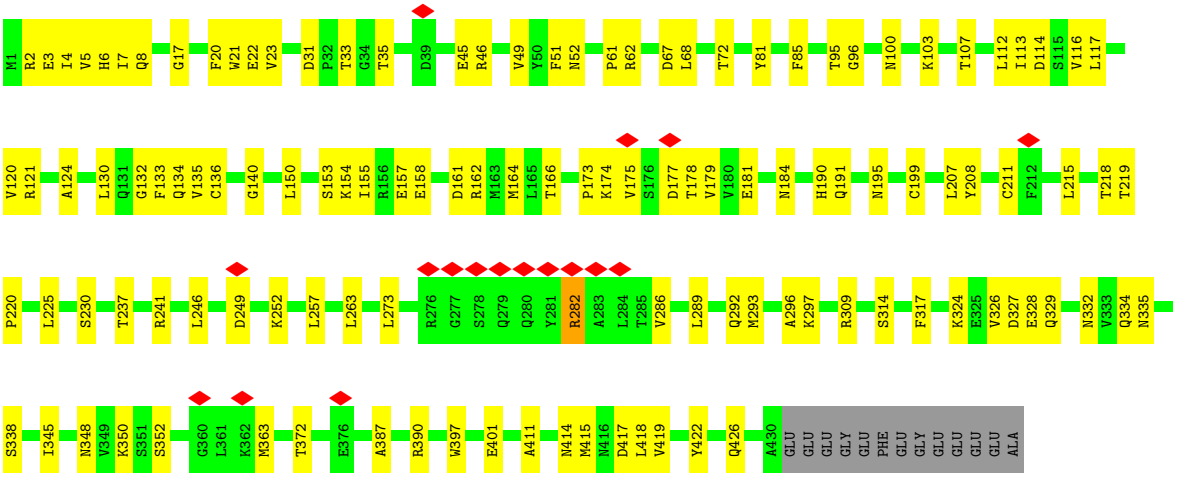
- Molecule 1: Tubulin beta

Chain U6:



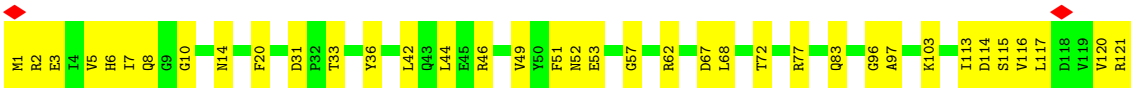
- Molecule 1: Tubulin beta

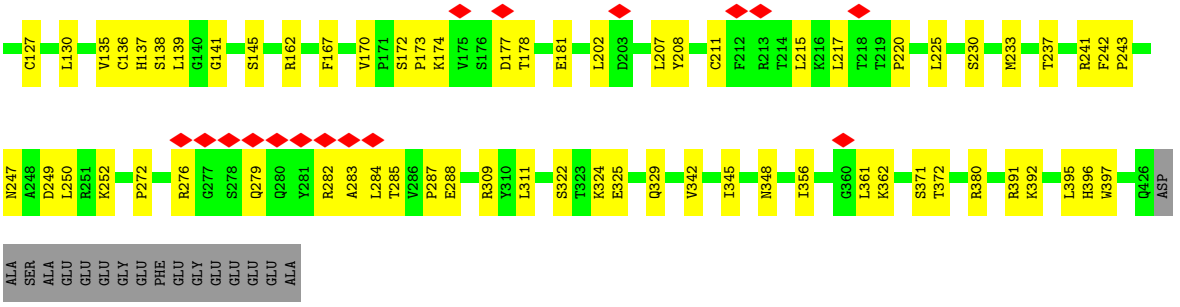
Chain U8:



- Molecule 1: Tubulin beta

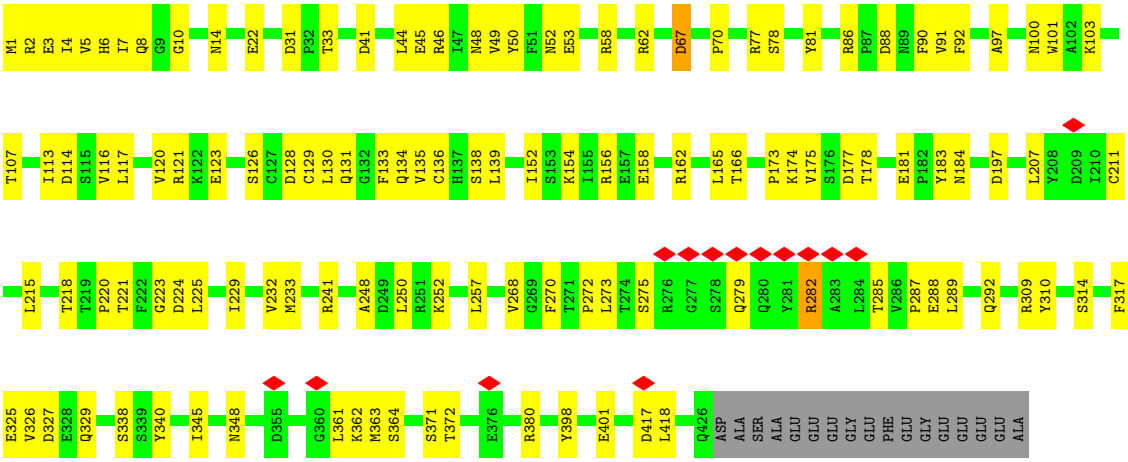
Chain V0:





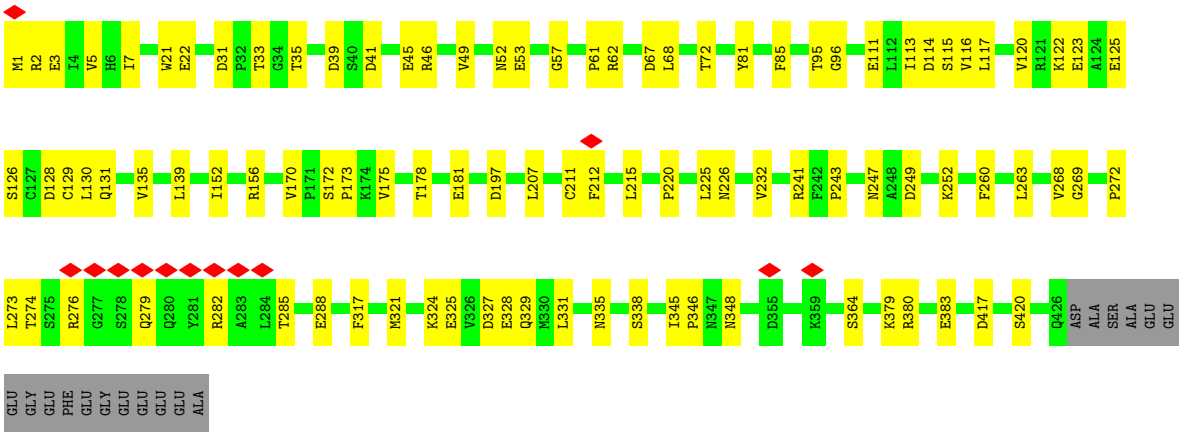
- Molecule 1: Tubulin beta

Chain V2:



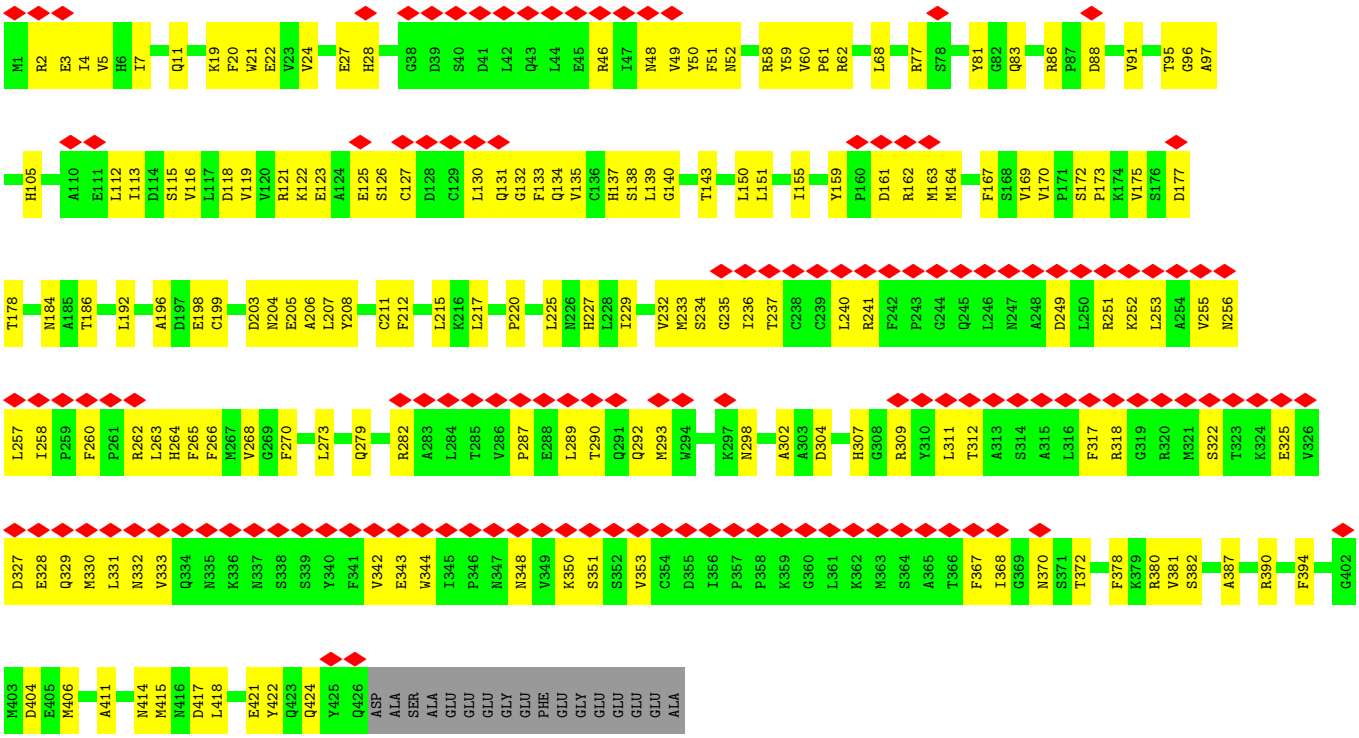
- Molecule 1: Tubulin beta

Chain V4:



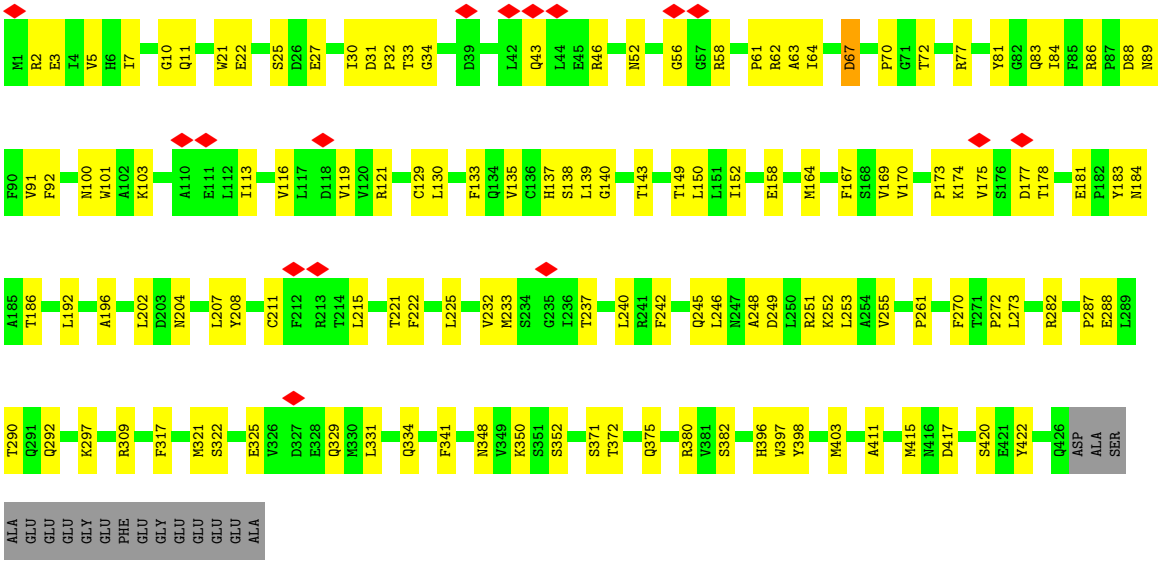
- Molecule 1: Tubulin beta

Chain V6:



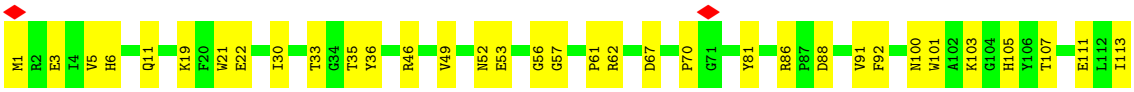
- Molecule 1: Tubulin beta

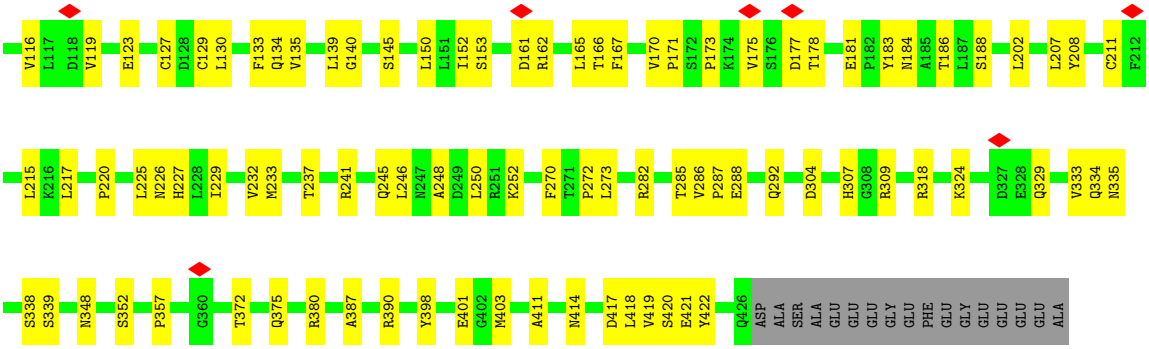
Chain V8:



- Molecule 1: Tubulin beta

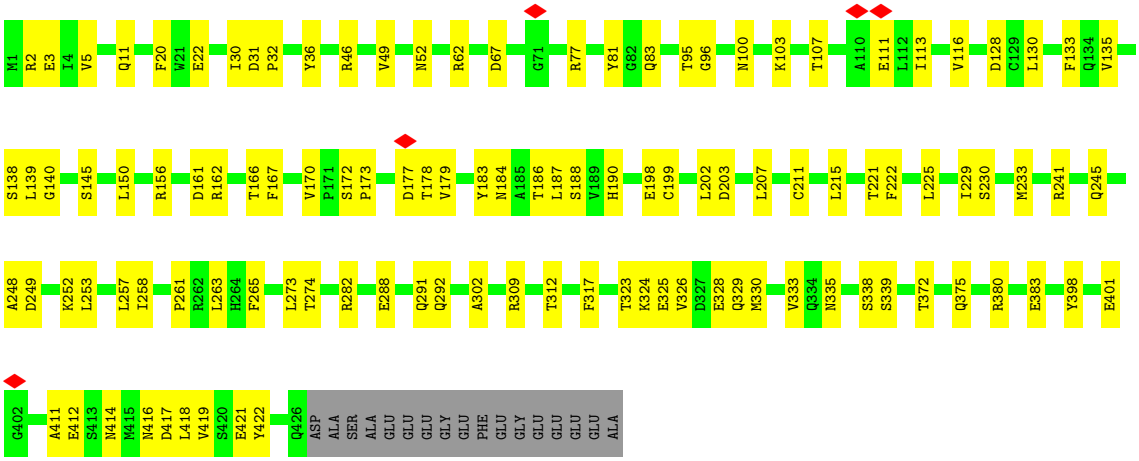
Chain W0:





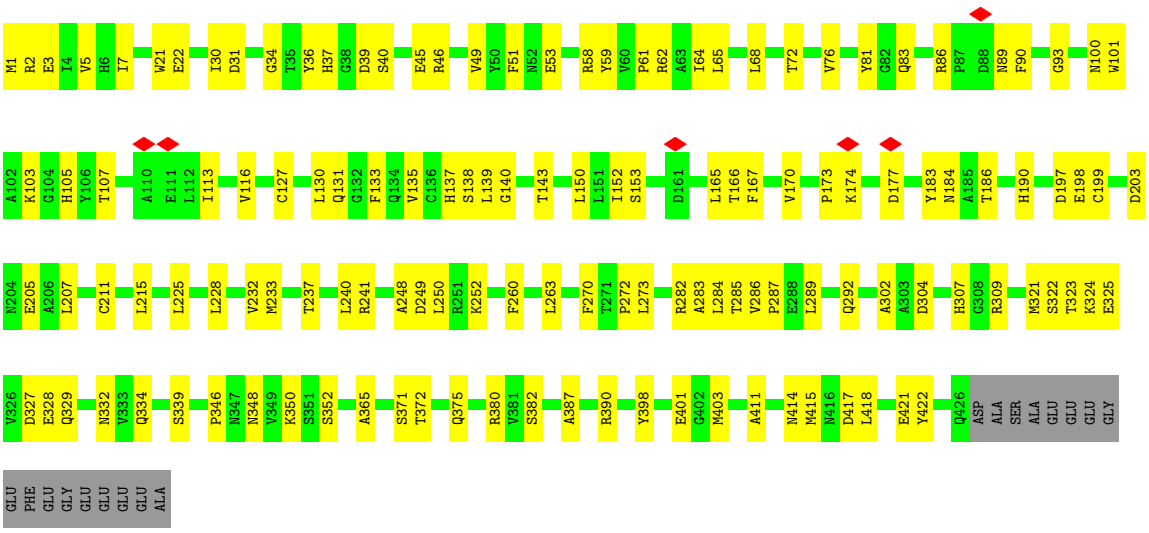
- Molecule 1: Tubulin beta

Chain W2:



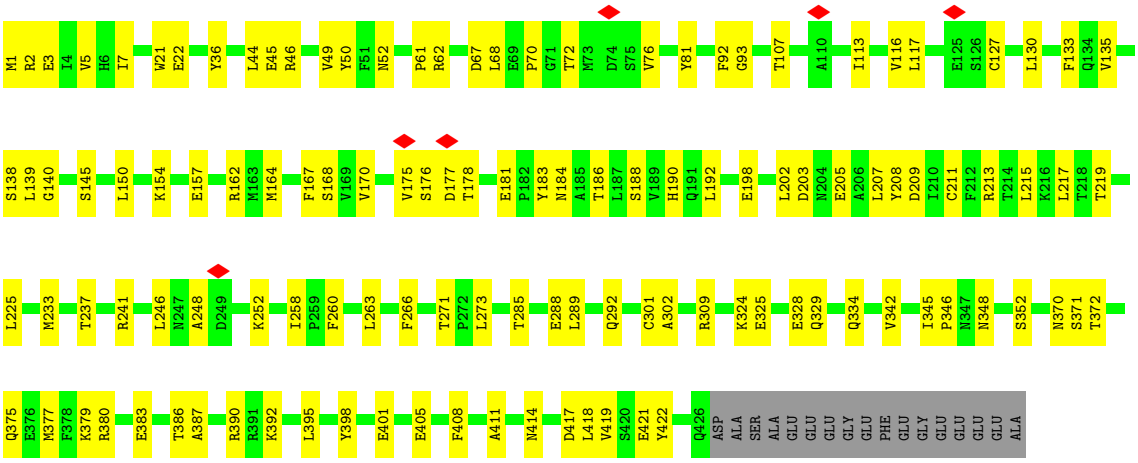
- Molecule 1: Tubulin beta

Chain W4:



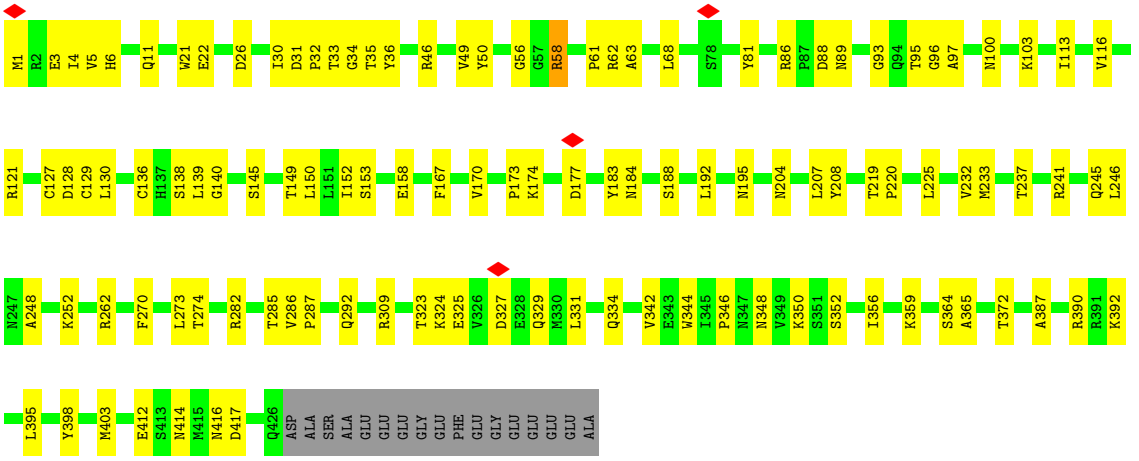
- Molecule 1: Tubulin beta

Chain W6:



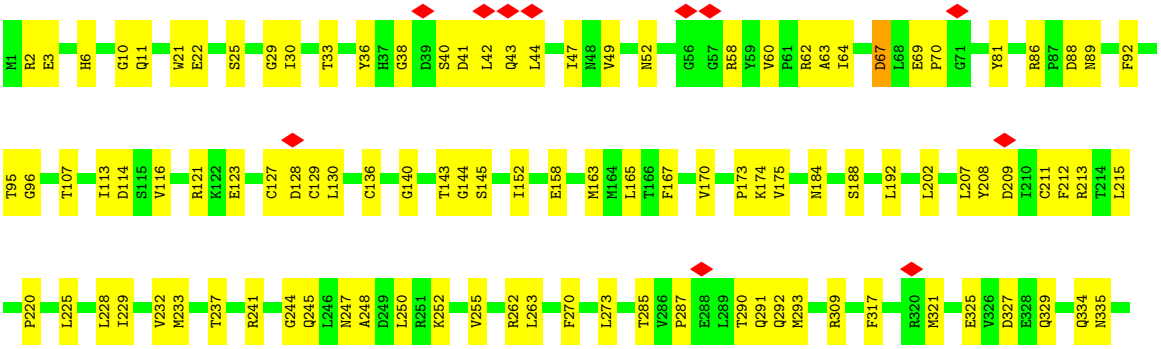
- Molecule 1: Tubulin beta

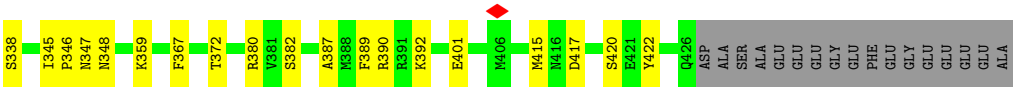
Chain W8:



- Molecule 1: Tubulin beta

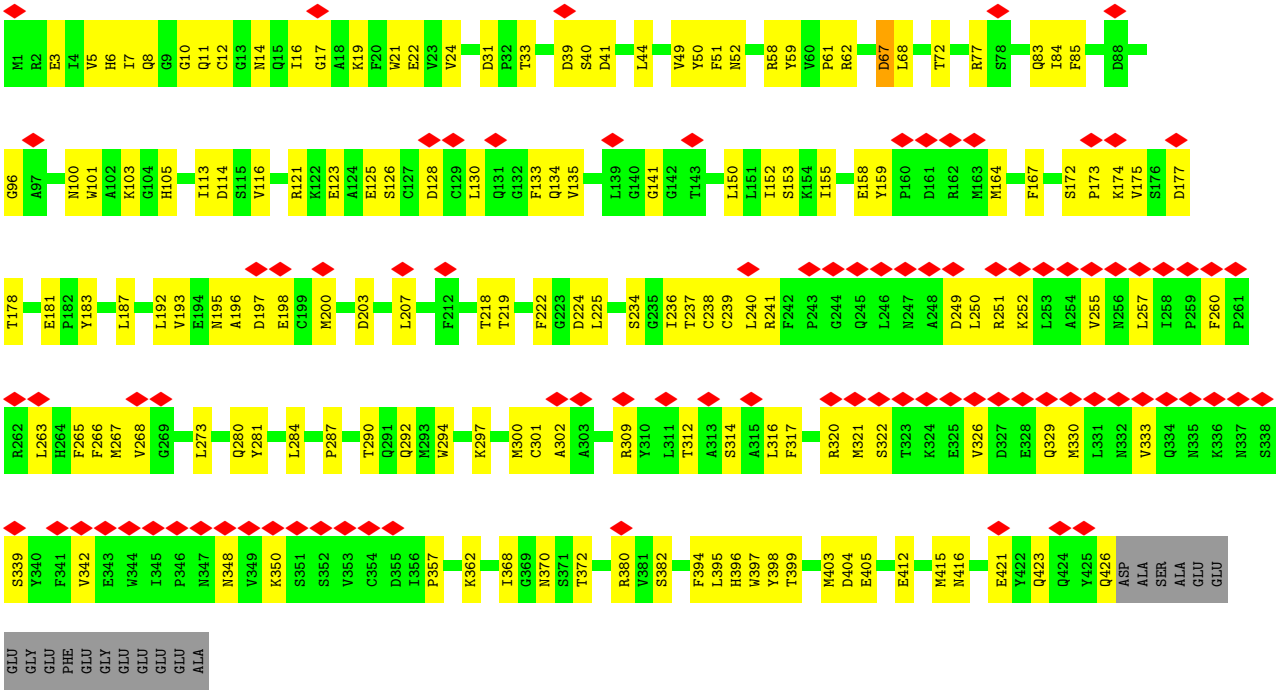
Chain X0:





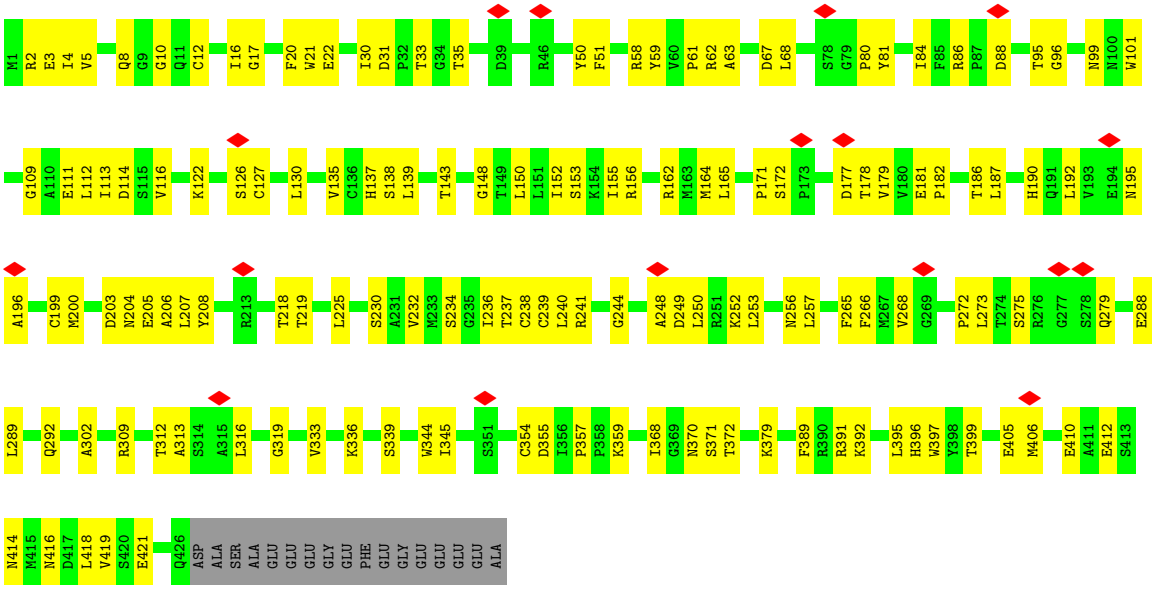
• Molecule 1: Tubulin beta

Chain X2:



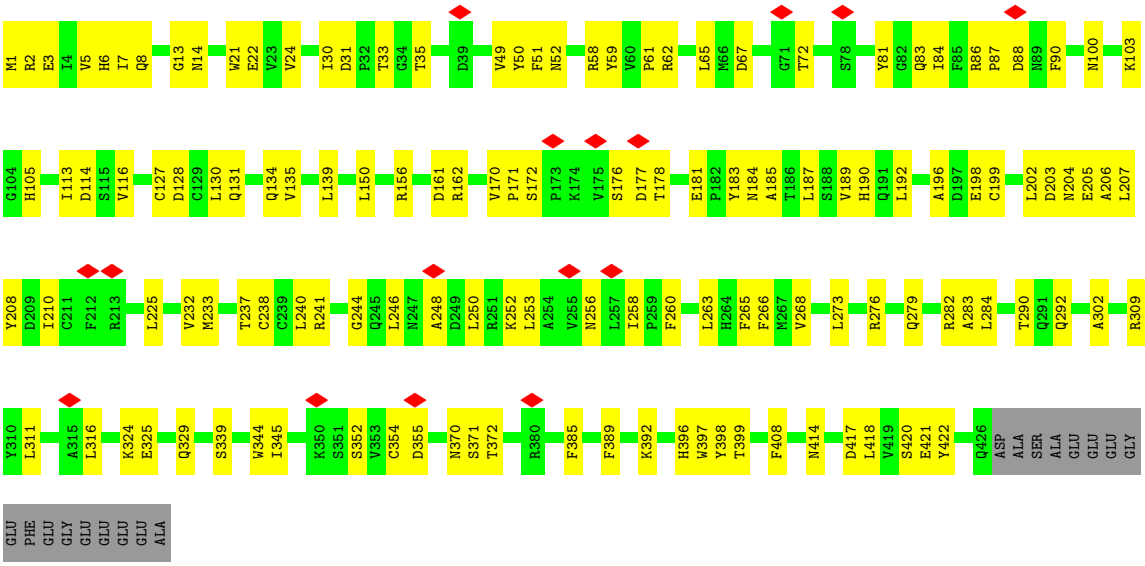
• Molecule 1: Tubulin beta

Chain X4:



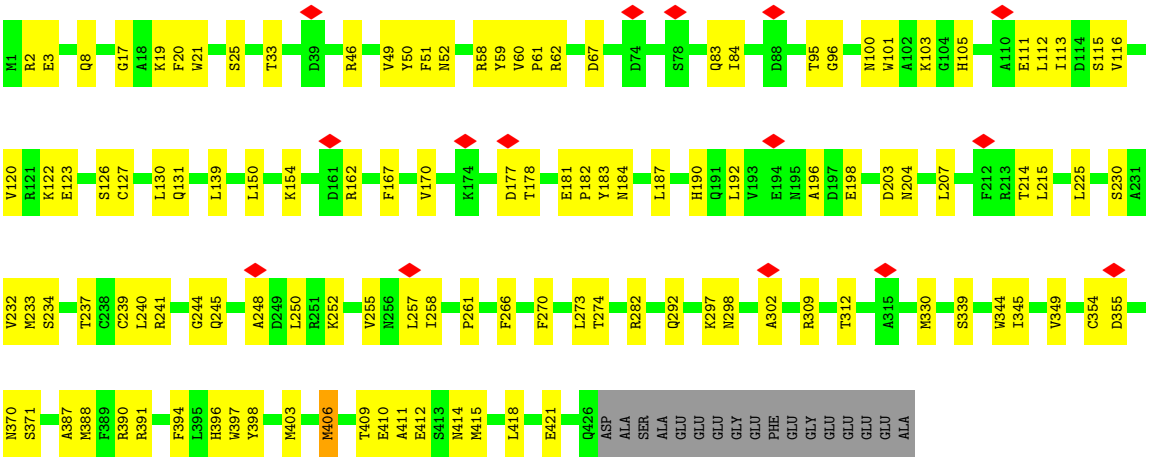
• Molecule 1: Tubulin beta

Chain X6:



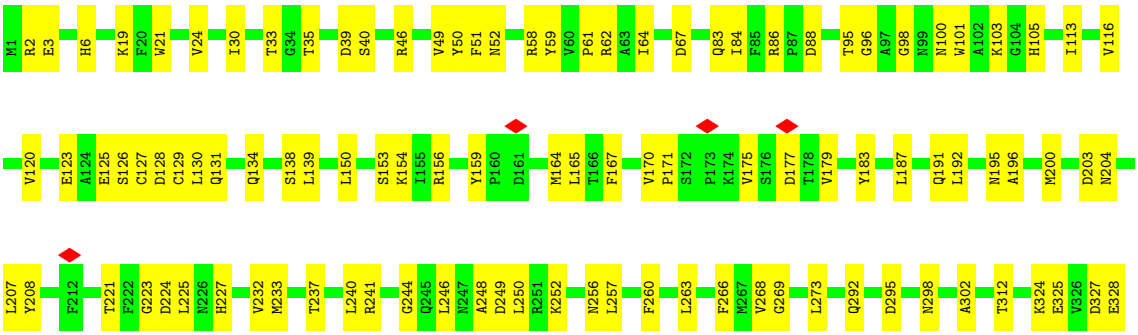
• Molecule 1: Tubulin beta

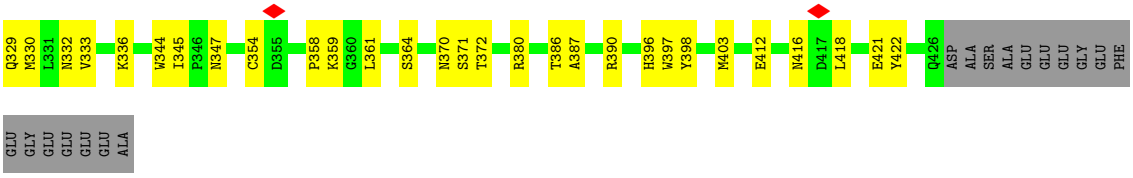
Chain X8:



• Molecule 1: Tubulin beta

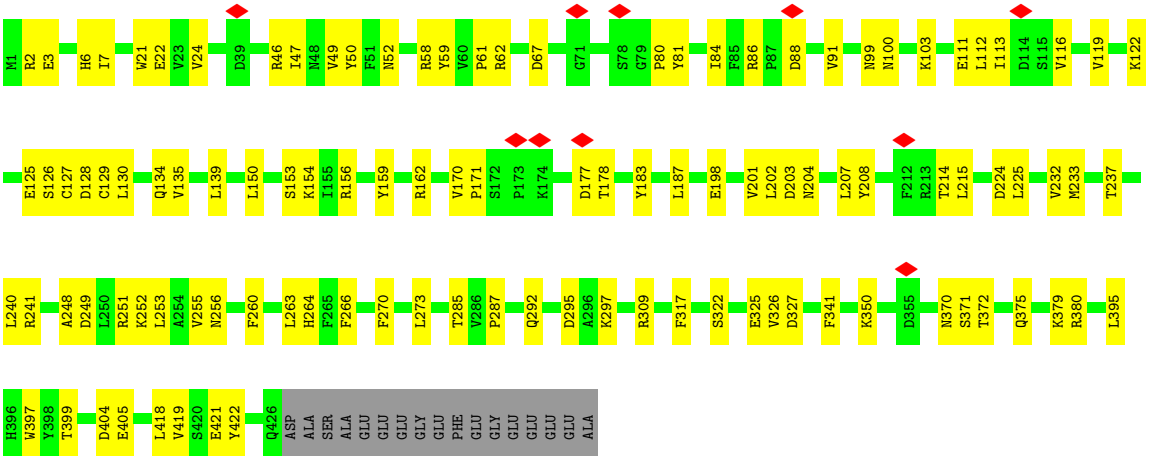
Chain Y0:





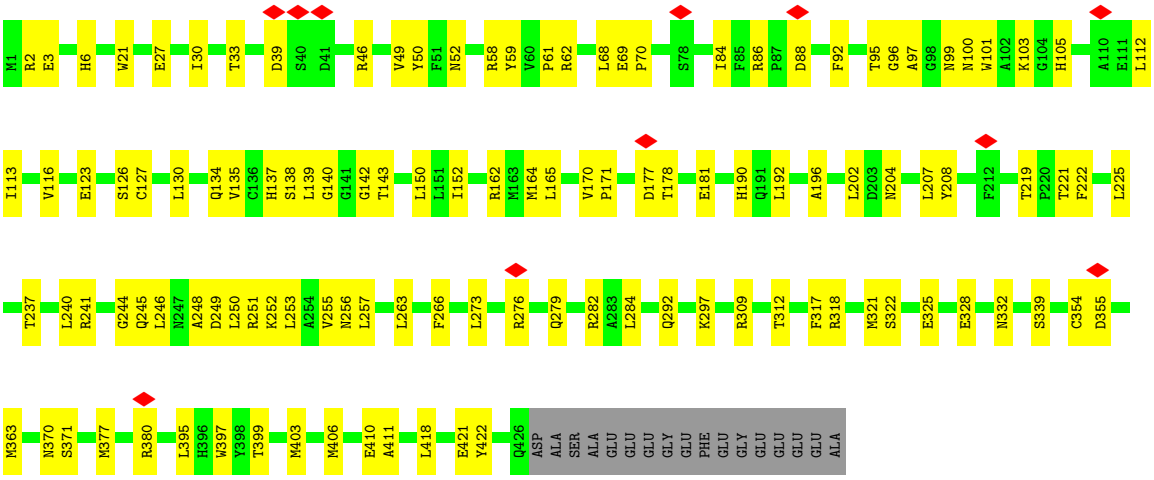
- Molecule 1: Tubulin beta

Chain Y2:



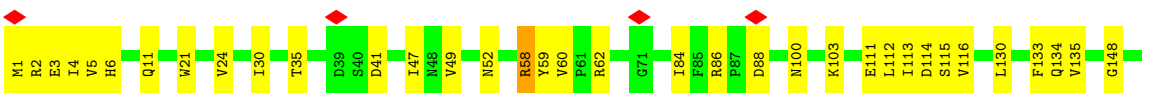
- Molecule 1: Tubulin beta

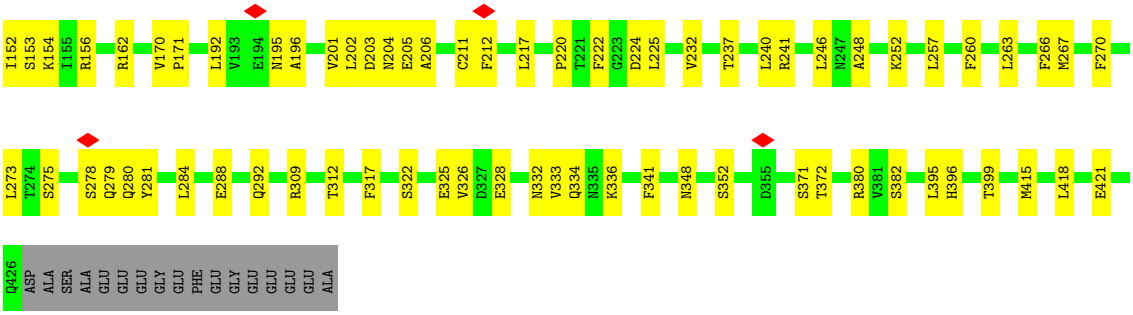
Chain Y4:



- Molecule 1: Tubulin beta

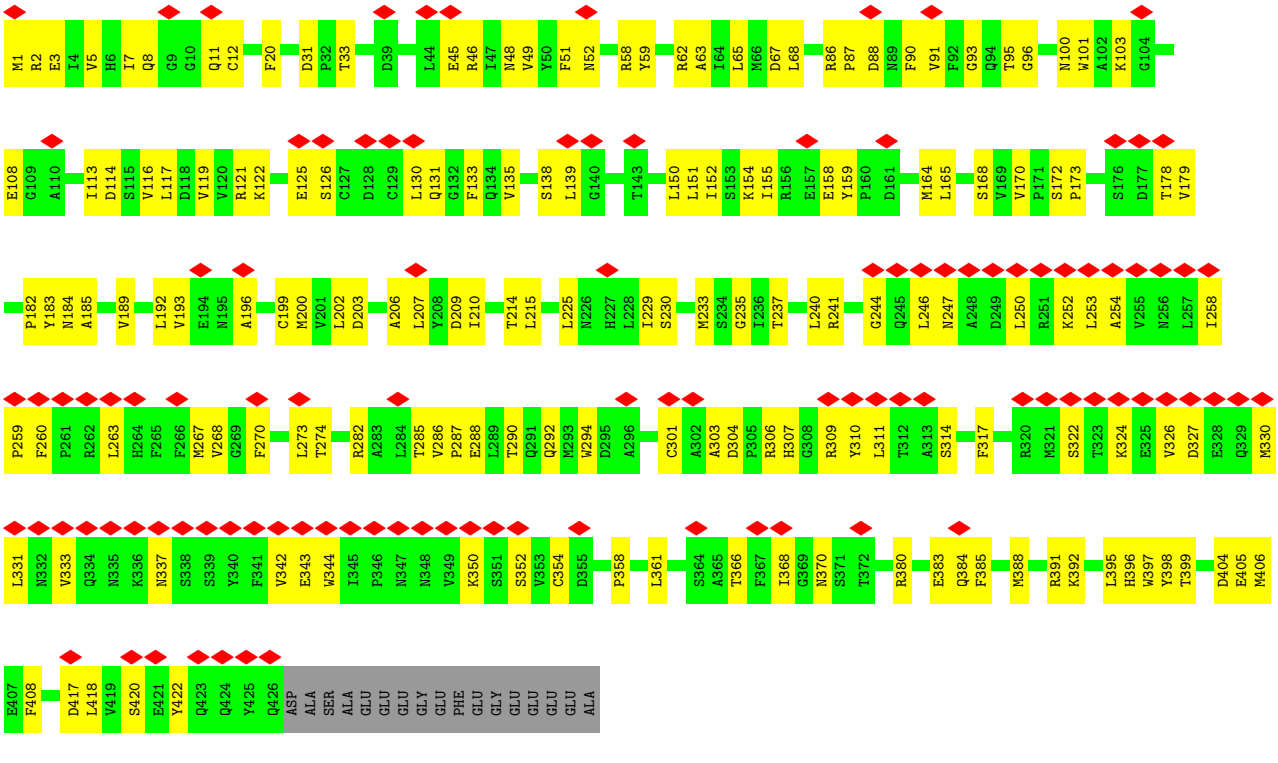
Chain Y6:





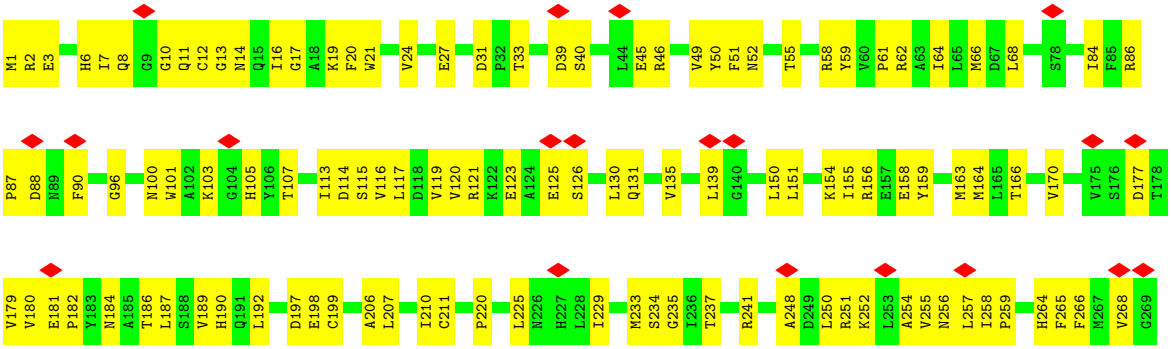
- Molecule 1: Tubulin beta

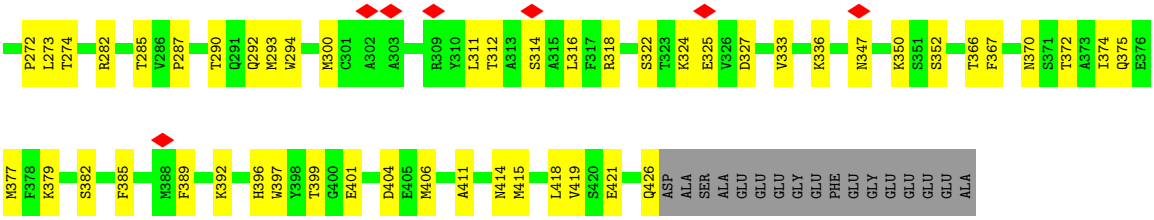
Chain Y8:



- Molecule 1: Tubulin beta

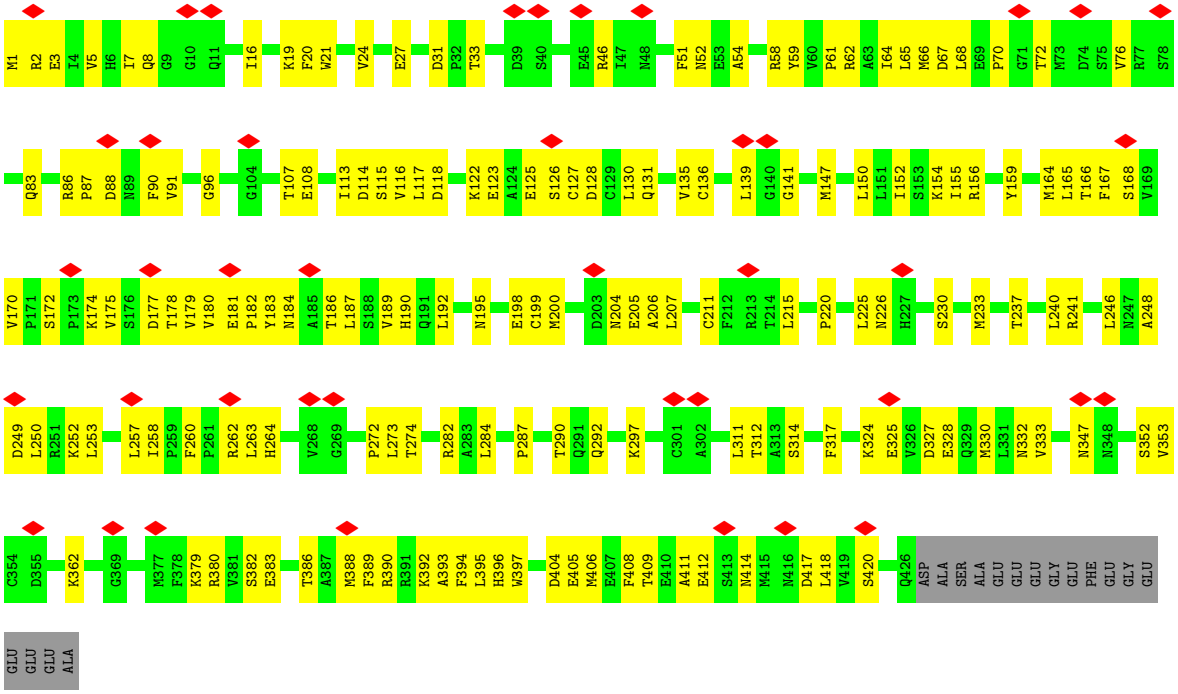
Chain Z0:





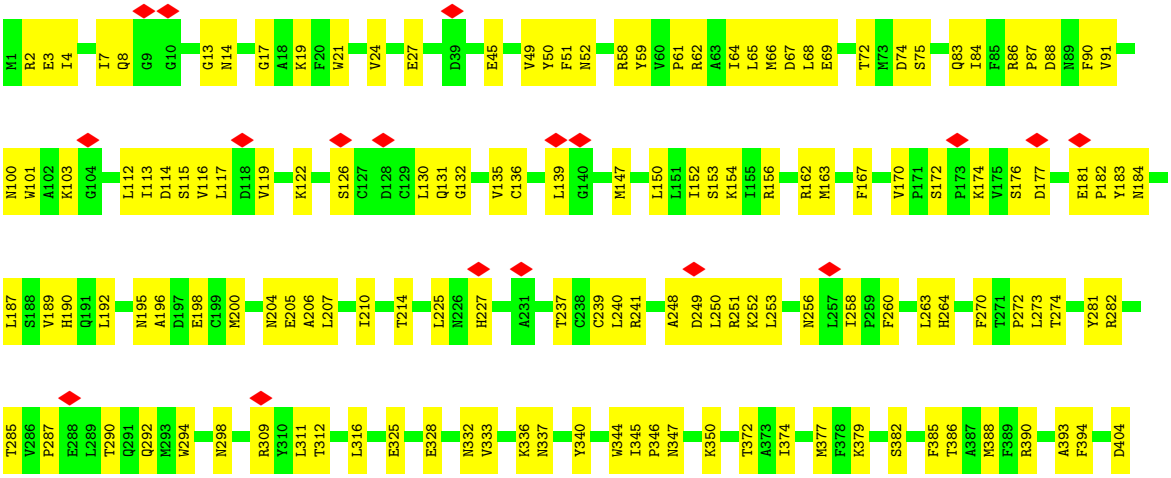
• Molecule 1: Tubulin beta

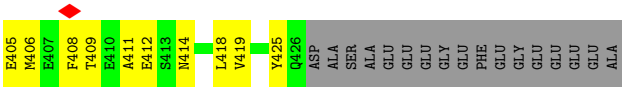
Chain Z2:



• Molecule 1: Tubulin beta

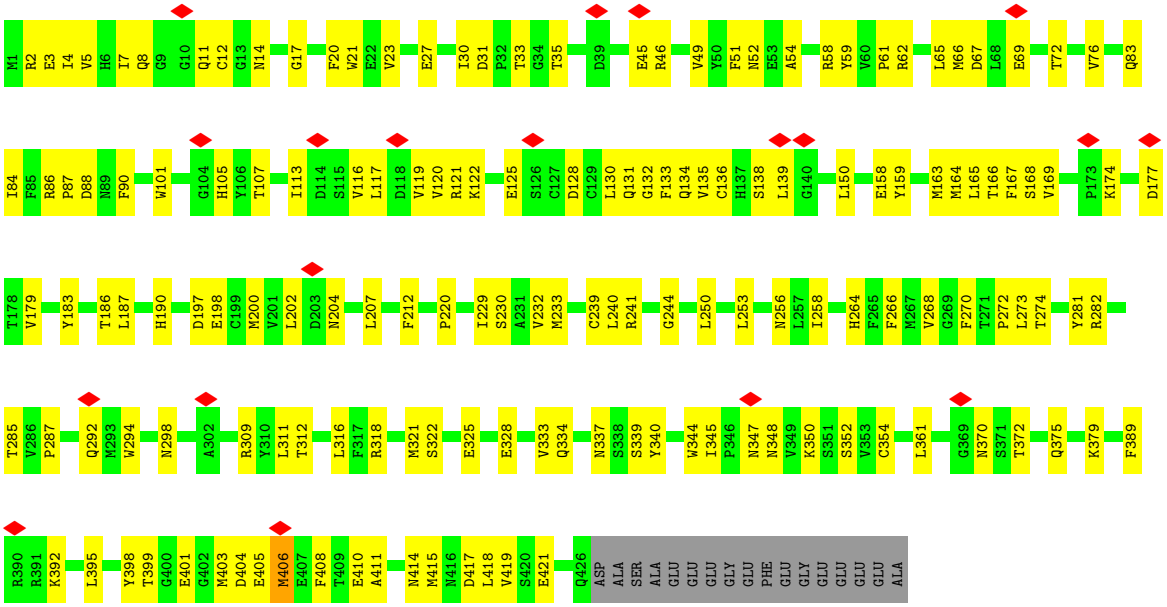
Chain Z4:





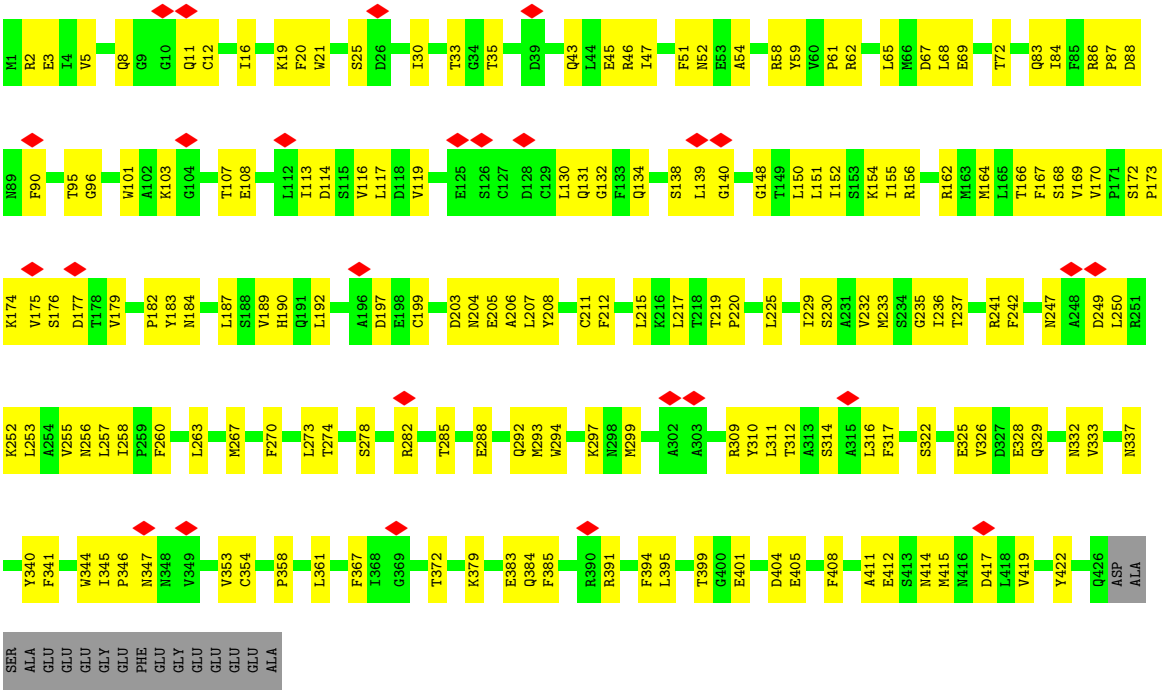
- Molecule 1: Tubulin beta

Chain Z6:



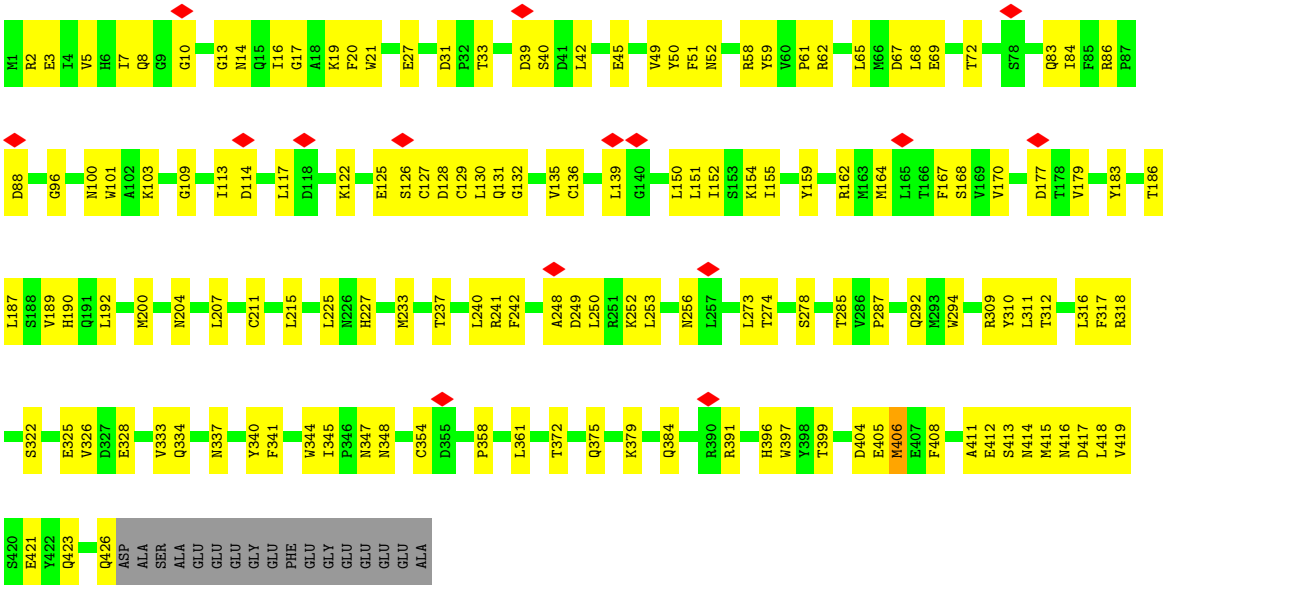
- Molecule 1: Tubulin beta

Chain Z8:



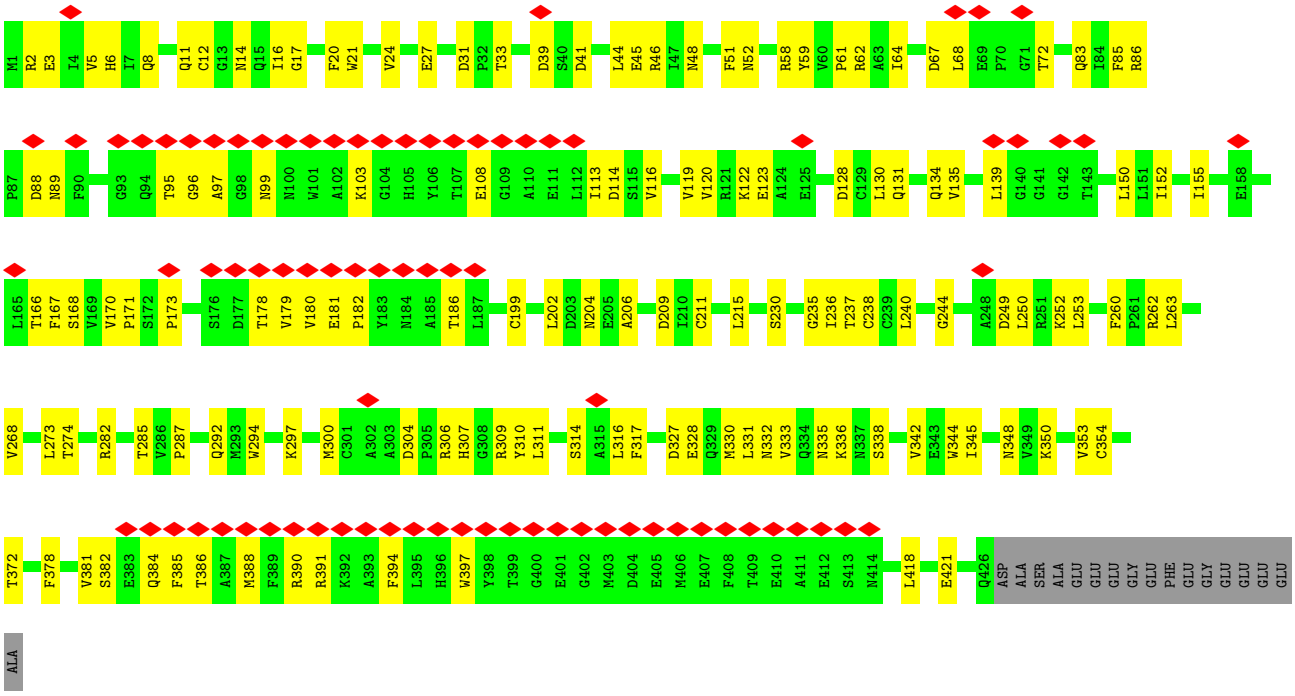
- Molecule 1: Tubulin beta

Chain 0A:



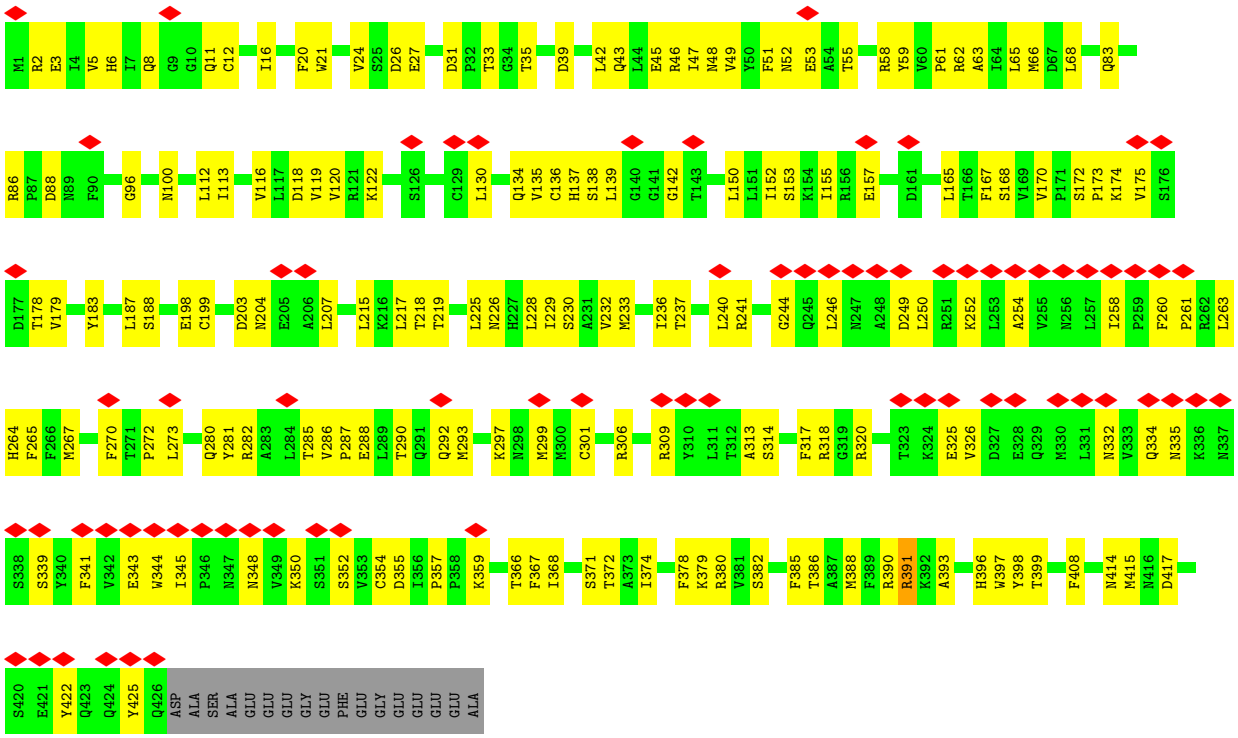
- Molecule 1: Tubulin beta

Chain 0C:



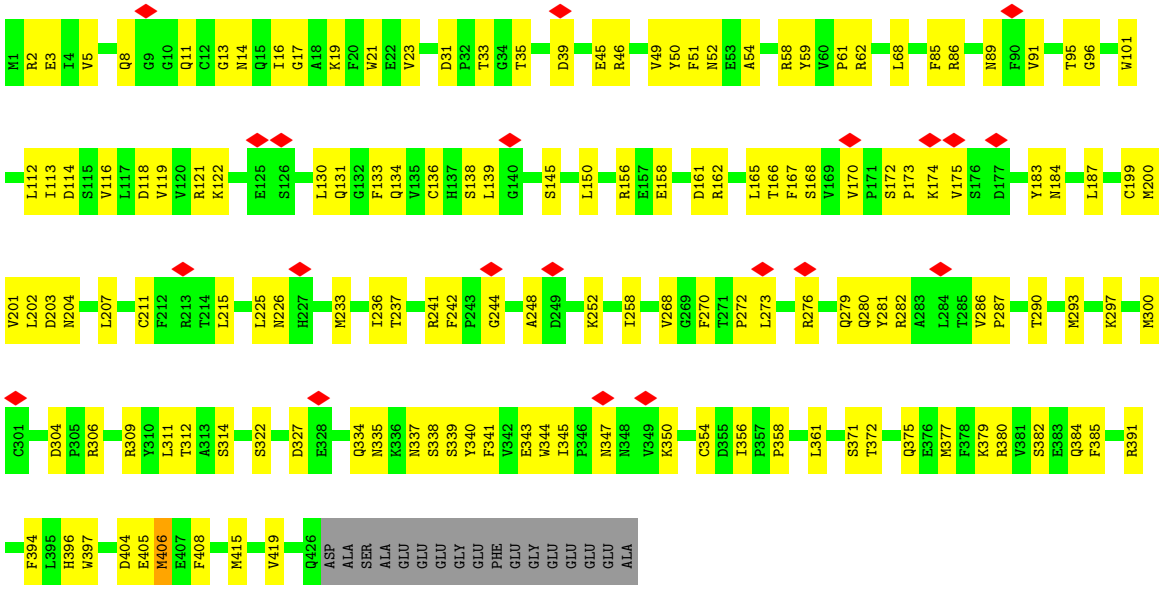
- Molecule 1: Tubulin beta

Chain 0E:



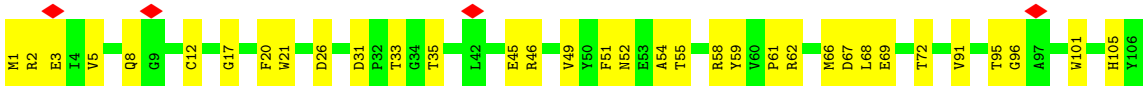
- Molecule 1: Tubulin beta

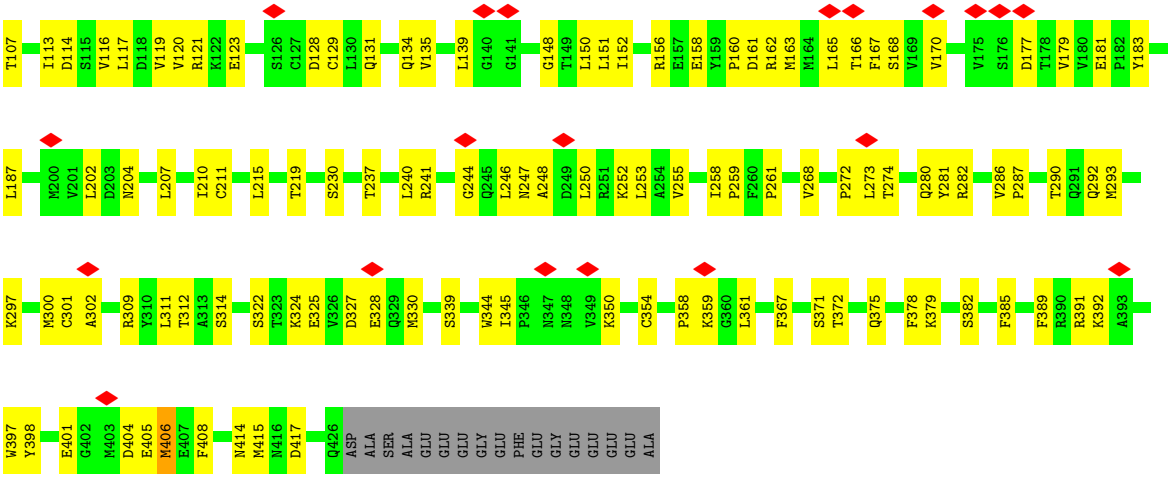
Chain 0G:



- Molecule 1: Tubulin beta

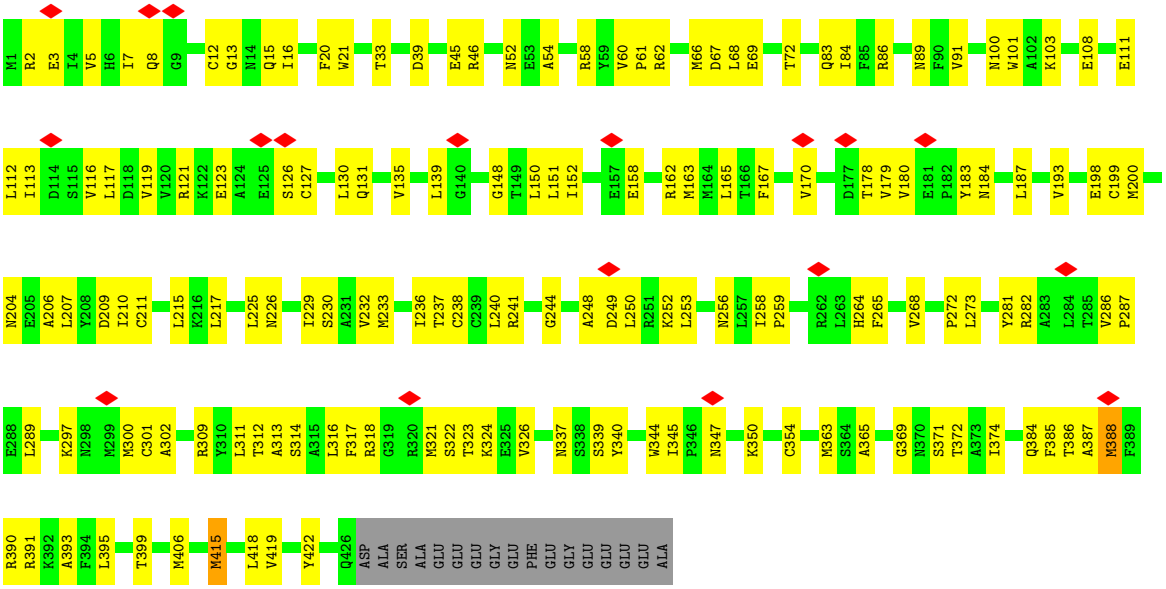
Chain 0I:





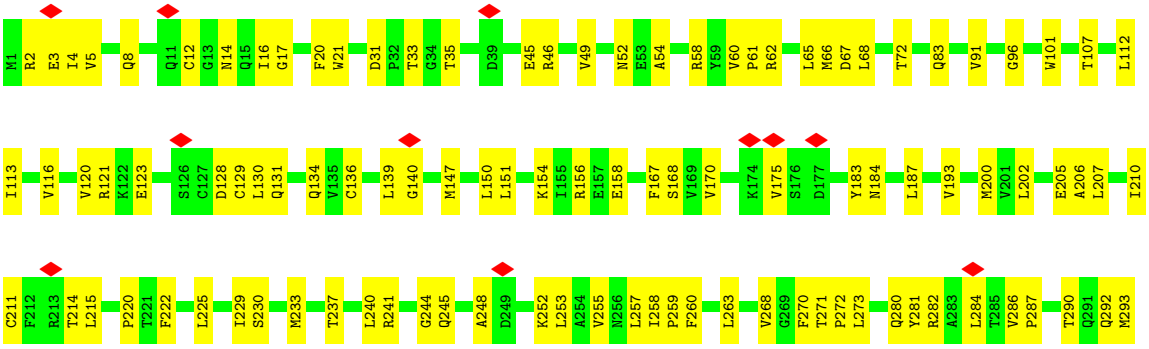
- Molecule 1: Tubulin beta

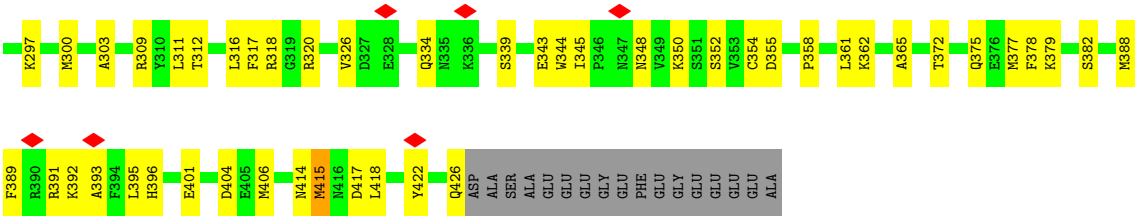
Chain 0K:



- Molecule 1: Tubulin beta

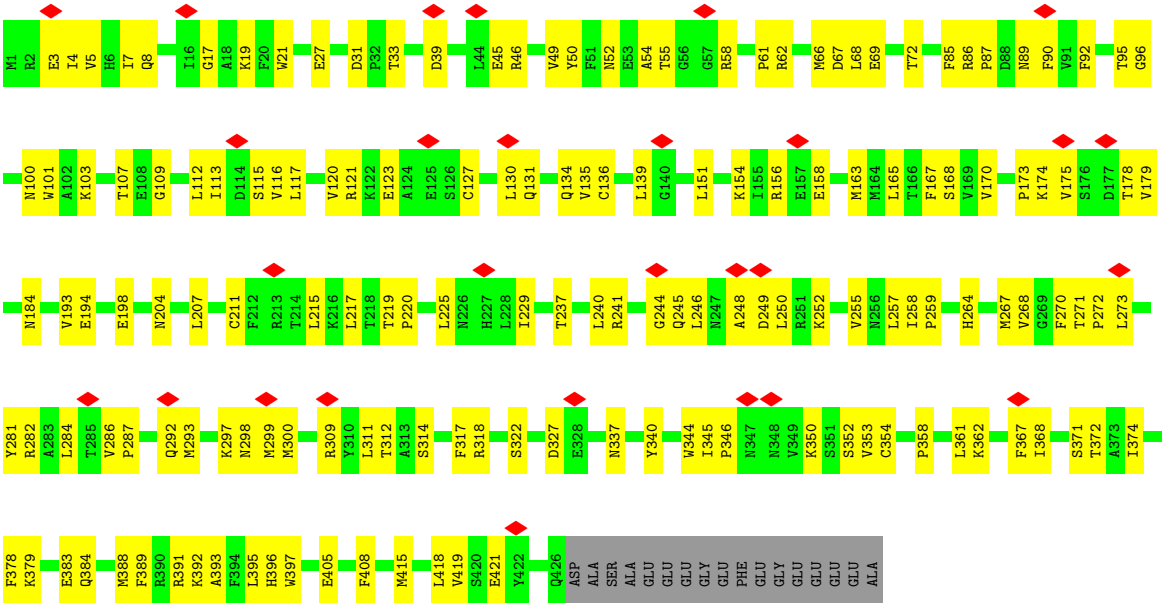
Chain 0M:





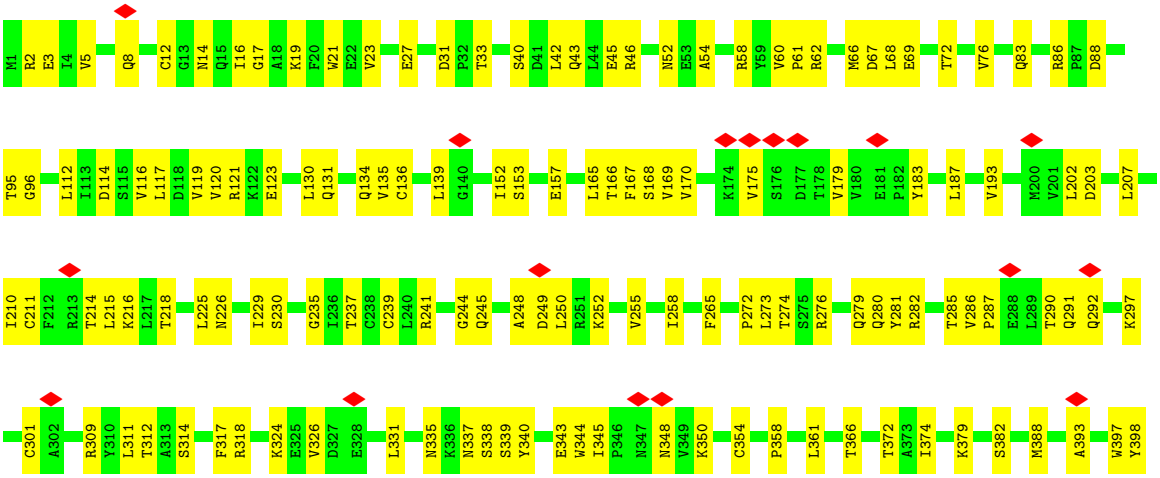
• Molecule 1: Tubulin beta

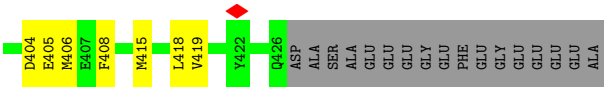
Chain 0O:



• Molecule 1: Tubulin beta

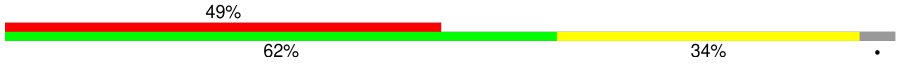
Chain 0Q:

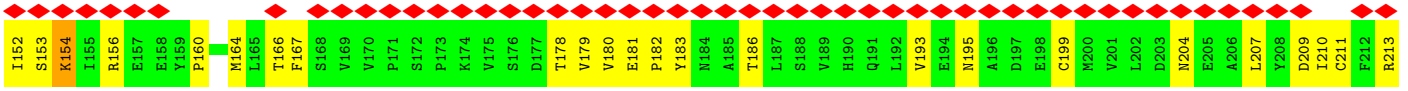


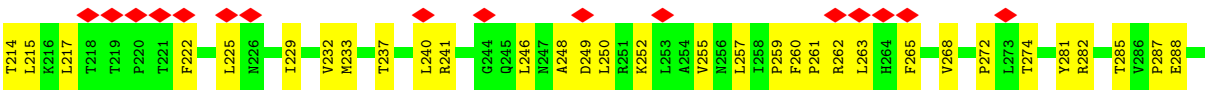


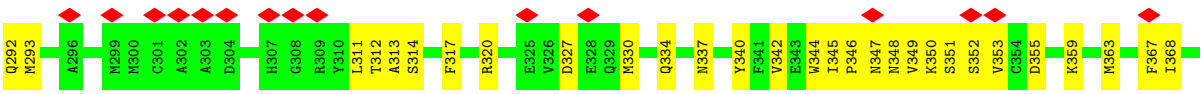
• Molecule 1: Tubulin beta

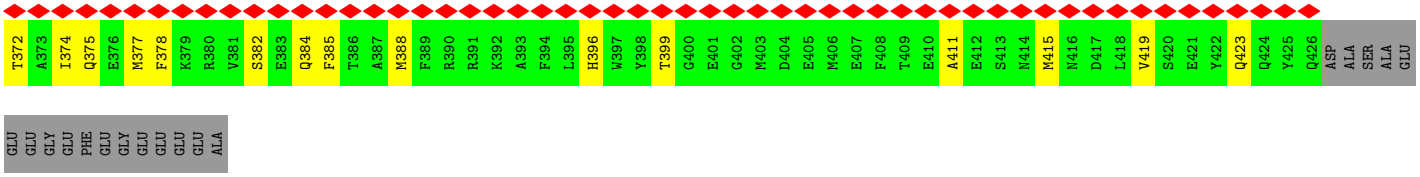
Chain 0S:





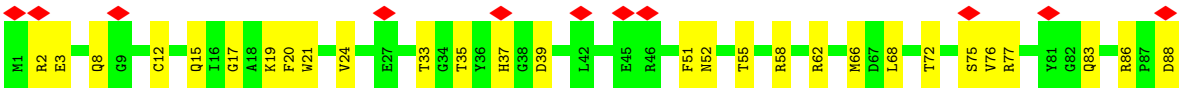


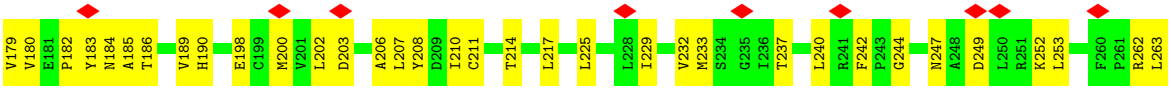


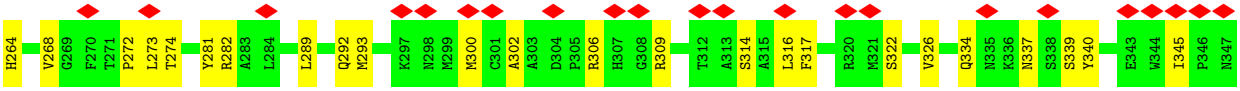


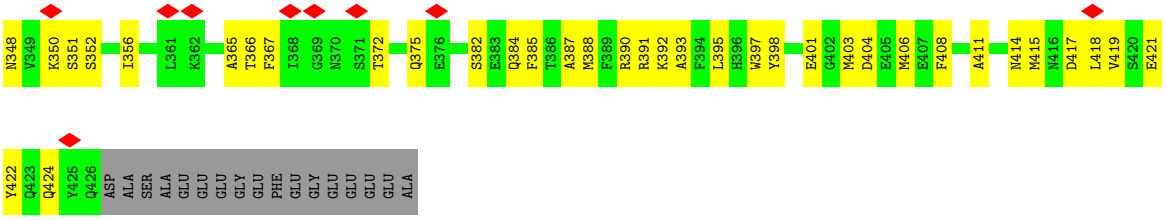
• Molecule 1: Tubulin beta

Chain 0U:



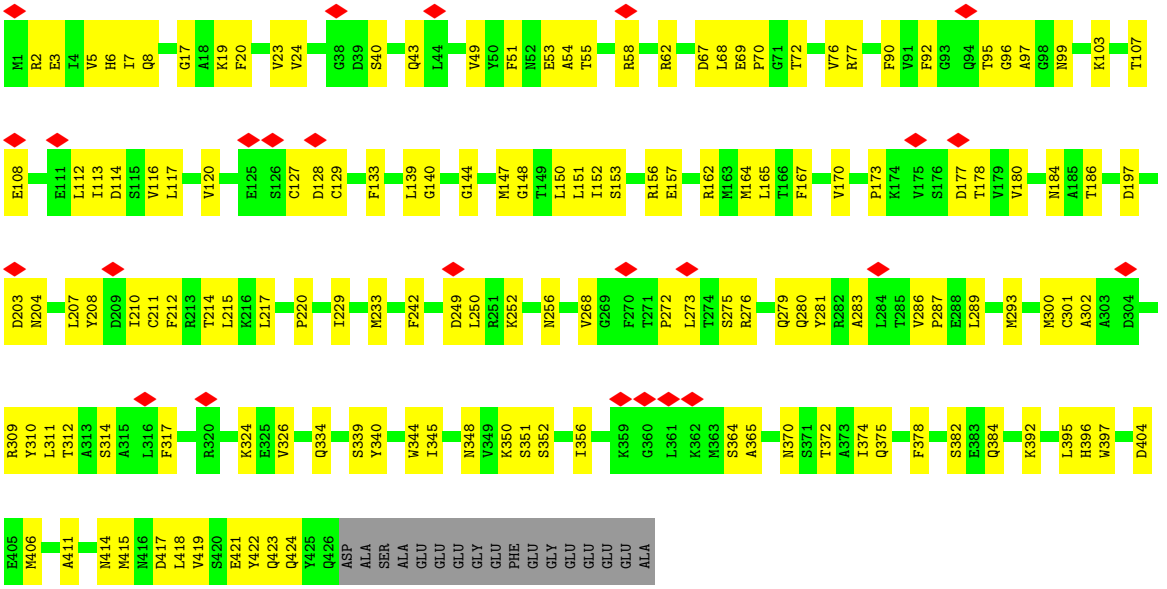






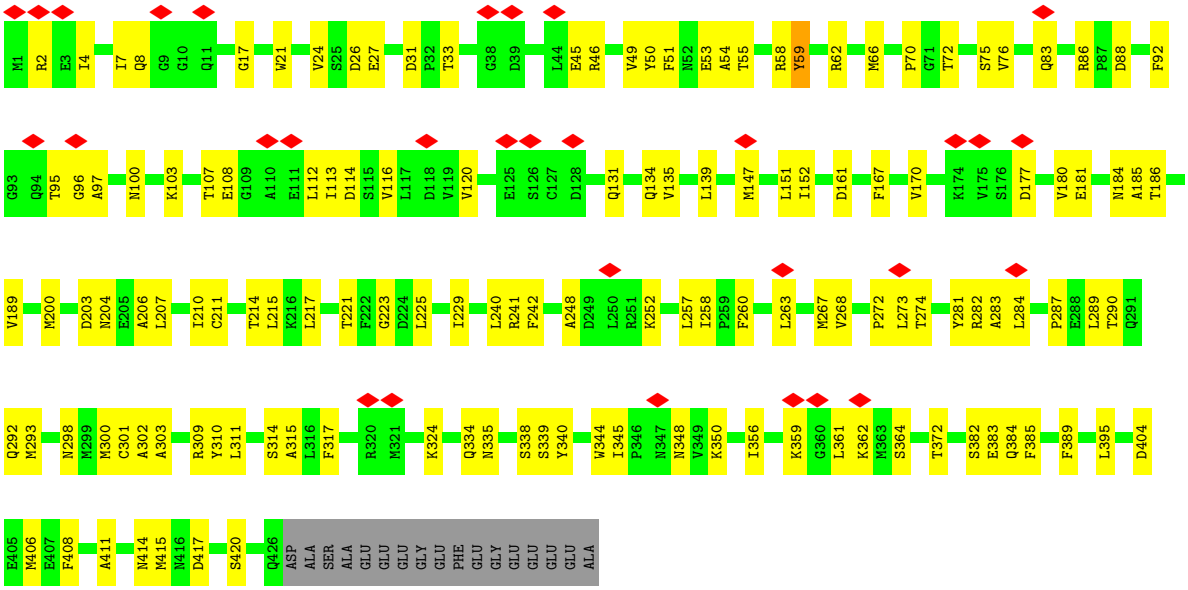
• Molecule 1: Tubulin beta

Chain 0W:



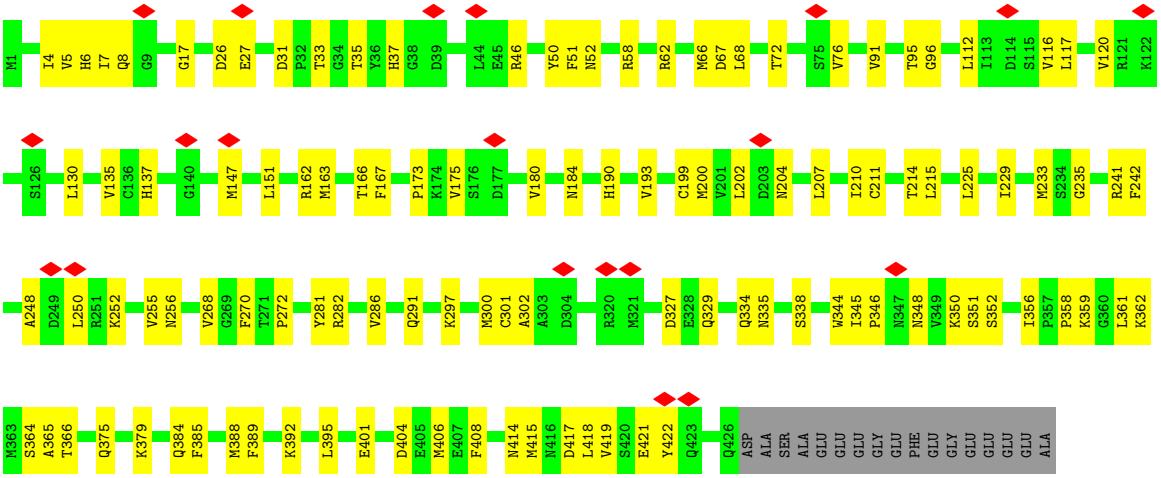
• Molecule 1: Tubulin beta

Chain 0Y:



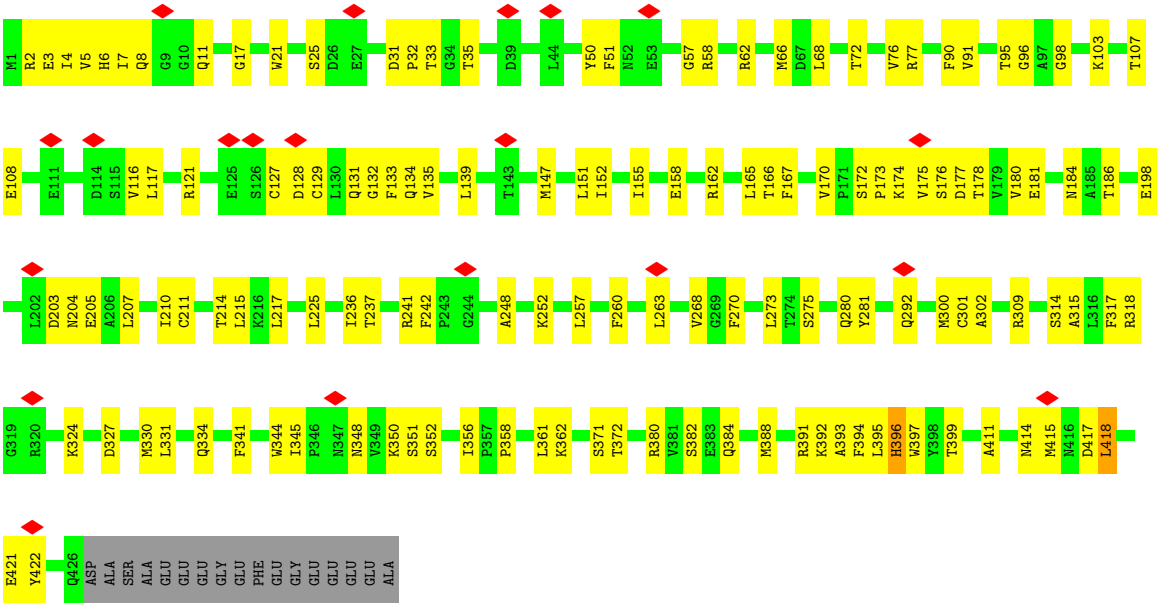
- Molecule 1: Tubulin beta

Chain 1A:



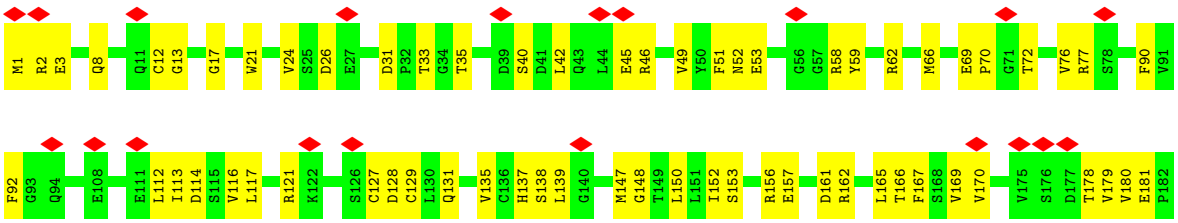
- Molecule 1: Tubulin beta

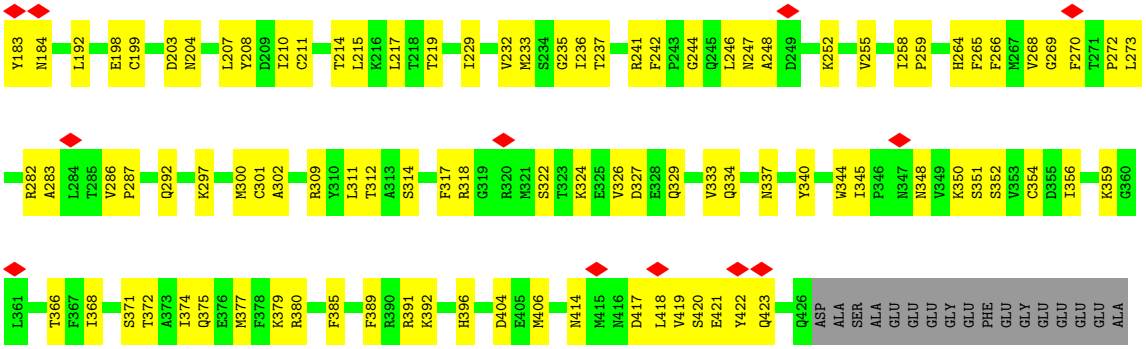
Chain 1C:



- Molecule 1: Tubulin beta

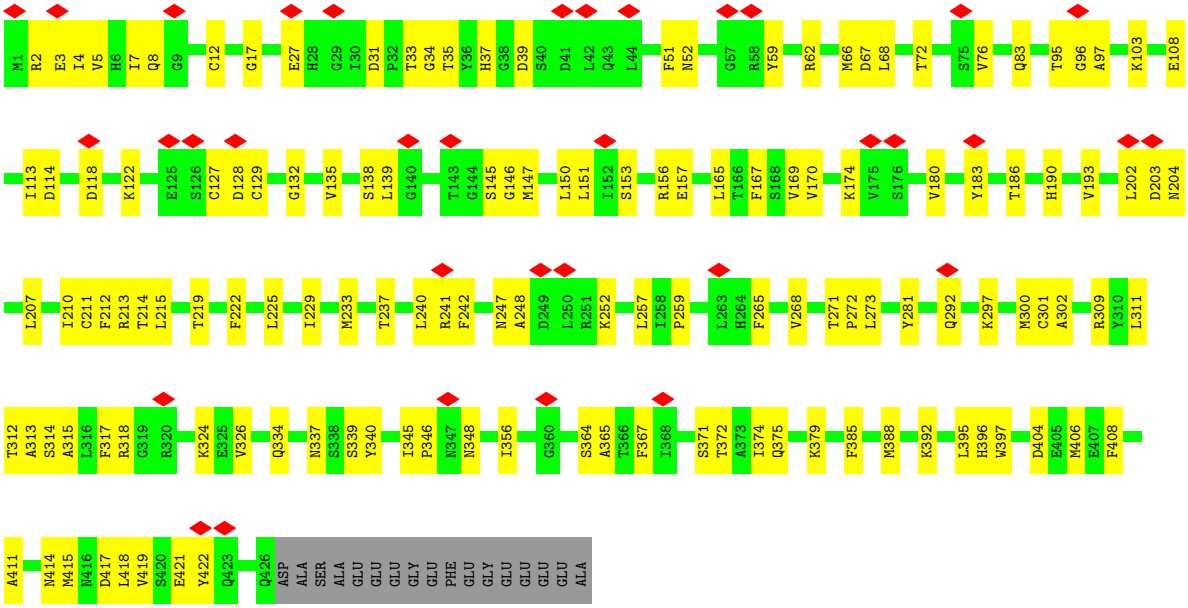
Chain 1E:





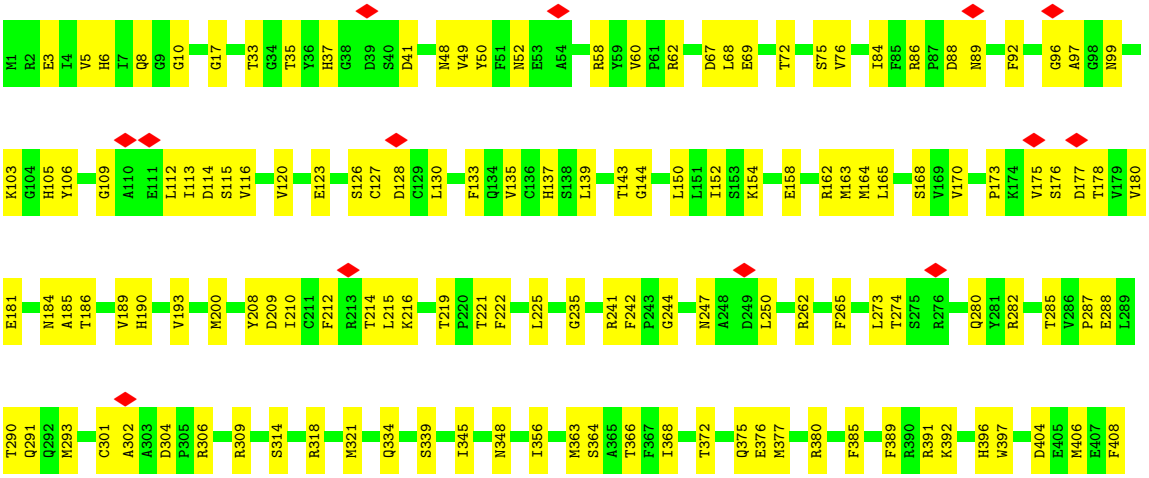
• Molecule 1: Tubulin beta

Chain 1G:



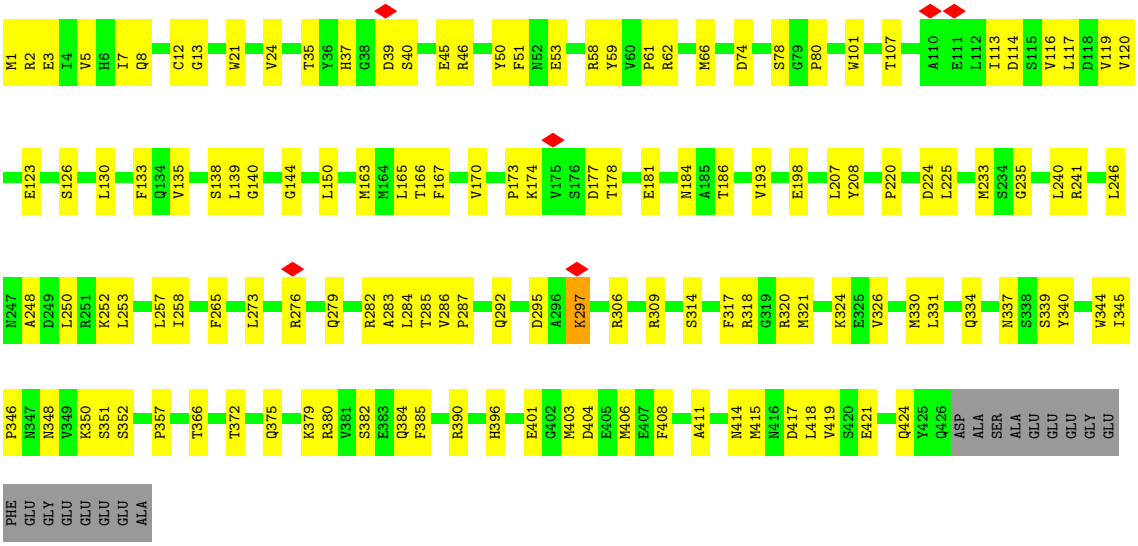
• Molecule 1: Tubulin beta

Chain 1K:



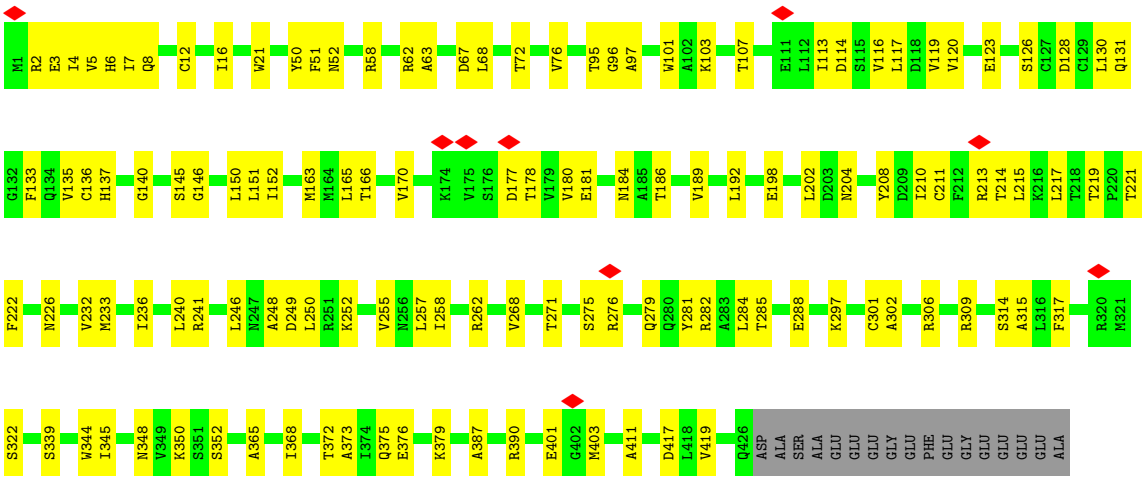
• Molecule 1: Tubulin beta

Chain 1M:



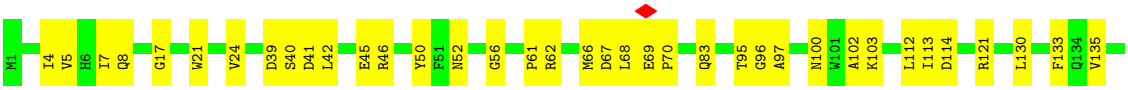
• Molecule 1: Tubulin beta

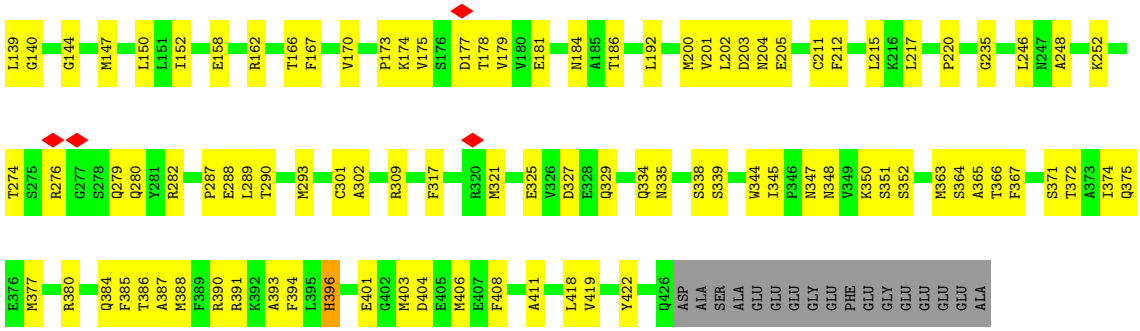
Chain 1O:



• Molecule 1: Tubulin beta

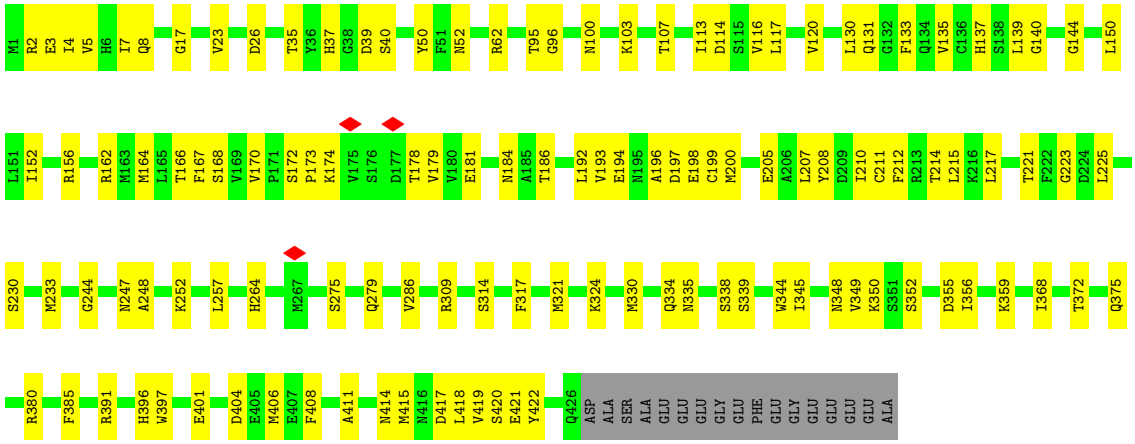
Chain 1Q:





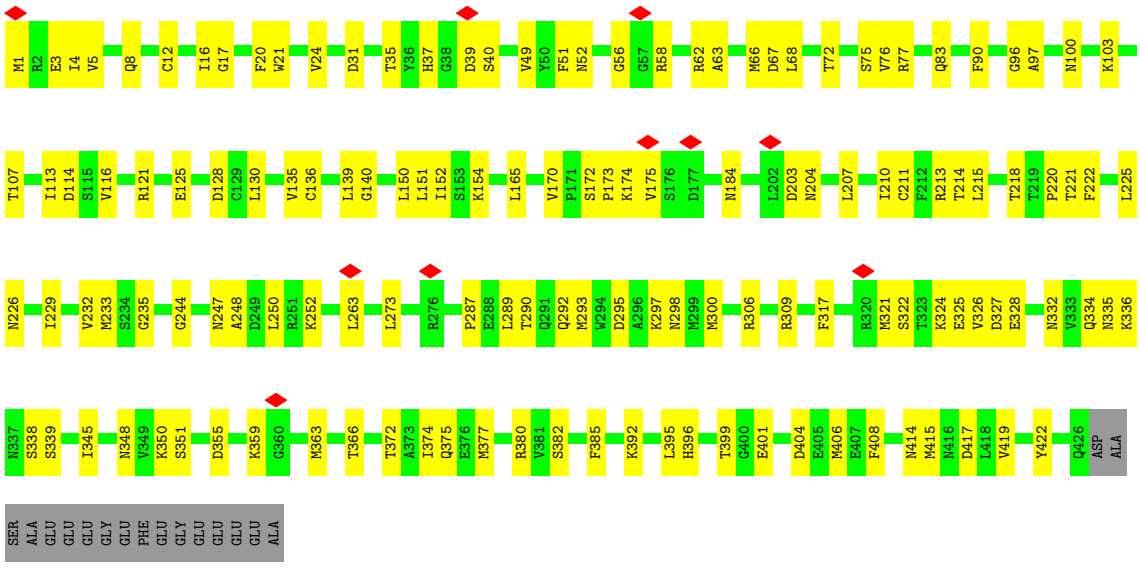
• Molecule 1: Tubulin beta

Chain 1S:



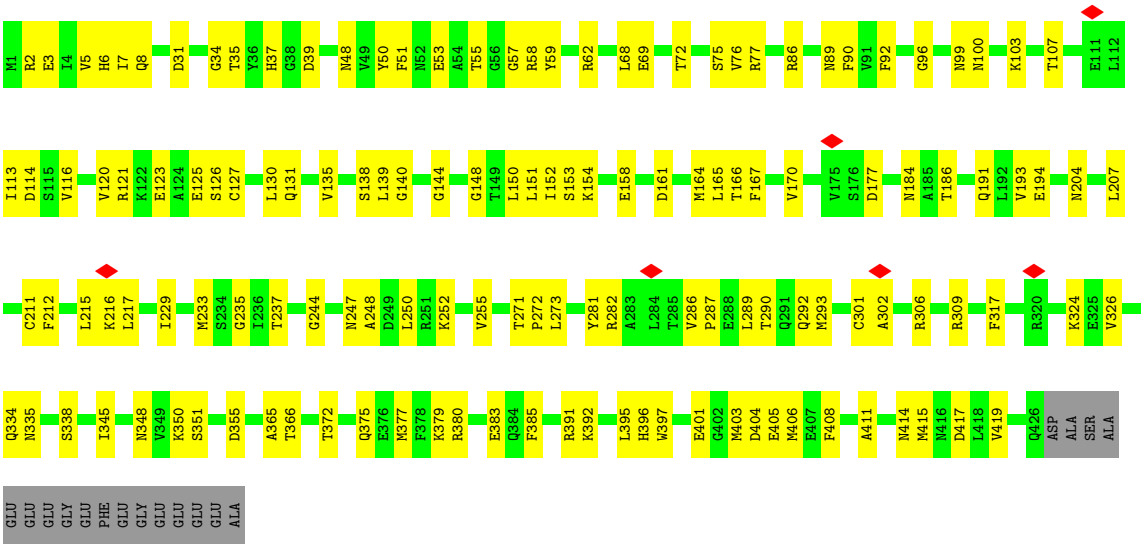
• Molecule 1: Tubulin beta

Chain 1U:



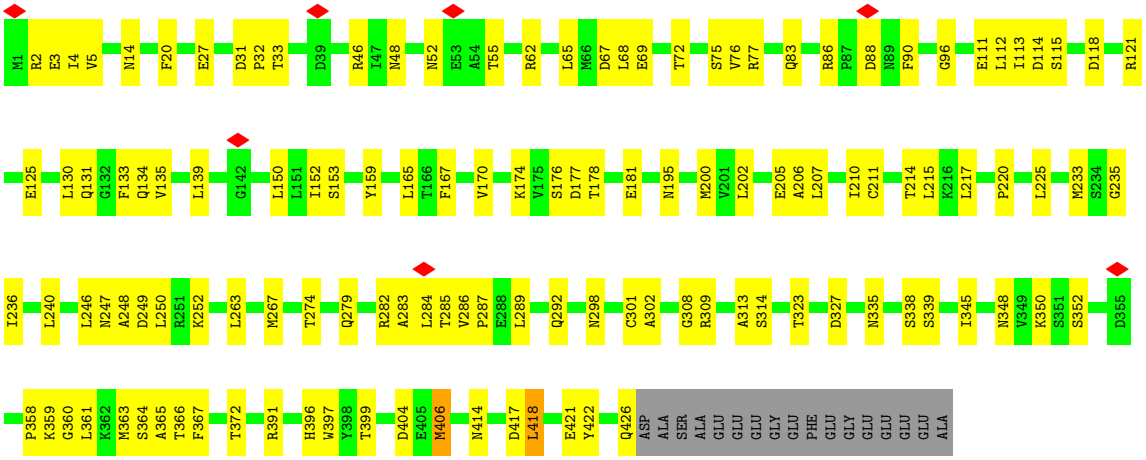
• Molecule 1: Tubulin beta

Chain 1W:



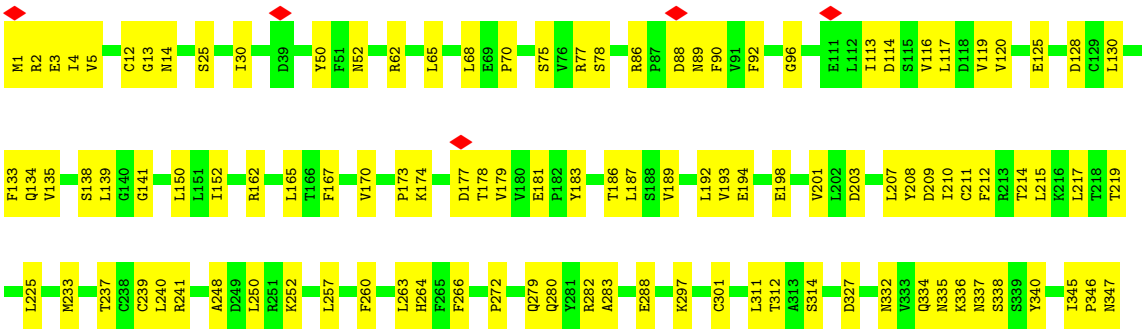
- Molecule 1: Tubulin beta

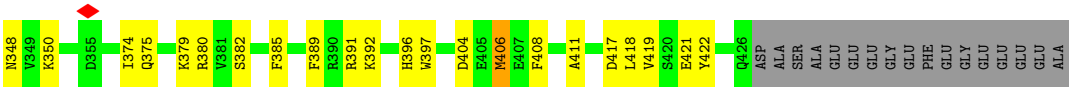
Chain 2A:



- Molecule 1: Tubulin beta

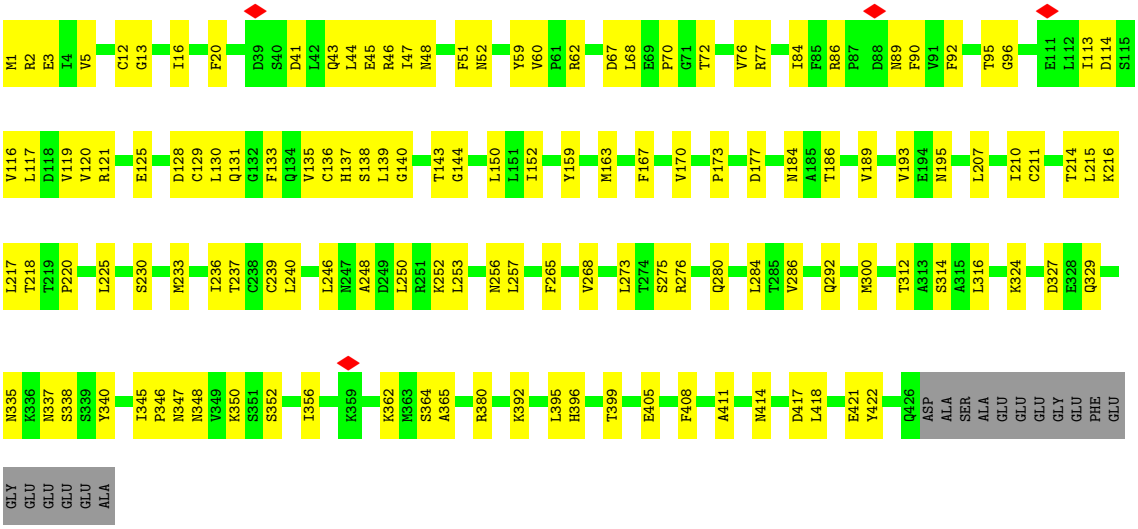
Chain 2C:





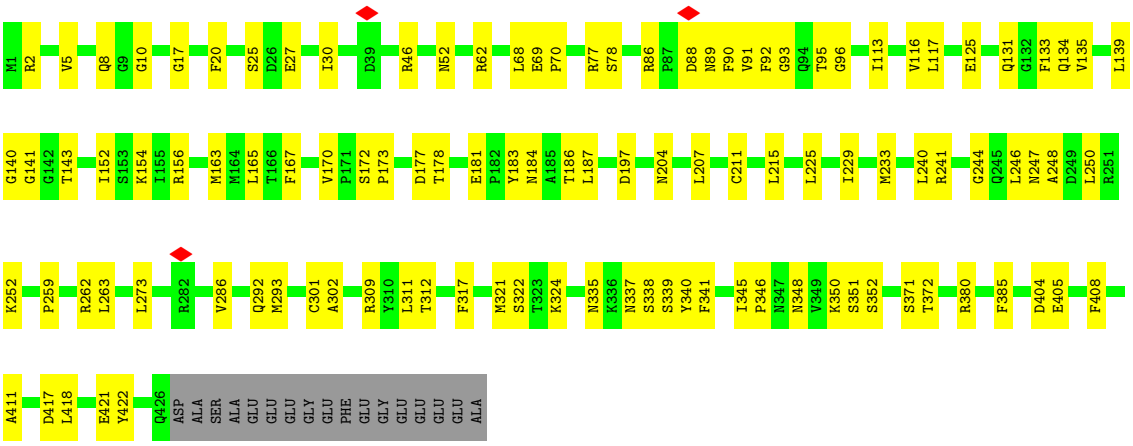
- Molecule 1: Tubulin beta

Chain 2E:



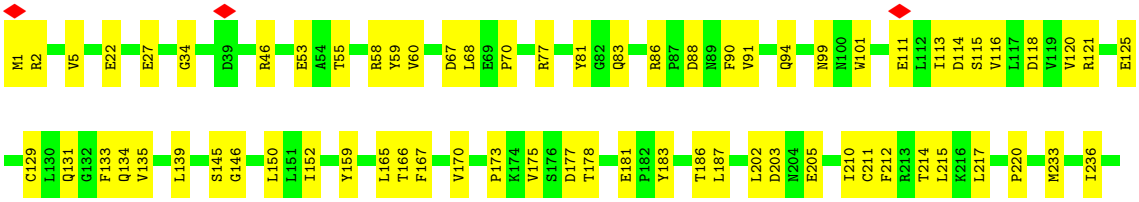
- Molecule 1: Tubulin beta

Chain 2G:



- Molecule 1: Tubulin beta

Chain 2I:



C239 L240 R241 G244 N247 A248 K252 P259 F270 L273 T274 S275 Q279 T285 V286 P287 E288 Q292 M300 C301 A302 R309 Y310 L311 T312 A313 S314 K324 D327 N335 K336 N337 S338 S339 Y340 F341 P346 K350 S351 D355 K359

F367 Q375 R380 F385 F389 R390 R391 L395 H396 W397 Y398 T399 M403 D404 E405 M406 E407 F408 A411 L418 V419 Y422 Q426 ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain 2K:

M1 R2 E3 I4 V5 G10 W21 G38 D39 N48 V49 Y50 F51 N52 G56 G57 P61 R62 L68 T72 S75 V76 R77 S78 R86 P87 D88 T95 G96 E111 L112 I113 D114 S115 V116 R121 E125 D128 C129 L130 F133 Q134 L139

G140 G141 G142 T143 G144 L151 I152 R156 E157 E158 R162 M163 M164 F167 V170 P173 K174 V175 S176 D177 T178 V179 N184 D197 E198 C199 M200 V201 L202 L207 Y208 C211 L215 K216 L217 L225 M233 S234 G235 L240 R241 A248 K252

F265 F266 L273 T274 S275 R276 Q280 Y281 R282 V286 P287 Q292 R309 S314 F317 M321 E325 Q334 S339 I345 P346 N347 N348 V349 K350 S351 S352 V353 P358 L361 T366 T372 R380 H396 T399 D404 E405 M406 Q426

ASP ALA SER ALA GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain 2M:

M1 R2 V5 H6 I7 Q8 C12 G17 F20 D31 P32 T33 G34 T35 Y36 H37 G38 D39 Q43 L44 E45 R46 I47 N48 V49 N52 R62 M66 D67 L68 D74 R77 S78 Q83 D88 N89 F90 Q94 T95 G96 A110 I113 D114 S115

V116 L117 D118 V119 V120 R121 K122 E123 A124 E125 S126 C129 Q134 V135 S138 L139 G140 G144 G148 I152 M164 L165 T166 F167 V170 P171 S172 P173 K174 V175 S176 D177 T178 E181 P182 Y183 N184 A185 T186 V189 E194 M200 V201 L202 D203 N204 L207

I210 C211 T214 L215 P220 D224 L225 M233 I236 R241 G244 N247 A248 D249 L250 R251 K252 L253 N256 R262 V268 T274 R282 A283 L284 T285 V286 P287 C301 A302 R309 T312 A313 S314 A315 L316 F317 T323 K324 E325 V326 D327

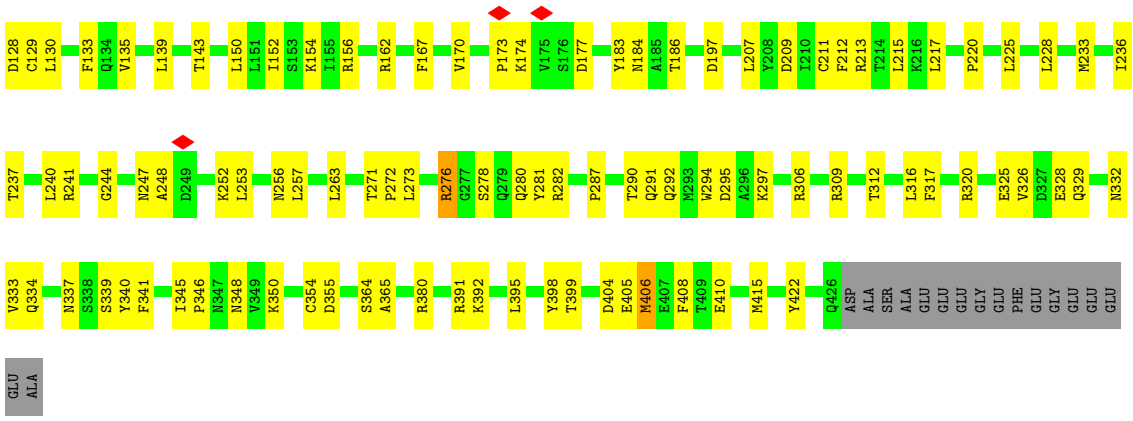
E328 N335 K336 N337 S338 S339 Y340 F341 I345 P346 N347 N348 V349 K350 D355 F367 I368 S371 T372 R380 V381 S382 F385 R391 L395 H396 W397 Y398 T399 D404 E405 M406 E407 F408 A411 N414 M415 E421 Q424 Y425 Q426 ASP ALA SER ALA GLU

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

- Molecule 1: Tubulin beta

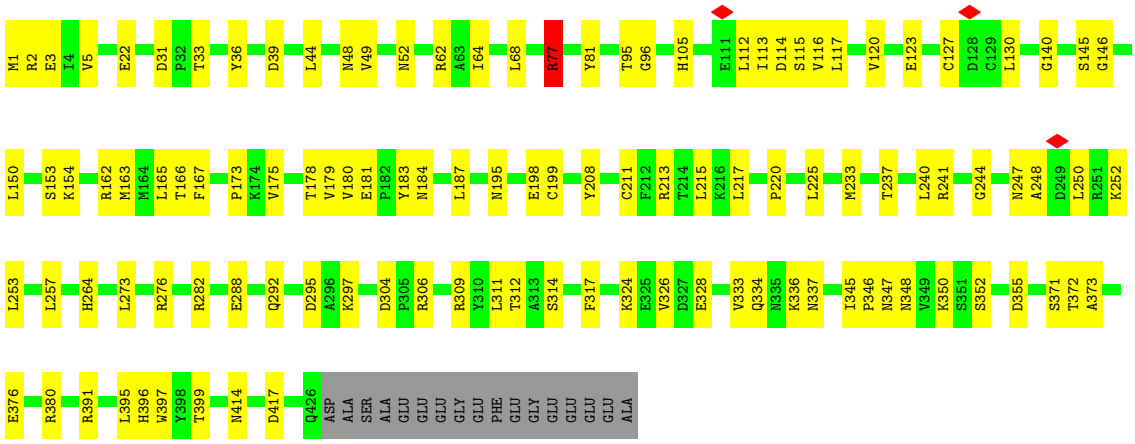
Chain 2Q:

M1 R2 E3 I4 V5 H6 I7 G10 D31 T35 D39 S40 E45 R46 V49 N52 T55 R58 R62 E69 R77 R86 N89 F90 V91 T95 G96 W101 T107 E108 E111 L112 I113 D114 S115 V116 R121 E125 S126 C127



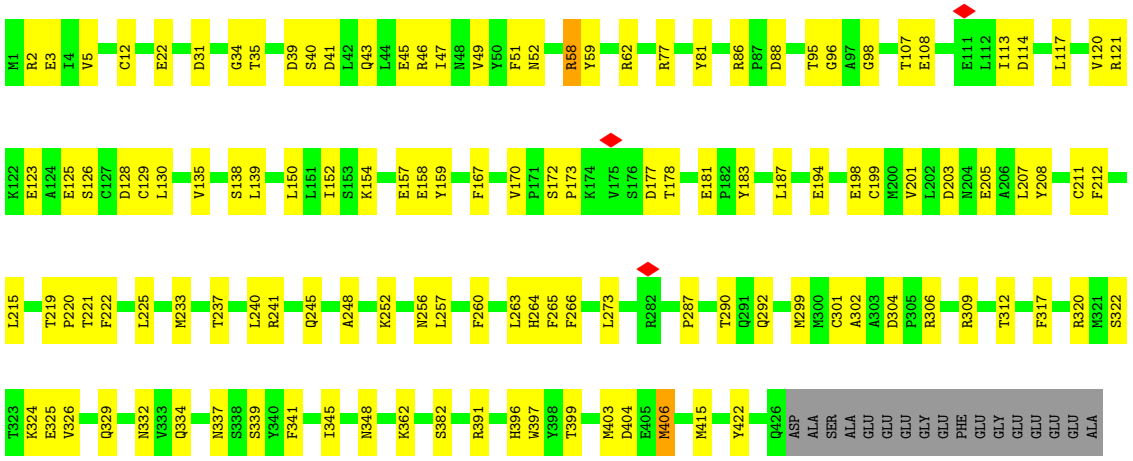
• Molecule 1: Tubulin beta

Chain 2S:



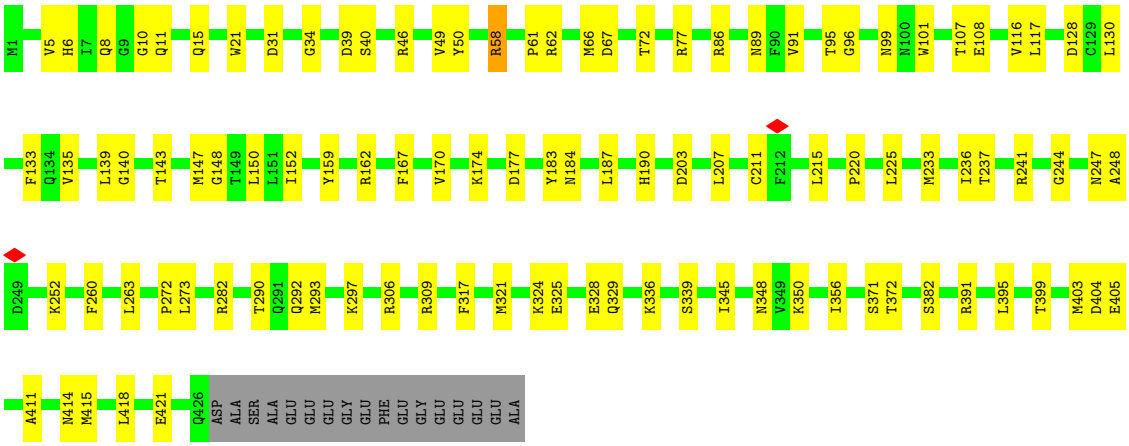
• Molecule 1: Tubulin beta

Chain 2U:



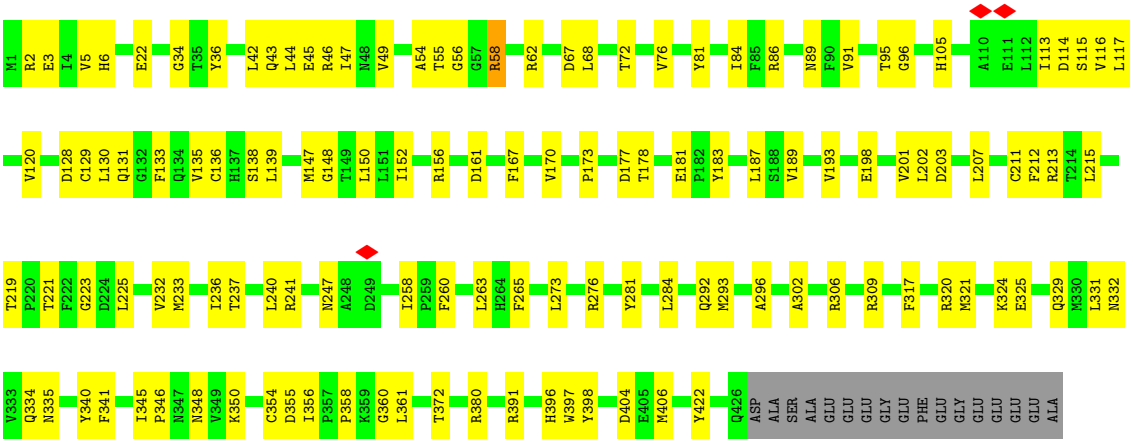
• Molecule 1: Tubulin beta

Chain 2W:



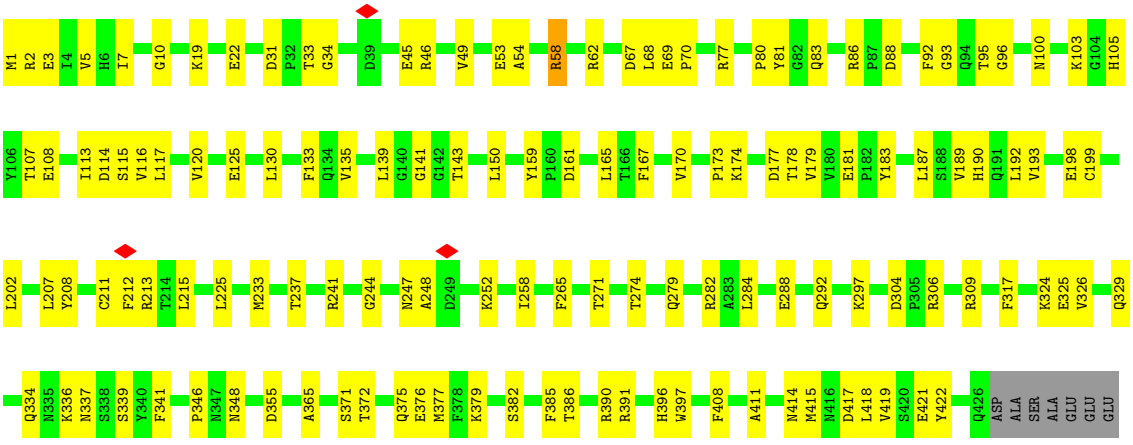
- Molecule 1: Tubulin beta

Chain 2Y:



- Molecule 1: Tubulin beta

Chain 3A:



GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain 3C:

M1 R2 E3 I4 V5 H6 I7 C12 G13 E22 G34 T35 L42 Q43 L44 E45 R46 I47 N48 V49 Y50 F51 N52 E53 A54 T55 R58 Y59 R62 R77 Y81 R86 P87 D88 N89 T95 G96 A97 G98 N99 N100 K103 G104 H105 A110 E111 L112 I113

V116 L117 D118 V119 V120 R121 D128 C129 L130 V135 C136 H137 S138 L139 G140 G141 S145 G146 M147 G148 T149 L150 L151 I152 S153 D161 R162 L165 T166 F167 S168 V169 V170 P171 S172 P173 K174 V175 S176 D177 T178 V179 V180 E181 P182 Y183 N184 A185 T186 L187 S188 V189 V201

L202 D203 N204 E205 A206 L207 Y208 C211 F212 R213 T214 L215 K216 L217 M233 I236 T237 C238 C239 L240 R241 G244 Q245 L246 N247 A248 D249 L250 R251 K252 V255 N256 L257 F266 T274 S275 Q279 T285 V286 P287 Q291 M299 M300 C301 A302 R306 R309

T312 L316 F317 R320 T323 K324 E325 V326 Q329 N332 V333 Q334 N337 S338 S339 I345 P346 N347 N348 V349 K350 S351 S352 D355 K359 G360 L361 K362 M363 S371 T372 Q375 E376 K379 R380 V381 S382 T386 A387 M388 F389 R390 R391 K392 A393 F394

L395 H396 W397 Y398 T399 M406 E410 M415 Q426 ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain 3G:

M1 R2 E3 H6 I7 Q8 I30 G34 D39 S40 R46 V49 Y50 F51 N52 E53 G57 R58 Y59 V60 P61 R62 L65 M66 T72 V76 R77 Q83 R86 P87 D88 N89 F90 Q94 T95 N99 N100 K103 E111 L112 I113 D114 S115 V116

L117 V120 R121 K122 D128 C129 L130 Q134 V135 S138 L139 G140 M147 L150 L151 I152 R156 P160 D161 M164 F167 V170 P171 S172 P173 K174 V175 S176 D177 T178 E181 N184 L192 N195 A196 D197 E198 L202 D203 N204 E205 D209 I210

C211 L215 T218 T219 I229 M233 T237 L240 R241 G244 N247 A248 K252 L253 H264 T271 P272 L273 T274 S275 R276 Q280 Y281 R282 V286 P287 M293 A302 R309 L316 F317 K324 E325 V326 Q334 I345 P346 N347 N348 V349

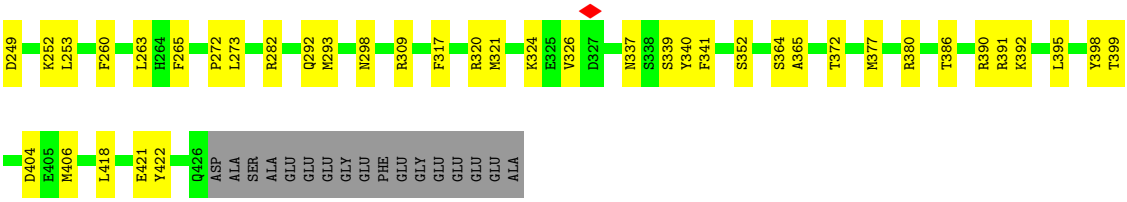
K350 S351 T372 R380 V381 S382 R391 M406 E410 M415 Q426 ASP ALA SER ALA GLU GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain 3I:

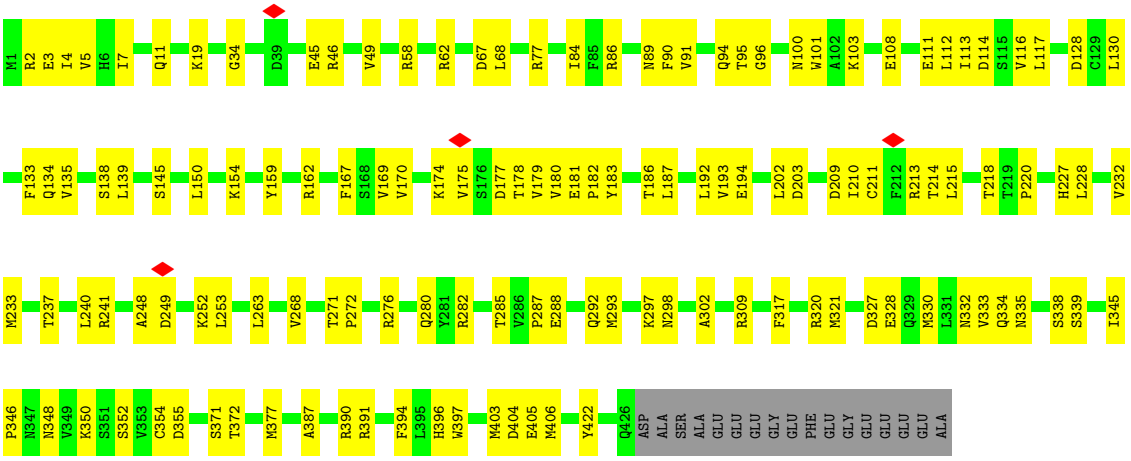
M1 R2 E3 I4 V5 H6 I7 Q8 Q11 W21 I30 D31 P32 T33 G34 D39 Y50 F51 N52 R58 Y59 V60 P61 R62 D67 L68 E69 P70 R77 Y81 F90 Q94 T95 L112 I113 D114 S115 V116 L117 D118 V119 V120 R121 D128 C129 Q134

V135 C136 H137 S138 L139 G140 S145 D161 R162 T166 F167 V170 P173 D177 P182 Y183 N184 A185 T186 L187 L192 C199 L202 D203 N204 E205 Y208 D209 I210 C211 L215 K216 L217 T218 T219 P220 L225 M233 T237 G244 Q245 L246 N247 A248



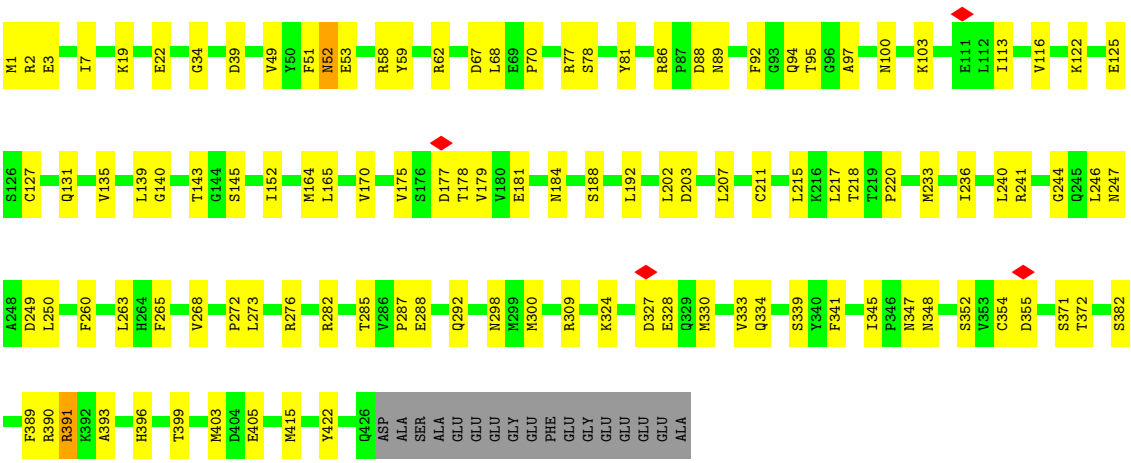
• Molecule 1: Tubulin beta

Chain 3K:



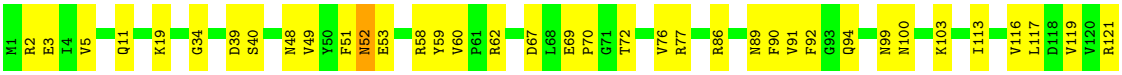
• Molecule 1: Tubulin beta

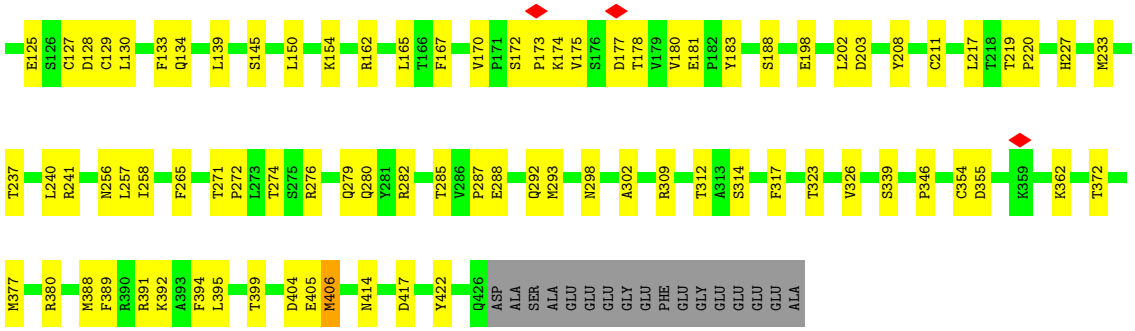
Chain 3M:



• Molecule 1: Tubulin beta

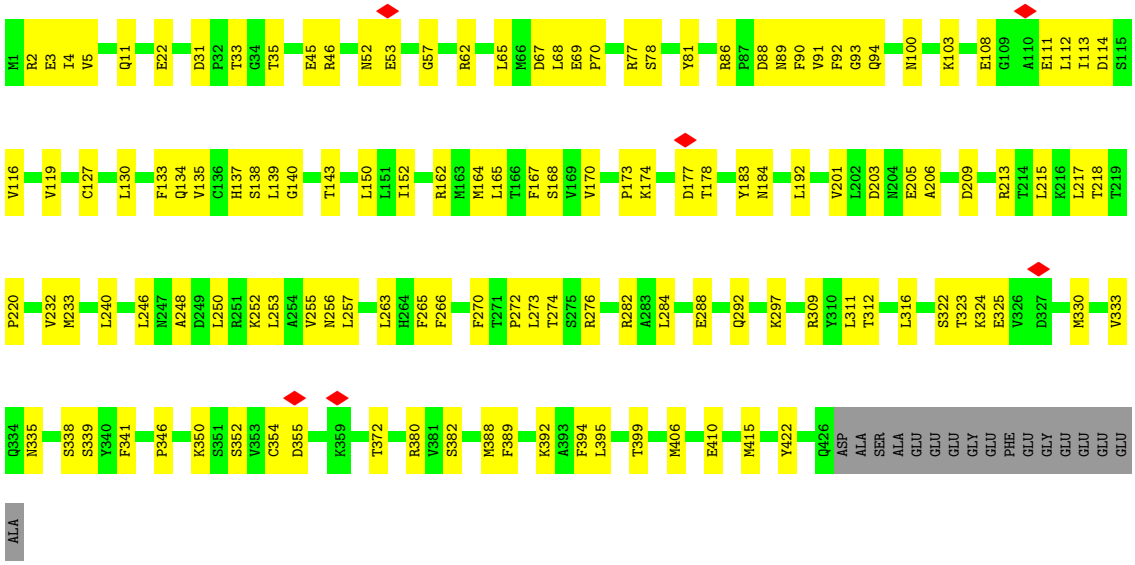
Chain 3O:





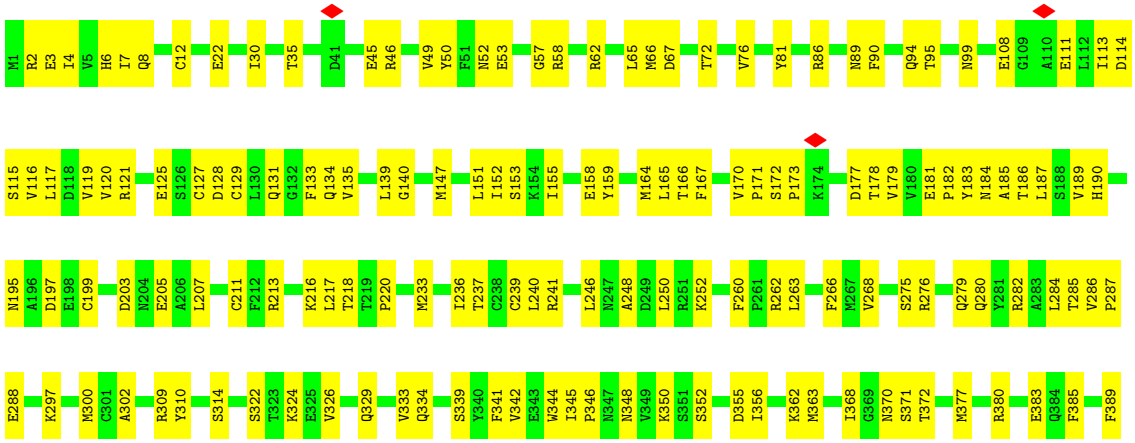
• Molecule 1: Tubulin beta

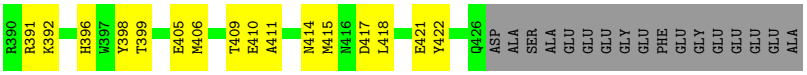
Chain 3Q:



• Molecule 1: Tubulin beta

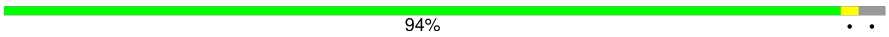
Chain 3S:

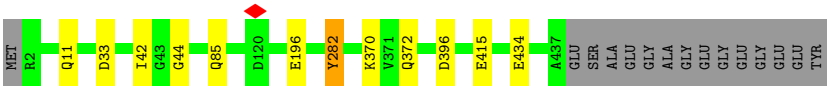




• Molecule 2: Tubulin alpha

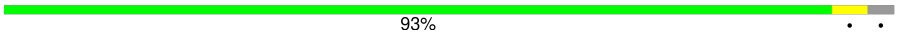
Chain 2:

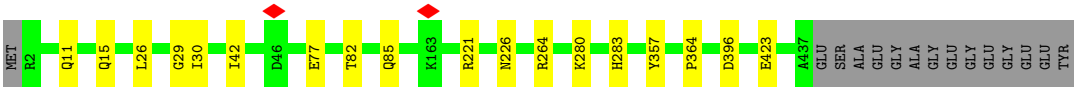




• Molecule 2: Tubulin alpha

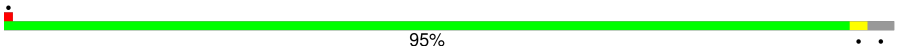
Chain 4:

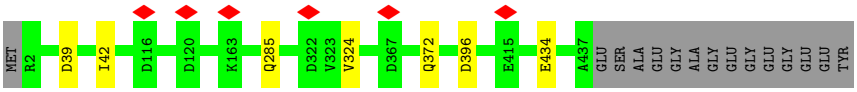




• Molecule 2: Tubulin alpha

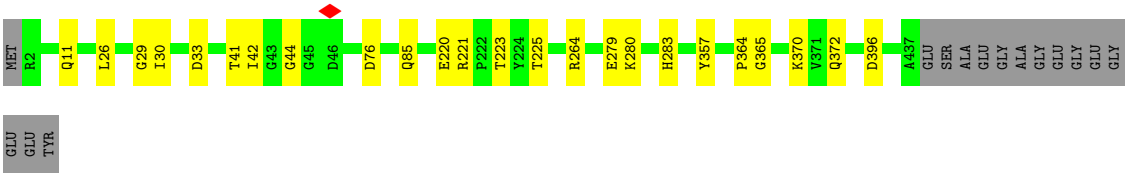
Chain 6:





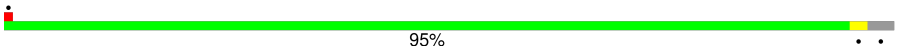
• Molecule 2: Tubulin alpha

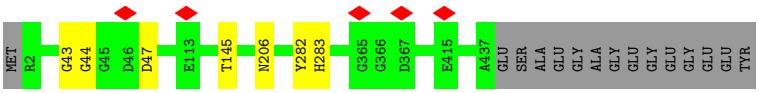
Chain 8:



• Molecule 2: Tubulin alpha

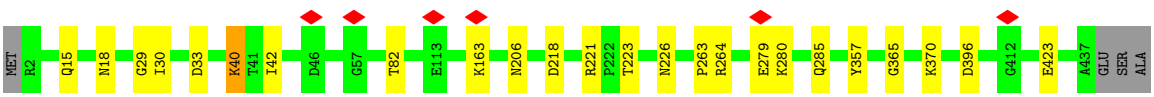
Chain A0:

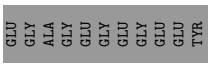




• Molecule 2: Tubulin alpha

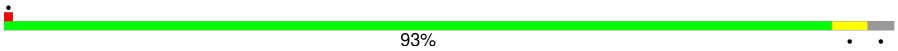
Chain A2:

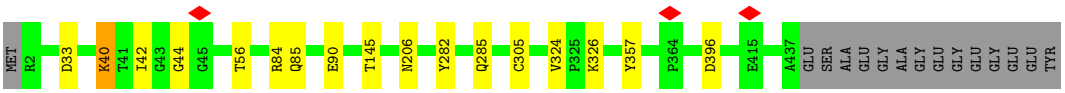




• Molecule 2: Tubulin alpha

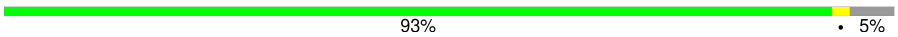
Chain A4:

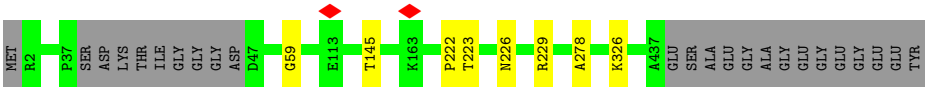




• Molecule 2: Tubulin alpha

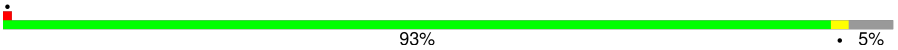
Chain A8:





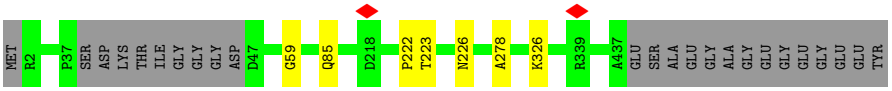
• Molecule 2: Tubulin alpha

Chain B0:



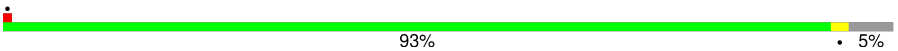
• Molecule 2: Tubulin alpha

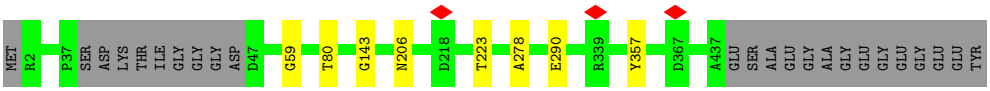
Chain B2:



• Molecule 2: Tubulin alpha

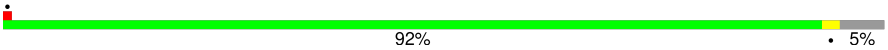
Chain B4:

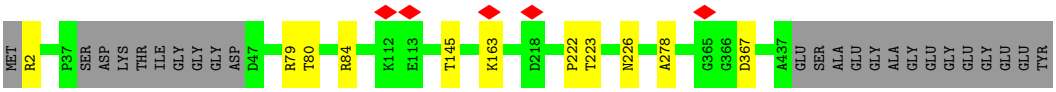




• Molecule 2: Tubulin alpha

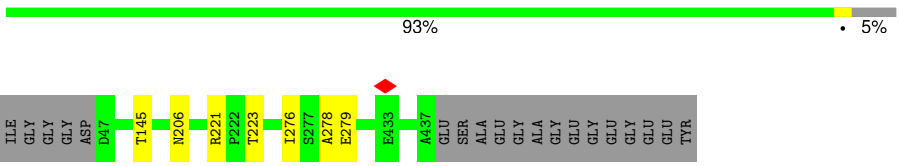
Chain B7:





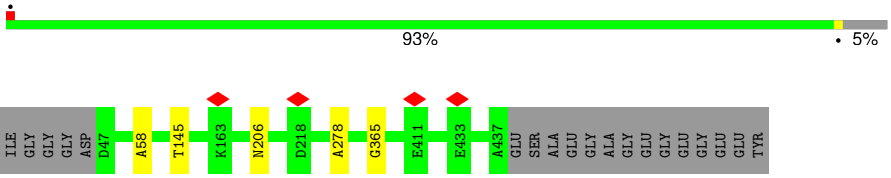
• Molecule 2: Tubulin alpha

Chain B9:



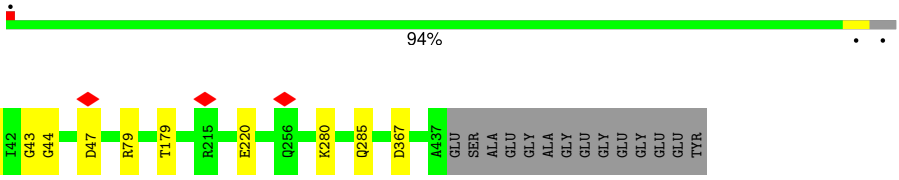
• Molecule 2: Tubulin alpha

Chain C1:



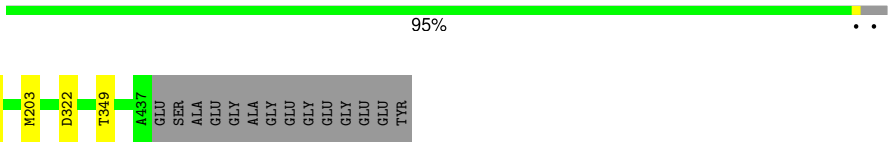
• Molecule 2: Tubulin alpha

Chain C5:



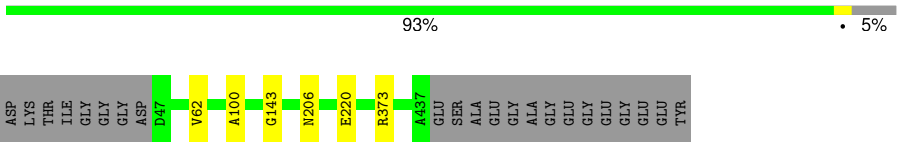
• Molecule 2: Tubulin alpha

Chain C7:



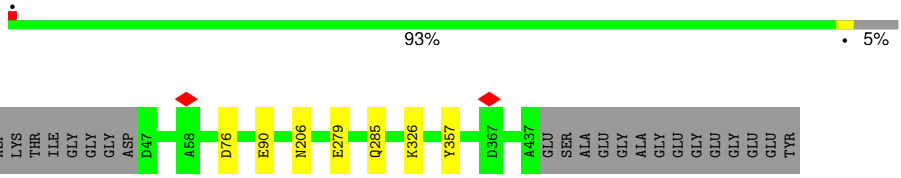
• Molecule 2: Tubulin alpha

Chain C9:



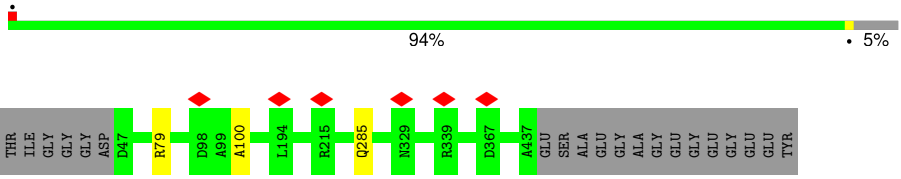
• Molecule 2: Tubulin alpha

Chain D1:



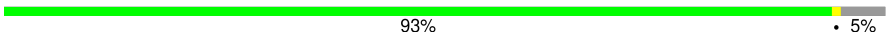
• Molecule 2: Tubulin alpha

Chain D3:



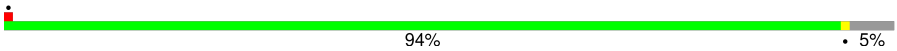
- Molecule 2: Tubulin alpha

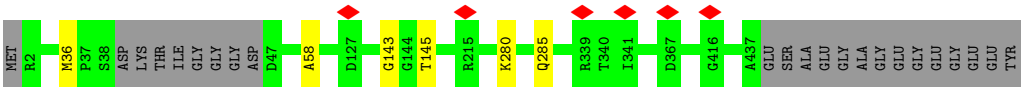
Chain D5:



- Molecule 2: Tubulin alpha

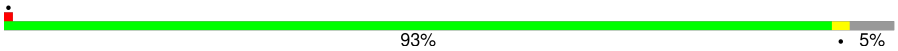
Chain D7:

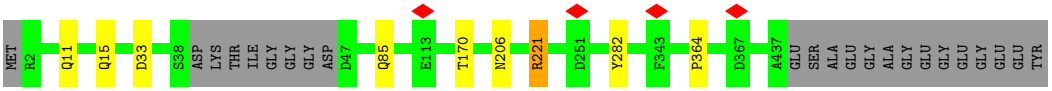




- Molecule 2: Tubulin alpha

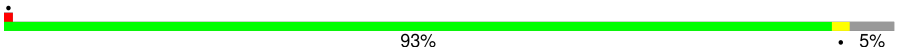
Chain E1:

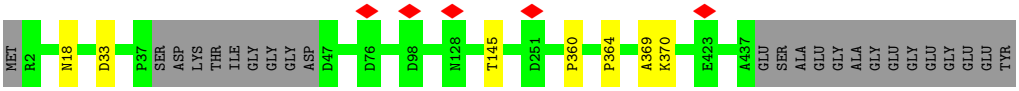




- Molecule 2: Tubulin alpha

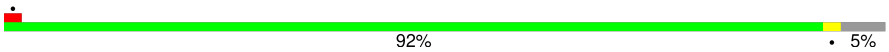
Chain E3:

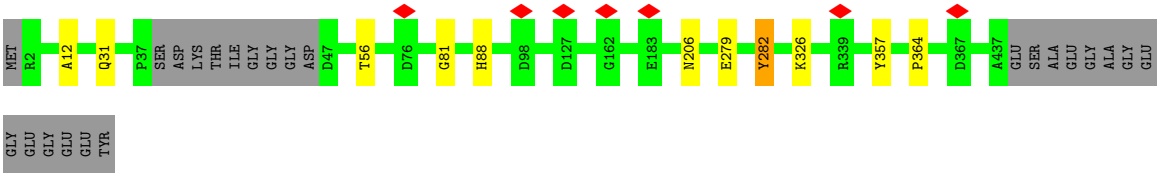




- Molecule 2: Tubulin alpha

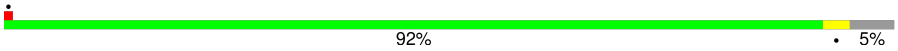
Chain E5:

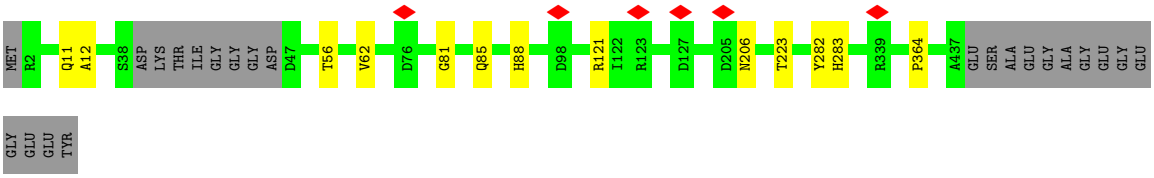




- Molecule 2: Tubulin alpha

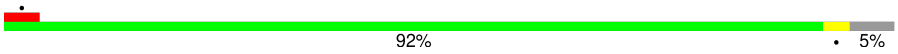
Chain E7:

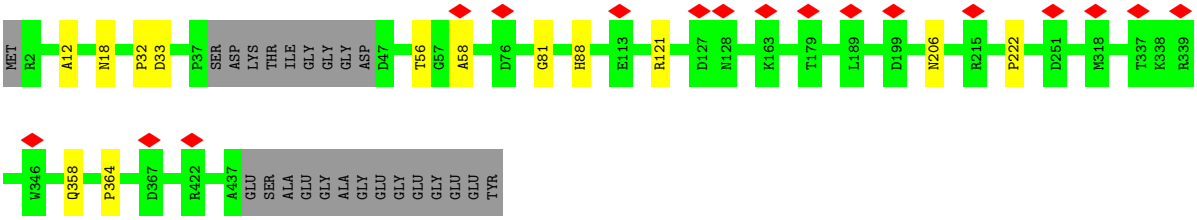




- Molecule 2: Tubulin alpha

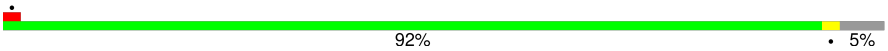
Chain E9:

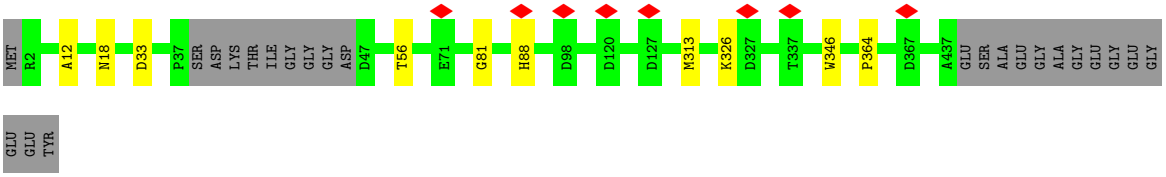




- Molecule 2: Tubulin alpha

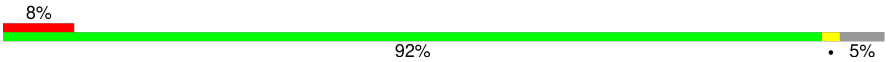
Chain F1:

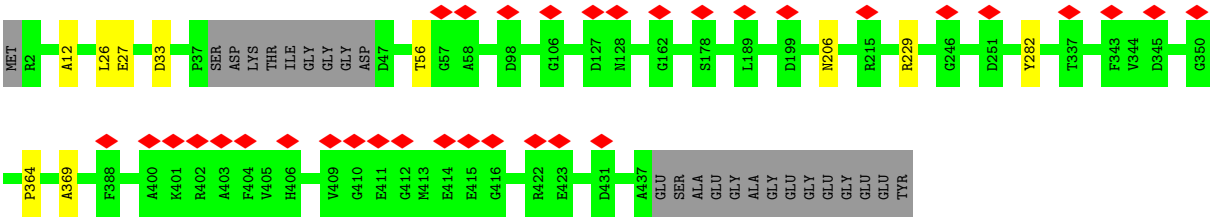




- Molecule 2: Tubulin alpha

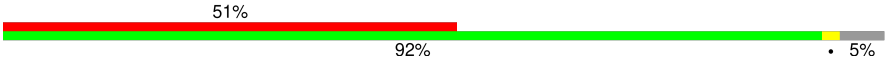
Chain F3:

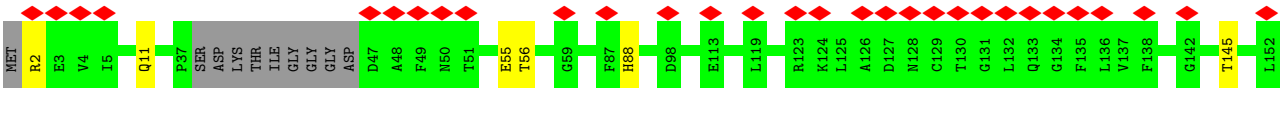


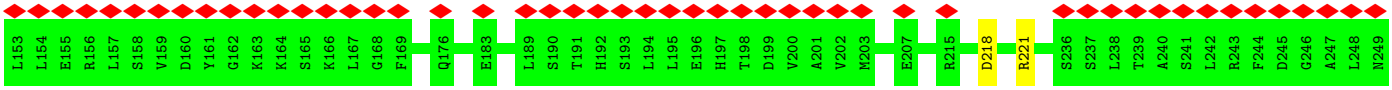


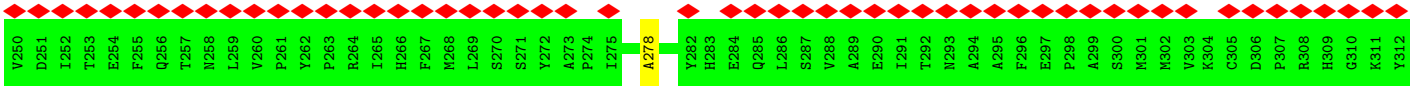
- Molecule 2: Tubulin alpha

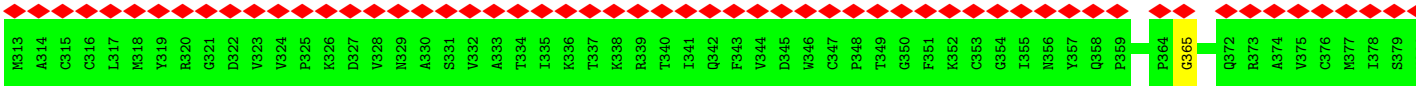
Chain F5:

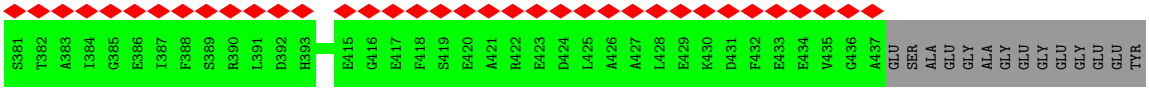






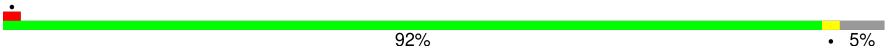


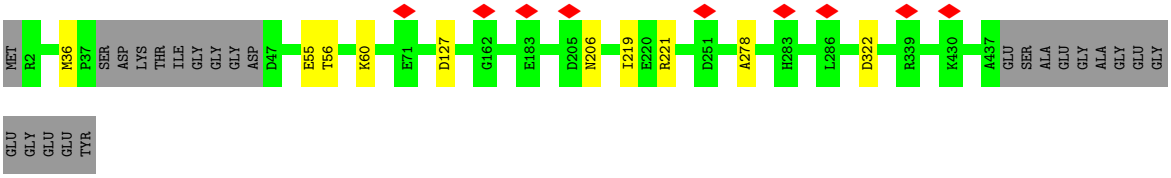




• Molecule 2: Tubulin alpha

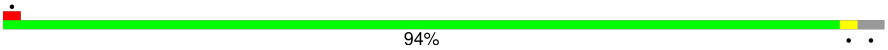
Chain F7:

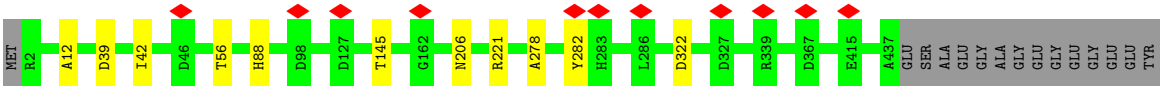




• Molecule 2: Tubulin alpha

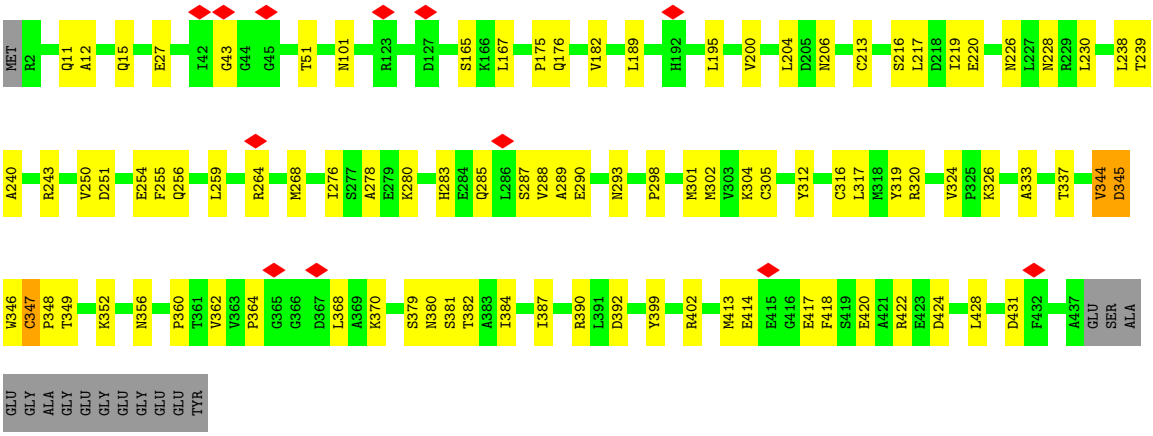
Chain F9:





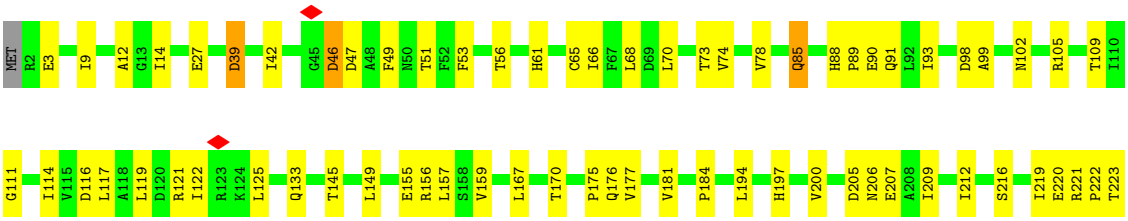
• Molecule 2: Tubulin alpha

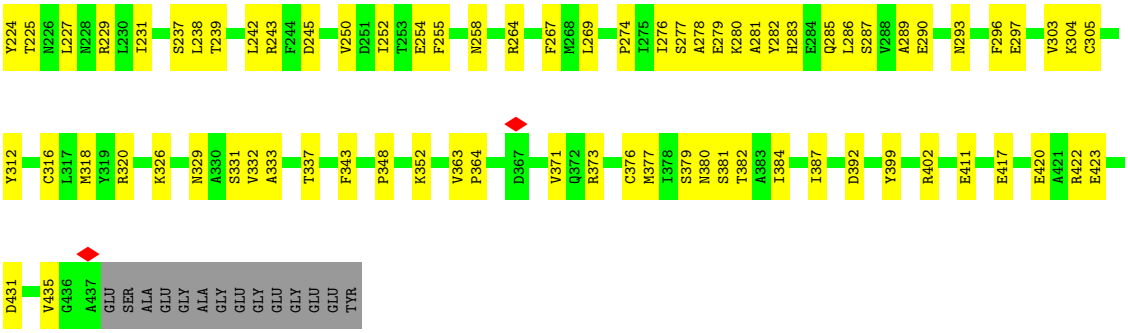
Chain G1:



• Molecule 2: Tubulin alpha

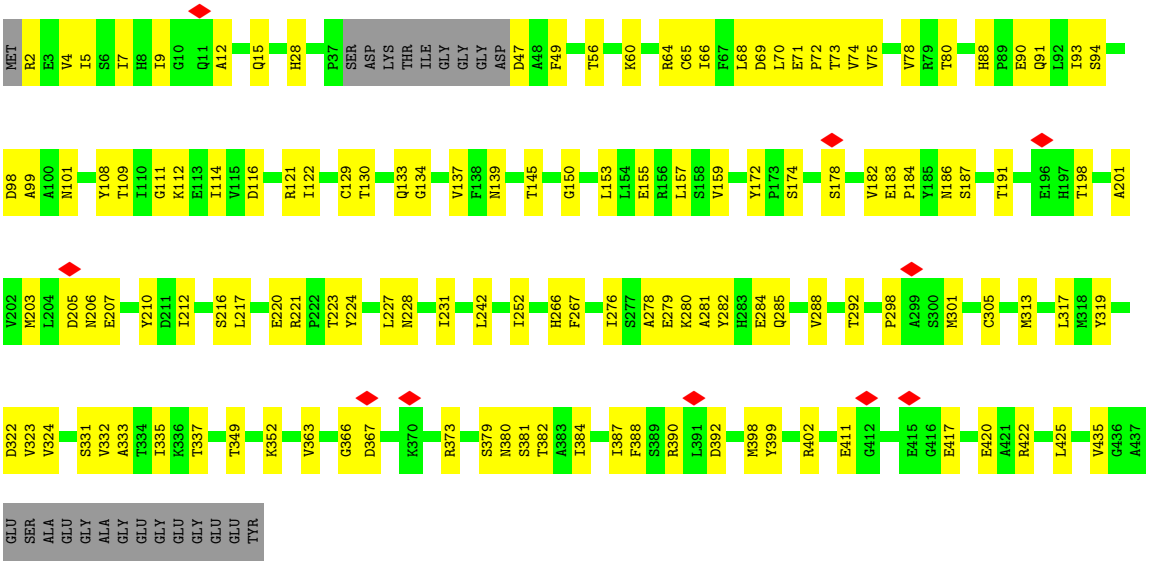
Chain G3:





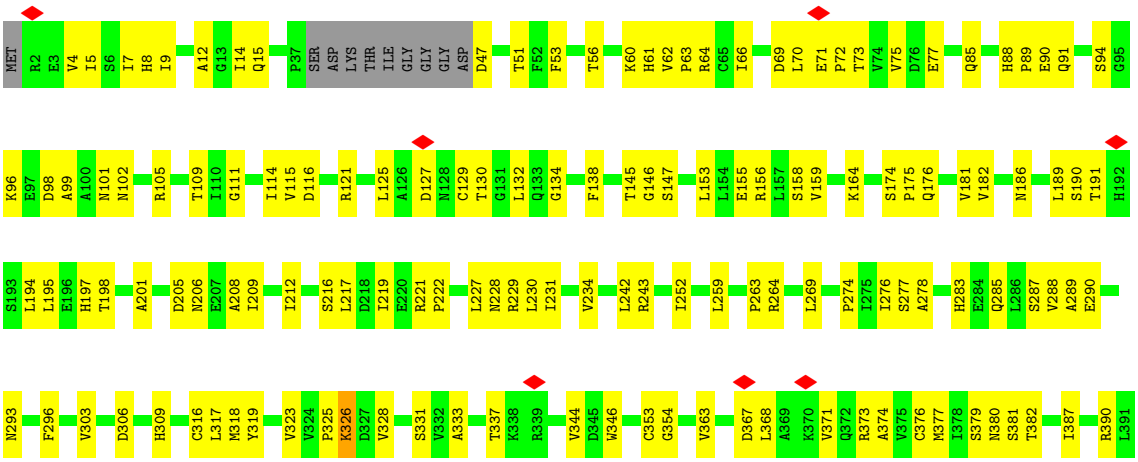
• Molecule 2: Tubulin alpha

Chain G5:



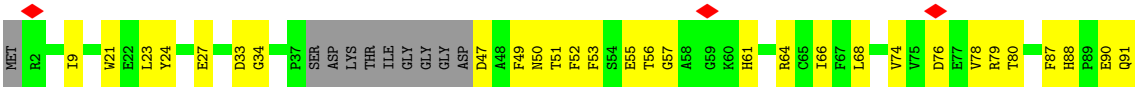
• Molecule 2: Tubulin alpha

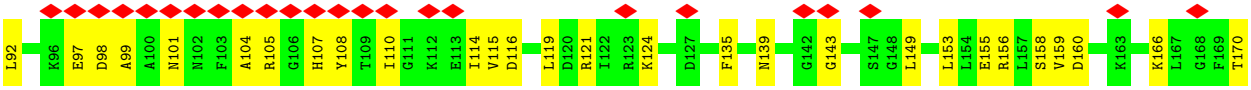
Chain G7:

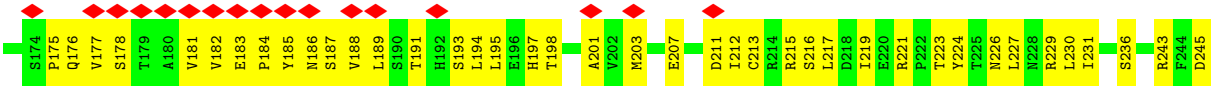


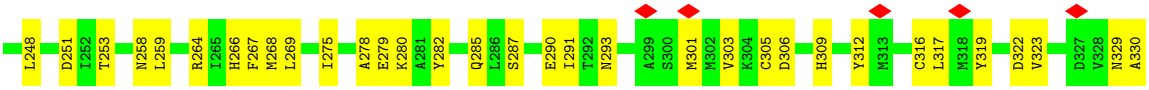
• Molecule 2: Tubulin alpha

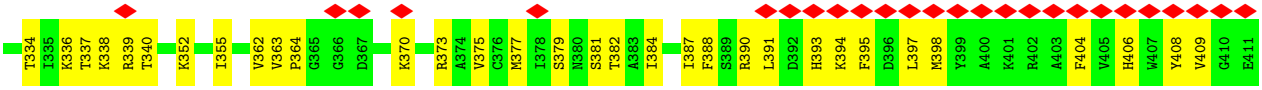
Chain G9:

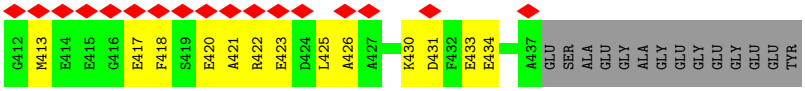






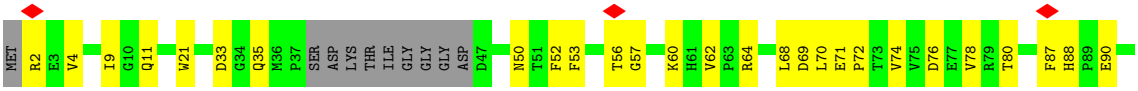


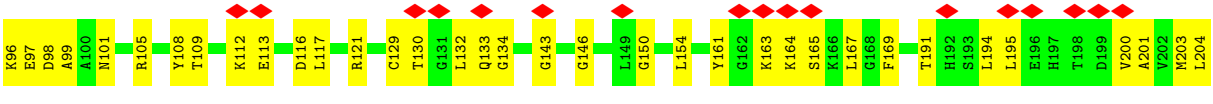


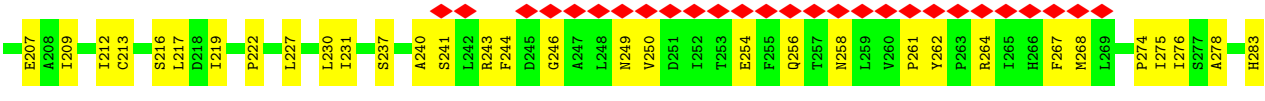


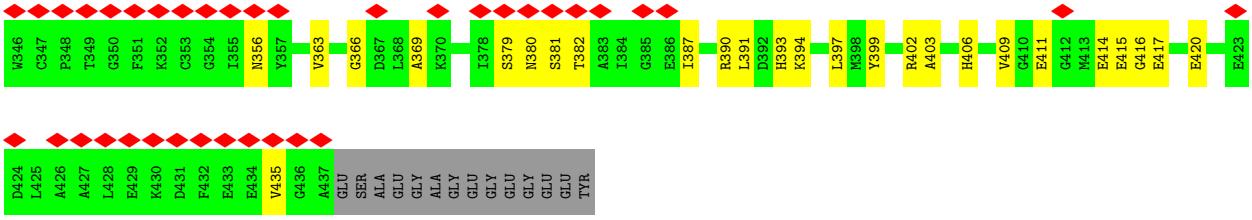
• Molecule 2: Tubulin alpha

Chain H1:



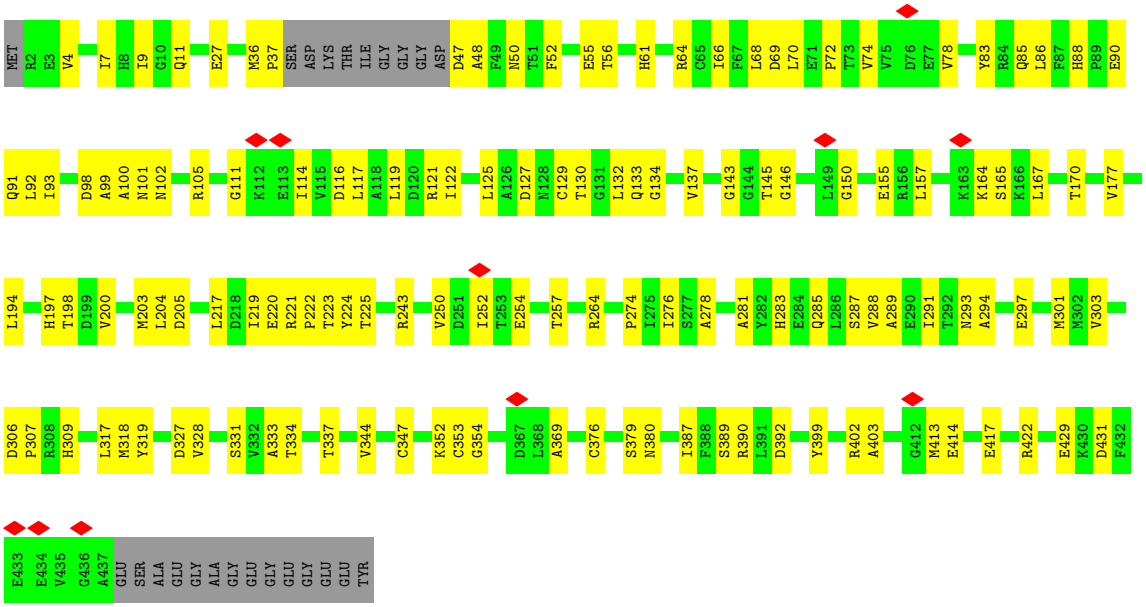






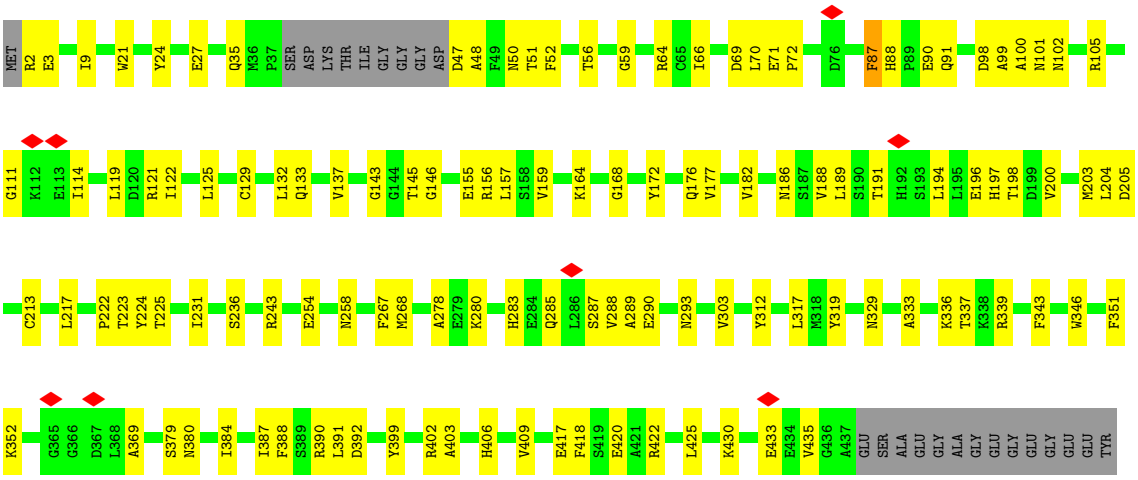
• Molecule 2: Tubulin alpha

Chain H3:



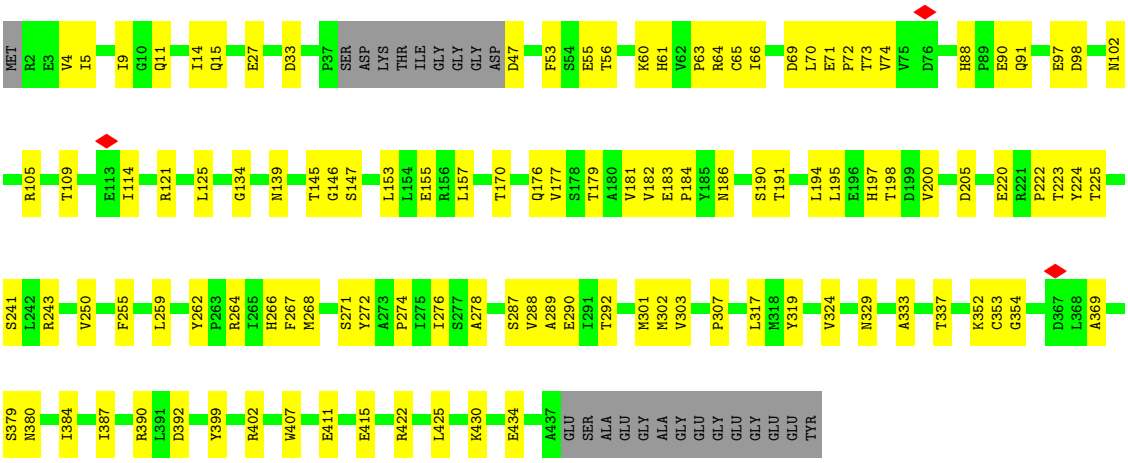
• Molecule 2: Tubulin alpha

Chain H5:



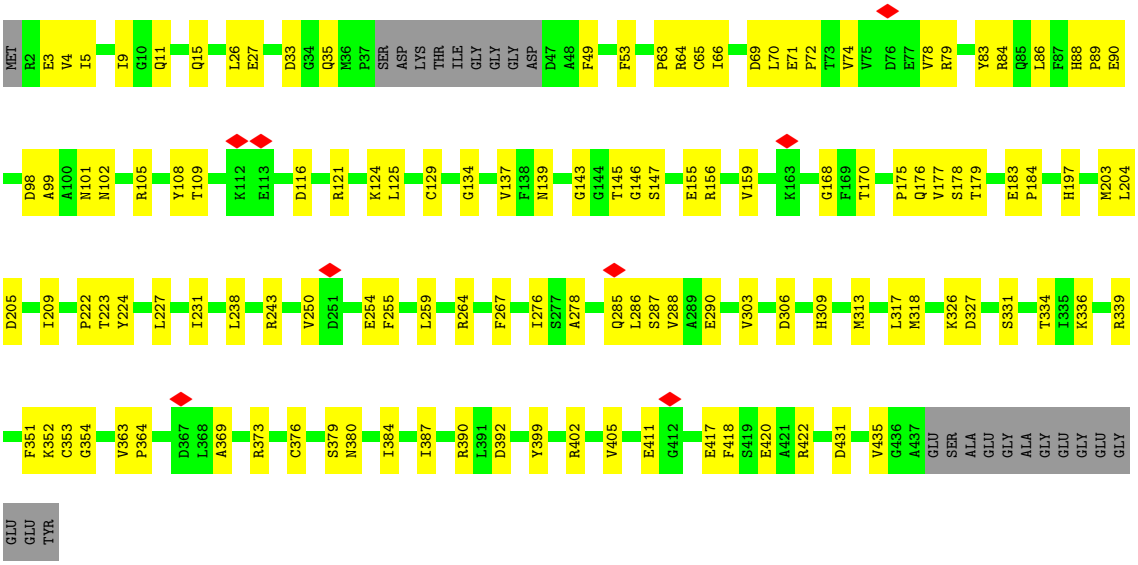
• Molecule 2: Tubulin alpha

Chain H7:



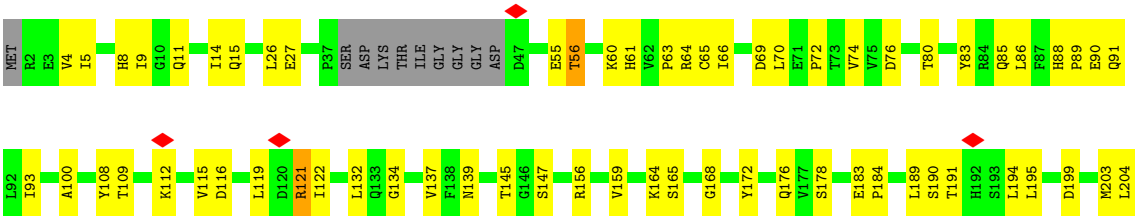
- Molecule 2: Tubulin alpha

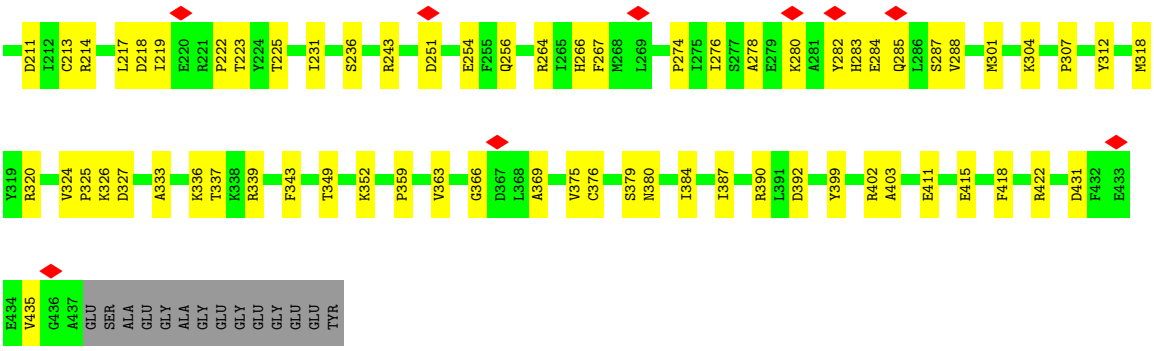
Chain H9:



- Molecule 2: Tubulin alpha

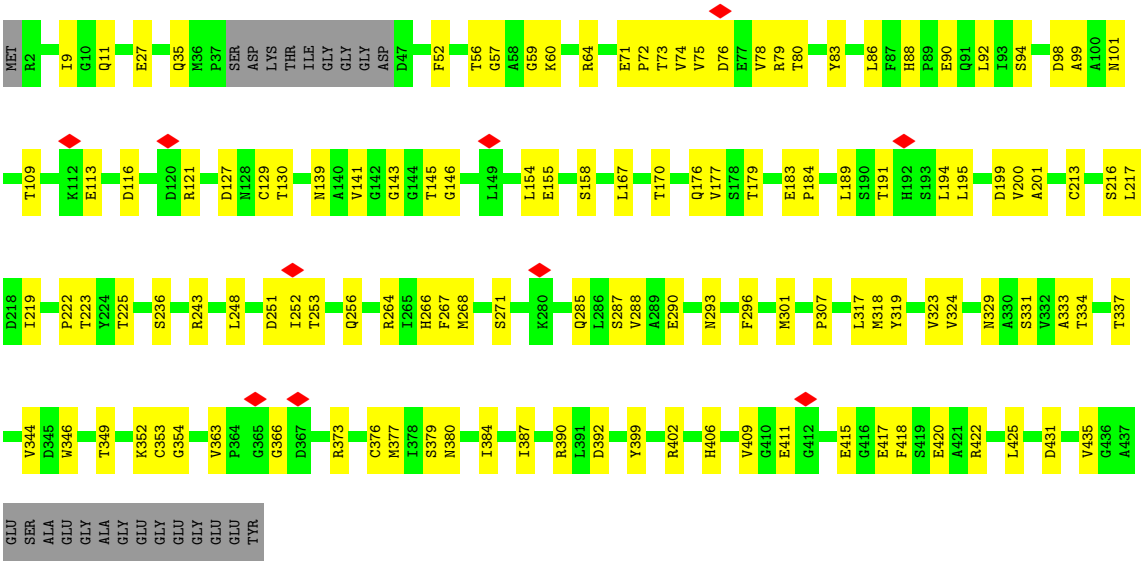
Chain I1:





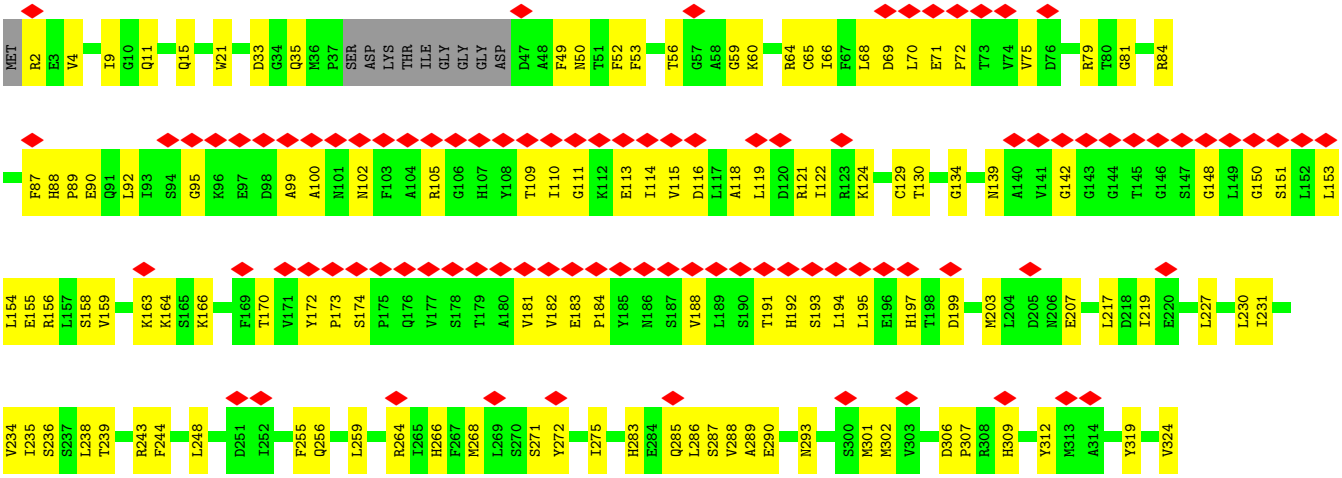
• Molecule 2: Tubulin alpha

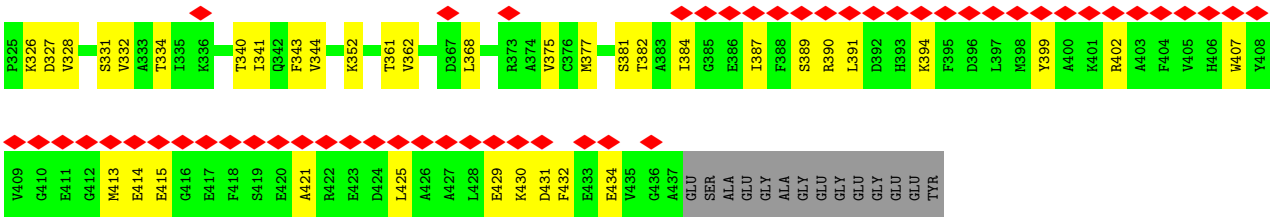
Chain I3:



• Molecule 2: Tubulin alpha

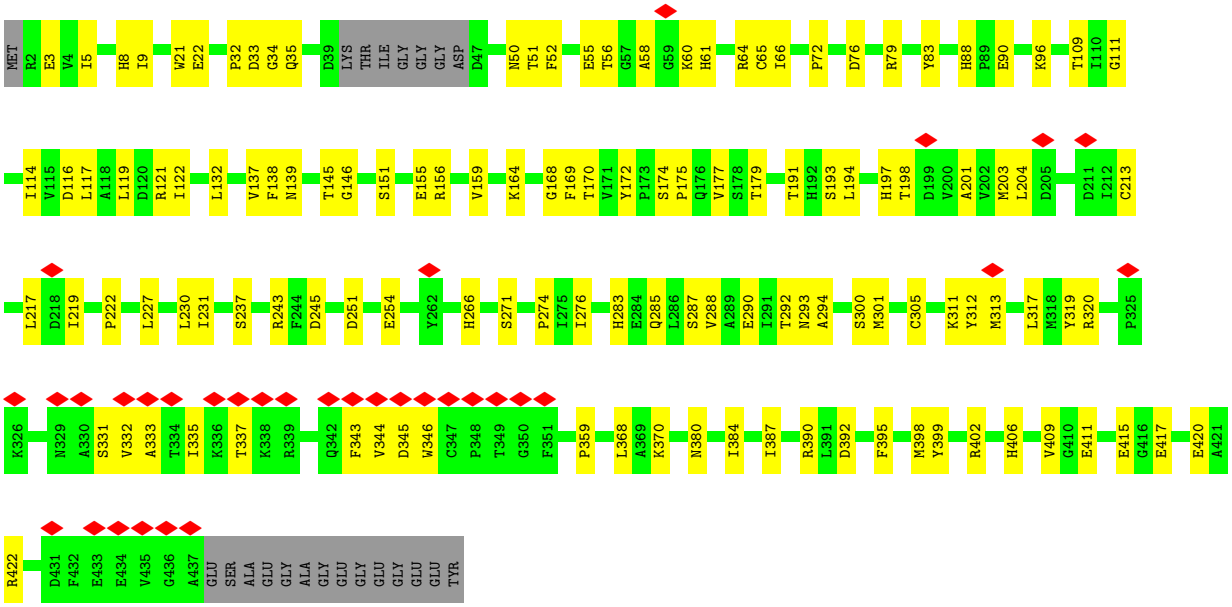
Chain I5:





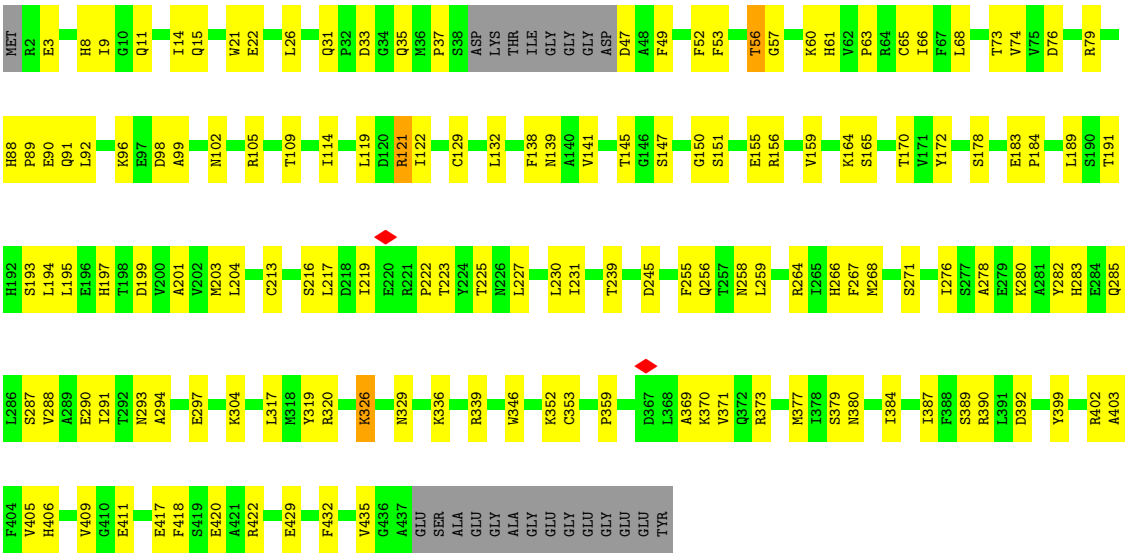
• Molecule 2: Tubulin alpha

Chain I7:



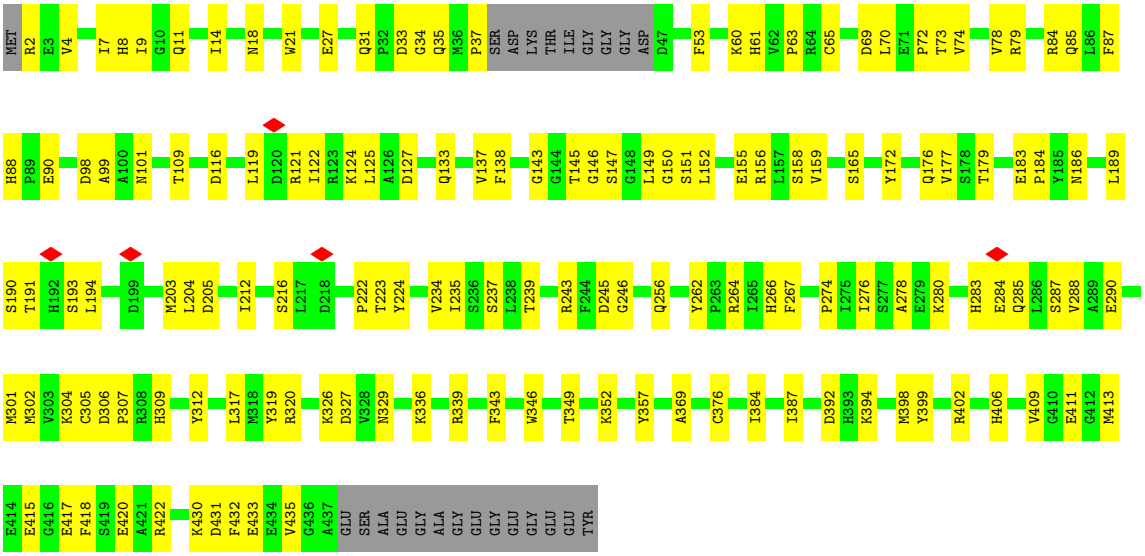
• Molecule 2: Tubulin alpha

Chain I9:



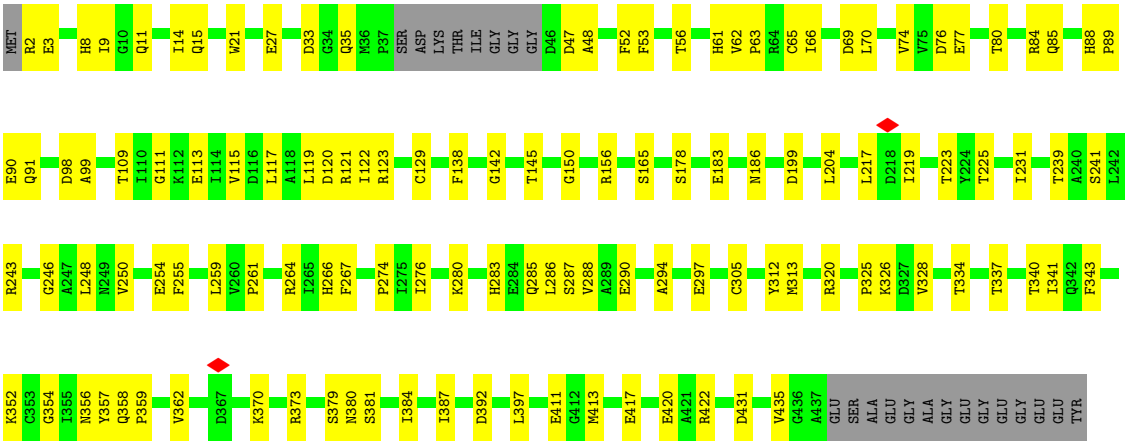
- Molecule 2: Tubulin alpha

Chain J1:



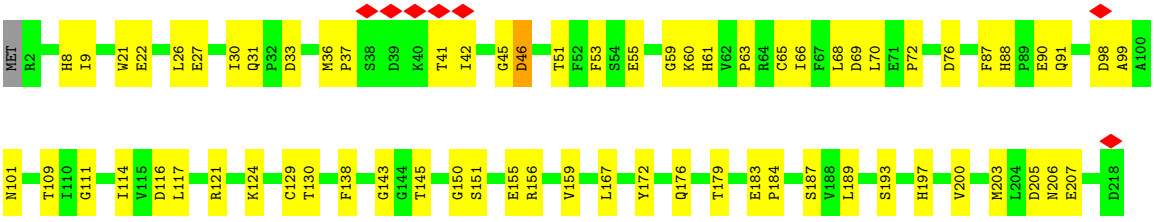
- Molecule 2: Tubulin alpha

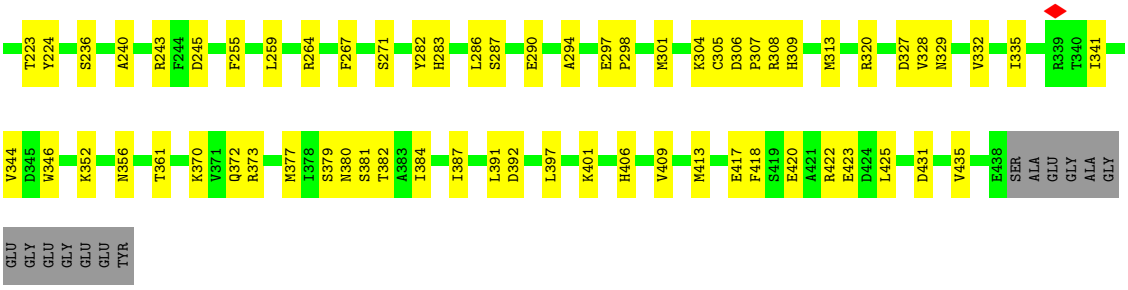
Chain J3:



- Molecule 2: Tubulin alpha

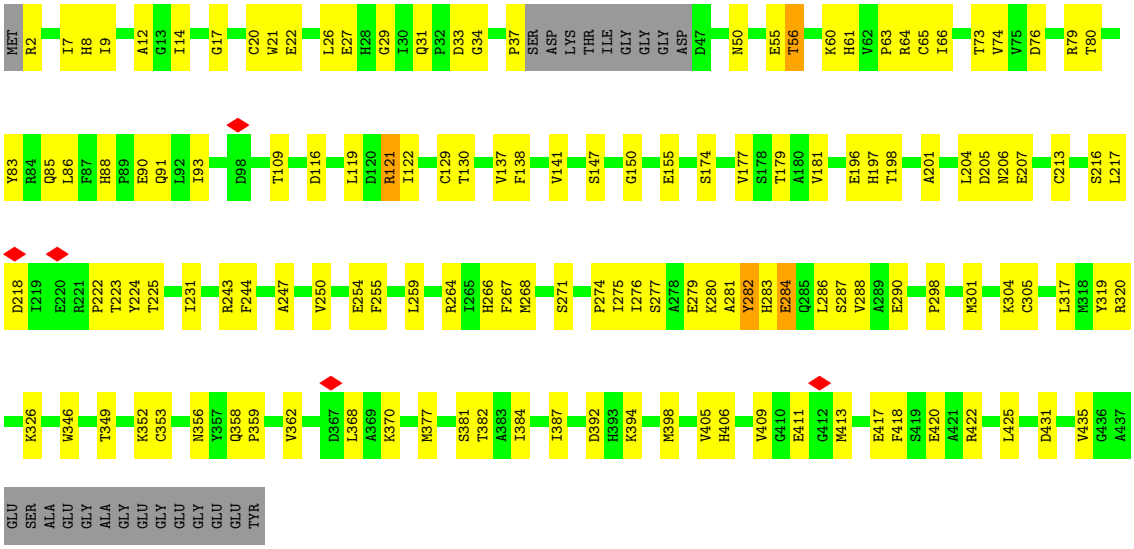
Chain J5:





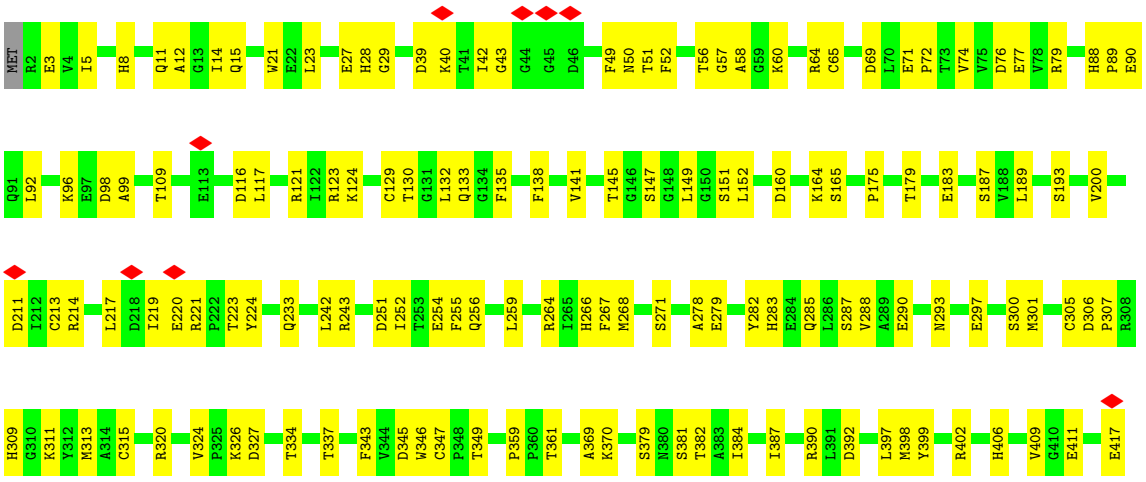
- Molecule 2: Tubulin alpha

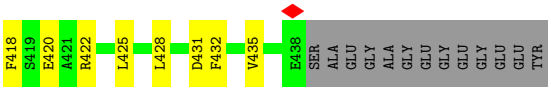
Chain J7:



- Molecule 2: Tubulin alpha

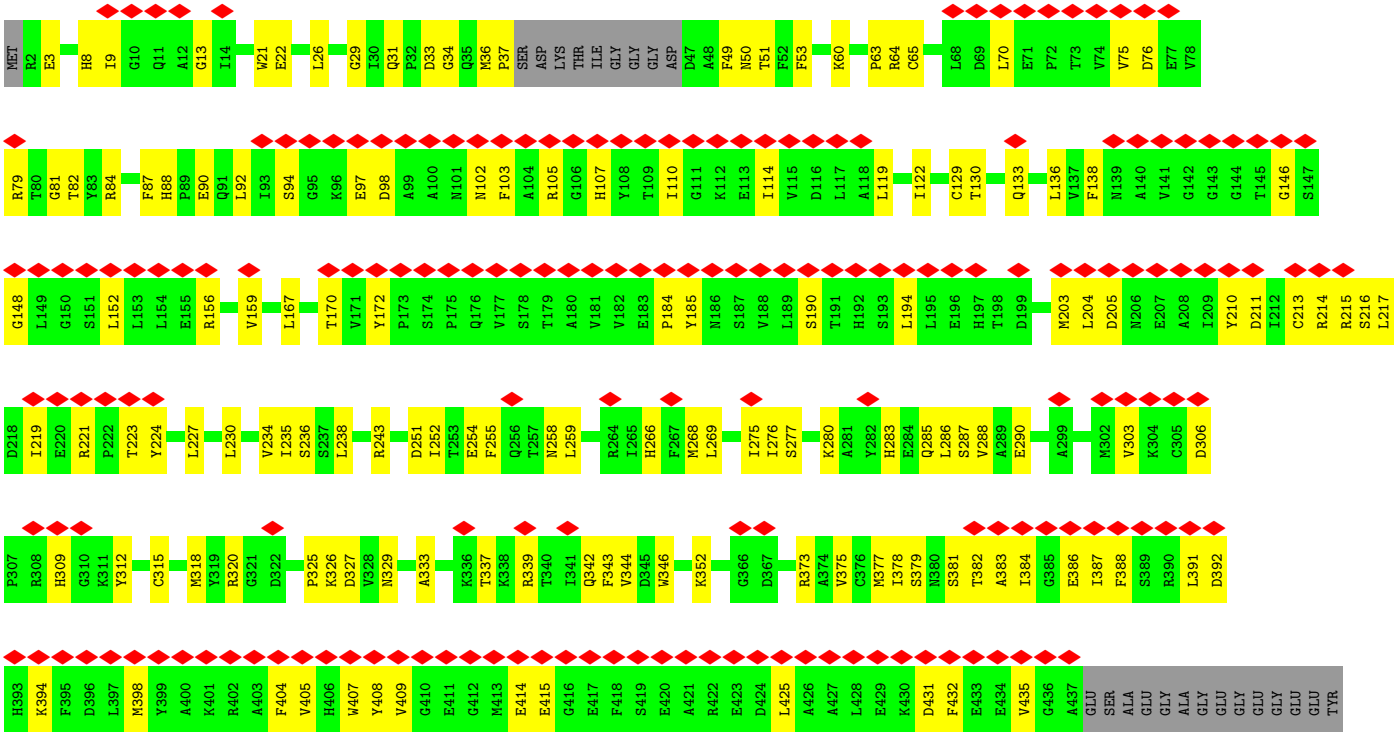
Chain J9:





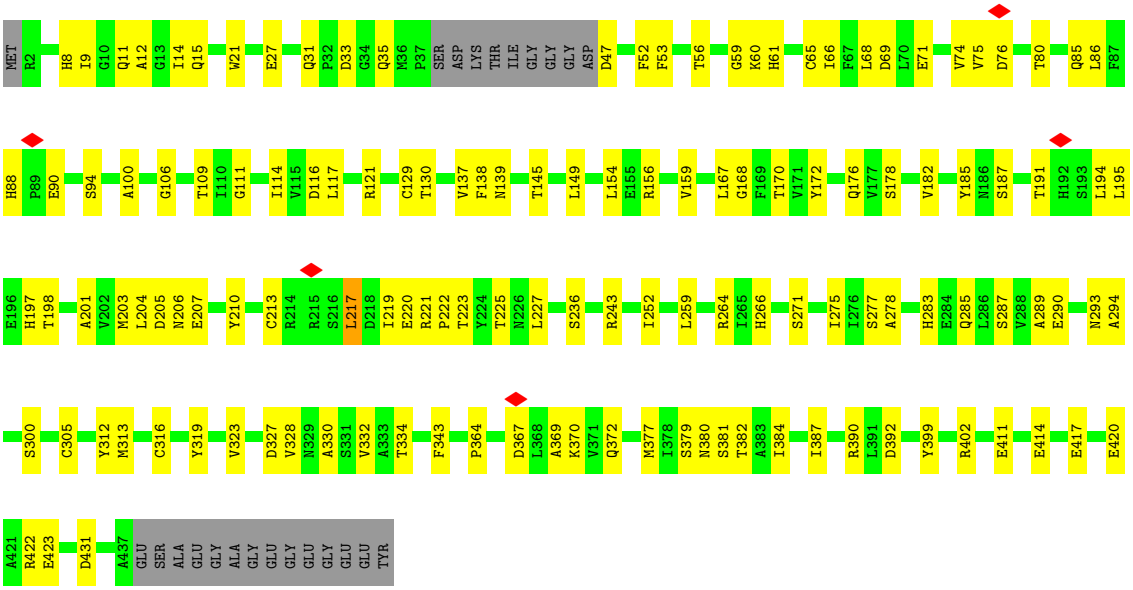
• Molecule 2: Tubulin alpha

Chain K1:



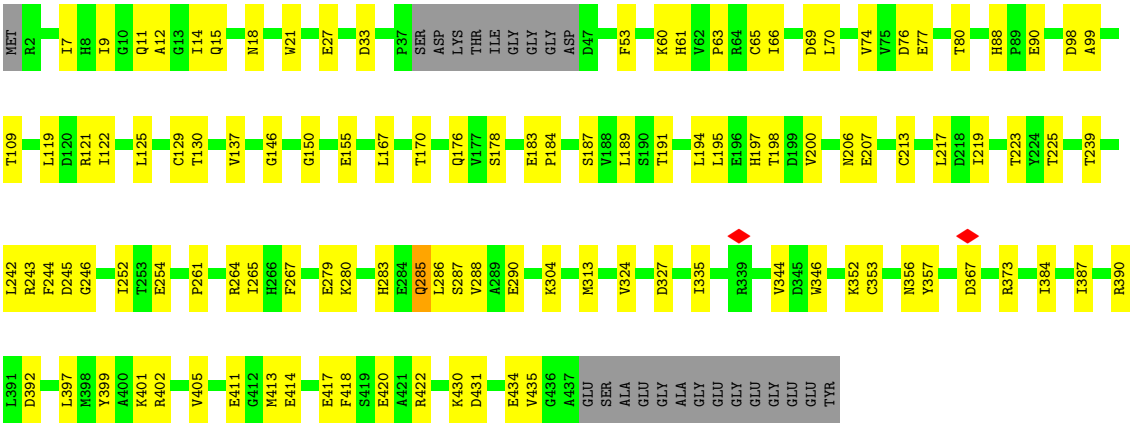
• Molecule 2: Tubulin alpha

Chain K3:



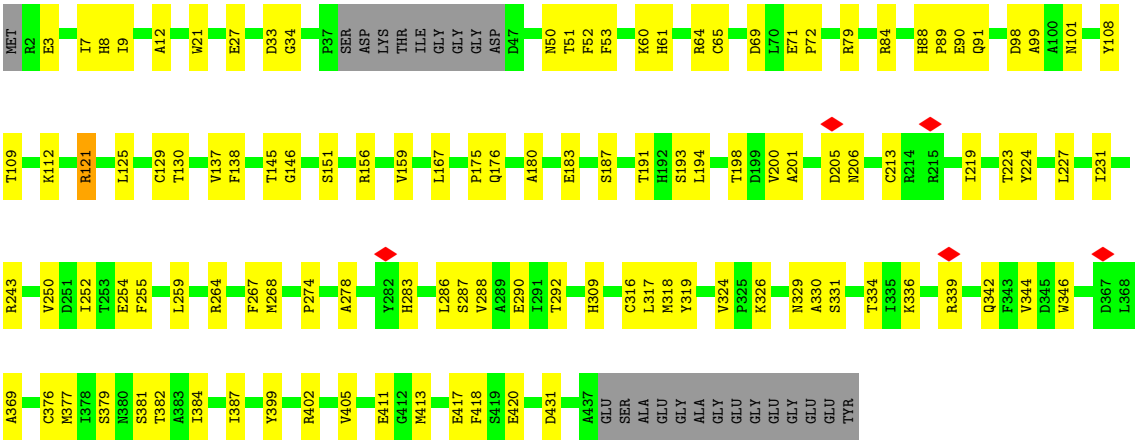
- Molecule 2: Tubulin alpha

Chain K5: 70% 24% 5%



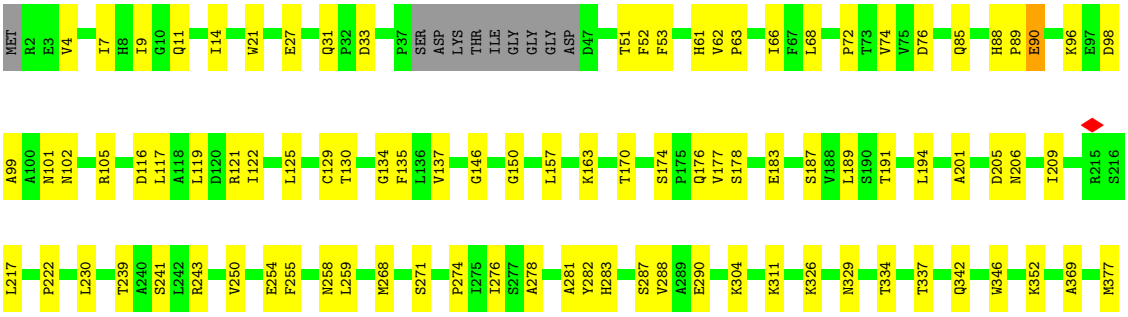
- Molecule 2: Tubulin alpha

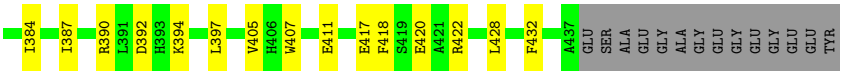
Chain K7: 70% 25% 5%



- Molecule 2: Tubulin alpha

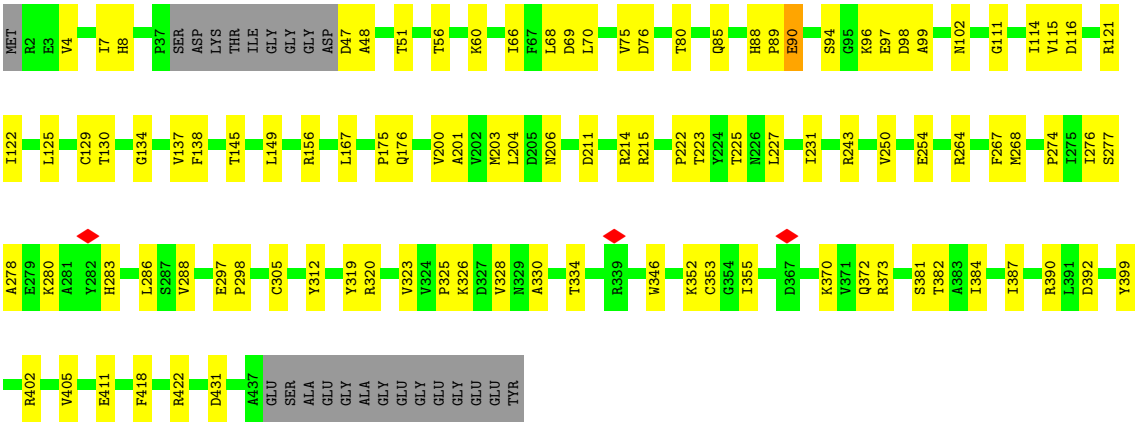
Chain K9: 71% 24% 5%





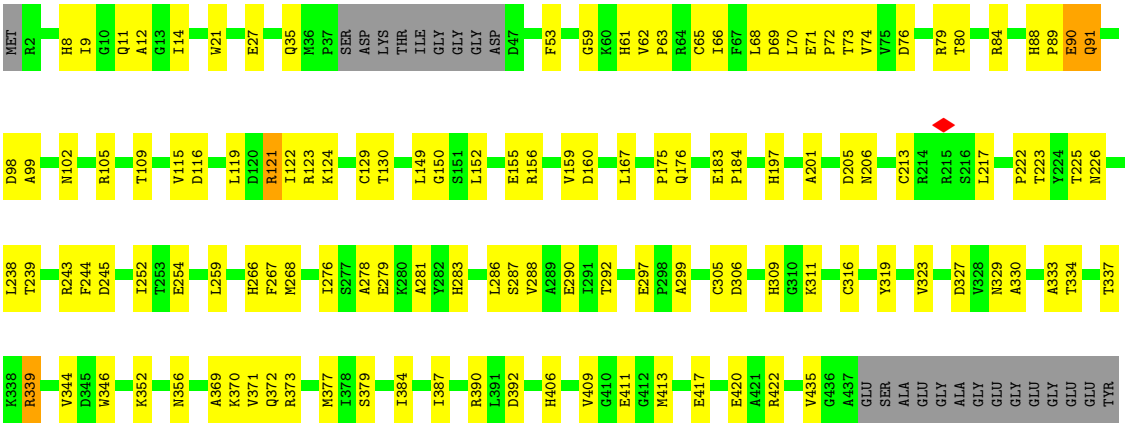
• Molecule 2: Tubulin alpha

Chain L1:



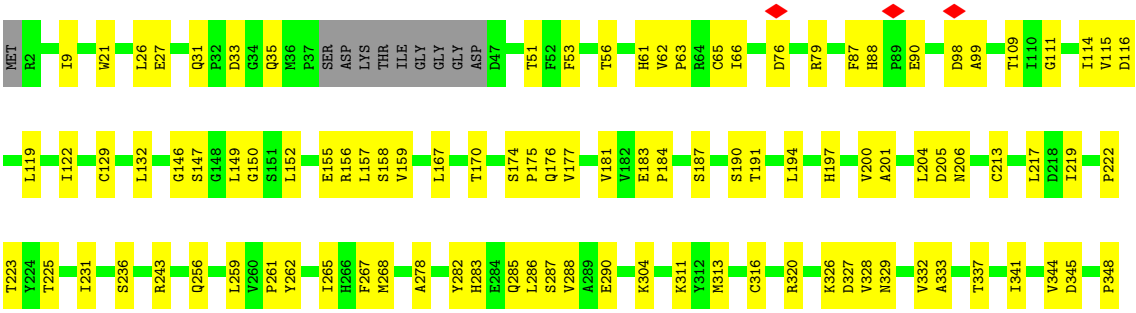
• Molecule 2: Tubulin alpha

Chain L3:



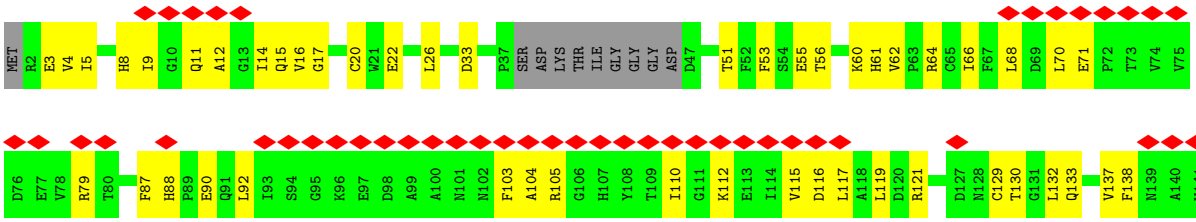
• Molecule 2: Tubulin alpha

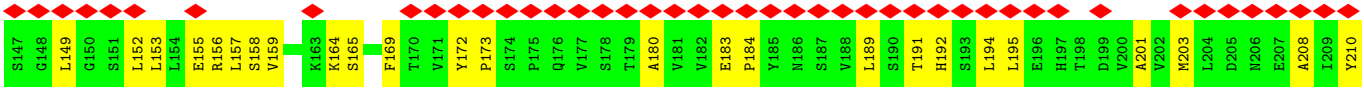
Chain L5:

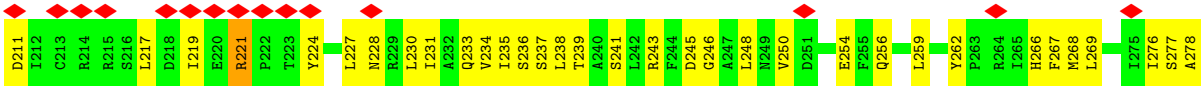


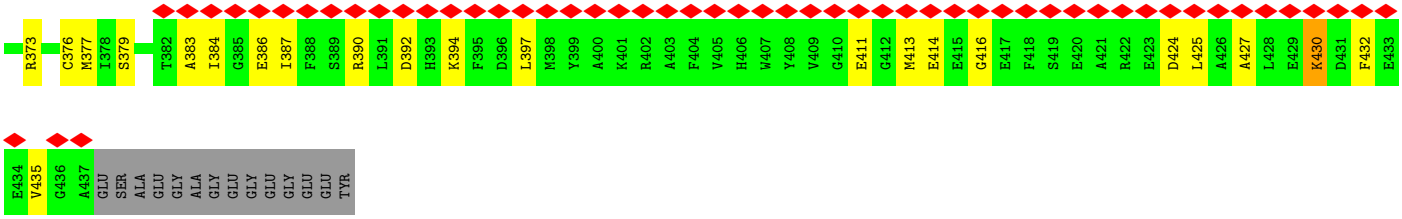
• Molecule 2: Tubulin alpha

Chain L7:



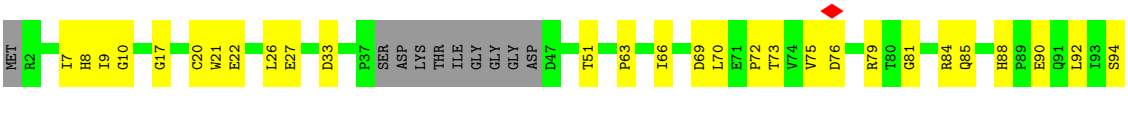


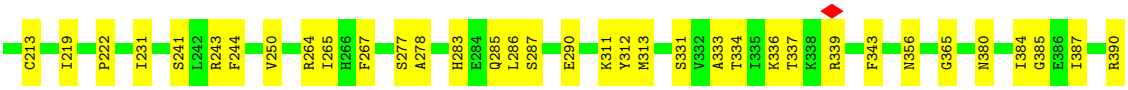


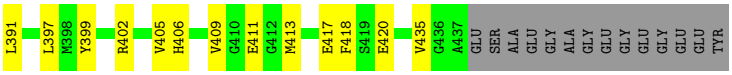


• Molecule 2: Tubulin alpha

Chain L9:

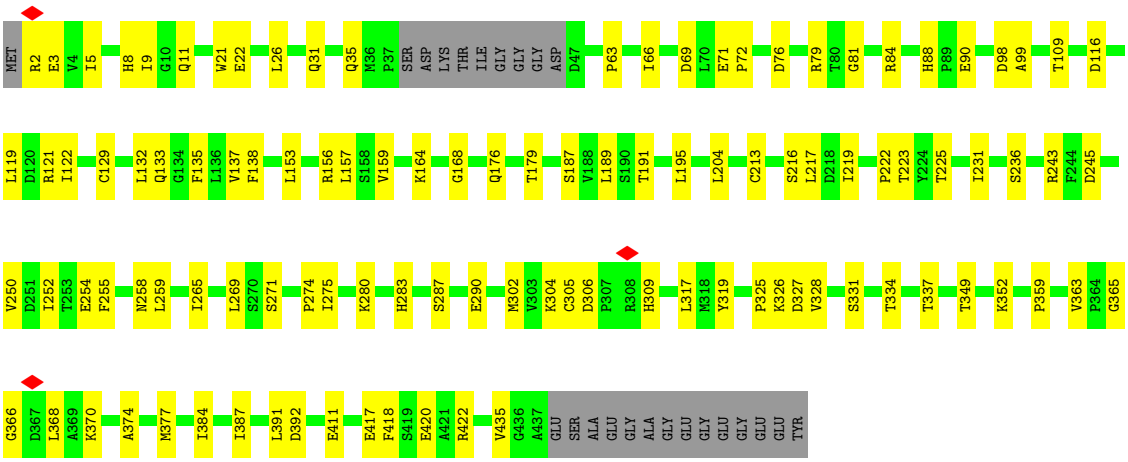






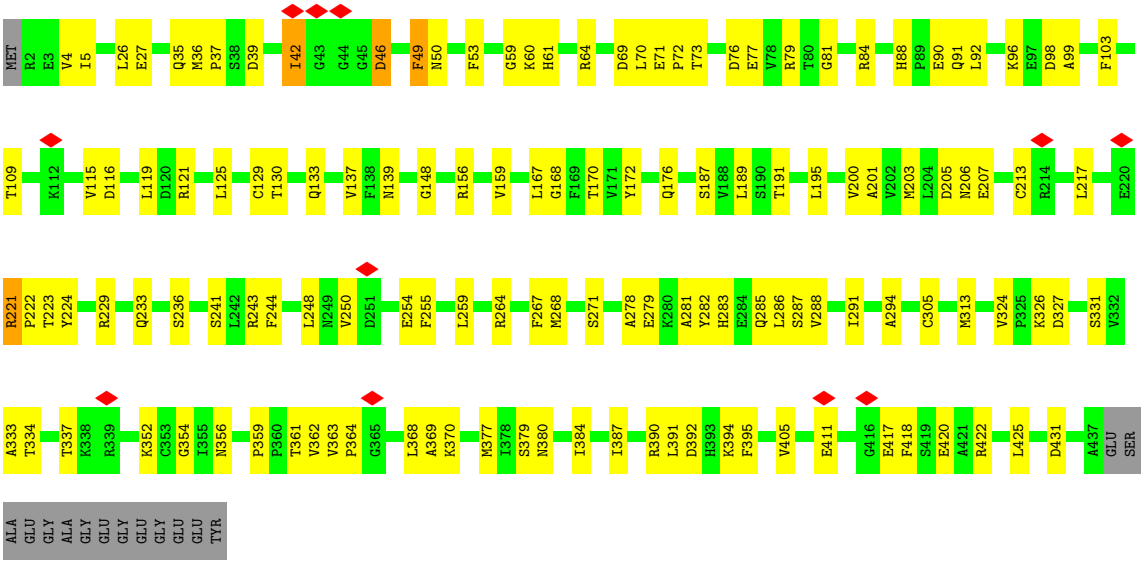
• Molecule 2: Tubulin alpha

Chain M1:



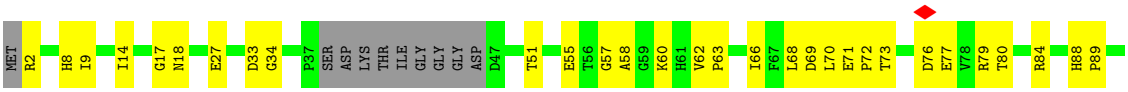
• Molecule 2: Tubulin alpha

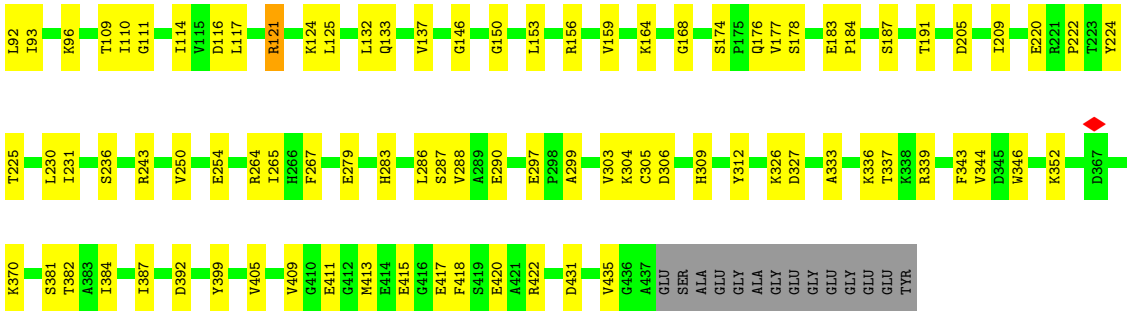
Chain M3:



• Molecule 2: Tubulin alpha

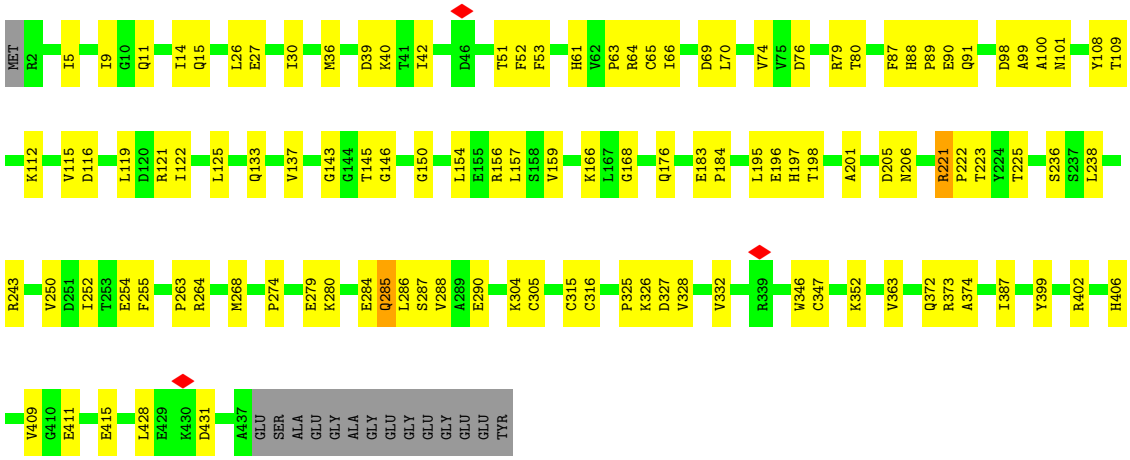
Chain M5:





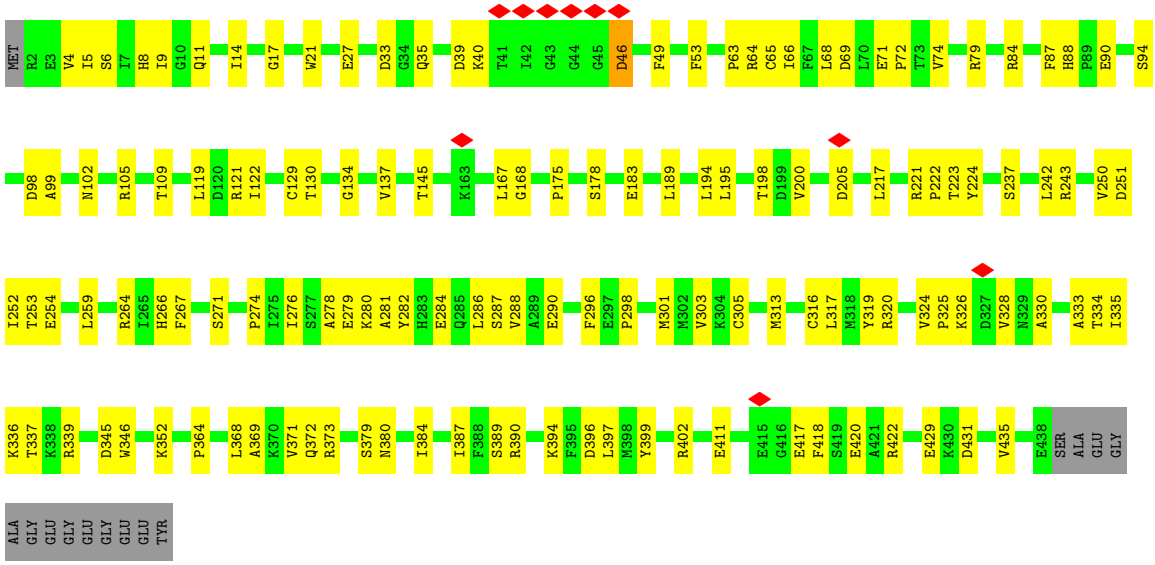
- Molecule 2: Tubulin alpha

Chain M7:



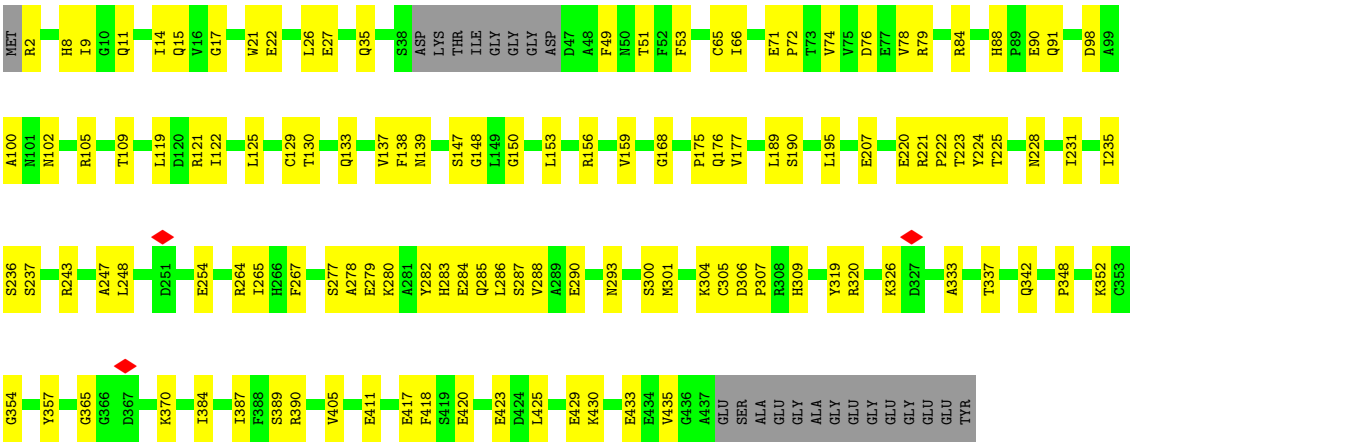
- Molecule 2: Tubulin alpha

Chain M9:



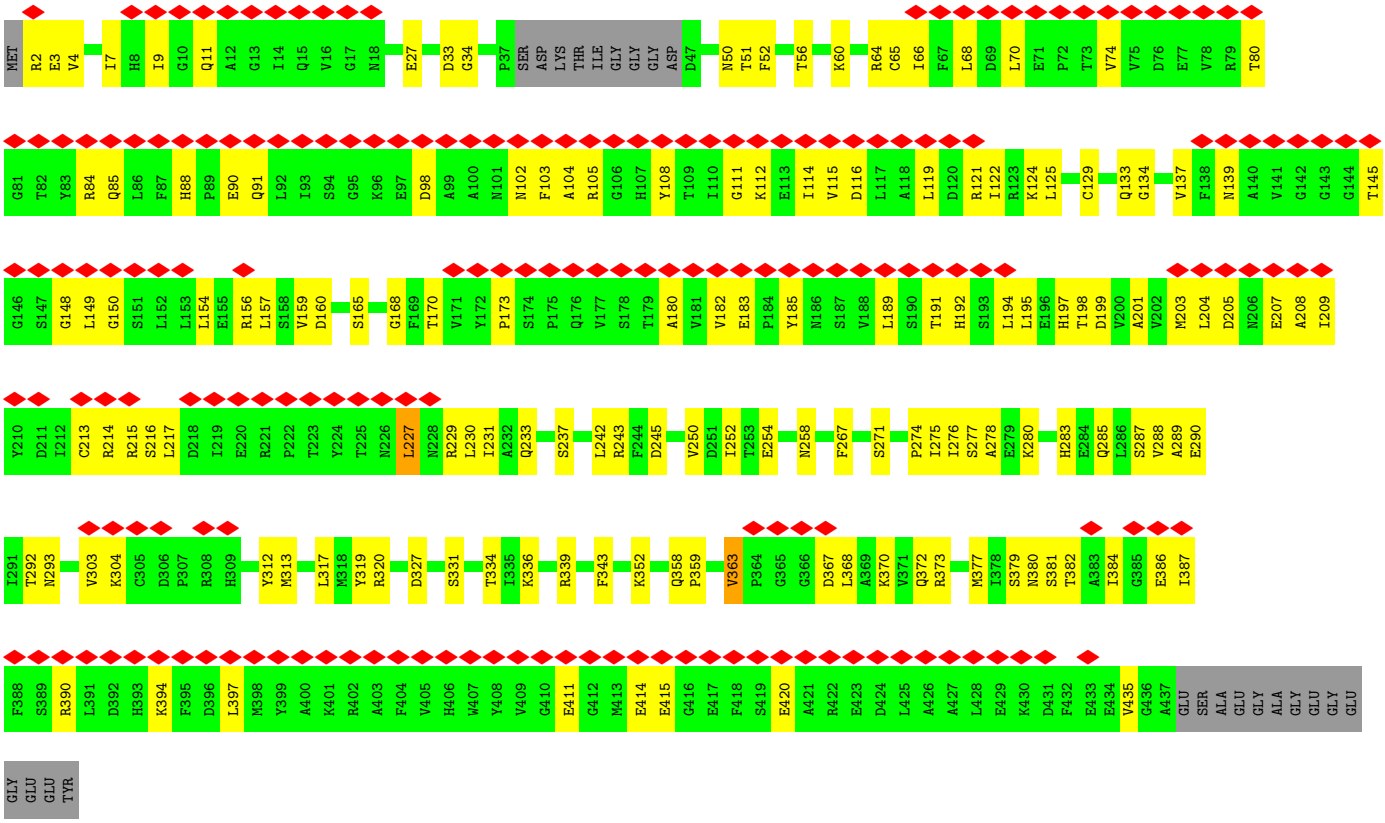
- Molecule 2: Tubulin alpha

Chain N1: 68% 27% 5%



- Molecule 2: Tubulin alpha

Chain N3: 42% 61% 33% 5%

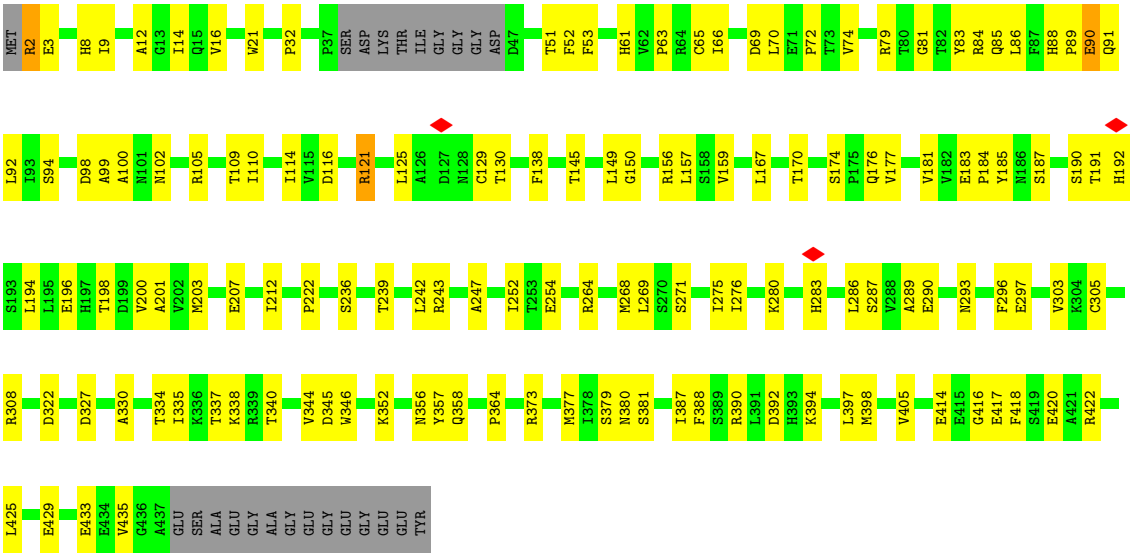


- Molecule 2: Tubulin alpha

Chain N5: 66% 28% 5%

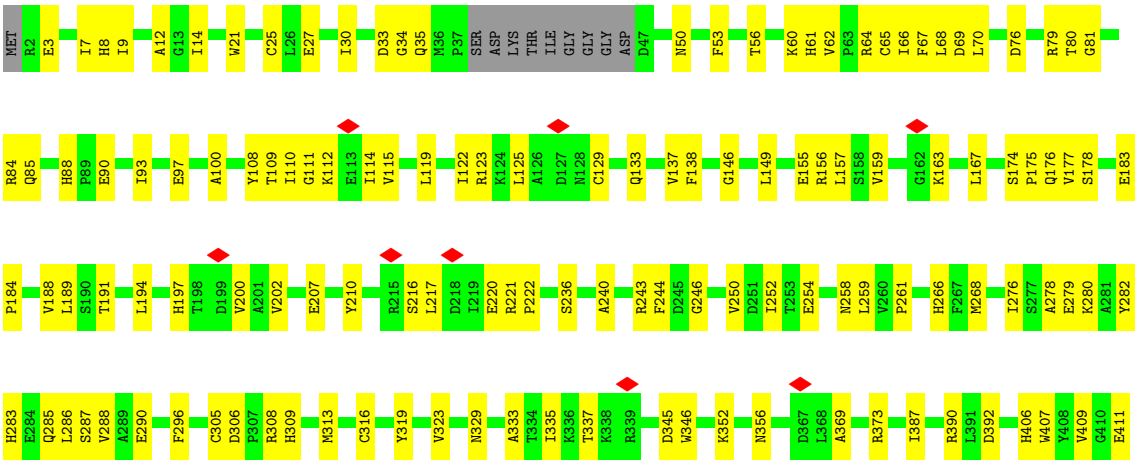
- Molecule 2: Tubulin alpha

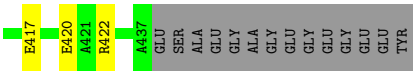
Chain N7:



- Molecule 2: Tubulin alpha

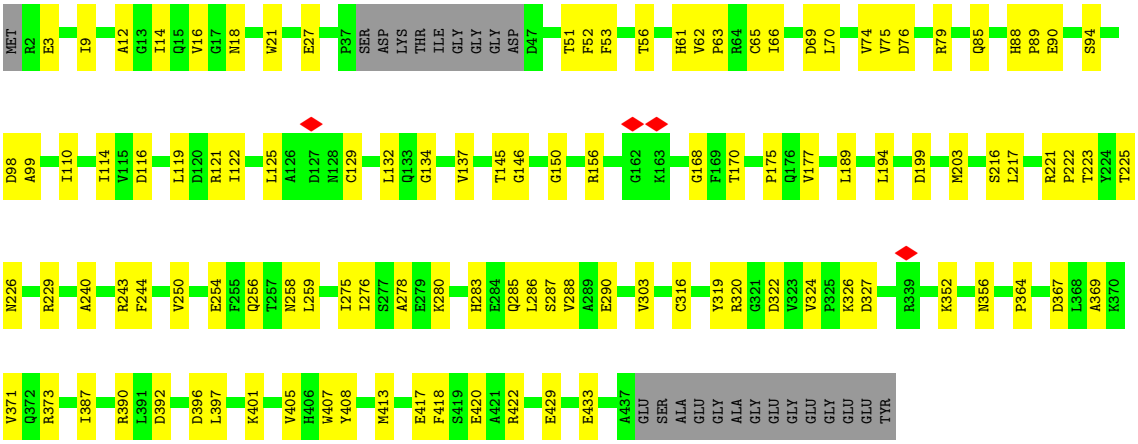
Chain N9:





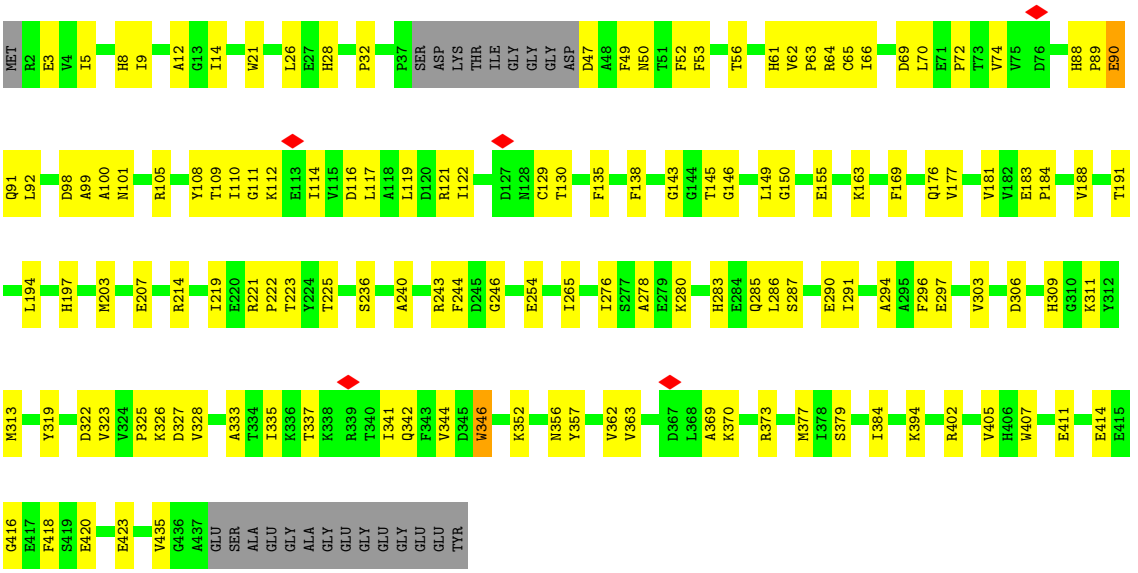
• Molecule 2: Tubulin alpha

Chain O1:



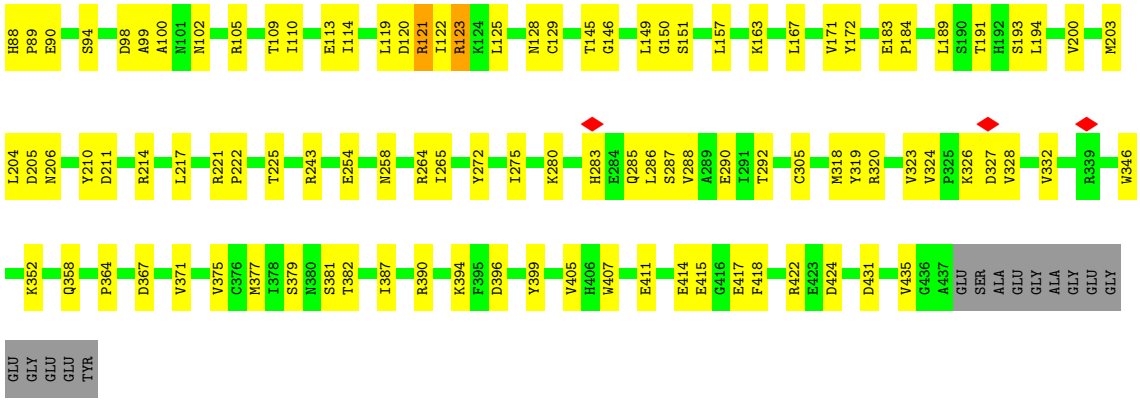
• Molecule 2: Tubulin alpha

Chain O3:



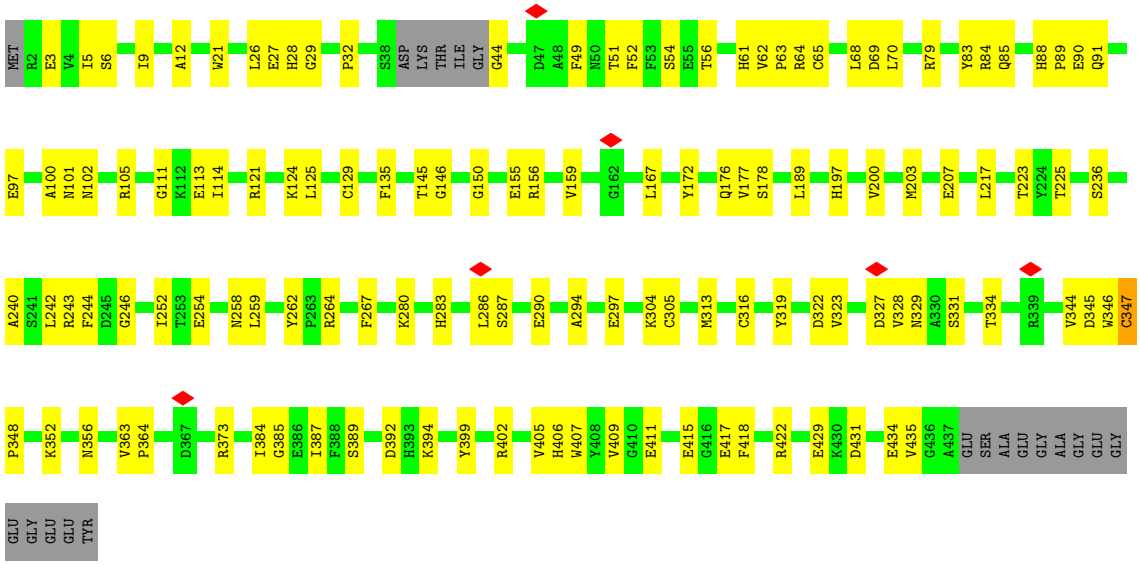
• Molecule 2: Tubulin alpha

Chain O5:



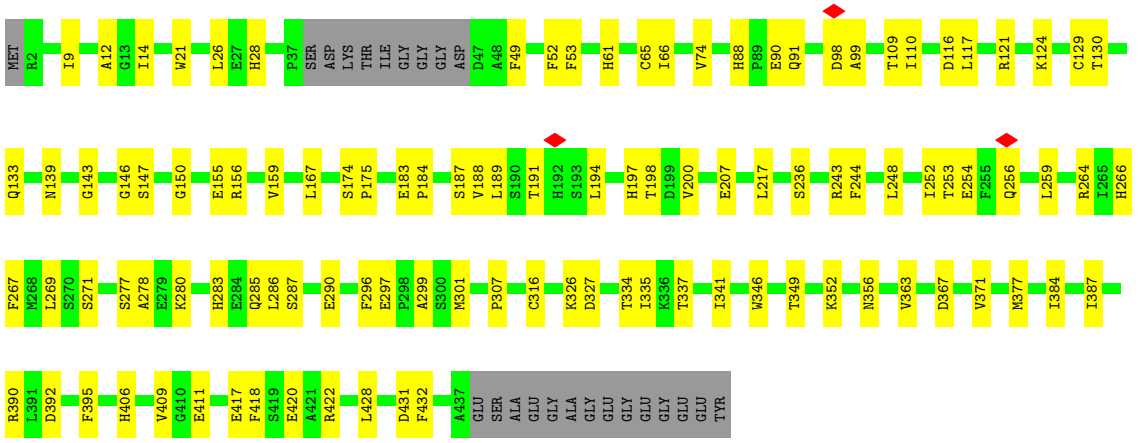
• Molecule 2: Tubulin alpha

Chain O7:



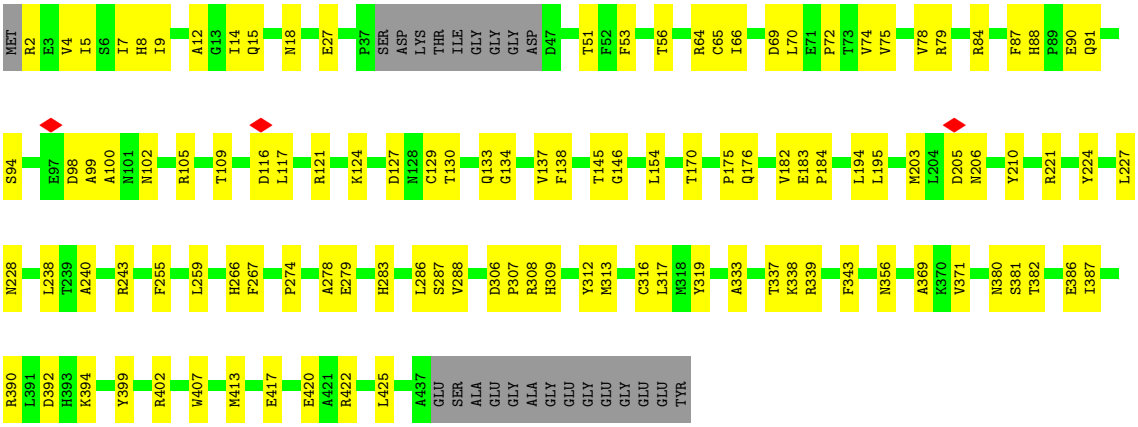
• Molecule 2: Tubulin alpha

Chain O9:



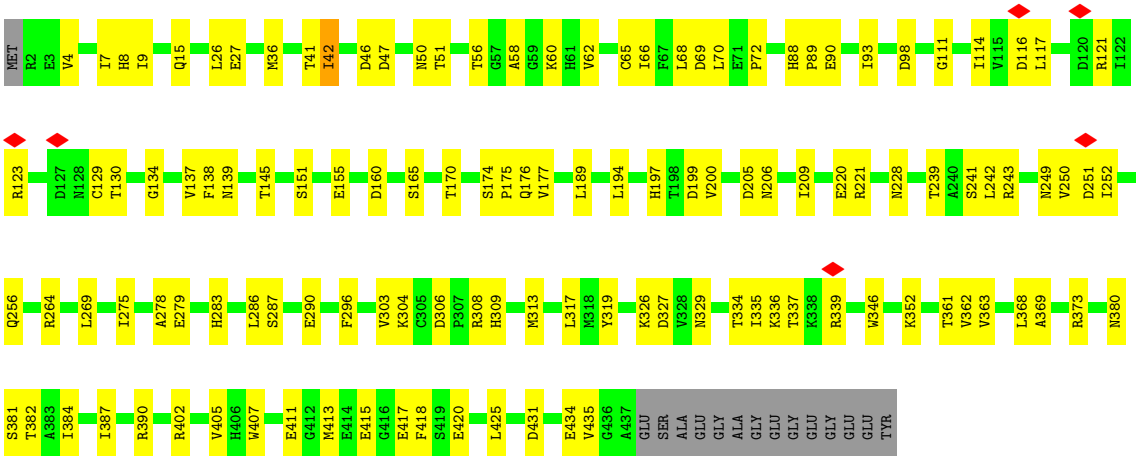
- Molecule 2: Tubulin alpha

Chain P3:



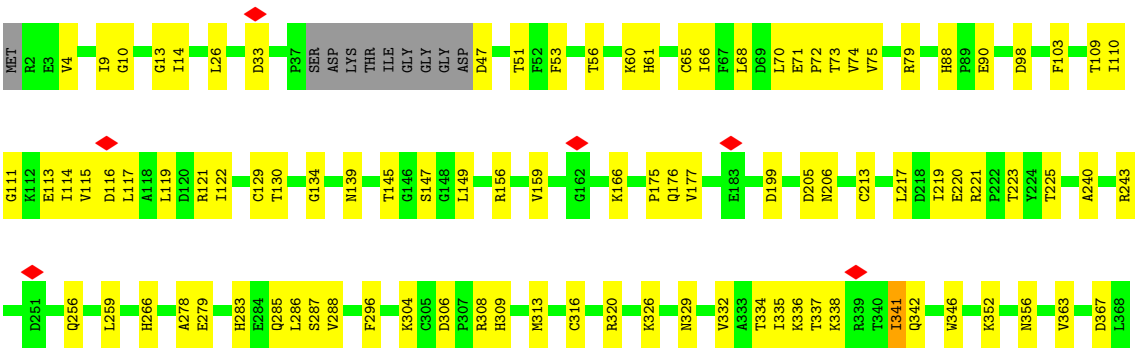
- Molecule 2: Tubulin alpha

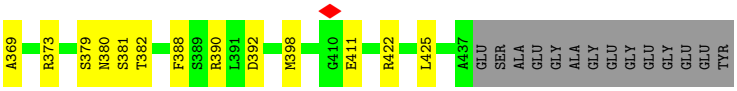
Chain P5:



- Molecule 2: Tubulin alpha

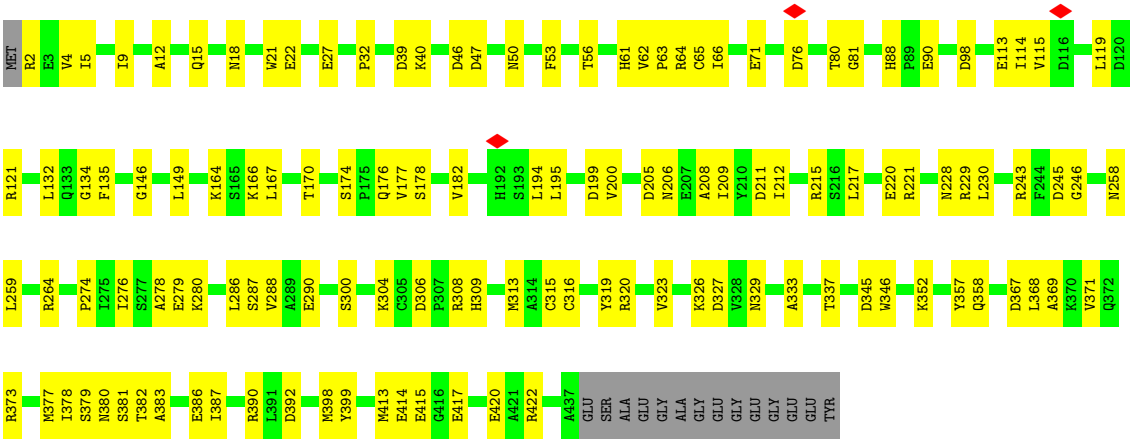
Chain P7:





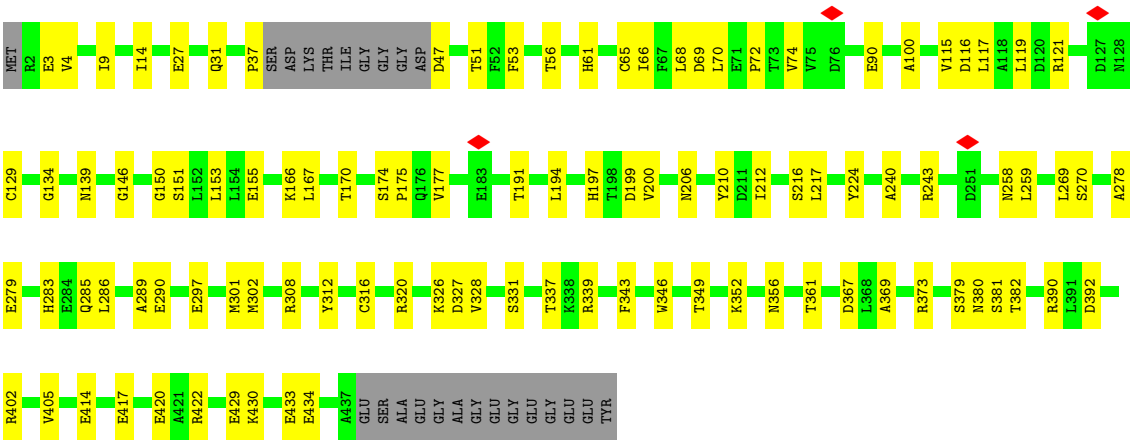
• Molecule 2: Tubulin alpha

Chain P9:



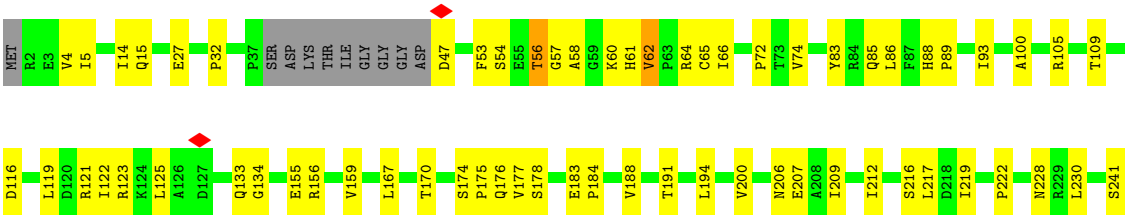
• Molecule 2: Tubulin alpha

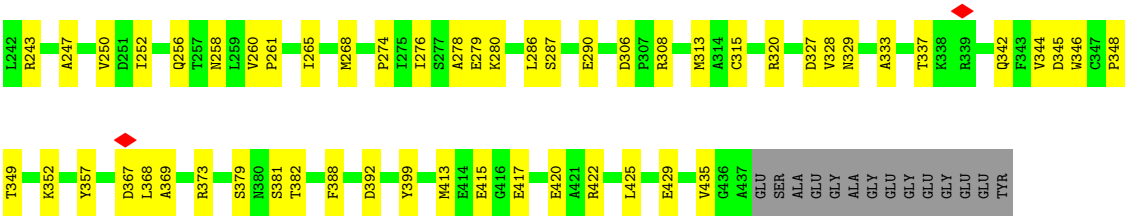
Chain Q1:



• Molecule 2: Tubulin alpha

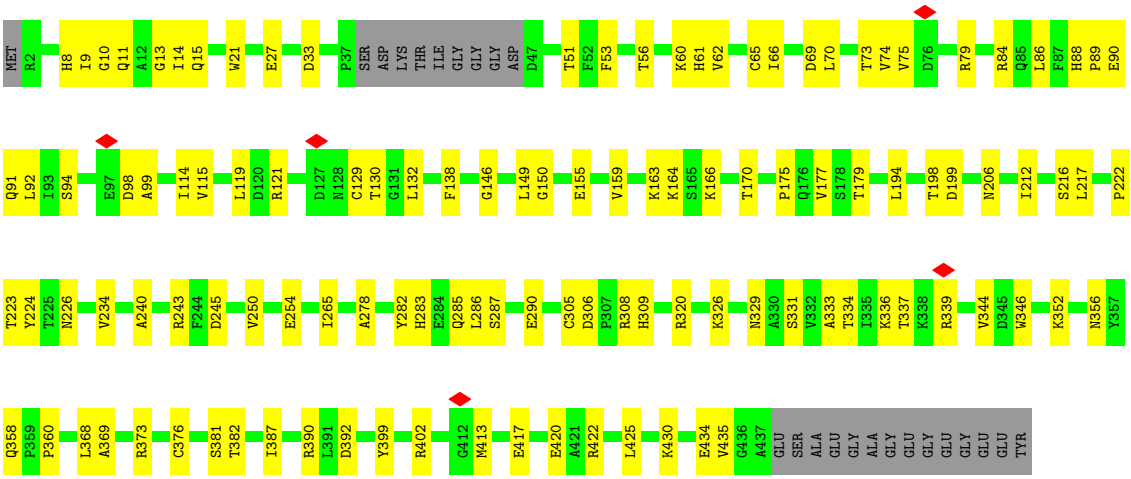
Chain Q3:





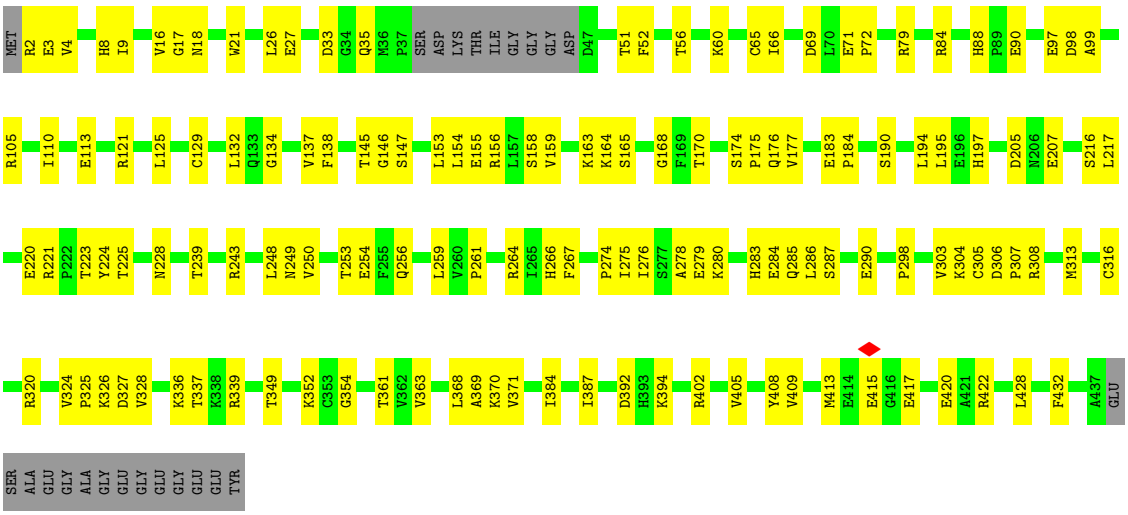
- Molecule 2: Tubulin alpha

Chain Q5:



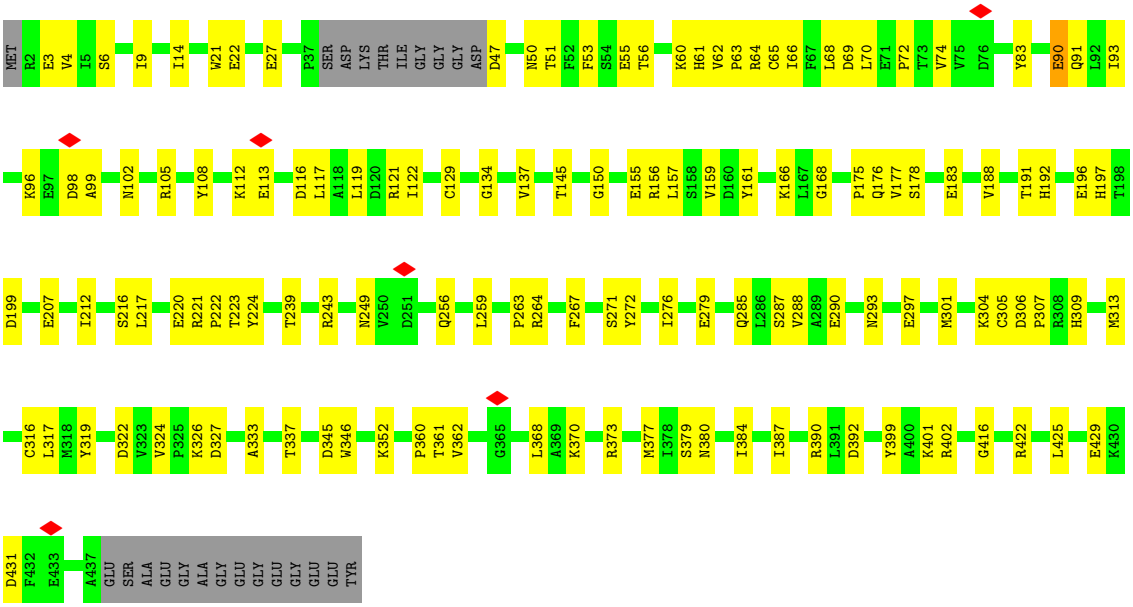
- Molecule 2: Tubulin alpha

Chain Q9:



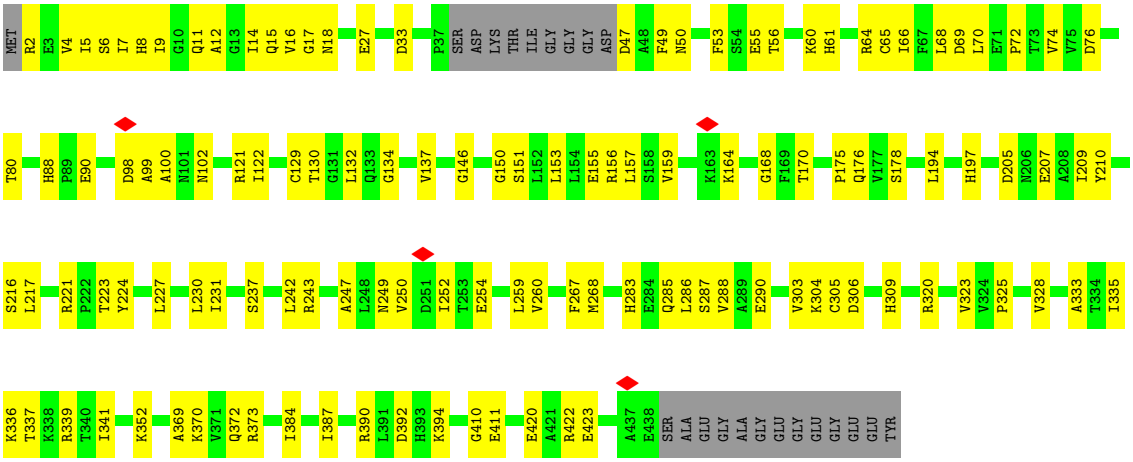
- Molecule 2: Tubulin alpha

Chain R1:



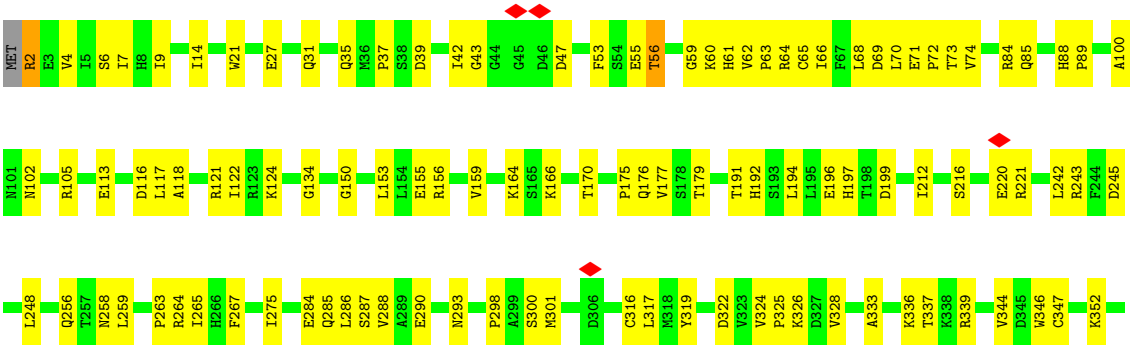
- Molecule 2: Tubulin alpha

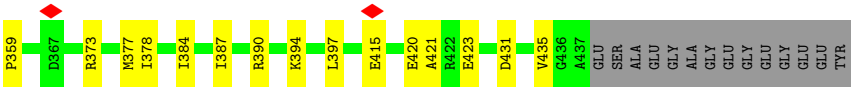
Chain R3:



- Molecule 2: Tubulin alpha

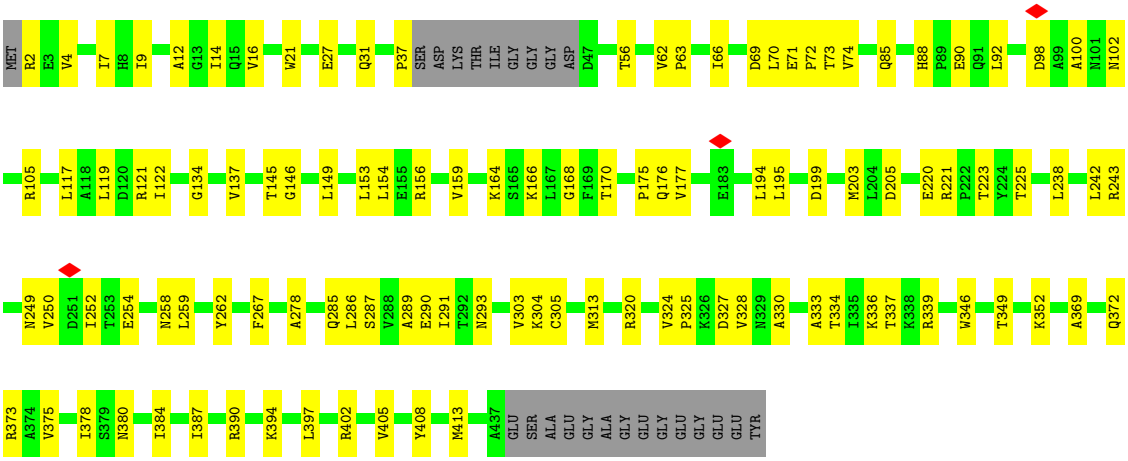
Chain R5:





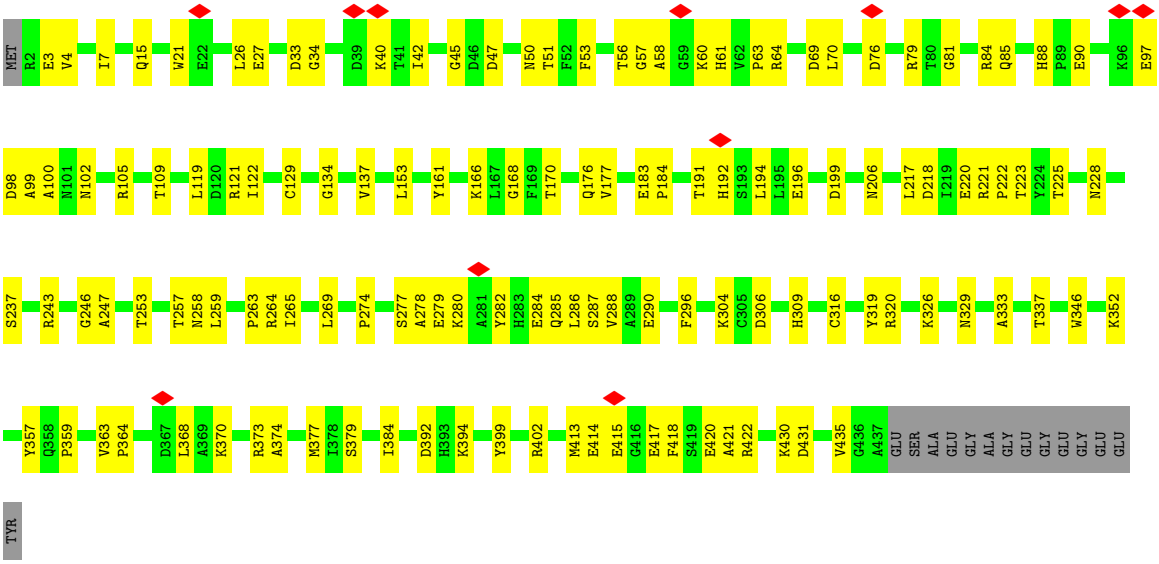
- Molecule 2: Tubulin alpha

Chain R7:



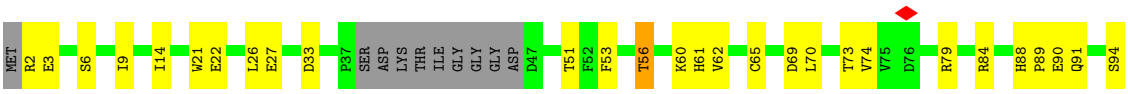
- Molecule 2: Tubulin alpha

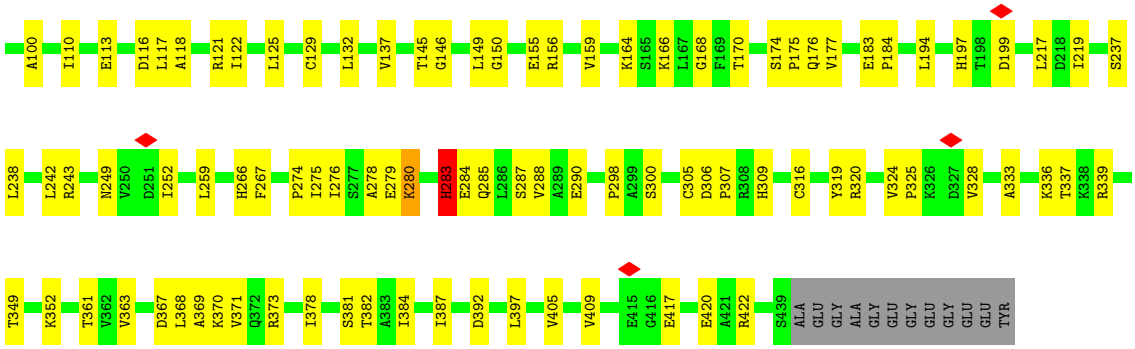
Chain R9:



- Molecule 2: Tubulin alpha

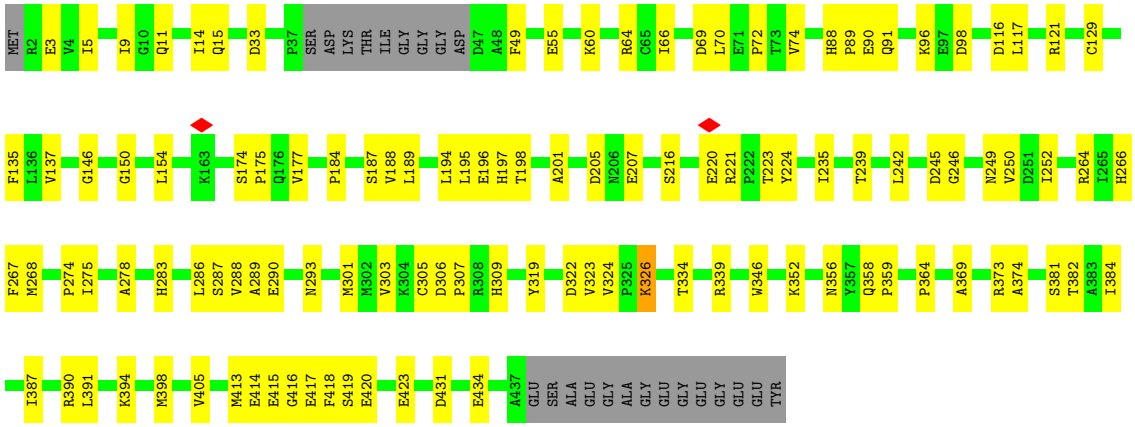
Chain S1:





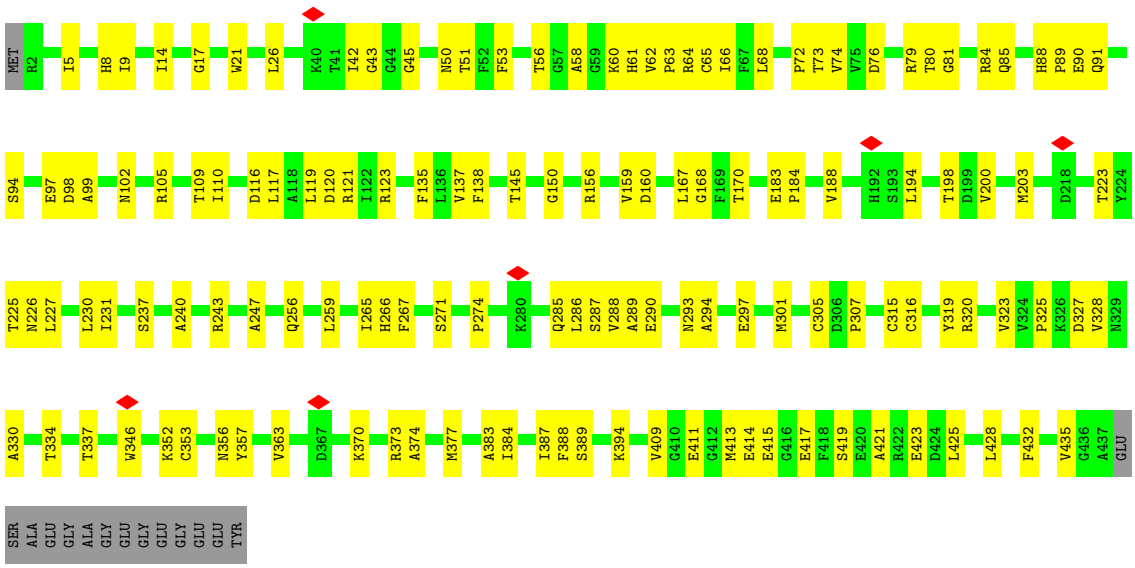
• Molecule 2: Tubulin alpha

Chain S5:



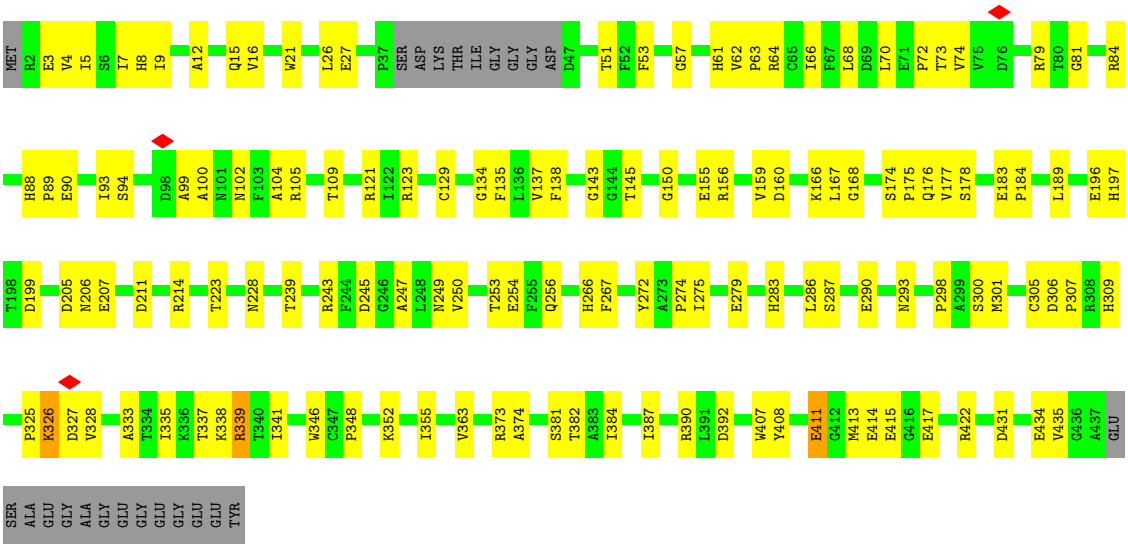
• Molecule 2: Tubulin alpha

Chain S7:



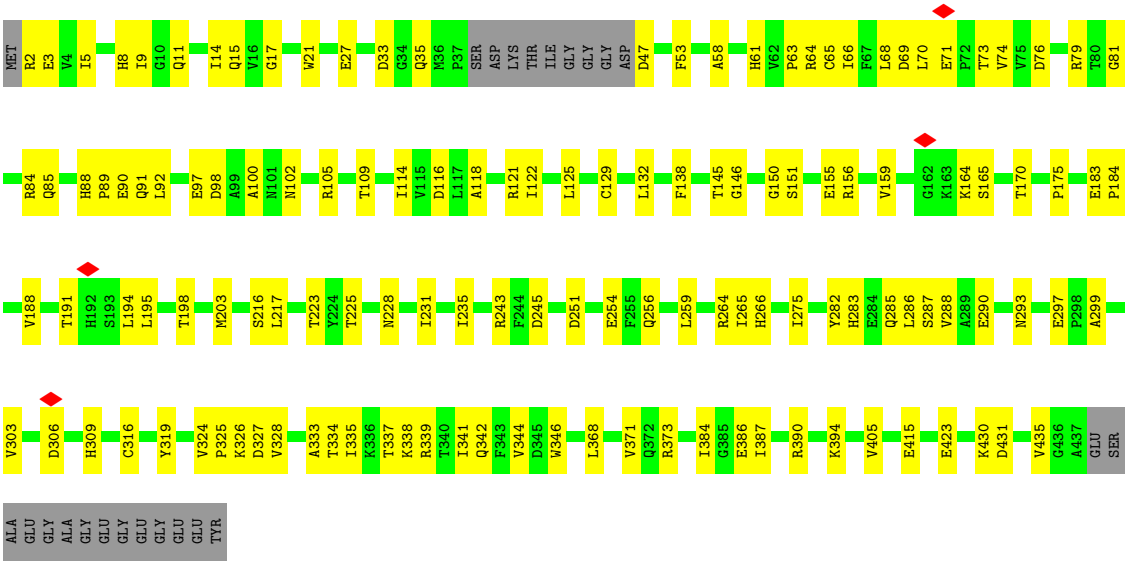
• Molecule 2: Tubulin alpha

Chain S9:



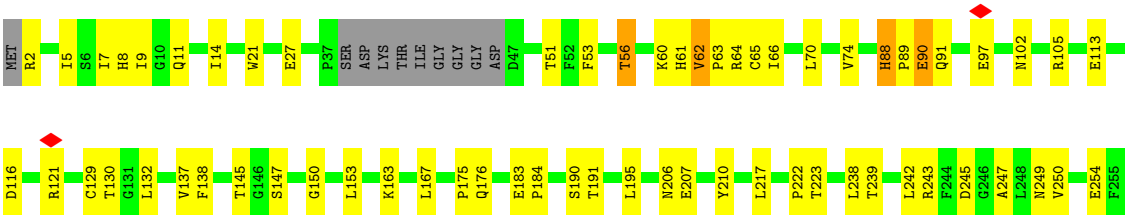
- Molecule 2: Tubulin alpha

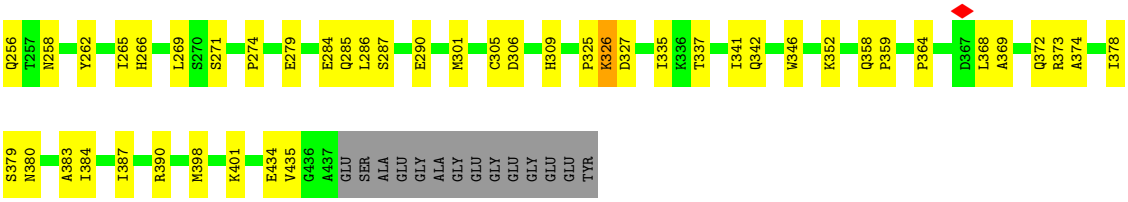
Chain T1:



- Molecule 2: Tubulin alpha

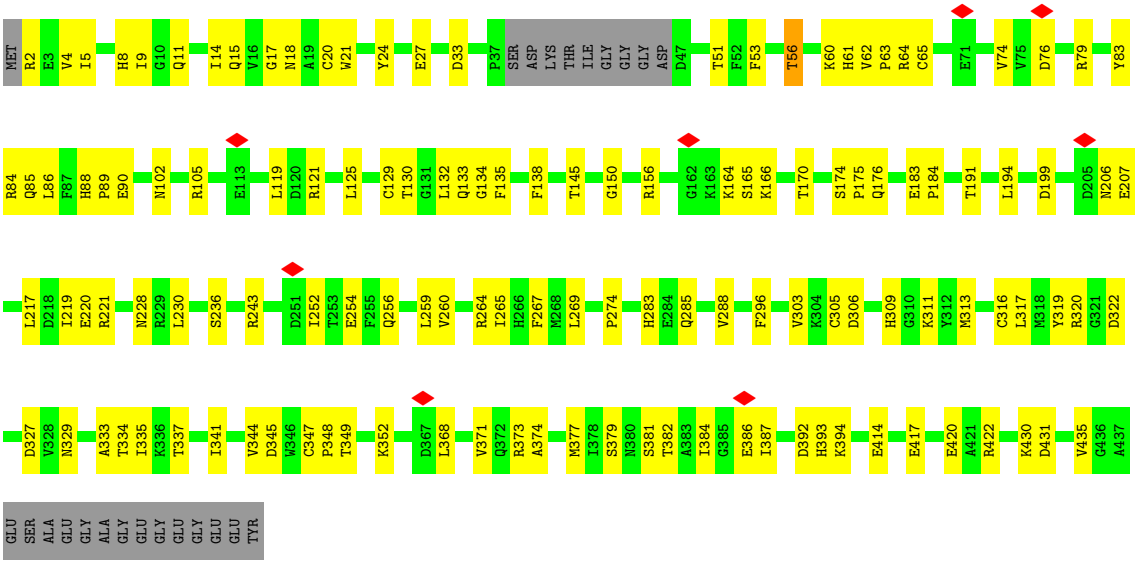
Chain T3:





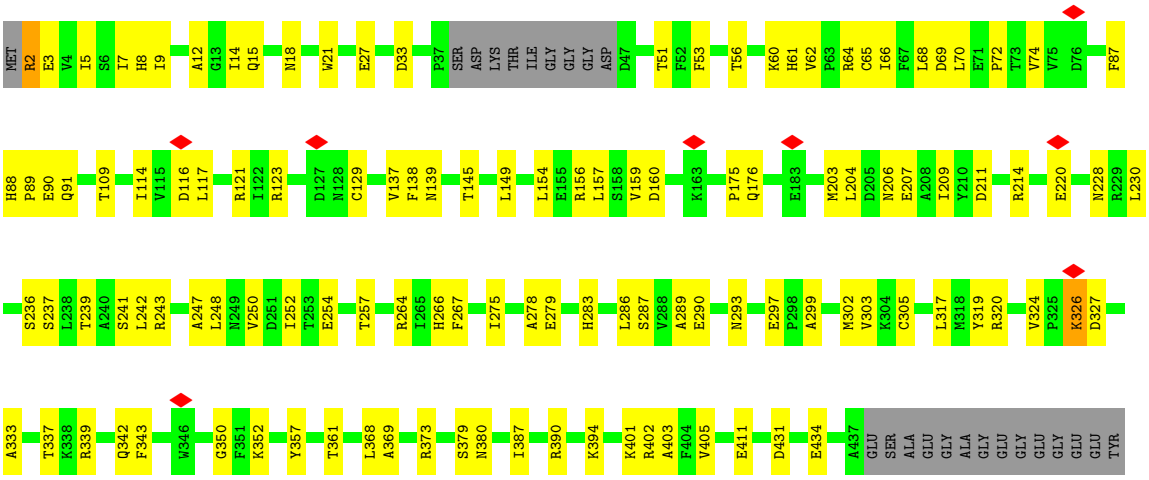
• Molecule 2: Tubulin alpha

Chain T5:



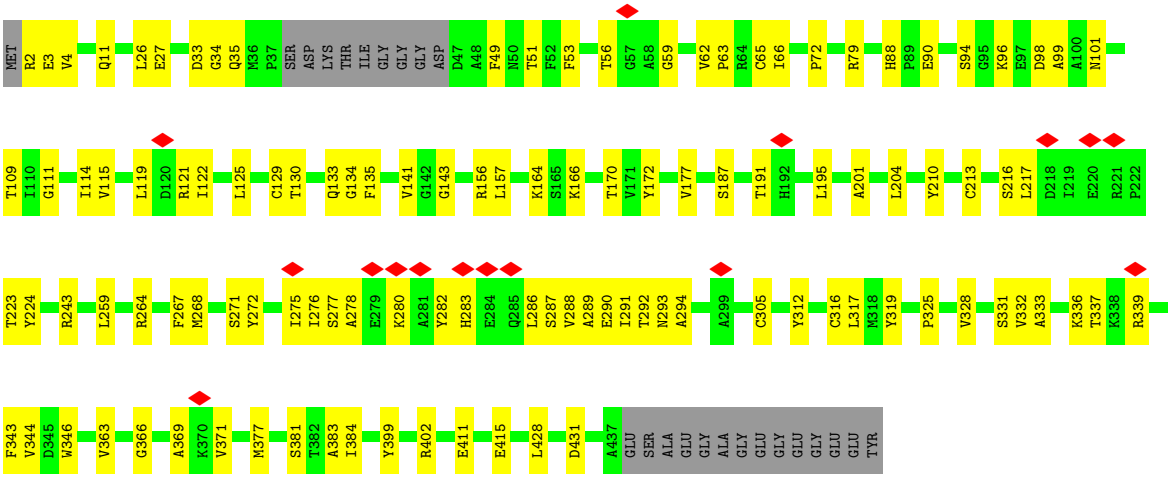
• Molecule 2: Tubulin alpha

Chain T7:



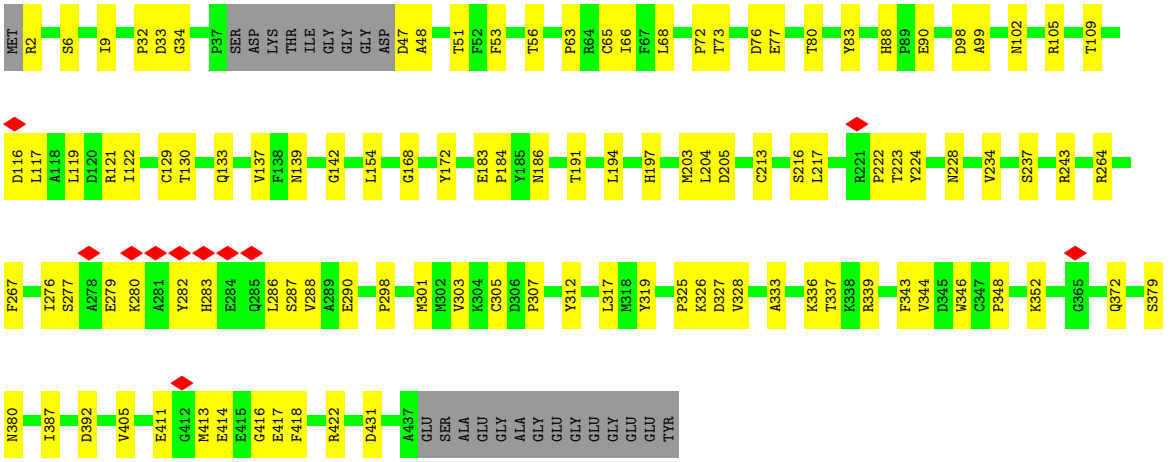
• Molecule 2: Tubulin alpha

Chain U1:



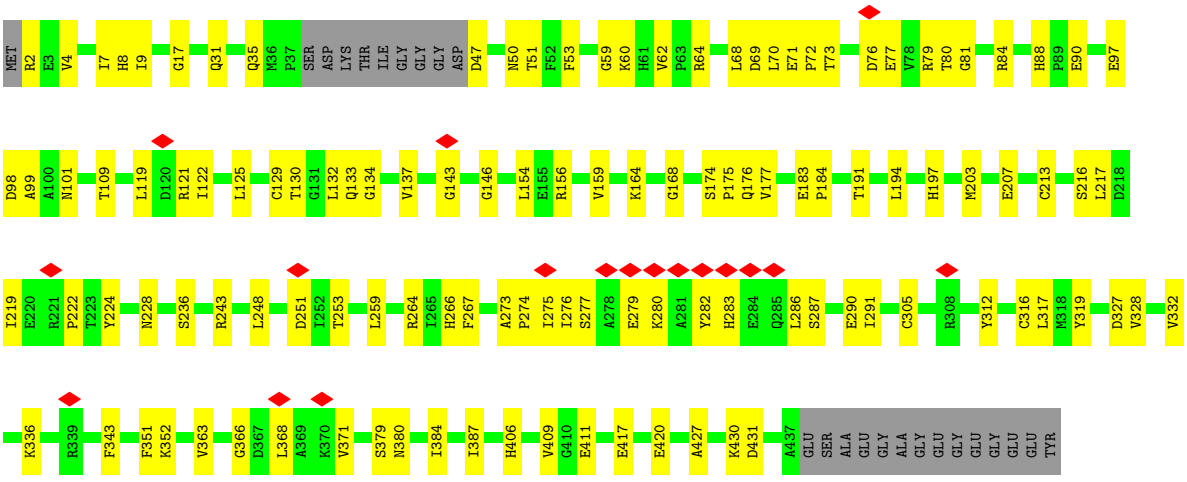
- Molecule 2: Tubulin alpha

Chain U3:



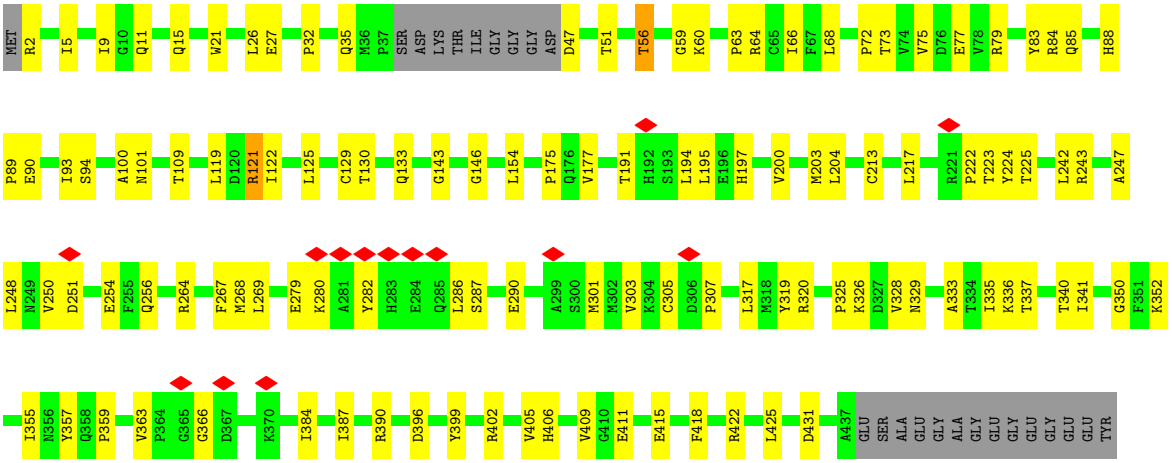
- Molecule 2: Tubulin alpha

Chain U5:



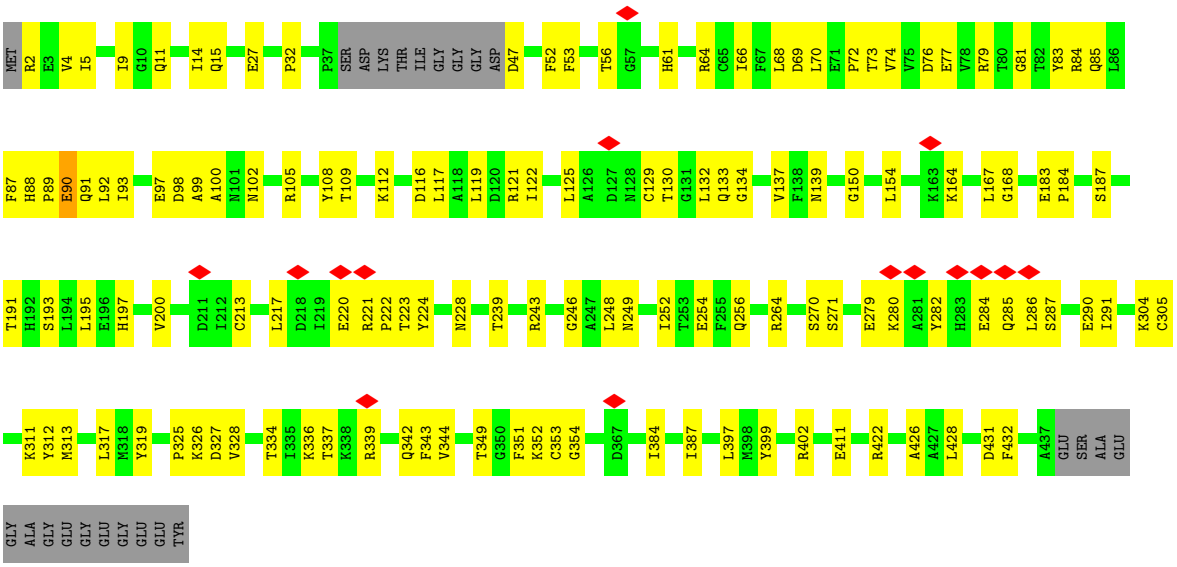
- Molecule 2: Tubulin alpha

Chain U7:



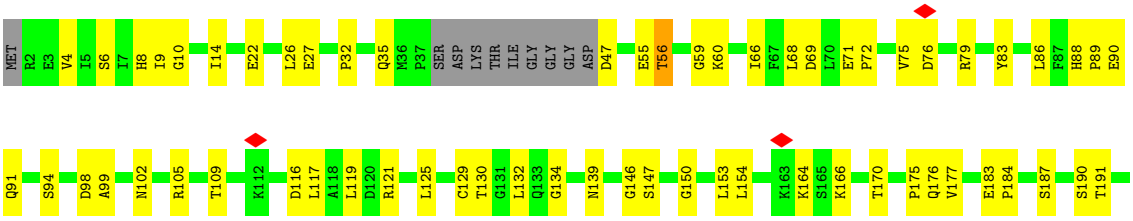
- Molecule 2: Tubulin alpha

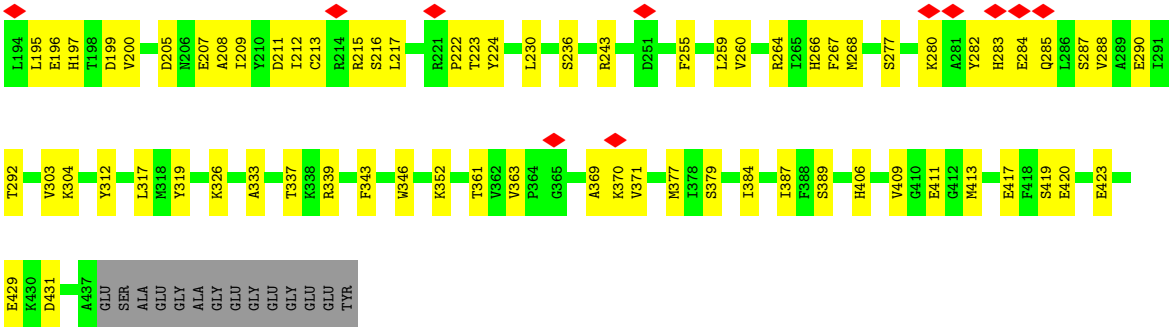
Chain U9:



- Molecule 2: Tubulin alpha

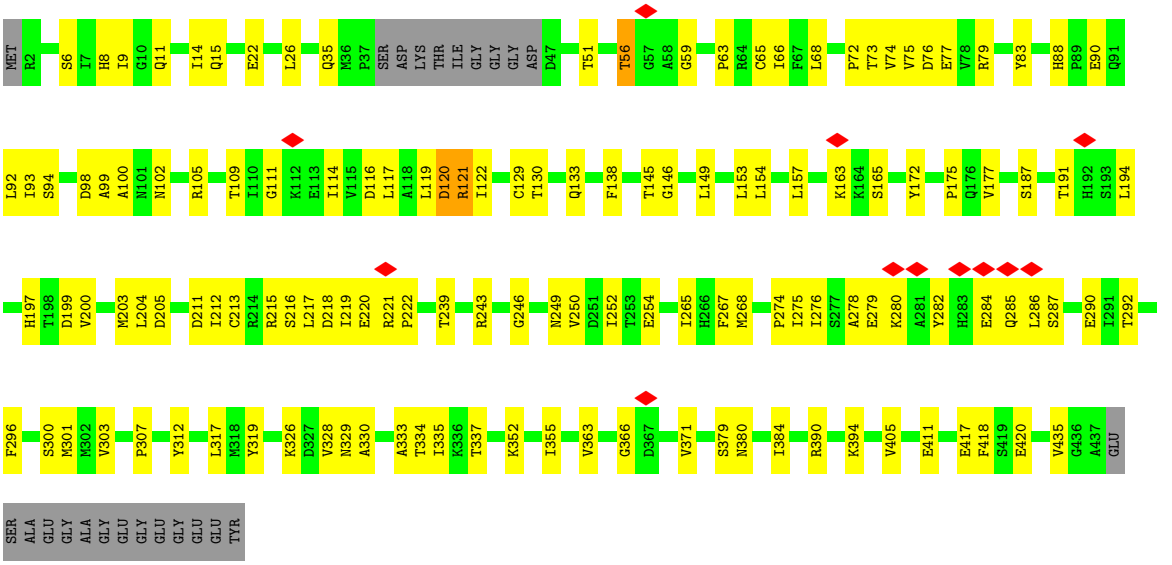
Chain V1:





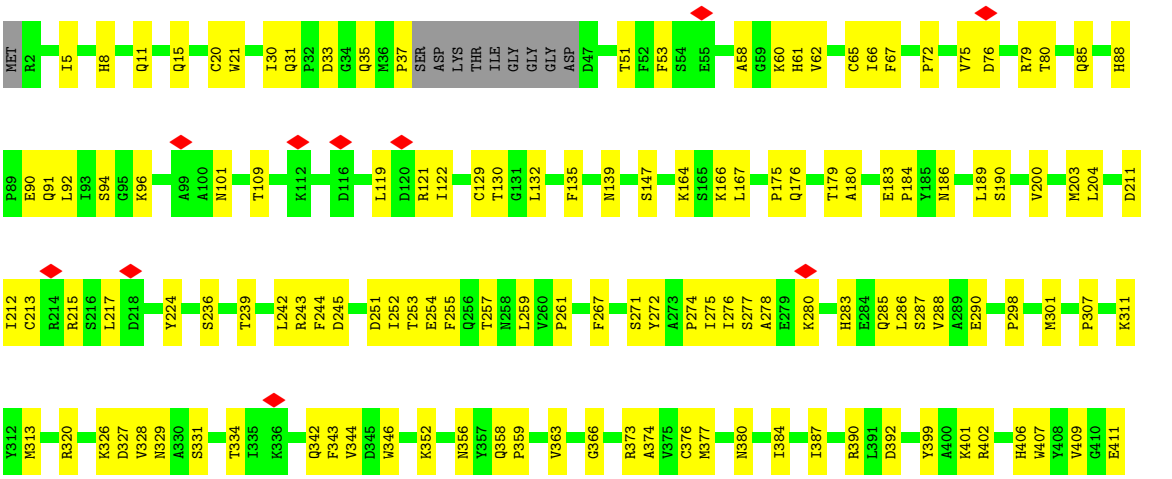
• Molecule 2: Tubulin alpha

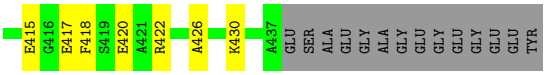
Chain V3:



• Molecule 2: Tubulin alpha

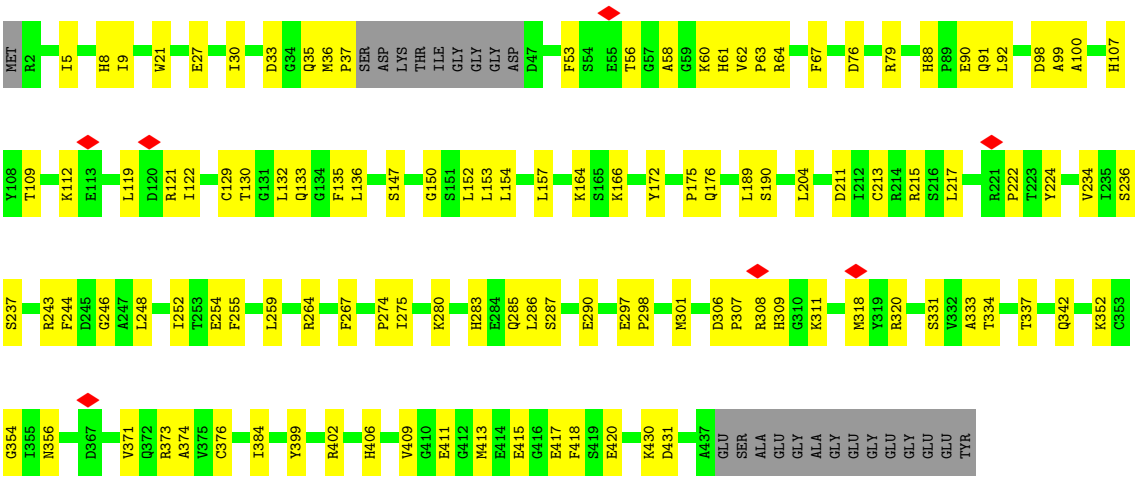
Chain V7:





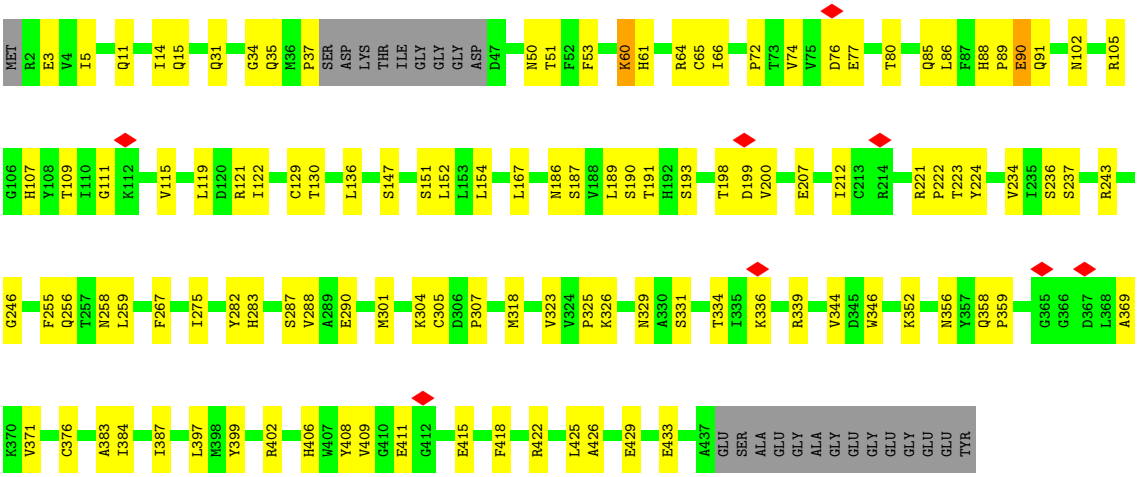
• Molecule 2: Tubulin alpha

Chain V9:



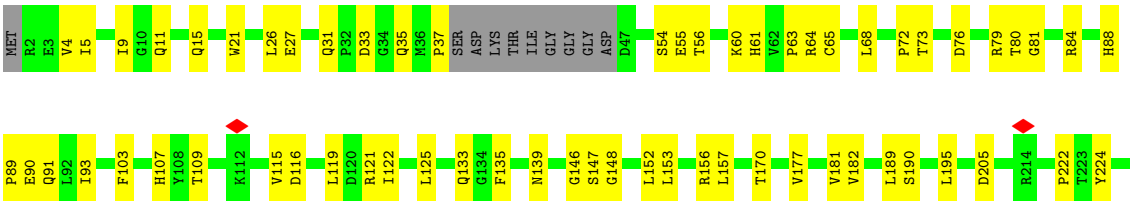
• Molecule 2: Tubulin alpha

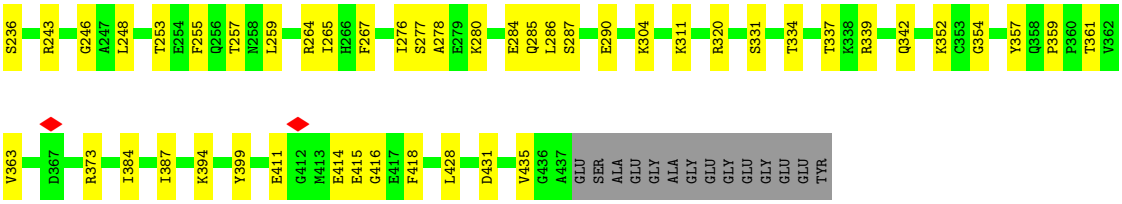
Chain W1:



• Molecule 2: Tubulin alpha

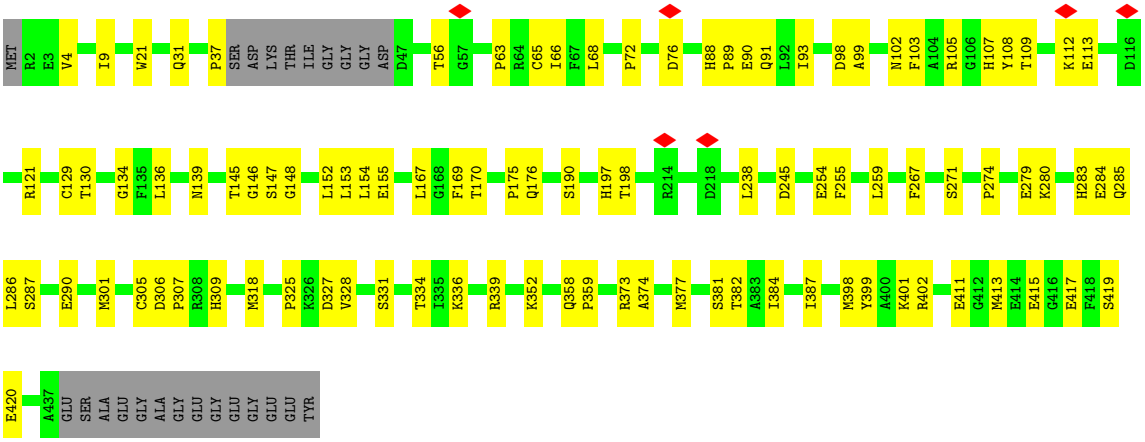
Chain W3:





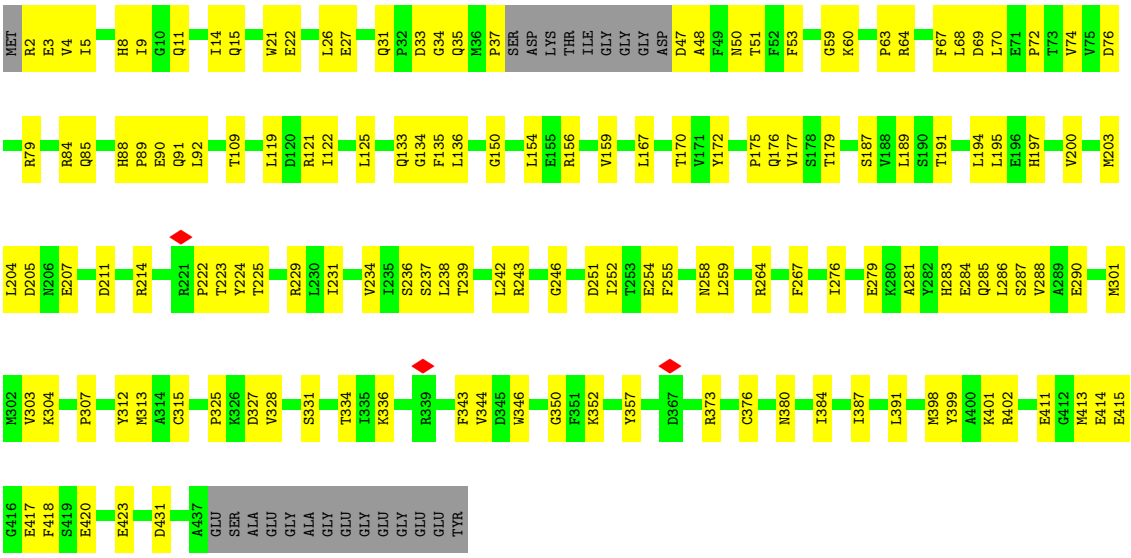
- Molecule 2: Tubulin alpha

Chain W5:



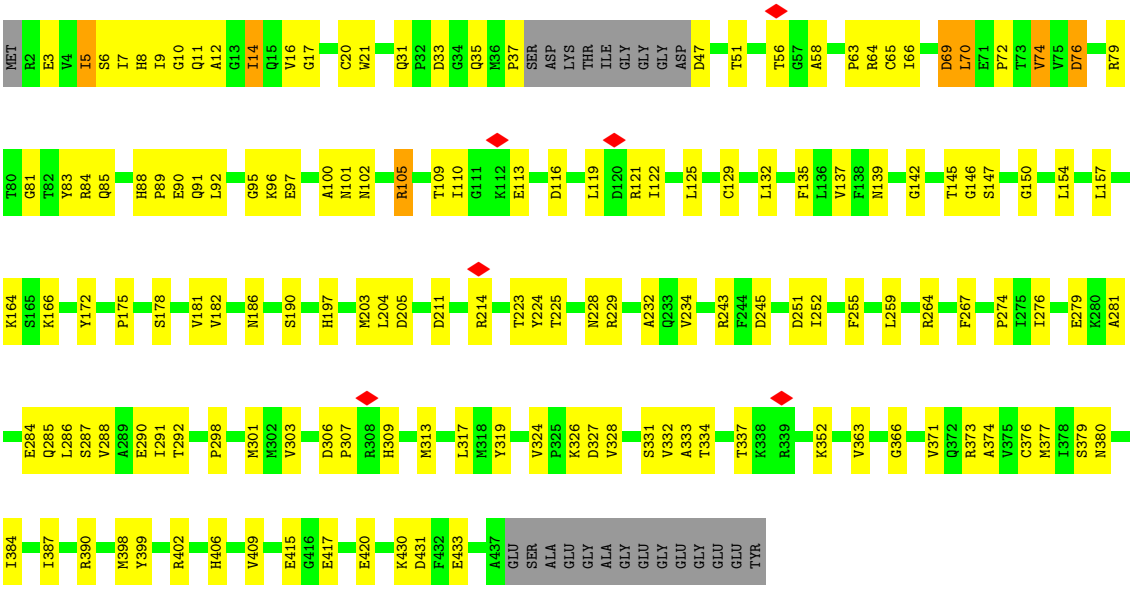
- Molecule 2: Tubulin alpha

Chain W7:



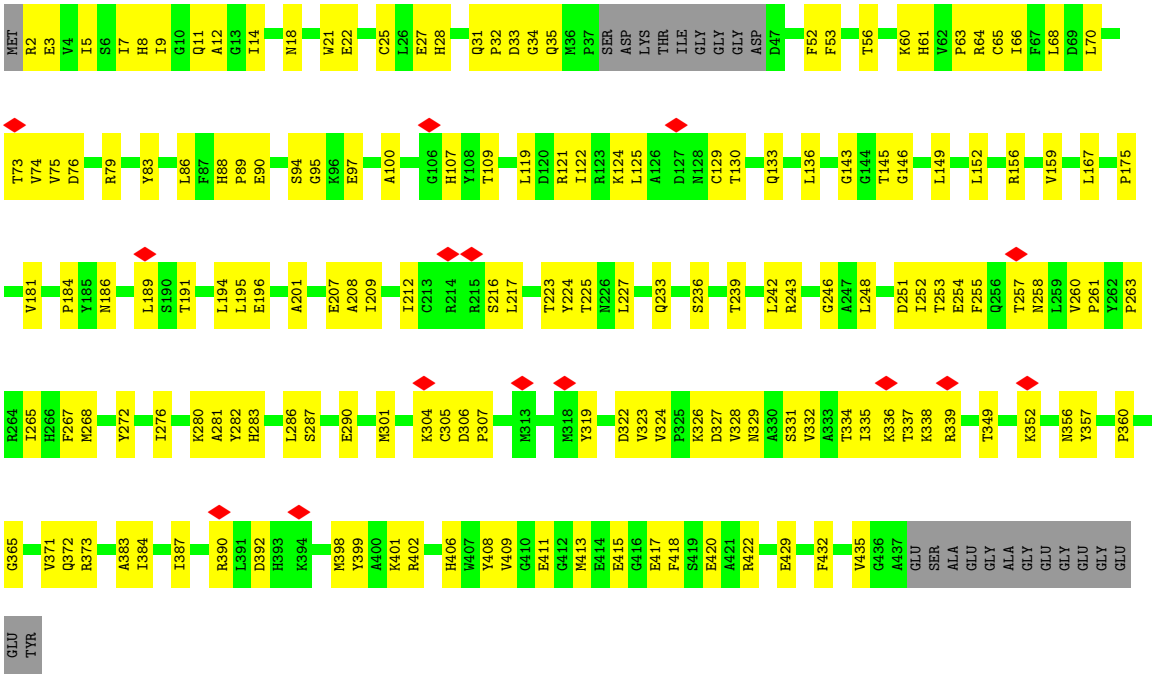
- Molecule 2: Tubulin alpha

Chain W9:



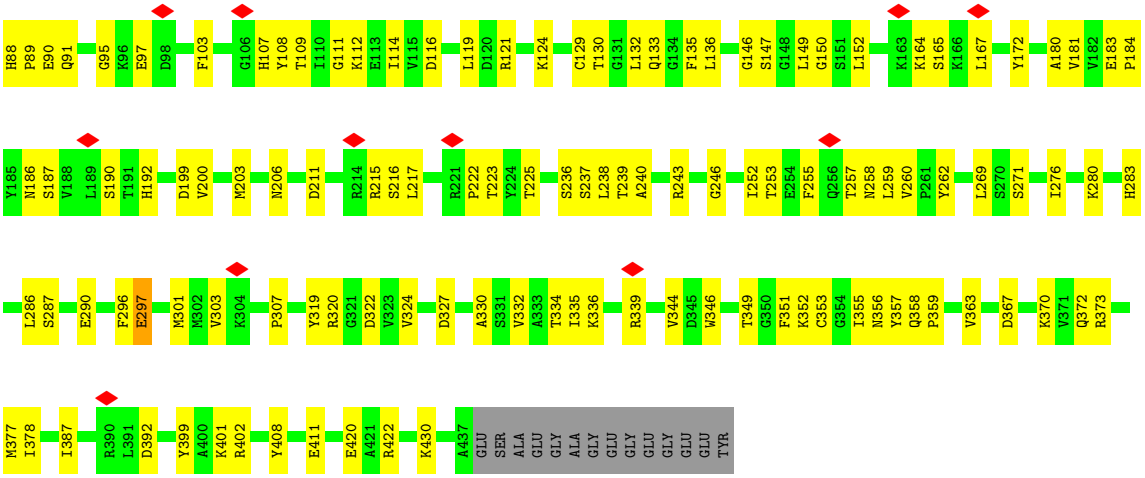
- Molecule 2: Tubulin alpha

Chain X3:



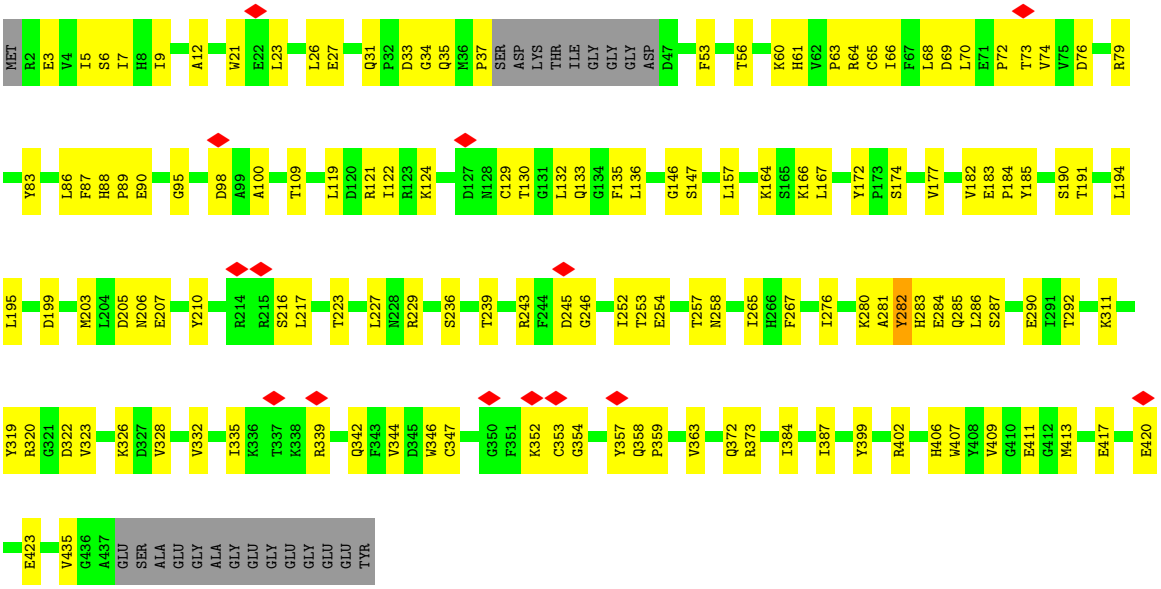
- Molecule 2: Tubulin alpha

Chain X5:



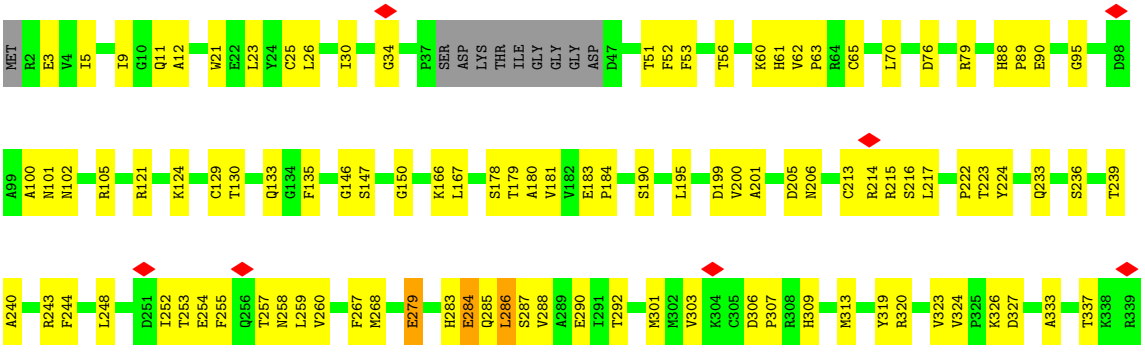
- Molecule 2: Tubulin alpha

Chain X7:



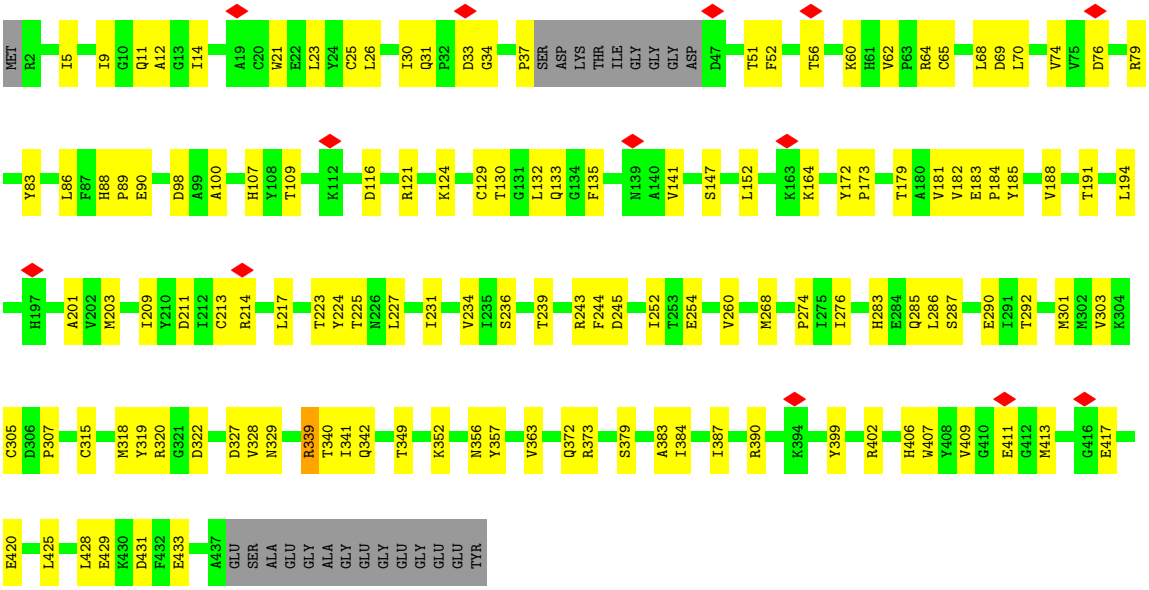
- Molecule 2: Tubulin alpha

Chain X9:



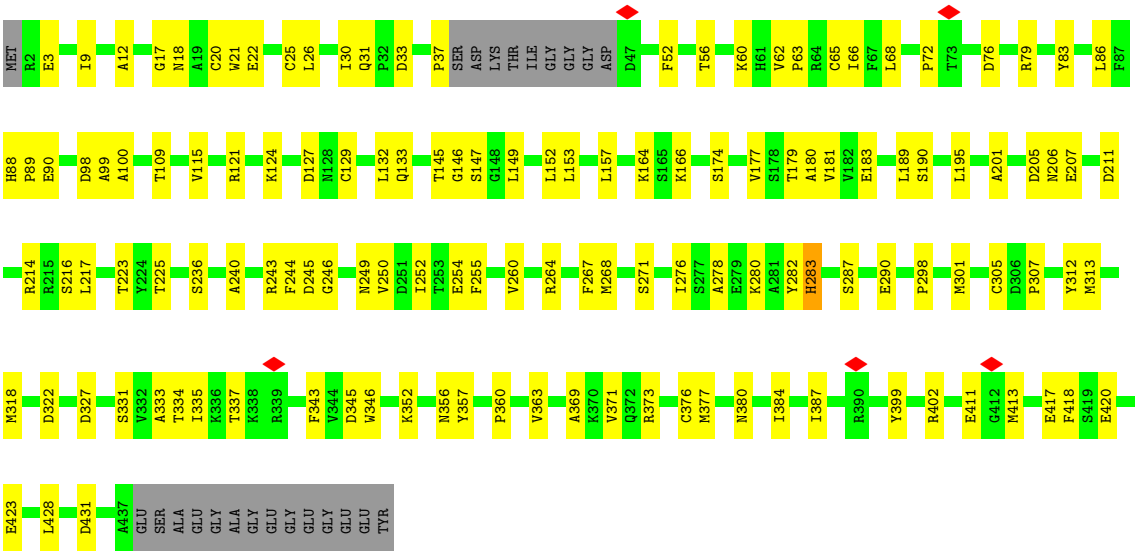
• Molecule 2: Tubulin alpha

Chain Y1:



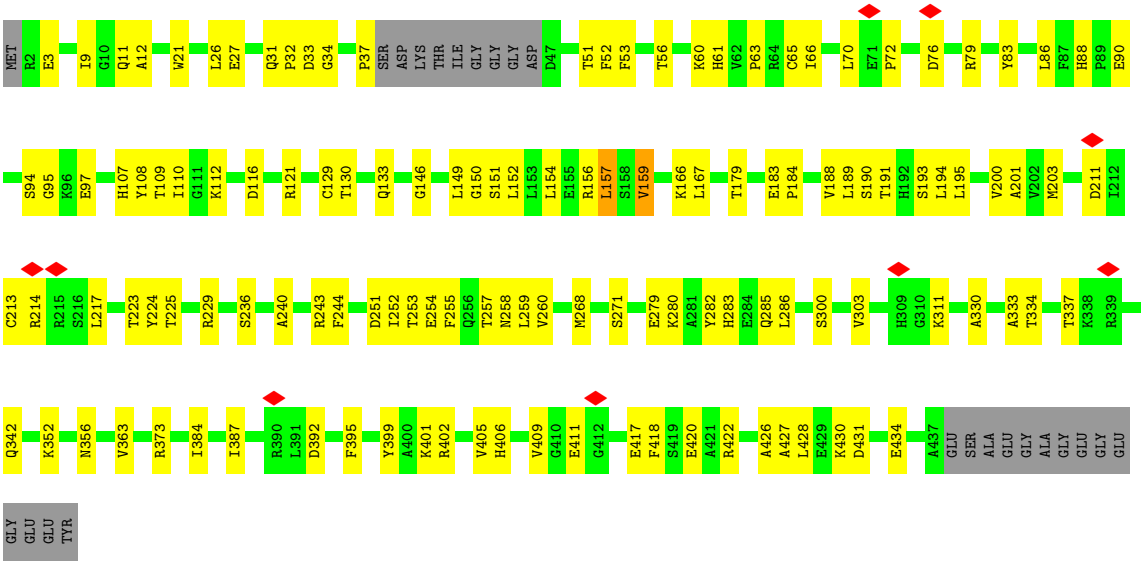
• Molecule 2: Tubulin alpha

Chain Y3:



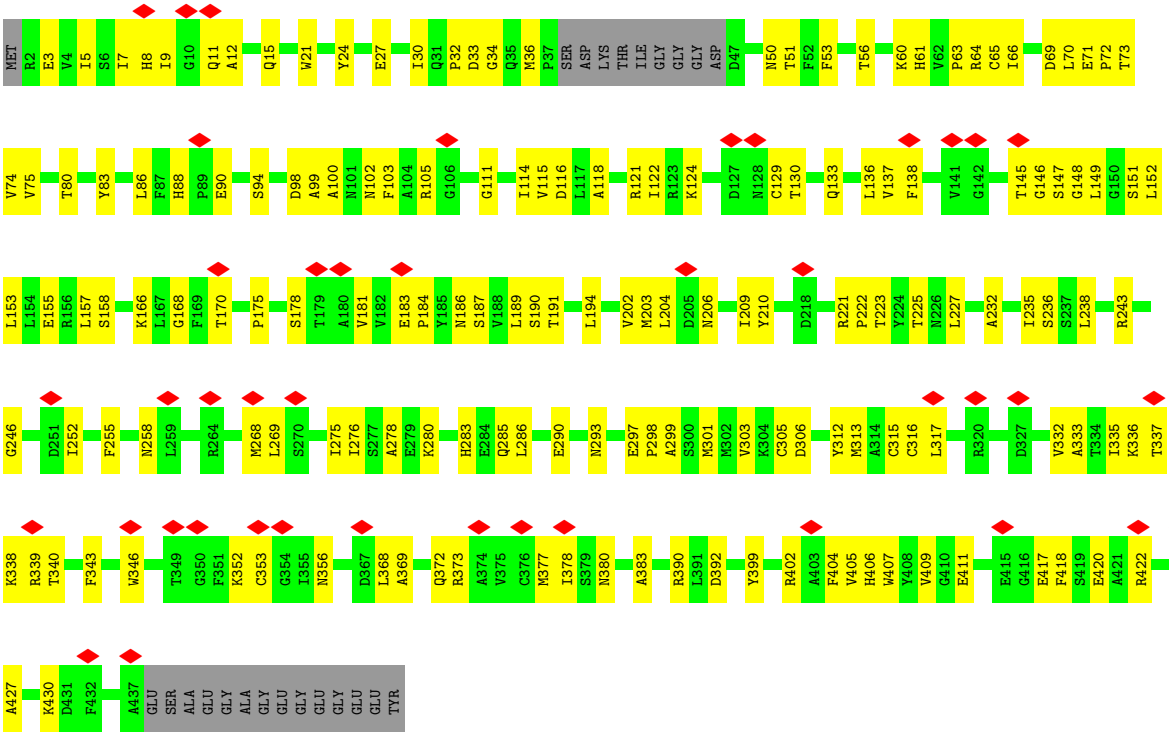
• Molecule 2: Tubulin alpha

Chain Y5:



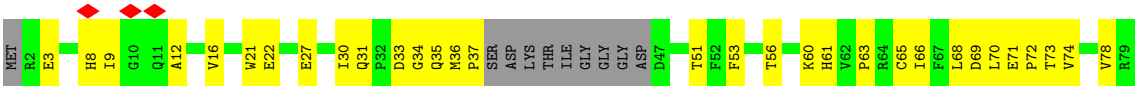
- Molecule 2: Tubulin alpha

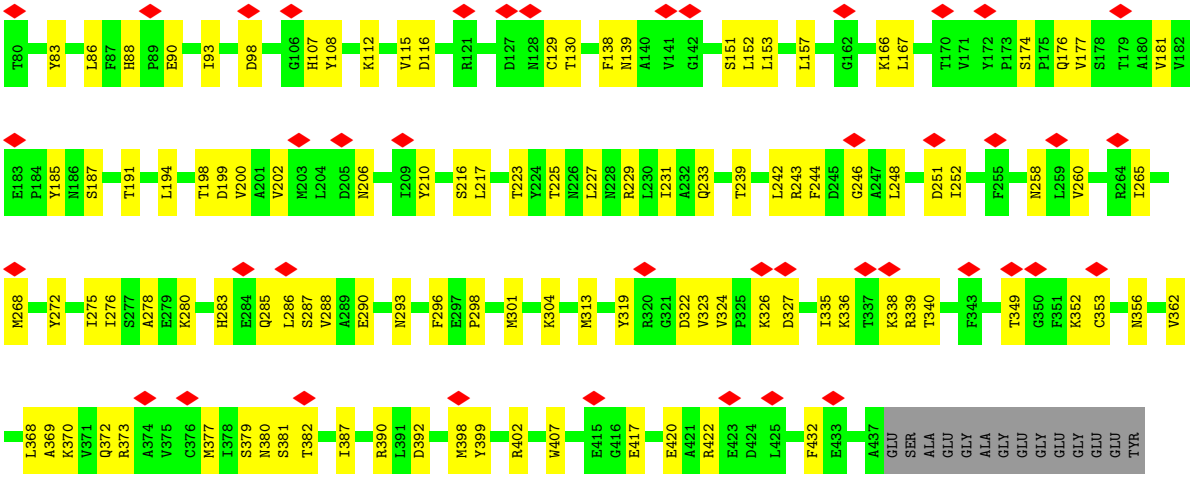
Chain Y9:



- Molecule 2: Tubulin alpha

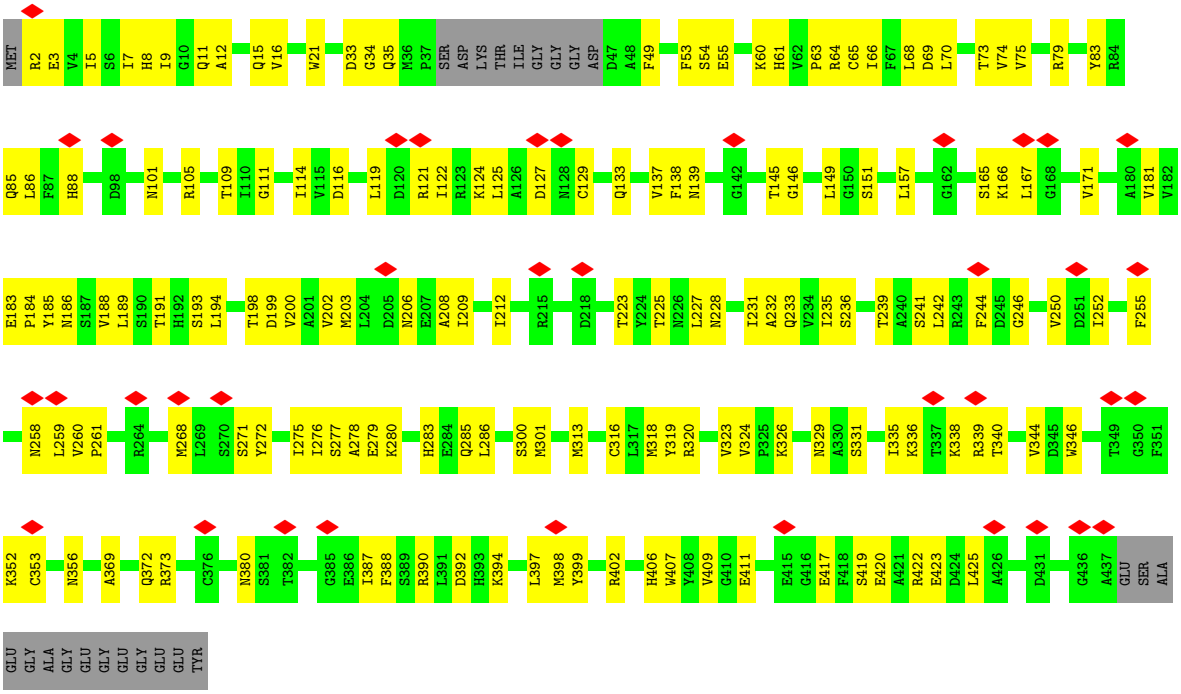
Chain Z1:





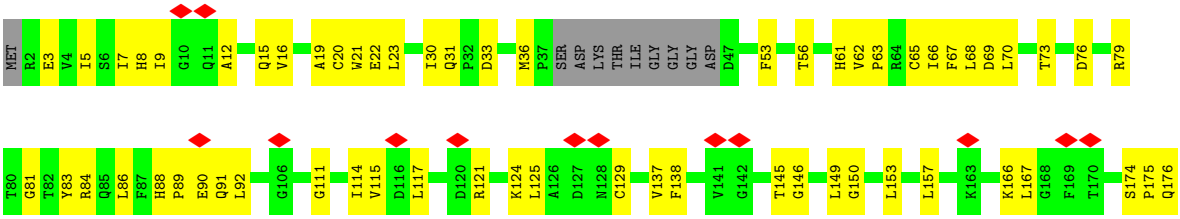
• Molecule 2: Tubulin alpha

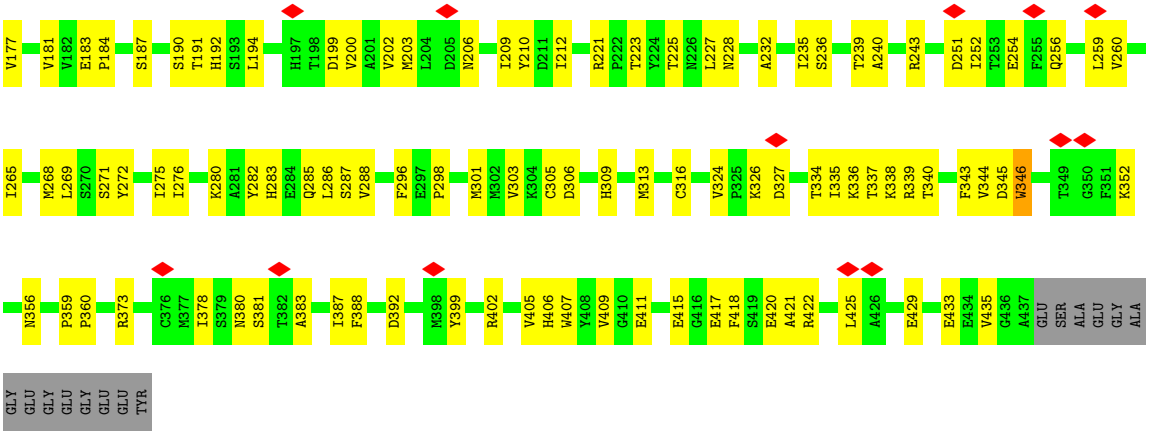
Chain Z3:



• Molecule 2: Tubulin alpha

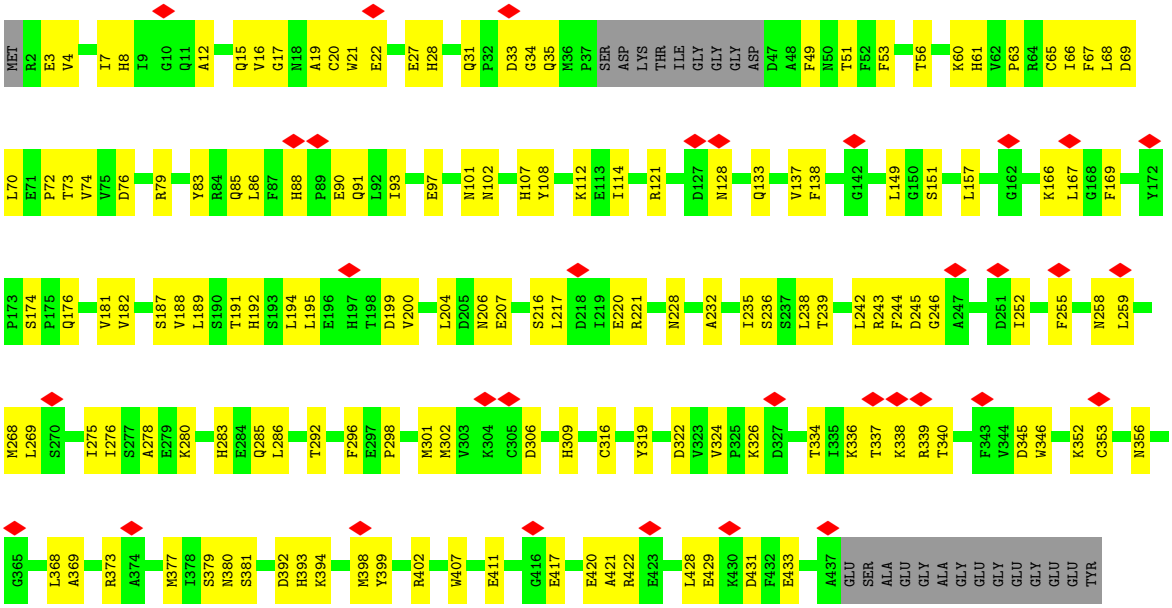
Chain Z5:





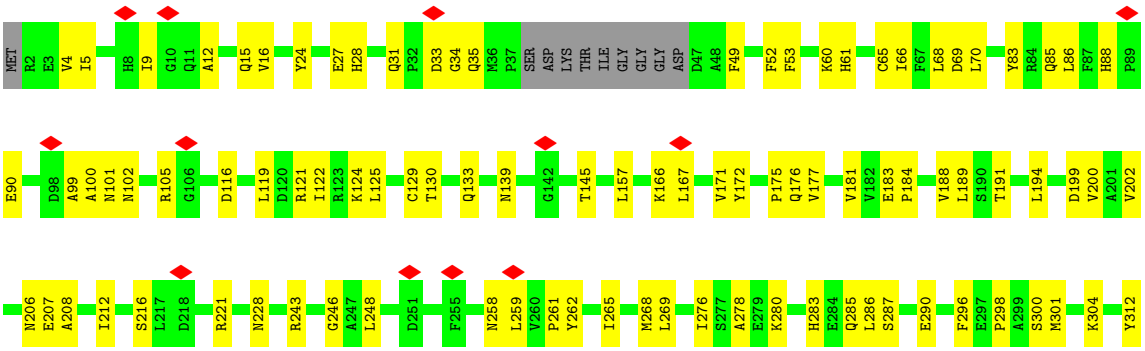
- Molecule 2: Tubulin alpha

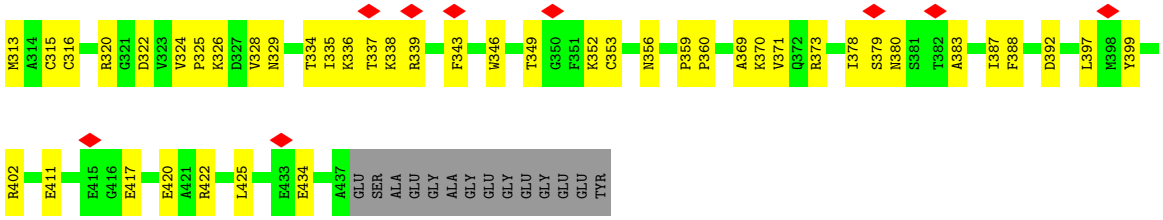
Chain Z7:



- Molecule 2: Tubulin alpha

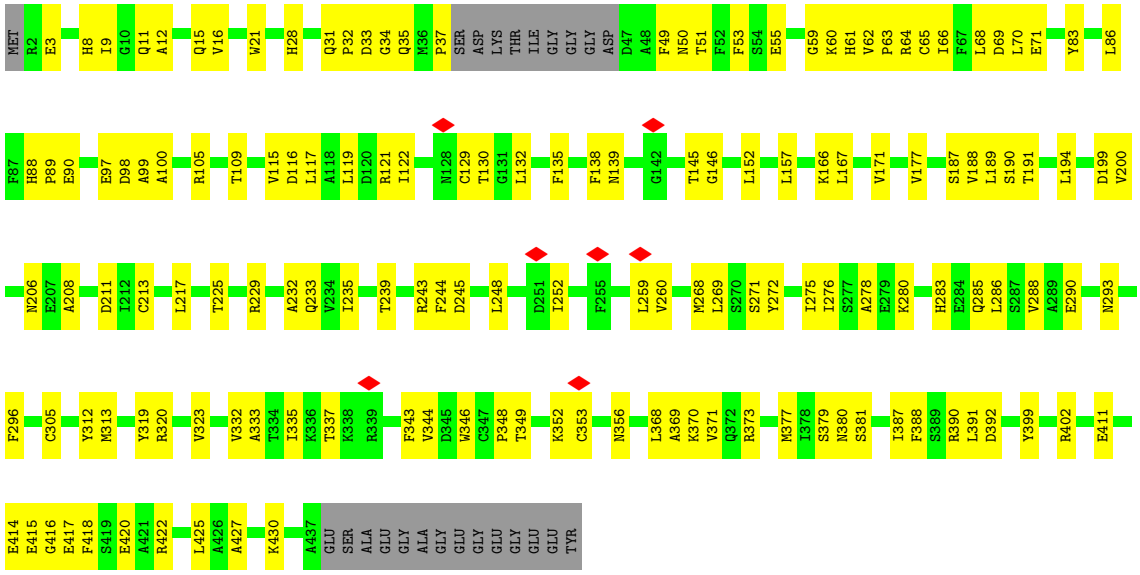
Chain Z9:





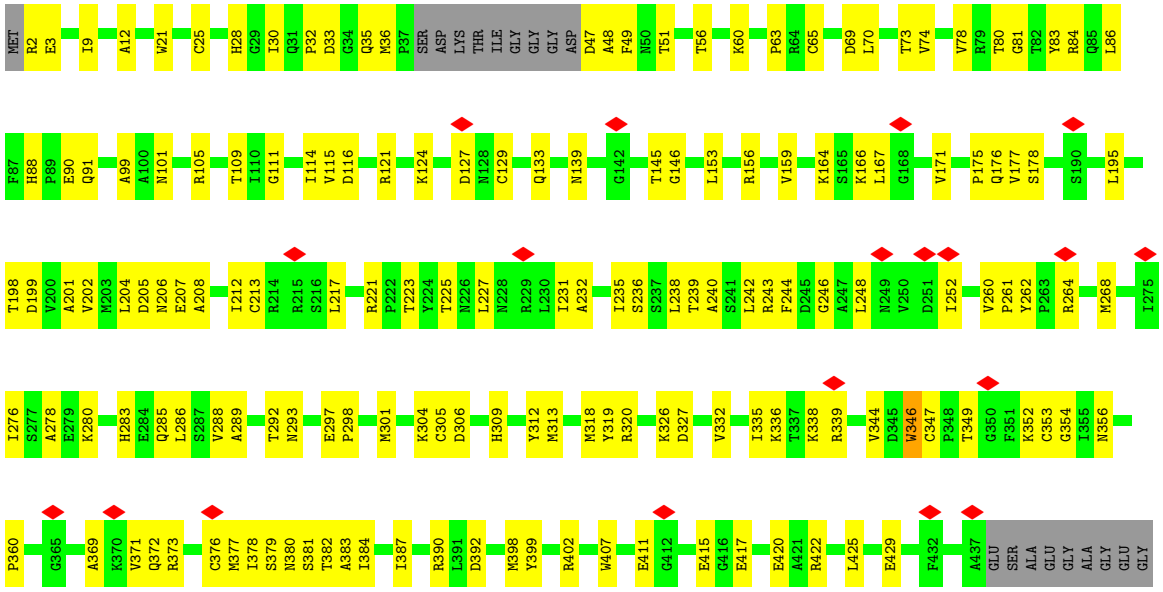
• Molecule 2: Tubulin alpha

Chain 0B:



• Molecule 2: Tubulin alpha

Chain 0F:



GLU GLY GLU GLU TYR

- Molecule 2: Tubulin alpha

Chain 0H:

MET R2 E3 I7 H8 I9 A12 Q15 C20 W21 E27 H28 G29 I30 M36 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 A48 F49 N50 T51 E55 T56 K60 P63 R64 C65 I66 F67 L68 D69 L70 E71 P72 T73 V74 V78 G81 T82 Y83

R84 Q85 L86 F87 H88 P89 E90 A100 N101 N102 R105 T109 I110 V115 R121 I122 R123 K124 L132 Q133 V137 G142 T145 G146 S147 G148 L149 G150 L153 R156 V159 K166 L167 V171 P175 Q176 E183 P184 S190 T191 L194

T198 A201 V202 M203 L204 D205 N206 E207 A208 I209 Y210 D211 I212 C213 R214 L217 R221 P222 L227 N228 R229 V234 T239 L242 R243 F244 D245 G246 D251 I252 T257 N258 L259 V260 R264 F267 S271 Y272 A273 P274 A278 E279 K280 H283 E284 Q285

L286 S287 V288 A289 E290 I291 T292 N293 E297 P298 A299 S300 M301 K304 C305 D306 H309 C316 R320 G321 D322 D327 A330 S331 V332 A333 T334 I335 K336 T337 K338 R339 W346 C347 G350 C353 G354 I355 N356 D367 L368 A369 K370 R373 C376 M377 I378

S381 T382 A383 I384 I387 R390 L391 D392 L397 M398 Y399 A400 K401 R402 A403 H406 W407 E411 G412 E417 E420 A421 R422 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

- Molecule 2: Tubulin alpha

Chain 0J:

MET R2 E3 V4 I5 I9 A12 Q15 V16 W21 C25 H28 G29 I30 Q31 P32 D33 G34 Q35 M36 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 A48 F49 N50 T51 S54 E55 T56 G57 K60 H61 R64 C65 I66 F67 L68 D69 L70 T73 V74

V75 R79 T82 Y83 R84 Q85 L86 F87 H88 P89 E90 I93 S94 D98 A99 A100 T109 I110 G111 I114 V115 D116 L117 A118 L119 D120 R121 I122 R123 K124 L125 A126 D127 F135 L136 V137 G142 G146 S147 L153 R156 V159 G162 L167 G168 F169

S174 P175 Q176 V177 S178 V181 S187 S190 T198 A201 V202 M203 L204 D205 N206 E207 A208 I209 Y210 D211 I212 R215 S216 L217 R221 P222 N228 R229 A232 I235 L242 R243 F244 D245 G246 A247 D251 I252 F255 Q256 T257 N258 L259 V260 R264

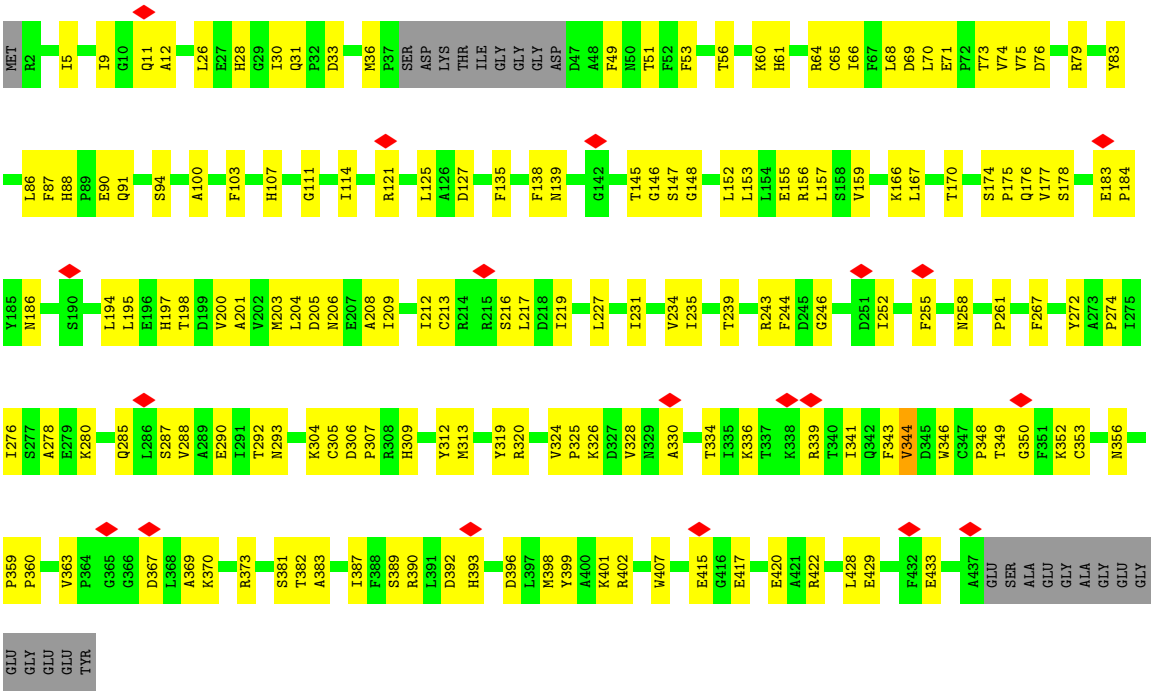
F267 M268 L269 S270 S271 P274 I275 I276 S277 A278 H283 L286 S287 V288 T292 N293 E297 P298 A299 S300 M301 K304 M313 M318 Y319 R320 G321 D322 P325 V328 N329 A330 S331 V332 A333 T334 I335 K336 T337 K338 R339 T340 F343 W346 T349 G350

N356 P360 T361 V362 G365 G366 D367 L368 A369 K370 R373 C376 N380 S381 T382 A383 I384 I387 R390 L391 D392 H393 M398 Y399 R402 W407 E411 R422 E429 F432 E433 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU

GLU TYR

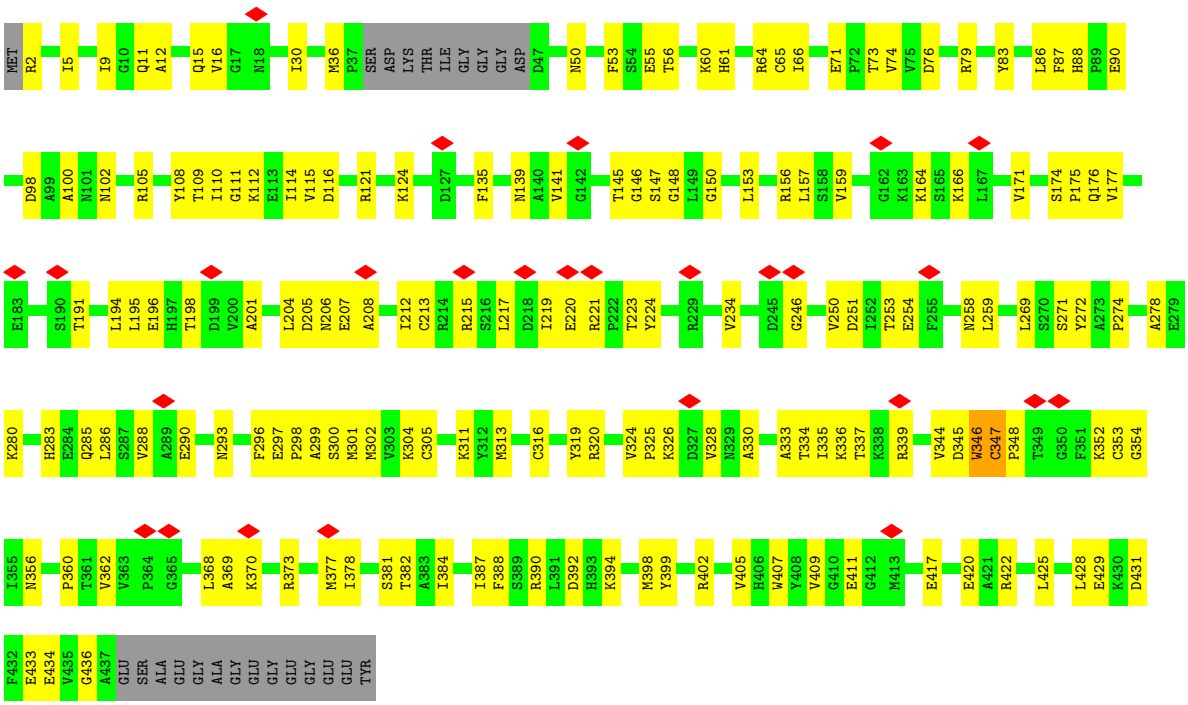
- Molecule 2: Tubulin alpha

Chain 0L: 59% 36% 5%



- Molecule 2: Tubulin alpha

Chain 0N: 6% 57% 37% 5%



- Molecule 2: Tubulin alpha

Chain 0P: 65% 30% 5%

MET R2 I5 H8 I9 A12 Q15 N18 C25 H28 Q31 P32 D33 G34 Q35 M36 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 A48 F49 E55 T56 K60 R64 C65 I66 D69 L70 D76 R79 Y83 L86 F87 H88 F89

E90 N102 R105 T109 I110 G111 I114 V115 D116 R121 C129 L132 F138 N139 A140 V141 G142 T145 G146 L152 L153 R156 V159 G162 K163 K164 S165 K166 L167 S174 P175 Q176 V177 E183 T191 L194 T198 D199 V200 A201 D205

N206 I212 C213 S216 L217 D218 I219 E220 R221 P222 T223 Y224 N228 V234 T239 R243 F244 D245 G246 D251 I252 F255 Q256 T257 N258 L259 Y262 I265 M268 Y272 A273 P274 I275 I276 S277 A278 E279 K280 H283 L286 S287 V288 A289 E290 I291 T292

F296 E297 P298 M301 Y312 C316 Y319 R320 P325 K326 D327 V328 N329 A330 A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 K352 C353 N356 A369 Q372 R373 S381 T382 I387 R390 L391 D392 L397

M398 Y399 R402 A403 F404 V405 H406 W407 Y408 V409 G410 E411 G412 M413 E417 E420 A421 R422 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

- Molecule 2: Tubulin alpha

Chain 0R: 5% 59% 36% 5%

MET R2 I5 S6 I7 H8 I9 A12 G17 N18 A19 C20 Y24 C25 L26 E27 H28 D33 G34 Q35 M36 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 A48 F49 N50 T51 F52 F53 S54 E55 T56 G57 K60 R64 C65 I66 E71 P72 T73 V74 V75 D76

E77 V78 R79 Y83 R84 Q85 L86 F87 H88 P89 E90 D98 A99 A100 H107 Y108 T109 I110 G111 K112 E113 I114 V115 D116 R121 I122 R123 K124 Q133 F138 N139 G142 T145 G146 S147 G148 L149 L152 L153 L154 E155 R156 L157 S158 V159 G162 K163 K164 S165 K166

L167 S174 P175 Q176 V177 E183 P184 Y185 V188 L189 S190 T191 H192 S193 L194 L195 E196 H197 T198 D199 V200 A201 V202 M203 E207 C213 R214 R215 S216 L217 Q233 S237 L238 T239 A240 R243 F244 D245 G246 N249 F255 N258 L259 V260 H266 S271

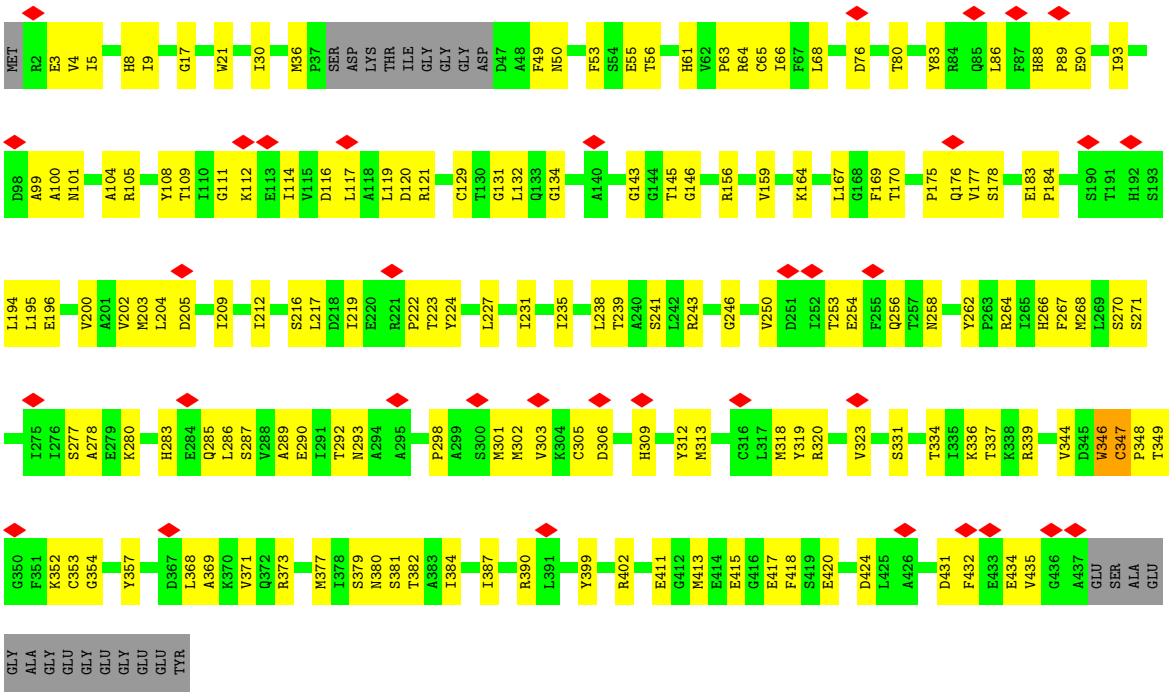
P274 I275 I276 S277 A278 E279 K280 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 F296 E297 P298 M301 K304 C305 D306 H309 Y312 M318 Y319 R320 V323 V324 P325 K326 D327 V328 N329 A330 T334 I335 K336 T337 K338 R339 T340 I341 G350 F351 K352 C353

G354 I355 N356 V363 P364 G365 G366 D367 L368 A369 K370 V371 Q372 R373 G376 M377 I378 S379 N380 S381 T382 I387 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 R402 A403 H406 W407 E411 E417 F418 S419 E420 A421 R422 A437 GLU SER ALA GLU GLY ALA GLY

GLU GLY GLU GLY GLU GLU TYR

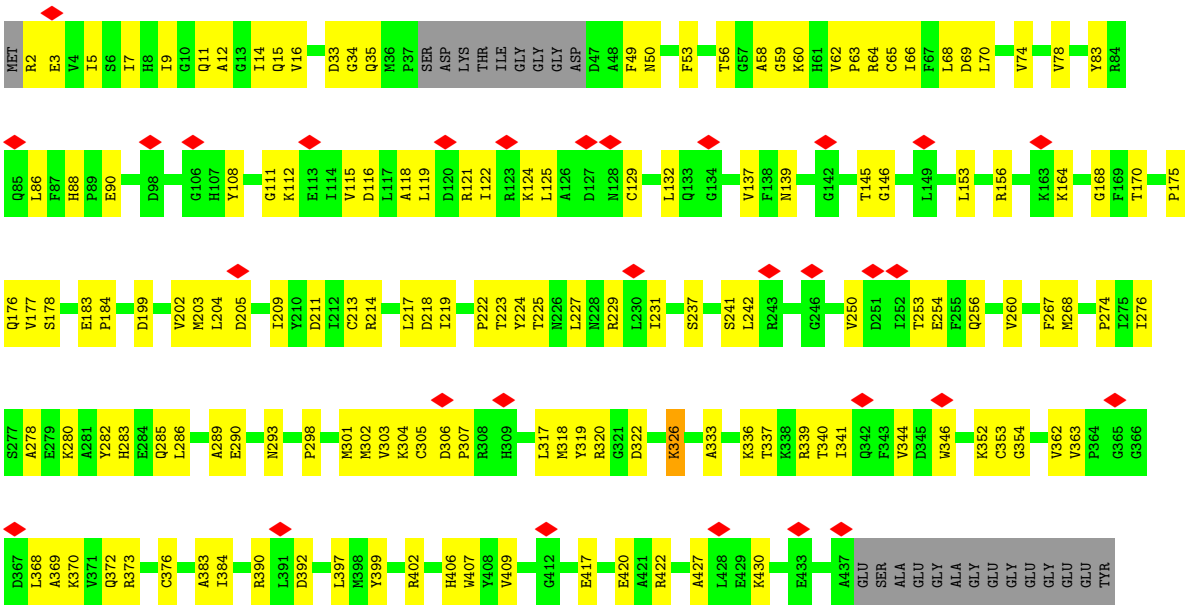
- Molecule 2: Tubulin alpha

Chain 0V: 8% 59% 35% 5%



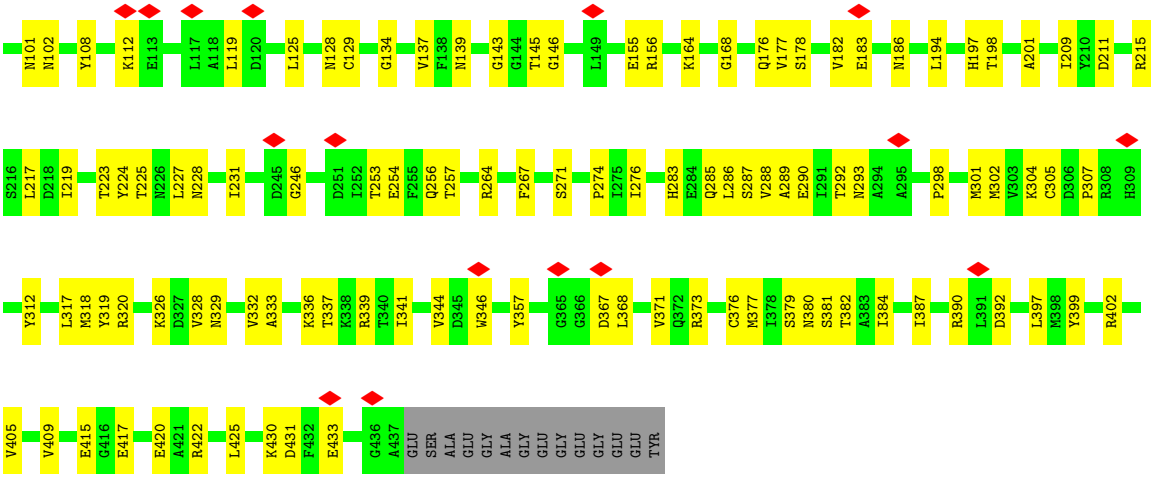
- Molecule 2: Tubulin alpha

Chain 0X:



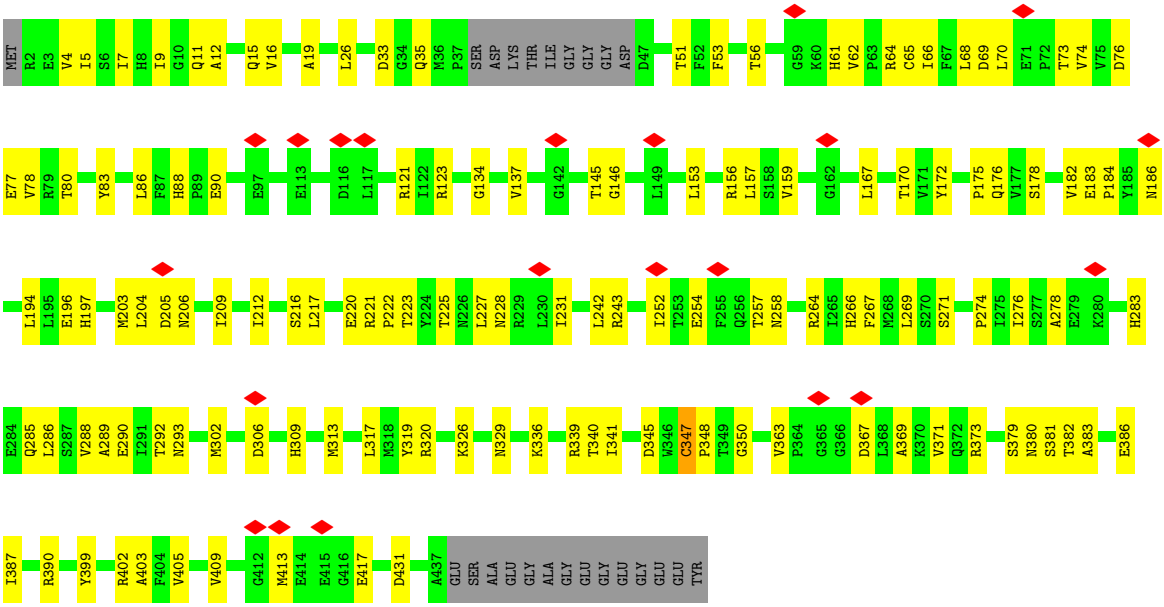
- Molecule 2: Tubulin alpha

Chain 0Z:



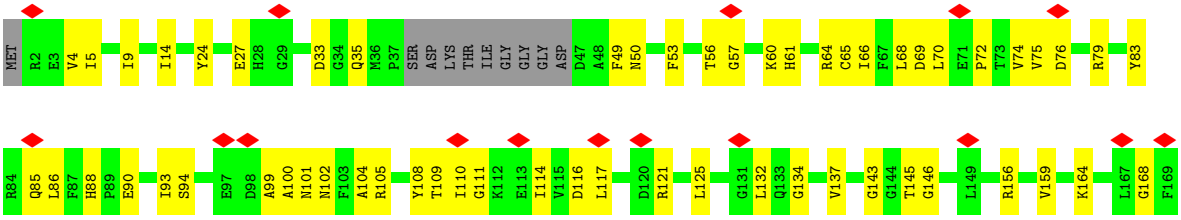
- Molecule 2: Tubulin alpha

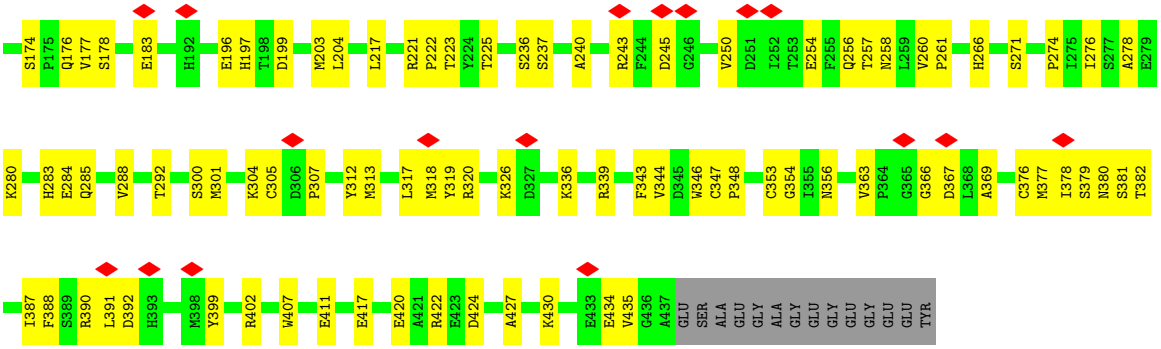
Chain 1B:



- Molecule 2: Tubulin alpha

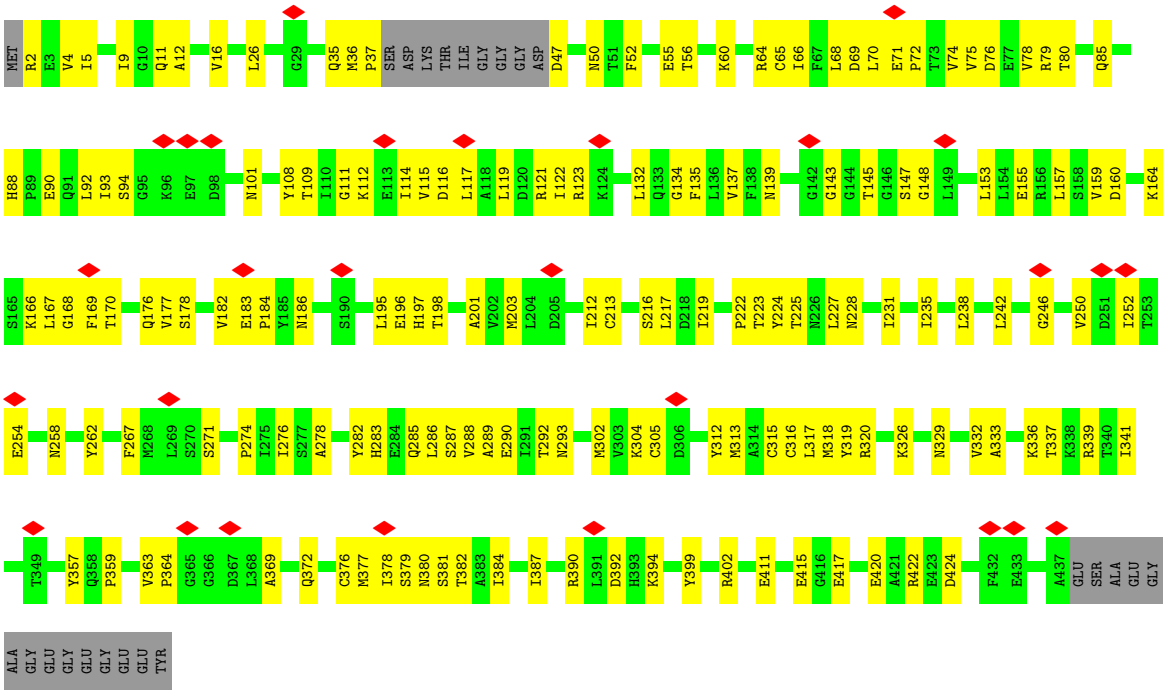
Chain 1D:





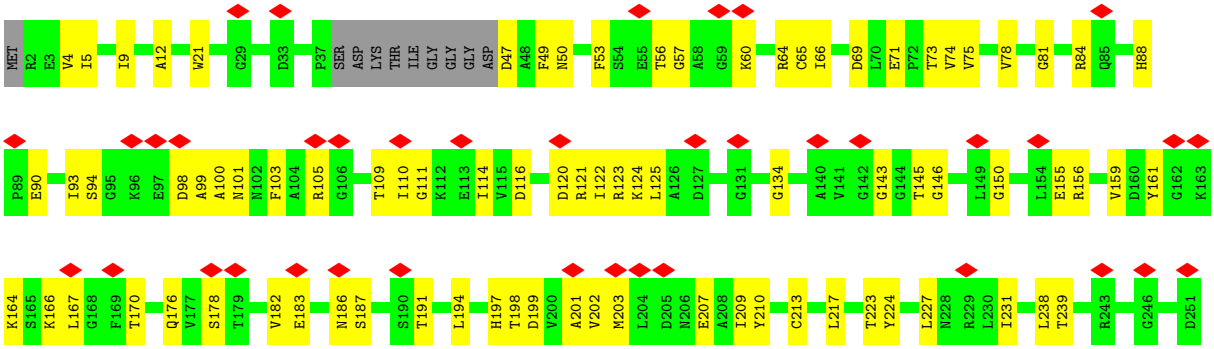
- Molecule 2: Tubulin alpha

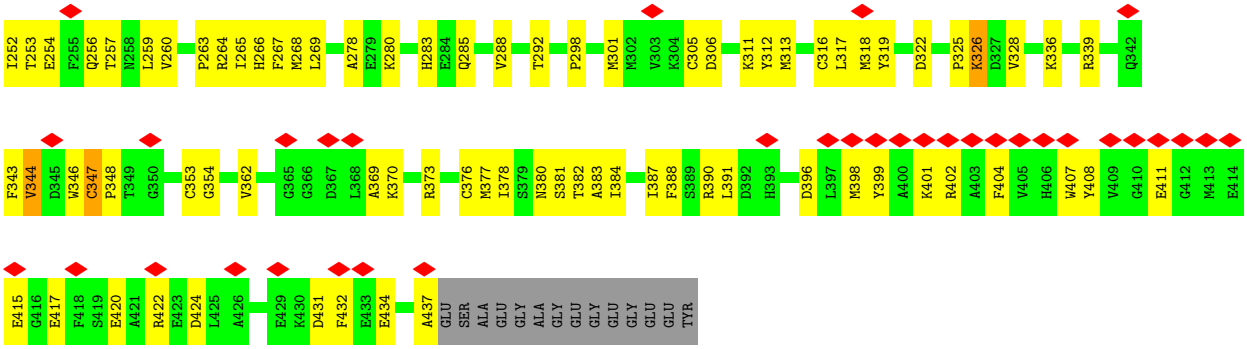
Chain 1F:



- Molecule 2: Tubulin alpha

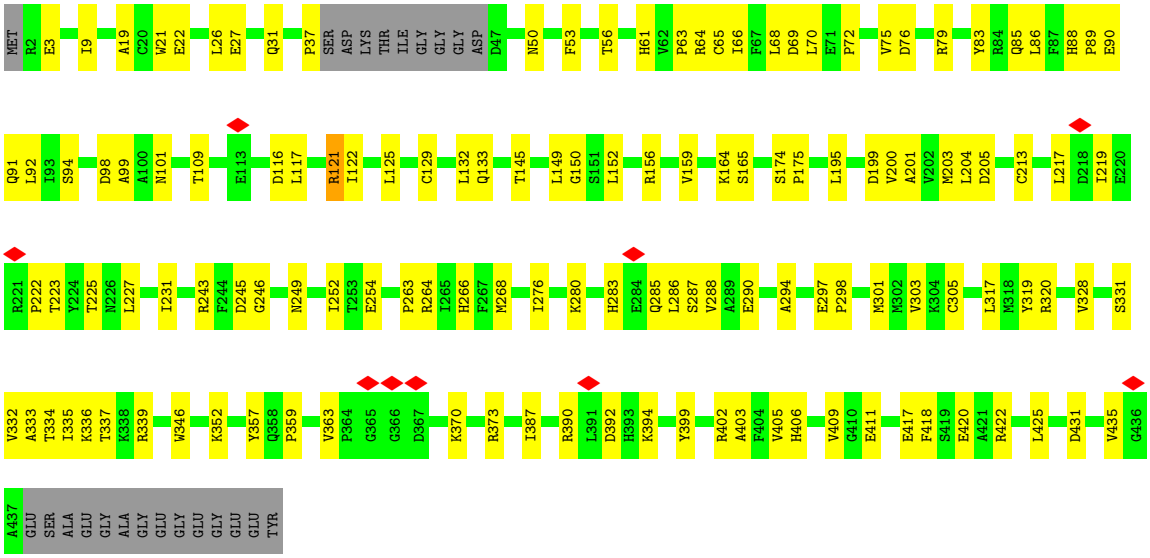
Chain 1H:





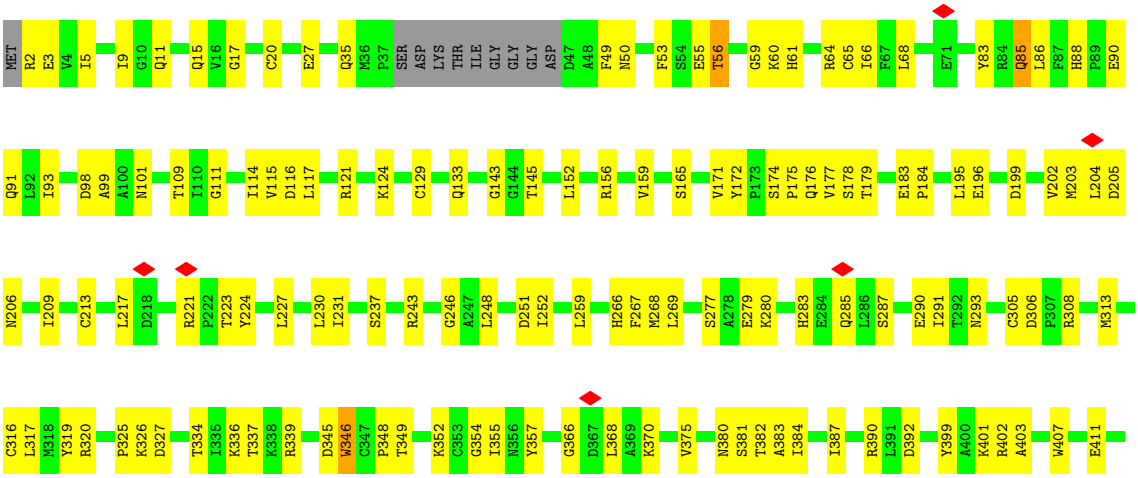
- Molecule 2: Tubulin alpha

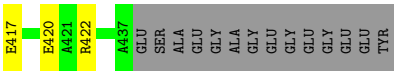
Chain 1L:



- Molecule 2: Tubulin alpha

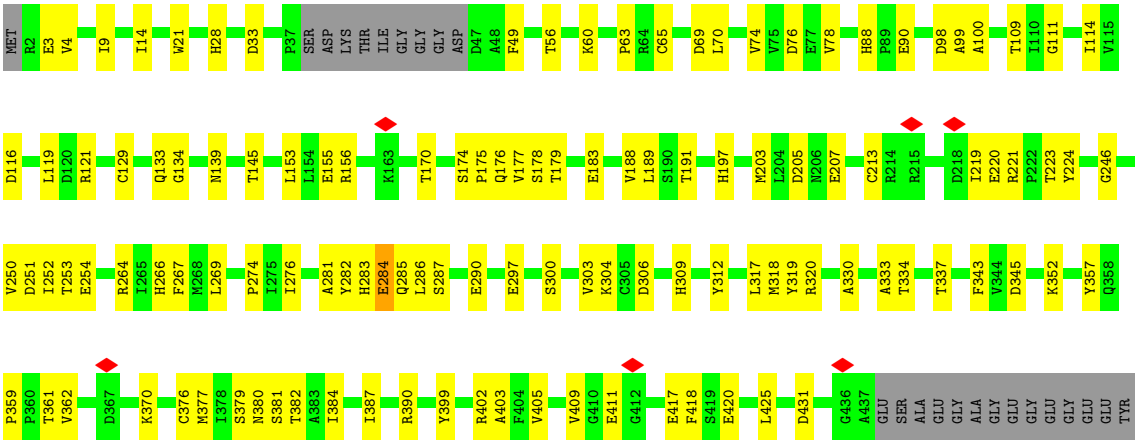
Chain 1N:





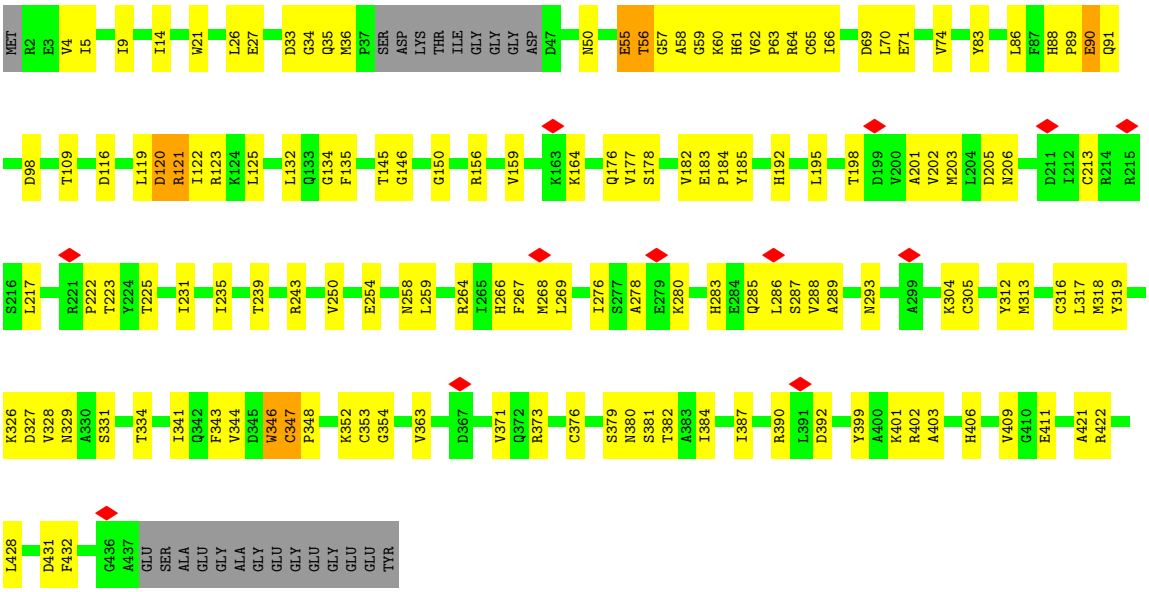
• Molecule 2: Tubulin alpha

Chain 1P:



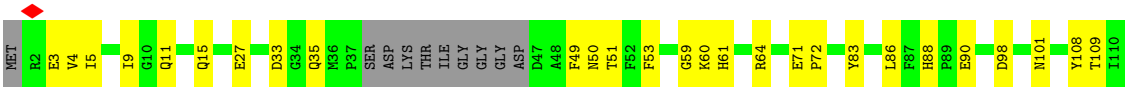
• Molecule 2: Tubulin alpha

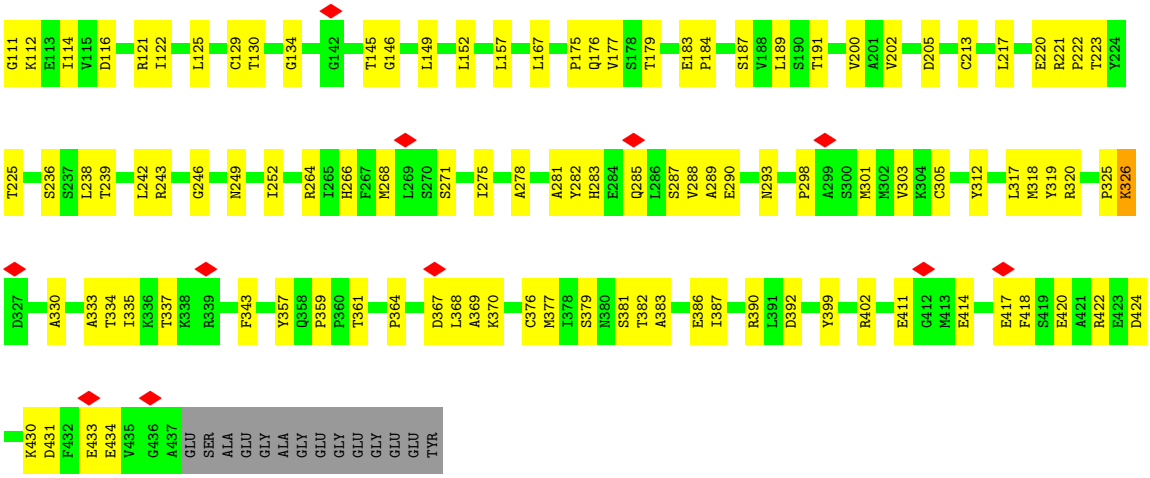
Chain 1R:



• Molecule 2: Tubulin alpha

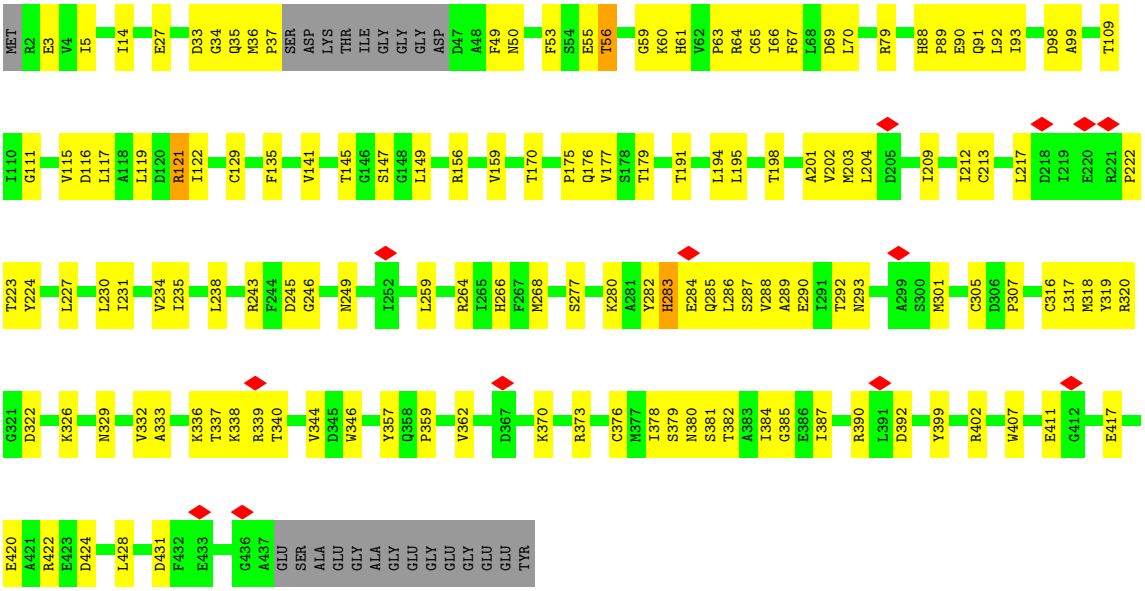
Chain 1T:





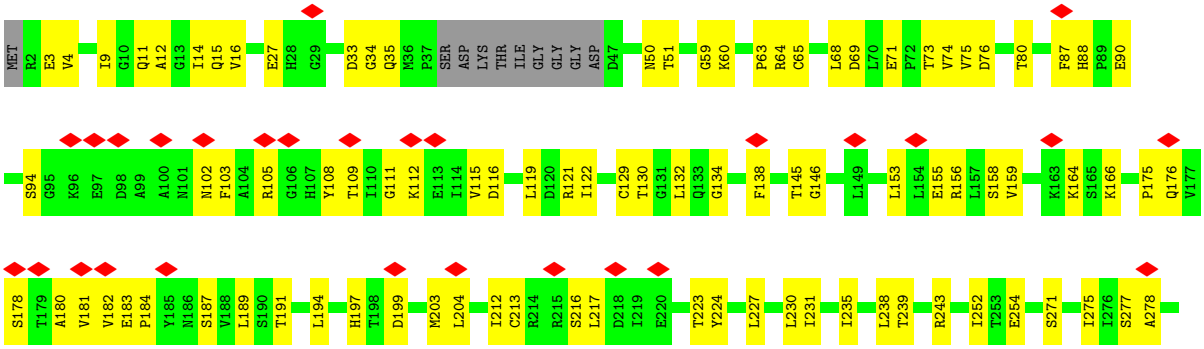
- Molecule 2: Tubulin alpha

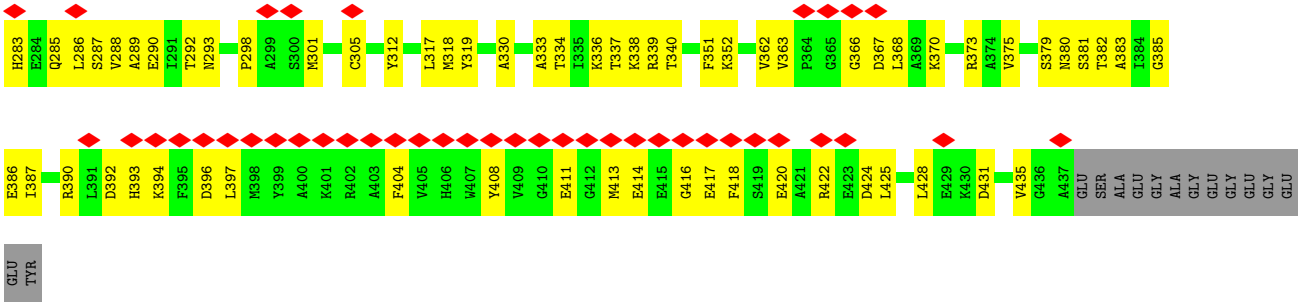
Chain 1V:



- Molecule 2: Tubulin alpha

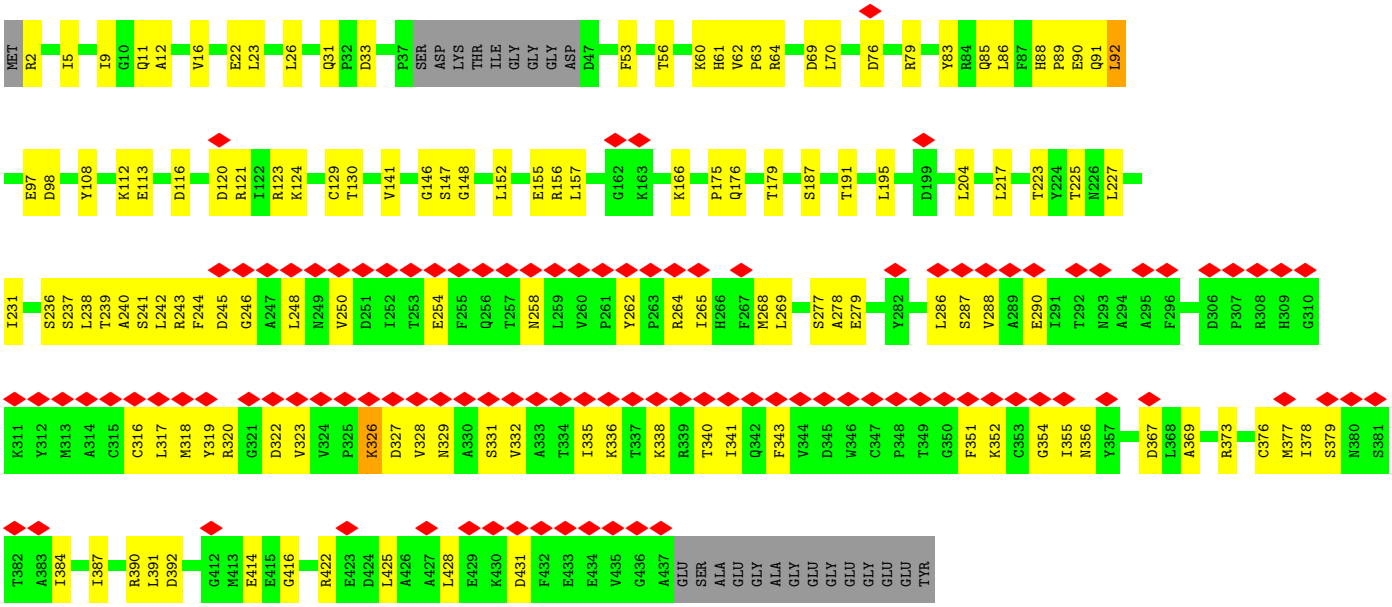
Chain 1X:





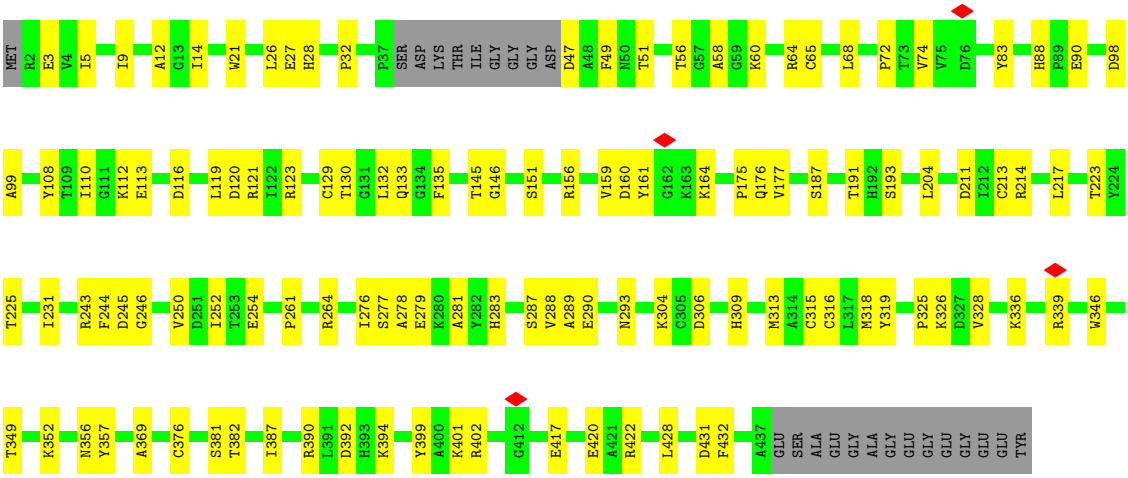
- Molecule 2: Tubulin alpha

Chain 1Z:



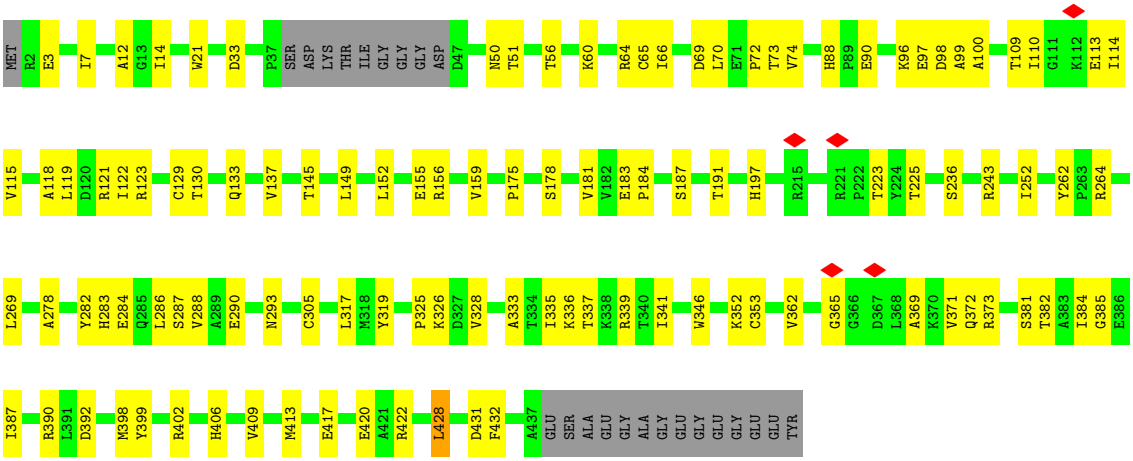
- Molecule 2: Tubulin alpha

Chain 2B:



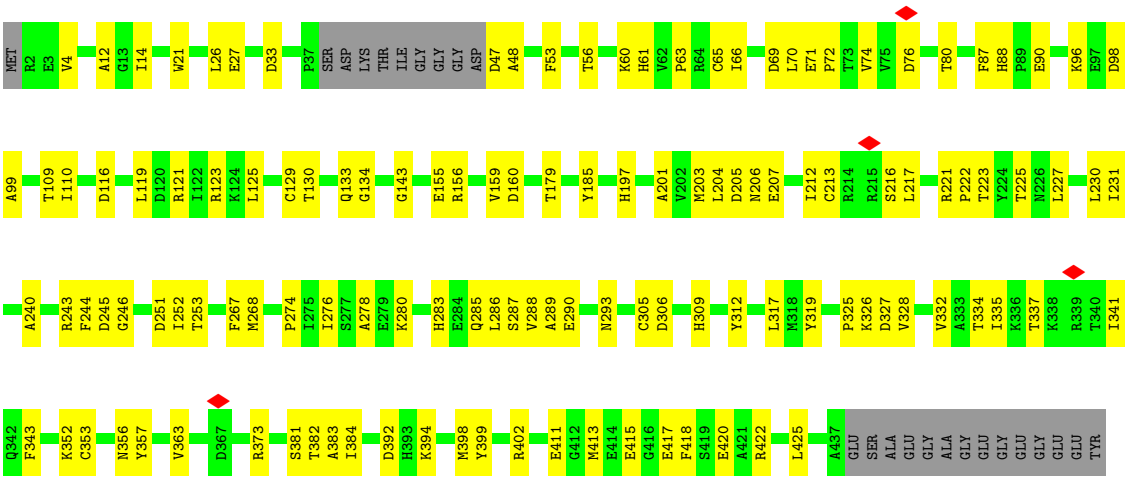
- Molecule 2: Tubulin alpha

Chain 2D:



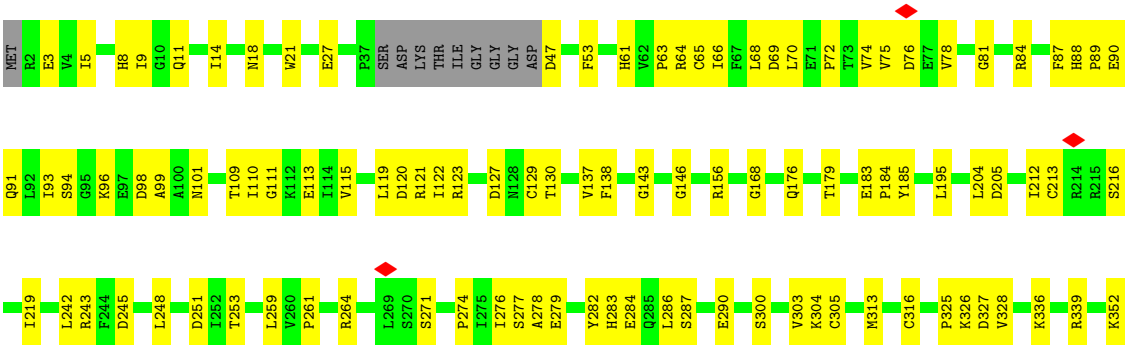
- Molecule 2: Tubulin alpha

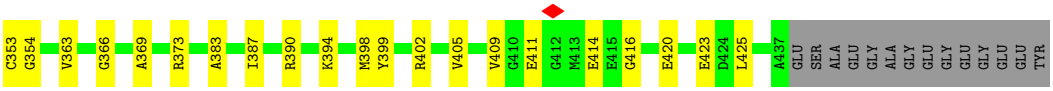
Chain 2F:



- Molecule 2: Tubulin alpha

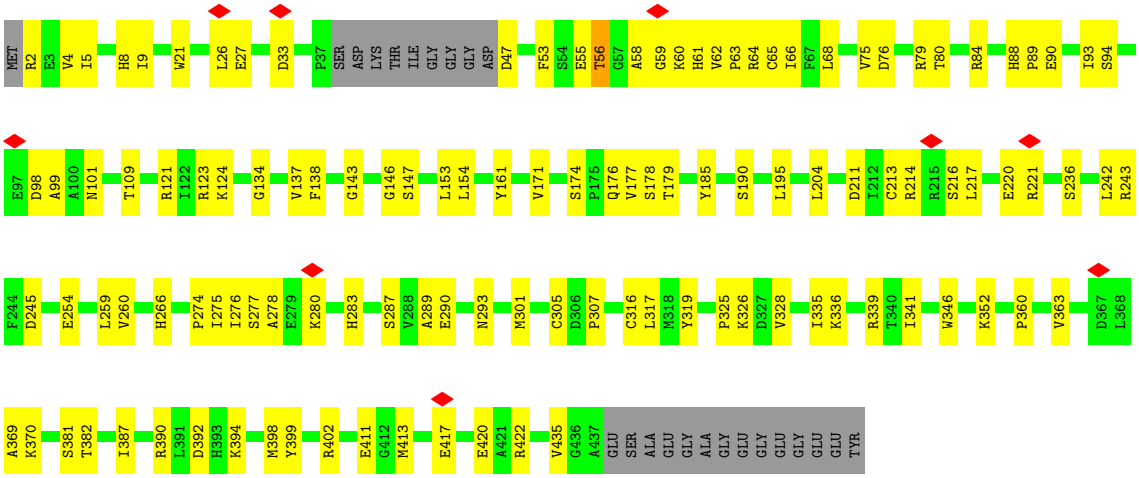
Chain 2H:





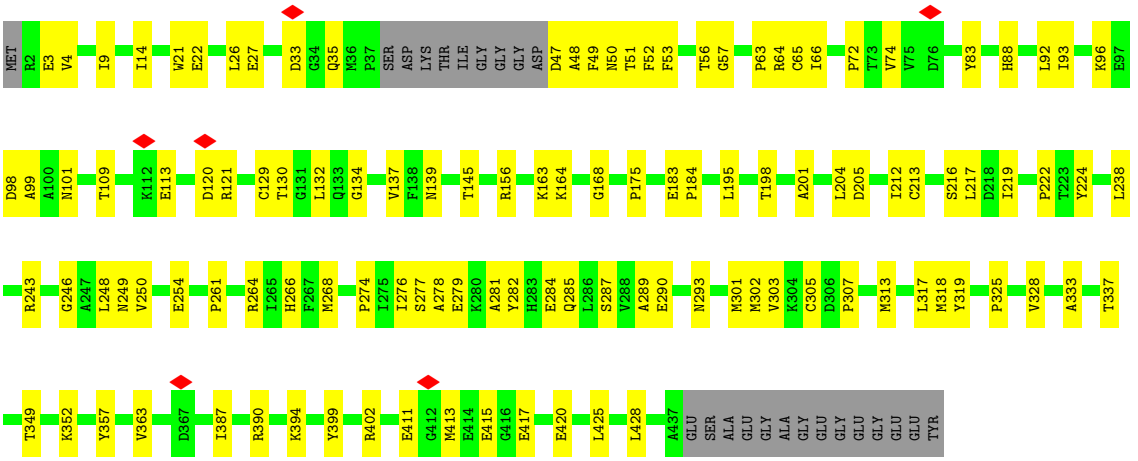
• Molecule 2: Tubulin alpha

Chain 2J:



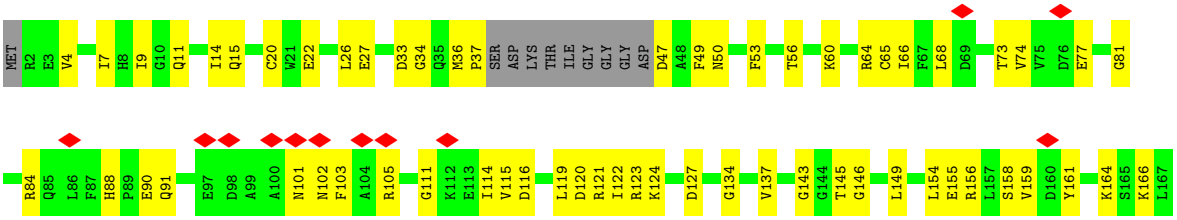
• Molecule 2: Tubulin alpha

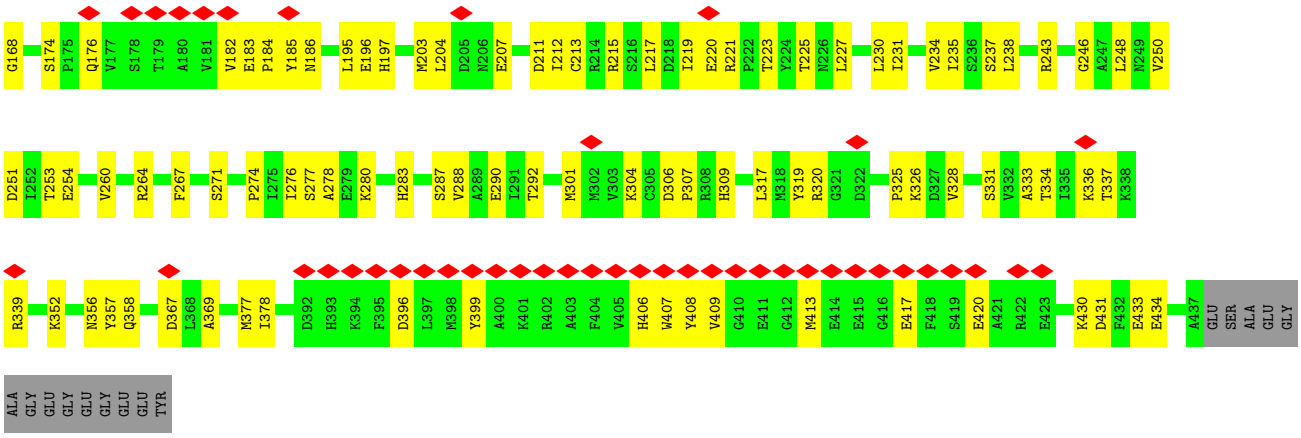
Chain 2L:



• Molecule 2: Tubulin alpha

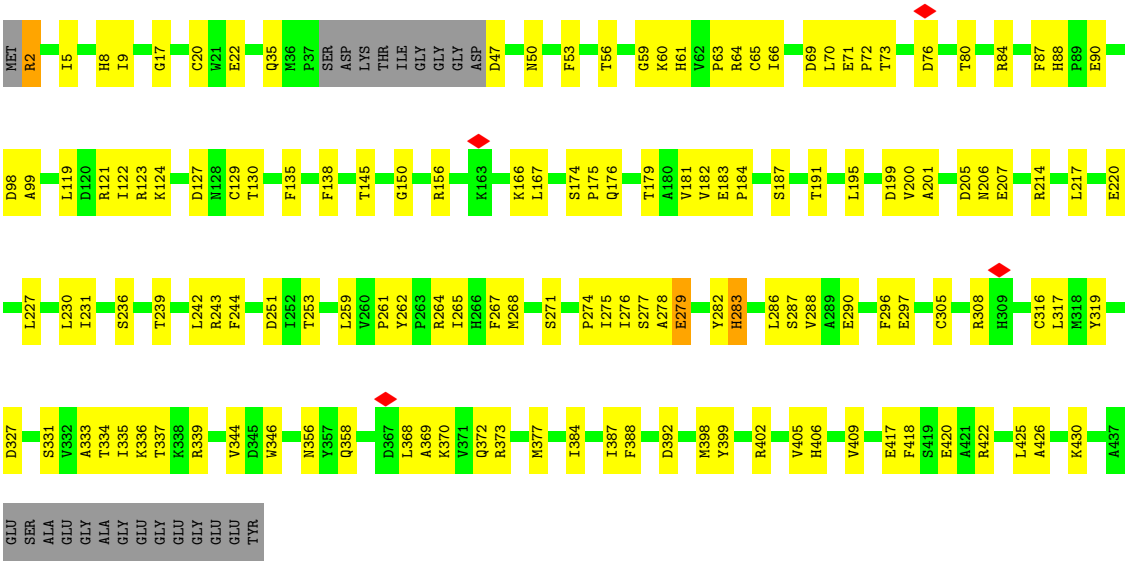
Chain 2N:





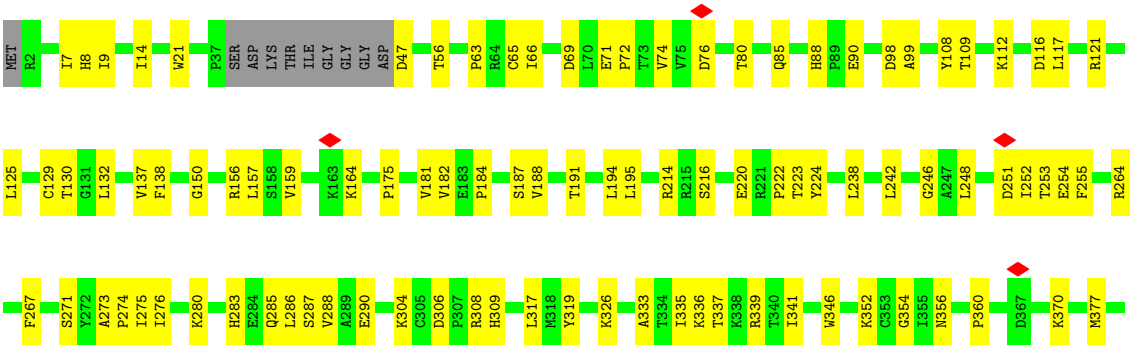
- Molecule 2: Tubulin alpha

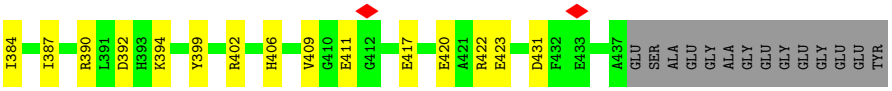
Chain 2P:



- Molecule 2: Tubulin alpha

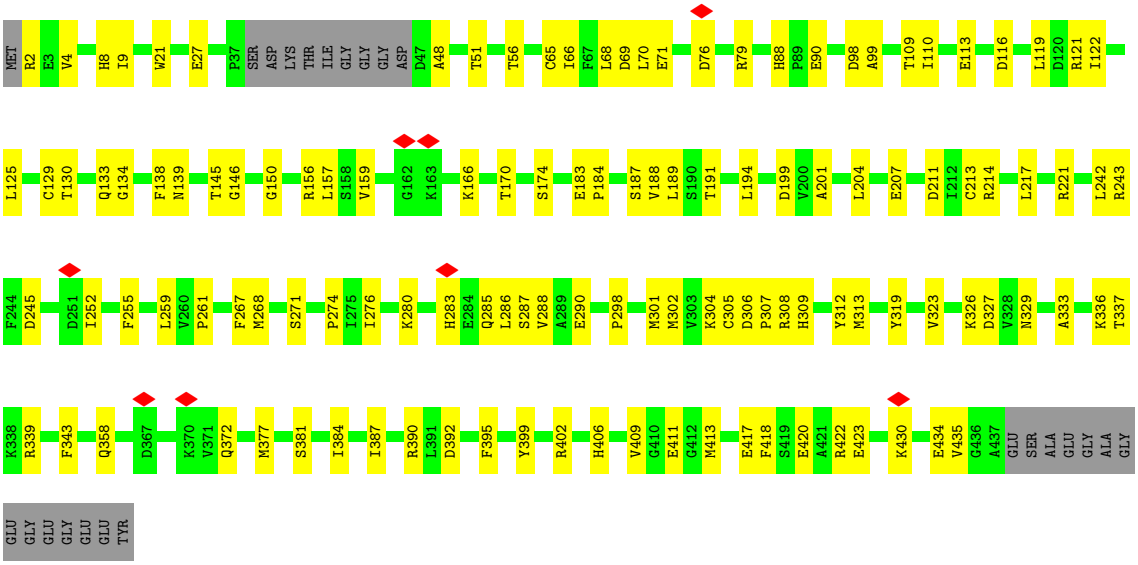
Chain 2R:





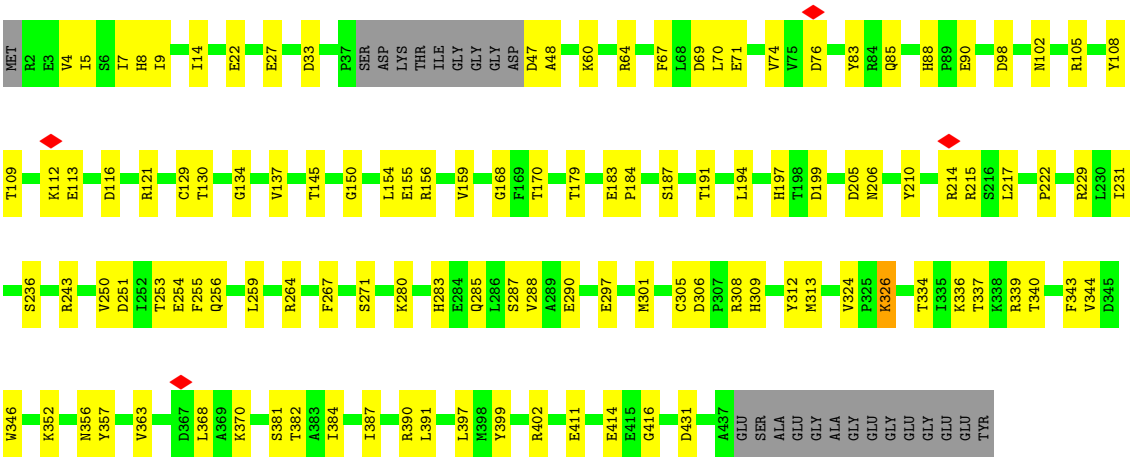
• Molecule 2: Tubulin alpha

Chain 2T:



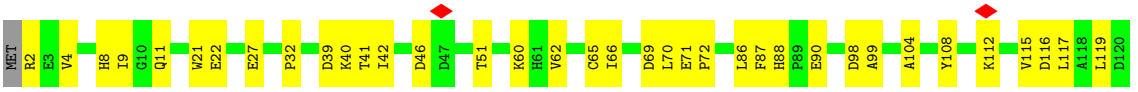
• Molecule 2: Tubulin alpha

Chain 2V:



• Molecule 2: Tubulin alpha

Chain 2X:



R121 I122 L125 C129 T130 Q133 G134 V137 F138 N139 A140 V141 G142 G143 S147 G150 S151 L152 R156 L157 S158 V159 D160 Y161 G162 K163 G168 F169 T170 V171 S174 T179 E183 P184 S187 T191 H192 S193 L194 L195 V200 D205 N206 E207

R214 D218 P222 T223 Y224 R243 F244 D245 L248 N249 V250 D251 E254 I265 H266 F267 M268 S271 Y272 A273 P274 I275 I276 E279 K280 A281 Y282 L286 S287 E290 P298 K304 C305 D306 M313 K326 I335 I341 W346 C347 K352 C353

G354 I355 N356 Y357 Q358 V371 Q372 R373 N380 S381 T382 A383 I384 I387 K394 Y399 R402 H406 V409 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 L428 D431 E434 V435 E438 SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU

TYR

- Molecule 2: Tubulin alpha

Chain 2Z:

MET R2 E3 H8 I9 G10 G17 W21 L26 E27 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 T56 K60 H61 V62 P63 R64 C65 I66 F72 D76 R79 Q85 L86 F87 H88 P89 E90 Q91 L92 K96 E97 D98 A99 A100 N101 N102

R105 G106 H107 Y108 T109 I110 G111 K112 E113 L119 D120 R121 I122 L125 C129 F135 L136 V137 G143 G144 T145 G146 S147 G150 S151 L152 L153 L154 E155 R156 V159 G168 S178 V182 E183 P184 Y185 V188 L189 S190 D199 M203 L204 C213 R214 R215

S216 L217 P222 T223 Y224 T225 N228 I235 S236 S237 L238 T239 R243 F244 D251 N258 Y262 F267 Y272 A273 P274 I275 I276 S277 A278 E279 Y282 Q285 L286 E297 M301 D306 P307 R308 H309 Y312 R320 V324 P325 V328 S331

V332 A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 K352 N356 V363 D367 L368 A369 K370 R373 I378 S381 T382 A383 I384 I387 D392 H393 K394 F395 D396 L397 M398 Y399 R402 E411 G412 E415 G416 E417 F418 S419 E420 A421 R422 E423 A426

E429 K430 E433 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

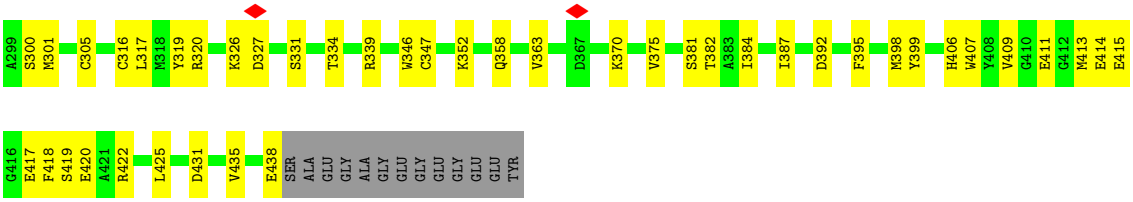
- Molecule 2: Tubulin alpha

Chain 3B:

MET R2 I5 S6 I9 G10 Q11 Q15 W21 E22 L26 E27 H28 G29 I30 D33 K40 T41 I42 D46 D47 A48 F49 N50 T51 F52 F53 S54 E55 T56 K60 H61 V62 P63 R64 C65 I66 F67 L68 E71 D76 E77 V78 R79 T80 R84 Q85

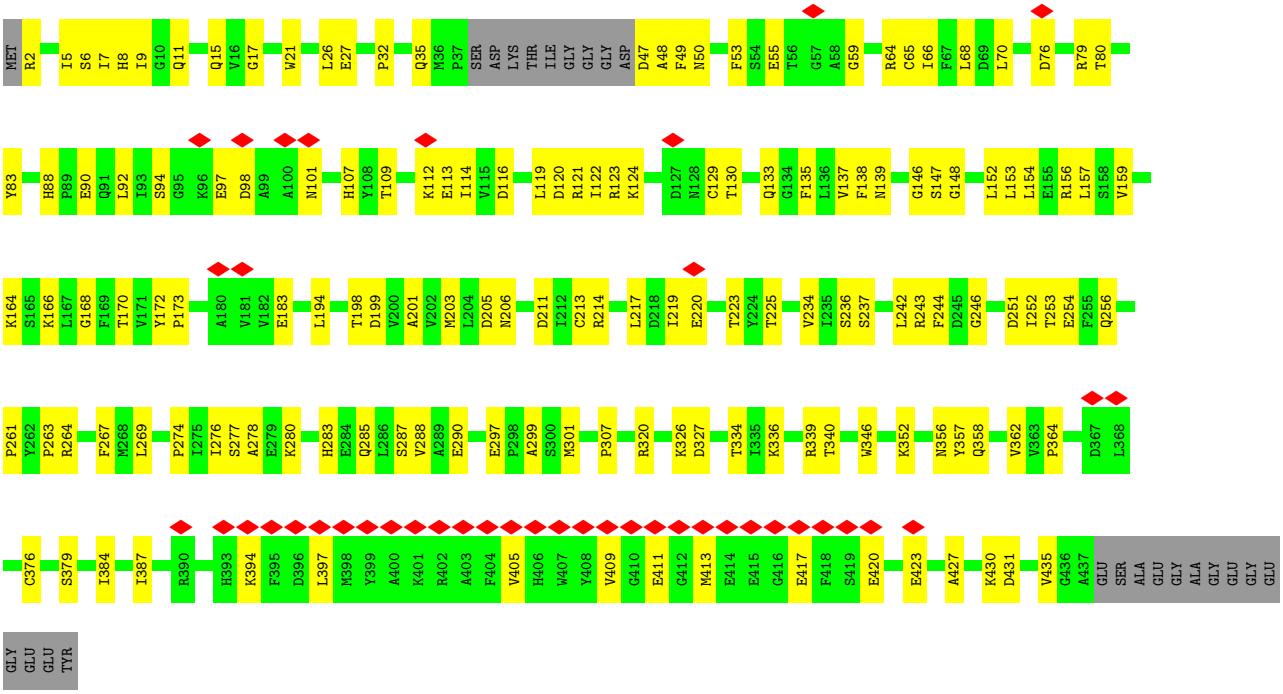
E90 Q91 L92 I93 E97 D98 N102 R105 T109 I110 G111 K112 V115 L119 D120 R121 L125 C129 T130 F135 N139 A140 V141 S147 L152 L153 R156 V159 V171 S178 T179 E183 P184 L189 M203 L204 D205 N206 D211 I212

C213 R214 L217 E220 R221 P222 T223 Y224 N228 I231 V234 I235 S236 S237 S241 L242 R243 F244 V250 D251 I252 T253 E254 L259 Y262 P263 R264 I265 L269 I276 S277 A278 E279 K280 A281 Y282 H283 L286 S287 V288 A289 E290 I291 A294 E297 P298



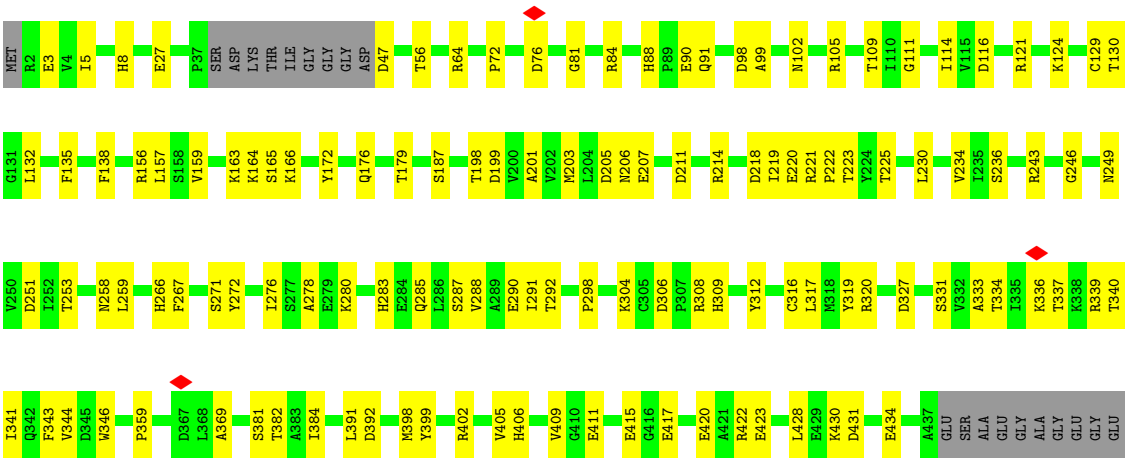
• Molecule 2: Tubulin alpha

Chain 3D:



• Molecule 2: Tubulin alpha

Chain 3F:



GLY GLU GLU TYR

- Molecule 2: Tubulin alpha

Chain 3H: 67% 27% 5%

MET R2 E3 V4 I5 I9 I14 W21 L26 E27 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 T51 T56 P63 R64 C65 I66 P72 T73 V74 V75 D76 T80 R84 E90 Q91 D98 A99 V115 D116 L117 R121 K124

D127 N128 C129 F135 G146 S147 L152 L153 R156 V159 K163 K164 L167 S174 P175 Q176 V177 V182 E183 P184 Y185 S190 D199 V200 A201 V202 M203 L204 D205 N206 I219 E220 R221 P222 I231 S236 A240 R243 F244 D245 G246 V250 D251

E254 F255 Q256 P261 R264 F267 M268 L269 P274 I275 I276 S277 A278 E279 K280 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 M301 C305 D306 P307 R308 H309 Y312 M313 R320 V324 D327 R339 T340 I341 Q342 F343 V344 D345 W346 T349

K352 N356 Y357 Q358 P359 V363 P364 G365 G366 D367 L368 A369 R373 A374 I384 R390 L391 D392 L397 M398 Y399 R402 E417 E420 A421 R422 D431 E434 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

- Molecule 2: Tubulin alpha

Chain 3J: 70% 25% 5%

MET R2 E3 H8 I9 I14 W21 E27 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 N50 T51 T56 R64 C65 L70 E71 P72 T73 V74 V75 D76 R79 H88 P89 E90 Q91 S94 D98 D116 L117 R121 I122 R123 K124 L125

A126 D127 N128 C129 Q133 F138 G146 R156 V159 S165 V177 S178 T179 E183 P184 H192 S193 L194 T198 D199 V200 C213 L217 E220 R221 P222 T223 Y224 S236 R243 G246 N249 I252 T253 E254 F255 Q256 T257 N258 L259 R264

F267 S271 Y272 I276 S277 A278 E279 K280 H283 E284 Q285 L286 S287 V288 A289 N293 M301 C305 D306 P307 L317 M318 Y319 K326 A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 T349 K352 N356 Y357 A369 R373

I384 I387 D392 H393 K394 L397 M398 Y399 R402 V405 E415 G416 E417 F418 S419 E420 A421 R422 D431 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

- Molecule 2: Tubulin alpha

Chain 3L: 71% 24% 5%

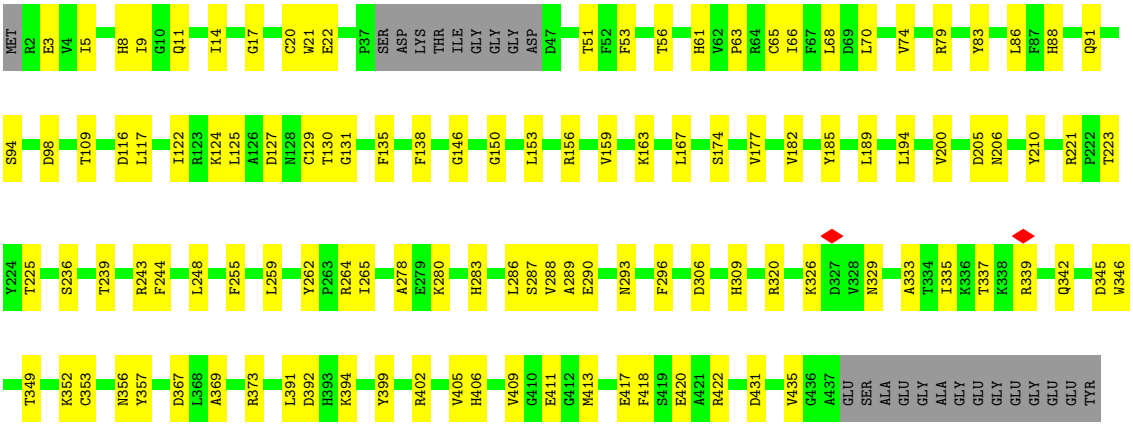
MET R2 E3 V4 I5 H8 I9 G10 Q11 I14 W21 E27 D33 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 T51 T56 P63 R64 C65 E71 P72 D76 R79 R84 H88 Q91 D98 T109 L119 I122 R123

K124 L125 N128 C129 T130 G131 L132 Q133 G134 F135 F138 R156 V159 K163 K164 V177 S178 V182 E183 P184 Y185 V188 L189 L195 V200 C213 L217 D218 I219 E220 R221 P222 T223 Y224 S236 S237 L238 T239 R243 D251 I252 T253 E254 F255

L259 F267 M268 L269 S270 S271 K280 H283 L286 S287 V288 A289 E290 N293 F296 M301 C305 D306 P307 K326 A333 T334 I335 K336 T337 K338 R339 Q342 W346 T349 K352 N356 Y357 D367 R373 M377 I378 A383 I384 L391

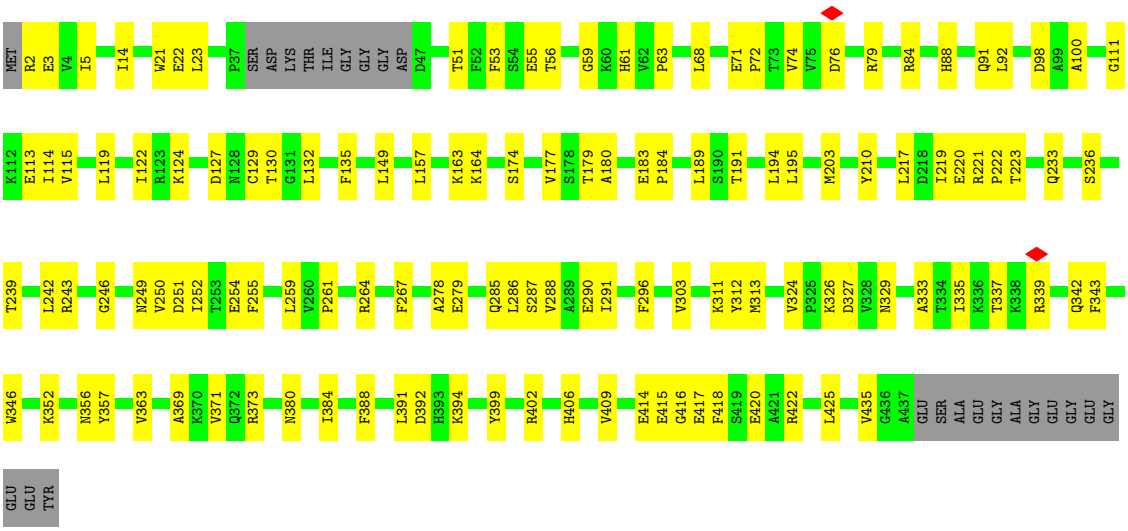
• Molecule 2: Tubulin alpha

Chain 3N:



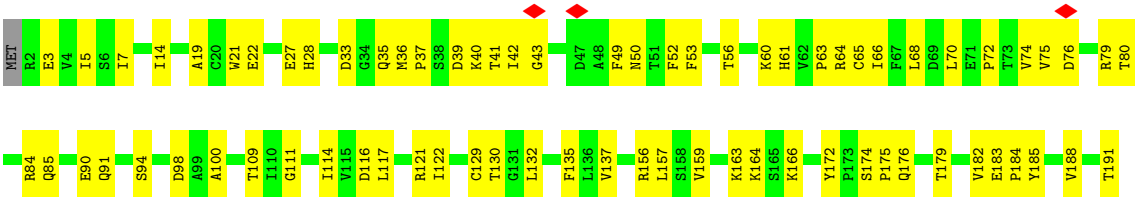
• Molecule 2: Tubulin alpha

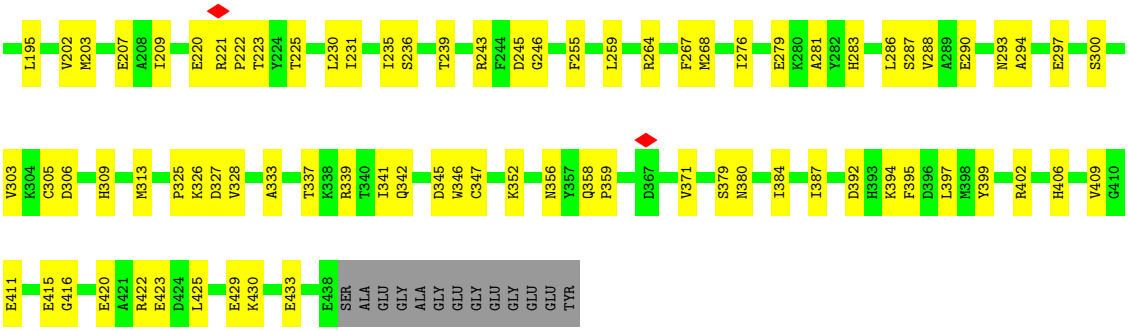
Chain 3P:



• Molecule 2: Tubulin alpha

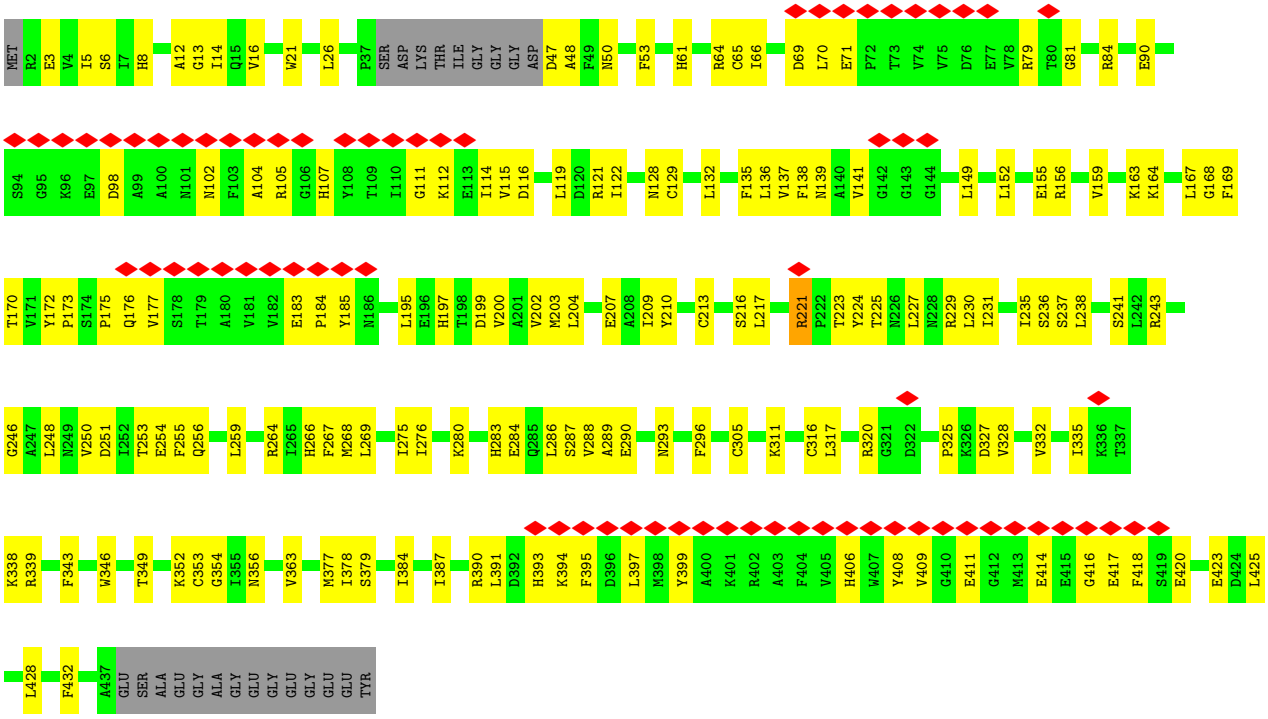
Chain 3R:





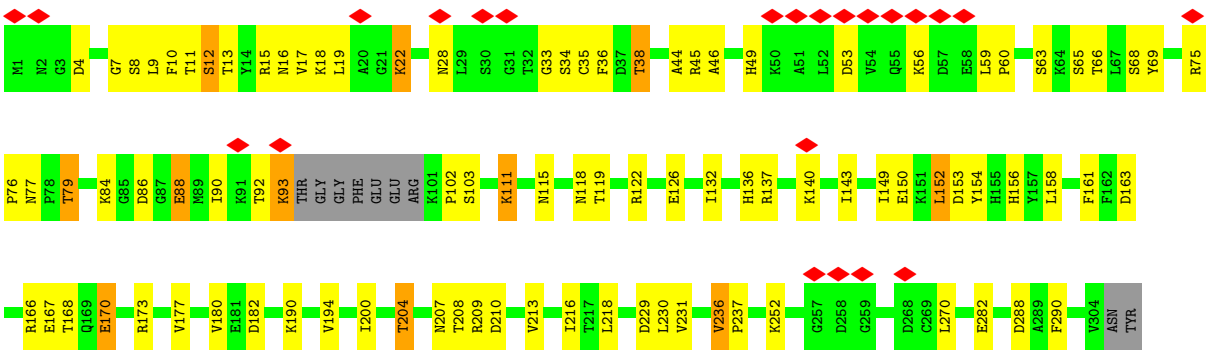
- Molecule 2: Tubulin alpha

Chain 3T:



- Molecule 3: PACRG

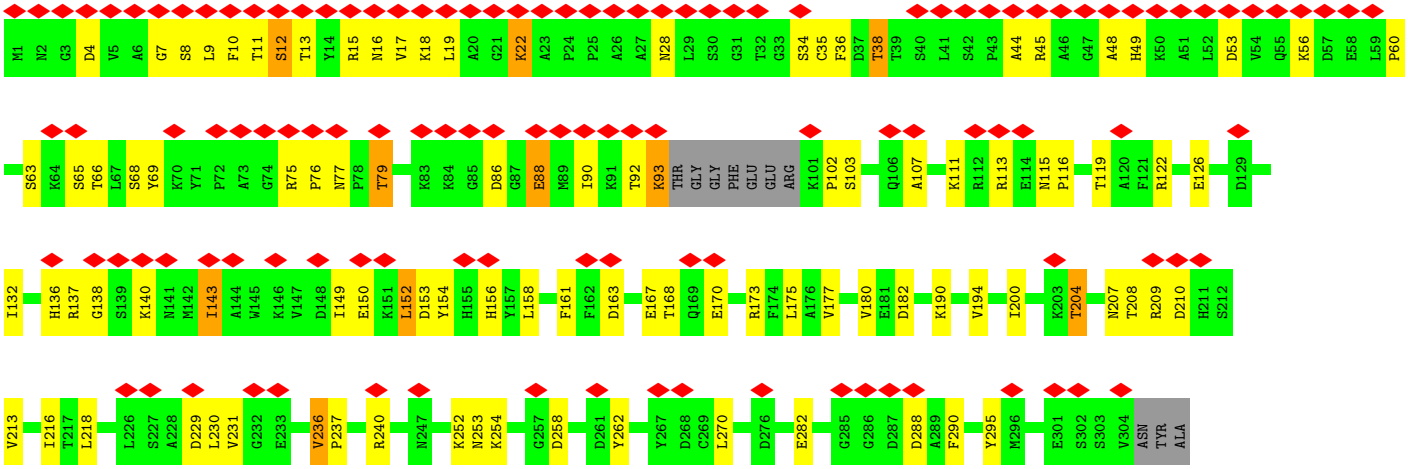
Chain 3V:



ALA

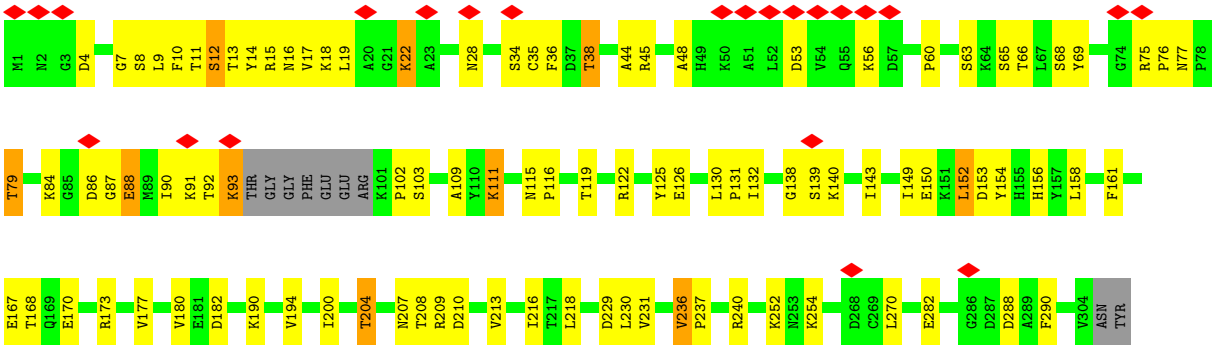
• Molecule 3: PACRG

Chain 3X:



• Molecule 3: PACRG

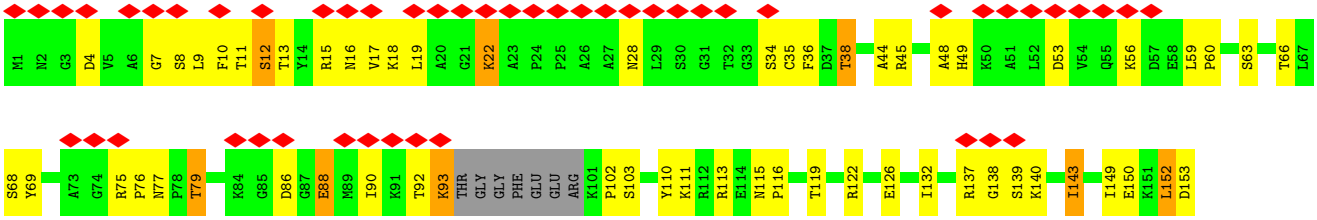
Chain 3Z:

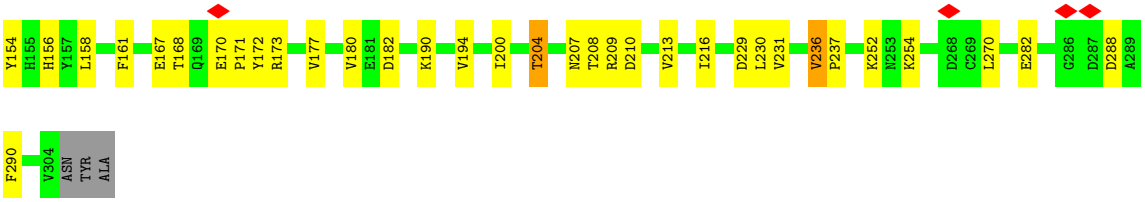


ALA

• Molecule 3: PACRG

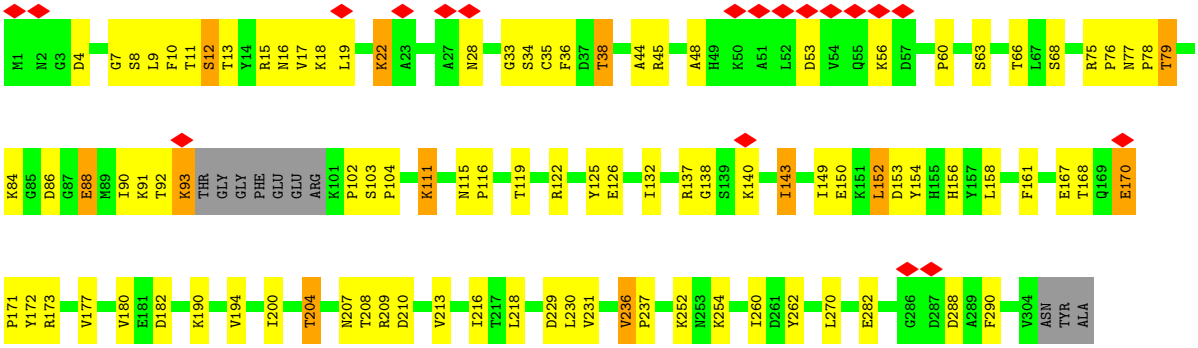
Chain 4B:





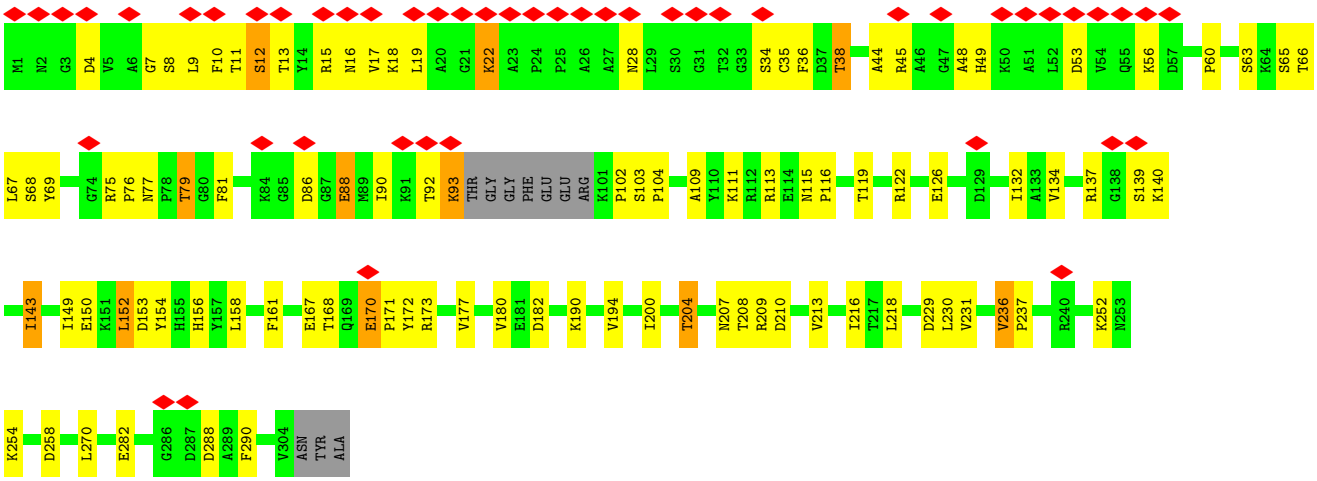
• Molecule 3: PACRG

Chain 4D:



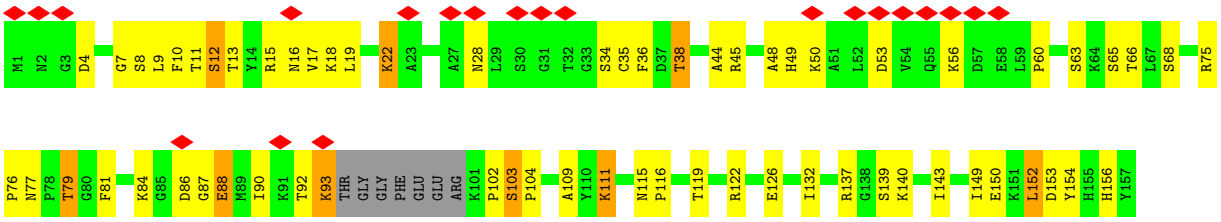
• Molecule 3: PACRG

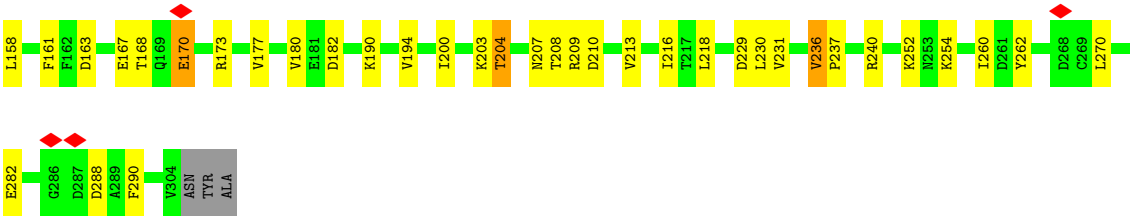
Chain 4F:



• Molecule 3: PACRG

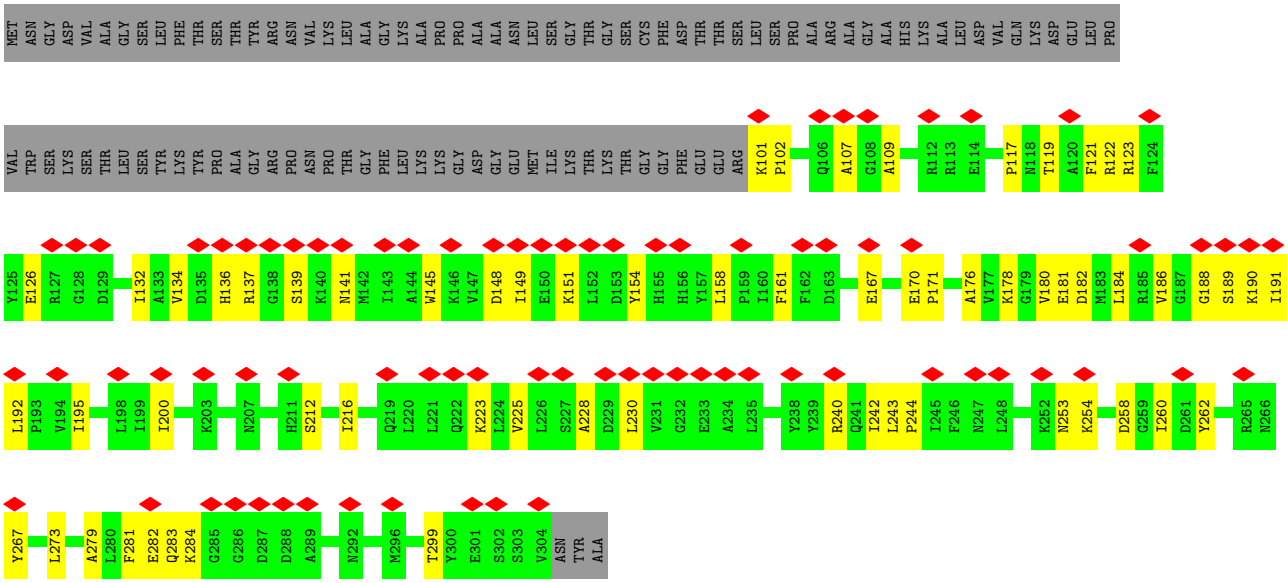
Chain 4H:





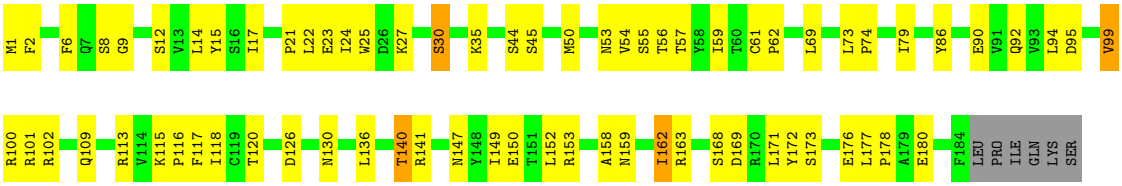
• Molecule 3: PACRG

Chain 4J:



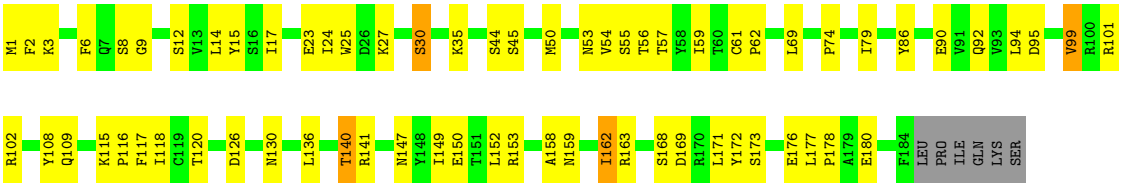
• Molecule 4: FAP20

Chain 3W:



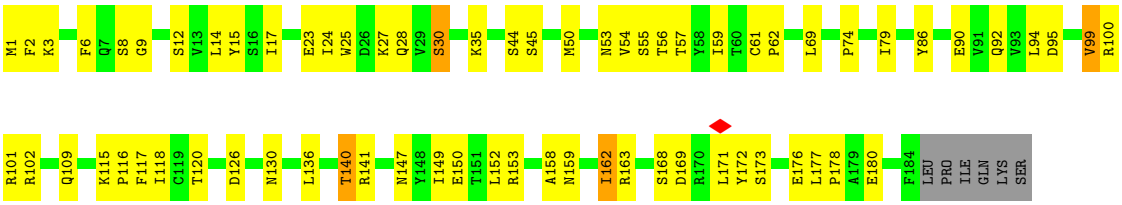
• Molecule 4: FAP20

Chain 3Y:



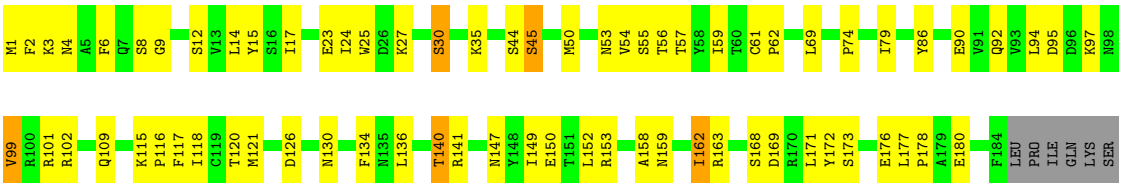
• Molecule 4: FAP20

Chain 4A:



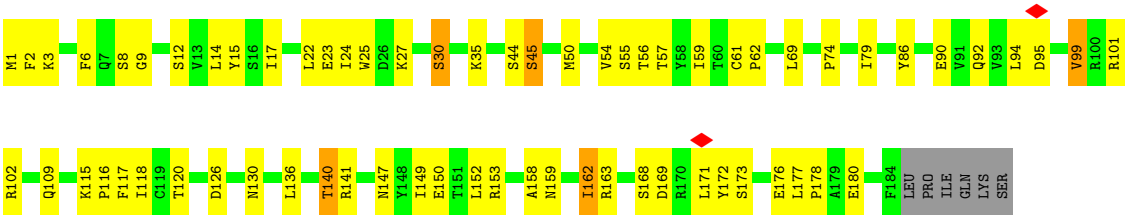
• Molecule 4: FAP20

Chain 4C:



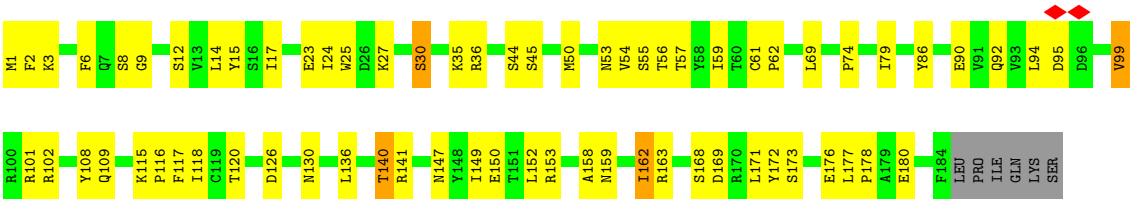
• Molecule 4: FAP20

Chain 4E:



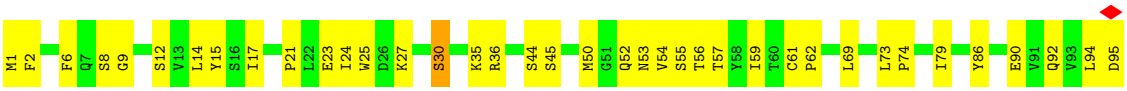
• Molecule 4: FAP20

Chain 4G:



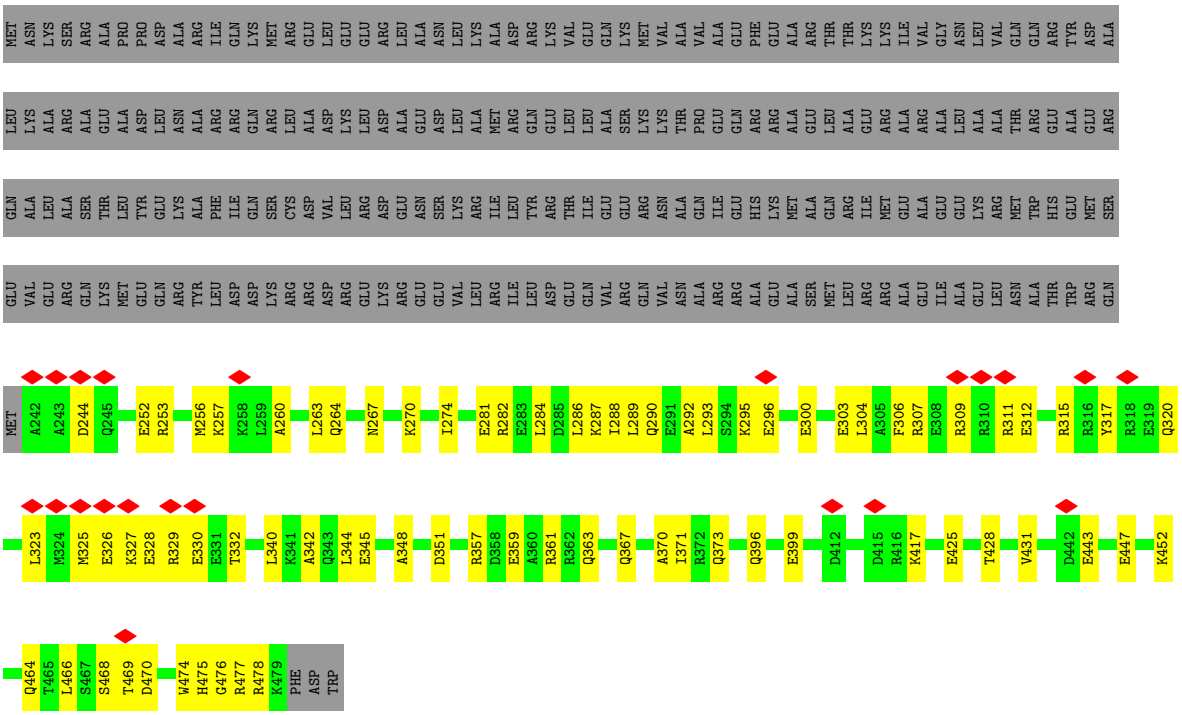
• Molecule 4: FAP20

Chain 4I:



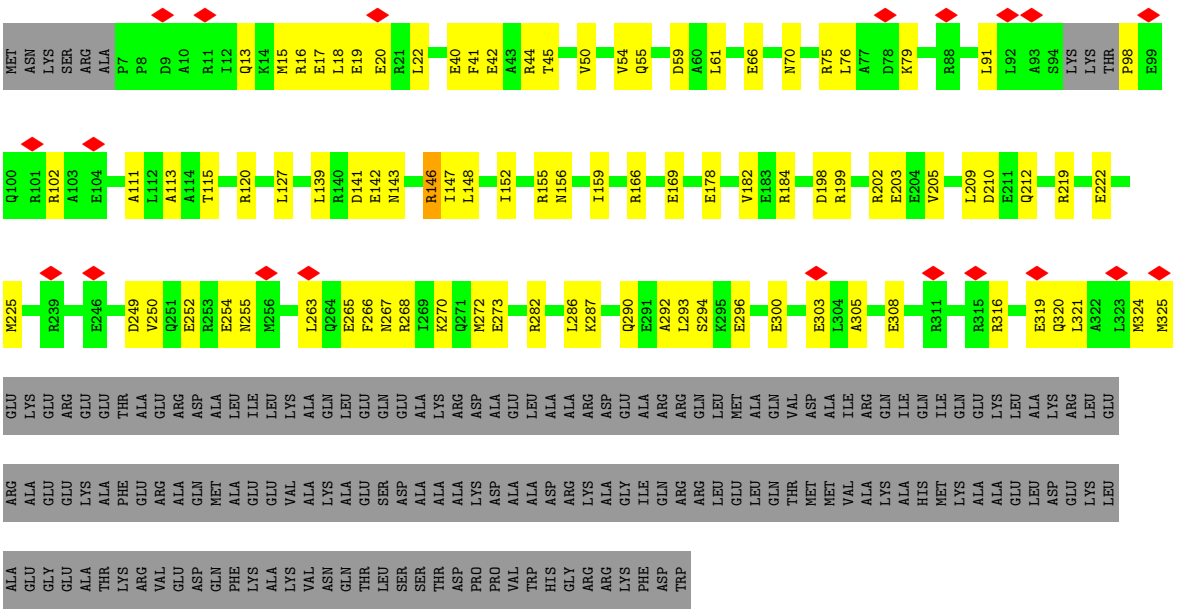
• Molecule 5: FAP53

Chain 4L:



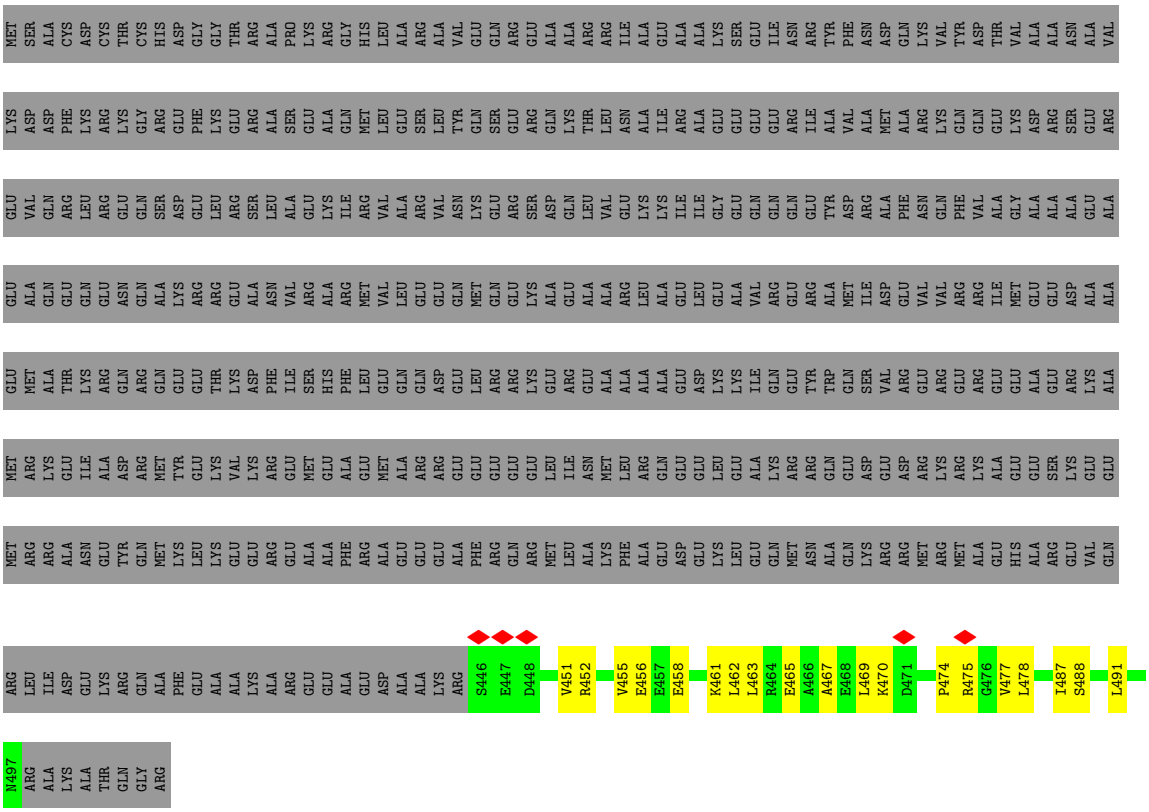
• Molecule 5: FAP53

Chain 4M:



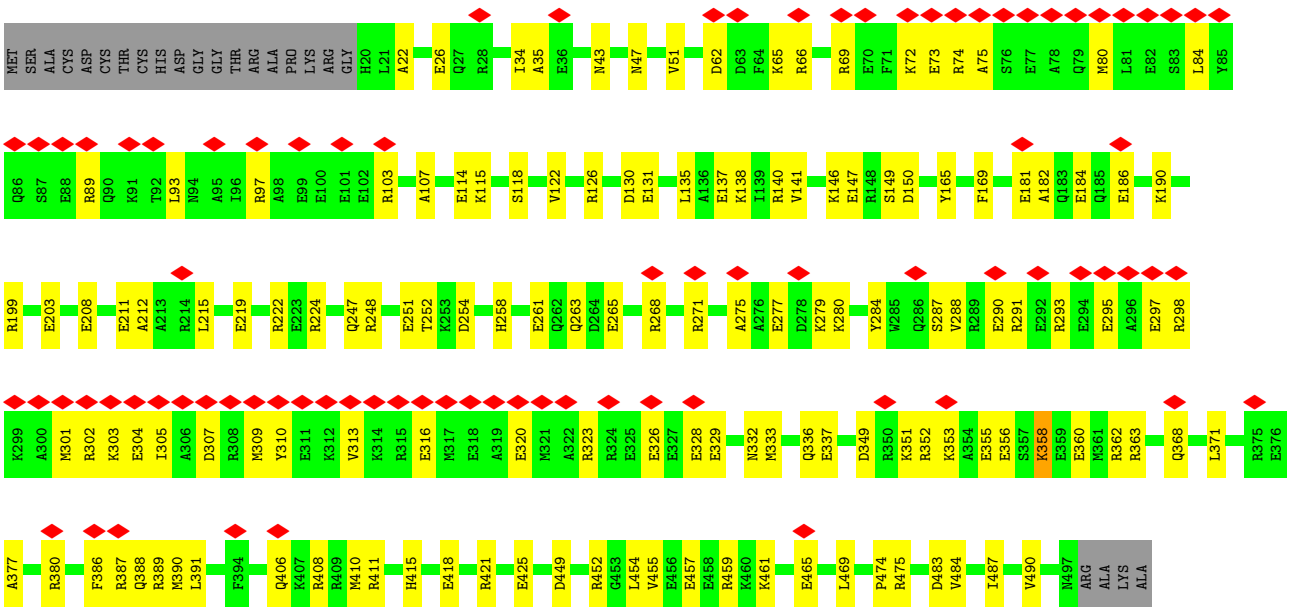
- Molecule 6: FAP127

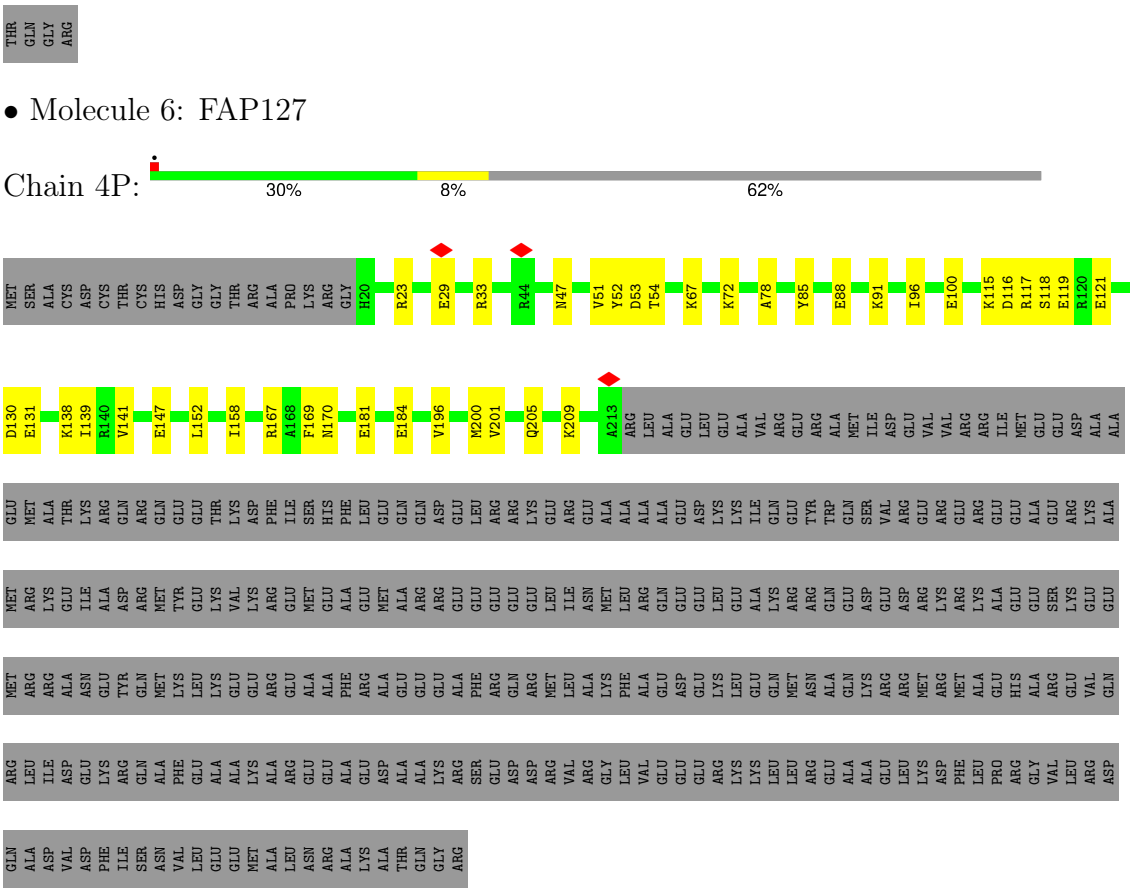
Chain 4N:



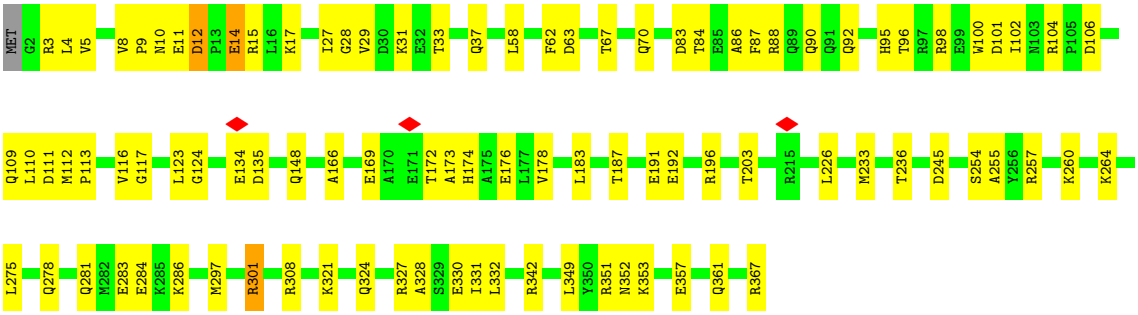
- Molecule 6: FAP127

Chain 4O:



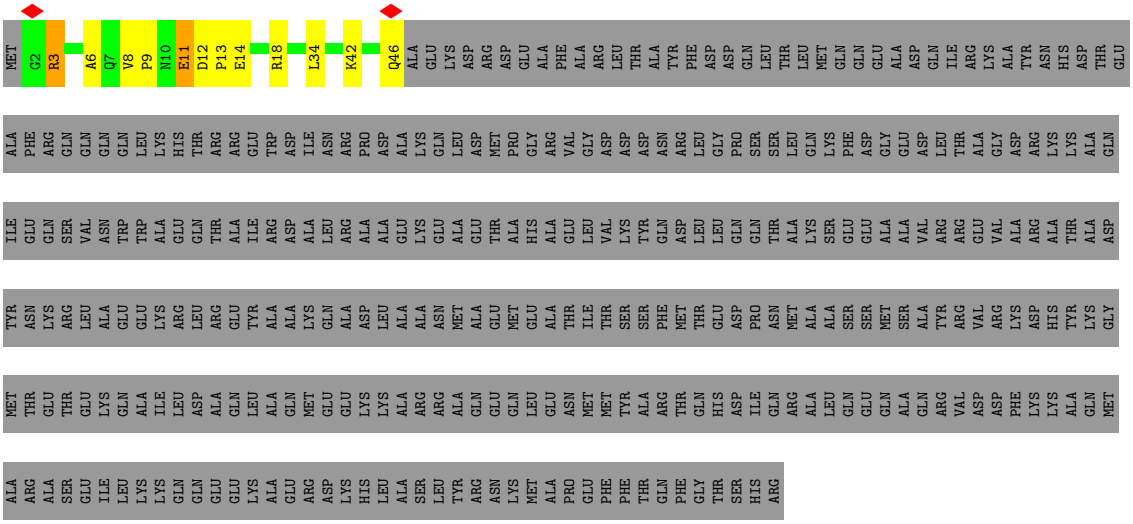

THR GLN GLY ARG
• Molecule 6: FAP127
Chain 4P:
30%
8%
62%
MET SER ALA CYS ASP CYS THR CYS HIS ASP GLY GLY THR ARG ALA PRO LYS ARG GLY H20 R23 E29 R33 R44 N47 V51 Y52 D53 T54 K67 K72 A78 Y85 E88 K91 I96 E100 K115 D116 R117 S118 E119 R120 E121
D130 E131 K138 I139 R140 V141 E147 L152 I158 R167 A168 F169 N170 E181 E184 V196 M200 V201 Q205 K209 A213 ARG LEU ALA GLU LEU GLU ALA VAL ARG GLU ARG ALA MET ILE ASP GLU VAL VAL ARG ILE MET GLU GLU ASP ALA ALA
GLU MET ALA THR LYS ARG GLN ARG GLN GLU GLU GLU THR LYS ASP PHE ILE SER HIS PHE LEU GLU GLN GLN GLN ASP GLU GLU LEU ARG ARG LYS GLU ARG GLU GLU ALA ALA ALA ALA GLU ASP LYS LYS LYS ILE GLN GLU TYR TRP GLN SER VAL ARG GLU ARG GLU GLU ARG GLU GLU ALA LYS ARG
MET ARG LYS GLU ILE ALA ASP ARG MET TYR GLU LYS VAL LYS ARG GLU MET GLU ALA GLU MET ALA ARG ARG GLU GLU GLU GLU GLU LEU ILE ASN MET LEU ARG GLN GLU GLU LEU GLU ALA LYS ARG ARG GLN GLU ASP GLU ASP ARG LYS ARG LYS ALA GLU GLU SER LYS GLU GLU
MET ARG ARG ALA ASN GLU TYR GLN MET LYS LEU LYS GLU GLU ARG GLU ALA ALA ALA PHE ARG ALA GLU GLU GLU ALA PHE ARG GLN ARG MET LEU ALA LYS PHE ALA GLU ASP GLU LYS LEU GLU GLN MET ASN ALA GLN GLN LYS ARG ARG MET ARG MET ALA GLU HIS ALA ARG GLU VAL GLN
ARG LEU ILE ASP GLU LYS ARG GLN ALA PHE GLU ALA ALA LYS ALA ARG GLU GLU GLU ALA GLU ASP ALA ALA ALA LYS ARG SER GLU ASP ASP ARG VAL ARG GLY LEU VAL GLU GLU GLU ARG LYS LYS LEU LEU ARG GLU ALA ALA GLU LEU LYS ASP PHE LEU PRO ARG GLY VAL LEU ARG ASP
GLN ALA ASP VAL ASP PHE ILE SER ASN VAL LEU GLU GLU MET ALA LEU ASN ARG ALA LYS ALA THR GLN GLY ARG
• Molecule 7: RIB43a
Chain 4Q:
15%
83%
MET GLY ARG LEU VAL ALA GLN VAL PRO ASN GLU ASP PRO GLU ARG LEU LYS ARG VAL LEU ASP ALA LYS TRP ARG THR ILE GLY VAL ASP LYS GLU THR LEU GLU LEU GLN ALA GLN GLU LYS LYS LYS ASP ARG GLU GLN ALA GLU LYS ASP ARG ASP GLU ALA PHE ALA ARG LEU THR ALA
TYR PHE ASP ASP GLN LEU THR LEU MET GLN GLN GLU ALA ASP GLN ILE ARG LYS ALA TYR ASN HIS ASP THR GLU ALA PHE ARG GLN GLN GLN GLN LEU LYS HIS THR ARG ARG GLU TRP ASP ILE ASN ARG PRO ASP ALA LYS GLN LEU ASP MET PRO GLY ARG VAL GLY ASP ASP
ASN ARG LEU GLY PRO SER SER LEU GLN LYS PHE ASP GLY GLU ASP LEU THR ALA GLY ASP ARG LYS LYS ALA GLN ILE GLU GLN SER VAL ASN TRP TRP ALA GLU GLN THR ALA ILE ARG ASP ALA LEU ARG ALA ALA GLU LYS GLU ALA GLU THR ALA HIS ALA GLU LEU VAL LYS TYR
GLN ASP LEU LEU GLN GLN THR ALA LYS SER GLU GLU ALA VAL ARG ARG GLU VAL ALA ARG ALA THR ALA ASP TYR ASN LYS ARG LEU ALA GLU GLU LYS ARG LEU ARG GLU TYR ALA ALA LYS GLN ALA ASP LEU ALA ALA ALA ASN MET ALA GLU MET GLU ALA THR ILE THR SER SER
PHE MET THR GLU ASP PRO ASN MET ALA ALA SER SER MET SER ALA TYR ARG VAL ARG LYS ASP HIS TYR LYS GLY MET THR GLU THR GLU LYS GLN ALA ILE LEU ASP ALA GLN LEU ALA GLN MET GLU GLU LYS LYS ALA ARG ARG ALA GLN GLU GLN LEU GLU ASN MET MET TYR ALA
ARG THR GLN HIS D305 I306 F320 K321 K322 A323 Q324 Q336 N352 S365 H366 R367

• Molecule 7: RIB43a
Chain 4R:
74%
25%



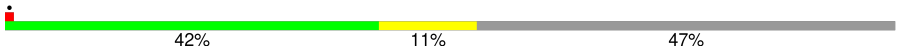
- Molecule 7: RIB43a

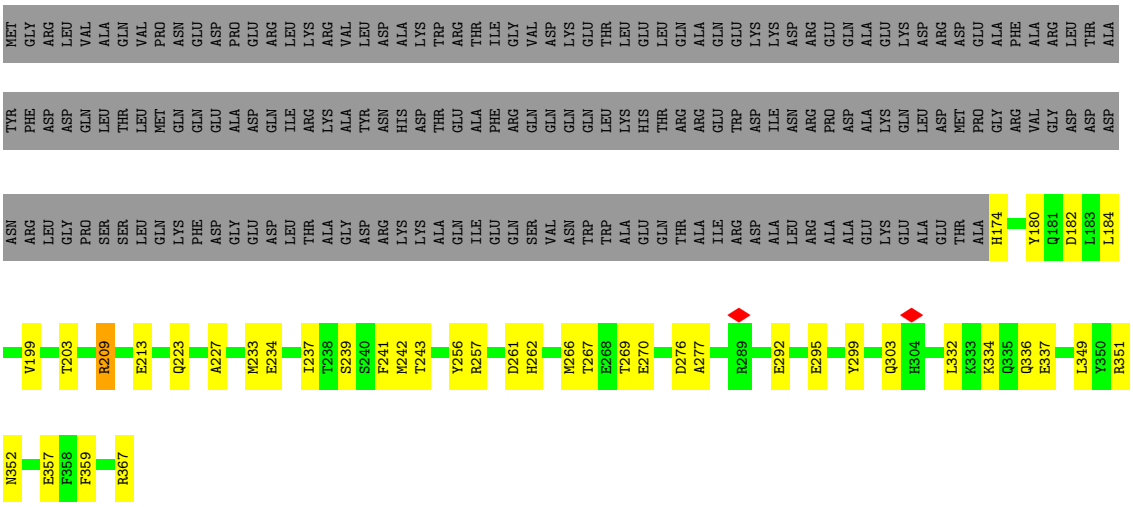
Chain 4S:



- Molecule 7: RIB43a

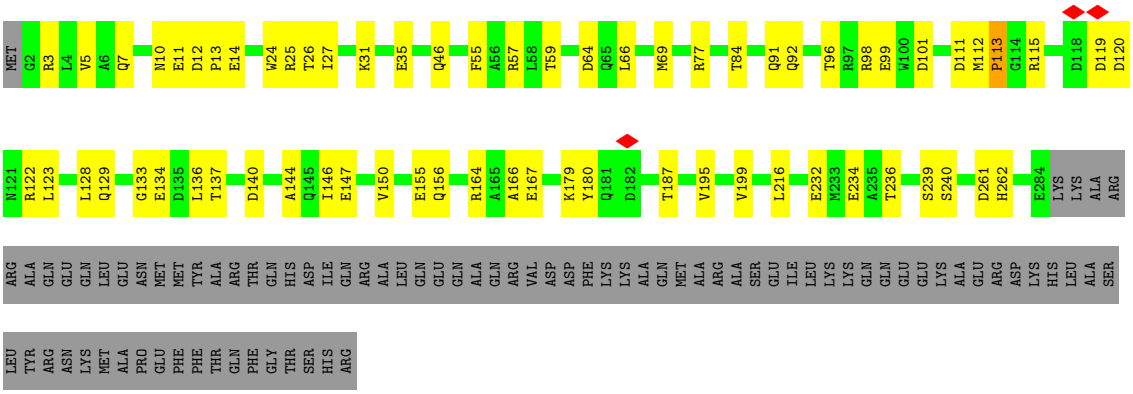
Chain 4T:





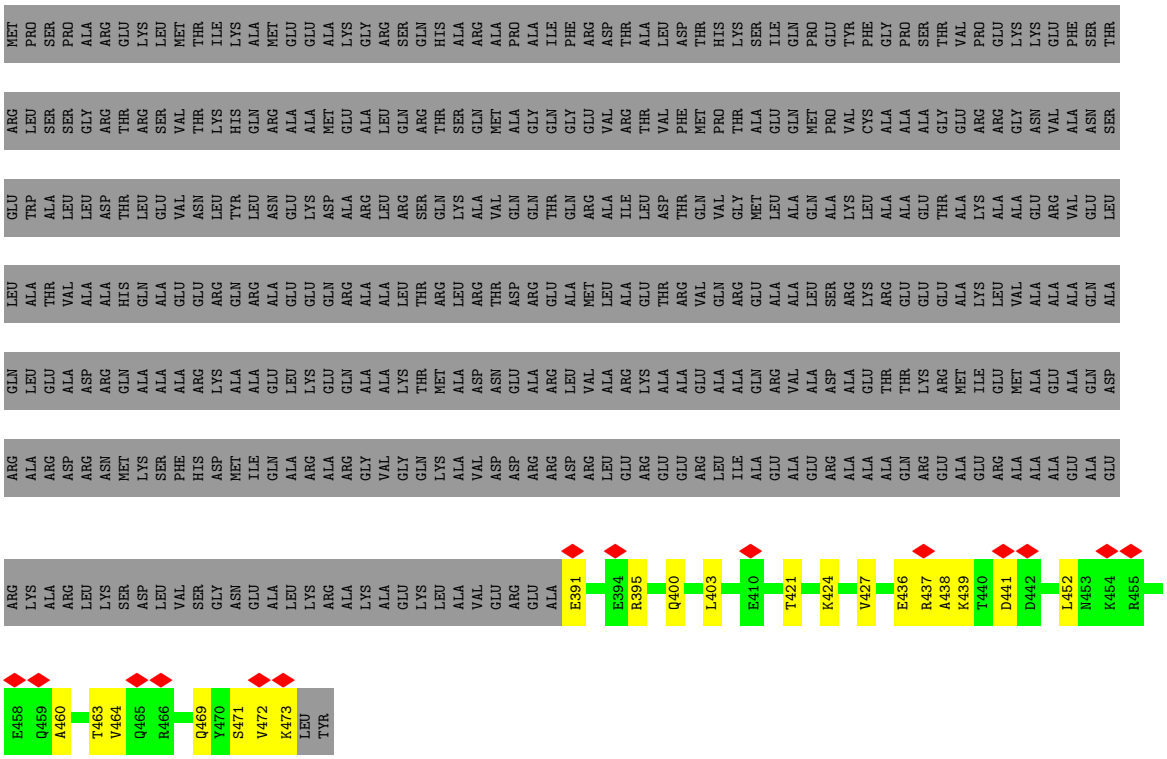
- Molecule 7: RIB43a

Chain 4U:



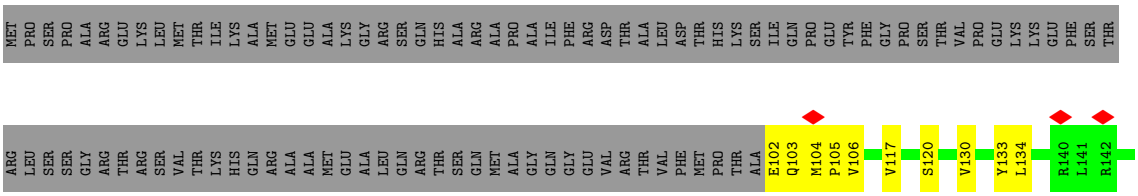
- Molecule 8: FAP112

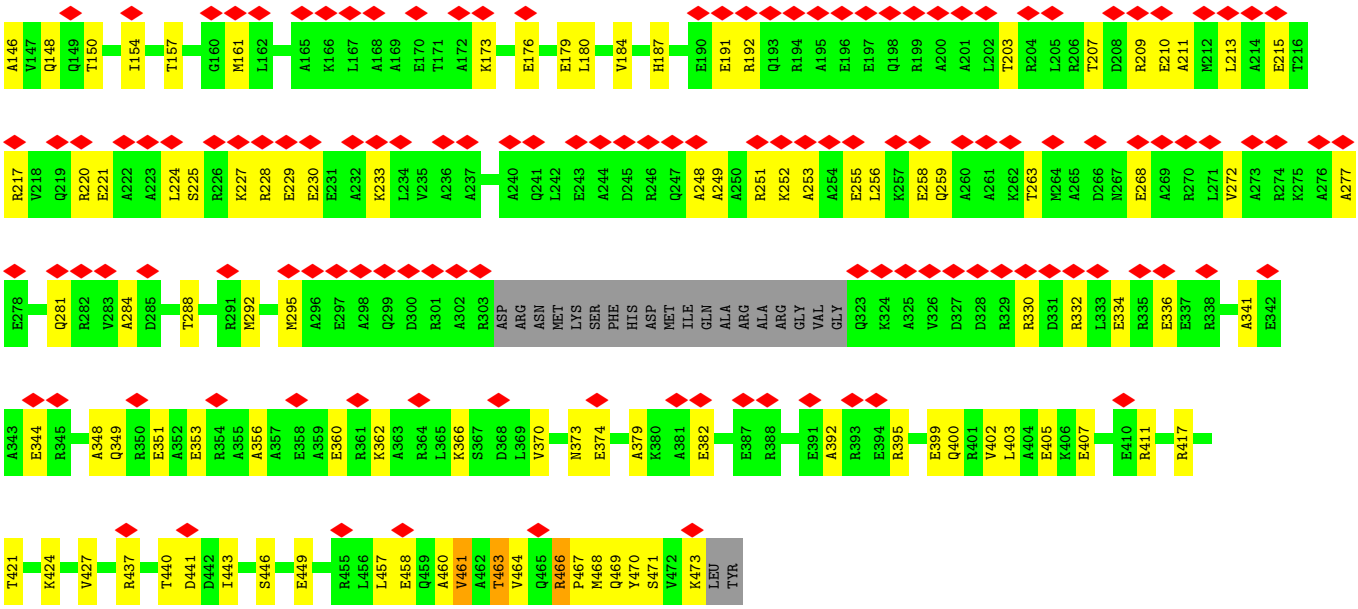
Chain 4V:



- Molecule 8: FAP112

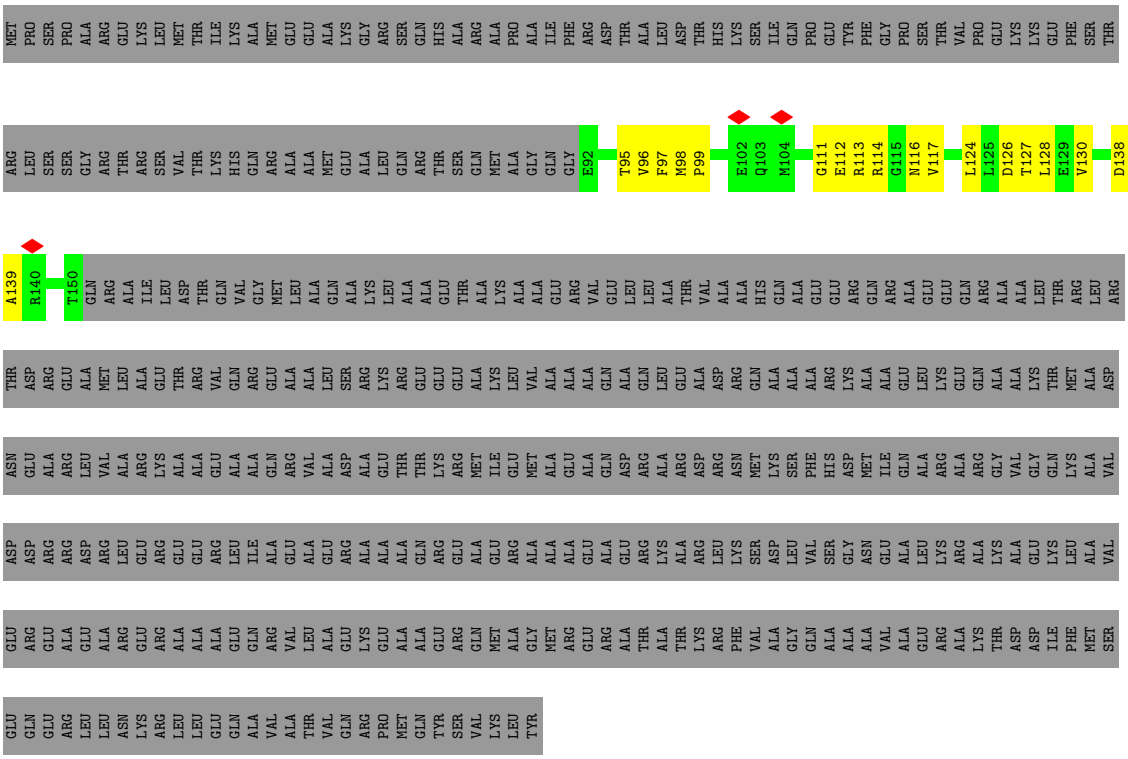
Chain 4W:





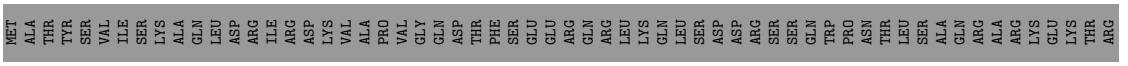
- Molecule 8: FAP112

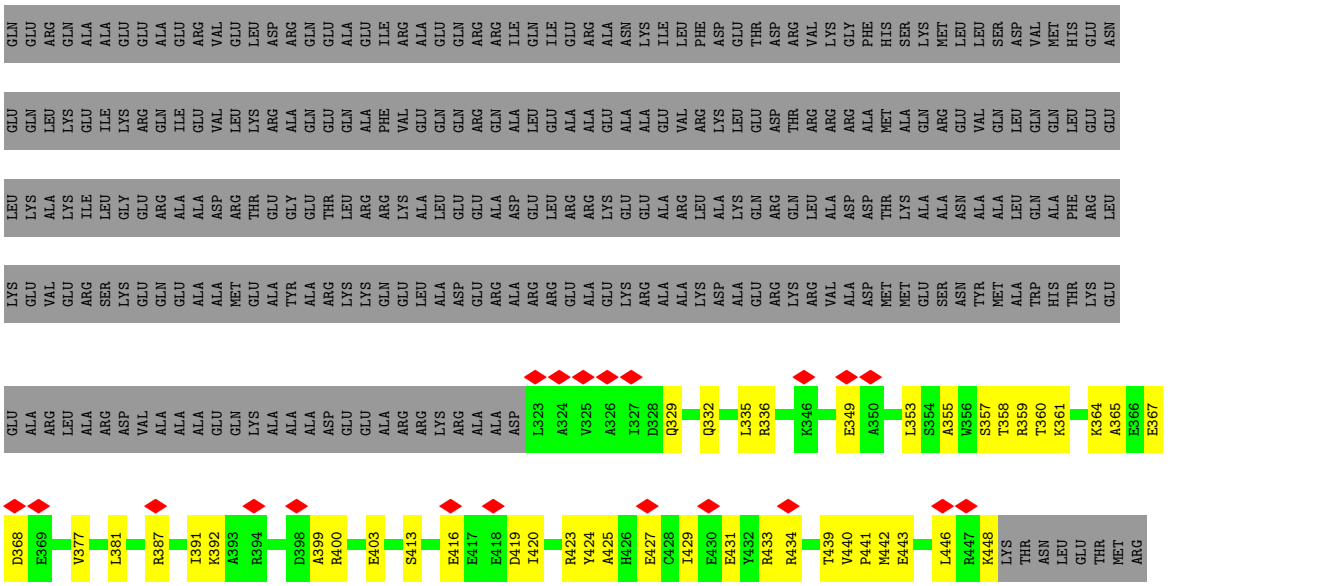
Chain 4X:



- Molecule 9: FAP210

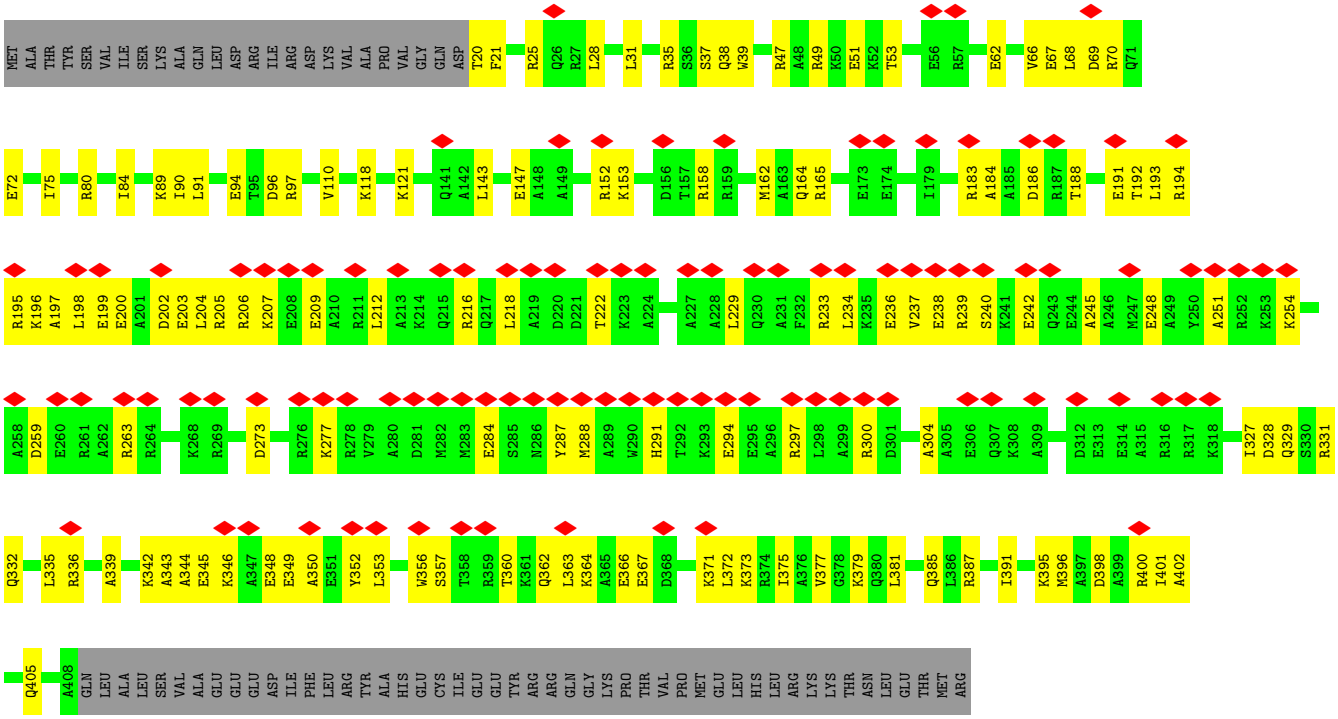
Chain 4Y:





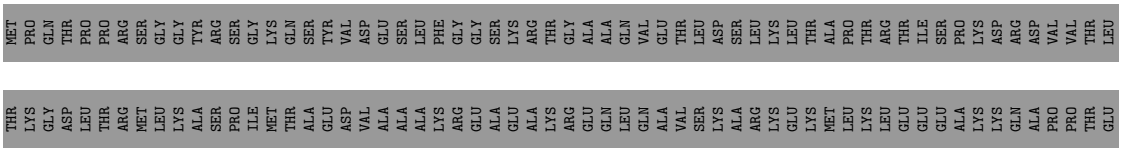
- Molecule 9: FAP210

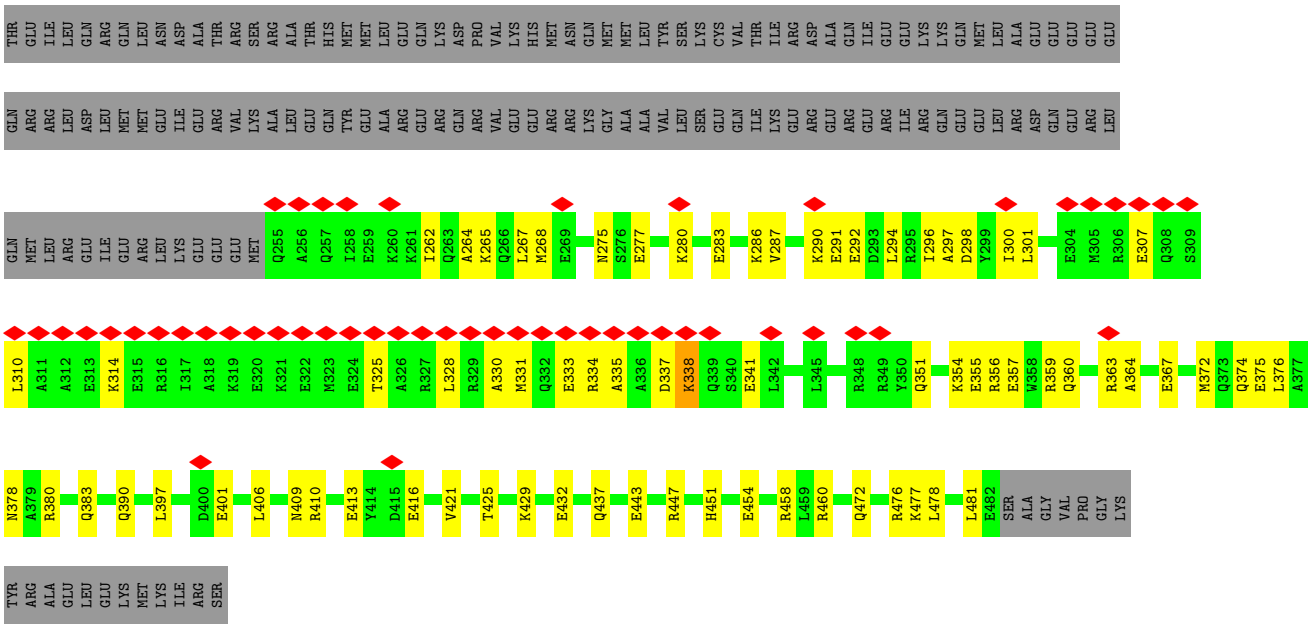
Chain 4Z:



- Molecule 10: FAP45

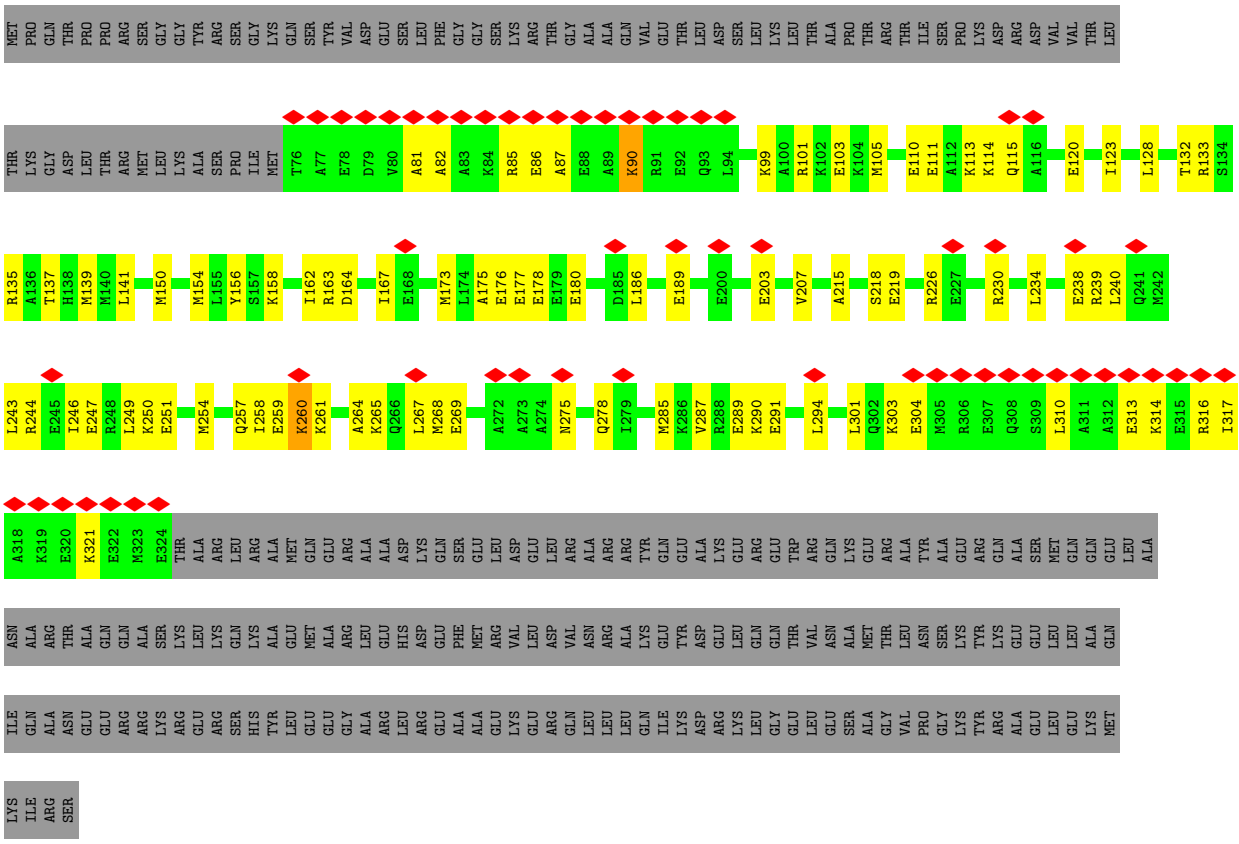
Chain 5A:





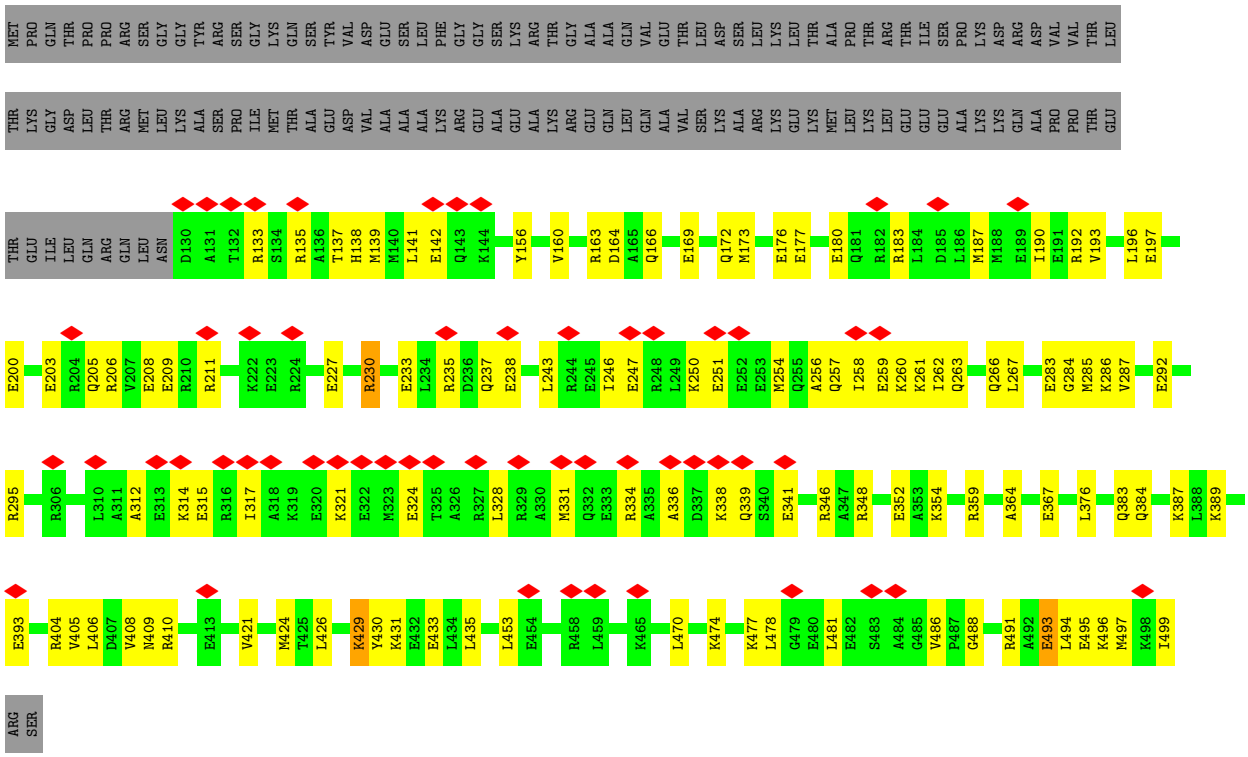
- Molecule 10: FAP45

Chain 5B:



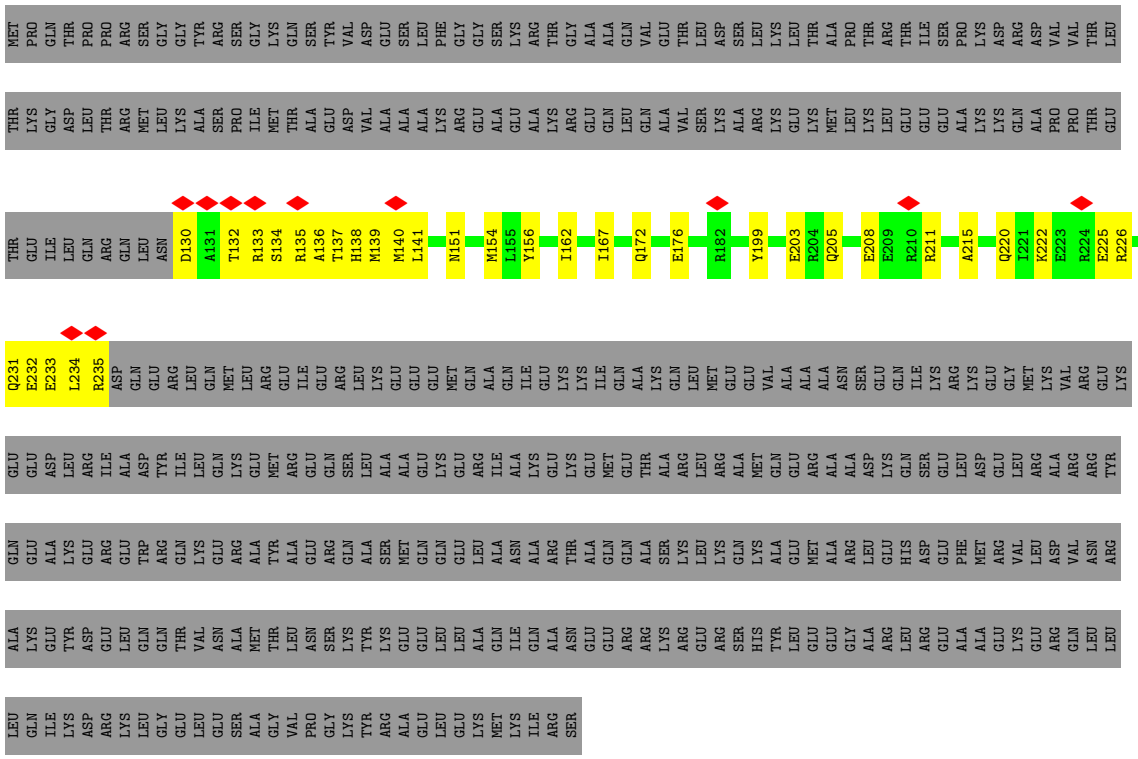
- Molecule 10: FAP45

Chain 5C:



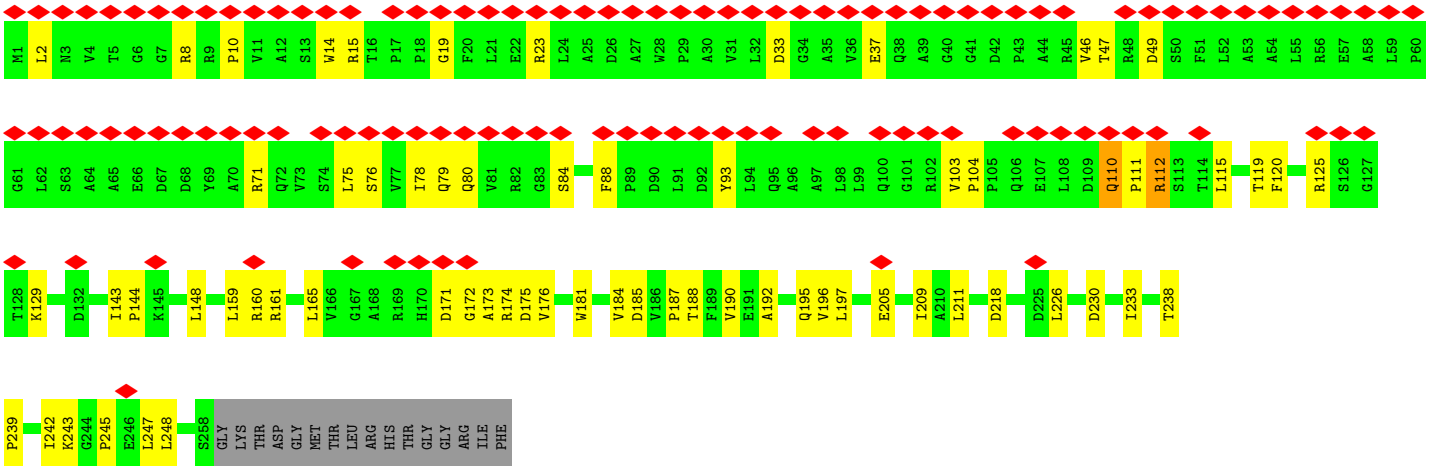
- Molecule 10: FAP45

Chain 5D:



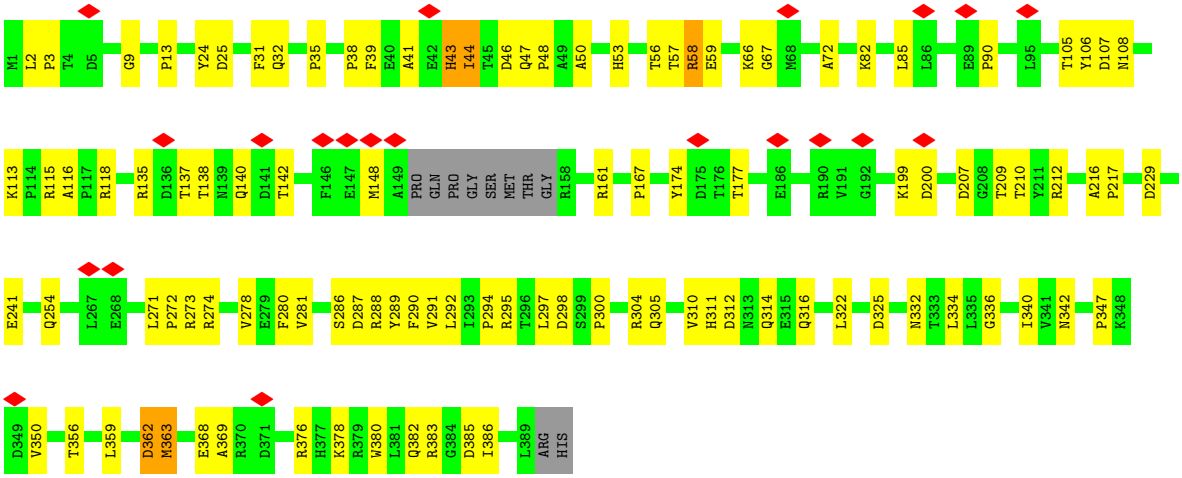
- Molecule 11: RIB30

Chain 5E:



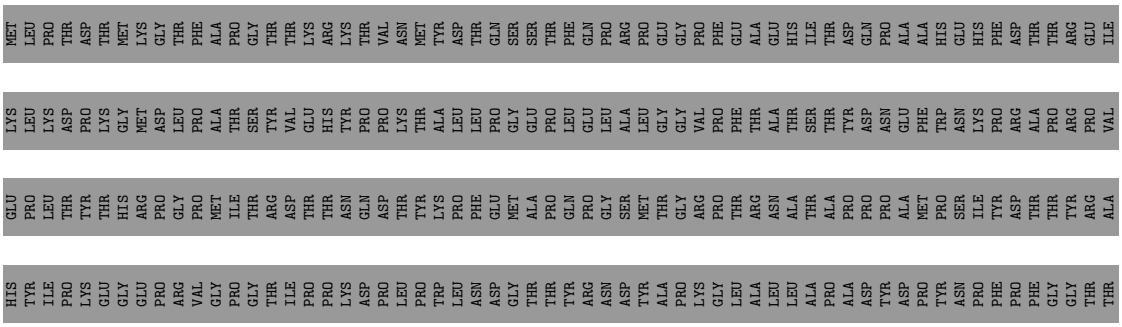
- Molecule 12: FAP363

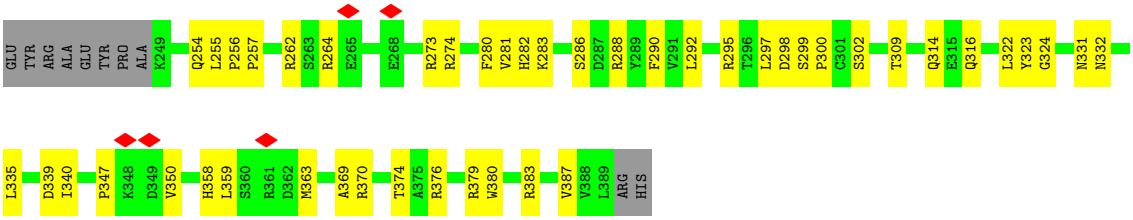
Chain 5F:



- Molecule 12: FAP363

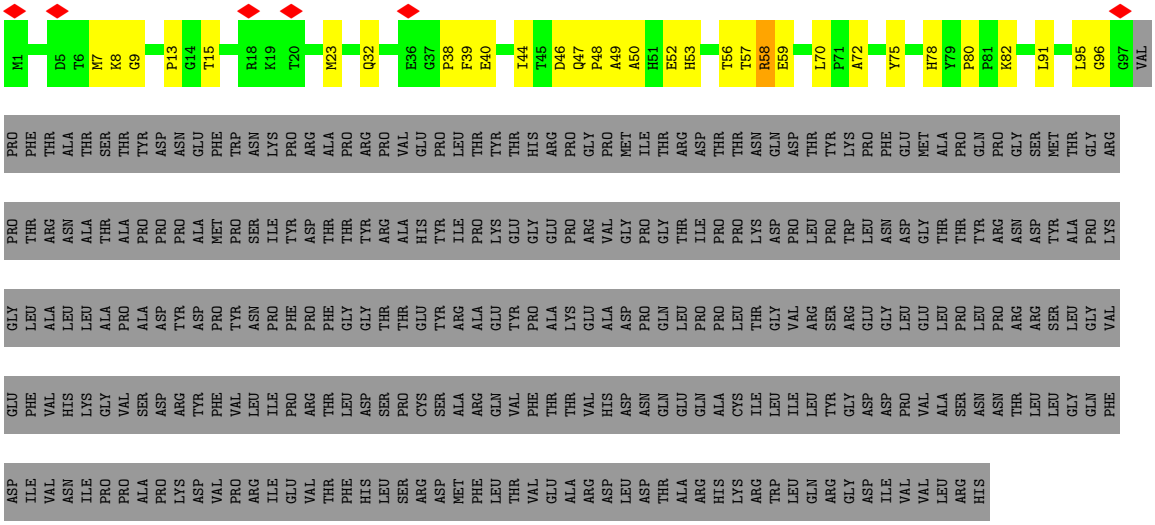
Chain 5G:





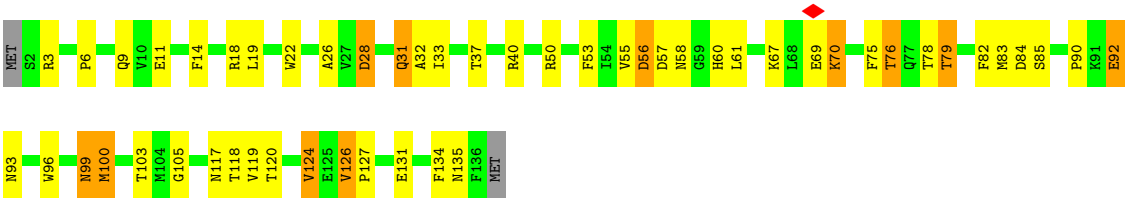
- Molecule 12: FAP363

Chain 7B:



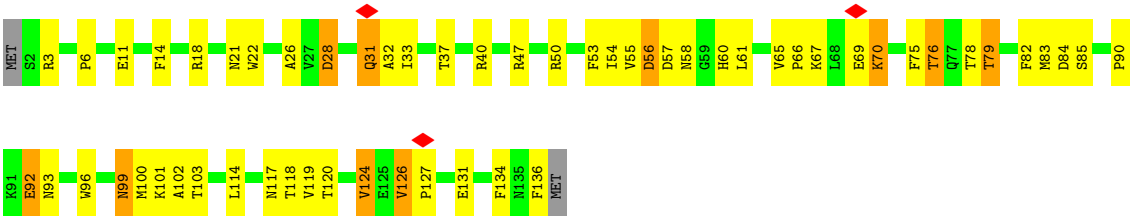
- Molecule 13: FAP126

Chain 5H:



- Molecule 13: FAP126

Chain 5I:



- Molecule 13: FAP126

Chain 5J: 60% 31% 8%

MET S2 R3 P6 G7 E8 E11 F14 R18 N21 W22 D28 Q31 A32 I33 T37 R40 I54 V55 D56 D57 N58 L61 K67 L68 E69 K70 N74 F75 T76 Q77 T78 T79 F82 M83 D84 S85 P90 K91 E92 N93 P94 T95 W96

N99 M100 K101 A102 T103 M104 G105 Y106 T118 V119 T120 V124 E125 V126 P127 G128 E131 F134 N135 F136 MET

- Molecule 13: FAP126

Chain 5K: 58% 33% 8%

MET S2 R3 S4 Y5 P6 E11 K17 R18 W22 E23 V24 P25 A26 V27 D28 Q31 A32 I33 T37 R40 T43 R50 T51 Q52 F53 I54 V55 D56 D57 N58 G59 H60 L61 K67 L68 E69 K70 N74 F75 T76 Q77 T78 T79 F82 M83 D84 S85 A86

P87 R88 W89 E92 N93 W96 N99 M100 K101 A102 T103 Y106 L114 V119 T120 V124 E125 V126 P127 E131 F136 MET

- Molecule 14: FAP52

Chain 5L: 50% 44% 5%

MET A2 L5 V6 L7 N8 S9 V10 I11 G12 F13 E18 N19 G20 L21 I22 A23 H24 P25 R28 T29 I30 I31 Y32 P33 L34 G35 S36 T37 I38 R41 A44 D45 L52 H55 S56 D57 K58 V59 L64 I76 T77 Y78 F81 I86 I87 W88 D89 L90

E91 S92 K93 Q94 L95 I96 H97 R98 M99 V104 K105 V106 Q107 D110 F111 S112 C113 D114 E115 R116 F117 L121 G122 G123 Q124 D125 D126 N127 L131 W132 D133 V134 A135 S136 G137 N138 A139 N146 T147 N148 F149 T150 V153 K154 F155 F156 N157 N158 S159 K162 L163 I164 T165

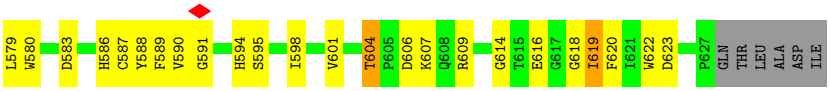
A166 G167 N168 F169 N170 M171 N172 V173 W174 D177 N180 P185 T186 D187 A188 T189 V196 S199 V200 V201 W202 D203 A204 N205 D206 E207 Y208 A209 Y210 T213 T214 D217 V218 L219 Q220 I221 A222 V226 L227 F228 K229 N230 T231 G232 P233 A234 N237 V238 Q239 M240 G241

V242 T243 A244 T245 C246 E247 V248 G251 D252 I253 L265 R266 T267 S272 S273 T274 K277 R280 K281 M282 A286 Q287 E291 S296 I297 M302 F307 F310 M315 G316 N317 I318 Y319 T322 L330 K331 E332 E333 L334 T337 A338 H339 N340 D341 K342

A347 F348 P349 N350 E351 Y352 S353 E354 V355 F356 A357 T358 C359 G360 T361 I364 R365 L366 W367 H368 L369 T370 T371 E374 R377 I378 P381 N382 L383 E384 C385 F386 C387 T392 S395 S399 G400 W401 S402 D403 G404 K405 P411 K415 I416 I417 F418 N421 D422

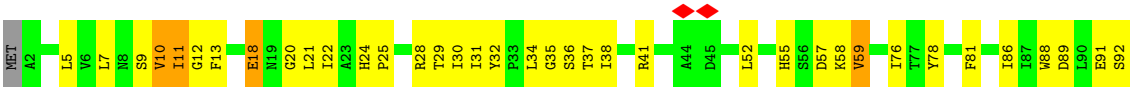
Q425 K426 A427 V428 T429 A430 I431 A432 S433 T434 A435 R439 G444 E445 E446 R450 V451 W452 R453 I454 G455 R456 T457 S458 Q459 T460 L461 E462 A463 S464 M465 K466 D467 G470 I477 K478 G479 S480 G481 D482 E483 C484 V485 S489 D490 G491 S492 C493 I494 L495 W496 D497 L498

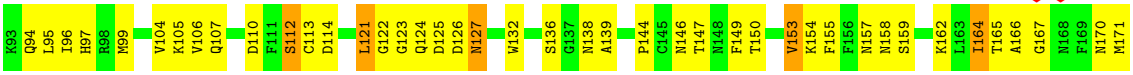
H499 T500 F501 K502 R503 R504 T505 S506 L507 F508 A509 N510 T511 F512 F513 K514 S515 V516 V517 Y518 H519 P520 Q524 L525 V526 T527 A528 G529 T530 D531 R532 Y540 D541 I548 D549 G550 S551 D552 L553 D554 E555 V556 N557 A558 V561 D562 R563 D564 G565 G573 D574 K575 L576 V577 K578

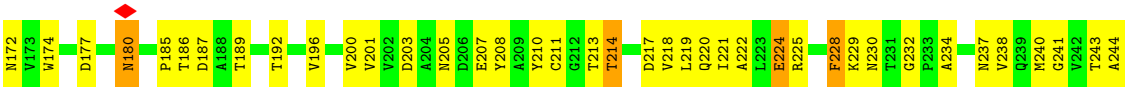


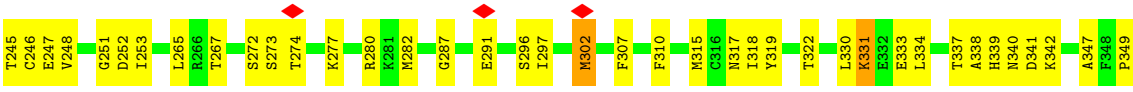
- Molecule 14: FAP52

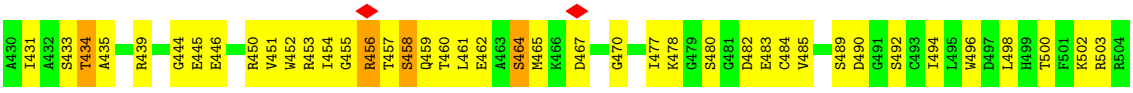
Chain 5M:

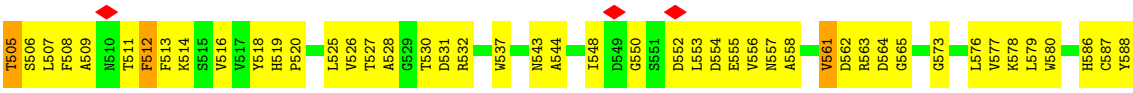


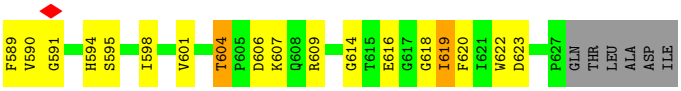






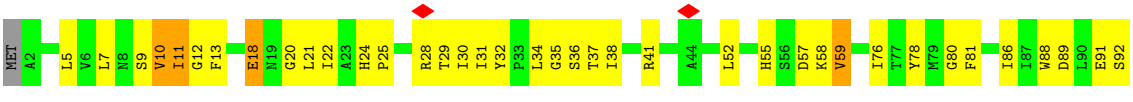


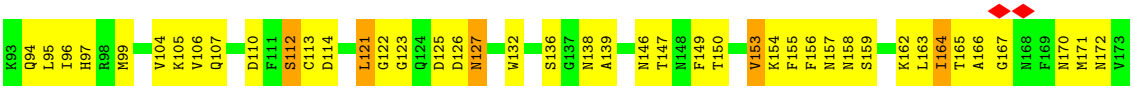


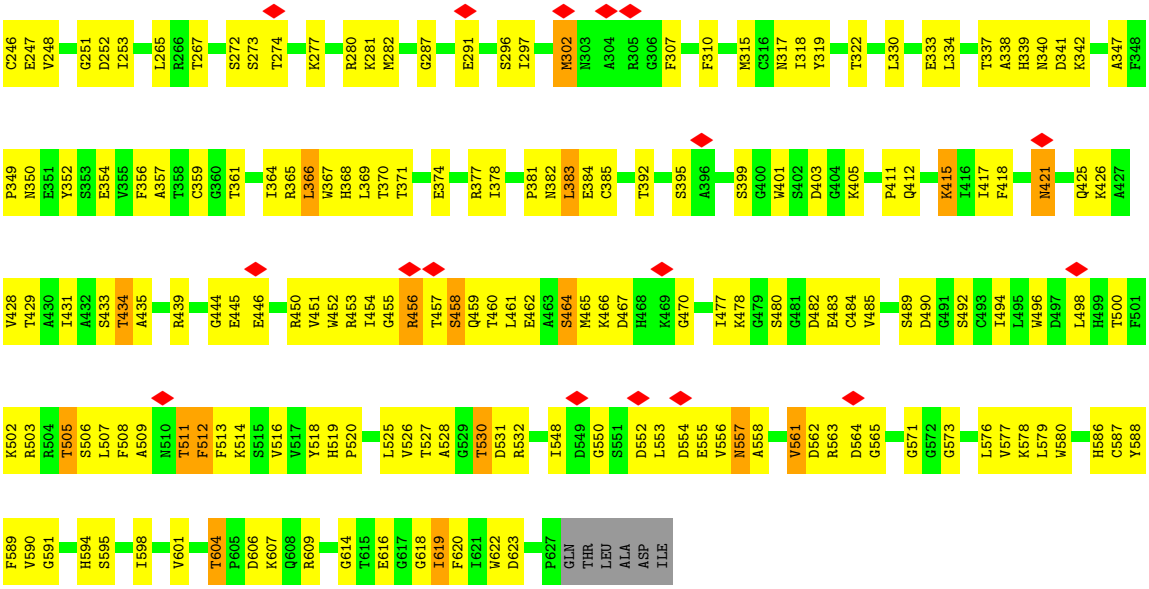


- Molecule 14: FAP52

Chain 5N:

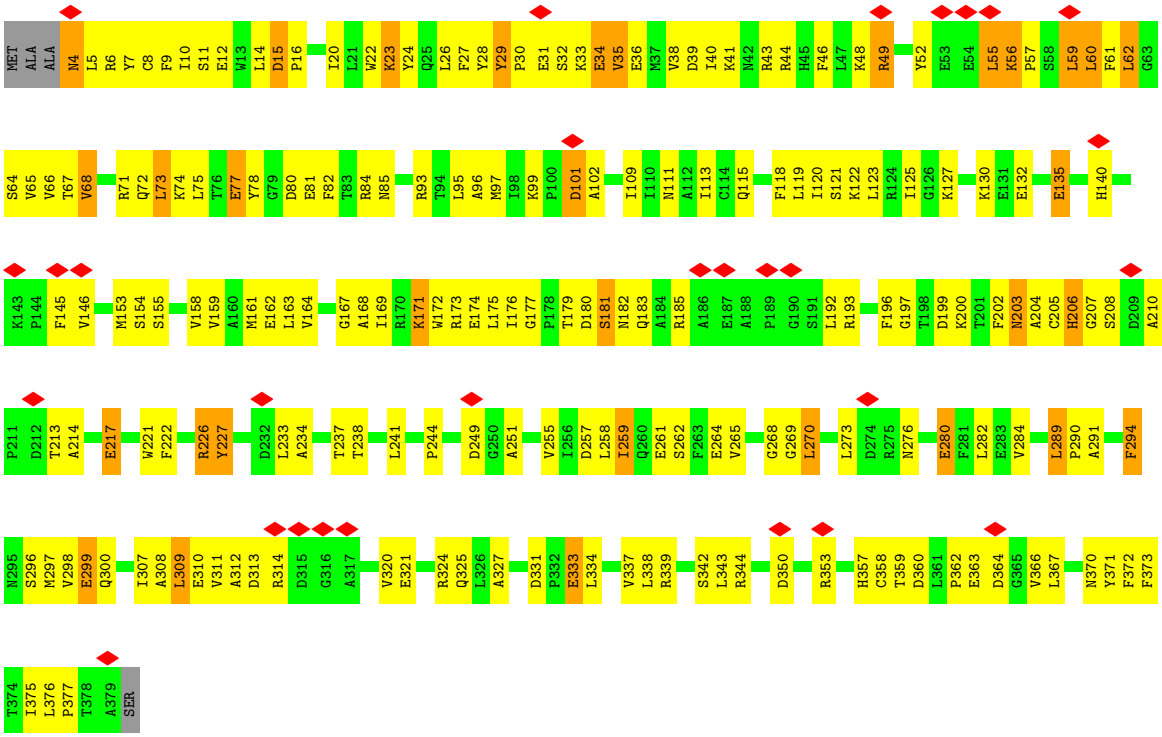






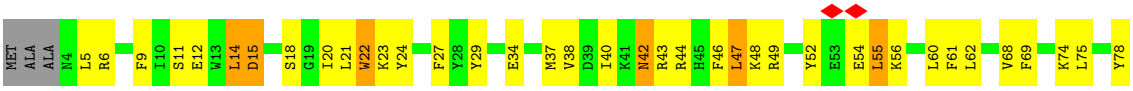
• Molecule 15: FAP67

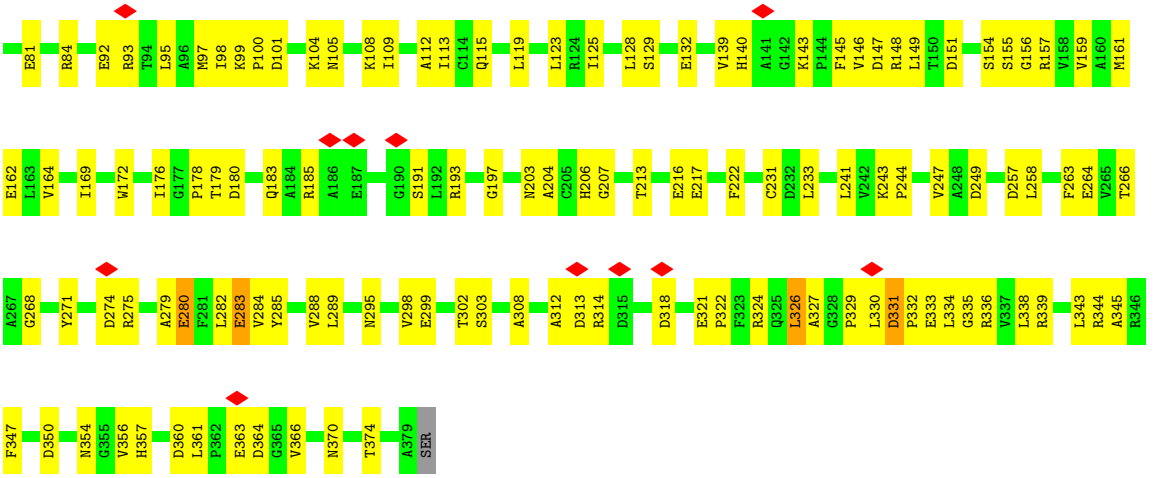
Chain 5O:



• Molecule 15: FAP67

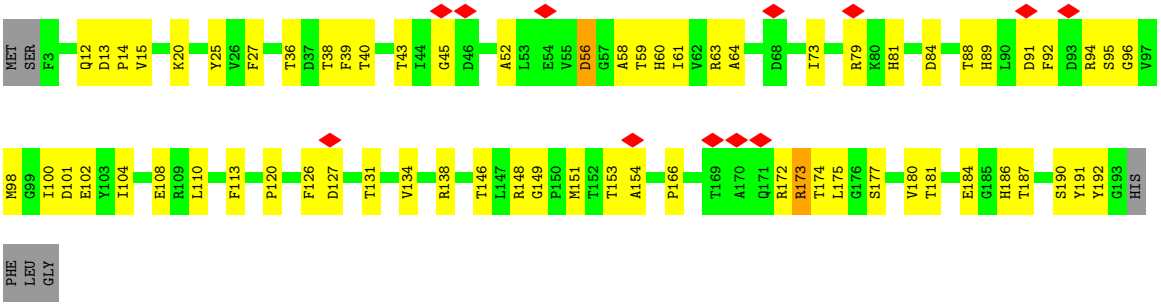
Chain 5P:





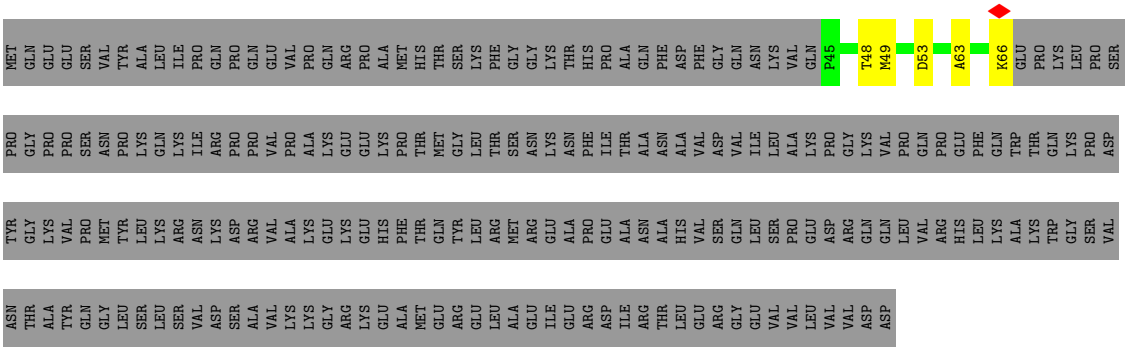
- Molecule 16: FAP85

Chain 5Q:



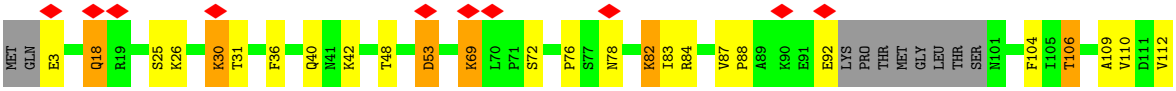
- Molecule 17: FAP106

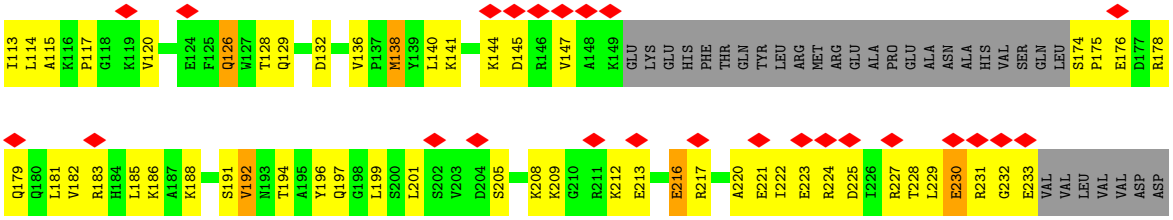
Chain 5R:



- Molecule 17: FAP106

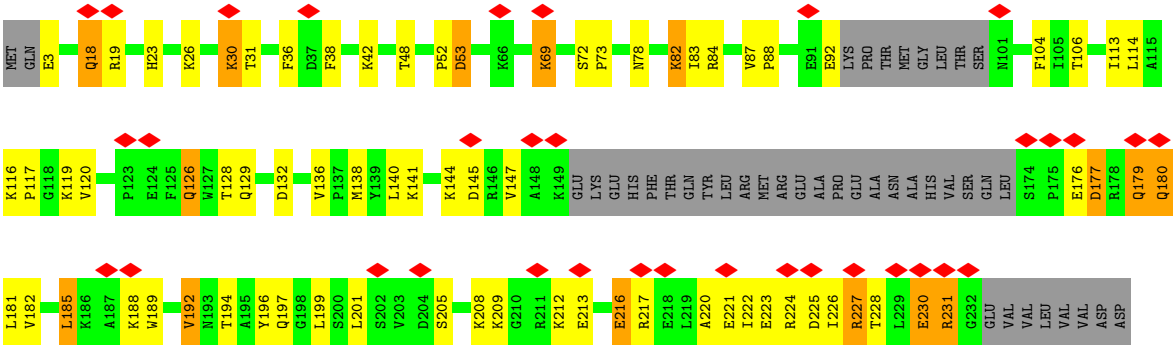
Chain 5S:





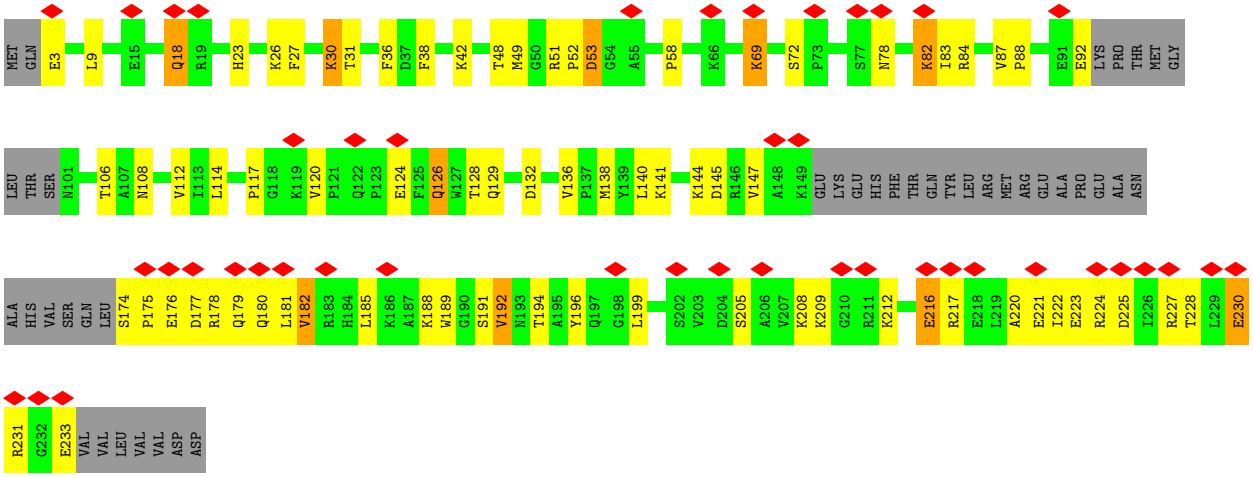
• Molecule 17: FAP106

Chain 5T:



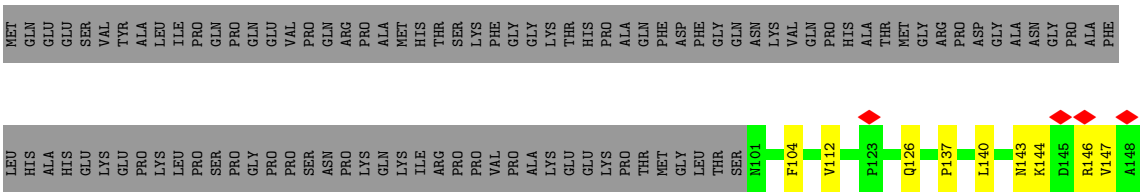
• Molecule 17: FAP106

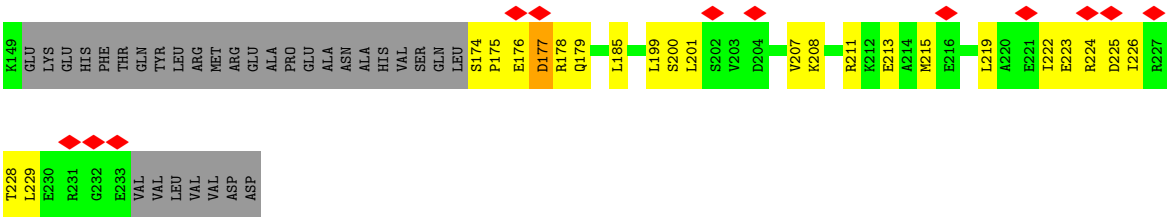
Chain 5U:



• Molecule 17: FAP106

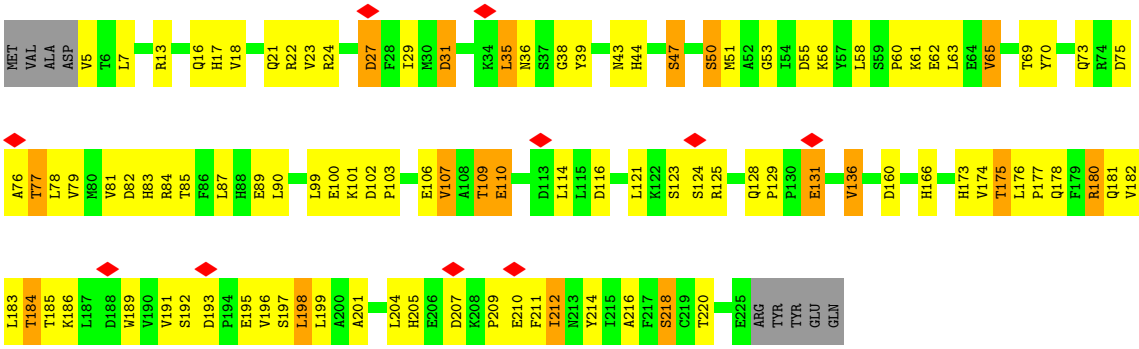
Chain 5V:





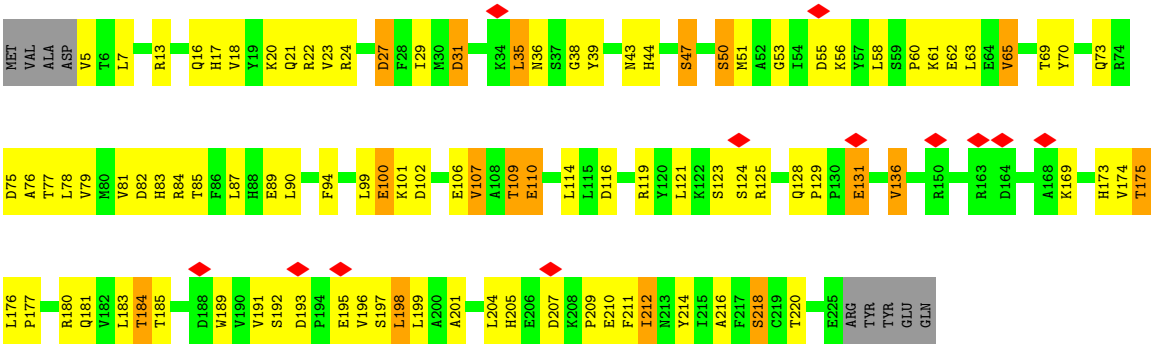
• Molecule 18: FAP115

Chain 5X:



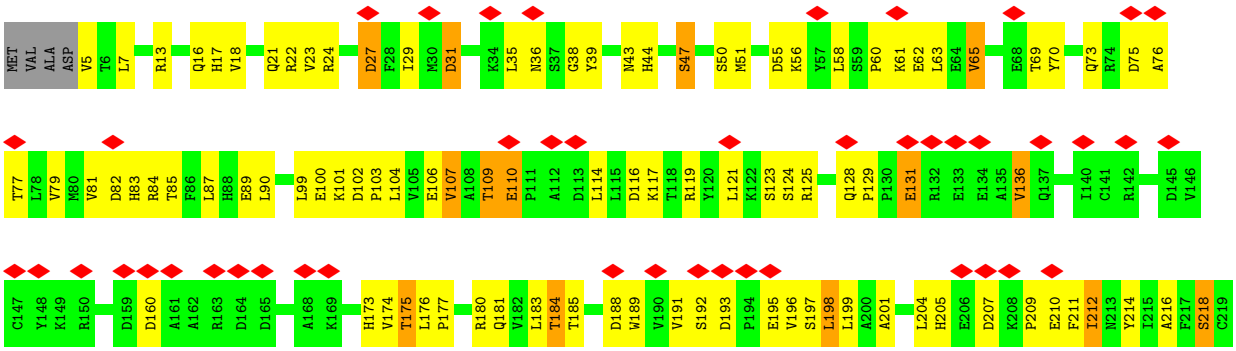
• Molecule 18: FAP115

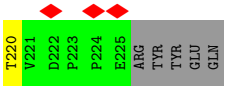
Chain 5Y:



• Molecule 18: FAP115

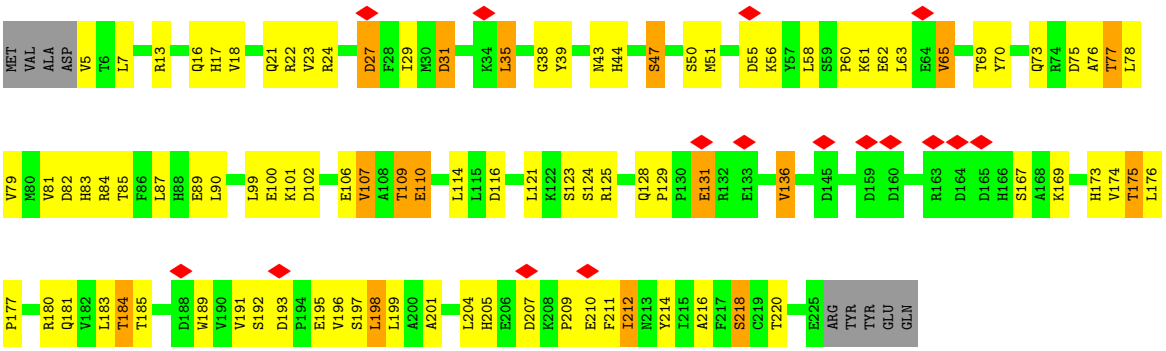
Chain 5Z:





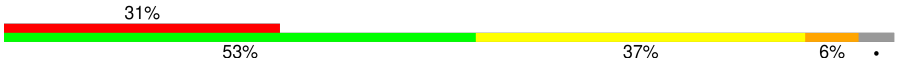
• Molecule 18: FAP115

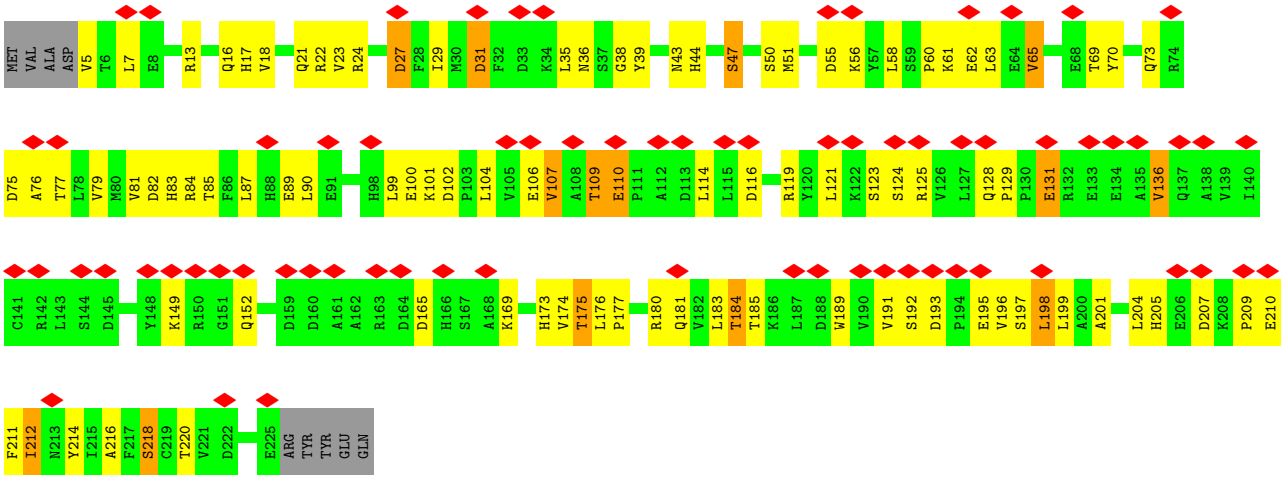
Chain 6A:



• Molecule 18: FAP115

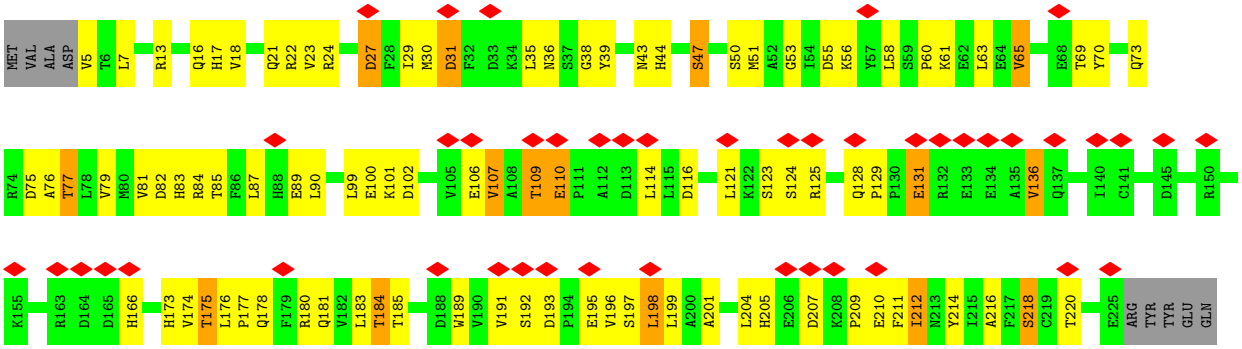
Chain 6B:





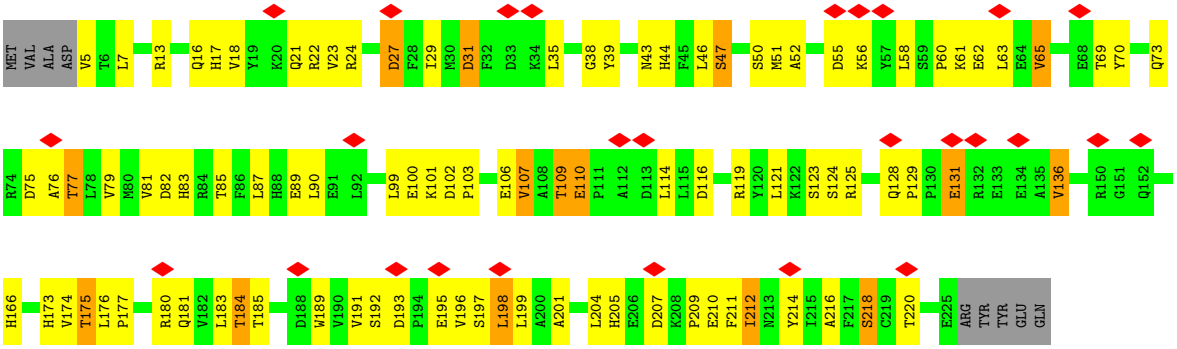
• Molecule 18: FAP115

Chain 6C:



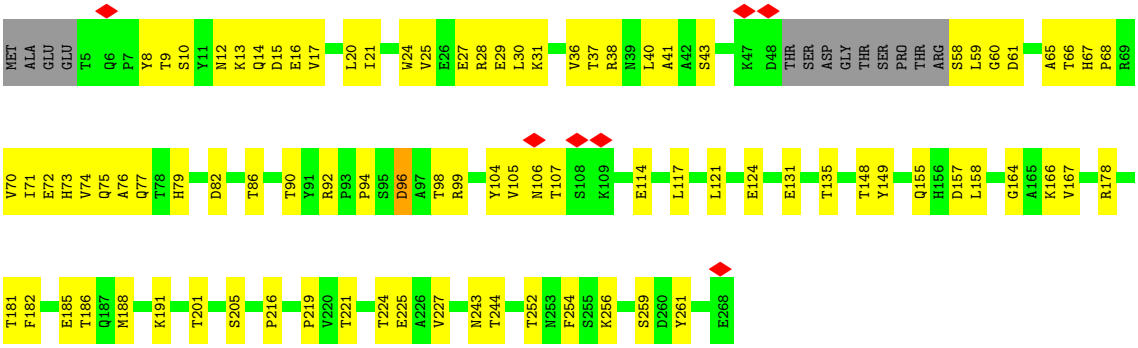
- Molecule 18: FAP115

Chain 6D:



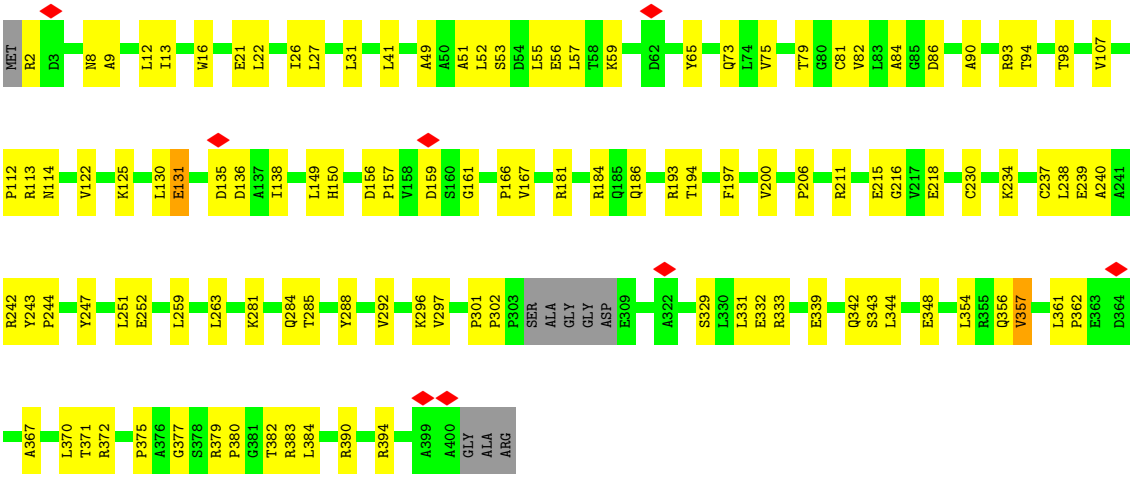
- Molecule 19: FAP143

Chain 6E:



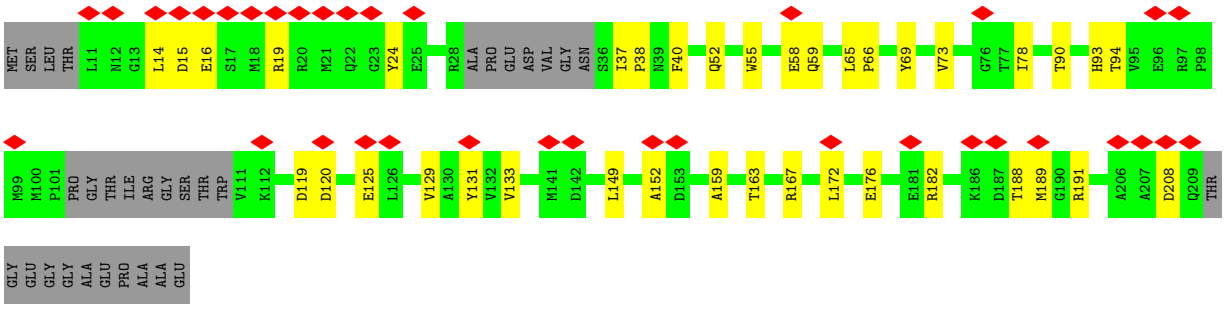
- Molecule 20: FAP161

Chain 6F:



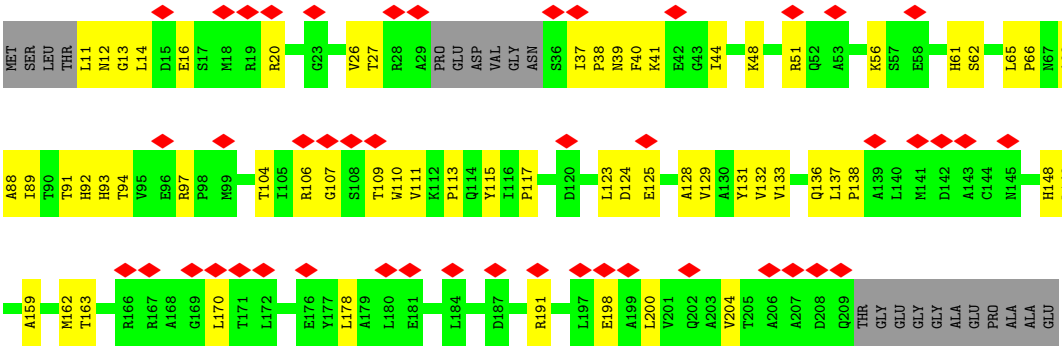
- Molecule 21: FAP166

Chain 6G:



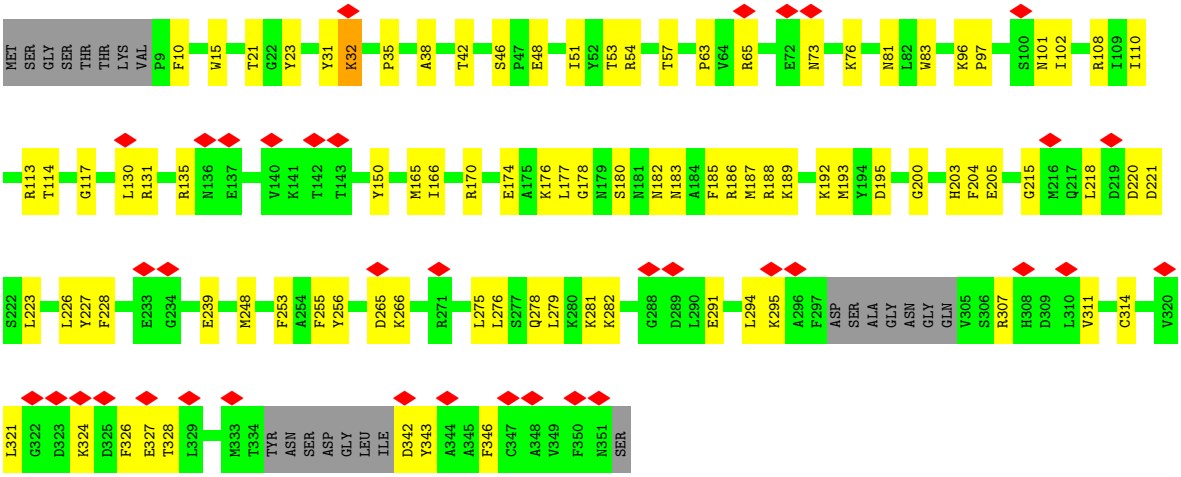
- Molecule 21: FAP166

Chain 6H:



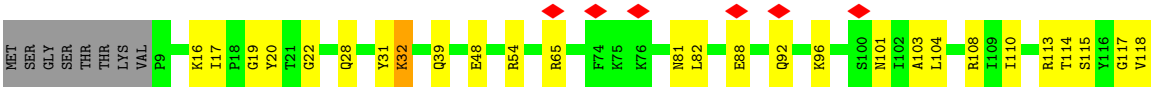
- Molecule 22: FAP252

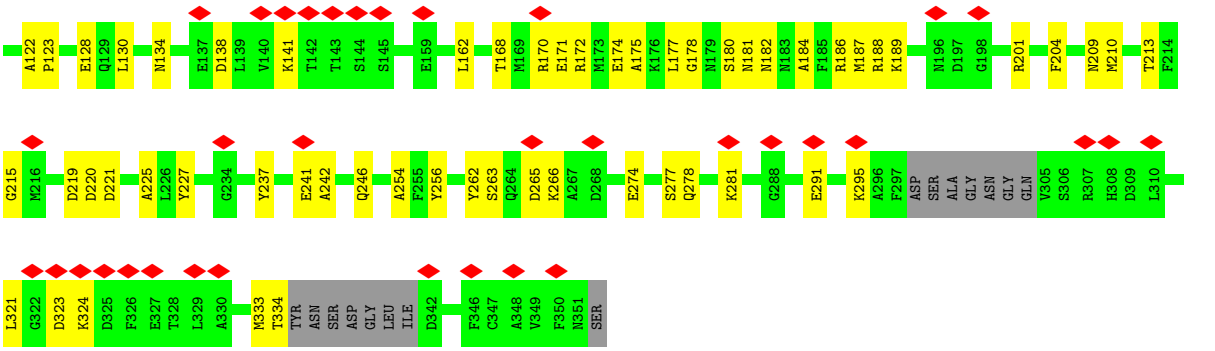
Chain 6I:



- Molecule 22: FAP252

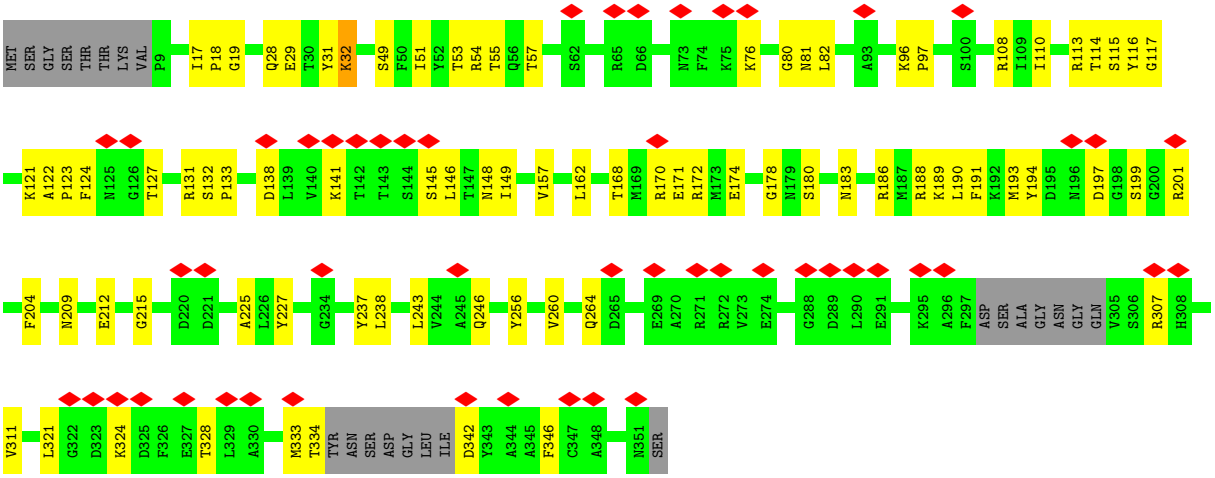
Chain 6J:





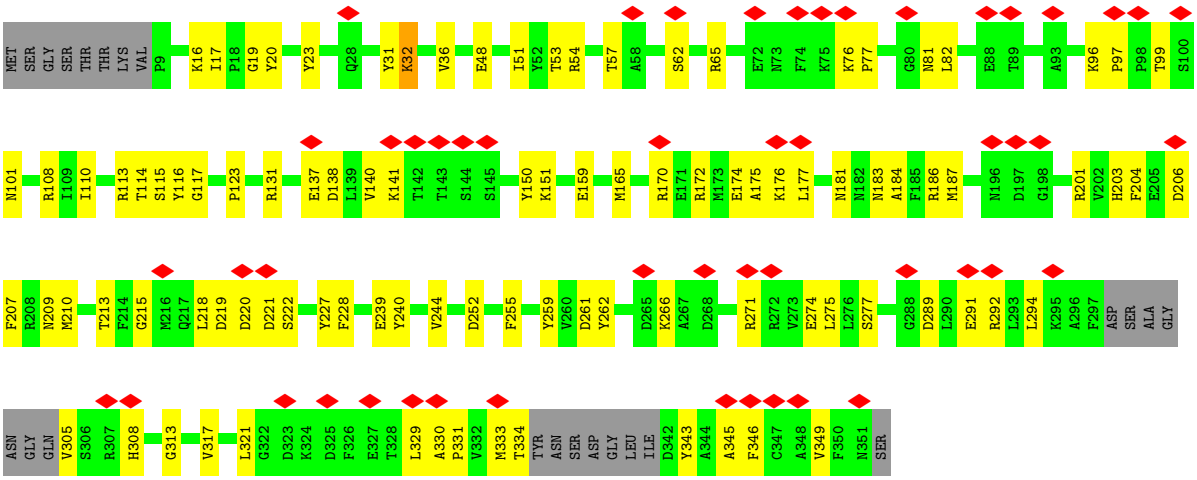
- Molecule 22: FAP252

Chain 6K:



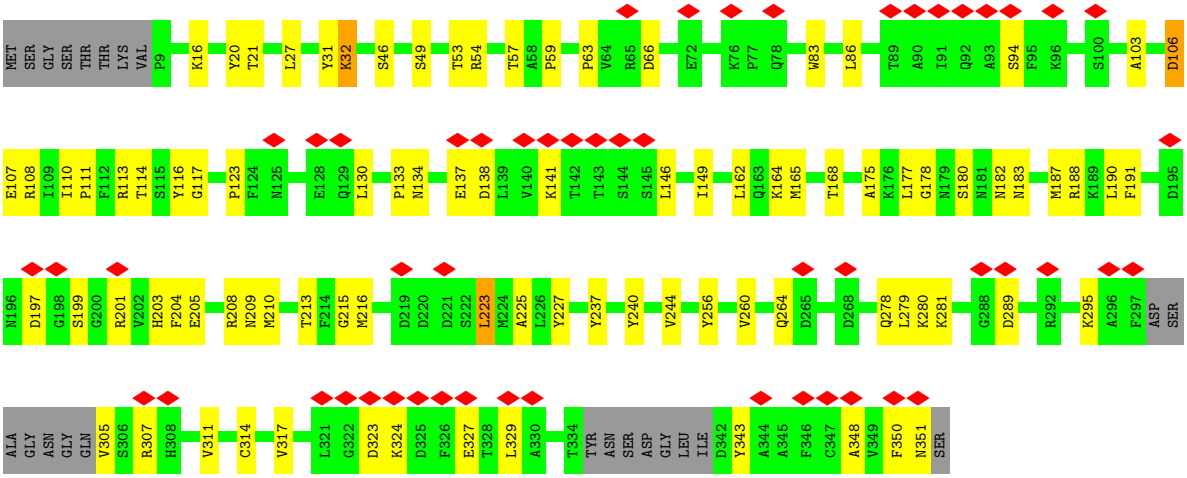
- Molecule 22: FAP252

Chain 6L:



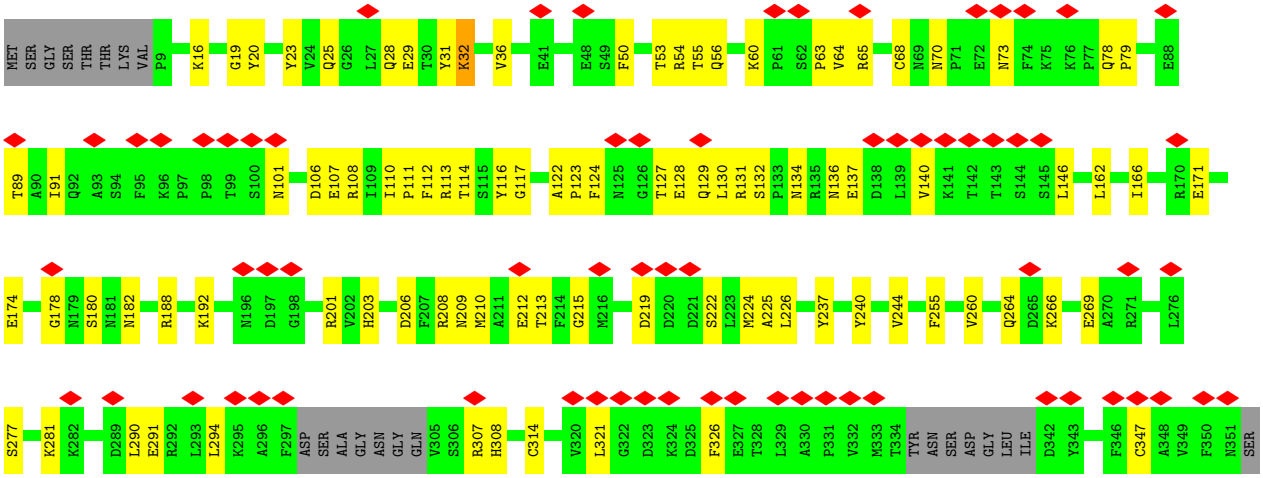
- Molecule 22: FAP252

Chain 6M:



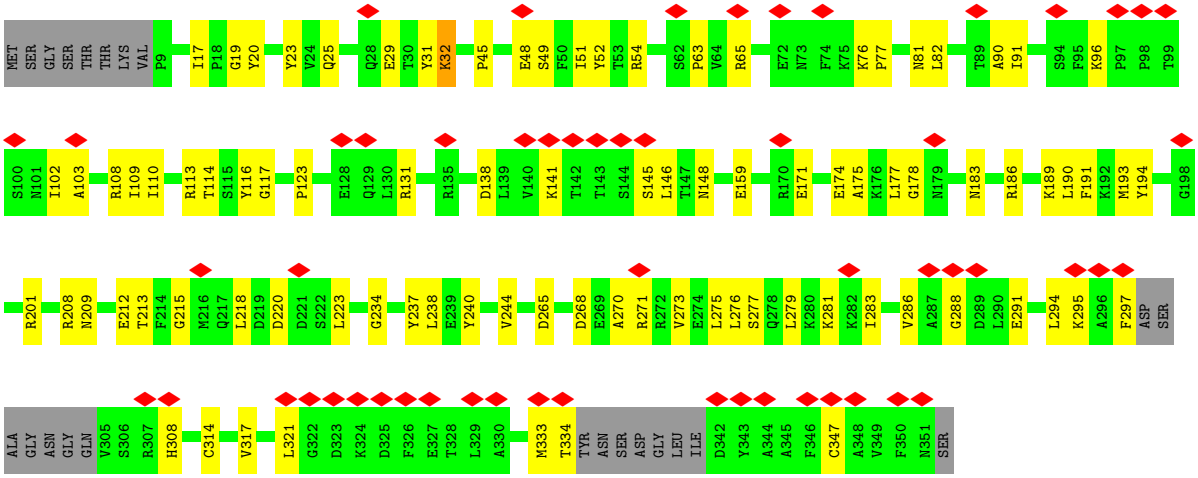
- Molecule 22: FAP252

Chain 6N:



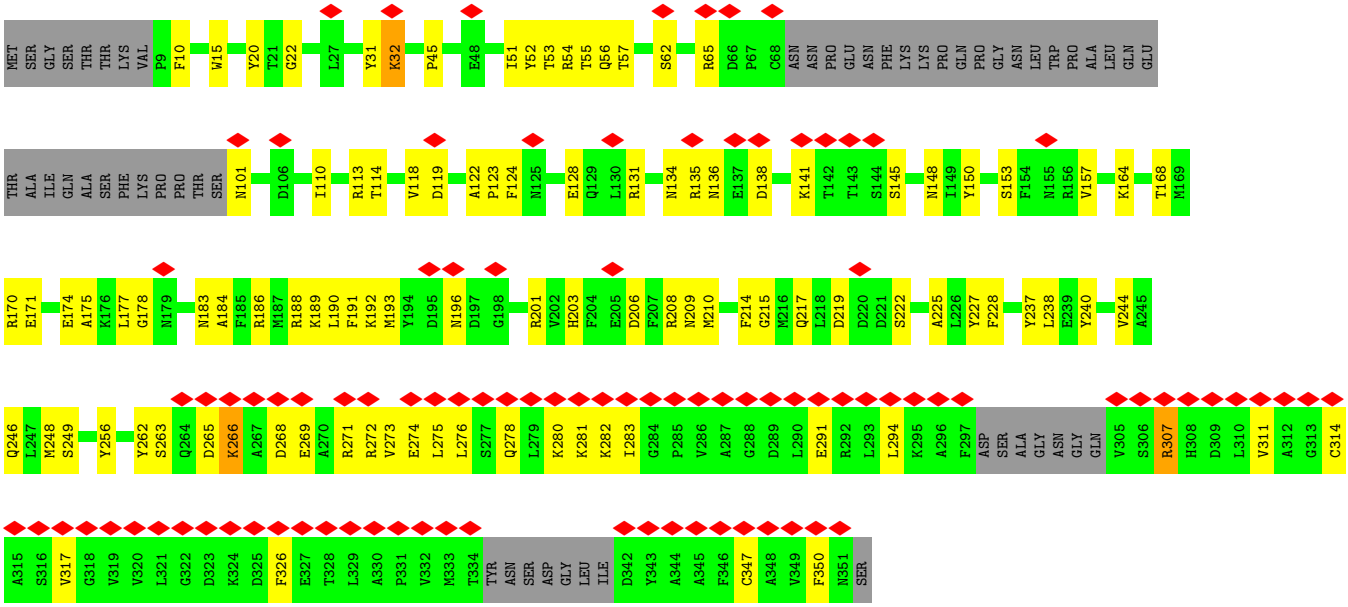
- Molecule 22: FAP252

Chain 6O:



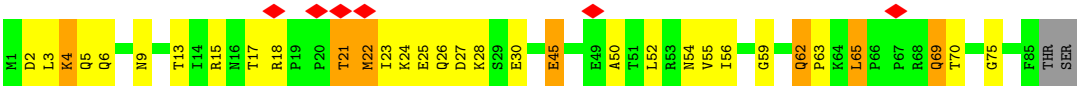
- Molecule 22: FAP252

Chain 6P:



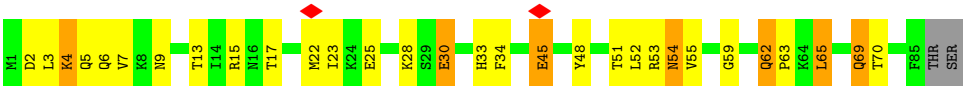
- Molecule 23: FAP276

Chain 6Q:



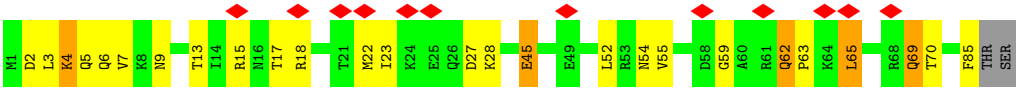
- Molecule 23: FAP276

Chain 6R:



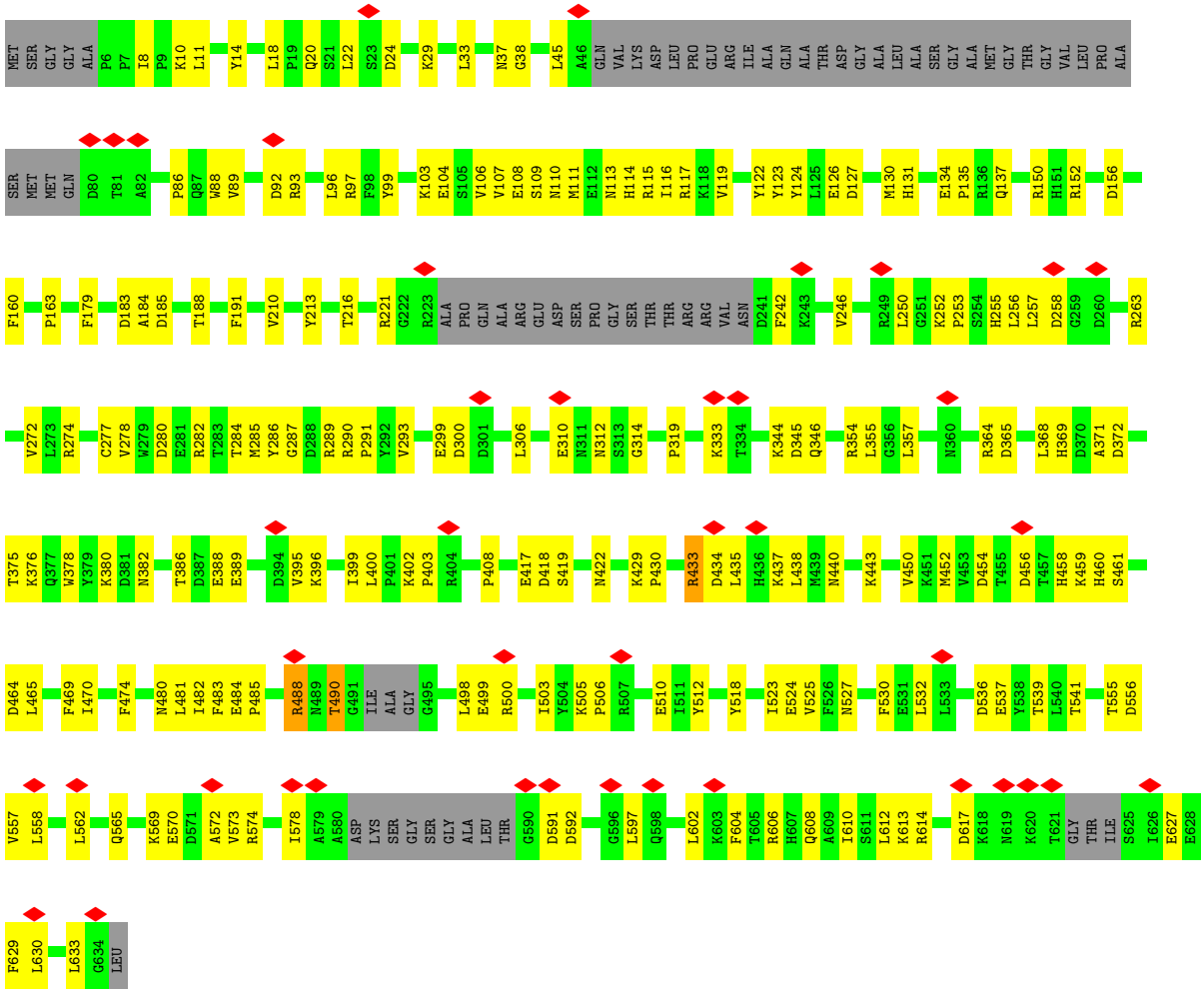
- Molecule 23: FAP276

Chain 6S:



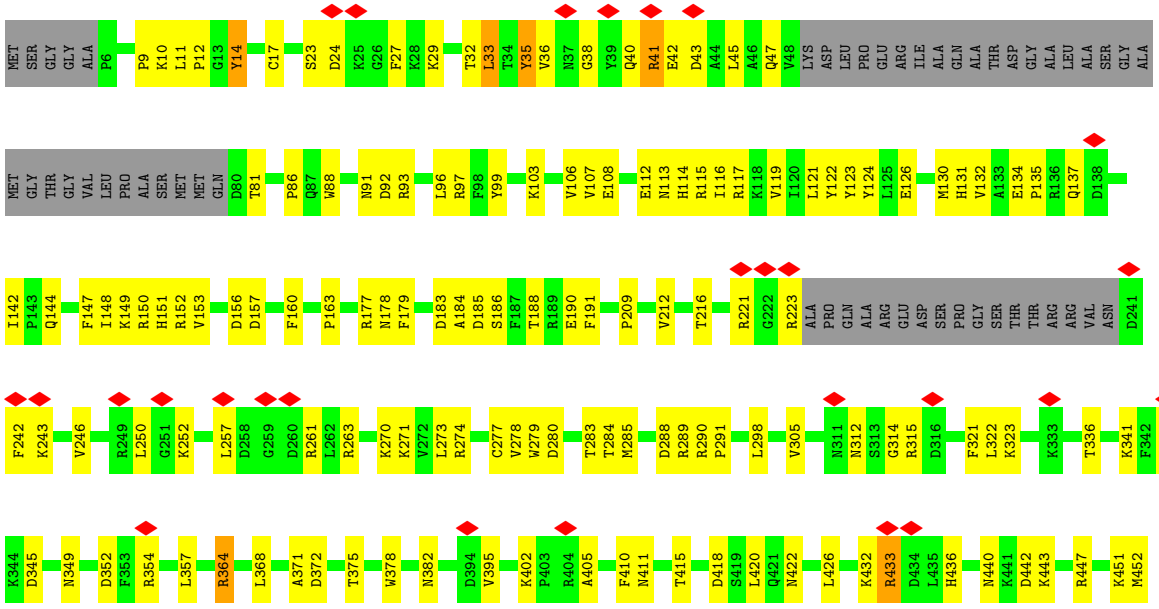
- Molecule 24: RIB72

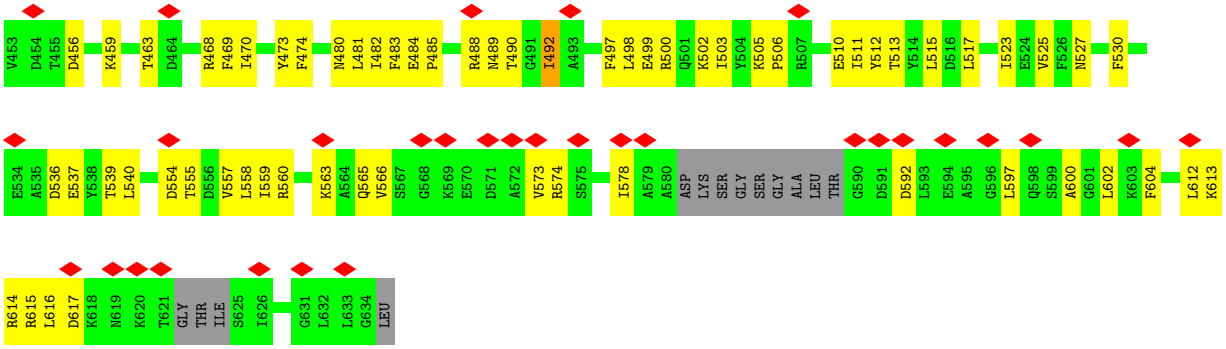
Chain 6T:



- Molecule 24: RIB72

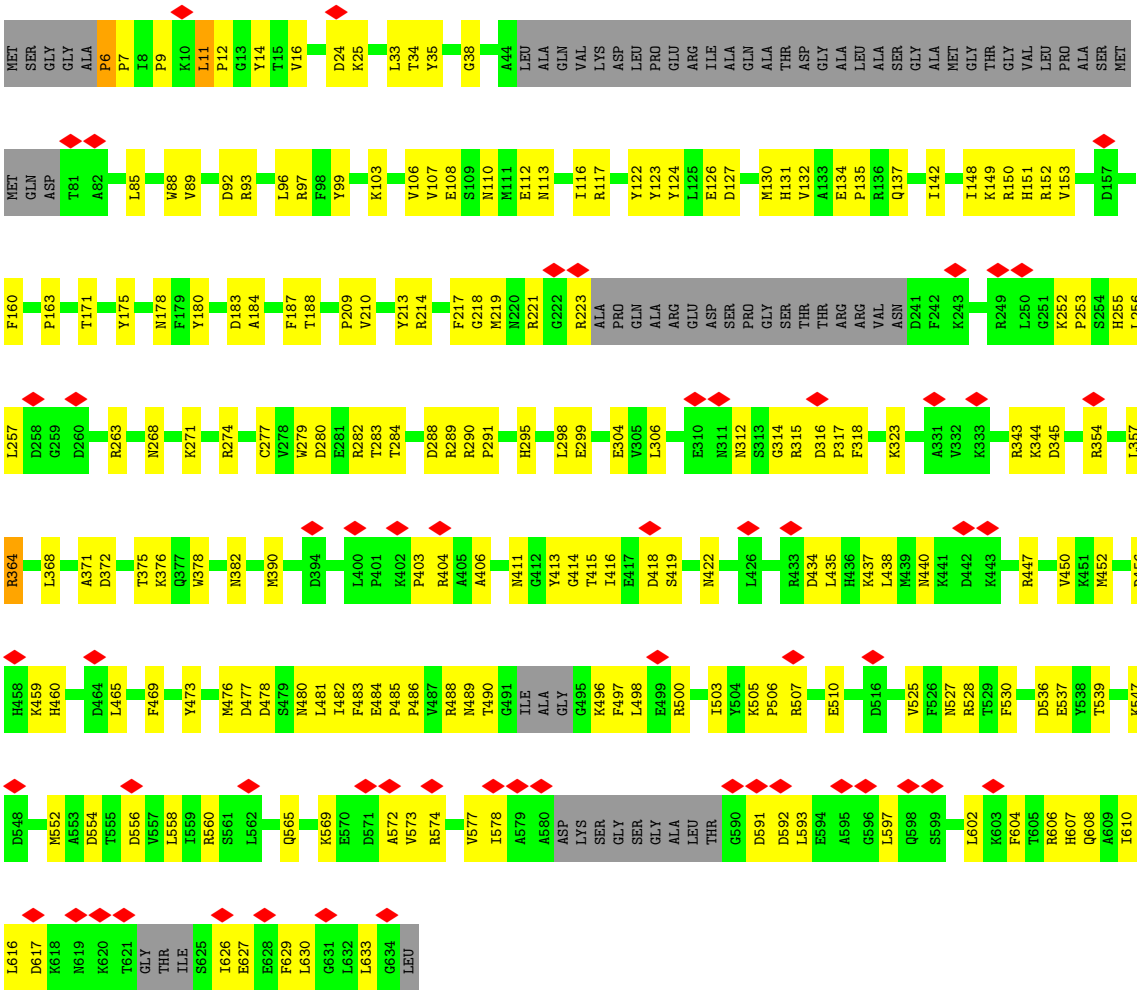
Chain 6U:





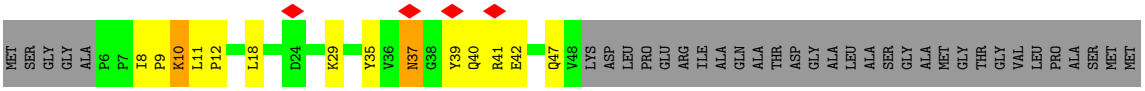
- Molecule 24: RIB72

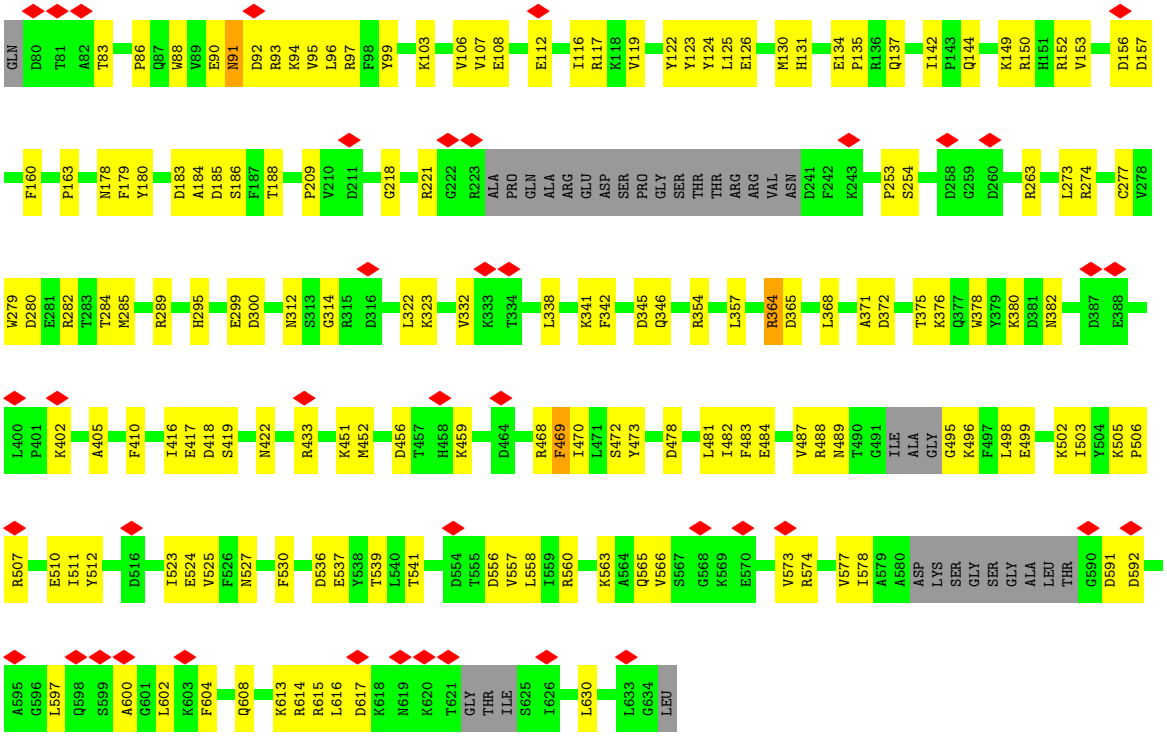
Chain 6V:



- Molecule 24: RIB72

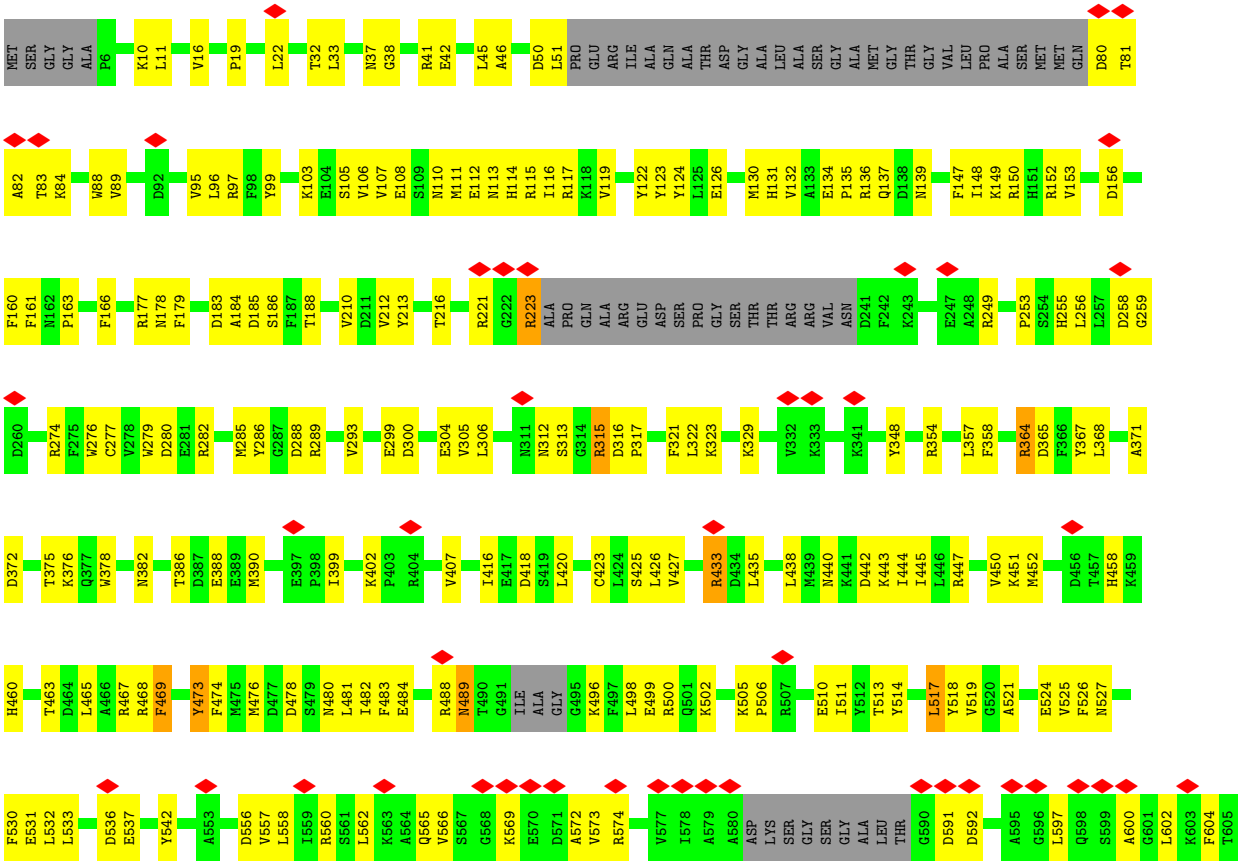
Chain 6W:

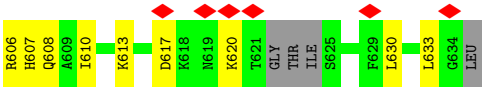




- Molecule 24: RIB72

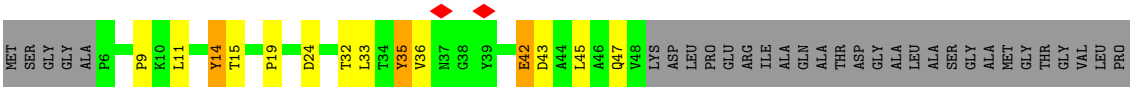
Chain 6X:

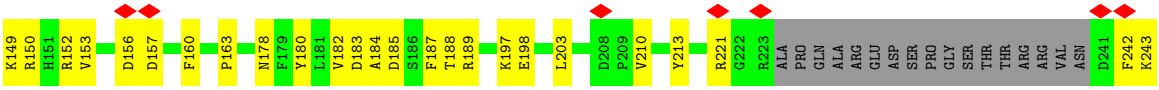


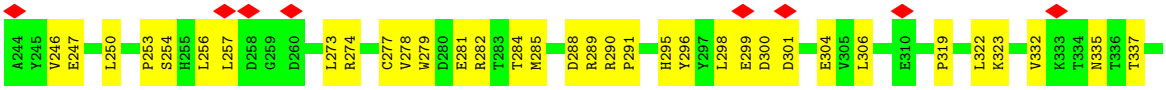


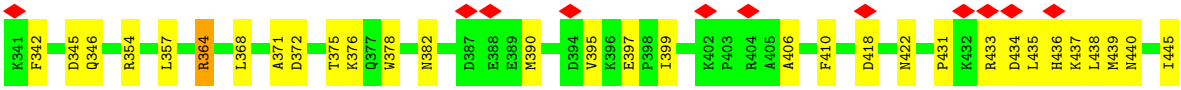
• Molecule 24: RIB72

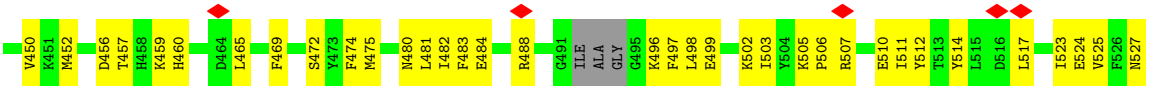
Chain 6Y:

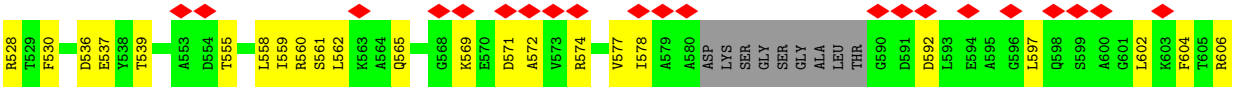


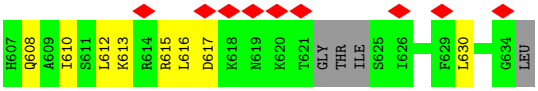






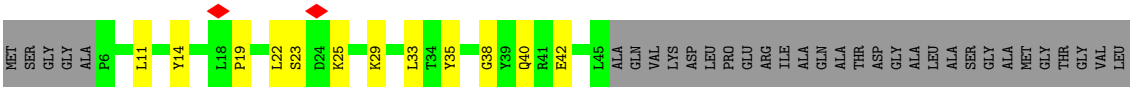


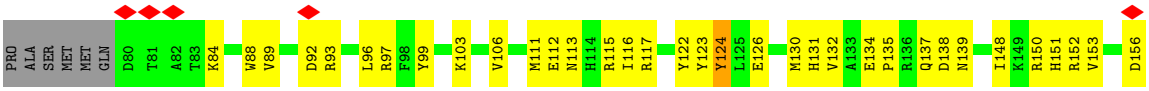


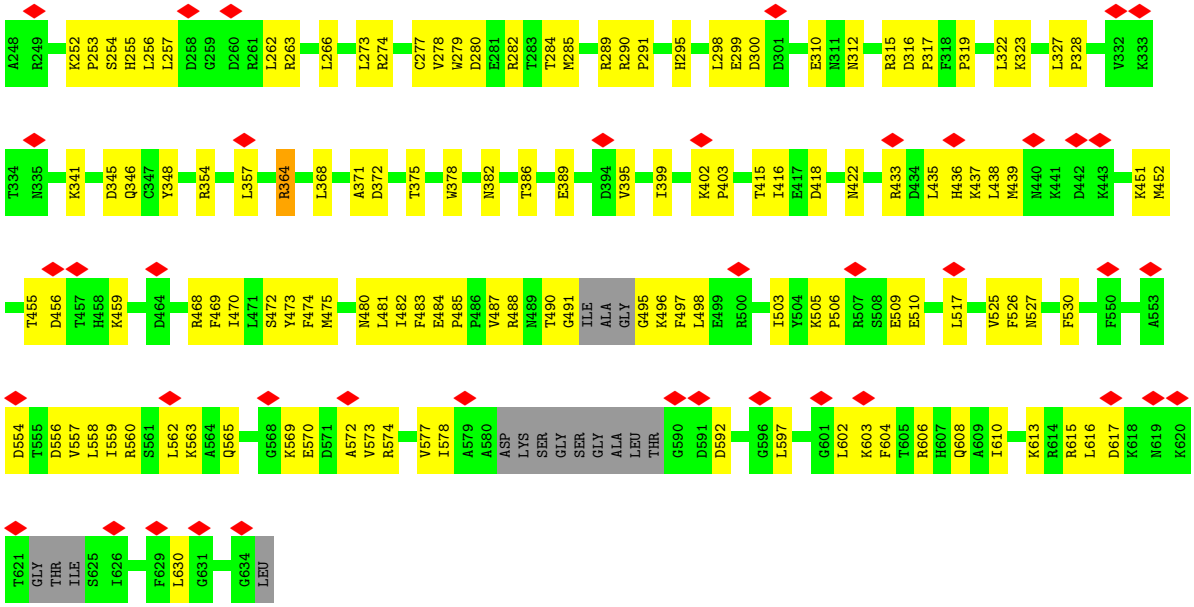


• Molecule 24: RIB72

Chain 6Z:

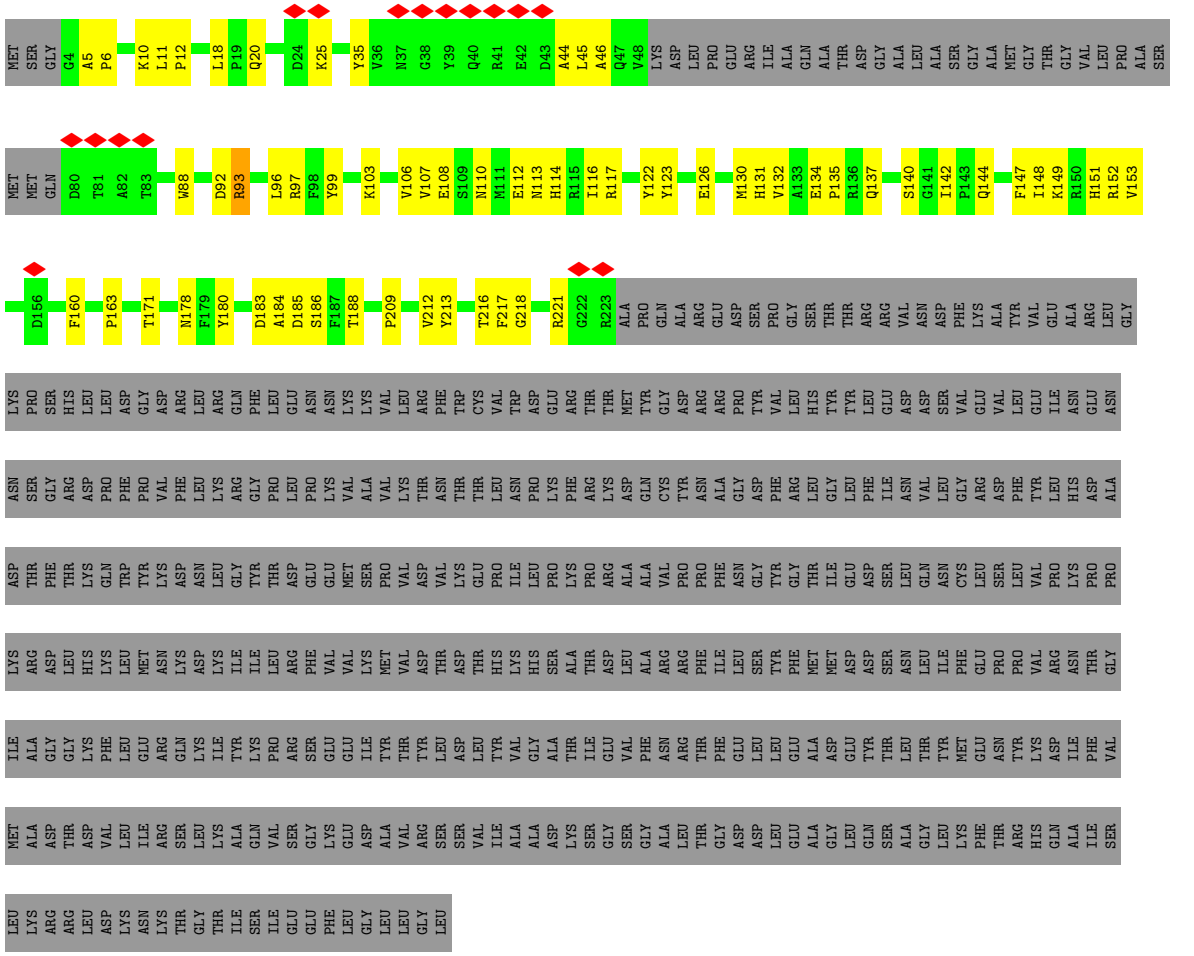






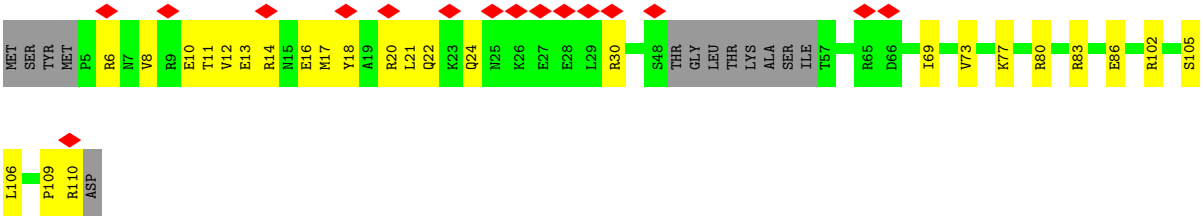
- Molecule 24: RIB72

Chain 7A:



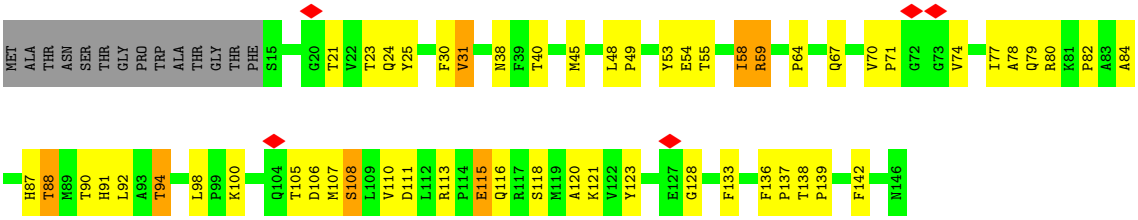
- Molecule 25: FAP141

Chain 7C:



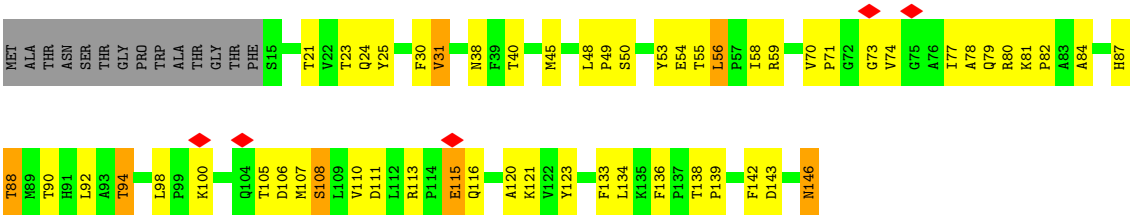
- Molecule 26: FAP222

Chain 7D:



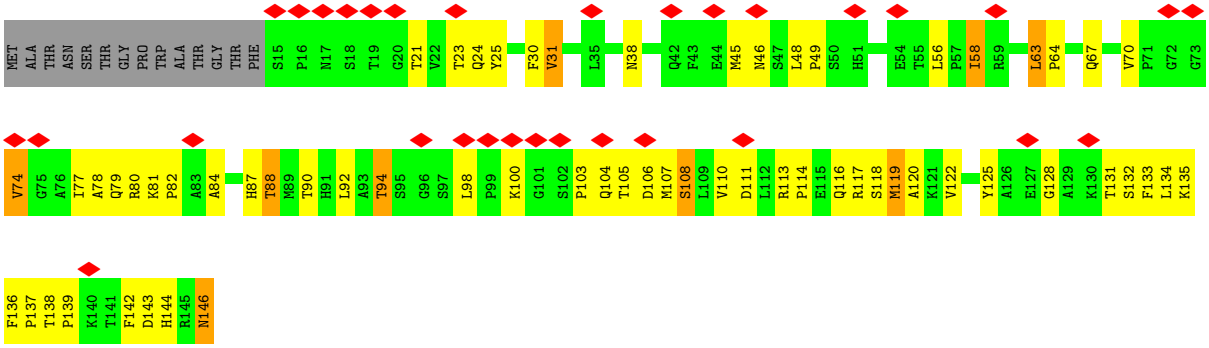
- Molecule 26: FAP222

Chain 7E:



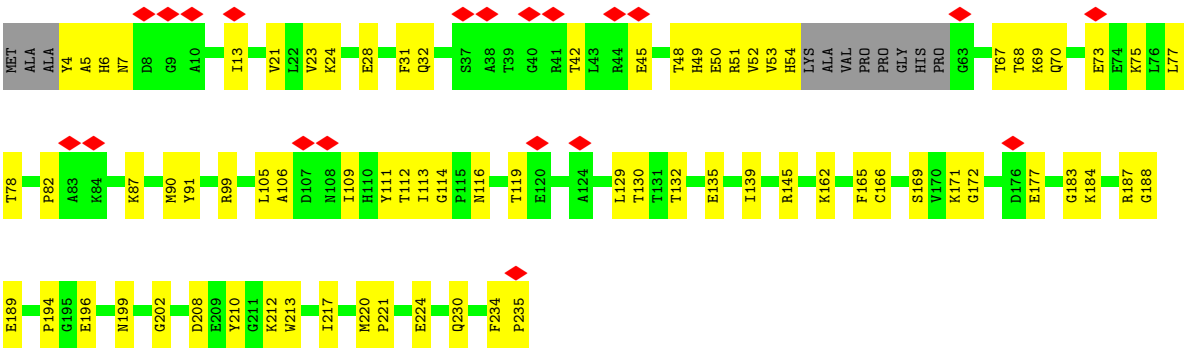
- Molecule 26: FAP222

Chain 7F:



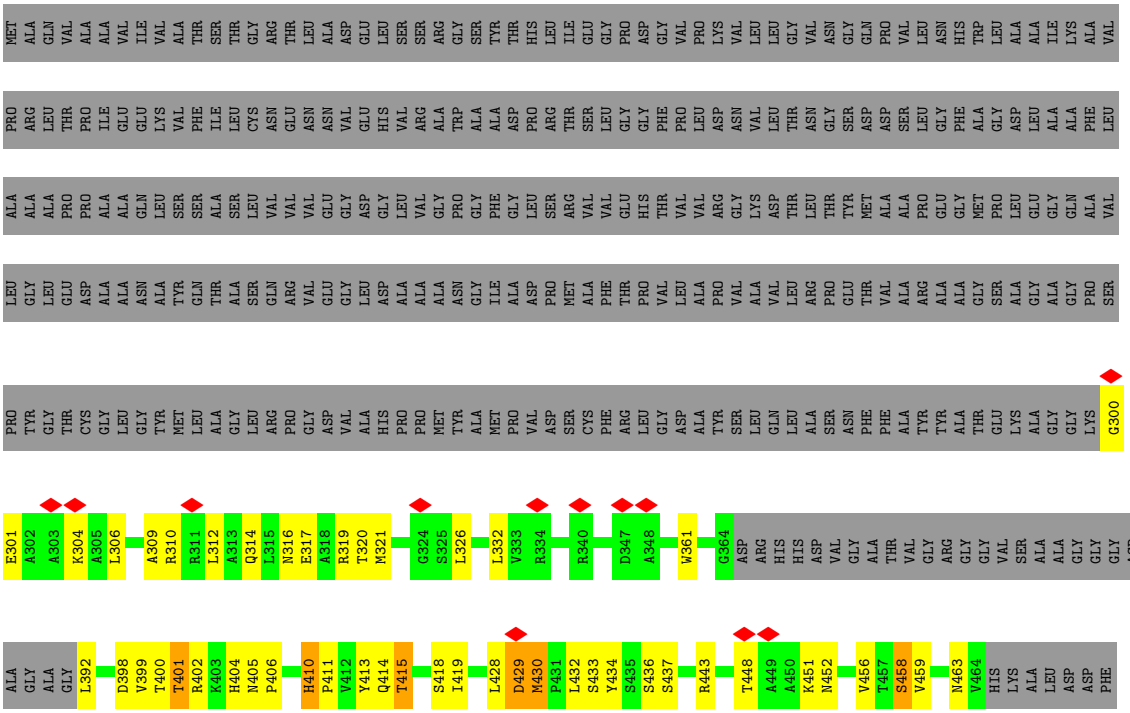
- Molecule 27: FAP95

Chain 7G:



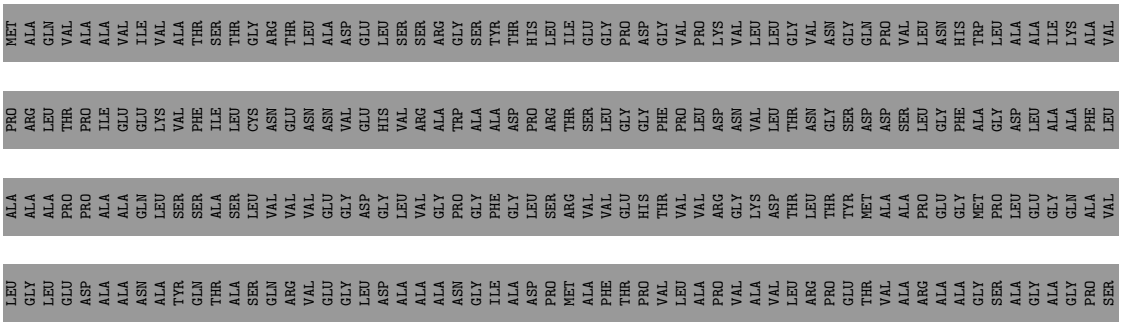
- Molecule 28: FAP182

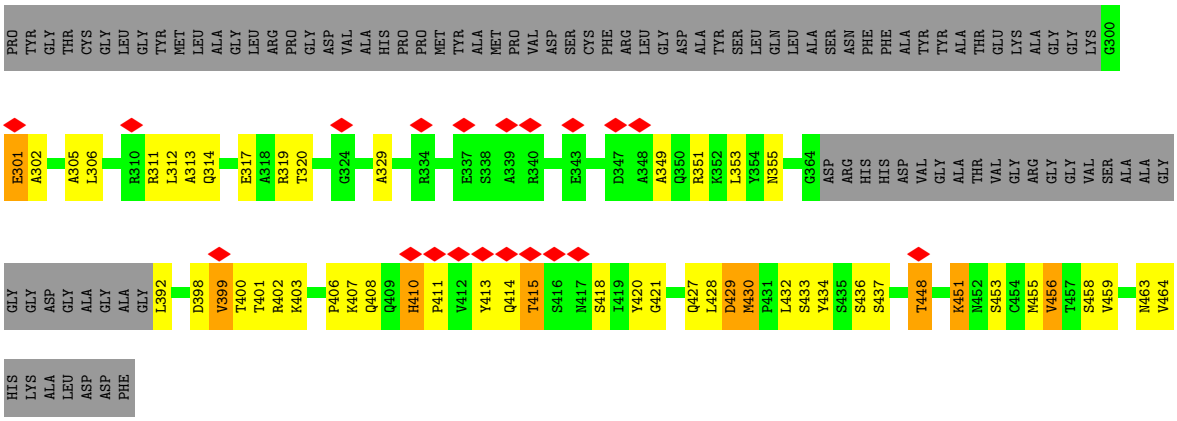
Chain 7H:



- Molecule 28: FAP182

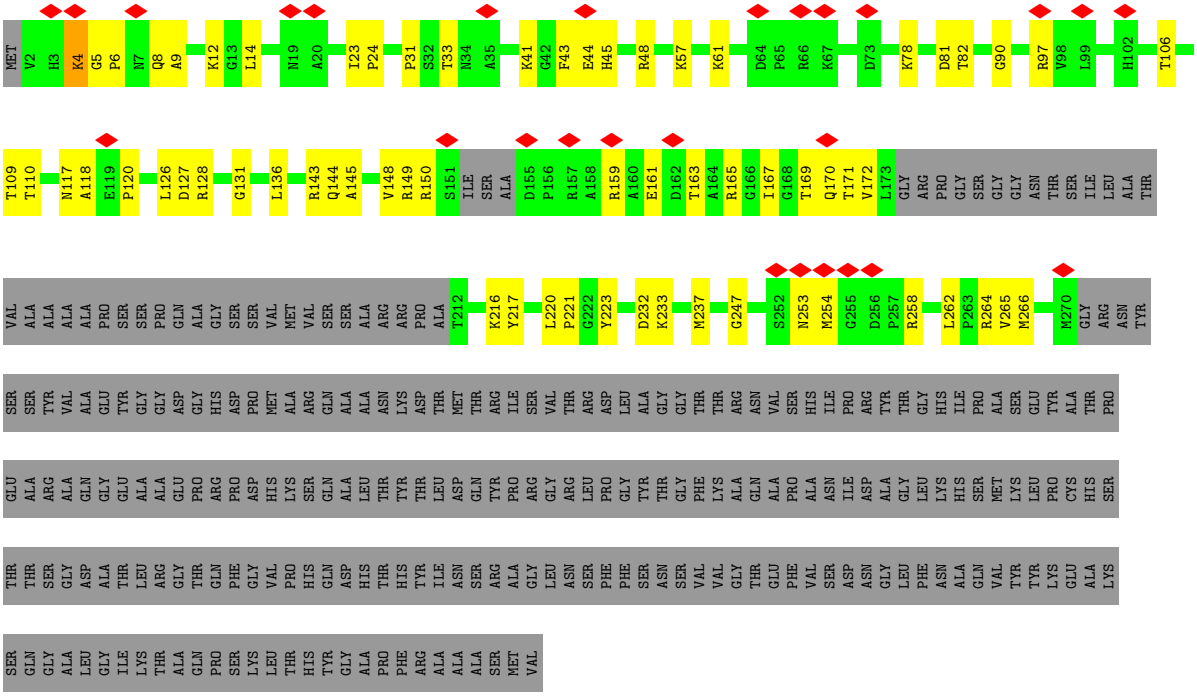
Chain 7X:





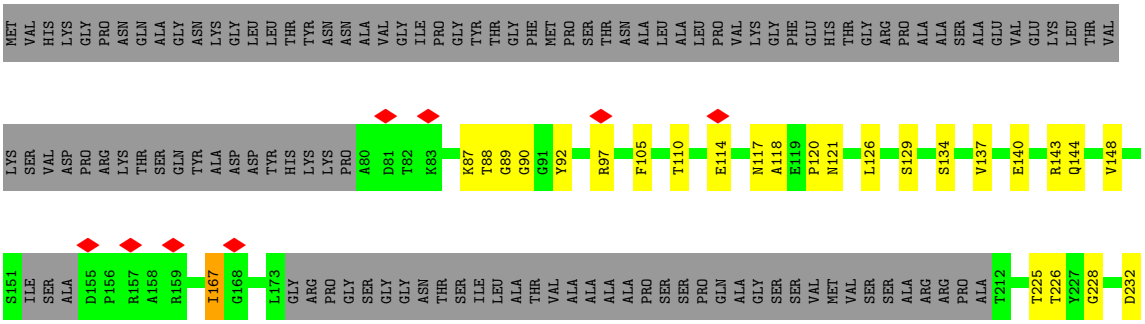
• Molecule 29: FAP129

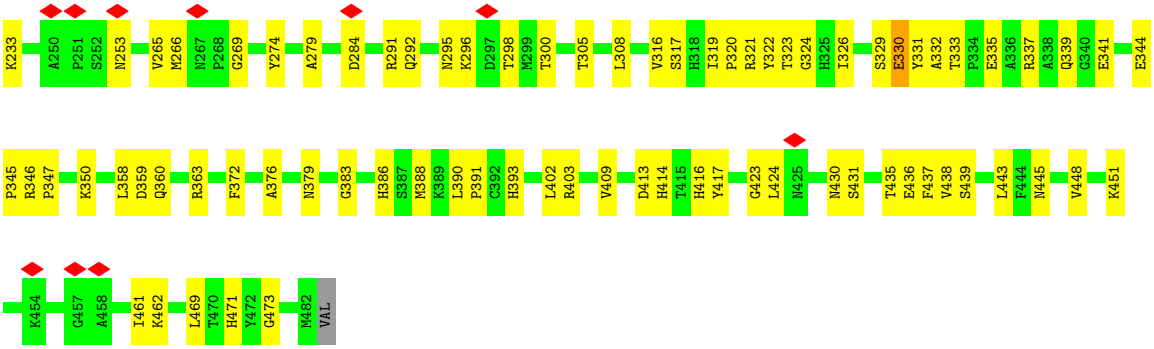
Chain 7I:



• Molecule 29: FAP129

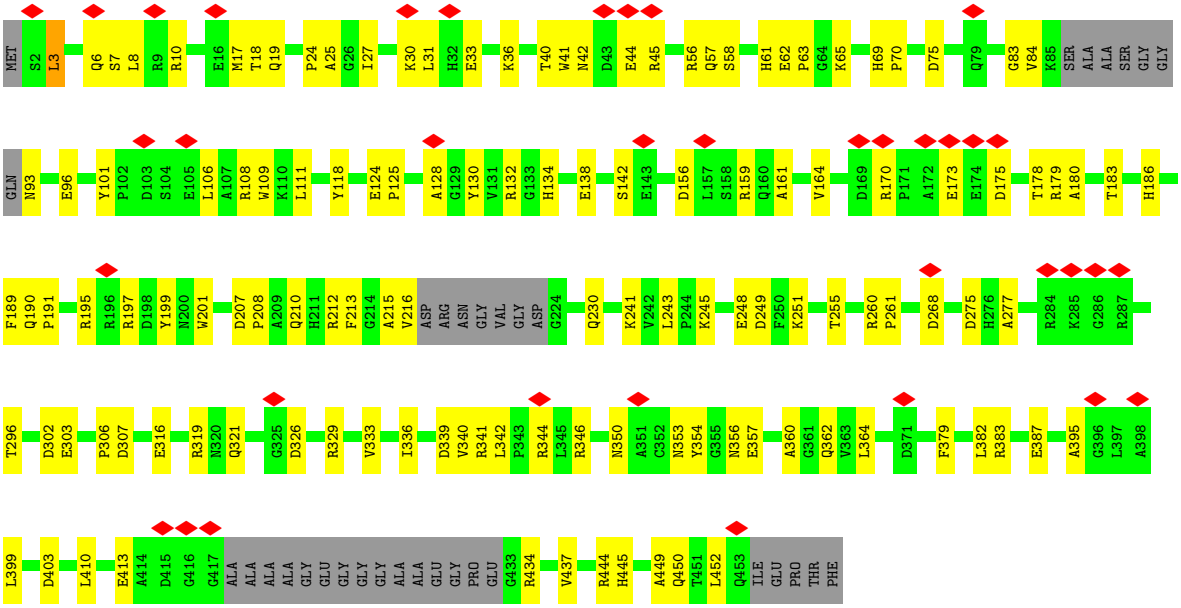
Chain 7J:





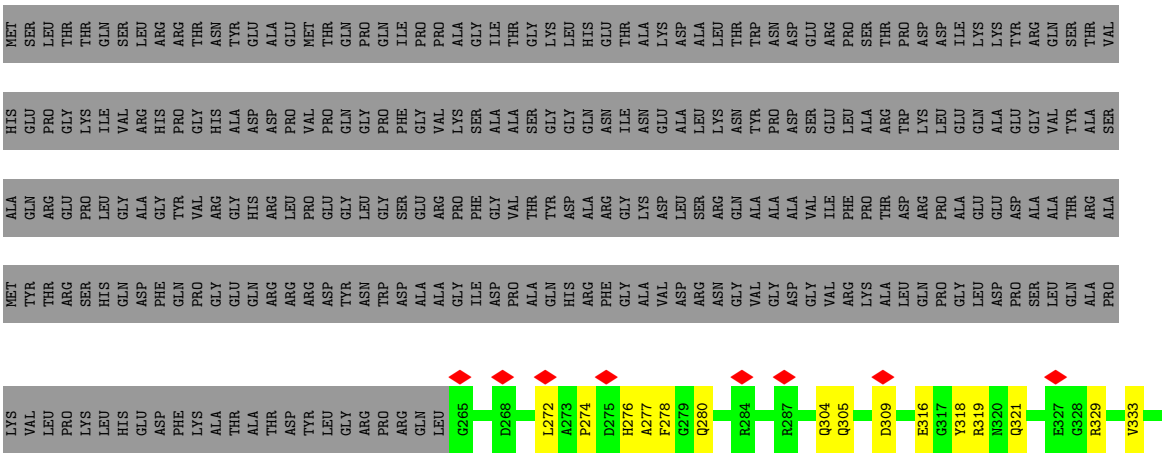
• Molecule 30: FAP21

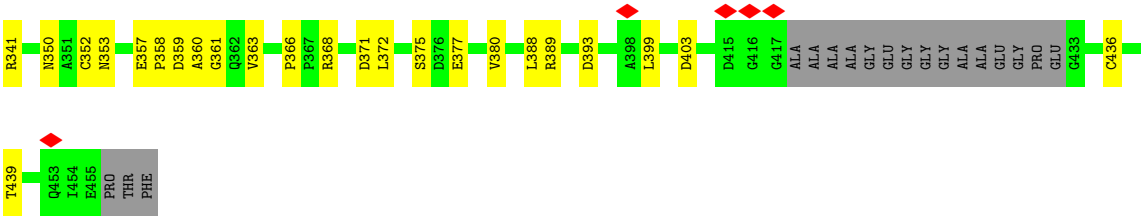
Chain 7K:



• Molecule 30: FAP21

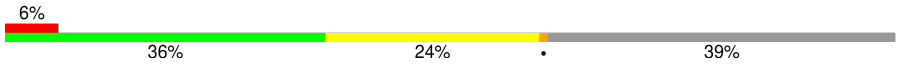
Chain 7L:

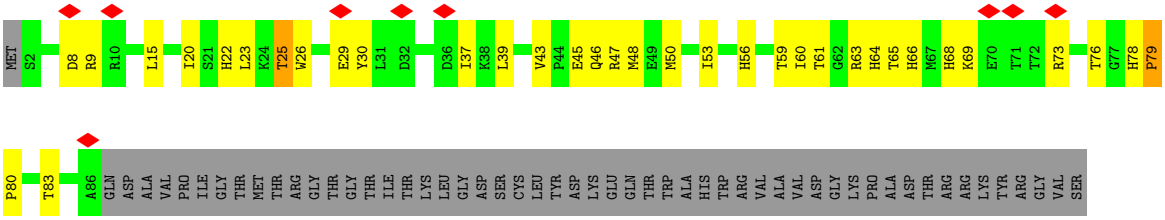




• Molecule 31: FAP273

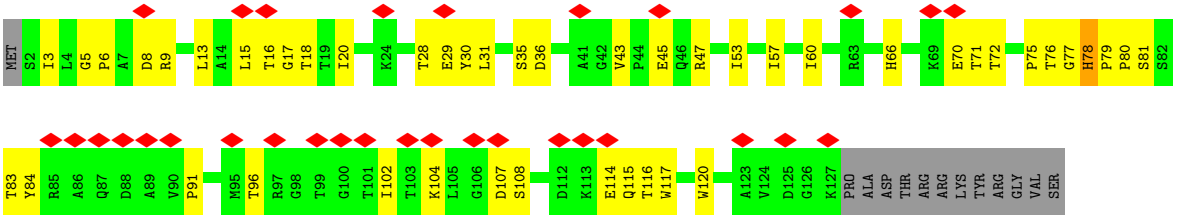
Chain 7M:





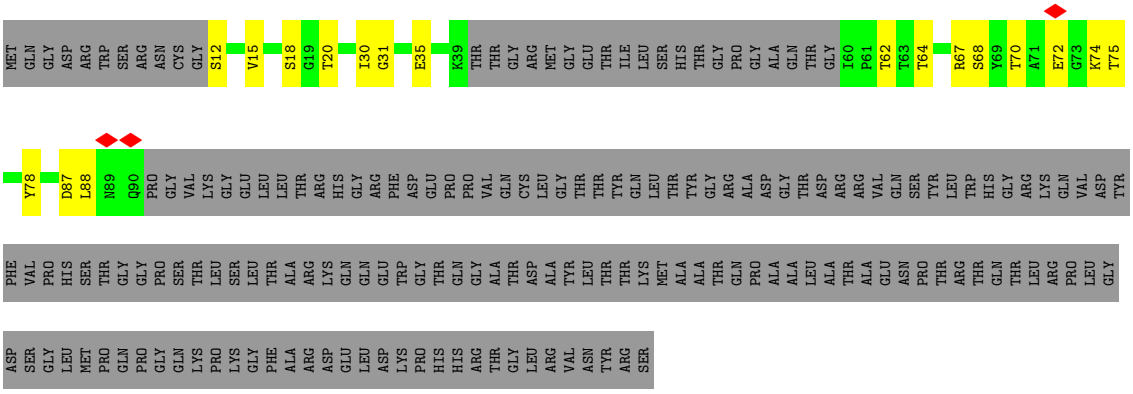
• Molecule 31: FAP273

Chain 7N:



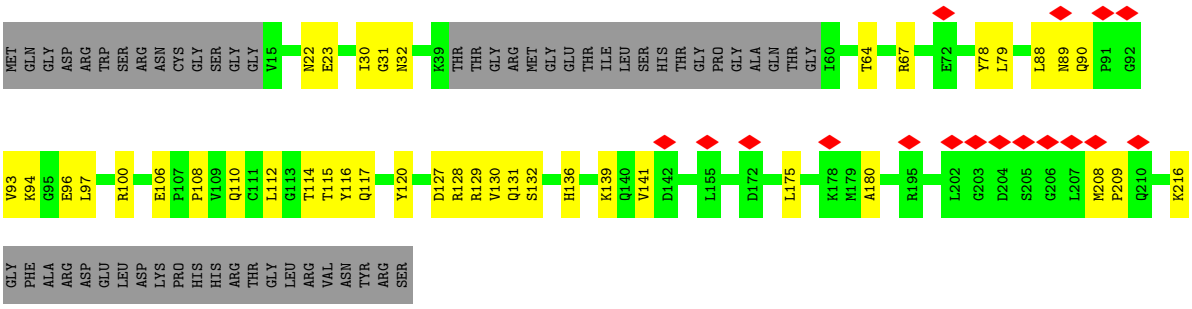
• Molecule 32: FAP107

Chain 7O:



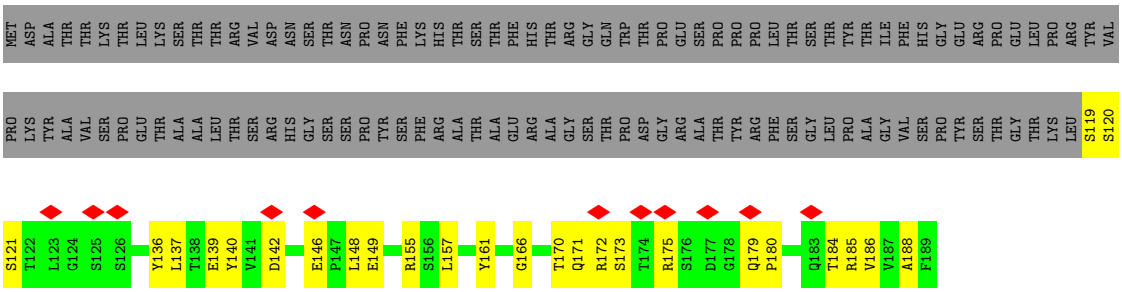
• Molecule 32: FAP107

Chain 7P:



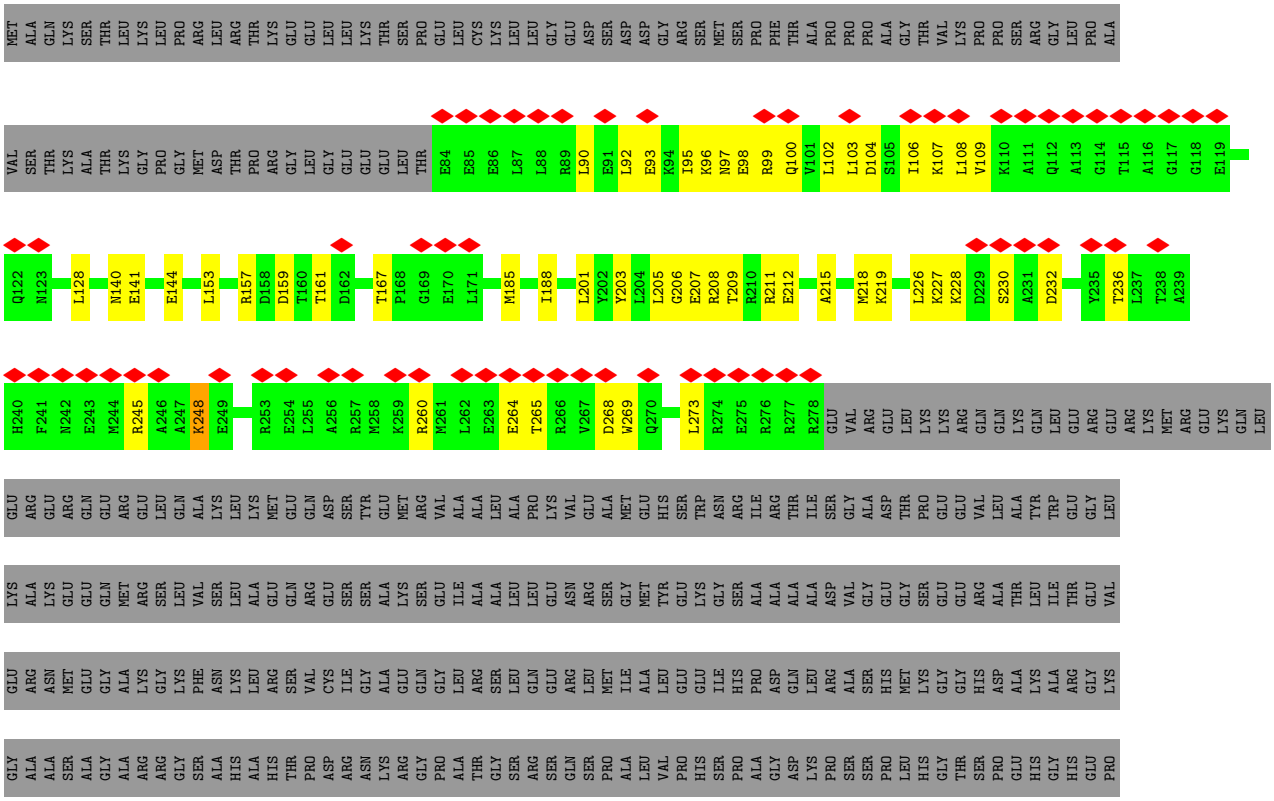
- Molecule 33: RIB21

Chain 7Q:



- Molecule 34: DC1

Chain 7R:



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

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

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

VAL VAL ASP ARG ASP TYR ILE LYS LEU ARG ALA LEU LYS MET SER GLN ARG LEU ALA ASN GLN GLN ARG ALA ILE LYS VAL

- Molecule 34: DC1

Chain 7S: 5% 16% 5% 79%

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

VAL SER THR LYS ALA THR LYS GLY PRO GLY MET ASP THR PRO ARG GLY LEU GLY GLU GLU GLU LEU THR GLU GLU GLU LEU LEU ARG LEU GLU LEU GLU LYS ILE LYS ASN GLU ARG GLN VAL LEU LEU ASP SER ILE LYS LEU VAL LYS ALA GLN ALA GLY THR ALA GLY GLY E119

N123 K126 R129 R130 L134 N140 K149 V152 Q156 T160 G169 E170 L171 I188 L201 L205 R210 R211 E212 H213 L214 A215 M216 D217 V220 L226 K227 K228 D229 D232 Y235 T238 A239 H240 F241 N242 E243 M244 R245 A246 A247 K248

E249 Q250 A251 E252 R253 E254 L255 A256 R257 M258 K259 R260 M261 L262 E263 E264 T265 R266 V267 D268 W269 Q270 K271 K272 L273 R274 E275 R276 R277 R278 GLU VAL ARG GLU LEU LYS LYS ARG GLN GLN LYS GLN LEU GLU ARG GLU ARG LYS MET ARG GLU LYS GLN LEU GLU ARG GLU ARG GLN GLU

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

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

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

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

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

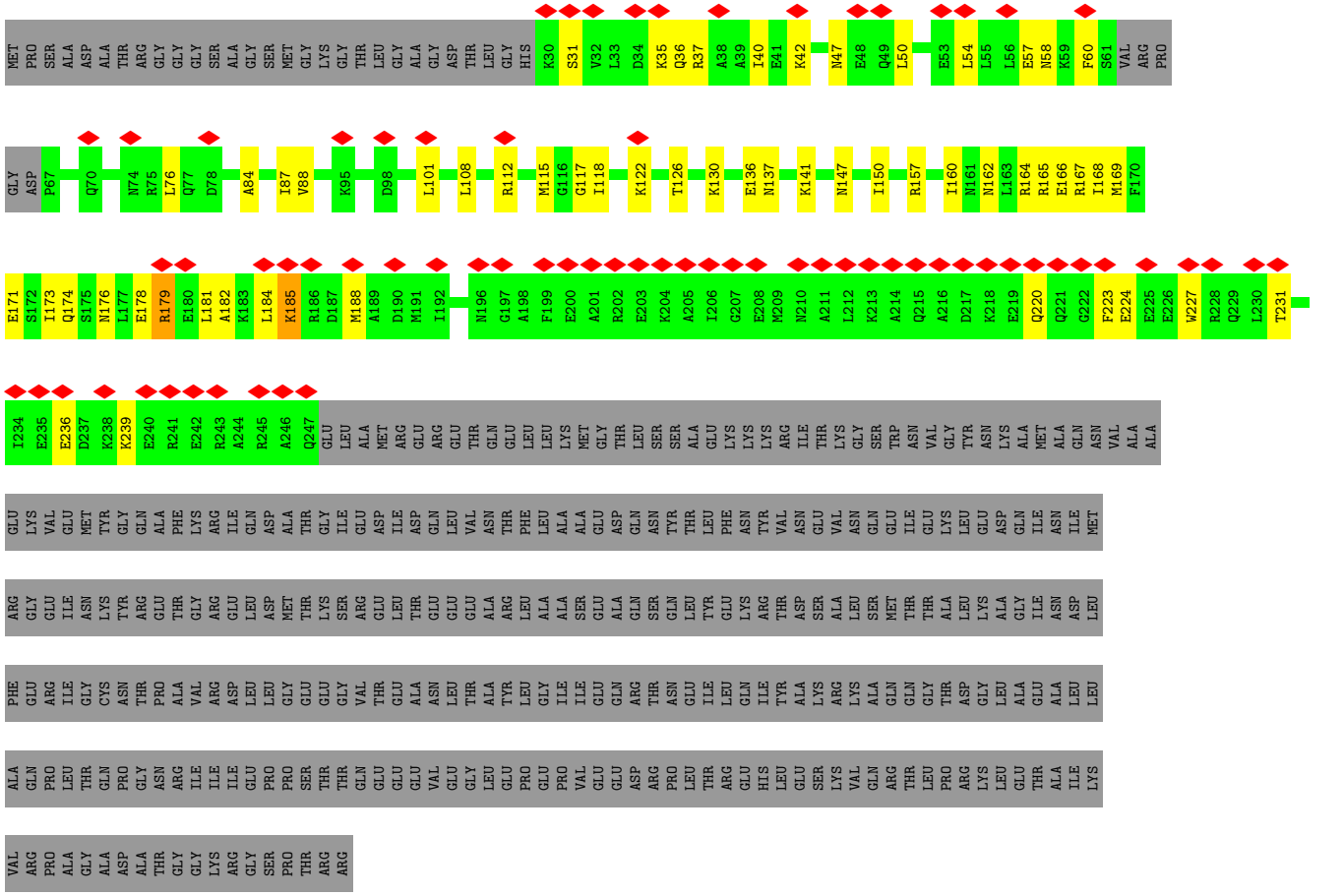
GLY LEU PRO LEU SER GLY GLU PRO GLY ALA ASP GLY ALA GLU GLY ALA ALA PRO ALA SER PRO SER ARG GLY ALA PRO GLU GLY LEU SER GLU SER GLU ARG THR LEU VAL LYS GLY MET ASN ARG ARG THR TRP THR GLY ALA PRO LEU LEU GLU THR ILE ASN ALA SER PRO GLU GLU

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

ILE LYS LEU ARG ALA LEU LYS MET SER GLN ARG LEU ALA ASN GLN GLN ARG ALA ILE LYS VAL

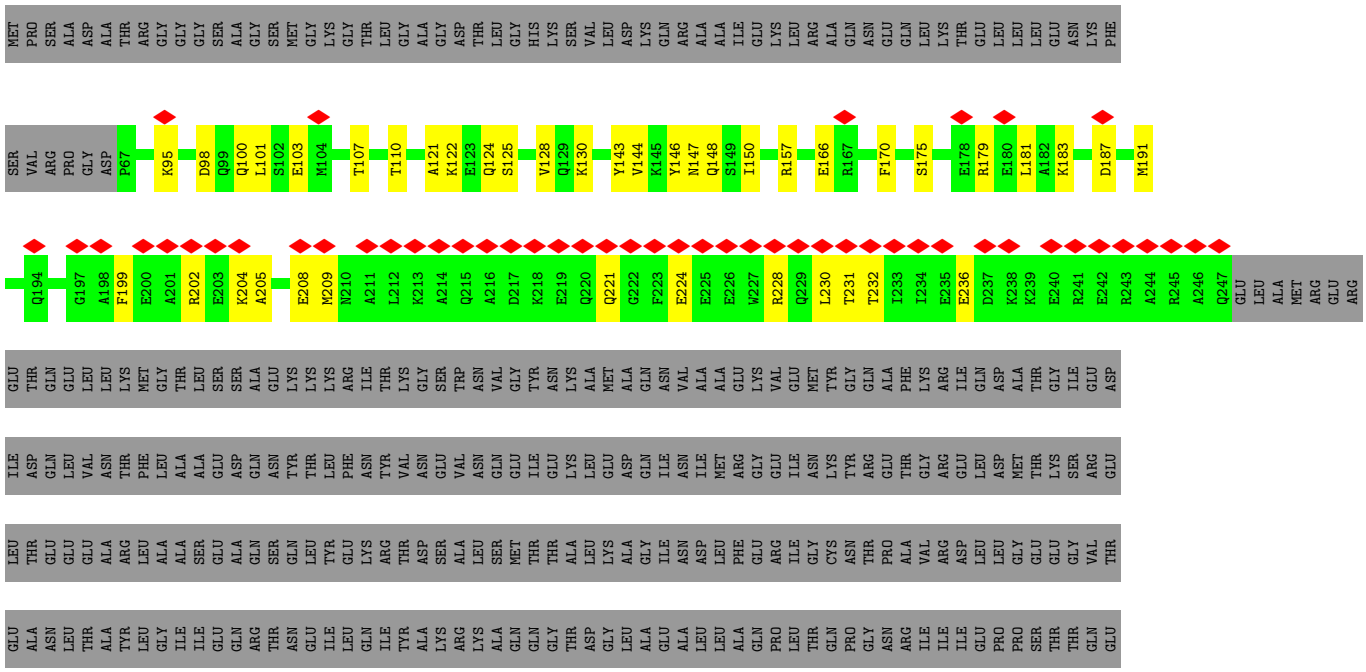
- Molecule 35: DC2

Chain 7T: 13% 28% 10% 61%



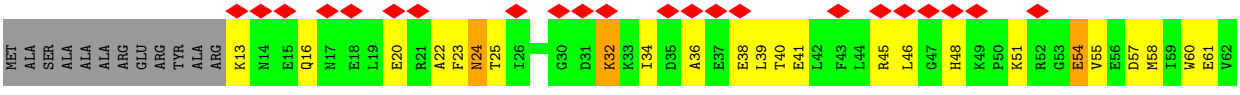
- Molecule 35: DC2

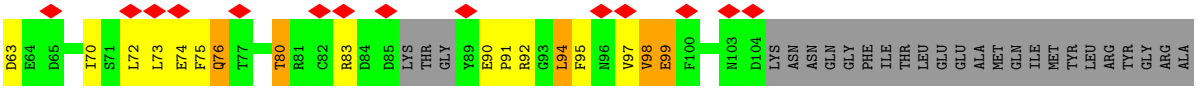
Chain 7U:



- Molecule 36: DC3

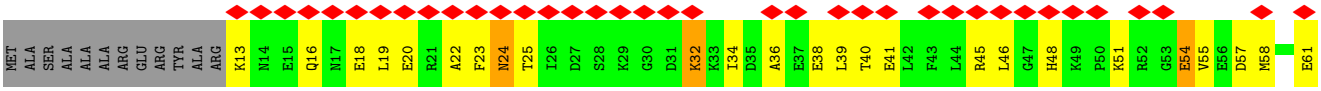
Chain 7V:

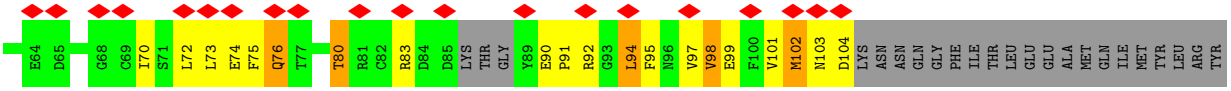




- Molecule 36: DC3

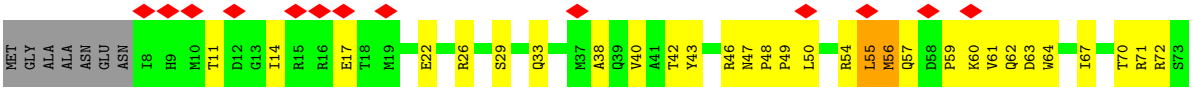
Chain 7W:

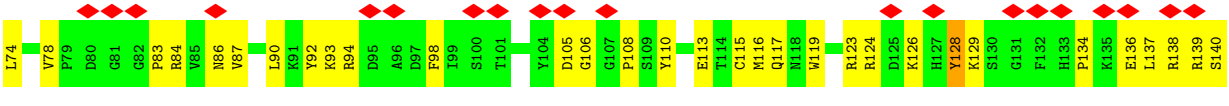


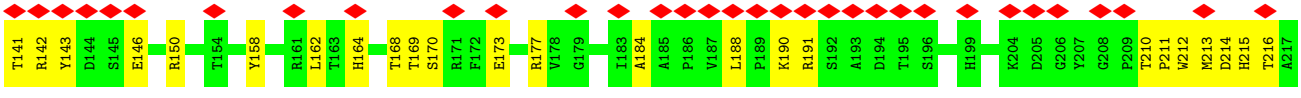


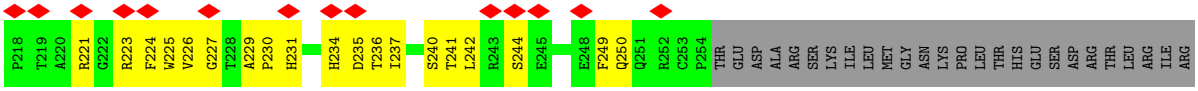
- Molecule 37: FAP68

Chain 7Y:



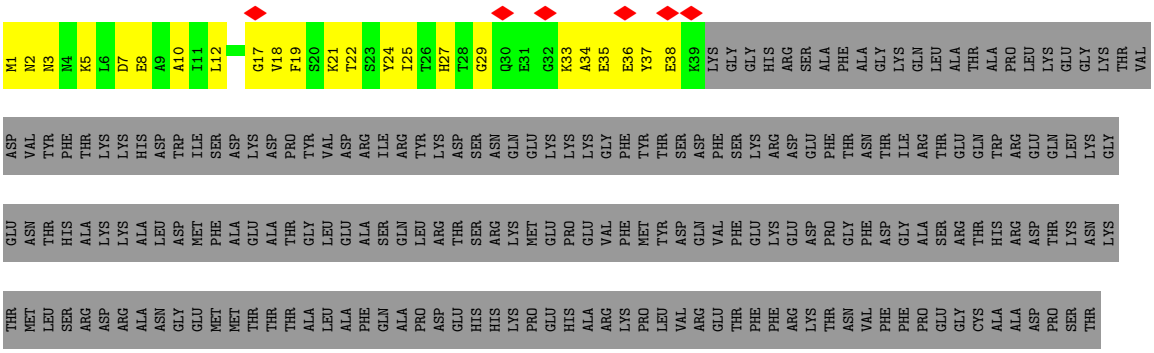






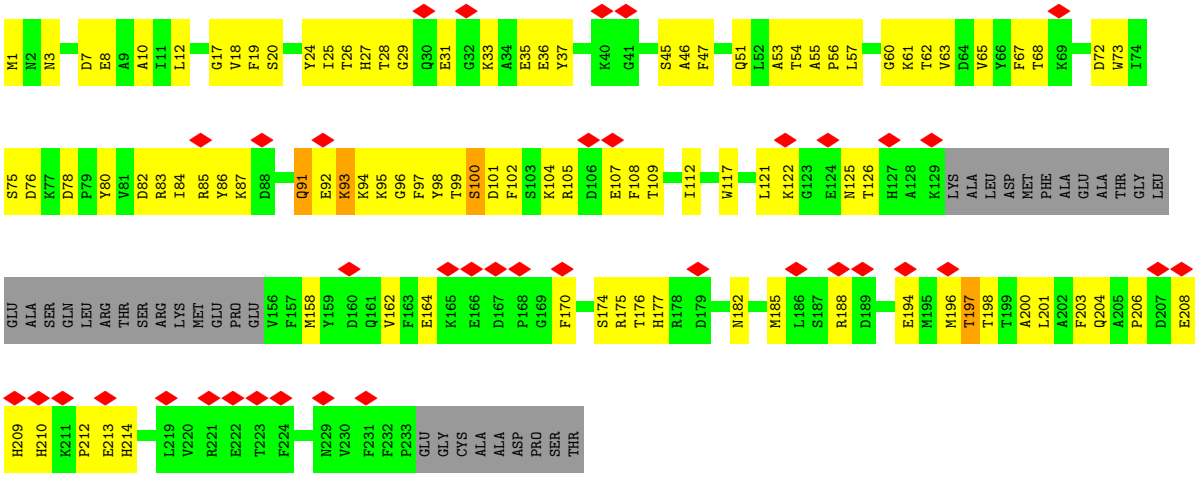
- Molecule 38: FAP90

Chain 7Z:



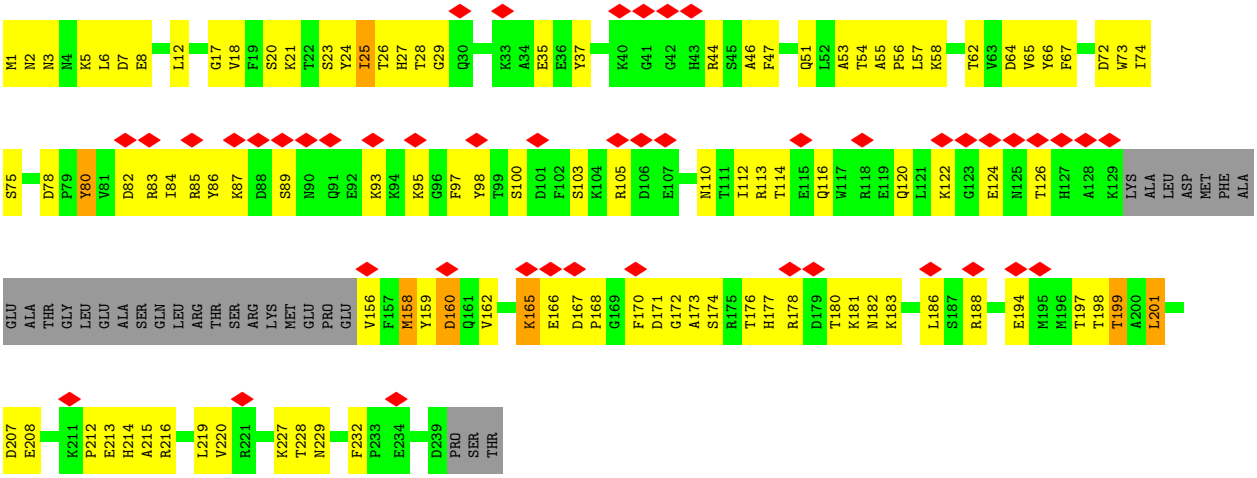
- Molecule 38: FAP90

Chain 8A:



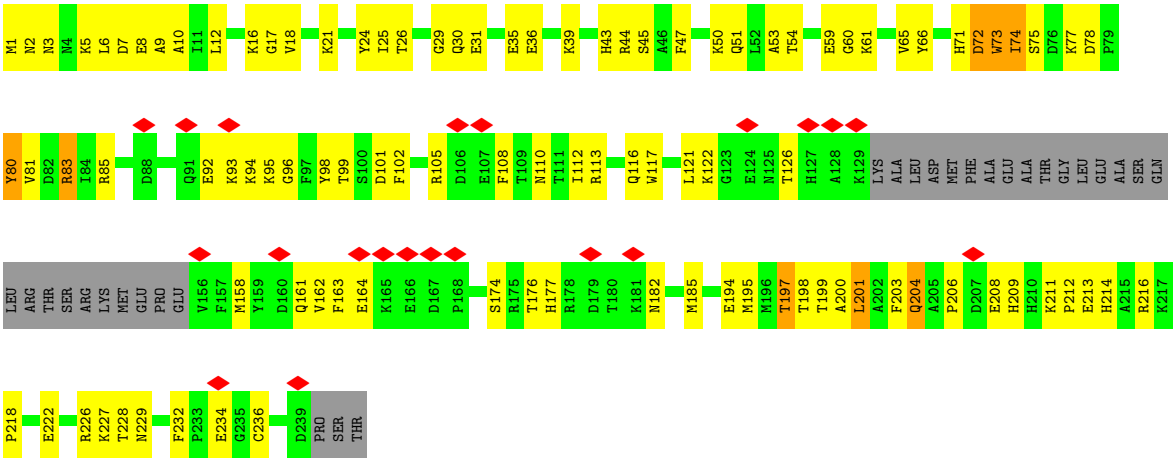
- Molecule 38: FAP90

Chain 8B:



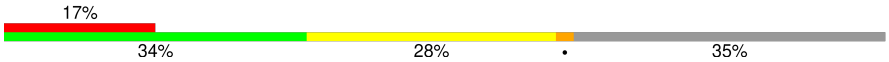
- Molecule 38: FAP90

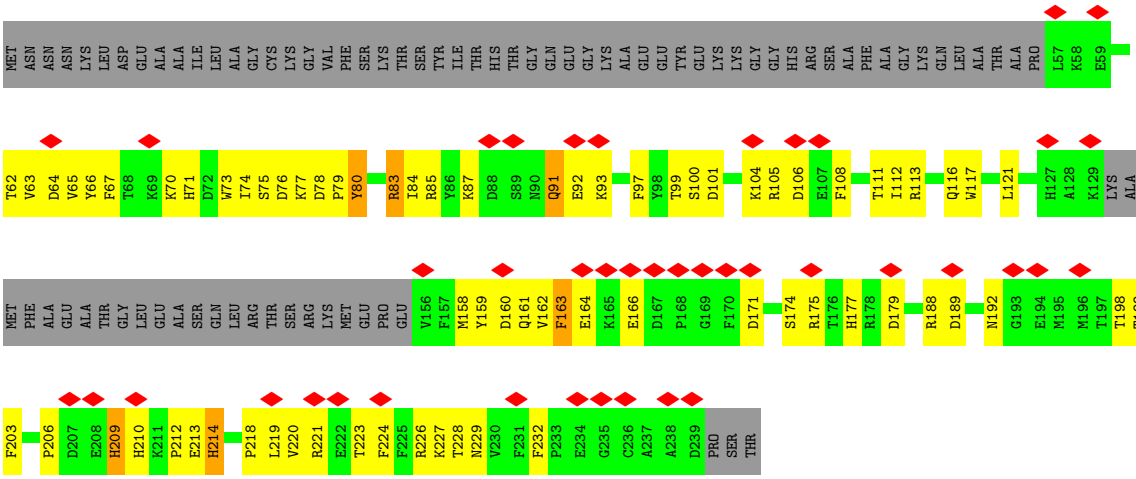
Chain 8C:



- Molecule 38: FAP90

Chain 8D:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143765	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.122	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	718.336, 718.336, 718.336	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.403, 1.403, 1.403	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: GDP, GTP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0A	0.33	0/3420	0.46	0/4628
1	0C	0.30	0/3420	0.45	0/4628
1	0E	0.31	0/3420	0.45	0/4628
1	0G	0.32	0/3420	0.45	0/4628
1	0I	0.32	0/3420	0.45	0/4628
1	0K	0.35	0/3420	0.47	0/4628
1	0M	0.34	0/3420	0.46	0/4628
1	0O	0.33	0/3420	0.46	0/4628
1	0Q	0.32	0/3420	0.44	0/4628
1	0S	0.30	0/3420	0.47	0/4628
1	0U	0.31	0/3420	0.46	0/4628
1	0W	0.33	0/3420	0.47	0/4628
1	0Y	0.33	0/3420	0.47	0/4628
1	1	0.43	0/1144	0.50	0/1538
1	1A	0.35	0/3420	0.47	0/4628
1	1C	0.35	0/3420	0.47	1/4628 (0.0%)
1	1E	0.33	0/3420	0.47	0/4628
1	1G	0.33	0/3420	0.46	0/4628
1	1K	0.32	0/3420	0.44	0/4628
1	1M	0.34	0/3420	0.45	0/4628
1	1O	0.34	0/3420	0.45	0/4628
1	1Q	0.37	0/3420	0.46	0/4628
1	1S	0.35	0/3420	0.45	0/4628
1	1U	0.34	0/3420	0.47	0/4628
1	1W	0.33	0/3420	0.44	0/4628
1	2A	0.35	0/3420	0.47	1/4628 (0.0%)
1	2C	0.37	0/3420	0.46	0/4628
1	2E	0.35	0/3420	0.45	0/4628
1	2G	0.38	0/3420	0.46	0/4628
1	2I	0.37	0/3420	0.46	0/4628
1	2K	0.37	0/3420	0.45	0/4628
1	2M	0.36	0/3420	0.46	0/4628

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	2Q	0.39	0/3420	0.48	0/4628
1	2S	0.39	0/3420	0.48	1/4628 (0.0%)
1	2U	0.39	0/3420	0.47	0/4628
1	2W	0.41	0/3420	0.47	0/4628
1	2Y	0.40	0/3420	0.48	0/4628
1	3	0.42	0/3471	0.48	0/4697
1	3A	0.41	0/3420	0.48	0/4628
1	3C	0.40	0/3420	0.47	0/4628
1	3G	0.38	0/3420	0.47	0/4628
1	3I	0.39	0/3420	0.47	0/4628
1	3K	0.40	0/3420	0.48	0/4628
1	3M	0.42	0/3420	0.50	1/4628 (0.0%)
1	3O	0.39	0/3420	0.50	0/4628
1	3Q	0.40	0/3420	0.50	0/4628
1	3S	0.43	0/3420	0.55	0/4628
1	5	0.41	0/3496	0.48	0/4730
1	7	0.43	0/3505	0.49	0/4742
1	9	0.44	0/3496	0.52	1/4730 (0.0%)
1	A1	0.40	0/3462	0.48	0/4685
1	A3	0.32	0/3484	0.44	0/4714
1	A5	0.38	0/3444	0.45	0/4661
1	A7	0.37	0/3420	0.46	0/4628
1	A9	0.40	0/3420	0.47	0/4628
1	B1	0.38	0/3420	0.45	0/4628
1	B3	0.40	0/3420	0.46	0/4628
1	B5	0.41	0/3420	0.47	0/4628
1	B8	0.37	0/3420	0.47	0/4628
1	C0	0.38	0/3420	0.46	0/4628
1	C2	0.35	0/3420	0.44	0/4628
1	C4	0.35	0/3420	0.45	0/4628
1	C6	0.40	0/3420	0.48	0/4628
1	C8	0.38	0/3420	0.48	0/4628
1	D0	0.41	0/3420	0.47	0/4628
1	D2	0.41	0/3420	0.49	1/4628 (0.0%)
1	D4	0.38	0/3420	0.48	0/4628
1	D6	0.38	0/3420	0.47	0/4628
1	D8	0.32	0/3420	0.46	0/4628
1	E0	0.34	0/3420	0.46	0/4628
1	E2	0.39	0/3420	0.48	0/4628
1	E4	0.35	0/3420	0.47	0/4628
1	E6	0.37	0/3420	0.47	0/4628
1	E8	0.38	0/3420	0.48	0/4628
1	F0	0.35	0/3420	0.47	0/4628

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	F2	0.36	0/3420	0.47	0/4628
1	F6	0.32	0/3420	0.47	1/4628 (0.0%)
1	F8	0.36	0/3420	0.46	0/4628
1	G0	0.34	0/3420	0.46	0/4628
1	G2	0.38	0/3420	0.47	0/4628
1	G4	0.35	0/3420	0.45	0/4628
1	G6	0.37	0/3420	0.48	0/4628
1	G8	0.34	0/3420	0.46	0/4628
1	H2	0.33	0/3420	0.46	0/4628
1	H4	0.36	0/3420	0.48	0/4628
1	H6	0.34	0/3420	0.45	0/4628
1	H8	0.38	0/3420	0.46	0/4628
1	I0	0.36	0/3420	0.46	0/4628
1	I2	0.36	0/3420	0.46	0/4628
1	I4	0.36	0/3420	0.47	0/4628
1	I8	0.37	0/3420	0.45	0/4628
1	J0	0.39	0/3420	0.46	0/4628
1	J2	0.38	0/3420	0.46	0/4628
1	J4	0.40	0/3420	0.46	0/4628
1	J6	0.38	0/3420	0.46	0/4628
1	J8	0.38	0/3420	0.45	0/4628
1	K0	0.35	0/3420	0.45	0/4628
1	K4	0.37	0/3420	0.46	0/4628
1	K6	0.38	0/3420	0.46	0/4628
1	K8	0.38	0/3420	0.45	0/4628
1	L0	0.40	0/3420	0.46	0/4628
1	L2	0.37	0/3420	0.46	0/4628
1	L4	0.39	0/3420	0.46	0/4628
1	L6	0.37	0/3420	0.46	0/4628
1	M0	0.37	0/3420	0.46	0/4628
1	M2	0.37	0/3420	0.46	0/4628
1	M4	0.36	0/3420	0.46	0/4628
1	M6	0.39	0/3420	0.47	0/4628
1	M8	0.36	0/3420	0.48	0/4628
1	N0	0.39	0/3420	0.47	0/4628
1	N2	0.36	0/3420	0.48	1/4628 (0.0%)
1	N6	0.40	0/3420	0.46	0/4628
1	N8	0.41	0/3420	0.47	0/4628
1	O0	0.37	0/3420	0.47	0/4628
1	O2	0.42	0/3420	0.49	0/4628
1	O4	0.42	0/3420	0.48	0/4628
1	O6	0.43	0/3420	0.47	0/4628
1	O8	0.41	1/3420 (0.0%)	0.46	0/4628

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	P4	0.42	0/3420	0.47	0/4628
1	P6	0.40	0/3420	0.46	0/4628
1	P8	0.41	0/3420	0.46	0/4628
1	Q0	0.42	0/3420	0.48	1/4628 (0.0%)
1	Q2	0.41	0/3420	0.46	0/4628
1	Q4	0.42	0/3420	0.47	0/4628
1	Q6	0.40	0/3420	0.46	0/4628
1	Q8	0.33	0/3366	0.49	0/4556
1	R0	0.42	0/3475	0.48	0/4702
1	R2	0.40	0/3420	0.50	1/4628 (0.0%)
1	R4	0.43	0/3444	0.48	0/4661
1	R6	0.42	0/3420	0.47	0/4628
1	R8	0.41	0/3453	0.47	0/4673
1	S0	0.41	0/3420	0.48	0/4628
1	S2	0.41	0/3453	0.49	0/4673
1	S4	0.37	0/3428	0.49	0/4639
1	S6	0.41	0/3420	0.48	1/4628 (0.0%)
1	S8	0.41	0/3420	0.48	0/4628
1	T0	0.42	0/3420	0.49	0/4628
1	T2	0.44	0/3420	0.49	0/4628
1	T4	0.40	0/3420	0.46	0/4628
1	T6	0.44	1/3420 (0.0%)	0.54	0/4628
1	T8	0.38	0/3420	0.46	0/4628
1	U2	0.36	0/3420	0.47	0/4628
1	U4	0.37	0/3420	0.46	0/4628
1	U6	0.37	0/3420	0.47	0/4628
1	U8	0.39	0/3444	0.49	0/4661
1	V0	0.37	0/3420	0.45	0/4628
1	V2	0.37	0/3420	0.47	0/4628
1	V4	0.36	0/3420	0.45	0/4628
1	V6	0.33	0/3420	0.46	0/4628
1	V8	0.36	0/3420	0.47	0/4628
1	W0	0.37	0/3420	0.46	0/4628
1	W2	0.37	0/3420	0.46	0/4628
1	W4	0.40	0/3420	0.48	0/4628
1	W6	0.36	0/3420	0.45	0/4628
1	W8	0.38	0/3420	0.48	0/4628
1	X0	0.36	0/3420	0.46	0/4628
1	X2	0.31	0/3420	0.45	0/4628
1	X4	0.34	0/3420	0.46	0/4628
1	X6	0.35	0/3420	0.46	0/4628
1	X8	0.36	0/3420	0.47	0/4628
1	Y0	0.37	0/3420	0.47	0/4628

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	Y2	0.34	0/3420	0.46	0/4628
1	Y4	0.39	0/3420	0.47	0/4628
1	Y6	0.33	0/3420	0.45	0/4628
1	Y8	0.29	0/3420	0.46	0/4628
1	Z0	0.32	0/3420	0.46	0/4628
1	Z2	0.32	0/3420	0.46	0/4628
1	Z4	0.34	0/3420	0.48	0/4628
1	Z6	0.34	0/3420	0.47	0/4628
1	Z8	0.32	0/3420	0.46	0/4628
2	0B	0.32	0/3389	0.46	0/4595
2	0F	0.32	0/3389	0.47	0/4595
2	0H	0.32	0/3389	0.46	0/4595
2	0J	0.34	0/3389	0.48	0/4595
2	0L	0.35	0/3389	0.49	1/4595 (0.0%)
2	0N	0.33	0/3389	0.47	0/4595
2	0P	0.34	0/3389	0.48	0/4595
2	0R	0.32	0/3389	0.47	0/4595
2	0V	0.35	0/3389	0.47	0/4595
2	0X	0.33	0/3389	0.47	0/4595
2	0Z	0.36	0/3389	0.47	0/4595
2	1B	0.35	0/3389	0.47	0/4595
2	1D	0.34	0/3389	0.48	0/4595
2	1F	0.34	0/3389	0.47	0/4595
2	1H	0.32	0/3389	0.47	0/4595
2	1L	0.34	0/3389	0.48	0/4595
2	1N	0.36	0/3389	0.48	0/4595
2	1P	0.37	0/3389	0.48	0/4595
2	1R	0.38	0/3389	0.49	0/4595
2	1T	0.34	0/3389	0.47	0/4595
2	1V	0.35	0/3389	0.48	0/4595
2	1X	0.32	0/3389	0.47	0/4595
2	1Z	0.33	0/3389	0.47	0/4595
2	2	0.41	0/3448	0.49	1/4675 (0.0%)
2	2B	0.38	0/3389	0.49	0/4595
2	2D	0.35	0/3389	0.47	1/4595 (0.0%)
2	2F	0.37	0/3389	0.48	1/4595 (0.0%)
2	2H	0.38	0/3389	0.50	0/4595
2	2J	0.38	0/3389	0.50	0/4595
2	2L	0.39	0/3389	0.48	0/4595
2	2N	0.33	0/3389	0.49	0/4595
2	2P	0.38	0/3389	0.49	0/4595
2	2R	0.40	0/3389	0.48	0/4595
2	2T	0.39	0/3389	0.48	0/4595

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	2V	0.41	0/3389	0.49	0/4595
2	2X	0.41	0/3457	0.49	1/4687 (0.0%)
2	2Z	0.41	0/3389	0.49	0/4595
2	3B	0.43	0/3455	0.52	0/4684
2	3D	0.36	0/3389	0.48	0/4595
2	3F	0.37	0/3389	0.49	0/4595
2	3H	0.39	0/3389	0.49	0/4595
2	3J	0.39	0/3389	0.48	0/4595
2	3L	0.41	0/3389	0.49	0/4595
2	3N	0.41	0/3389	0.50	0/4595
2	3P	0.39	0/3389	0.50	0/4595
2	3R	0.40	0/3457	0.53	0/4687
2	3T	0.36	0/3389	0.55	0/4595
2	4	0.43	0/3448	0.52	0/4675
2	6	0.41	0/3448	0.49	0/4675
2	8	0.44	0/3448	0.51	0/4675
2	A0	0.41	0/3448	0.49	0/4675
2	A2	0.35	0/3448	0.50	0/4675
2	A4	0.41	0/3448	0.49	0/4675
2	A8	0.39	0/3389	0.48	0/4595
2	B0	0.39	0/3389	0.48	0/4595
2	B2	0.40	0/3389	0.47	0/4595
2	B4	0.42	0/3389	0.48	0/4595
2	B7	0.38	0/3389	0.50	0/4595
2	B9	0.40	0/3389	0.48	1/4595 (0.0%)
2	C1	0.37	0/3389	0.47	0/4595
2	C5	0.39	0/3448	0.48	0/4675
2	C7	0.40	0/3448	0.48	0/4675
2	C9	0.41	0/3389	0.50	0/4595
2	D1	0.42	0/3389	0.51	1/4595 (0.0%)
2	D3	0.37	0/3395	0.47	0/4603
2	D5	0.40	0/3389	0.49	0/4595
2	D7	0.37	0/3395	0.48	0/4603
2	E1	0.37	0/3395	0.48	0/4603
2	E3	0.37	0/3389	0.47	0/4595
2	E5	0.39	0/3389	0.49	0/4595
2	E7	0.38	0/3395	0.50	0/4603
2	E9	0.35	0/3389	0.49	0/4595
2	F1	0.37	0/3389	0.49	0/4595
2	F3	0.34	0/3389	0.49	0/4595
2	F5	0.31	0/3389	0.46	0/4595
2	F7	0.36	0/3389	0.47	0/4595
2	F9	0.35	0/3448	0.46	0/4675

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	G1	0.38	0/3448	0.50	0/4675
2	G3	0.39	0/3448	0.51	0/4675
2	G5	0.34	0/3389	0.47	0/4595
2	G7	0.35	0/3389	0.47	0/4595
2	G9	0.33	0/3389	0.47	0/4595
2	H1	0.31	0/3389	0.47	0/4595
2	H3	0.38	0/3389	0.48	0/4595
2	H5	0.35	0/3389	0.47	1/4595 (0.0%)
2	H7	0.38	0/3389	0.48	0/4595
2	H9	0.38	0/3389	0.48	0/4595
2	I1	0.35	0/3389	0.49	0/4595
2	I3	0.36	0/3389	0.47	0/4595
2	I5	0.31	0/3389	0.46	0/4595
2	I7	0.35	0/3403	0.47	0/4614
2	I9	0.40	0/3395	0.49	0/4603
2	J1	0.37	0/3389	0.47	0/4595
2	J3	0.43	0/3397	0.52	0/4606
2	J5	0.42	0/3457	0.52	2/4687 (0.0%)
2	J7	0.39	0/3389	0.48	0/4595
2	J9	0.37	0/3457	0.48	0/4687
2	K1	0.32	0/3389	0.46	0/4595
2	K3	0.35	0/3389	0.48	0/4595
2	K5	0.39	0/3389	0.48	0/4595
2	K7	0.36	0/3389	0.47	0/4595
2	K9	0.41	0/3389	0.50	0/4595
2	L1	0.38	0/3389	0.47	0/4595
2	L3	0.39	0/3389	0.49	0/4595
2	L5	0.39	0/3389	0.49	0/4595
2	L7	0.31	0/3389	0.47	0/4595
2	L9	0.35	0/3389	0.47	0/4595
2	M1	0.37	0/3389	0.49	0/4595
2	M3	0.37	0/3448	0.48	0/4675
2	M5	0.40	0/3389	0.49	0/4595
2	M7	0.38	0/3448	0.49	0/4675
2	M9	0.41	0/3457	0.50	0/4687
2	N1	0.40	0/3395	0.53	0/4603
2	N3	0.30	0/3389	0.47	0/4595
2	N5	0.38	0/3389	0.50	0/4595
2	N7	0.41	0/3389	0.50	0/4595
2	N9	0.39	0/3389	0.50	0/4595
2	O1	0.41	0/3389	0.50	0/4595
2	O3	0.42	0/3389	0.51	0/4595
2	O5	0.41	0/3389	0.50	0/4595

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	O7	0.42	0/3411	0.52	0/4624
2	O9	0.38	0/3389	0.47	0/4595
2	P3	0.41	0/3389	0.49	1/4595 (0.0%)
2	P5	0.42	0/3448	0.51	0/4675
2	P7	0.41	0/3389	0.48	0/4595
2	P9	0.42	0/3448	0.49	0/4675
2	Q1	0.42	0/3389	0.50	0/4595
2	Q3	0.42	0/3389	0.51	0/4595
2	Q5	0.43	0/3389	0.50	0/4595
2	Q9	0.40	0/3389	0.48	0/4595
2	R1	0.41	0/3389	0.50	0/4595
2	R3	0.41	0/3398	0.51	0/4607
2	R5	0.42	0/3448	0.51	0/4675
2	R7	0.42	0/3389	0.49	0/4595
2	R9	0.42	0/3448	0.49	0/4675
2	S1	0.43	0/3404	0.55	2/4615 (0.0%)
2	S5	0.40	0/3389	0.48	0/4595
2	S7	0.42	0/3448	0.55	1/4675 (0.0%)
2	S9	0.41	0/3389	0.49	0/4595
2	T1	0.43	0/3389	0.50	0/4595
2	T3	0.44	0/3389	0.50	0/4595
2	T5	0.41	0/3389	0.49	0/4595
2	T7	0.41	0/3389	0.50	0/4595
2	U1	0.35	0/3389	0.47	0/4595
2	U3	0.37	0/3389	0.48	0/4595
2	U5	0.36	0/3389	0.48	0/4595
2	U7	0.39	0/3389	0.50	0/4595
2	U9	0.38	0/3389	0.49	0/4595
2	V1	0.38	0/3389	0.50	0/4595
2	V3	0.38	0/3389	0.49	0/4595
2	V7	0.36	0/3389	0.47	0/4595
2	V9	0.37	0/3389	0.48	0/4595
2	W1	0.38	0/3389	0.49	0/4595
2	W3	0.41	0/3389	0.50	0/4595
2	W5	0.39	0/3389	0.49	0/4595
2	W7	0.39	0/3389	0.50	0/4595
2	W9	0.43	0/3389	0.55	0/4595
2	X3	0.33	0/3389	0.49	0/4595
2	X5	0.36	0/3389	0.49	0/4595
2	X7	0.34	0/3389	0.50	1/4595 (0.0%)
2	X9	0.37	0/3389	0.49	0/4595
2	Y1	0.35	0/3389	0.49	1/4595 (0.0%)
2	Y3	0.35	0/3389	0.48	0/4595

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	Y5	0.35	0/3389	0.48	0/4595
2	Y9	0.32	0/3389	0.47	0/4595
2	Z1	0.31	0/3389	0.47	0/4595
2	Z3	0.34	0/3389	0.48	0/4595
2	Z5	0.36	0/3389	0.49	0/4595
2	Z7	0.33	0/3389	0.47	0/4595
2	Z9	0.32	0/3389	0.46	0/4595
3	3V	0.39	0/2383	0.50	0/3226
3	3X	0.38	0/2383	0.49	0/3226
3	3Z	0.38	0/2383	0.49	0/3226
3	4B	0.38	0/2383	0.49	0/3226
3	4D	0.38	0/2383	0.49	0/3226
3	4F	0.39	0/2383	0.49	0/3226
3	4H	0.38	0/2383	0.49	0/3226
3	4J	0.30	0/1682	0.47	0/2279
4	3W	0.41	0/1548	0.48	0/2090
4	3Y	0.41	0/1548	0.48	0/2090
4	4A	0.41	0/1548	0.48	0/2090
4	4C	0.41	0/1548	0.48	0/2090
4	4E	0.41	0/1548	0.48	0/2090
4	4G	0.41	0/1548	0.48	0/2090
4	4I	0.41	0/1548	0.48	0/2090
5	4L	0.34	0/1931	0.46	0/2570
5	4M	0.35	0/2638	0.45	0/3512
6	4N	0.30	0/424	0.46	0/567
6	4O	0.32	0/4020	0.43	0/5336
6	4P	0.35	0/1597	0.40	0/2126
7	4Q	0.35	0/532	0.39	0/706
7	4R	0.39	0/3021	0.47	0/4049
7	4S	0.41	0/374	0.50	0/501
7	4T	0.36	0/1592	0.43	0/2125
7	4U	0.38	1/2314 (0.0%)	0.47	1/3110 (0.0%)
8	4V	0.29	0/656	0.43	0/875
8	4W	0.30	0/2757	0.43	0/3687
8	4X	0.32	0/467	0.51	0/632
9	4Y	0.31	0/1014	0.42	0/1357
9	4Z	0.31	0/3176	0.47	0/4229
10	5A	0.33	0/1912	0.46	0/2536
10	5B	0.31	0/2081	0.44	0/2756
10	5C	0.33	0/3120	0.43	0/4136
10	5D	0.32	0/905	0.42	0/1198
11	5E	0.34	0/2021	0.51	0/2754
12	5F	0.38	0/3116	0.54	3/4267 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
12	5G	0.35	0/1148	0.54	0/1564
12	7B	0.37	0/775	0.55	0/1055
13	5H	0.39	0/1098	0.54	0/1490
13	5I	0.39	0/1098	0.54	0/1490
13	5J	0.39	0/1098	0.54	0/1490
13	5K	0.39	0/1098	0.54	0/1490
14	5L	0.40	0/4851	0.57	0/6582
14	5M	0.40	0/4851	0.57	1/6582 (0.0%)
14	5N	0.40	0/4851	0.59	1/6582 (0.0%)
15	5O	0.43	0/2991	0.62	0/4048
15	5P	0.38	0/2991	0.53	0/4048
16	5Q	0.38	0/1564	0.49	0/2126
17	5R	0.30	0/168	0.44	0/226
17	5S	0.38	0/1612	0.58	0/2177
17	5T	0.40	0/1603	0.56	0/2165
17	5U	0.37	0/1612	0.57	0/2177
17	5V	0.38	0/893	0.49	0/1198
18	5X	0.40	0/1835	0.51	0/2488
18	5Y	0.40	0/1835	0.50	0/2488
18	5Z	0.40	0/1835	0.50	0/2488
18	6A	0.40	0/1835	0.50	0/2488
18	6B	0.40	0/1835	0.50	0/2488
18	6C	0.40	0/1835	0.50	0/2488
18	6D	0.40	0/1835	0.50	0/2488
19	6E	0.42	0/1991	0.57	1/2713 (0.0%)
20	6F	0.44	0/3010	0.54	0/4102
21	6G	0.34	0/1450	0.51	0/1970
21	6H	0.31	0/1527	0.49	0/2078
22	6I	0.31	0/2678	0.46	0/3618
22	6J	0.34	0/2678	0.45	0/3618
22	6K	0.34	0/2678	0.46	0/3618
22	6L	0.37	0/2678	0.45	0/3618
22	6M	0.34	0/2678	0.45	0/3618
22	6N	0.33	0/2678	0.45	0/3618
22	6O	0.35	0/2678	0.46	0/3618
22	6P	0.31	0/2416	0.47	0/3256
23	6Q	0.42	0/710	0.55	0/957
23	6R	0.46	0/710	0.58	0/957
23	6S	0.44	0/710	0.55	0/957
24	6T	0.36	0/4696	0.49	0/6341
24	6U	0.39	0/4730	0.49	0/6389
24	6V	0.38	0/4675	0.51	0/6312
24	6W	0.40	0/4712	0.48	0/6363

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
24	6X	0.42	0/4737	0.53	0/6396
24	6Y	0.38	0/4685	0.50	0/6325
24	6Z	0.38	0/4691	0.49	0/6334
24	7A	0.37	0/1557	0.47	0/2105
25	7C	0.37	0/802	0.50	0/1074
26	7D	0.40	0/1045	0.60	1/1416 (0.1%)
26	7E	0.39	0/1045	0.58	0/1416
26	7F	0.45	0/1045	0.55	0/1416
27	7G	0.37	0/1771	0.48	0/2406
28	7H	0.37	0/1066	0.53	0/1444
28	7X	0.36	0/1066	0.53	0/1444
29	7I	0.35	0/1752	0.48	0/2377
29	7J	0.38	0/2803	0.49	0/3802
30	7K	0.34	0/3351	0.48	0/4541
30	7L	0.32	0/1358	0.46	0/1836
31	7M	0.34	0/678	0.56	1/921 (0.1%)
31	7N	0.35	0/1000	0.59	1/1359 (0.1%)
32	7O	0.33	0/448	0.53	0/603
32	7P	0.36	0/1428	0.49	0/1939
33	7Q	0.37	0/578	0.50	0/783
34	7R	0.28	0/1629	0.42	0/2171
34	7S	0.27	0/1357	0.41	0/1808
35	7T	0.29	0/1748	0.41	0/2324
35	7U	0.29	0/1486	0.40	0/1977
36	7V	0.33	0/745	0.54	0/999
36	7W	0.32	0/745	0.54	0/999
37	7Y	0.39	0/2025	0.56	0/2749
38	7Z	0.38	0/301	0.55	0/401
38	8A	0.40	0/1729	0.55	0/2316
38	8B	0.39	0/1766	0.51	0/2366
38	8C	0.40	0/1766	0.54	0/2366
38	8D	0.42	0/1342	0.57	0/1799
All	All	0.38	3/1377068 (0.0%)	0.48	37/1864119 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T6	60	VAL	CB-CG1	5.93	1.65	1.52
7	4U	113	PRO	N-CD	5.70	1.55	1.47
1	O8	281	TYR	CD2-CE2	-5.05	1.31	1.39

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D1	357	TYR	C-N-CA	-5.94	106.85	121.70
31	7N	78	HIS	CB-CA-C	5.91	122.21	110.40
2	B9	276	ILE	CG1-CB-CG2	-5.89	98.43	111.40
26	7D	128	GLY	N-CA-C	5.88	127.80	113.10
2	S1	283	HIS	CB-CA-C	5.79	121.98	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0A	3346	0	3238	108	0
1	0C	3346	0	3238	102	0
1	0E	3346	0	3240	136	0
1	0G	3346	0	3240	126	0
1	0I	3346	0	3238	117	0
1	0K	3346	0	3238	128	0
1	0M	3346	0	3238	120	0
1	0O	3346	0	3238	138	0
1	0Q	3346	0	3238	110	0
1	0S	3346	0	3238	125	0
1	0U	3346	0	3240	113	0
1	0W	3346	0	3240	113	0
1	0Y	3346	0	3238	97	0
1	1	1120	0	1071	15	0
1	1A	3346	0	3238	90	0
1	1C	3346	0	3238	106	0
1	1E	3346	0	3240	112	0
1	1G	3346	0	3238	106	0
1	1K	3346	0	3240	99	0
1	1M	3346	0	3240	97	0
1	1O	3346	0	3240	94	0
1	1Q	3346	0	3239	100	0
1	1S	3346	0	3238	83	0
1	1U	3346	0	3240	103	0
1	1W	3346	0	3238	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2A	3346	0	3238	108	0
1	2C	3346	0	3238	97	0
1	2E	3346	0	3238	103	0
1	2G	3346	0	3238	77	0
1	2I	3346	0	3238	108	0
1	2K	3346	0	3238	76	0
1	2M	3346	0	3240	109	0
1	2Q	3346	0	3236	157	0
1	2S	3346	0	3238	86	0
1	2U	3346	0	3238	99	0
1	2W	3346	0	3239	76	0
1	2Y	3346	0	3238	121	0
1	3	3397	0	3275	22	0
1	3A	3346	0	3238	113	0
1	3C	3346	0	3238	143	0
1	3G	3346	0	3238	92	0
1	3I	3346	0	3239	95	0
1	3K	3346	0	3239	114	0
1	3M	3346	0	3239	106	0
1	3O	3346	0	3239	103	0
1	3Q	3346	0	3240	106	0
1	3S	3346	0	3239	148	0
1	5	3421	0	3295	32	0
1	7	3430	0	3299	17	0
1	9	3421	0	3295	32	0
1	A1	3388	0	3268	14	0
1	A3	3410	0	3286	65	0
1	A5	3370	0	3259	11	0
1	A7	3346	0	3240	14	0
1	A9	3346	0	3238	9	0
1	B1	3346	0	3240	12	0
1	B3	3346	0	3240	9	0
1	B5	3346	0	3238	12	0
1	B8	3346	0	3240	19	0
1	C0	3346	0	3238	4	0
1	C2	3346	0	3240	9	0
1	C4	3346	0	3240	6	0
1	C6	3346	0	3240	7	0
1	C8	3346	0	3239	6	0
1	D0	3346	0	3240	8	0
1	D2	3346	0	3240	6	0
1	D4	3346	0	3240	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D6	3346	0	3240	10	0
1	D8	3346	0	3240	3	0
1	E0	3346	0	3240	11	0
1	E2	3346	0	3240	16	0
1	E4	3346	0	3238	9	0
1	E6	3346	0	3238	22	0
1	E8	3346	0	3239	12	0
1	F0	3346	0	3238	6	0
1	F2	3346	0	3240	10	0
1	F6	3346	0	3240	12	0
1	F8	3346	0	3238	11	0
1	G0	3346	0	3238	17	0
1	G2	3346	0	3240	123	0
1	G4	3346	0	3238	96	0
1	G6	3346	0	3240	127	0
1	G8	3346	0	3240	118	0
1	H2	3346	0	3238	98	0
1	H4	3346	0	3240	98	0
1	H6	3346	0	3238	99	0
1	H8	3346	0	3238	73	0
1	I0	3346	0	3238	98	0
1	I2	3346	0	3240	106	0
1	I4	3346	0	3237	126	0
1	I8	3346	0	3238	97	0
1	J0	3346	0	3238	89	0
1	J2	3346	0	3238	82	0
1	J4	3346	0	3238	79	0
1	J6	3346	0	3239	82	0
1	J8	3346	0	3239	70	0
1	K0	3346	0	3238	76	0
1	K4	3346	0	3239	83	0
1	K6	3346	0	3239	71	0
1	K8	3346	0	3240	83	0
1	L0	3346	0	3240	76	0
1	L2	3346	0	3238	82	0
1	L4	3346	0	3239	100	0
1	L6	3346	0	3238	110	0
1	M0	3346	0	3239	86	0
1	M2	3346	0	3238	84	0
1	M4	3346	0	3238	85	0
1	M6	3346	0	3238	119	0
1	M8	3346	0	3240	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N0	3346	0	3238	85	0
1	N2	3346	0	3240	104	0
1	N6	3346	0	3239	85	0
1	N8	3346	0	3239	86	0
1	O0	3346	0	3238	73	0
1	O2	3346	0	3239	97	0
1	O4	3346	0	3237	101	0
1	O6	3346	0	3239	76	0
1	O8	3346	0	3239	75	0
1	P4	3346	0	3238	103	0
1	P6	3346	0	3238	69	0
1	P8	3346	0	3239	80	0
1	Q0	3346	0	3240	73	0
1	Q2	3346	0	3238	86	0
1	Q4	3346	0	3238	85	0
1	Q6	3346	0	3239	77	0
1	Q8	3293	0	3182	122	0
1	R0	3401	0	3278	89	0
1	R2	3346	0	3238	97	0
1	R4	3370	0	3257	102	0
1	R6	3346	0	3238	91	0
1	R8	3379	0	3264	89	0
1	S0	3346	0	3239	100	0
1	S2	3379	0	3263	96	0
1	S4	3354	0	3244	144	0
1	S6	3346	0	3240	101	0
1	S8	3346	0	3239	116	0
1	T0	3346	0	3240	107	0
1	T2	3346	0	3239	122	0
1	T4	3346	0	3238	109	0
1	T6	3346	0	3239	157	0
1	T8	3346	0	3239	99	0
1	U2	3346	0	3239	87	0
1	U4	3346	0	3238	83	0
1	U6	3346	0	3238	99	0
1	U8	3370	0	3259	89	0
1	V0	3346	0	3240	80	0
1	V2	3346	0	3238	92	0
1	V4	3346	0	3240	79	0
1	V6	3346	0	3240	135	0
1	V8	3346	0	3238	93	0
1	W0	3346	0	3238	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W2	3346	0	3238	83	0
1	W4	3346	0	3238	93	0
1	W6	3346	0	3240	82	0
1	W8	3346	0	3238	86	0
1	X0	3346	0	3238	120	0
1	X2	3346	0	3240	124	0
1	X4	3346	0	3238	110	0
1	X6	3346	0	3238	105	0
1	X8	3346	0	3240	90	0
1	Y0	3346	0	3239	101	0
1	Y2	3346	0	3240	79	0
1	Y4	3346	0	3239	92	0
1	Y6	3346	0	3239	74	0
1	Y8	3346	0	3240	130	0
1	Z0	3346	0	3238	135	0
1	Z2	3346	0	3239	131	0
1	Z4	3346	0	3240	110	0
1	Z6	3346	0	3238	116	0
1	Z8	3346	0	3240	142	0
2	0B	3318	0	3259	112	0
2	0F	3318	0	3259	123	0
2	0H	3318	0	3259	118	0
2	0J	3318	0	3259	122	0
2	0L	3318	0	3259	129	0
2	0N	3318	0	3259	138	0
2	0P	3318	0	3259	101	0
2	0R	3318	0	3259	125	0
2	0V	3318	0	3259	122	0
2	0X	3318	0	3259	116	0
2	0Z	3318	0	3259	124	0
2	1B	3318	0	3259	96	0
2	1D	3318	0	3259	123	0
2	1F	3318	0	3259	125	0
2	1H	3318	0	3259	123	0
2	1L	3318	0	3259	101	0
2	1N	3318	0	3259	116	0
2	1P	3318	0	3259	93	0
2	1R	3318	0	3259	111	0
2	1T	3318	0	3259	95	0
2	1V	3318	0	3259	114	0
2	1X	3318	0	3259	110	0
2	1Z	3318	0	3259	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	3376	0	3313	19	0
2	2B	3318	0	3259	95	0
2	2D	3318	0	3259	85	0
2	2F	3318	0	3259	106	0
2	2H	3318	0	3259	124	0
2	2J	3318	0	3259	95	0
2	2L	3318	0	3259	96	0
2	2N	3318	0	3259	123	0
2	2P	3318	0	3259	118	0
2	2R	3318	0	3259	85	0
2	2T	3318	0	3259	107	0
2	2V	3318	0	3259	95	0
2	2X	3385	0	3319	112	0
2	2Z	3318	0	3259	130	0
2	3B	3383	0	3314	142	0
2	3D	3318	0	3259	124	0
2	3F	3318	0	3259	95	0
2	3H	3318	0	3259	96	0
2	3J	3318	0	3259	90	0
2	3L	3318	0	3259	82	0
2	3N	3318	0	3259	99	0
2	3P	3318	0	3259	102	0
2	3R	3385	0	3319	110	0
2	3T	3318	0	3259	139	0
2	4	3376	0	3313	32	0
2	6	3376	0	3313	10	0
2	8	3376	0	3312	56	0
2	A0	3376	0	3313	13	0
2	A2	3376	0	3312	69	0
2	A4	3376	0	3313	12	0
2	A8	3318	0	3259	8	0
2	B0	3318	0	3259	8	0
2	B2	3318	0	3259	8	0
2	B4	3318	0	3259	9	0
2	B7	3318	0	3259	10	0
2	B9	3318	0	3259	9	0
2	C1	3318	0	3259	7	0
2	C5	3376	0	3313	14	0
2	C7	3376	0	3313	4	0
2	C9	3318	0	3259	8	0
2	D1	3318	0	3259	6	0
2	D3	3324	0	3264	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D5	3318	0	3259	9	0
2	D7	3324	0	3264	10	0
2	E1	3324	0	3264	9	0
2	E3	3318	0	3259	7	0
2	E5	3318	0	3259	31	0
2	E7	3324	0	3264	26	0
2	E9	3318	0	3259	17	0
2	F1	3318	0	3259	11	0
2	F3	3318	0	3259	11	0
2	F5	3318	0	3259	11	0
2	F7	3318	0	3259	12	0
2	F9	3376	0	3313	12	0
2	G1	3376	0	3313	71	0
2	G3	3376	0	3313	133	0
2	G5	3318	0	3259	107	0
2	G7	3318	0	3259	116	0
2	G9	3318	0	3259	149	0
2	H1	3318	0	3259	117	0
2	H3	3318	0	3259	107	0
2	H5	3318	0	3259	86	0
2	H7	3318	0	3259	85	0
2	H9	3318	0	3259	83	0
2	I1	3318	0	3259	104	0
2	I3	3318	0	3259	96	0
2	I5	3318	0	3259	135	0
2	I7	3332	0	3268	106	0
2	I9	3324	0	3264	110	0
2	J1	3318	0	3259	108	0
2	J3	3326	0	3263	103	0
2	J5	3385	0	3319	101	0
2	J7	3318	0	3259	128	0
2	J9	3385	0	3319	127	0
2	K1	3318	0	3259	135	0
2	K3	3318	0	3259	106	0
2	K5	3318	0	3259	85	0
2	K7	3318	0	3259	86	0
2	K9	3318	0	3259	89	0
2	L1	3318	0	3259	72	0
2	L3	3318	0	3259	115	0
2	L5	3318	0	3259	99	0
2	L7	3318	0	3259	124	0
2	L9	3318	0	3259	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M1	3318	0	3259	86	0
2	M3	3376	0	3313	129	0
2	M5	3318	0	3259	110	0
2	M7	3376	0	3313	106	0
2	M9	3385	0	3319	115	0
2	N1	3324	0	3264	106	0
2	N3	3318	0	3259	128	0
2	N5	3318	0	3259	96	0
2	N7	3318	0	3259	105	0
2	N9	3318	0	3259	105	0
2	O1	3318	0	3259	92	0
2	O3	3318	0	3259	125	0
2	O5	3318	0	3259	108	0
2	O7	3340	0	3274	122	0
2	O9	3318	0	3259	78	0
2	P3	3318	0	3259	95	0
2	P5	3376	0	3313	112	0
2	P7	3318	0	3259	82	0
2	P9	3376	0	3313	92	0
2	Q1	3318	0	3259	70	0
2	Q3	3318	0	3259	96	0
2	Q5	3318	0	3259	94	0
2	Q9	3318	0	3259	111	0
2	R1	3318	0	3259	95	0
2	R3	3327	0	3265	83	0
2	R5	3376	0	3313	100	0
2	R7	3318	0	3259	81	0
2	R9	3376	0	3313	102	0
2	S1	3333	0	3270	98	0
2	S5	3318	0	3259	86	0
2	S7	3376	0	3313	105	0
2	S9	3318	0	3259	110	0
2	T1	3318	0	3259	107	0
2	T3	3318	0	3259	94	0
2	T5	3318	0	3259	100	0
2	T7	3318	0	3259	98	0
2	U1	3318	0	3259	83	0
2	U3	3318	0	3259	72	0
2	U5	3318	0	3259	89	0
2	U7	3318	0	3259	83	0
2	U9	3318	0	3259	113	0
2	V1	3318	0	3259	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V3	3318	0	3259	94	0
2	V7	3318	0	3259	102	0
2	V9	3318	0	3259	85	0
2	W1	3318	0	3259	98	0
2	W3	3318	0	3259	80	0
2	W5	3318	0	3259	76	0
2	W7	3318	0	3259	118	0
2	W9	3318	0	3259	150	0
2	X3	3318	0	3259	124	0
2	X5	3318	0	3259	115	0
2	X7	3318	0	3259	121	0
2	X9	3318	0	3259	98	0
2	Y1	3318	0	3259	95	0
2	Y3	3318	0	3259	116	0
2	Y5	3318	0	3259	102	0
2	Y9	3318	0	3259	118	0
2	Z1	3318	0	3259	105	0
2	Z3	3318	0	3259	119	0
2	Z5	3318	0	3259	128	0
2	Z7	3318	0	3259	116	0
2	Z9	3318	0	3259	108	0
3	3V	2329	0	2356	83	0
3	3X	2329	0	2356	90	0
3	3Z	2329	0	2356	79	0
3	4B	2329	0	2356	76	0
3	4D	2329	0	2356	84	0
3	4F	2329	0	2356	86	0
3	4H	2329	0	2356	84	0
3	4J	1643	0	1662	50	0
4	3W	1515	0	1526	49	0
4	3Y	1515	0	1526	46	0
4	4A	1515	0	1526	43	0
4	4C	1515	0	1526	47	0
4	4E	1515	0	1526	42	0
4	4G	1515	0	1526	51	0
4	4I	1515	0	1526	43	0
5	4L	1921	0	1936	75	0
5	4M	2622	0	2653	110	0
6	4N	422	0	422	13	0
6	4O	3995	0	3956	111	0
6	4P	1588	0	1574	37	0
7	4Q	525	0	521	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	4R	2982	0	2914	102	0
7	4S	371	0	380	20	0
7	4T	1574	0	1556	42	0
7	4U	2285	0	2221	66	0
8	4V	653	0	667	19	0
8	4W	2750	0	2805	116	0
8	4X	462	0	459	48	0
9	4Y	1004	0	1032	28	0
9	4Z	3158	0	3201	130	0
10	5A	1902	0	1930	65	0
10	5B	2074	0	2132	82	0
10	5C	3103	0	3156	110	0
10	5D	901	0	914	26	0
11	5E	1981	0	1969	58	0
12	5F	3020	0	2948	105	0
12	5G	1123	0	1132	34	0
12	7B	753	0	735	41	0
13	5H	1069	0	1048	45	0
13	5I	1069	0	1048	49	0
13	5J	1069	0	1048	44	0
13	5K	1069	0	1048	50	0
14	5L	4757	0	4692	251	0
14	5M	4757	0	4691	242	0
14	5N	4757	0	4692	244	0
15	5O	2927	0	2895	247	0
15	5P	2927	0	2895	188	0
16	5Q	1523	0	1453	78	0
17	5R	162	0	149	8	0
17	5S	1572	0	1577	63	0
17	5T	1563	0	1571	66	0
17	5U	1572	0	1577	62	0
17	5V	879	0	901	39	0
18	5X	1793	0	1800	78	0
18	5Y	1793	0	1800	72	0
18	5Z	1793	0	1800	66	0
18	6A	1793	0	1800	74	0
18	6B	1793	0	1800	72	0
18	6C	1793	0	1800	75	0
18	6D	1793	0	1800	66	0
19	6E	1952	0	1910	117	0
20	6F	2950	0	2946	111	0
21	6G	1420	0	1394	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	6H	1493	0	1466	64	0
22	6I	2617	0	2556	66	0
22	6J	2617	0	2556	70	0
22	6K	2617	0	2556	80	0
22	6L	2617	0	2556	98	0
22	6M	2617	0	2556	81	0
22	6N	2617	0	2556	79	0
22	6O	2617	0	2556	78	0
22	6P	2366	0	2311	84	0
23	6Q	694	0	690	30	0
23	6R	694	0	690	41	0
23	6S	694	0	690	27	0
24	6T	4590	0	4521	203	0
24	6U	4623	0	4558	209	0
24	6V	4569	0	4501	195	0
24	6W	4606	0	4538	187	0
24	6X	4631	0	4566	291	0
24	6Y	4579	0	4515	206	0
24	6Z	4585	0	4516	200	0
24	7A	1518	0	1462	61	0
25	7C	794	0	816	30	0
26	7D	1016	0	993	80	0
26	7E	1016	0	993	82	0
26	7F	1016	0	994	133	0
27	7G	1728	0	1670	91	0
28	7H	1046	0	1046	53	0
28	7X	1046	0	1046	64	0
29	7I	1716	0	1685	72	0
29	7J	2741	0	2638	165	0
30	7K	3276	0	3173	165	0
30	7L	1333	0	1289	36	0
31	7M	662	0	657	40	0
31	7N	977	0	965	54	0
32	7O	443	0	425	22	0
32	7P	1398	0	1368	40	0
33	7Q	567	0	551	27	0
34	7R	1619	0	1650	45	0
34	7S	1347	0	1357	33	0
35	7T	1738	0	1787	53	0
35	7U	1476	0	1506	34	0
36	7V	735	0	696	33	0
36	7W	735	0	696	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	7Y	1971	0	1898	143	0
38	7Z	298	0	291	35	0
38	8A	1691	0	1638	195	0
38	8B	1728	0	1666	168	0
38	8C	1728	0	1666	193	0
38	8D	1311	0	1252	139	0
39	0A	28	0	12	1	0
39	0C	28	0	12	2	0
39	0E	28	0	12	3	0
39	0G	28	0	12	2	0
39	0I	28	0	12	1	0
39	0K	28	0	12	1	0
39	0M	28	0	12	1	0
39	0O	28	0	12	1	0
39	0Q	28	0	12	1	0
39	0S	28	0	12	2	0
39	0U	28	0	12	1	0
39	0W	28	0	12	2	0
39	0Y	28	0	12	1	0
39	1A	28	0	12	2	0
39	1C	28	0	12	1	0
39	1E	28	0	12	0	0
39	1G	28	0	12	0	0
39	1K	28	0	12	1	0
39	1M	28	0	12	1	0
39	1O	28	0	12	1	0
39	1Q	28	0	12	1	0
39	1S	28	0	12	1	0
39	1U	28	0	12	0	0
39	1W	28	0	12	2	0
39	2	28	0	12	0	0
39	2A	28	0	12	0	0
39	2C	28	0	12	1	0
39	2E	28	0	12	1	0
39	2G	28	0	12	3	0
39	2I	28	0	12	0	0
39	2K	28	0	12	2	0
39	2M	28	0	12	2	0
39	2Q	28	0	12	0	0
39	2S	28	0	12	0	0
39	2U	28	0	12	0	0
39	2W	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	2Y	28	0	12	0	0
39	3	28	0	12	2	0
39	3A	28	0	12	1	0
39	3C	28	0	12	1	0
39	3G	28	0	12	0	0
39	3I	28	0	12	1	0
39	3K	28	0	12	1	0
39	3M	28	0	12	0	0
39	3O	28	0	12	1	0
39	3Q	28	0	12	1	0
39	3S	28	0	12	1	0
39	5	28	0	12	1	0
39	7	28	0	12	3	0
39	9	28	0	12	1	0
39	A1	28	0	12	0	0
39	A3	28	0	12	0	0
39	A5	28	0	12	1	0
39	A7	28	0	12	2	0
39	A9	28	0	12	0	0
39	B1	28	0	12	1	0
39	B3	28	0	12	1	0
39	B5	28	0	12	0	0
39	B8	28	0	12	2	0
39	C0	28	0	12	0	0
39	C2	28	0	12	0	0
39	C4	28	0	12	3	0
39	C6	28	0	12	3	0
39	C8	28	0	12	3	0
39	D0	28	0	12	5	0
39	D2	28	0	12	2	0
39	D4	28	0	12	3	0
39	D6	28	0	12	3	0
39	D8	28	0	12	1	0
39	E0	28	0	12	4	0
39	E2	28	0	12	2	0
39	E4	28	0	12	0	0
39	E6	28	0	12	1	0
39	E8	28	0	12	1	0
39	F0	28	0	12	2	0
39	F2	28	0	12	3	0
39	F6	28	0	12	0	0
39	F8	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	G0	28	0	12	0	0
39	G2	28	0	12	0	0
39	G4	28	0	12	1	0
39	G6	28	0	12	0	0
39	G8	28	0	12	1	0
39	H2	28	0	12	1	0
39	H4	28	0	12	1	0
39	H6	28	0	12	1	0
39	H8	28	0	12	0	0
39	I0	28	0	12	0	0
39	I2	28	0	12	0	0
39	I4	28	0	12	0	0
39	I8	28	0	12	0	0
39	J0	28	0	12	0	0
39	J2	28	0	12	1	0
39	J4	28	0	12	0	0
39	J6	28	0	12	1	0
39	J8	28	0	12	1	0
39	K0	28	0	12	0	0
39	K4	28	0	12	1	0
39	K6	28	0	12	0	0
39	K8	28	0	12	0	0
39	L0	28	0	12	0	0
39	L2	28	0	12	1	0
39	L4	28	0	12	2	0
39	L6	28	0	12	1	0
39	M0	28	0	12	0	0
39	M2	28	0	12	0	0
39	M4	28	0	12	0	0
39	M6	28	0	12	0	0
39	M8	28	0	12	0	0
39	N0	28	0	12	0	0
39	N2	28	0	12	1	0
39	N6	28	0	12	2	0
39	N8	28	0	12	3	0
39	O0	28	0	12	0	0
39	O2	28	0	12	2	0
39	O4	28	0	12	0	0
39	O6	28	0	12	1	0
39	O8	28	0	12	1	0
39	P4	28	0	12	1	0
39	P6	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	P8	28	0	12	2	0
39	Q0	28	0	12	0	0
39	Q2	28	0	12	1	0
39	Q4	28	0	12	1	0
39	Q6	28	0	12	2	0
39	Q8	28	0	12	0	0
39	R0	28	0	12	0	0
39	R2	28	0	12	0	0
39	R4	28	0	12	1	0
39	R6	28	0	12	1	0
39	R8	28	0	12	0	0
39	S0	28	0	12	0	0
39	S2	28	0	12	1	0
39	S4	28	0	12	1	0
39	S6	28	0	12	0	0
39	S8	28	0	12	1	0
39	T0	28	0	12	2	0
39	T2	28	0	12	0	0
39	T4	28	0	12	0	0
39	T6	28	0	12	3	0
39	T8	28	0	12	0	0
39	U2	28	0	12	1	0
39	U4	28	0	12	0	0
39	U6	28	0	12	0	0
39	U8	28	0	12	0	0
39	V0	28	0	12	0	0
39	V2	28	0	12	0	0
39	V4	28	0	12	1	0
39	V6	28	0	12	1	0
39	V8	28	0	12	1	0
39	W0	28	0	12	2	0
39	W2	28	0	12	1	0
39	W4	28	0	12	0	0
39	W6	28	0	12	0	0
39	W8	28	0	12	2	0
39	X0	28	0	12	2	0
39	X2	28	0	12	3	0
39	X4	28	0	12	2	0
39	X6	28	0	12	3	0
39	X8	28	0	12	1	0
39	Y0	28	0	12	2	0
39	Y2	28	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Y4	28	0	12	3	0
39	Y6	28	0	12	2	0
39	Y8	28	0	12	2	0
39	Z0	28	0	12	2	0
39	Z2	28	0	12	3	0
39	Z4	28	0	12	1	0
39	Z6	28	0	12	2	0
39	Z8	28	0	12	3	0
40	0A	1	0	0	0	0
40	0B	1	0	0	0	0
40	0F	1	0	0	0	0
40	0H	1	0	0	0	0
40	0J	1	0	0	0	0
40	0L	1	0	0	0	0
40	0N	1	0	0	0	0
40	0P	1	0	0	0	0
40	0R	1	0	0	0	0
40	0W	1	0	0	0	0
40	0X	1	0	0	0	0
40	1A	1	0	0	0	0
40	1B	1	0	0	0	0
40	1D	1	0	0	0	0
40	1F	1	0	0	0	0
40	1H	1	0	0	0	0
40	1L	1	0	0	0	0
40	1N	1	0	0	0	0
40	1P	1	0	0	0	0
40	1R	1	0	0	0	0
40	1T	1	0	0	0	0
40	1V	1	0	0	0	0
40	1X	1	0	0	0	0
40	1Z	1	0	0	0	0
40	2	1	0	0	0	0
40	2B	1	0	0	0	0
40	2D	1	0	0	0	0
40	2F	1	0	0	0	0
40	2H	1	0	0	0	0
40	2J	1	0	0	0	0
40	2L	1	0	0	0	0
40	2N	1	0	0	0	0
40	2P	1	0	0	0	0
40	2R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2T	1	0	0	0	0
40	2V	1	0	0	0	0
40	2X	1	0	0	0	0
40	2Z	1	0	0	0	0
40	3B	1	0	0	0	0
40	3D	1	0	0	0	0
40	3F	1	0	0	0	0
40	3H	1	0	0	0	0
40	3K	1	0	0	0	0
40	3L	1	0	0	0	0
40	3N	1	0	0	0	0
40	3P	1	0	0	0	0
40	3R	1	0	0	0	0
40	3T	1	0	0	0	0
40	4	1	0	0	0	0
40	6	1	0	0	0	0
40	8	1	0	0	0	0
40	A0	1	0	0	0	0
40	A2	1	0	0	0	0
40	A4	1	0	0	0	0
40	A8	1	0	0	0	0
40	B0	1	0	0	0	0
40	B2	1	0	0	0	0
40	B4	1	0	0	0	0
40	B7	1	0	0	0	0
40	B9	1	0	0	0	0
40	C1	1	0	0	0	0
40	C5	1	0	0	0	0
40	C7	1	0	0	0	0
40	C9	1	0	0	0	0
40	D1	1	0	0	0	0
40	D3	1	0	0	0	0
40	D5	1	0	0	0	0
40	D7	1	0	0	0	0
40	E1	1	0	0	0	0
40	E3	1	0	0	0	0
40	E5	1	0	0	0	0
40	E7	1	0	0	0	0
40	E9	1	0	0	0	0
40	F1	1	0	0	0	0
40	F3	1	0	0	0	0
40	F5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	F7	1	0	0	0	0
40	F9	1	0	0	0	0
40	G1	1	0	0	0	0
40	G3	1	0	0	0	0
40	G5	1	0	0	0	0
40	G7	1	0	0	0	0
40	G9	1	0	0	0	0
40	H2	1	0	0	0	0
40	H3	1	0	0	0	0
40	H5	1	0	0	0	0
40	H8	1	0	0	0	0
40	H9	1	0	0	0	0
40	I1	1	0	0	0	0
40	I3	1	0	0	0	0
40	I5	1	0	0	0	0
40	I7	1	0	0	0	0
40	I9	1	0	0	0	0
40	J1	1	0	0	0	0
40	J4	1	0	0	0	0
40	J5	1	0	0	0	0
40	J7	1	0	0	0	0
40	J9	1	0	0	0	0
40	K1	1	0	0	0	0
40	K3	1	0	0	0	0
40	K5	1	0	0	0	0
40	K7	1	0	0	0	0
40	K9	1	0	0	0	0
40	L1	1	0	0	0	0
40	L3	1	0	0	0	0
40	L5	1	0	0	0	0
40	L7	1	0	0	0	0
40	L9	1	0	0	0	0
40	M1	1	0	0	0	0
40	M3	1	0	0	0	0
40	M5	1	0	0	0	0
40	M7	1	0	0	0	0
40	M9	1	0	0	0	0
40	N1	1	0	0	0	0
40	N3	1	0	0	0	0
40	N6	1	0	0	0	0
40	N7	1	0	0	0	0
40	O0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	O1	1	0	0	0	0
40	O3	1	0	0	0	0
40	O5	1	0	0	0	0
40	O8	1	0	0	0	0
40	O9	1	0	0	0	0
40	P4	1	0	0	0	0
40	P6	1	0	0	0	0
40	P7	1	0	0	0	0
40	P9	1	0	0	0	0
40	Q1	1	0	0	0	0
40	Q3	1	0	0	0	0
40	Q5	1	0	0	0	0
40	Q9	1	0	0	0	0
40	R1	1	0	0	0	0
40	R3	1	0	0	0	0
40	R6	1	0	0	0	0
40	R7	1	0	0	0	0
40	R9	1	0	0	0	0
40	S1	1	0	0	0	0
40	S5	1	0	0	0	0
40	S7	1	0	0	0	0
40	S9	1	0	0	0	0
40	T1	1	0	0	0	0
40	T3	1	0	0	0	0
40	T5	1	0	0	0	0
40	T7	1	0	0	0	0
40	U1	1	0	0	0	0
40	U3	1	0	0	0	0
40	U5	1	0	0	0	0
40	U7	1	0	0	0	0
40	U9	1	0	0	0	0
40	V2	1	0	0	0	0
40	V3	1	0	0	0	0
40	V7	1	0	0	0	0
40	V9	1	0	0	0	0
40	W2	1	0	0	0	0
40	W3	1	0	0	0	0
40	W5	1	0	0	0	0
40	W8	1	0	0	0	0
40	W9	1	0	0	0	0
40	X3	1	0	0	0	0
40	X5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	X7	1	0	0	0	0
40	X9	1	0	0	0	0
40	Y1	1	0	0	0	0
40	Y3	1	0	0	0	0
40	Y5	1	0	0	0	0
40	Y9	1	0	0	0	0
40	Z2	1	0	0	0	0
40	Z3	1	0	0	0	0
40	Z5	1	0	0	0	0
40	Z7	1	0	0	0	0
41	0A	32	0	12	2	0
41	0C	32	0	12	3	0
41	0F	32	0	12	3	0
41	0I	32	0	12	3	0
41	0K	32	0	12	2	0
41	0M	32	0	12	3	0
41	0O	32	0	12	2	0
41	0Q	32	0	12	3	0
41	0S	32	0	12	2	0
41	0V	32	0	12	1	0
41	0Y	32	0	12	1	0
41	1A	32	0	12	1	0
41	1C	32	0	12	1	0
41	1D	32	0	12	1	0
41	1G	32	0	12	1	0
41	1H	32	0	12	2	0
41	1L	32	0	12	1	0
41	1N	32	0	12	1	0
41	1Q	32	0	12	1	0
41	1S	32	0	12	1	0
41	1T	32	0	12	1	0
41	1W	32	0	12	1	0
41	1X	32	0	12	1	0
41	2A	32	0	12	0	0
41	2C	32	0	12	2	0
41	2E	32	0	12	2	0
41	2G	32	0	12	2	0
41	2I	32	0	12	1	0
41	2K	32	0	12	0	0
41	2L	32	0	12	1	0
41	2N	32	0	12	1	0
41	2Q	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	2S	32	0	12	0	0
41	2U	32	0	12	1	0
41	2W	32	0	12	1	0
41	2Y	32	0	12	0	0
41	3	32	0	12	1	0
41	3A	32	0	12	0	0
41	3C	32	0	12	0	0
41	3D	32	0	12	2	0
41	3G	32	0	12	0	0
41	3I	32	0	12	0	0
41	3K	32	0	12	0	0
41	3M	32	0	12	1	0
41	3O	32	0	12	1	0
41	3P	32	0	12	0	0
41	3S	32	0	12	0	0
41	3T	32	0	12	0	0
41	4	32	0	12	1	0
41	7	32	0	12	0	0
41	8	32	0	12	1	0
41	A1	32	0	12	2	0
41	A2	32	0	12	1	0
41	A4	32	0	12	2	0
41	A9	32	0	12	1	0
41	B0	32	0	12	2	0
41	B2	32	0	12	0	0
41	B5	32	0	12	2	0
41	B7	32	0	12	1	0
41	C0	32	0	12	2	0
41	C1	32	0	12	2	0
41	C5	32	0	12	2	0
41	C8	32	0	12	1	0
41	C9	32	0	12	5	0
41	D1	32	0	12	1	0
41	D3	32	0	12	2	0
41	D5	32	0	12	1	0
41	D7	32	0	12	2	0
41	E1	32	0	12	3	0
41	E4	32	0	12	1	0
41	E6	32	0	12	2	0
41	E8	32	0	12	3	0
41	F0	32	0	12	2	0
41	F1	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	F3	32	0	12	2	0
41	F5	32	0	12	2	0
41	F8	32	0	12	1	0
41	G0	32	0	12	3	0
41	G1	32	0	12	2	0
41	G4	32	0	12	2	0
41	G5	32	0	12	3	0
41	G7	32	0	12	2	0
41	G9	32	0	12	1	0
41	H2	32	0	12	1	0
41	H3	32	0	12	1	0
41	H6	32	0	12	1	0
41	H8	32	0	12	1	0
41	I0	32	0	12	1	0
41	I1	32	0	12	1	0
41	I4	32	0	12	2	0
41	I5	32	0	12	0	0
41	I8	32	0	12	1	0
41	J0	32	0	12	1	0
41	J2	32	0	12	1	0
41	J4	32	0	12	1	0
41	J6	32	0	12	1	0
41	J8	32	0	12	1	0
41	K0	32	0	12	2	0
41	K1	32	0	12	0	0
41	K4	32	0	12	2	0
41	K6	32	0	12	3	0
41	K7	32	0	12	2	0
41	K9	32	0	12	2	0
41	L2	32	0	12	2	0
41	L4	32	0	12	3	0
41	L6	32	0	12	1	0
41	L7	32	0	12	0	0
41	M0	32	0	12	0	0
41	M2	32	0	12	0	0
41	M4	32	0	12	0	0
41	M6	32	0	12	0	0
41	M7	32	0	12	1	0
41	N0	32	0	12	1	0
41	N1	32	0	12	0	0
41	N3	32	0	12	0	0
41	N6	32	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	N8	32	0	12	2	0
41	O0	32	0	12	1	0
41	O2	32	0	12	0	0
41	O4	32	0	12	2	0
41	O6	32	0	12	1	0
41	O8	32	0	12	1	0
41	O9	32	0	12	1	0
41	P4	32	0	12	3	0
41	P6	32	0	12	2	0
41	P8	32	0	12	2	0
41	P9	32	0	12	2	0
41	Q2	32	0	12	1	0
41	Q4	32	0	12	1	0
41	Q6	32	0	12	1	0
41	R0	32	0	12	1	0
41	R2	32	0	12	1	0
41	R4	32	0	12	0	0
41	R6	32	0	12	1	0
41	R8	32	0	12	0	0
41	S0	32	0	12	1	0
41	S2	32	0	12	1	0
41	S5	32	0	12	0	0
41	S8	32	0	12	1	0
41	S9	32	0	12	2	0
41	T2	32	0	12	2	0
41	T4	32	0	12	3	0
41	T6	32	0	12	3	0
41	T8	32	0	12	2	0
41	U2	32	0	12	0	0
41	U4	32	0	12	1	0
41	U6	32	0	12	1	0
41	U7	32	0	12	0	0
41	U9	32	0	12	0	0
41	V2	32	0	12	0	0
41	V3	32	0	12	0	0
41	V8	32	0	12	0	0
41	W0	32	0	12	0	0
41	W2	32	0	12	0	0
41	W4	32	0	12	0	0
41	W5	32	0	12	1	0
41	W8	32	0	12	0	0
41	X0	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	X4	32	0	12	3	0
41	X6	32	0	12	3	0
41	X7	32	0	12	2	0
41	Y0	32	0	12	3	0
41	Y1	32	0	12	2	0
41	Y4	32	0	12	2	0
41	Y6	32	0	12	2	0
41	Z0	32	0	12	1	0
41	Z2	32	0	12	2	0
41	Z3	32	0	12	2	0
41	Z6	32	0	12	2	0
41	Z7	32	0	12	2	0
All	All	1358547	0	1321887	33426	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 12.

The worst 5 of 33426 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)
1:3S:362:LYS:CE	38:8D:166:GLU:HG3	1.25	1.64
2:E5:282:TYR:CZ	22:6K:82:LEU:HD23	1.38	1.57
24:6X:451:LYS:CD	24:6X:468:ARG:HH12	1.02	1.56
2:S1:88:HIS:CD2	2:S1:89:PRO:HD2	1.42	1.51
2:E5:282:TYR:CE1	22:6K:82:LEU:CD2	1.93	1.49

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0A	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	0C	367/379 (97%)	367 (100%)	0	100	100
1	0E	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	0G	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	0I	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	0K	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	0M	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	0O	367/379 (97%)	367 (100%)	0	100	100
1	0Q	367/379 (97%)	367 (100%)	0	100	100
1	0S	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	0U	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	0W	367/379 (97%)	367 (100%)	0	100	100
1	0Y	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	1	122/379 (32%)	118 (97%)	4 (3%)	33	58
1	1A	367/379 (97%)	367 (100%)	0	100	100
1	1C	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	1E	367/379 (97%)	367 (100%)	0	100	100
1	1G	367/379 (97%)	367 (100%)	0	100	100
1	1K	367/379 (97%)	367 (100%)	0	100	100
1	1M	367/379 (97%)	364 (99%)	3 (1%)	79	87
1	1O	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	1Q	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	1S	367/379 (97%)	367 (100%)	0	100	100
1	1U	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	1W	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	2A	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	2C	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	2E	367/379 (97%)	367 (100%)	0	100	100
1	2G	367/379 (97%)	367 (100%)	0	100	100
1	2I	367/379 (97%)	367 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2K	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	2M	367/379 (97%)	367 (100%)	0	100	100
1	2Q	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	2S	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	2U	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	2W	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	2Y	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	3	372/379 (98%)	370 (100%)	2 (0%)	86	91
1	3A	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	3C	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	3G	367/379 (97%)	367 (100%)	0	100	100
1	3I	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	3K	367/379 (97%)	367 (100%)	0	100	100
1	3M	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	3O	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	3Q	367/379 (97%)	367 (100%)	0	100	100
1	3S	367/379 (97%)	367 (100%)	0	100	100
1	5	374/379 (99%)	372 (100%)	2 (0%)	86	91
1	7	375/379 (99%)	373 (100%)	2 (0%)	86	91
1	9	374/379 (99%)	373 (100%)	1 (0%)	91	95
1	A1	371/379 (98%)	370 (100%)	1 (0%)	91	95
1	A3	373/379 (98%)	372 (100%)	1 (0%)	91	95
1	A5	369/379 (97%)	369 (100%)	0	100	100
1	A7	367/379 (97%)	367 (100%)	0	100	100
1	A9	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	B1	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	B3	367/379 (97%)	367 (100%)	0	100	100
1	B5	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	B8	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	C0	367/379 (97%)	367 (100%)	0	100	100
1	C2	367/379 (97%)	366 (100%)	1 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C4	367/379 (97%)	367 (100%)	0	100	100
1	C6	367/379 (97%)	367 (100%)	0	100	100
1	C8	367/379 (97%)	367 (100%)	0	100	100
1	D0	367/379 (97%)	367 (100%)	0	100	100
1	D2	367/379 (97%)	367 (100%)	0	100	100
1	D4	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	D6	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	D8	367/379 (97%)	367 (100%)	0	100	100
1	E0	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	E2	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	E4	367/379 (97%)	367 (100%)	0	100	100
1	E6	367/379 (97%)	367 (100%)	0	100	100
1	E8	367/379 (97%)	367 (100%)	0	100	100
1	F0	367/379 (97%)	367 (100%)	0	100	100
1	F2	367/379 (97%)	367 (100%)	0	100	100
1	F6	367/379 (97%)	367 (100%)	0	100	100
1	F8	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	G0	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	G2	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	G4	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	G6	367/379 (97%)	367 (100%)	0	100	100
1	G8	367/379 (97%)	367 (100%)	0	100	100
1	H2	367/379 (97%)	367 (100%)	0	100	100
1	H4	367/379 (97%)	367 (100%)	0	100	100
1	H6	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	H8	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	I0	367/379 (97%)	367 (100%)	0	100	100
1	I2	367/379 (97%)	367 (100%)	0	100	100
1	I4	367/379 (97%)	367 (100%)	0	100	100
1	I8	367/379 (97%)	367 (100%)	0	100	100
1	J0	367/379 (97%)	367 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J2	367/379 (97%)	367 (100%)	0	100	100
1	J4	367/379 (97%)	367 (100%)	0	100	100
1	J6	367/379 (97%)	367 (100%)	0	100	100
1	J8	367/379 (97%)	367 (100%)	0	100	100
1	K0	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	K4	367/379 (97%)	367 (100%)	0	100	100
1	K6	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	K8	367/379 (97%)	367 (100%)	0	100	100
1	L0	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	L2	367/379 (97%)	367 (100%)	0	100	100
1	L4	367/379 (97%)	367 (100%)	0	100	100
1	L6	367/379 (97%)	367 (100%)	0	100	100
1	M0	367/379 (97%)	367 (100%)	0	100	100
1	M2	367/379 (97%)	367 (100%)	0	100	100
1	M4	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	M6	367/379 (97%)	367 (100%)	0	100	100
1	M8	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	N0	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	N2	367/379 (97%)	367 (100%)	0	100	100
1	N6	367/379 (97%)	367 (100%)	0	100	100
1	N8	367/379 (97%)	367 (100%)	0	100	100
1	O0	367/379 (97%)	367 (100%)	0	100	100
1	O2	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	O4	367/379 (97%)	367 (100%)	0	100	100
1	O6	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	O8	367/379 (97%)	367 (100%)	0	100	100
1	P4	367/379 (97%)	367 (100%)	0	100	100
1	P6	367/379 (97%)	367 (100%)	0	100	100
1	P8	367/379 (97%)	367 (100%)	0	100	100
1	Q0	367/379 (97%)	367 (100%)	0	100	100
1	Q2	367/379 (97%)	366 (100%)	1 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q4	367/379 (97%)	367 (100%)	0	100	100
1	Q6	367/379 (97%)	367 (100%)	0	100	100
1	Q8	361/379 (95%)	359 (99%)	2 (1%)	84	90
1	R0	372/379 (98%)	372 (100%)	0	100	100
1	R2	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	R4	369/379 (97%)	368 (100%)	1 (0%)	91	95
1	R6	367/379 (97%)	367 (100%)	0	100	100
1	R8	370/379 (98%)	370 (100%)	0	100	100
1	S0	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	S2	370/379 (98%)	370 (100%)	0	100	100
1	S4	368/379 (97%)	368 (100%)	0	100	100
1	S6	367/379 (97%)	367 (100%)	0	100	100
1	S8	367/379 (97%)	367 (100%)	0	100	100
1	T0	367/379 (97%)	367 (100%)	0	100	100
1	T2	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	T4	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	T6	367/379 (97%)	364 (99%)	3 (1%)	79	87
1	T8	367/379 (97%)	367 (100%)	0	100	100
1	U2	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	U4	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	U6	367/379 (97%)	367 (100%)	0	100	100
1	U8	369/379 (97%)	367 (100%)	2 (0%)	86	91
1	V0	367/379 (97%)	367 (100%)	0	100	100
1	V2	367/379 (97%)	364 (99%)	3 (1%)	79	87
1	V4	367/379 (97%)	367 (100%)	0	100	100
1	V6	367/379 (97%)	367 (100%)	0	100	100
1	V8	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	W0	367/379 (97%)	367 (100%)	0	100	100
1	W2	367/379 (97%)	367 (100%)	0	100	100
1	W4	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	W6	367/379 (97%)	367 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W8	367/379 (97%)	364 (99%)	3 (1%)	79	87
1	X0	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	X2	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	X4	367/379 (97%)	367 (100%)	0	100	100
1	X6	367/379 (97%)	367 (100%)	0	100	100
1	X8	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	Y0	367/379 (97%)	367 (100%)	0	100	100
1	Y2	367/379 (97%)	367 (100%)	0	100	100
1	Y4	367/379 (97%)	367 (100%)	0	100	100
1	Y6	367/379 (97%)	365 (100%)	2 (0%)	86	91
1	Y8	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	Z0	367/379 (97%)	367 (100%)	0	100	100
1	Z2	367/379 (97%)	367 (100%)	0	100	100
1	Z4	367/379 (97%)	367 (100%)	0	100	100
1	Z6	367/379 (97%)	366 (100%)	1 (0%)	91	95
1	Z8	367/379 (97%)	367 (100%)	0	100	100
2	0B	359/374 (96%)	359 (100%)	0	100	100
2	0F	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	0H	359/374 (96%)	359 (100%)	0	100	100
2	0J	359/374 (96%)	359 (100%)	0	100	100
2	0L	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	0N	359/374 (96%)	356 (99%)	3 (1%)	79	87
2	0P	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	0R	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	0V	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	0X	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	0Z	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	1B	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	1D	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	1F	359/374 (96%)	359 (100%)	0	100	100
2	1H	359/374 (96%)	356 (99%)	3 (1%)	79	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1L	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	1N	359/374 (96%)	356 (99%)	3 (1%)	79	87
2	1P	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	1R	359/374 (96%)	351 (98%)	8 (2%)	47	68
2	1T	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	1V	359/374 (96%)	355 (99%)	4 (1%)	70	81
2	1X	359/374 (96%)	359 (100%)	0	100	100
2	1Z	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	2	365/374 (98%)	365 (100%)	0	100	100
2	2B	359/374 (96%)	359 (100%)	0	100	100
2	2D	359/374 (96%)	359 (100%)	0	100	100
2	2F	359/374 (96%)	359 (100%)	0	100	100
2	2H	359/374 (96%)	359 (100%)	0	100	100
2	2J	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	2L	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	2N	359/374 (96%)	359 (100%)	0	100	100
2	2P	359/374 (96%)	356 (99%)	3 (1%)	79	87
2	2R	359/374 (96%)	359 (100%)	0	100	100
2	2T	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	2V	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	2X	366/374 (98%)	366 (100%)	0	100	100
2	2Z	359/374 (96%)	356 (99%)	3 (1%)	79	87
2	3B	365/374 (98%)	362 (99%)	3 (1%)	79	87
2	3D	359/374 (96%)	359 (100%)	0	100	100
2	3F	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	3H	359/374 (96%)	359 (100%)	0	100	100
2	3J	359/374 (96%)	359 (100%)	0	100	100
2	3L	359/374 (96%)	359 (100%)	0	100	100
2	3N	359/374 (96%)	359 (100%)	0	100	100
2	3P	359/374 (96%)	359 (100%)	0	100	100
2	3R	366/374 (98%)	366 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3T	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	4	365/374 (98%)	365 (100%)	0	100	100
2	6	365/374 (98%)	365 (100%)	0	100	100
2	8	365/374 (98%)	365 (100%)	0	100	100
2	A0	365/374 (98%)	365 (100%)	0	100	100
2	A2	365/374 (98%)	363 (100%)	2 (0%)	86	91
2	A4	365/374 (98%)	357 (98%)	8 (2%)	47	68
2	A8	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	B0	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	B2	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	B4	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	B7	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	B9	359/374 (96%)	359 (100%)	0	100	100
2	C1	359/374 (96%)	359 (100%)	0	100	100
2	C5	365/374 (98%)	365 (100%)	0	100	100
2	C7	365/374 (98%)	363 (100%)	2 (0%)	86	91
2	C9	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	D1	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	D3	360/374 (96%)	360 (100%)	0	100	100
2	D5	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	D7	360/374 (96%)	360 (100%)	0	100	100
2	E1	360/374 (96%)	358 (99%)	2 (1%)	84	90
2	E3	359/374 (96%)	359 (100%)	0	100	100
2	E5	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	E7	360/374 (96%)	358 (99%)	2 (1%)	84	90
2	E9	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	F1	359/374 (96%)	356 (99%)	3 (1%)	79	87
2	F3	359/374 (96%)	359 (100%)	0	100	100
2	F5	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	F7	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	F9	365/374 (98%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G1	365/374 (98%)	362 (99%)	3 (1%)	79	87
2	G3	365/374 (98%)	362 (99%)	3 (1%)	79	87
2	G5	359/374 (96%)	359 (100%)	0	100	100
2	G7	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	G9	359/374 (96%)	359 (100%)	0	100	100
2	H1	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	H3	359/374 (96%)	359 (100%)	0	100	100
2	H5	359/374 (96%)	359 (100%)	0	100	100
2	H7	359/374 (96%)	359 (100%)	0	100	100
2	H9	359/374 (96%)	359 (100%)	0	100	100
2	I1	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	I3	359/374 (96%)	359 (100%)	0	100	100
2	I5	359/374 (96%)	359 (100%)	0	100	100
2	I7	361/374 (96%)	361 (100%)	0	100	100
2	I9	360/374 (96%)	356 (99%)	4 (1%)	70	81
2	J1	359/374 (96%)	359 (100%)	0	100	100
2	J3	360/374 (96%)	359 (100%)	1 (0%)	91	95
2	J5	366/374 (98%)	366 (100%)	0	100	100
2	J7	359/374 (96%)	354 (99%)	5 (1%)	62	77
2	J9	366/374 (98%)	366 (100%)	0	100	100
2	K1	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	K3	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	K5	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	K7	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	K9	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	L1	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	L3	359/374 (96%)	355 (99%)	4 (1%)	70	81
2	L5	359/374 (96%)	359 (100%)	0	100	100
2	L7	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	L9	359/374 (96%)	359 (100%)	0	100	100
2	M1	359/374 (96%)	359 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M3	365/374 (98%)	361 (99%)	4 (1%)	70	81
2	M5	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	M7	365/374 (98%)	363 (100%)	2 (0%)	86	91
2	M9	366/374 (98%)	365 (100%)	1 (0%)	91	95
2	N1	360/374 (96%)	360 (100%)	0	100	100
2	N3	359/374 (96%)	356 (99%)	3 (1%)	79	87
2	N5	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	N7	359/374 (96%)	356 (99%)	3 (1%)	79	87
2	N9	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	O1	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	O3	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	O5	359/374 (96%)	356 (99%)	3 (1%)	79	87
2	O7	361/374 (96%)	360 (100%)	1 (0%)	91	95
2	O9	359/374 (96%)	359 (100%)	0	100	100
2	P3	359/374 (96%)	359 (100%)	0	100	100
2	P5	365/374 (98%)	362 (99%)	3 (1%)	79	87
2	P7	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	P9	365/374 (98%)	365 (100%)	0	100	100
2	Q1	359/374 (96%)	359 (100%)	0	100	100
2	Q3	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	Q5	359/374 (96%)	359 (100%)	0	100	100
2	Q9	359/374 (96%)	359 (100%)	0	100	100
2	R1	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	R3	360/374 (96%)	360 (100%)	0	100	100
2	R5	365/374 (98%)	363 (100%)	2 (0%)	86	91
2	R7	359/374 (96%)	359 (100%)	0	100	100
2	R9	365/374 (98%)	365 (100%)	0	100	100
2	S1	361/374 (96%)	358 (99%)	3 (1%)	79	87
2	S5	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	S7	365/374 (98%)	364 (100%)	1 (0%)	91	95
2	S9	359/374 (96%)	355 (99%)	4 (1%)	70	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T1	359/374 (96%)	359 (100%)	0	100	100
2	T3	359/374 (96%)	354 (99%)	5 (1%)	62	77
2	T5	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	T7	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	U1	359/374 (96%)	359 (100%)	0	100	100
2	U3	359/374 (96%)	359 (100%)	0	100	100
2	U5	359/374 (96%)	359 (100%)	0	100	100
2	U7	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	U9	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	V1	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	V3	359/374 (96%)	355 (99%)	4 (1%)	70	81
2	V7	359/374 (96%)	359 (100%)	0	100	100
2	V9	359/374 (96%)	359 (100%)	0	100	100
2	W1	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	W3	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	W5	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	W7	359/374 (96%)	359 (100%)	0	100	100
2	W9	359/374 (96%)	350 (98%)	9 (2%)	42	65
2	X3	359/374 (96%)	359 (100%)	0	100	100
2	X5	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	X7	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	X9	359/374 (96%)	356 (99%)	3 (1%)	79	87
2	Y1	359/374 (96%)	358 (100%)	1 (0%)	91	95
2	Y3	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	Y5	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	Y9	359/374 (96%)	359 (100%)	0	100	100
2	Z1	359/374 (96%)	359 (100%)	0	100	100
2	Z3	359/374 (96%)	359 (100%)	0	100	100
2	Z5	359/374 (96%)	357 (99%)	2 (1%)	84	90
2	Z7	359/374 (96%)	359 (100%)	0	100	100
2	Z9	359/374 (96%)	359 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3V	251/258 (97%)	229 (91%)	22 (9%)	8	28
3	3X	251/258 (97%)	229 (91%)	22 (9%)	8	28
3	3Z	251/258 (97%)	229 (91%)	22 (9%)	8	28
3	4B	251/258 (97%)	229 (91%)	22 (9%)	8	28
3	4D	251/258 (97%)	229 (91%)	22 (9%)	8	28
3	4F	251/258 (97%)	229 (91%)	22 (9%)	8	28
3	4H	251/258 (97%)	229 (91%)	22 (9%)	8	28
3	4J	178/258 (69%)	178 (100%)	0	100	100
4	3W	170/176 (97%)	159 (94%)	11 (6%)	14	39
4	3Y	170/176 (97%)	159 (94%)	11 (6%)	14	39
4	4A	170/176 (97%)	159 (94%)	11 (6%)	14	39
4	4C	170/176 (97%)	159 (94%)	11 (6%)	14	39
4	4E	170/176 (97%)	159 (94%)	11 (6%)	14	39
4	4G	170/176 (97%)	159 (94%)	11 (6%)	14	39
4	4I	170/176 (97%)	159 (94%)	11 (6%)	14	39
5	4L	191/399 (48%)	190 (100%)	1 (0%)	86	91
5	4M	267/399 (67%)	266 (100%)	1 (0%)	89	93
6	4N	46/422 (11%)	45 (98%)	1 (2%)	47	68
6	4O	403/422 (96%)	402 (100%)	1 (0%)	92	96
6	4P	159/422 (38%)	159 (100%)	0	100	100
7	4Q	54/306 (18%)	54 (100%)	0	100	100
7	4R	305/306 (100%)	300 (98%)	5 (2%)	58	75
7	4S	40/306 (13%)	38 (95%)	2 (5%)	20	46
7	4T	160/306 (52%)	159 (99%)	1 (1%)	84	90
7	4U	234/306 (76%)	234 (100%)	0	100	100
8	4V	63/362 (17%)	63 (100%)	0	100	100
8	4W	261/362 (72%)	258 (99%)	3 (1%)	70	81
8	4X	49/362 (14%)	48 (98%)	1 (2%)	50	70
9	4Y	98/374 (26%)	98 (100%)	0	100	100
9	4Z	309/374 (83%)	309 (100%)	0	100	100
10	5A	194/433 (45%)	193 (100%)	1 (0%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	5B	220/433 (51%)	218 (99%)	2 (1%)	75	86
10	5C	323/433 (75%)	320 (99%)	3 (1%)	75	86
10	5D	97/433 (22%)	97 (100%)	0	100	100
11	5E	211/223 (95%)	209 (99%)	2 (1%)	75	86
12	5F	332/340 (98%)	328 (99%)	4 (1%)	67	80
12	5G	127/340 (37%)	126 (99%)	1 (1%)	79	87
12	7B	83/340 (24%)	82 (99%)	1 (1%)	67	80
13	5H	119/121 (98%)	100 (84%)	19 (16%)	2	8
13	5I	119/121 (98%)	100 (84%)	19 (16%)	2	8
13	5J	119/121 (98%)	100 (84%)	19 (16%)	2	8
13	5K	119/121 (98%)	100 (84%)	19 (16%)	2	8
14	5L	511/517 (99%)	450 (88%)	61 (12%)	4	16
14	5M	511/517 (99%)	453 (89%)	58 (11%)	4	17
14	5N	511/517 (99%)	450 (88%)	61 (12%)	4	16
15	5O	307/309 (99%)	262 (85%)	45 (15%)	2	10
15	5P	307/309 (99%)	291 (95%)	16 (5%)	19	45
16	5Q	162/167 (97%)	160 (99%)	2 (1%)	67	80
17	5R	15/206 (7%)	15 (100%)	0	100	100
17	5S	169/206 (82%)	141 (83%)	28 (17%)	2	7
17	5T	168/206 (82%)	137 (82%)	31 (18%)	1	4
17	5U	169/206 (82%)	139 (82%)	30 (18%)	1	5
17	5V	94/206 (46%)	92 (98%)	2 (2%)	48	69
18	5X	202/210 (96%)	169 (84%)	33 (16%)	2	7
18	5Y	202/210 (96%)	170 (84%)	32 (16%)	2	8
18	5Z	202/210 (96%)	170 (84%)	32 (16%)	2	8
18	6A	202/210 (96%)	170 (84%)	32 (16%)	2	8
18	6B	202/210 (96%)	170 (84%)	32 (16%)	2	8
18	6C	202/210 (96%)	170 (84%)	32 (16%)	2	8
18	6D	202/210 (96%)	170 (84%)	32 (16%)	2	8
19	6E	211/222 (95%)	209 (99%)	2 (1%)	75	86
20	6F	310/314 (99%)	308 (99%)	2 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	6G	150/171 (88%)	150 (100%)	0	100	100
21	6H	157/171 (92%)	157 (100%)	0	100	100
22	6I	285/303 (94%)	283 (99%)	2 (1%)	81	88
22	6J	285/303 (94%)	284 (100%)	1 (0%)	89	93
22	6K	285/303 (94%)	283 (99%)	2 (1%)	81	88
22	6L	285/303 (94%)	284 (100%)	1 (0%)	89	93
22	6M	285/303 (94%)	282 (99%)	3 (1%)	70	81
22	6N	285/303 (94%)	284 (100%)	1 (0%)	89	93
22	6O	285/303 (94%)	283 (99%)	2 (1%)	81	88
22	6P	257/303 (85%)	254 (99%)	3 (1%)	67	80
23	6Q	76/78 (97%)	68 (90%)	8 (10%)	5	21
23	6R	76/78 (97%)	69 (91%)	7 (9%)	7	26
23	6S	76/78 (97%)	71 (93%)	5 (7%)	14	39
24	6T	500/549 (91%)	495 (99%)	5 (1%)	73	83
24	6U	503/549 (92%)	496 (99%)	7 (1%)	62	77
24	6V	498/549 (91%)	493 (99%)	5 (1%)	73	83
24	6W	502/549 (91%)	494 (98%)	8 (2%)	58	75
24	6X	505/549 (92%)	495 (98%)	10 (2%)	50	70
24	6Y	499/549 (91%)	492 (99%)	7 (1%)	62	77
24	6Z	500/549 (91%)	495 (99%)	5 (1%)	73	83
24	7A	162/549 (30%)	161 (99%)	1 (1%)	84	90
25	7C	84/95 (88%)	84 (100%)	0	100	100
26	7D	112/122 (92%)	97 (87%)	15 (13%)	3	12
26	7E	112/122 (92%)	96 (86%)	16 (14%)	2	10
26	7F	112/122 (92%)	96 (86%)	16 (14%)	2	10
27	7G	179/186 (96%)	179 (100%)	0	100	100
28	7H	110/347 (32%)	99 (90%)	11 (10%)	6	22
28	7X	110/347 (32%)	97 (88%)	13 (12%)	4	16
29	7I	177/371 (48%)	176 (99%)	1 (1%)	84	90
29	7J	280/371 (76%)	278 (99%)	2 (1%)	81	88
30	7K	332/350 (95%)	329 (99%)	3 (1%)	75	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	7L	132/350 (38%)	132 (100%)	0	100	100
31	7M	71/115 (62%)	70 (99%)	1 (1%)	62	77
31	7N	104/115 (90%)	104 (100%)	0	100	100
32	7O	47/191 (25%)	47 (100%)	0	100	100
32	7P	148/191 (78%)	148 (100%)	0	100	100
33	7Q	64/165 (39%)	64 (100%)	0	100	100
34	7R	172/618 (28%)	171 (99%)	1 (1%)	84	90
34	7S	143/618 (23%)	142 (99%)	1 (1%)	81	88
35	7T	186/462 (40%)	184 (99%)	2 (1%)	70	81
35	7U	157/462 (34%)	157 (100%)	0	100	100
36	7V	82/162 (51%)	71 (87%)	11 (13%)	3	12
36	7W	82/162 (51%)	70 (85%)	12 (15%)	2	10
37	7Y	209/267 (78%)	205 (98%)	4 (2%)	52	71
38	7Z	31/206 (15%)	31 (100%)	0	100	100
38	8A	179/206 (87%)	174 (97%)	5 (3%)	38	62
38	8B	182/206 (88%)	175 (96%)	7 (4%)	28	54
38	8C	182/206 (88%)	172 (94%)	10 (6%)	18	44
38	8D	141/206 (68%)	128 (91%)	13 (9%)	7	26
All	All	146455/160298 (91%)	145005 (99%)	1450 (1%)	71	83

5 of 1450 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	5S	225	ASP
18	6B	184	THR
17	5T	192	VAL
17	5S	217	ARG
18	5Y	110	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 2787 such sidechains are listed below:

Mol	Chain	Res	Type
2	0H	356	ASN
1	3C	332	ASN
2	0P	309	HIS

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Mol	Chain	Res	Type
2	0H	293	ASN
2	1R	293	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 510 ligands modelled in this entry, 170 are monoatomic - leaving 340 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	$\#\|Z\| > 2$
41	GTP	8	501	40	29,34,34	1.27	2 (6%)	35,54,54	1.29	4 (11%)
39	GDP	W8	503	-	25,30,30	0.93	1 (4%)	30,47,47	1.06	2 (6%)
41	GTP	K0	501	40	29,34,34	1.22	2 (6%)	35,54,54	1.31	4 (11%)
41	GTP	Q4	501	40	29,34,34	1.28	2 (6%)	35,54,54	1.38	5 (14%)
41	GTP	A4	501	40	29,34,34	1.21	2 (6%)	35,54,54	1.36	6 (17%)
41	GTP	L4	501	40	29,34,34	1.22	2 (6%)	35,54,54	1.30	4 (11%)
39	GDP	2Y	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.20	3 (10%)
41	GTP	G5	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
41	GTP	N0	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
41	GTP	F5	501	40	29,34,34	1.23	1 (3%)	35,54,54	1.24	4 (11%)
41	GTP	C8	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.36	4 (11%)
41	GTP	1L	501	40	29,34,34	1.24	1 (3%)	35,54,54	1.28	4 (11%)
39	GDP	W4	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.21	5 (16%)
41	GTP	2Y	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.33	4 (11%)
39	GDP	1Q	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.16	3 (10%)
41	GTP	B7	501	40	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
41	GTP	Y0	501	40	29,34,34	1.19	2 (6%)	35,54,54	1.37	4 (11%)
39	GDP	1E	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
39	GDP	H4	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.16	2 (6%)
39	GDP	I8	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.12	2 (6%)
41	GTP	O4	501	40	29,34,34	1.23	2 (6%)	35,54,54	1.35	4 (11%)
39	GDP	C4	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.21	3 (10%)
41	GTP	L6	501	40	29,34,34	1.23	2 (6%)	35,54,54	1.33	4 (11%)
39	GDP	K4	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.12	2 (6%)
41	GTP	M4	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
39	GDP	T4	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.16	3 (10%)
41	GTP	D3	501	40	29,34,34	1.23	2 (6%)	35,54,54	1.33	3 (8%)
39	GDP	G2	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.17	2 (6%)
41	GTP	2A	501	40	29,34,34	1.17	1 (3%)	35,54,54	1.27	3 (8%)
39	GDP	G6	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.19	2 (6%)
39	GDP	Q8	501	-	25,30,30	0.92	1 (4%)	30,47,47	1.26	4 (13%)
39	GDP	F0	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
39	GDP	A3	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.24	4 (13%)
39	GDP	2M	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.13	2 (6%)
41	GTP	Y4	501	40	29,34,34	1.22	2 (6%)	35,54,54	1.30	4 (11%)
41	GTP	Z3	501	40	29,34,34	1.26	1 (3%)	35,54,54	1.33	4 (11%)
41	GTP	N3	501	40	29,34,34	1.25	3 (10%)	35,54,54	1.26	4 (11%)
39	GDP	9	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.13	2 (6%)
41	GTP	V3	501	40	29,34,34	1.22	2 (6%)	35,54,54	1.32	4 (11%)
41	GTP	P8	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.33	4 (11%)
39	GDP	X2	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.14	2 (6%)
39	GDP	1K	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.15	3 (10%)
39	GDP	0Y	502	-	25,30,30	0.92	1 (4%)	30,47,47	1.19	2 (6%)
39	GDP	2E	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
39	GDP	L2	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
39	GDP	X6	502	-	25,30,30	0.91	1 (4%)	30,47,47	1.10	2 (6%)
39	GDP	A7	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.08	2 (6%)
39	GDP	P6	503	-	25,30,30	0.98	1 (4%)	30,47,47	1.15	2 (6%)
41	GTP	O8	501	40	29,34,34	1.23	2 (6%)	35,54,54	1.29	3 (8%)
39	GDP	C8	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
39	GDP	5	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.14	2 (6%)
39	GDP	0U	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.20	4 (13%)
41	GTP	F8	501	40	29,34,34	1.23	1 (3%)	35,54,54	1.29	4 (11%)
41	GTP	C9	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.36	3 (8%)
39	GDP	1A	503	-	25,30,30	0.96	1 (4%)	30,47,47	1.13	4 (13%)
41	GTP	2N	501	40	29,34,34	1.20	2 (6%)	35,54,54	1.28	4 (11%)
41	GTP	O9	501	40	29,34,34	1.22	2 (6%)	35,54,54	1.32	3 (8%)
39	GDP	2S	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.23	5 (16%)
39	GDP	R2	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.17	3 (10%)
41	GTP	2G	501	40	29,34,34	1.20	2 (6%)	35,54,54	1.27	4 (11%)
41	GTP	A9	501	40	29,34,34	1.22	2 (6%)	35,54,54	1.34	5 (14%)
41	GTP	M2	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.32	4 (11%)
39	GDP	N6	503	-	25,30,30	0.93	1 (4%)	30,47,47	1.13	2 (6%)
39	GDP	0S	502	-	25,30,30	1.03	2 (8%)	30,47,47	1.13	2 (6%)
41	GTP	I0	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.30	4 (11%)
39	GDP	L6	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.13	2 (6%)
39	GDP	2K	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.12	2 (6%)
39	GDP	Z6	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	2 (6%)
39	GDP	N0	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	2 (6%)
41	GTP	Q6	501	40	29,34,34	1.27	2 (6%)	35,54,54	1.34	4 (11%)
39	GDP	V0	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.13	2 (6%)
41	GTP	2L	501	40	29,34,34	1.20	2 (6%)	35,54,54	1.28	4 (11%)
39	GDP	0C	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.10	2 (6%)
41	GTP	B5	501	40	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
41	GTP	3A	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.35	4 (11%)
41	GTP	3M	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.37	4 (11%)
39	GDP	X0	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.10	1 (3%)
41	GTP	H3	501	40	29,34,34	1.24	1 (3%)	35,54,54	1.28	4 (11%)
41	GTP	W8	501	40	29,34,34	1.22	1 (3%)	35,54,54	1.30	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
41	GTP	P9	501	40	29,34,34	1.28	2 (6%)	35,54,54	1.42	5 (14%)
41	GTP	K1	501	40	29,34,34	1.29	2 (6%)	35,54,54	1.28	3 (8%)
41	GTP	R4	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.33	4 (11%)
39	GDP	U4	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.13	3 (10%)
39	GDP	0G	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	2 (6%)
39	GDP	N2	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.15	3 (10%)
41	GTP	Y1	501	40	29,34,34	1.19	1 (3%)	35,54,54	1.39	4 (11%)
39	GDP	K6	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.17	2 (6%)
39	GDP	V4	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.19	3 (10%)
39	GDP	S2	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.09	2 (6%)
41	GTP	B0	501	40	29,34,34	1.21	2 (6%)	35,54,54	1.31	4 (11%)
39	GDP	2G	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	2 (6%)
39	GDP	J2	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.14	2 (6%)
39	GDP	3I	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.17	3 (10%)
41	GTP	2S	501	40	29,34,34	1.29	2 (6%)	35,54,54	1.34	4 (11%)
39	GDP	0Q	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.16	3 (10%)
39	GDP	1U	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.13	2 (6%)
41	GTP	G7	501	40	29,34,34	1.22	1 (3%)	35,54,54	1.28	4 (11%)
39	GDP	S4	501	-	25,30,30	0.91	1 (4%)	30,47,47	1.17	3 (10%)
39	GDP	K8	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.15	2 (6%)
41	GTP	1G	501	40	29,34,34	1.21	1 (3%)	35,54,54	1.26	4 (11%)
41	GTP	X4	501	40	29,34,34	1.25	1 (3%)	35,54,54	1.43	5 (14%)
39	GDP	0O	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.19	4 (13%)
39	GDP	Q2	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.14	2 (6%)
39	GDP	S8	502	-	25,30,30	0.92	1 (4%)	30,47,47	1.19	2 (6%)
41	GTP	1T	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
39	GDP	3A	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.19	3 (10%)
39	GDP	1O	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
41	GTP	G9	501	40	29,34,34	1.22	1 (3%)	35,54,54	1.24	4 (11%)
41	GTP	P4	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.34	4 (11%)
41	GTP	K6	501	40	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
41	GTP	K4	501	40	29,34,34	1.21	1 (3%)	35,54,54	1.23	4 (11%)
39	GDP	2C	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.16	2 (6%)
41	GTP	S9	501	40	29,34,34	1.00	3 (10%)	35,54,54	1.13	2 (5%)
39	GDP	F6	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.13	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
39	GDP	Z0	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.15	3 (10%)
39	GDP	C2	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	3 (10%)
41	GTP	F1	501	40	29,34,34	1.23	1 (3%)	35,54,54	1.28	4 (11%)
39	GDP	K0	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.18	4 (13%)
41	GTP	D1	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.47	6 (17%)
41	GTP	J8	501	40	29,34,34	1.19	2 (6%)	35,54,54	1.33	4 (11%)
39	GDP	B5	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.15	2 (6%)
39	GDP	T2	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.16	2 (6%)
39	GDP	X4	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.11	3 (10%)
41	GTP	E8	501	40	29,34,34	1.22	1 (3%)	35,54,54	1.33	3 (8%)
39	GDP	A5	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.11	2 (6%)
39	GDP	M2	502	-	25,30,30	0.91	1 (4%)	30,47,47	1.15	2 (6%)
41	GTP	U7	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
39	GDP	W6	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.17	3 (10%)
41	GTP	H8	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
39	GDP	3C	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.16	4 (13%)
39	GDP	1C	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.17	2 (6%)
41	GTP	3O	501	40	29,34,34	1.27	3 (10%)	35,54,54	1.36	4 (11%)
41	GTP	Z6	501	40	29,34,34	1.26	1 (3%)	35,54,54	1.30	4 (11%)
39	GDP	D4	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.23	3 (10%)
41	GTP	S5	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.42	6 (17%)
39	GDP	Y8	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.14	2 (6%)
41	GTP	1Q	501	40	29,34,34	1.26	3 (10%)	35,54,54	1.32	4 (11%)
41	GTP	K9	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.30	4 (11%)
39	GDP	P4	503	-	25,30,30	0.98	1 (4%)	30,47,47	1.20	3 (10%)
39	GDP	U2	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
41	GTP	I8	501	40	29,34,34	1.21	2 (6%)	35,54,54	1.28	4 (11%)
41	GTP	1S	501	40	29,34,34	1.24	1 (3%)	35,54,54	1.29	4 (11%)
39	GDP	2Q	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.24	5 (16%)
41	GTP	T8	501	40	29,34,34	1.23	2 (6%)	35,54,54	1.36	4 (11%)
41	GTP	C1	501	40	29,34,34	1.18	2 (6%)	35,54,54	1.31	4 (11%)
41	GTP	G1	501	40	29,34,34	1.23	2 (6%)	35,54,54	1.36	4 (11%)
41	GTP	0S	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
41	GTP	2U	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
41	GTP	0I	501	40	29,34,34	1.22	1 (3%)	35,54,54	1.26	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
39	GDP	7	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.14	2 (6%)
41	GTP	E1	501	40	29,34,34	1.24	1 (3%)	35,54,54	1.30	4 (11%)
39	GDP	0W	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.19	2 (6%)
41	GTP	D7	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.30	3 (8%)
41	GTP	L7	501	40	29,34,34	1.30	2 (6%)	35,54,54	1.30	4 (11%)
41	GTP	C5	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.31	4 (11%)
41	GTP	W4	501	40	29,34,34	1.18	2 (6%)	35,54,54	1.26	4 (11%)
39	GDP	2I	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.15	3 (10%)
41	GTP	3T	501	40	29,34,34	1.27	2 (6%)	35,54,54	1.27	4 (11%)
41	GTP	Y6	501	40	29,34,34	1.16	1 (3%)	35,54,54	1.29	3 (8%)
39	GDP	I2	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.13	3 (10%)
39	GDP	Q0	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.15	4 (13%)
39	GDP	Y4	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.12	2 (6%)
41	GTP	N6	501	40	29,34,34	1.22	2 (6%)	35,54,54	1.32	4 (11%)
39	GDP	3	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.16	2 (6%)
41	GTP	3D	501	40	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
41	GTP	W5	501	40	29,34,34	1.20	2 (6%)	35,54,54	1.31	4 (11%)
41	GTP	0Y	501	40	29,34,34	1.18	2 (6%)	35,54,54	1.26	4 (11%)
41	GTP	Z2	501	40	29,34,34	1.23	1 (3%)	35,54,54	1.27	4 (11%)
41	GTP	I4	501	40	29,34,34	1.26	3 (10%)	35,54,54	1.27	4 (11%)
39	GDP	F8	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	2 (6%)
39	GDP	T8	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.16	2 (6%)
41	GTP	3P	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.44	6 (17%)
41	GTP	M6	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.35	4 (11%)
39	GDP	D8	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	2 (6%)
41	GTP	I5	501	40	29,34,34	1.21	1 (3%)	35,54,54	1.30	4 (11%)
39	GDP	M0	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.13	3 (10%)
41	GTP	L2	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.31	4 (11%)
39	GDP	3M	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.18	2 (6%)
39	GDP	0I	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	2 (6%)
39	GDP	3K	503	-	25,30,30	0.94	1 (4%)	30,47,47	1.13	2 (6%)
39	GDP	T0	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	3 (10%)
41	GTP	0O	501	40	29,34,34	1.24	1 (3%)	35,54,54	1.29	4 (11%)
41	GTP	Q2	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.38	5 (14%)
41	GTP	S8	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.33	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
39	GDP	R6	503	-	25,30,30	0.95	1 (4%)	30,47,47	1.26	5 (16%)
41	GTP	U9	501	40	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
41	GTP	1H	501	40	29,34,34	1.17	2 (6%)	35,54,54	1.26	4 (11%)
41	GTP	T6	501	40	29,34,34	1.27	2 (6%)	35,54,54	1.39	4 (11%)
41	GTP	2E	501	40	29,34,34	1.19	2 (6%)	35,54,54	1.27	3 (8%)
39	GDP	N8	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	2 (6%)
41	GTP	V8	501	40	29,34,34	1.17	1 (3%)	35,54,54	1.29	3 (8%)
41	GTP	1W	501	40	29,34,34	1.25	1 (3%)	35,54,54	1.28	4 (11%)
39	GDP	T6	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.15	2 (6%)
41	GTP	J6	501	40	29,34,34	1.22	1 (3%)	35,54,54	1.33	4 (11%)
41	GTP	S2	501	40	29,34,34	1.27	2 (6%)	35,54,54	1.35	5 (14%)
39	GDP	3Q	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.12	2 (6%)
41	GTP	J2	501	40	29,34,34	1.21	1 (3%)	35,54,54	1.31	4 (11%)
41	GTP	0Q	501	40	29,34,34	1.25	1 (3%)	35,54,54	1.28	4 (11%)
39	GDP	E0	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
39	GDP	2U	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.20	4 (13%)
41	GTP	R8	501	40	29,34,34	1.27	2 (6%)	35,54,54	1.32	4 (11%)
39	GDP	0E	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.17	3 (10%)
39	GDP	I4	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.13	2 (6%)
39	GDP	Q4	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	2 (6%)
41	GTP	3G	501	40	29,34,34	1.25	3 (10%)	35,54,54	1.34	4 (11%)
39	GDP	M6	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.25	5 (16%)
41	GTP	0F	501	40	29,34,34	1.21	1 (3%)	35,54,54	1.29	3 (8%)
41	GTP	G0	501	40	29,34,34	1.22	1 (3%)	35,54,54	1.27	4 (11%)
39	GDP	Y6	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
39	GDP	C6	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.13	2 (6%)
39	GDP	3S	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.15	2 (6%)
41	GTP	U4	501	40	29,34,34	1.21	2 (6%)	35,54,54	1.25	4 (11%)
39	GDP	Z2	503	-	25,30,30	0.98	1 (4%)	30,47,47	1.14	2 (6%)
41	GTP	E4	501	40	29,34,34	1.21	1 (3%)	35,54,54	1.26	4 (11%)
39	GDP	H6	502	-	25,30,30	0.92	1 (4%)	30,47,47	1.09	2 (6%)
39	GDP	R8	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.18	4 (13%)
39	GDP	V6	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
39	GDP	H2	503	-	25,30,30	0.94	1 (4%)	30,47,47	1.05	2 (6%)
41	GTP	K7	501	40	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
39	GDP	1W	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.16	2 (6%)
39	GDP	X8	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.11	2 (6%)
39	GDP	E6	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	2 (6%)
41	GTP	I1	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.31	4 (11%)
39	GDP	B8	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.25	4 (13%)
39	GDP	D0	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.21	3 (10%)
39	GDP	1G	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.16	2 (6%)
39	GDP	P8	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.17	3 (10%)
41	GTP	U2	501	40	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
41	GTP	A2	501	40	29,34,34	1.26	1 (3%)	35,54,54	1.47	5 (14%)
39	GDP	B1	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.11	2 (6%)
41	GTP	W0	501	40	29,34,34	1.19	2 (6%)	35,54,54	1.30	4 (11%)
39	GDP	J4	503	-	25,30,30	0.94	1 (4%)	30,47,47	1.14	3 (10%)
41	GTP	2C	501	40	29,34,34	1.20	1 (3%)	35,54,54	1.29	3 (8%)
41	GTP	G4	501	40	29,34,34	1.25	1 (3%)	35,54,54	1.28	4 (11%)
39	GDP	O0	503	-	25,30,30	0.96	1 (4%)	30,47,47	1.15	2 (6%)
39	GDP	Z4	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.16	2 (6%)
39	GDP	H8	503	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	2 (6%)
39	GDP	E4	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
39	GDP	O4	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.14	2 (6%)
41	GTP	7	501	40	29,34,34	1.27	2 (6%)	35,54,54	1.31	4 (11%)
39	GDP	V2	503	-	25,30,30	0.95	1 (4%)	30,47,47	1.13	3 (10%)
39	GDP	Z8	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	2 (6%)
41	GTP	0M	501	40	29,34,34	1.25	1 (3%)	35,54,54	1.34	4 (11%)
41	GTP	F0	501	40	29,34,34	1.21	1 (3%)	35,54,54	1.26	4 (11%)
41	GTP	2W	501	40	29,34,34	1.28	2 (6%)	35,54,54	1.36	4 (11%)
41	GTP	1X	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.29	4 (11%)
41	GTP	X7	501	40	29,34,34	1.22	2 (6%)	35,54,54	1.52	5 (14%)
41	GTP	H2	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.27	4 (11%)
41	GTP	A1	501	40	29,34,34	1.21	2 (6%)	35,54,54	1.31	4 (11%)
39	GDP	3O	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	2 (6%)
41	GTP	2Q	501	40	29,34,34	1.26	3 (10%)	35,54,54	1.34	4 (11%)
39	GDP	E8	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	2 (6%)
41	GTP	R0	501	40	29,34,34	1.28	2 (6%)	35,54,54	1.32	4 (11%)
39	GDP	V8	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
39	GDP	A9	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	2 (6%)
39	GDP	G4	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.13	2 (6%)
39	GDP	W0	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
39	GDP	Y0	502	-	25,30,30	0.90	1 (4%)	30,47,47	1.13	2 (6%)
41	GTP	3K	501	40	29,34,34	1.23	2 (6%)	35,54,54	1.34	4 (11%)
41	GTP	1N	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.30	4 (11%)
41	GTP	1A	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.28	4 (11%)
41	GTP	M0	501	40	29,34,34	1.20	1 (3%)	35,54,54	1.28	4 (11%)
41	GTP	C0	501	40	29,34,34	1.19	2 (6%)	35,54,54	1.27	4 (11%)
41	GTP	R6	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.39	5 (14%)
39	GDP	W2	503	-	25,30,30	0.95	1 (4%)	30,47,47	1.13	3 (10%)
39	GDP	M4	502	-	25,30,30	0.91	1 (4%)	30,47,47	1.12	2 (6%)
39	GDP	3G	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.19	3 (10%)
41	GTP	O6	501	40	29,34,34	1.20	2 (6%)	35,54,54	1.35	3 (8%)
41	GTP	U6	501	40	29,34,34	1.21	2 (6%)	35,54,54	1.26	4 (11%)
39	GDP	2	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.11	2 (6%)
39	GDP	G0	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.17	2 (6%)
41	GTP	E6	501	40	29,34,34	1.22	1 (3%)	35,54,54	1.30	3 (8%)
41	GTP	1D	501	40	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
39	GDP	G8	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
41	GTP	0V	501	40	29,34,34	1.20	2 (6%)	35,54,54	1.27	4 (11%)
41	GTP	0K	501	40	29,34,34	1.23	1 (3%)	35,54,54	1.26	4 (11%)
39	GDP	2W	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.22	4 (13%)
39	GDP	O2	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.17	2 (6%)
41	GTP	3	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
41	GTP	B2	501	40	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
41	GTP	F3	501	40	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
39	GDP	S0	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.23	4 (13%)
41	GTP	W2	501	40	29,34,34	1.19	2 (6%)	35,54,54	1.27	3 (8%)
39	GDP	M8	501	-	25,30,30	0.91	1 (4%)	30,47,47	1.13	2 (6%)
41	GTP	O2	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.47	6 (17%)
41	GTP	4	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.32	4 (11%)
41	GTP	Z7	501	40	29,34,34	1.26	1 (3%)	35,54,54	1.28	4 (11%)
41	GTP	T2	501	40	29,34,34	1.27	2 (6%)	35,54,54	1.39	4 (11%)
41	GTP	2K	501	40	29,34,34	1.21	1 (3%)	35,54,54	1.27	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
39	GDP	F2	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	2 (6%)
39	GDP	B3	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.17	3 (10%)
41	GTP	X6	501	40	29,34,34	1.23	2 (6%)	35,54,54	1.44	5 (14%)
41	GTP	3C	501	40	29,34,34	1.25	3 (10%)	35,54,54	1.33	4 (11%)
41	GTP	X0	501	40	29,34,34	1.21	1 (3%)	35,54,54	1.32	4 (11%)
41	GTP	0A	501	40	29,34,34	1.27	1 (3%)	35,54,54	1.29	4 (11%)
39	GDP	0M	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.18	1 (3%)
39	GDP	U8	501	-	25,30,30	0.92	1 (4%)	30,47,47	1.12	2 (6%)
41	GTP	2I	501	40	29,34,34	1.22	1 (3%)	35,54,54	1.28	4 (11%)
39	GDP	C0	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	2 (6%)
41	GTP	3S	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.31	4 (11%)
41	GTP	0C	501	40	29,34,34	1.25	1 (3%)	35,54,54	1.29	4 (11%)
39	GDP	O6	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.22	3 (10%)
41	GTP	N1	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.32	4 (11%)
41	GTP	N8	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.34	4 (11%)
41	GTP	3I	501	40	29,34,34	1.22	2 (6%)	35,54,54	1.37	3 (8%)
39	GDP	R4	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.15	2 (6%)
39	GDP	O8	503	-	25,30,30	0.94	1 (4%)	30,47,47	1.22	3 (10%)
39	GDP	D2	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
39	GDP	L0	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.16	2 (6%)
39	GDP	R0	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	2 (6%)
39	GDP	0A	503	-	25,30,30	0.96	1 (4%)	30,47,47	1.21	1 (3%)
39	GDP	0K	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.18	1 (3%)
41	GTP	M7	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.29	4 (11%)
41	GTP	P6	501	40	29,34,34	1.28	2 (6%)	35,54,54	1.34	4 (11%)
39	GDP	J8	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.23	3 (10%)
41	GTP	J0	501	40	29,34,34	1.23	1 (3%)	35,54,54	1.32	5 (14%)
39	GDP	S6	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.13	2 (6%)
41	GTP	R2	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.31	4 (11%)
39	GDP	I0	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.15	2 (6%)
39	GDP	J6	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.18	4 (13%)
39	GDP	J0	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.14	2 (6%)
41	GTP	D5	501	40	29,34,34	1.27	2 (6%)	35,54,54	1.32	4 (11%)
39	GDP	D6	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.18	2 (6%)
41	GTP	J4	501	40	29,34,34	1.24	2 (6%)	35,54,54	1.33	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
39	GDP	1M	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.18	3 (10%)
41	GTP	1C	501	40	29,34,34	1.23	1 (3%)	35,54,54	1.27	4 (11%)
39	GDP	Q6	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.15	2 (6%)
39	GDP	U6	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.10	2 (6%)
41	GTP	O0	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
39	GDP	A1	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.12	2 (6%)
41	GTP	S0	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.32	4 (11%)
39	GDP	2A	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.15	2 (6%)
41	GTP	V2	501	40	29,34,34	1.19	1 (3%)	35,54,54	1.29	4 (11%)
39	GDP	L4	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.12	3 (10%)
39	GDP	E2	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.12	2 (6%)
39	GDP	1S	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.20	2 (6%)
41	GTP	H6	501	40	29,34,34	1.25	1 (3%)	35,54,54	1.28	4 (11%)
41	GTP	Z0	501	40	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
41	GTP	T4	501	40	29,34,34	1.26	2 (6%)	35,54,54	1.34	4 (11%)
39	GDP	Y2	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.12	3 (10%)

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
41	GTP	8	501	40	-	5/18/38/38	0/3/3/3
39	GDP	W8	503	-	-	2/12/32/32	0/3/3/3
41	GTP	K0	501	40	-	8/18/38/38	0/3/3/3
41	GTP	Q4	501	40	-	8/18/38/38	0/3/3/3
41	GTP	A4	501	40	-	6/18/38/38	0/3/3/3
41	GTP	L4	501	40	-	7/18/38/38	0/3/3/3
39	GDP	2Y	502	-	-	7/12/32/32	0/3/3/3
41	GTP	G5	501	40	-	7/18/38/38	0/3/3/3
41	GTP	N0	501	40	-	9/18/38/38	0/3/3/3
41	GTP	F5	501	40	-	7/18/38/38	0/3/3/3
41	GTP	C8	501	40	-	2/18/38/38	0/3/3/3
41	GTP	1L	501	40	-	6/18/38/38	0/3/3/3
39	GDP	W4	502	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	2Y	501	40	-	8/18/38/38	0/3/3/3
39	GDP	1Q	502	-	-	1/12/32/32	0/3/3/3
41	GTP	B7	501	40	-	8/18/38/38	0/3/3/3
41	GTP	Y0	501	40	-	8/18/38/38	0/3/3/3
39	GDP	1E	501	-	-	1/12/32/32	0/3/3/3
39	GDP	H4	501	-	-	4/12/32/32	0/3/3/3
39	GDP	I8	502	-	-	1/12/32/32	0/3/3/3
41	GTP	O4	501	40	-	8/18/38/38	0/3/3/3
39	GDP	C4	501	-	-	2/12/32/32	0/3/3/3
41	GTP	L6	501	40	-	6/18/38/38	0/3/3/3
39	GDP	K4	502	-	-	1/12/32/32	0/3/3/3
41	GTP	M4	501	40	-	8/18/38/38	0/3/3/3
39	GDP	T4	502	-	-	4/12/32/32	0/3/3/3
41	GTP	D3	501	40	-	6/18/38/38	0/3/3/3
39	GDP	G2	501	-	-	3/12/32/32	0/3/3/3
41	GTP	2A	501	40	-	8/18/38/38	0/3/3/3
39	GDP	G6	501	-	-	5/12/32/32	0/3/3/3
39	GDP	Q8	501	-	-	3/12/32/32	0/3/3/3
39	GDP	F0	502	-	-	3/12/32/32	0/3/3/3
39	GDP	A3	501	-	-	5/12/32/32	0/3/3/3
39	GDP	2M	501	-	-	1/12/32/32	0/3/3/3
41	GTP	Y4	501	40	-	9/18/38/38	0/3/3/3
41	GTP	Z3	501	40	-	8/18/38/38	0/3/3/3
41	GTP	N3	501	40	-	9/18/38/38	0/3/3/3
39	GDP	9	501	-	-	0/12/32/32	0/3/3/3
41	GTP	V3	501	40	-	7/18/38/38	0/3/3/3
41	GTP	P8	501	40	-	7/18/38/38	0/3/3/3
39	GDP	X2	501	-	-	4/12/32/32	0/3/3/3
39	GDP	1K	501	-	-	4/12/32/32	0/3/3/3
39	GDP	0Y	502	-	-	1/12/32/32	0/3/3/3
39	GDP	2E	502	-	-	1/12/32/32	0/3/3/3
39	GDP	L2	502	-	-	3/12/32/32	0/3/3/3
39	GDP	X6	502	-	-	4/12/32/32	0/3/3/3
39	GDP	A7	501	-	-	5/12/32/32	0/3/3/3
39	GDP	P6	503	-	-	4/12/32/32	0/3/3/3
41	GTP	O8	501	40	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	C8	502	-	-	3/12/32/32	0/3/3/3
39	GDP	5	501	-	-	2/12/32/32	0/3/3/3
39	GDP	0U	501	-	-	6/12/32/32	0/3/3/3
41	GTP	F8	501	40	-	8/18/38/38	0/3/3/3
41	GTP	C9	501	40	-	5/18/38/38	0/3/3/3
39	GDP	1A	503	-	-	3/12/32/32	0/3/3/3
41	GTP	2N	501	40	-	8/18/38/38	0/3/3/3
41	GTP	O9	501	40	-	6/18/38/38	0/3/3/3
39	GDP	2S	502	-	-	4/12/32/32	0/3/3/3
39	GDP	R2	502	-	-	1/12/32/32	0/3/3/3
41	GTP	2G	501	40	-	7/18/38/38	0/3/3/3
41	GTP	A9	501	40	-	9/18/38/38	0/3/3/3
41	GTP	M2	501	40	-	8/18/38/38	0/3/3/3
39	GDP	N6	503	-	-	6/12/32/32	0/3/3/3
39	GDP	0S	502	-	-	2/12/32/32	0/3/3/3
41	GTP	I0	501	40	-	7/18/38/38	0/3/3/3
39	GDP	L6	502	-	-	6/12/32/32	0/3/3/3
39	GDP	2K	502	-	-	1/12/32/32	0/3/3/3
39	GDP	Z6	502	-	-	1/12/32/32	0/3/3/3
39	GDP	N0	502	-	-	1/12/32/32	0/3/3/3
41	GTP	Q6	501	40	-	6/18/38/38	0/3/3/3
39	GDP	V0	501	-	-	1/12/32/32	0/3/3/3
41	GTP	2L	501	40	-	8/18/38/38	0/3/3/3
39	GDP	0C	502	-	-	3/12/32/32	0/3/3/3
41	GTP	B5	501	40	-	7/18/38/38	0/3/3/3
41	GTP	3A	501	40	-	6/18/38/38	0/3/3/3
41	GTP	3M	501	40	-	6/18/38/38	0/3/3/3
39	GDP	X0	502	-	-	1/12/32/32	0/3/3/3
41	GTP	H3	501	40	-	8/18/38/38	0/3/3/3
41	GTP	W8	501	40	-	7/18/38/38	0/3/3/3
41	GTP	P9	501	40	-	8/18/38/38	0/3/3/3
41	GTP	K1	501	40	-	7/18/38/38	0/3/3/3
41	GTP	R4	501	40	-	8/18/38/38	0/3/3/3
39	GDP	U4	502	-	-	6/12/32/32	0/3/3/3
39	GDP	0G	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	N2	501	-	-	3/12/32/32	0/3/3/3
41	GTP	Y1	501	40	-	7/18/38/38	0/3/3/3
39	GDP	K6	502	-	-	2/12/32/32	0/3/3/3
39	GDP	V4	501	-	-	4/12/32/32	0/3/3/3
39	GDP	S2	502	-	-	5/12/32/32	0/3/3/3
41	GTP	B0	501	40	-	8/18/38/38	0/3/3/3
39	GDP	2G	502	-	-	4/12/32/32	0/3/3/3
39	GDP	J2	502	-	-	7/12/32/32	0/3/3/3
39	GDP	3I	502	-	-	4/12/32/32	0/3/3/3
41	GTP	2S	501	40	-	8/18/38/38	0/3/3/3
39	GDP	0Q	502	-	-	4/12/32/32	0/3/3/3
39	GDP	1U	501	-	-	4/12/32/32	0/3/3/3
41	GTP	G7	501	40	-	7/18/38/38	0/3/3/3
39	GDP	S4	501	-	-	1/12/32/32	0/3/3/3
39	GDP	K8	501	-	-	5/12/32/32	0/3/3/3
41	GTP	1G	501	40	-	9/18/38/38	0/3/3/3
41	GTP	X4	501	40	-	8/18/38/38	0/3/3/3
39	GDP	0O	502	-	-	1/12/32/32	0/3/3/3
39	GDP	Q2	502	-	-	3/12/32/32	0/3/3/3
39	GDP	S8	502	-	-	4/12/32/32	0/3/3/3
41	GTP	1T	501	40	-	7/18/38/38	0/3/3/3
39	GDP	3A	502	-	-	4/12/32/32	0/3/3/3
39	GDP	1O	501	-	-	1/12/32/32	0/3/3/3
41	GTP	G9	501	40	-	9/18/38/38	0/3/3/3
41	GTP	P4	501	40	-	8/18/38/38	0/3/3/3
41	GTP	K6	501	40	-	6/18/38/38	0/3/3/3
41	GTP	K4	501	40	-	8/18/38/38	0/3/3/3
39	GDP	2C	502	-	-	1/12/32/32	0/3/3/3
41	GTP	S9	501	40	-	3/18/38/38	0/3/3/3
39	GDP	F6	501	-	-	4/12/32/32	0/3/3/3
39	GDP	Z0	502	-	-	4/12/32/32	0/3/3/3
39	GDP	C2	501	-	-	2/12/32/32	0/3/3/3
41	GTP	F1	501	40	-	7/18/38/38	0/3/3/3
39	GDP	K0	502	-	-	4/12/32/32	0/3/3/3
41	GTP	D1	501	40	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	J8	501	40	-	6/18/38/38	0/3/3/3
39	GDP	B5	502	-	-	4/12/32/32	0/3/3/3
39	GDP	T2	502	-	-	4/12/32/32	0/3/3/3
39	GDP	X4	502	-	-	4/12/32/32	0/3/3/3
41	GTP	E8	501	40	-	5/18/38/38	0/3/3/3
39	GDP	A5	501	-	-	0/12/32/32	0/3/3/3
39	GDP	M2	502	-	-	1/12/32/32	0/3/3/3
41	GTP	U7	501	40	-	8/18/38/38	0/3/3/3
39	GDP	W6	501	-	-	0/12/32/32	0/3/3/3
41	GTP	H8	501	40	-	9/18/38/38	0/3/3/3
39	GDP	3C	502	-	-	3/12/32/32	0/3/3/3
39	GDP	1C	502	-	-	2/12/32/32	0/3/3/3
41	GTP	3O	501	40	-	6/18/38/38	0/3/3/3
41	GTP	Z6	501	40	-	9/18/38/38	0/3/3/3
39	GDP	D4	501	-	-	6/12/32/32	0/3/3/3
41	GTP	S5	501	40	-	4/18/38/38	0/3/3/3
39	GDP	Y8	501	-	-	3/12/32/32	0/3/3/3
41	GTP	1Q	501	40	-	6/18/38/38	0/3/3/3
41	GTP	K9	501	40	-	6/18/38/38	0/3/3/3
39	GDP	P4	503	-	-	4/12/32/32	0/3/3/3
39	GDP	U2	502	-	-	4/12/32/32	0/3/3/3
41	GTP	I8	501	40	-	7/18/38/38	0/3/3/3
41	GTP	1S	501	40	-	5/18/38/38	0/3/3/3
39	GDP	2Q	502	-	-	2/12/32/32	0/3/3/3
41	GTP	T8	501	40	-	8/18/38/38	0/3/3/3
41	GTP	C1	501	40	-	7/18/38/38	0/3/3/3
41	GTP	G1	501	40	-	9/18/38/38	0/3/3/3
41	GTP	0S	501	40	-	8/18/38/38	0/3/3/3
41	GTP	2U	501	40	-	8/18/38/38	0/3/3/3
41	GTP	0I	501	40	-	9/18/38/38	0/3/3/3
39	GDP	7	502	-	-	2/12/32/32	0/3/3/3
41	GTP	E1	501	40	-	6/18/38/38	0/3/3/3
39	GDP	0W	502	-	-	2/12/32/32	0/3/3/3
41	GTP	D7	501	40	-	4/18/38/38	0/3/3/3
41	GTP	L7	501	40	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	C5	501	40	-	7/18/38/38	0/3/3/3
41	GTP	W4	501	40	-	7/18/38/38	0/3/3/3
39	GDP	2I	502	-	-	5/12/32/32	0/3/3/3
41	GTP	3T	501	40	-	8/18/38/38	0/3/3/3
41	GTP	Y6	501	40	-	8/18/38/38	0/3/3/3
39	GDP	I2	501	-	-	1/12/32/32	0/3/3/3
39	GDP	Q0	501	-	-	4/12/32/32	0/3/3/3
39	GDP	Y4	502	-	-	6/12/32/32	0/3/3/3
41	GTP	N6	501	40	-	7/18/38/38	0/3/3/3
39	GDP	3	502	-	-	3/12/32/32	0/3/3/3
41	GTP	3D	501	40	-	8/18/38/38	0/3/3/3
41	GTP	W5	501	40	-	6/18/38/38	0/3/3/3
41	GTP	0Y	501	40	-	9/18/38/38	0/3/3/3
41	GTP	Z2	501	40	-	9/18/38/38	0/3/3/3
41	GTP	I4	501	40	-	8/18/38/38	0/3/3/3
39	GDP	F8	502	-	-	1/12/32/32	0/3/3/3
39	GDP	T8	502	-	-	3/12/32/32	0/3/3/3
41	GTP	3P	501	40	-	9/18/38/38	0/3/3/3
41	GTP	M6	501	40	-	8/18/38/38	0/3/3/3
39	GDP	D8	501	-	-	2/12/32/32	0/3/3/3
41	GTP	I5	501	40	-	9/18/38/38	0/3/3/3
39	GDP	M0	502	-	-	3/12/32/32	0/3/3/3
41	GTP	L2	501	40	-	7/18/38/38	0/3/3/3
39	GDP	3M	502	-	-	7/12/32/32	0/3/3/3
39	GDP	0I	502	-	-	1/12/32/32	0/3/3/3
39	GDP	3K	503	-	-	4/12/32/32	0/3/3/3
39	GDP	T0	501	-	-	4/12/32/32	0/3/3/3
41	GTP	0O	501	40	-	9/18/38/38	0/3/3/3
41	GTP	Q2	501	40	-	6/18/38/38	0/3/3/3
41	GTP	S8	501	40	-	7/18/38/38	0/3/3/3
39	GDP	R6	503	-	-	3/12/32/32	0/3/3/3
41	GTP	U9	501	40	-	8/18/38/38	0/3/3/3
41	GTP	1H	501	40	-	9/18/38/38	0/3/3/3
41	GTP	T6	501	40	-	5/18/38/38	0/3/3/3
41	GTP	2E	501	40	-	9/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	N8	502	-	-	7/12/32/32	0/3/3/3
41	GTP	V8	501	40	-	7/18/38/38	0/3/3/3
41	GTP	1W	501	40	-	7/18/38/38	0/3/3/3
39	GDP	T6	502	-	-	7/12/32/32	0/3/3/3
41	GTP	J6	501	40	-	8/18/38/38	0/3/3/3
41	GTP	S2	501	40	-	6/18/38/38	0/3/3/3
39	GDP	3Q	501	-	-	3/12/32/32	0/3/3/3
41	GTP	J2	501	40	-	8/18/38/38	0/3/3/3
41	GTP	0Q	501	40	-	8/18/38/38	0/3/3/3
39	GDP	E0	501	-	-	3/12/32/32	0/3/3/3
39	GDP	2U	502	-	-	5/12/32/32	0/3/3/3
41	GTP	R8	501	40	-	6/18/38/38	0/3/3/3
39	GDP	0E	501	-	-	2/12/32/32	0/3/3/3
39	GDP	I4	502	-	-	1/12/32/32	0/3/3/3
39	GDP	Q4	502	-	-	6/12/32/32	0/3/3/3
41	GTP	3G	501	40	-	8/18/38/38	0/3/3/3
39	GDP	M6	502	-	-	5/12/32/32	0/3/3/3
41	GTP	0F	501	40	-	9/18/38/38	0/3/3/3
41	GTP	G0	501	40	-	9/18/38/38	0/3/3/3
39	GDP	Y6	502	-	-	6/12/32/32	0/3/3/3
39	GDP	C6	501	-	-	4/12/32/32	0/3/3/3
39	GDP	3S	502	-	-	4/12/32/32	0/3/3/3
41	GTP	U4	501	40	-	7/18/38/38	0/3/3/3
39	GDP	Z2	503	-	-	1/12/32/32	0/3/3/3
41	GTP	E4	501	40	-	6/18/38/38	0/3/3/3
39	GDP	H6	502	-	-	1/12/32/32	0/3/3/3
39	GDP	R8	502	-	-	3/12/32/32	0/3/3/3
39	GDP	V6	501	-	-	4/12/32/32	0/3/3/3
39	GDP	H2	503	-	-	0/12/32/32	0/3/3/3
41	GTP	K7	501	40	-	9/18/38/38	0/3/3/3
39	GDP	1W	502	-	-	1/12/32/32	0/3/3/3
39	GDP	X8	501	-	-	3/12/32/32	0/3/3/3
39	GDP	E6	502	-	-	6/12/32/32	0/3/3/3
41	GTP	I1	501	40	-	9/18/38/38	0/3/3/3
39	GDP	B8	501	-	-	6/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	D0	501	-	-	8/12/32/32	0/3/3/3
39	GDP	1G	502	-	-	0/12/32/32	0/3/3/3
39	GDP	P8	502	-	-	3/12/32/32	0/3/3/3
41	GTP	U2	501	40	-	7/18/38/38	0/3/3/3
41	GTP	A2	501	40	-	2/18/38/38	0/3/3/3
39	GDP	B1	501	-	-	2/12/32/32	0/3/3/3
41	GTP	W0	501	40	-	8/18/38/38	0/3/3/3
39	GDP	J4	503	-	-	4/12/32/32	0/3/3/3
41	GTP	2C	501	40	-	9/18/38/38	0/3/3/3
41	GTP	G4	501	40	-	7/18/38/38	0/3/3/3
39	GDP	O0	503	-	-	3/12/32/32	0/3/3/3
39	GDP	Z4	501	-	-	1/12/32/32	0/3/3/3
39	GDP	H8	503	-	-	4/12/32/32	0/3/3/3
39	GDP	E4	502	-	-	5/12/32/32	0/3/3/3
39	GDP	O4	502	-	-	6/12/32/32	0/3/3/3
41	GTP	7	501	40	-	8/18/38/38	0/3/3/3
39	GDP	V2	503	-	-	3/12/32/32	0/3/3/3
39	GDP	Z8	501	-	-	1/12/32/32	0/3/3/3
41	GTP	0M	501	40	-	7/18/38/38	0/3/3/3
41	GTP	F0	501	40	-	6/18/38/38	0/3/3/3
41	GTP	2W	501	40	-	8/18/38/38	0/3/3/3
41	GTP	1X	501	40	-	7/18/38/38	0/3/3/3
41	GTP	X7	501	40	-	9/18/38/38	0/3/3/3
41	GTP	H2	501	40	-	8/18/38/38	0/3/3/3
41	GTP	A1	501	40	-	9/18/38/38	0/3/3/3
39	GDP	3O	502	-	-	5/12/32/32	0/3/3/3
41	GTP	2Q	501	40	-	8/18/38/38	0/3/3/3
39	GDP	E8	502	-	-	4/12/32/32	0/3/3/3
41	GTP	R0	501	40	-	8/18/38/38	0/3/3/3
39	GDP	V8	502	-	-	3/12/32/32	0/3/3/3
39	GDP	A9	502	-	-	3/12/32/32	0/3/3/3
39	GDP	G4	502	-	-	1/12/32/32	0/3/3/3
39	GDP	W0	502	-	-	5/12/32/32	0/3/3/3
39	GDP	Y0	502	-	-	5/12/32/32	0/3/3/3
41	GTP	3K	501	40	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	1N	501	40	-	8/18/38/38	0/3/3/3
41	GTP	1A	501	40	-	9/18/38/38	0/3/3/3
41	GTP	M0	501	40	-	8/18/38/38	0/3/3/3
41	GTP	C0	501	40	-	8/18/38/38	0/3/3/3
41	GTP	R6	501	40	-	6/18/38/38	0/3/3/3
39	GDP	W2	503	-	-	1/12/32/32	0/3/3/3
39	GDP	M4	502	-	-	4/12/32/32	0/3/3/3
39	GDP	3G	502	-	-	3/12/32/32	0/3/3/3
41	GTP	O6	501	40	-	7/18/38/38	0/3/3/3
41	GTP	U6	501	40	-	8/18/38/38	0/3/3/3
39	GDP	2	501	-	-	6/12/32/32	0/3/3/3
39	GDP	G0	502	-	-	1/12/32/32	0/3/3/3
41	GTP	E6	501	40	-	8/18/38/38	0/3/3/3
41	GTP	1D	501	40	-	7/18/38/38	0/3/3/3
39	GDP	G8	501	-	-	1/12/32/32	0/3/3/3
41	GTP	0V	501	40	-	9/18/38/38	0/3/3/3
41	GTP	0K	501	40	-	8/18/38/38	0/3/3/3
39	GDP	2W	502	-	-	5/12/32/32	0/3/3/3
39	GDP	O2	502	-	-	5/12/32/32	0/3/3/3
41	GTP	3	501	40	-	5/18/38/38	0/3/3/3
41	GTP	B2	501	40	-	4/18/38/38	0/3/3/3
41	GTP	F3	501	40	-	5/18/38/38	0/3/3/3
39	GDP	S0	502	-	-	4/12/32/32	0/3/3/3
41	GTP	W2	501	40	-	7/18/38/38	0/3/3/3
39	GDP	M8	501	-	-	4/12/32/32	0/3/3/3
41	GTP	O2	501	40	-	9/18/38/38	0/3/3/3
41	GTP	4	501	40	-	6/18/38/38	0/3/3/3
41	GTP	Z7	501	40	-	7/18/38/38	0/3/3/3
41	GTP	T2	501	40	-	6/18/38/38	0/3/3/3
41	GTP	2K	501	40	-	8/18/38/38	0/3/3/3
39	GDP	F2	501	-	-	3/12/32/32	0/3/3/3
39	GDP	B3	501	-	-	4/12/32/32	0/3/3/3
41	GTP	X6	501	40	-	7/18/38/38	0/3/3/3
41	GTP	3C	501	40	-	6/18/38/38	0/3/3/3
41	GTP	X0	501	40	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	0A	501	40	-	9/18/38/38	0/3/3/3
39	GDP	0M	502	-	-	2/12/32/32	0/3/3/3
39	GDP	U8	501	-	-	3/12/32/32	0/3/3/3
41	GTP	2I	501	40	-	7/18/38/38	0/3/3/3
39	GDP	C0	502	-	-	3/12/32/32	0/3/3/3
41	GTP	3S	501	40	-	7/18/38/38	0/3/3/3
41	GTP	0C	501	40	-	8/18/38/38	0/3/3/3
39	GDP	O6	502	-	-	4/12/32/32	0/3/3/3
41	GTP	N1	501	40	-	7/18/38/38	0/3/3/3
41	GTP	N8	501	40	-	8/18/38/38	0/3/3/3
41	GTP	3I	501	40	-	8/18/38/38	0/3/3/3
39	GDP	R4	502	-	-	7/12/32/32	0/3/3/3
39	GDP	O8	503	-	-	1/12/32/32	0/3/3/3
39	GDP	D2	501	-	-	4/12/32/32	0/3/3/3
39	GDP	L0	501	-	-	2/12/32/32	0/3/3/3
39	GDP	R0	502	-	-	4/12/32/32	0/3/3/3
39	GDP	0A	503	-	-	1/12/32/32	0/3/3/3
39	GDP	0K	502	-	-	2/12/32/32	0/3/3/3
41	GTP	M7	501	40	-	8/18/38/38	0/3/3/3
41	GTP	P6	501	40	-	8/18/38/38	0/3/3/3
39	GDP	J8	502	-	-	2/12/32/32	0/3/3/3
41	GTP	J0	501	40	-	8/18/38/38	0/3/3/3
39	GDP	S6	501	-	-	7/12/32/32	0/3/3/3
41	GTP	R2	501	40	-	6/18/38/38	0/3/3/3
39	GDP	I0	502	-	-	1/12/32/32	0/3/3/3
39	GDP	J6	502	-	-	1/12/32/32	0/3/3/3
39	GDP	J0	502	-	-	1/12/32/32	0/3/3/3
41	GTP	D5	501	40	-	4/18/38/38	0/3/3/3
39	GDP	D6	501	-	-	6/12/32/32	0/3/3/3
41	GTP	J4	501	40	-	6/18/38/38	0/3/3/3
39	GDP	1M	501	-	-	1/12/32/32	0/3/3/3
41	GTP	1C	501	40	-	8/18/38/38	0/3/3/3
39	GDP	Q6	502	-	-	6/12/32/32	0/3/3/3
39	GDP	U6	502	-	-	2/12/32/32	0/3/3/3
41	GTP	O0	501	40	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	A1	502	-	-	6/12/32/32	0/3/3/3
41	GTP	S0	501	40	-	8/18/38/38	0/3/3/3
39	GDP	2A	502	-	-	0/12/32/32	0/3/3/3
41	GTP	V2	501	40	-	6/18/38/38	0/3/3/3
39	GDP	L4	502	-	-	1/12/32/32	0/3/3/3
39	GDP	E2	501	-	-	5/12/32/32	0/3/3/3
39	GDP	1S	502	-	-	1/12/32/32	0/3/3/3
41	GTP	H6	501	40	-	9/18/38/38	0/3/3/3
41	GTP	Z0	501	40	-	8/18/38/38	0/3/3/3
41	GTP	T4	501	40	-	5/18/38/38	0/3/3/3
39	GDP	Y2	501	-	-	2/12/32/32	0/3/3/3

The worst 5 of 470 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	R0	501	GTP	C5-C6	-4.90	1.37	1.47
41	P4	501	GTP	C5-C6	-4.87	1.37	1.47
41	Z3	501	GTP	C5-C6	-4.86	1.37	1.47
41	P6	501	GTP	C5-C6	-4.86	1.37	1.47
41	2S	501	GTP	C5-C6	-4.83	1.37	1.47

The worst 5 of 1099 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	S9	501	GTP	C4'-O4'-C1'	-4.69	105.63	109.92
41	X7	501	GTP	C4'-O4'-C1'	-3.87	106.38	109.92
41	2C	501	GTP	C8-N7-C5	3.87	109.13	102.55
41	J8	501	GTP	C8-N7-C5	3.83	109.07	102.55
41	L4	501	GTP	C8-N7-C5	3.83	109.07	102.55

There are no chirality outliers.

5 of 1774 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	2	501	GDP	PA-O3A-PB-O3B
39	2	501	GDP	C5'-O5'-PA-O3A
39	2	501	GDP	C5'-O5'-PA-O1A
39	3	502	GDP	C5'-O5'-PA-O3A
39	3	502	GDP	C5'-O5'-PA-O2A

There are no ring outliers.

241 monomers are involved in 397 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	8	501	GTP	1	0
39	W8	503	GDP	2	0
41	K0	501	GTP	2	0
41	Q4	501	GTP	1	0
41	A4	501	GTP	2	0
41	L4	501	GTP	3	0
41	G5	501	GTP	3	0
41	N0	501	GTP	1	0
41	F5	501	GTP	2	0
41	C8	501	GTP	1	0
41	1L	501	GTP	1	0
39	1Q	502	GDP	1	0
41	B7	501	GTP	1	0
41	Y0	501	GTP	3	0
39	H4	501	GDP	1	0
41	O4	501	GTP	2	0
39	C4	501	GDP	3	0
41	L6	501	GTP	1	0
39	K4	502	GDP	1	0
41	D3	501	GTP	2	0
39	F0	502	GDP	2	0
39	2M	501	GDP	2	0
41	Y4	501	GTP	2	0
41	Z3	501	GTP	2	0
39	9	501	GDP	1	0
41	P8	501	GTP	2	0
39	X2	501	GDP	3	0
39	1K	501	GDP	1	0
39	0Y	502	GDP	1	0
39	2E	502	GDP	1	0
39	L2	502	GDP	1	0
39	X6	502	GDP	3	0
39	A7	501	GDP	2	0
41	O8	501	GTP	1	0
39	C8	502	GDP	3	0
39	5	501	GDP	1	0
39	0U	501	GDP	1	0
41	F8	501	GTP	1	0
41	C9	501	GTP	5	0
39	1A	503	GDP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	2N	501	GTP	1	0
41	O9	501	GTP	1	0
41	2G	501	GTP	2	0
41	A9	501	GTP	1	0
39	N6	503	GDP	2	0
39	0S	502	GDP	2	0
41	I0	501	GTP	1	0
39	L6	502	GDP	1	0
39	2K	502	GDP	2	0
39	Z6	502	GDP	2	0
41	Q6	501	GTP	1	0
41	2L	501	GTP	1	0
39	0C	502	GDP	2	0
41	B5	501	GTP	2	0
41	3M	501	GTP	1	0
39	X0	502	GDP	2	0
41	H3	501	GTP	1	0
41	P9	501	GTP	2	0
39	0G	501	GDP	2	0
39	N2	501	GDP	1	0
41	Y1	501	GTP	2	0
39	V4	501	GDP	1	0
39	S2	502	GDP	1	0
41	B0	501	GTP	2	0
39	2G	502	GDP	3	0
39	J2	502	GDP	1	0
39	3I	502	GDP	1	0
39	0Q	502	GDP	1	0
41	G7	501	GTP	2	0
39	S4	501	GDP	1	0
41	1G	501	GTP	1	0
41	X4	501	GTP	3	0
39	0O	502	GDP	1	0
39	Q2	502	GDP	1	0
39	S8	502	GDP	1	0
41	1T	501	GTP	1	0
39	3A	502	GDP	1	0
39	1O	501	GDP	1	0
41	G9	501	GTP	1	0
41	P4	501	GTP	3	0
41	K6	501	GTP	3	0
41	K4	501	GTP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	2C	502	GDP	1	0
41	S9	501	GTP	2	0
39	Z0	502	GDP	2	0
41	F1	501	GTP	1	0
41	D1	501	GTP	1	0
41	J8	501	GTP	1	0
39	X4	502	GDP	2	0
41	E8	501	GTP	3	0
39	A5	501	GDP	1	0
41	H8	501	GTP	1	0
39	3C	502	GDP	1	0
39	1C	502	GDP	1	0
41	3O	501	GTP	1	0
41	Z6	501	GTP	2	0
39	D4	501	GDP	3	0
39	Y8	501	GDP	2	0
41	1Q	501	GTP	1	0
41	K9	501	GTP	2	0
39	P4	503	GDP	1	0
39	U2	502	GDP	1	0
41	I8	501	GTP	1	0
41	1S	501	GTP	1	0
41	T8	501	GTP	2	0
41	C1	501	GTP	2	0
41	G1	501	GTP	2	0
41	0S	501	GTP	2	0
41	2U	501	GTP	1	0
41	0I	501	GTP	3	0
39	7	502	GDP	3	0
41	E1	501	GTP	3	0
39	0W	502	GDP	2	0
41	D7	501	GTP	2	0
41	C5	501	GTP	2	0
41	Y6	501	GTP	2	0
39	Y4	502	GDP	3	0
41	N6	501	GTP	3	0
39	3	502	GDP	2	0
41	3D	501	GTP	2	0
41	W5	501	GTP	1	0
41	0Y	501	GTP	1	0
41	Z2	501	GTP	2	0
41	I4	501	GTP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	D8	501	GDP	1	0
41	L2	501	GTP	2	0
39	0I	502	GDP	1	0
39	3K	503	GDP	1	0
39	T0	501	GDP	2	0
41	0O	501	GTP	2	0
41	Q2	501	GTP	1	0
41	S8	501	GTP	1	0
39	R6	503	GDP	1	0
41	1H	501	GTP	2	0
41	T6	501	GTP	3	0
41	2E	501	GTP	2	0
39	N8	502	GDP	3	0
41	1W	501	GTP	1	0
39	T6	502	GDP	3	0
41	J6	501	GTP	1	0
41	S2	501	GTP	1	0
39	3Q	501	GDP	1	0
41	J2	501	GTP	1	0
41	0Q	501	GTP	3	0
39	E0	501	GDP	4	0
39	0E	501	GDP	3	0
39	Q4	502	GDP	1	0
41	0F	501	GTP	3	0
41	G0	501	GTP	3	0
39	Y6	502	GDP	2	0
39	C6	501	GDP	3	0
39	3S	502	GDP	1	0
41	U4	501	GTP	1	0
39	Z2	503	GDP	3	0
41	E4	501	GTP	1	0
39	H6	502	GDP	1	0
39	V6	501	GDP	1	0
39	H2	503	GDP	1	0
41	K7	501	GTP	2	0
39	1W	502	GDP	2	0
39	X8	501	GDP	1	0
39	E6	502	GDP	1	0
41	I1	501	GTP	1	0
39	B8	501	GDP	2	0
39	D0	501	GDP	5	0
39	P8	502	GDP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	A2	501	GTP	1	0
39	B1	501	GDP	1	0
41	2C	501	GTP	2	0
41	G4	501	GTP	2	0
39	Z4	501	GDP	1	0
39	Z8	501	GDP	3	0
41	0M	501	GTP	3	0
41	F0	501	GTP	2	0
41	2W	501	GTP	1	0
41	1X	501	GTP	1	0
41	X7	501	GTP	2	0
41	H2	501	GTP	1	0
41	A1	501	GTP	2	0
39	3O	502	GDP	1	0
41	2Q	501	GTP	1	0
39	E8	502	GDP	1	0
41	R0	501	GTP	1	0
39	V8	502	GDP	1	0
39	G4	502	GDP	1	0
39	W0	502	GDP	2	0
39	Y0	502	GDP	2	0
41	1N	501	GTP	1	0
41	1A	501	GTP	1	0
41	C0	501	GTP	2	0
41	R6	501	GTP	1	0
39	W2	503	GDP	1	0
41	O6	501	GTP	1	0
41	U6	501	GTP	1	0
41	E6	501	GTP	2	0
41	1D	501	GTP	1	0
39	G8	501	GDP	1	0
41	0V	501	GTP	1	0
41	0K	501	GTP	2	0
39	O2	502	GDP	2	0
41	3	501	GTP	1	0
41	F3	501	GTP	2	0
41	4	501	GTP	1	0
41	Z7	501	GTP	2	0
41	T2	501	GTP	2	0
39	F2	501	GDP	3	0
39	B3	501	GDP	1	0
41	X6	501	GTP	3	0

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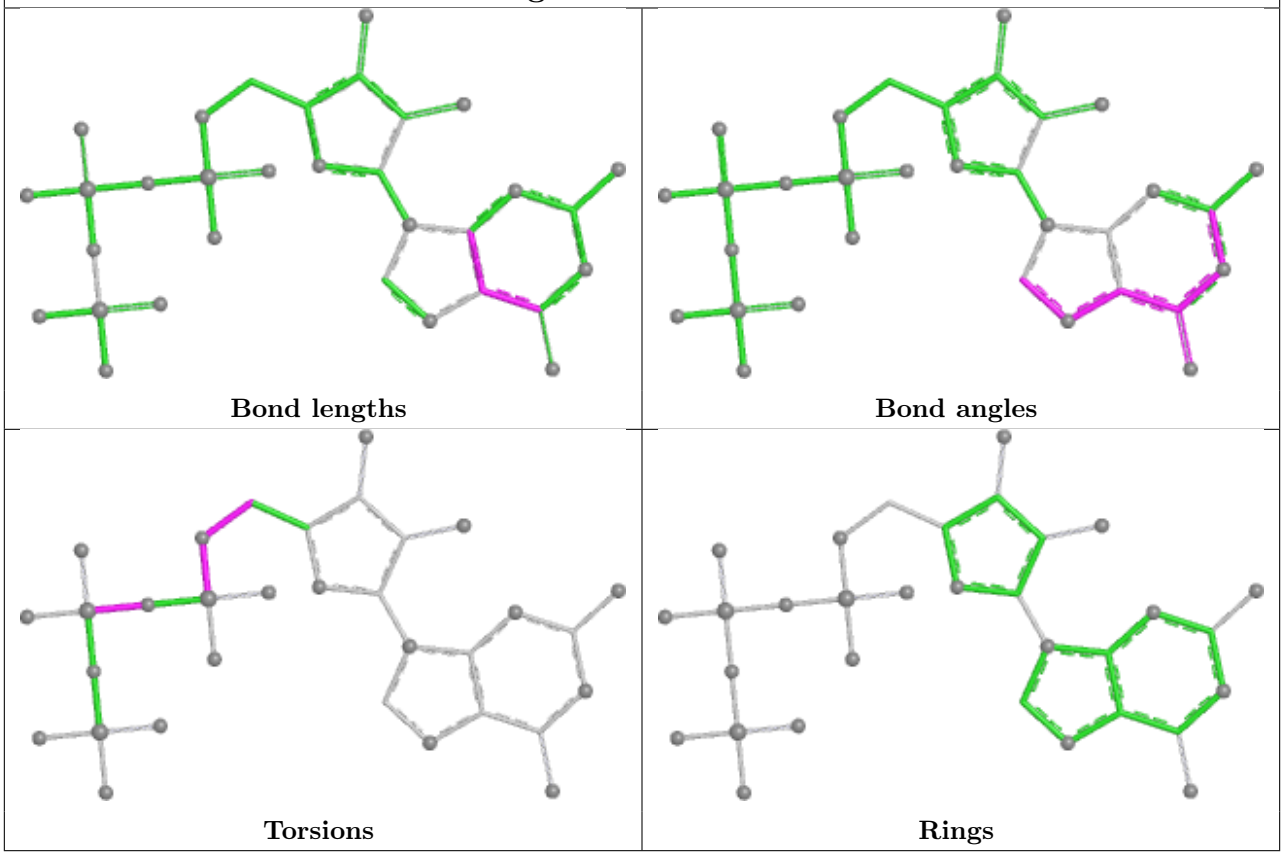
Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	X0	501	GTP	1	0
41	0A	501	GTP	2	0
39	0M	502	GDP	1	0
41	2I	501	GTP	1	0
41	0C	501	GTP	3	0
39	O6	502	GDP	1	0
41	N8	501	GTP	2	0
39	R4	502	GDP	1	0
39	O8	503	GDP	1	0
39	D2	501	GDP	2	0
39	0A	503	GDP	1	0
39	0K	502	GDP	1	0
41	M7	501	GTP	1	0
41	P6	501	GTP	2	0
39	J8	502	GDP	1	0
41	J0	501	GTP	1	0
41	R2	501	GTP	1	0
39	J6	502	GDP	1	0
41	D5	501	GTP	1	0
39	D6	501	GDP	3	0
41	J4	501	GTP	1	0
39	1M	501	GDP	1	0
41	1C	501	GTP	1	0
39	Q6	502	GDP	2	0
41	O0	501	GTP	1	0
41	S0	501	GTP	1	0
39	L4	502	GDP	2	0
39	E2	501	GDP	2	0
39	1S	502	GDP	1	0
41	H6	501	GTP	1	0
41	Z0	501	GTP	1	0
41	T4	501	GTP	3	0
39	Y2	501	GDP	2	0

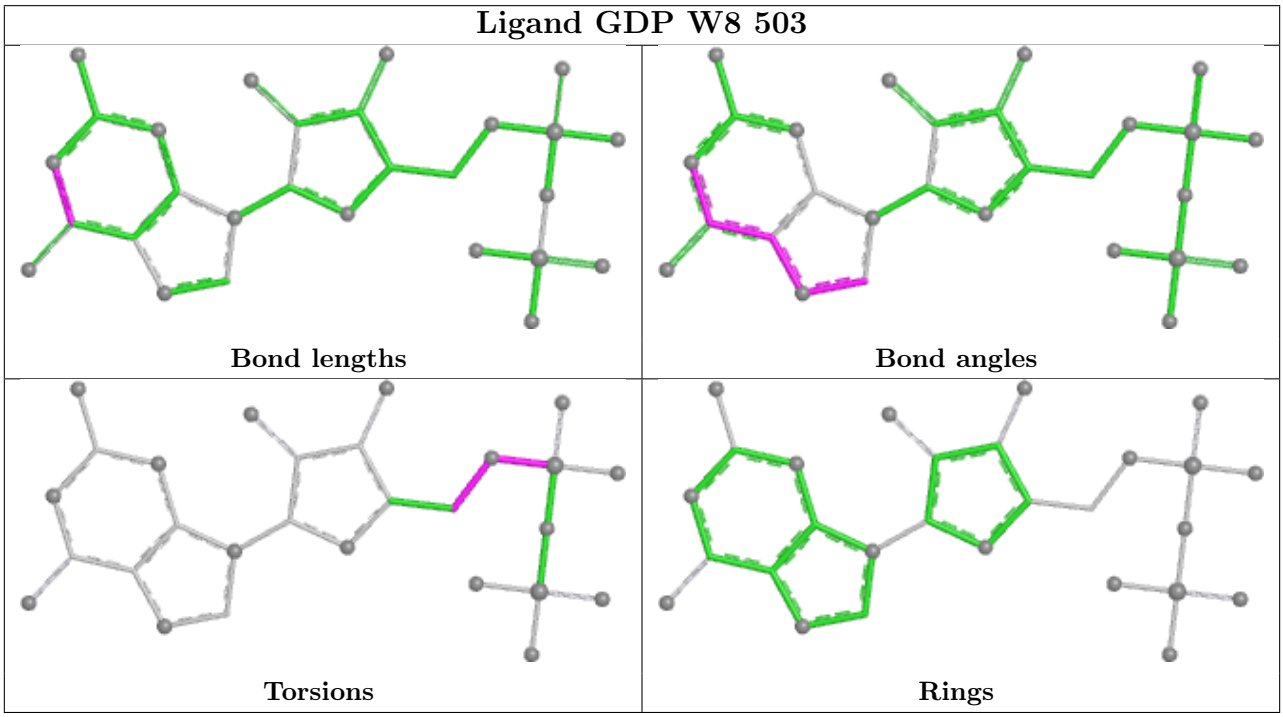
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

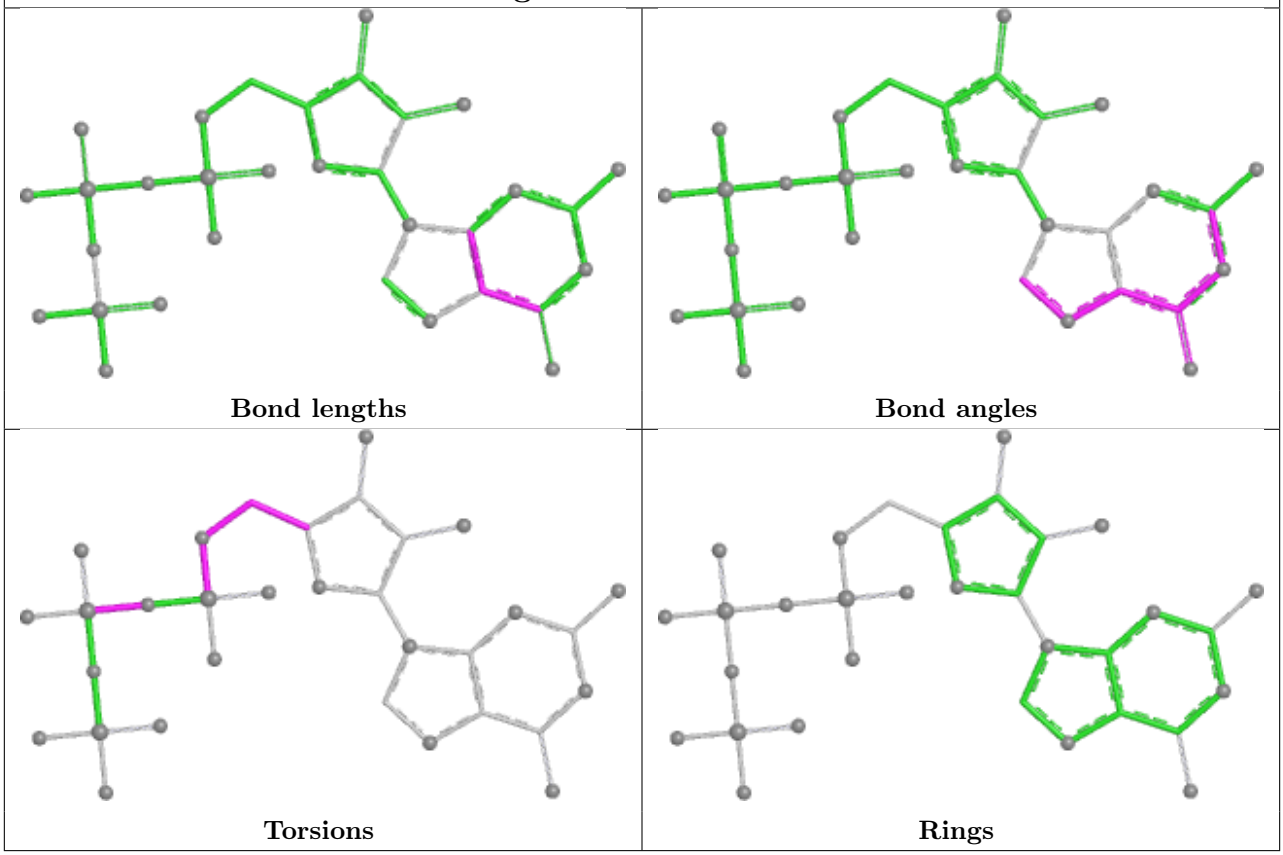
Ligand GTP 8 501



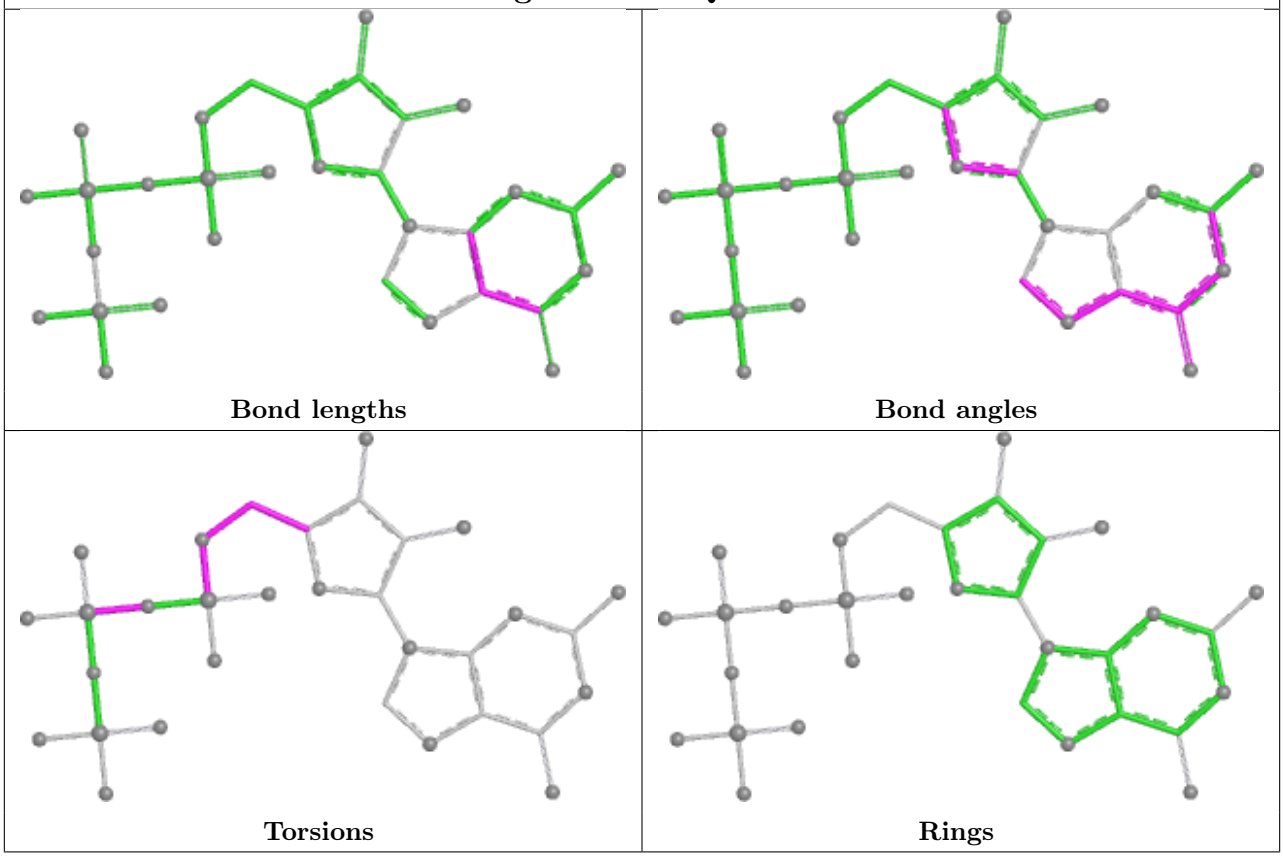
Ligand GDP W8 503



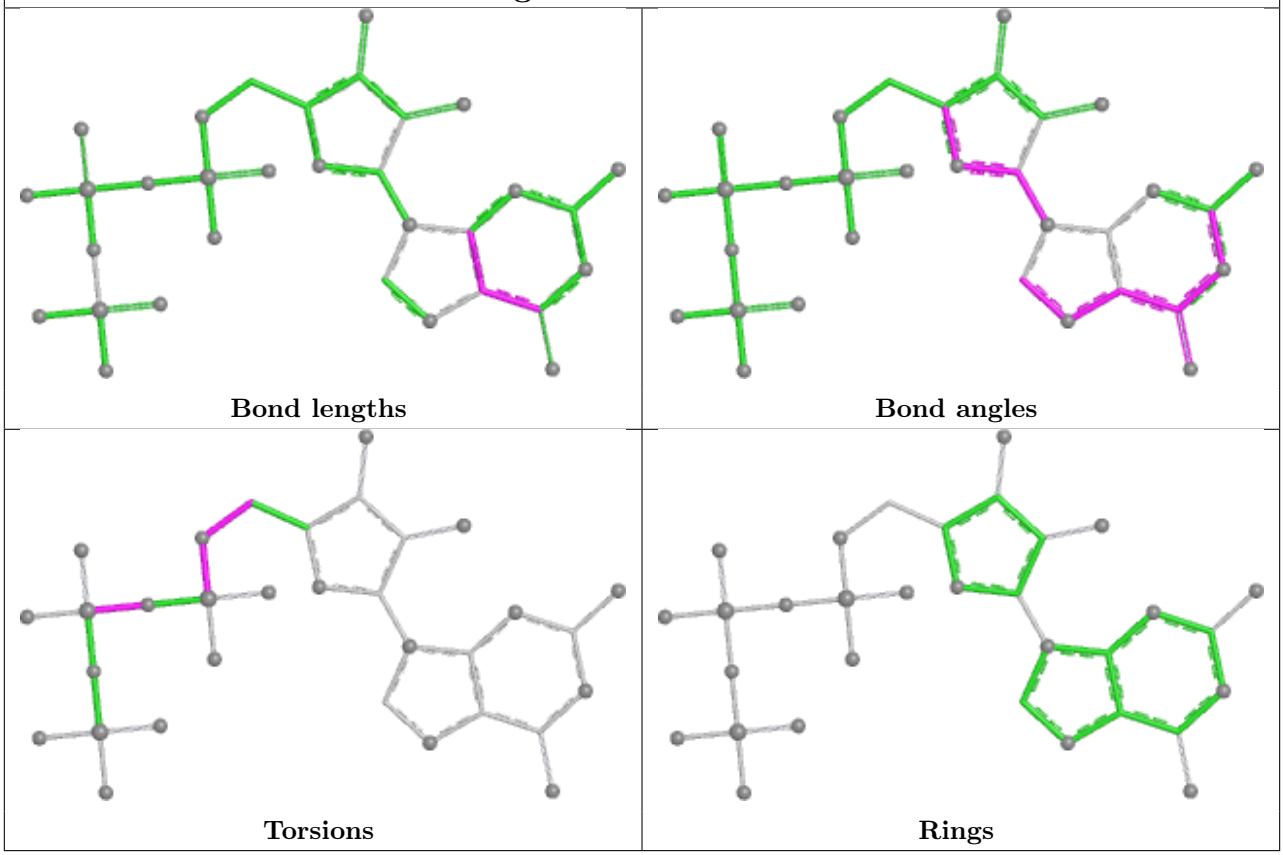
Ligand GTP K0 501



Ligand GTP Q4 501



Ligand GTP A4 501



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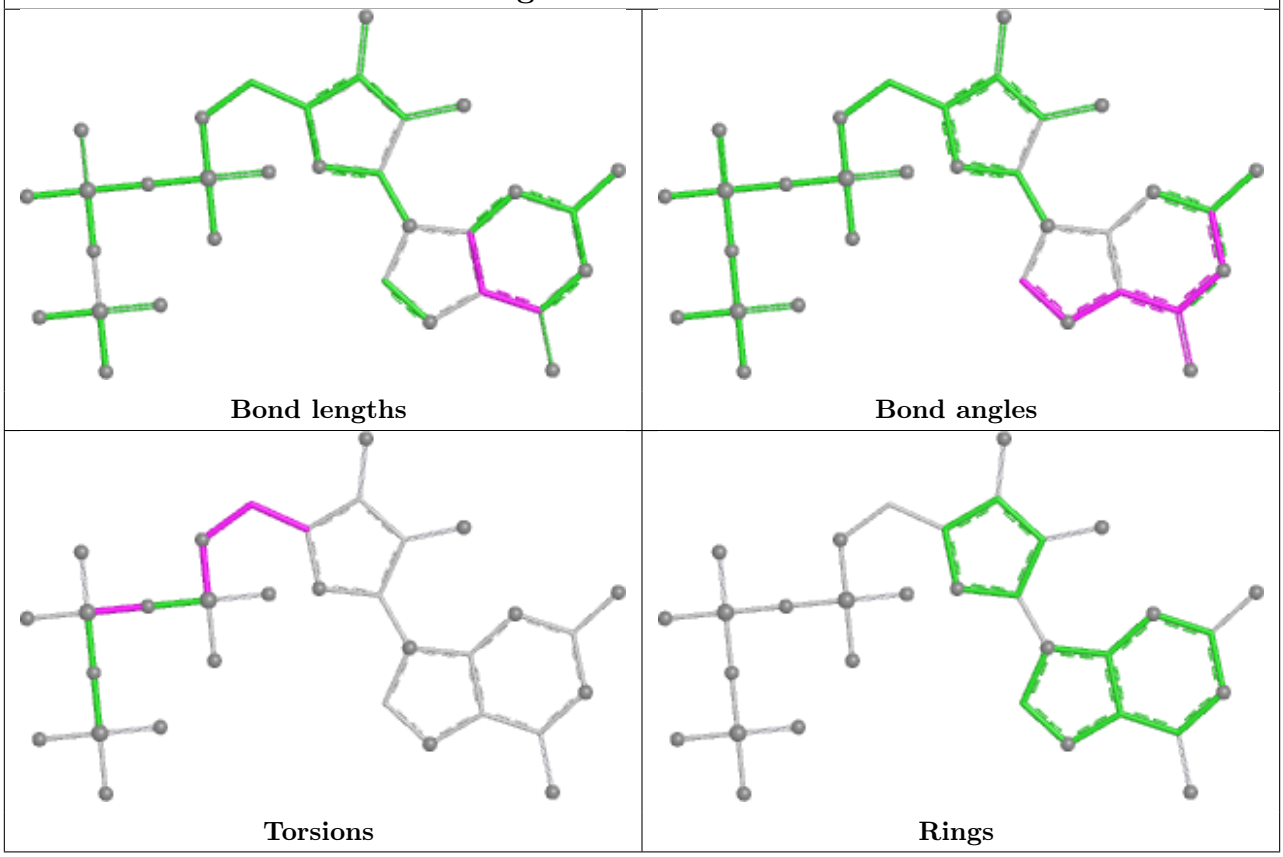
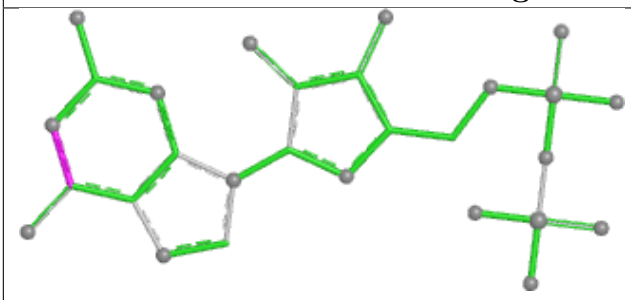


Ligand GDP 2Y 502



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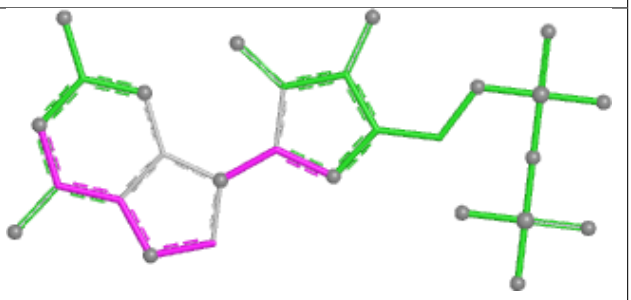
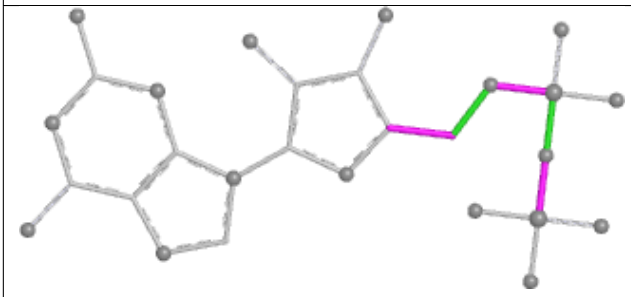
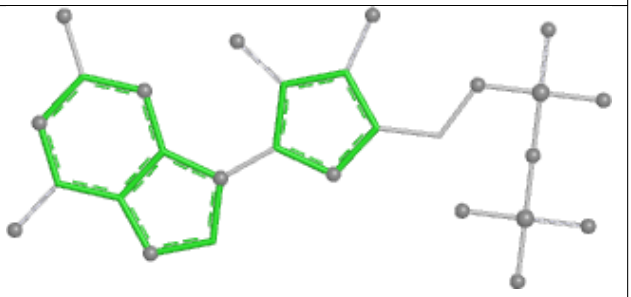


Bond angles

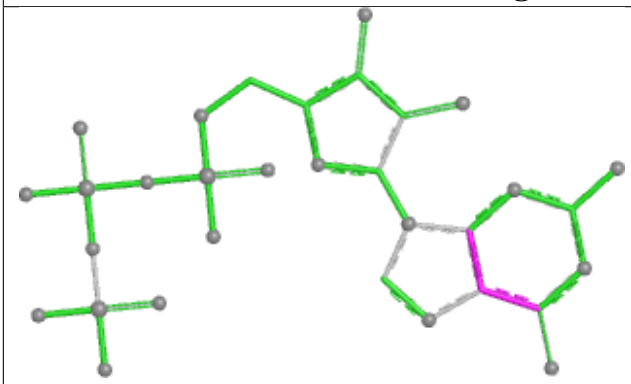


Torsions



Rings

Ligand GTP G5 501



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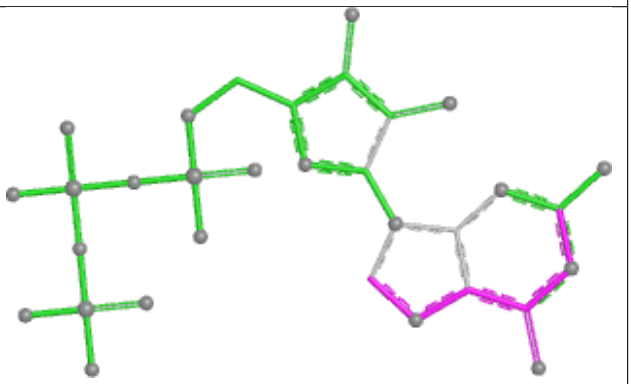
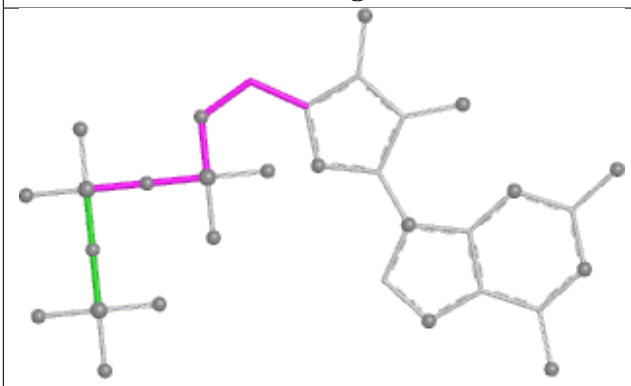
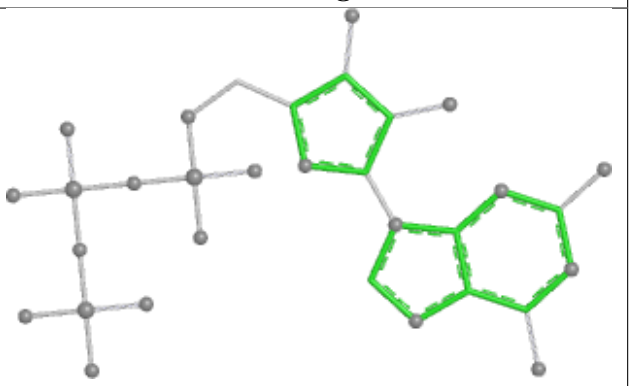


Bond angles

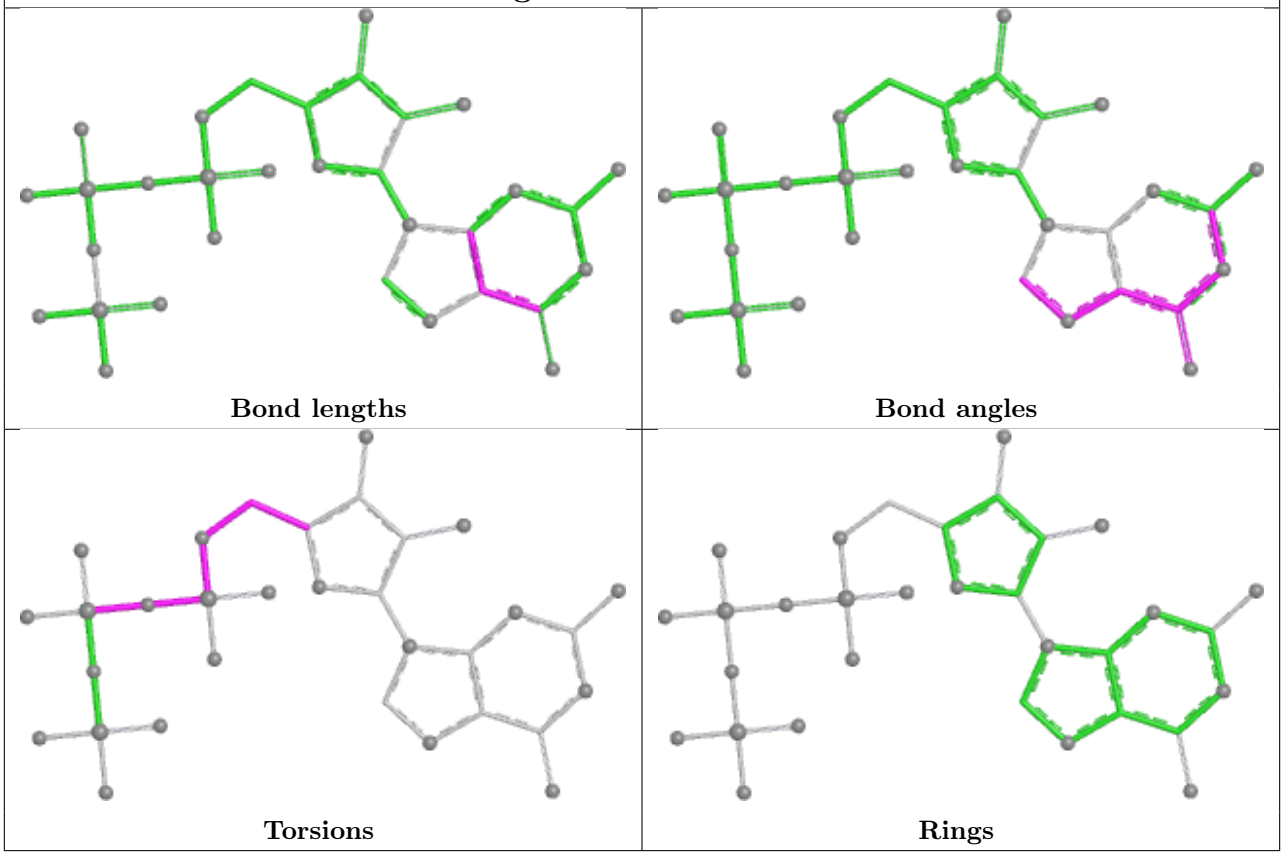


Torsions

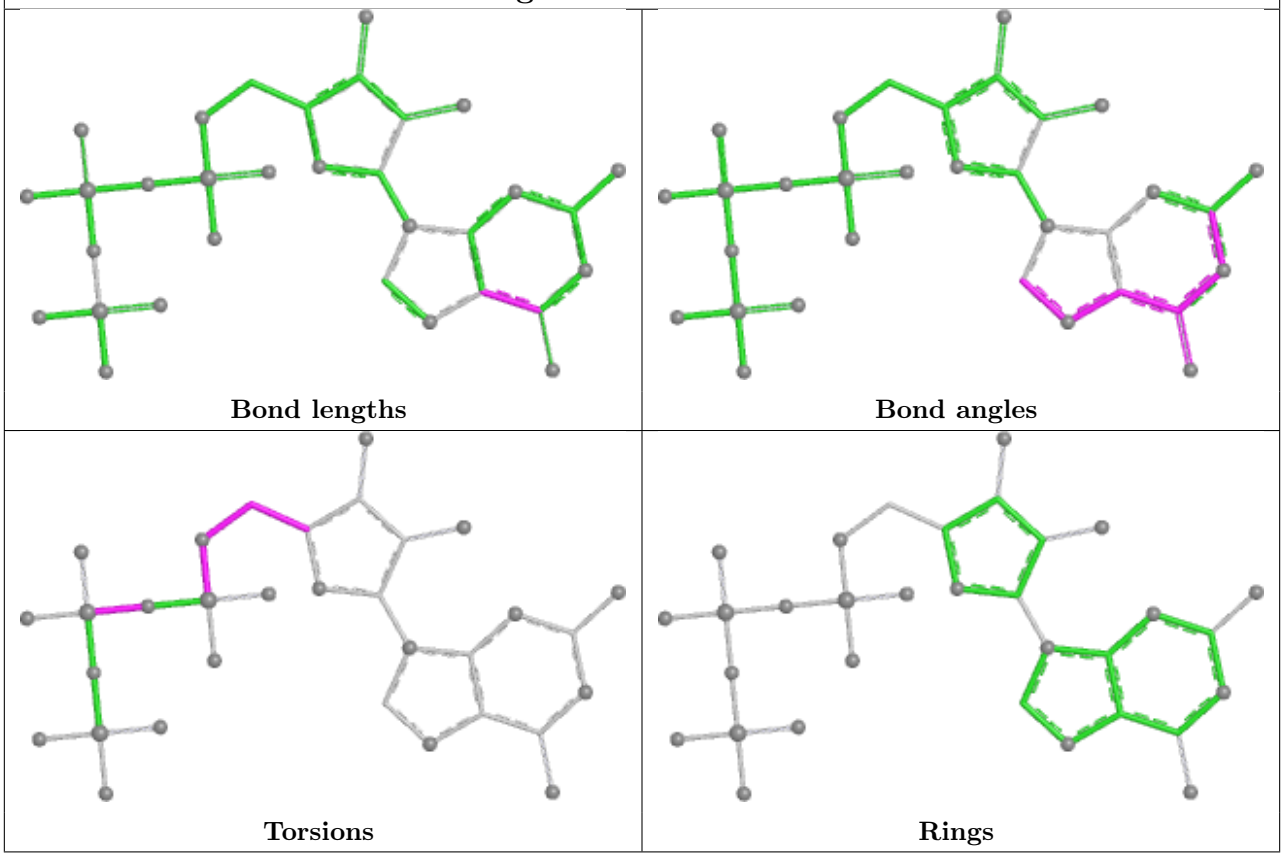


Rings

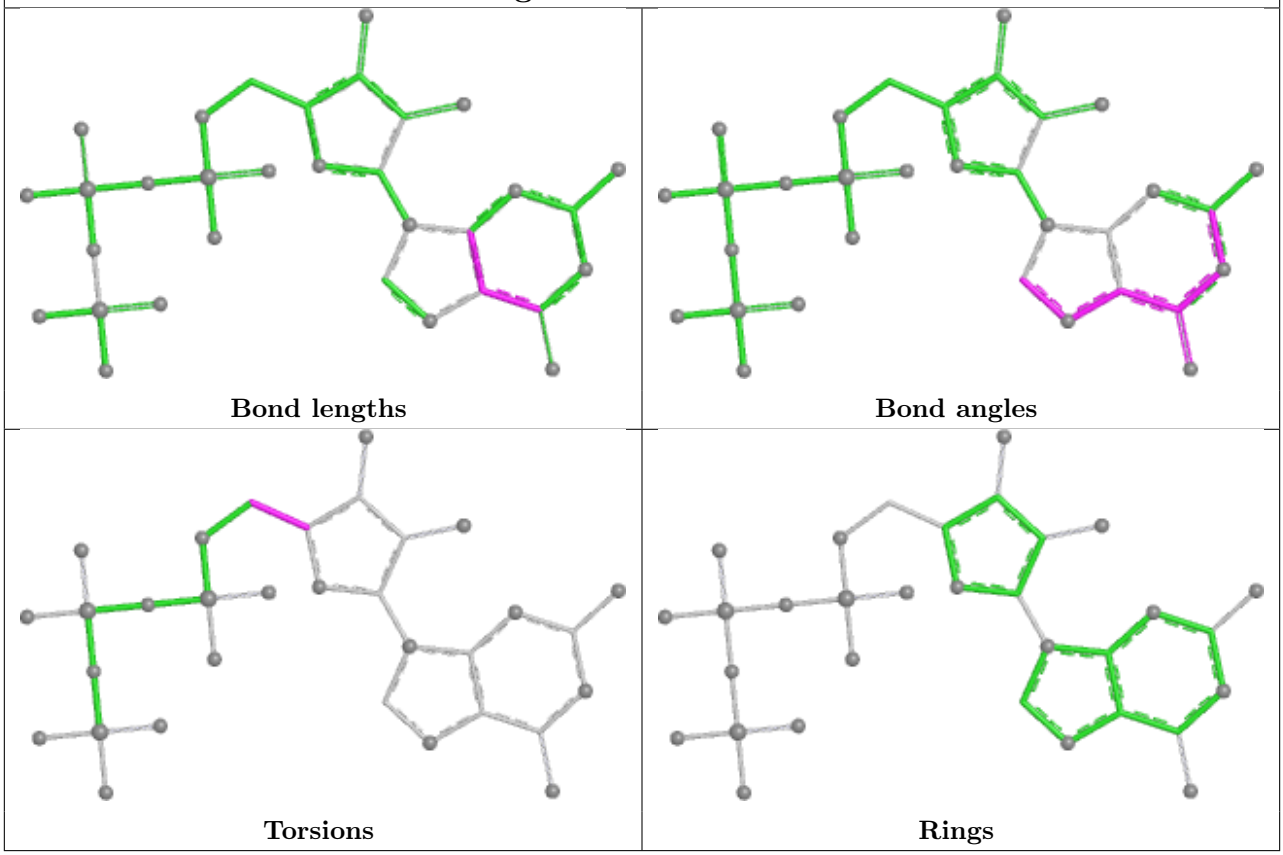
Ligand GTP N0 501



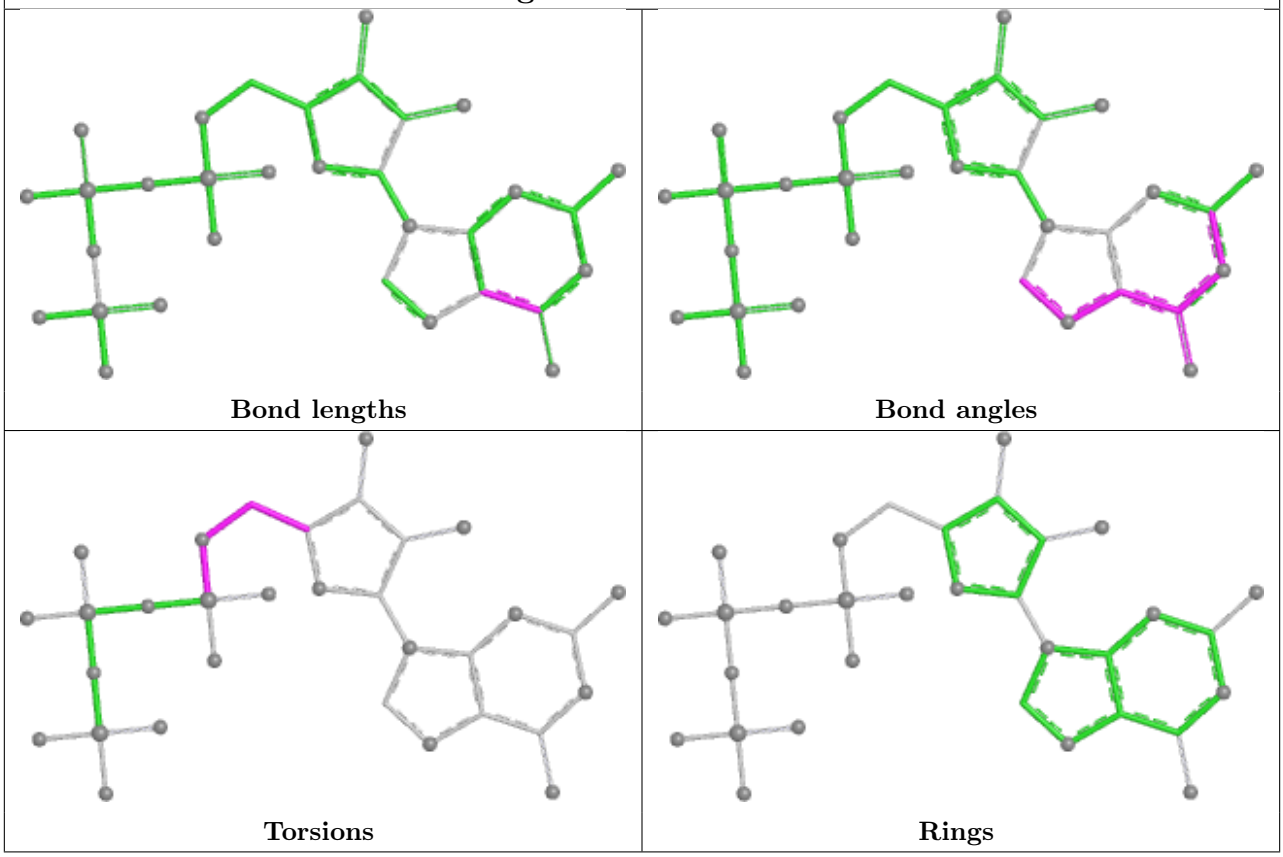
Ligand GTP F5 501



Ligand GTP C8 501



Ligand GTP 1L 501



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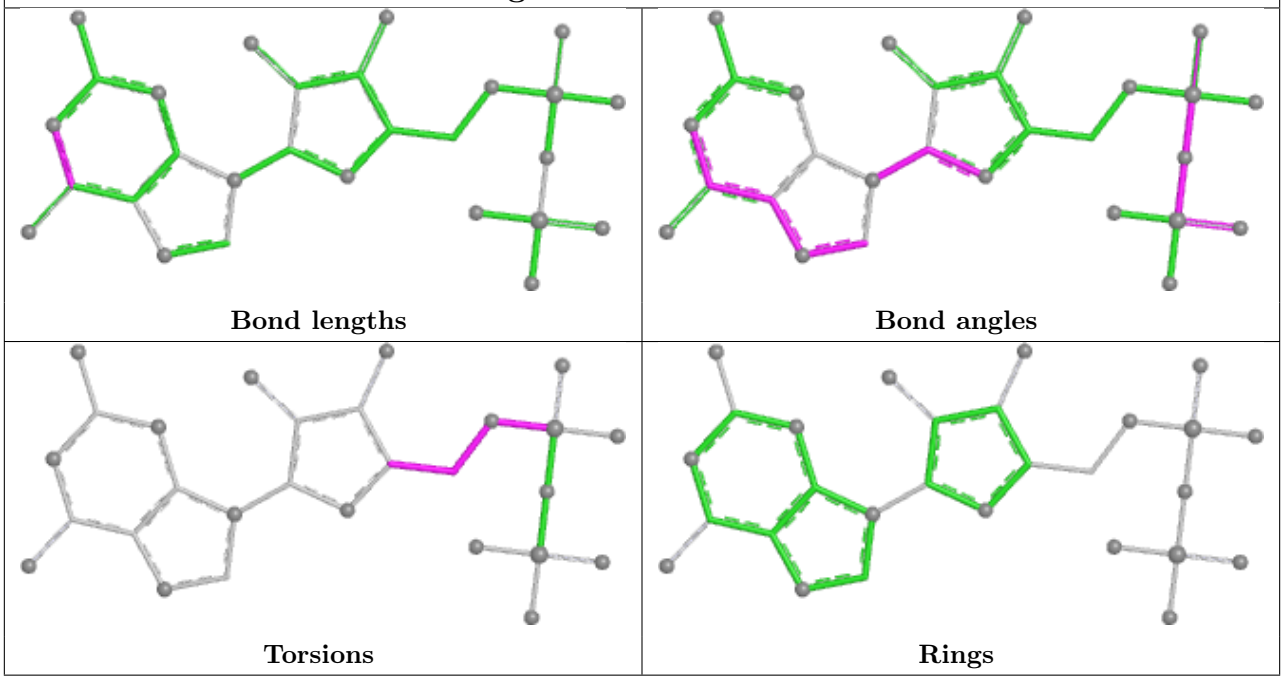

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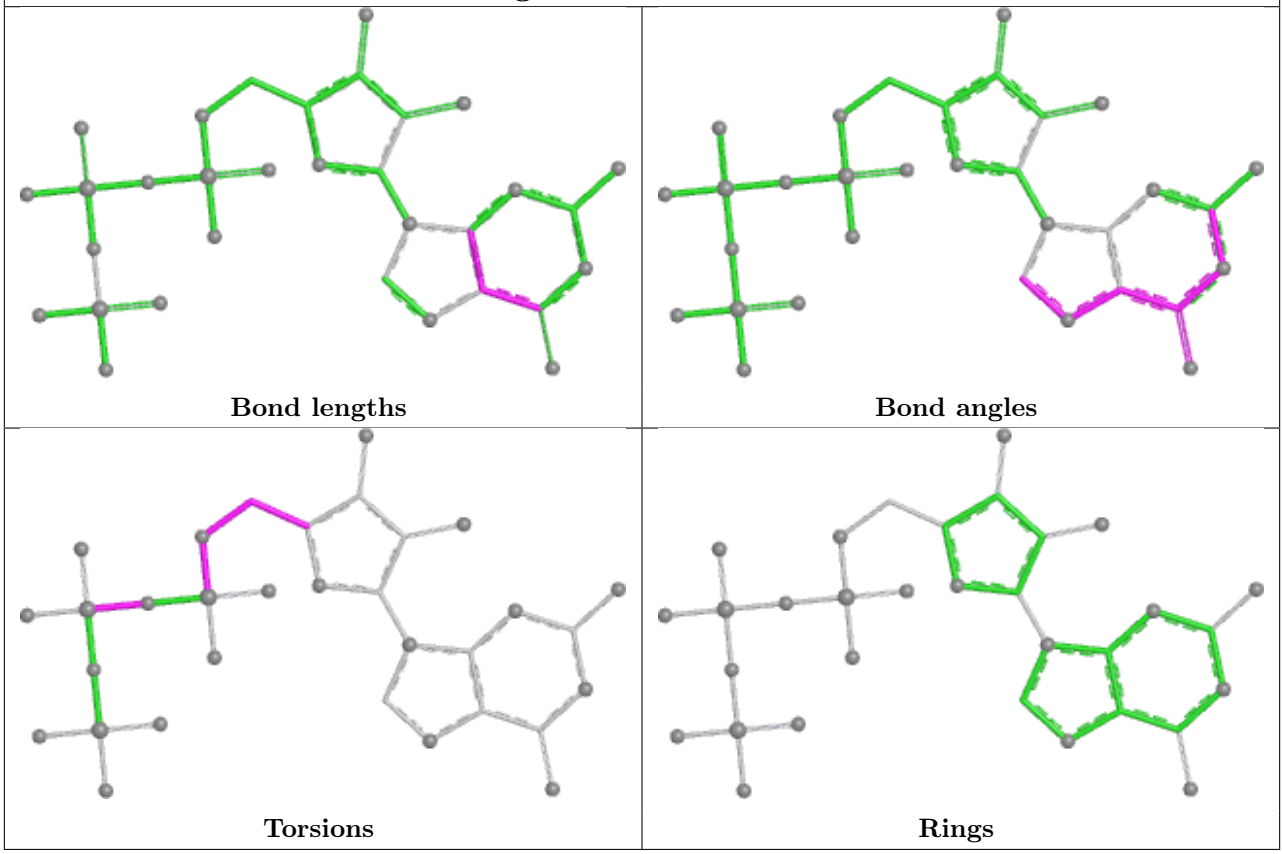

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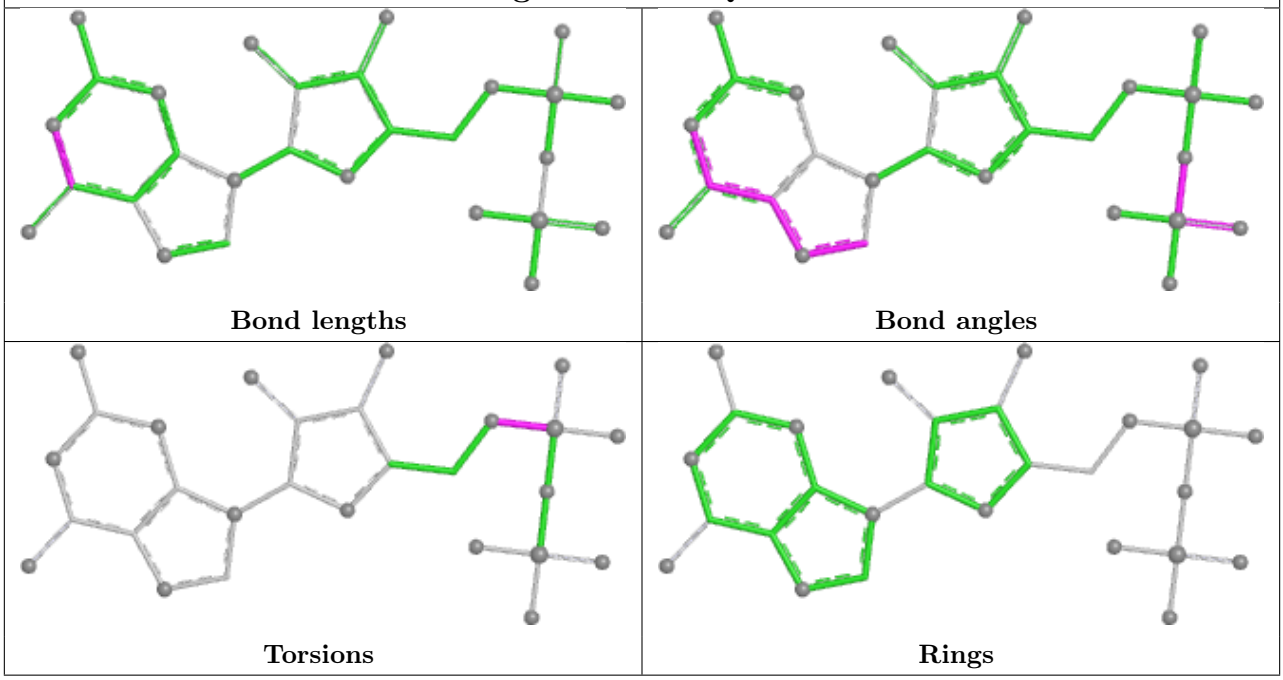

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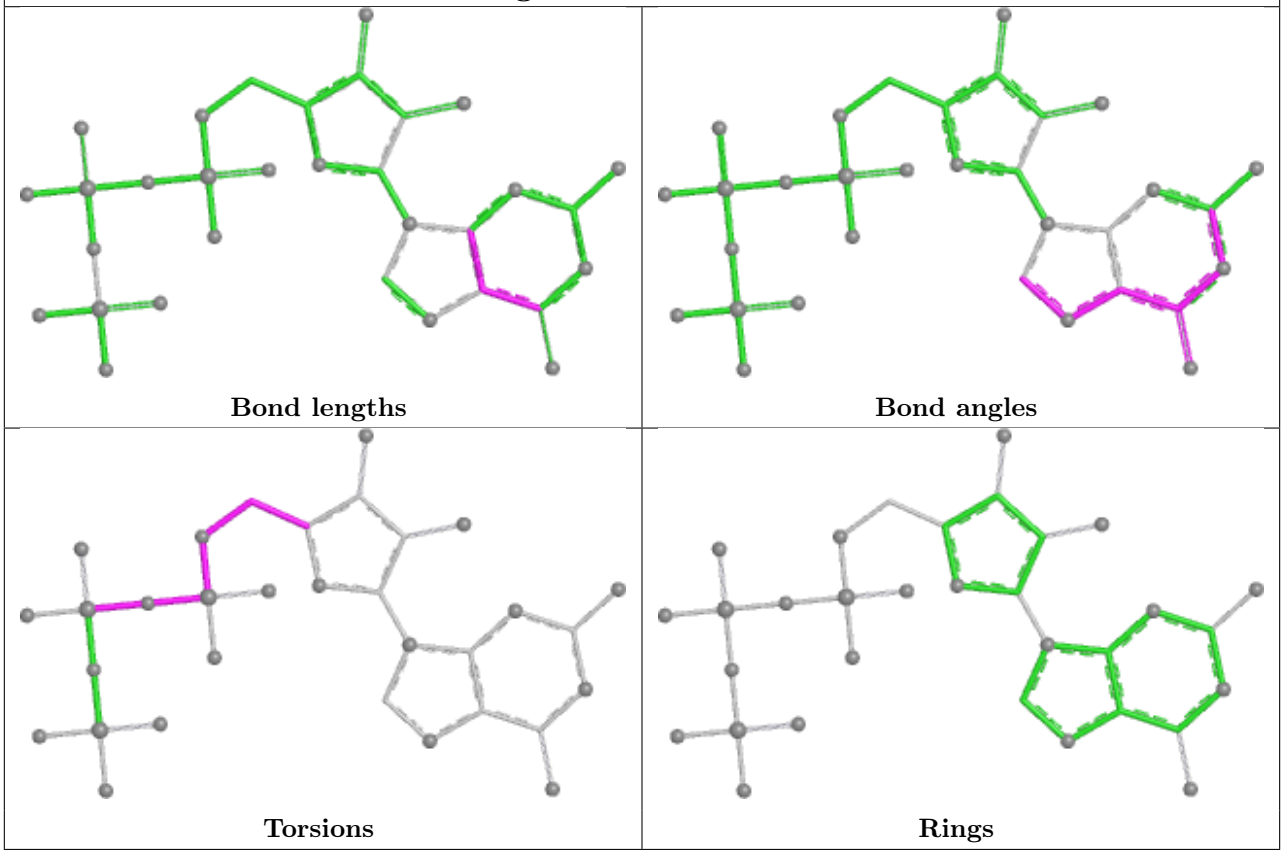

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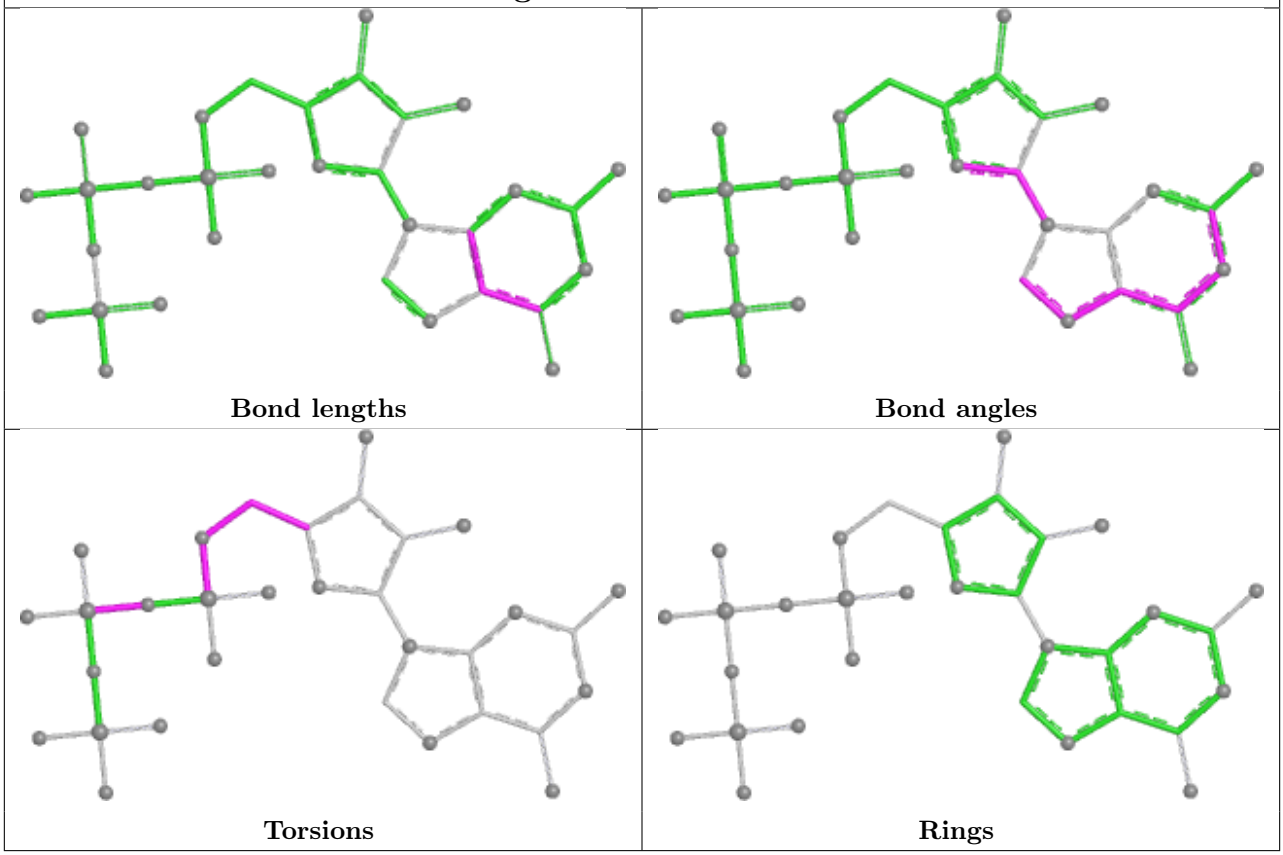

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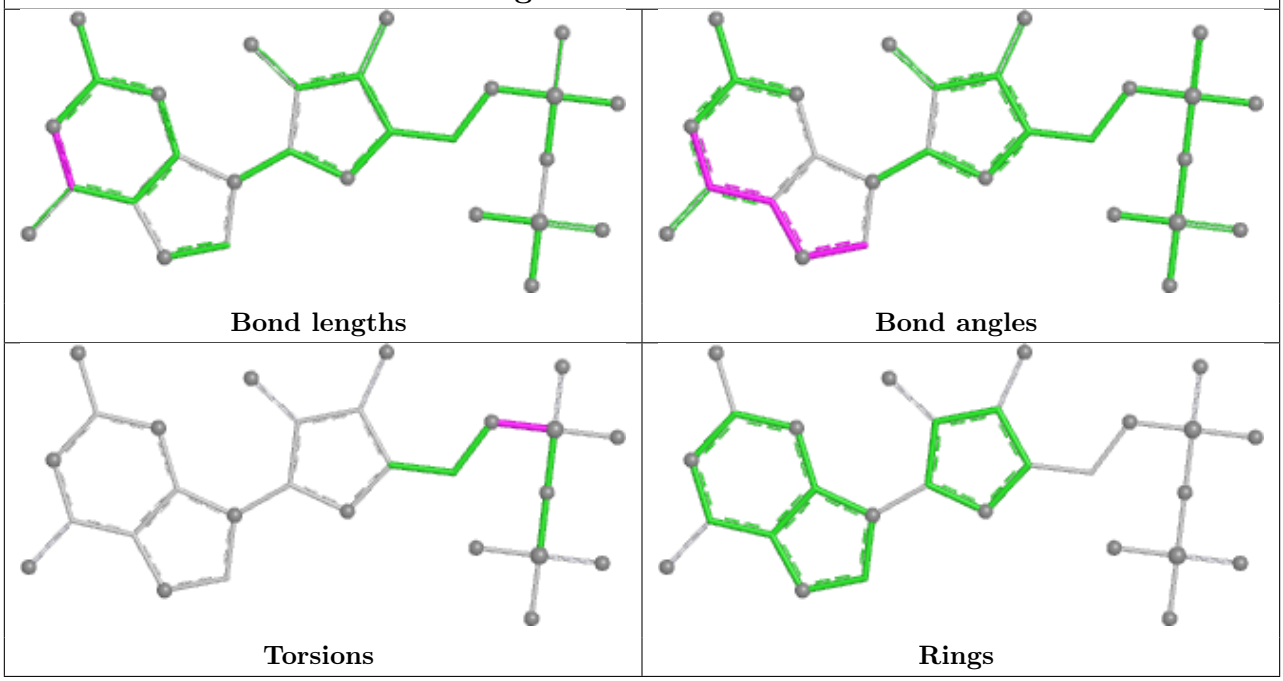

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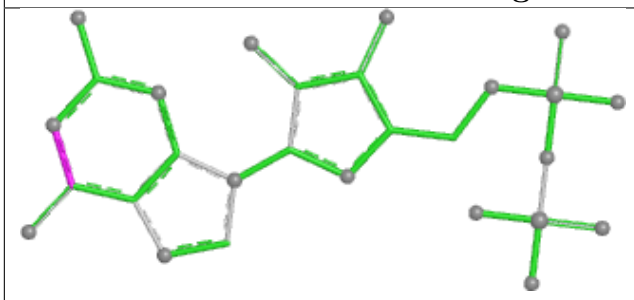

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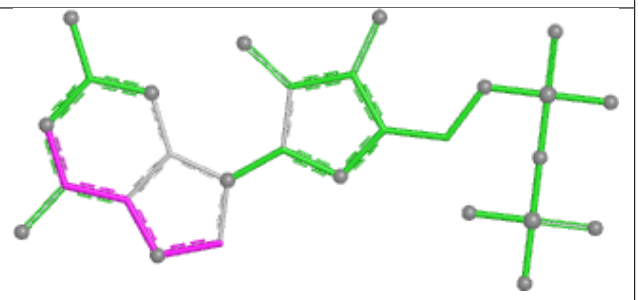
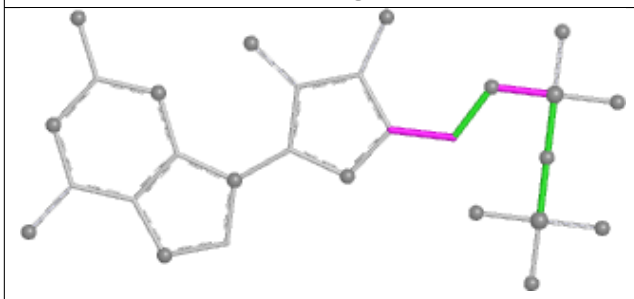
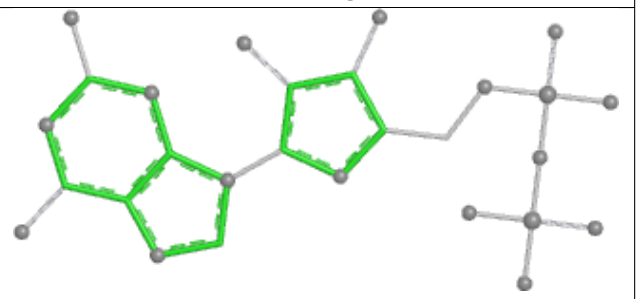


Bond angles

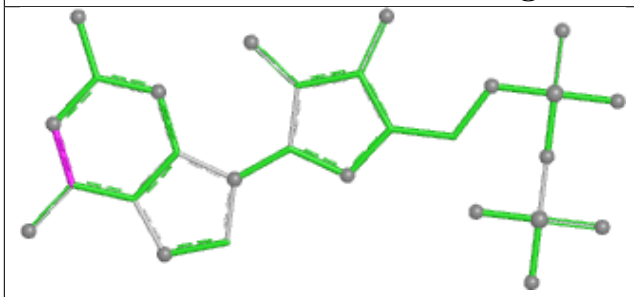


Torsions



Rings

Ligand GDP I8 502



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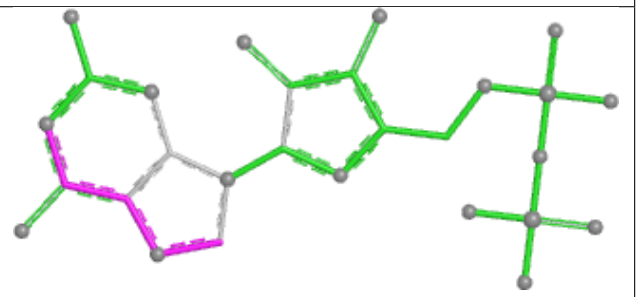

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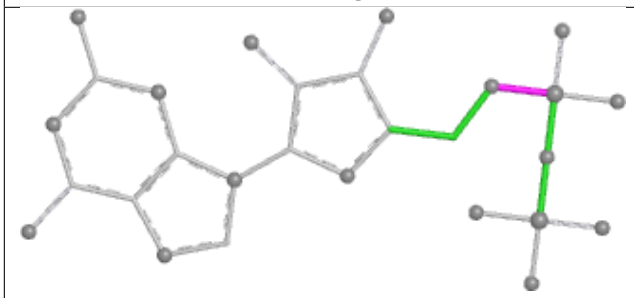
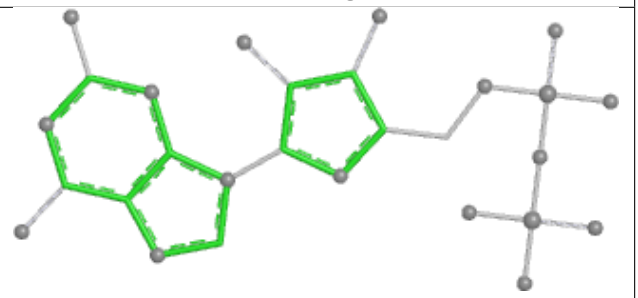
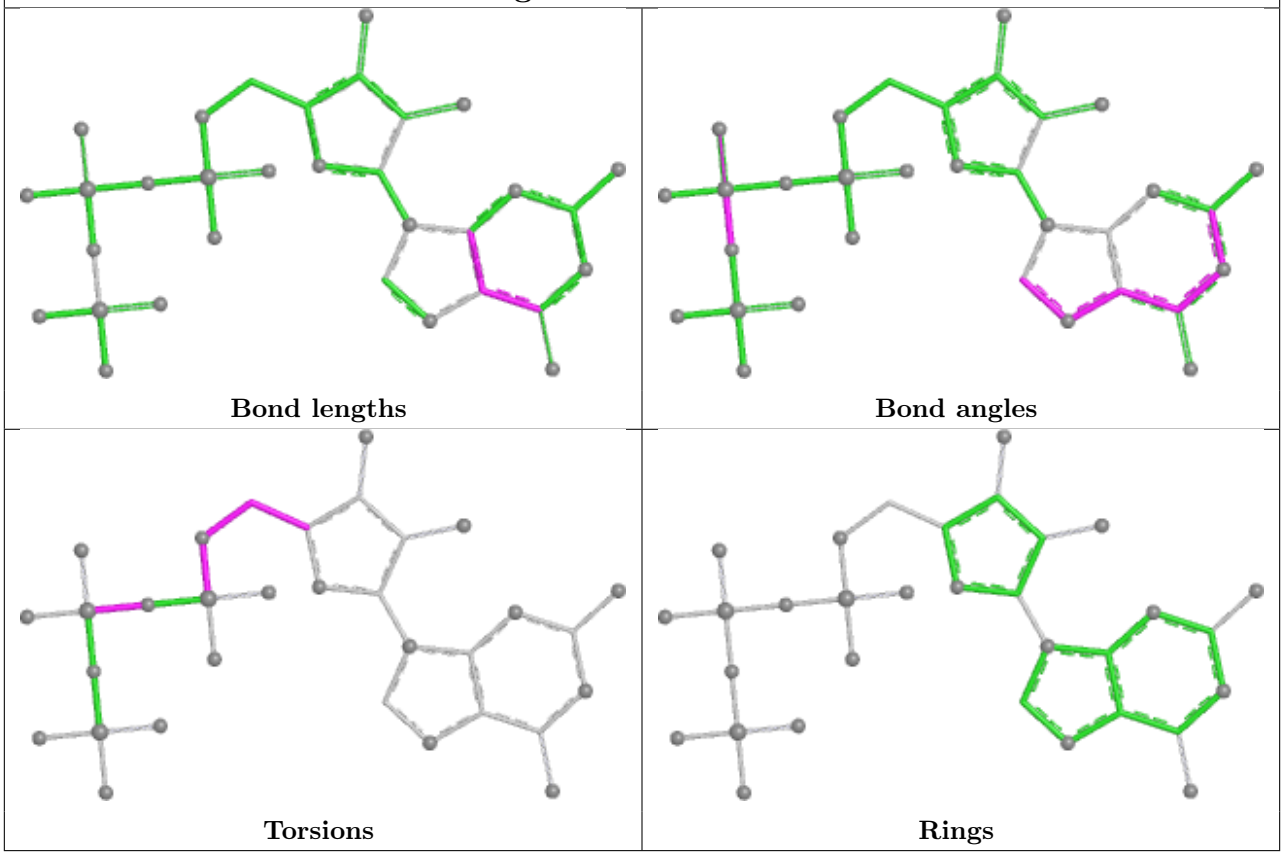


Torsions

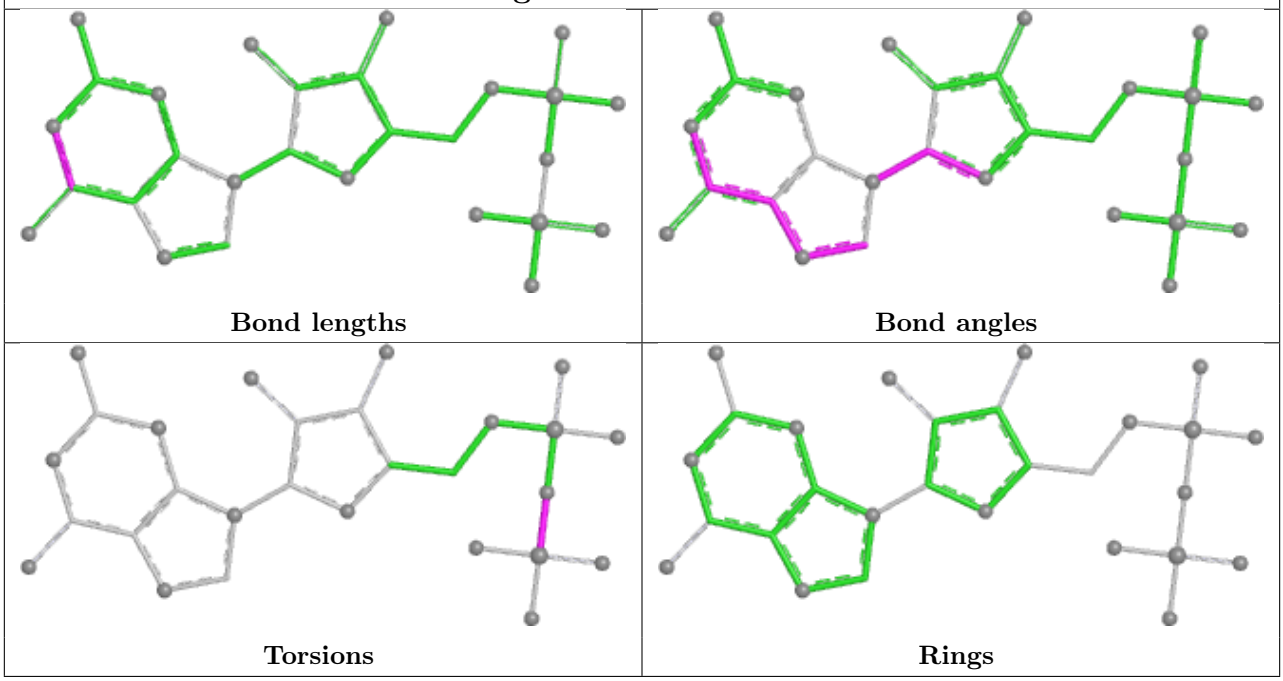


Rings

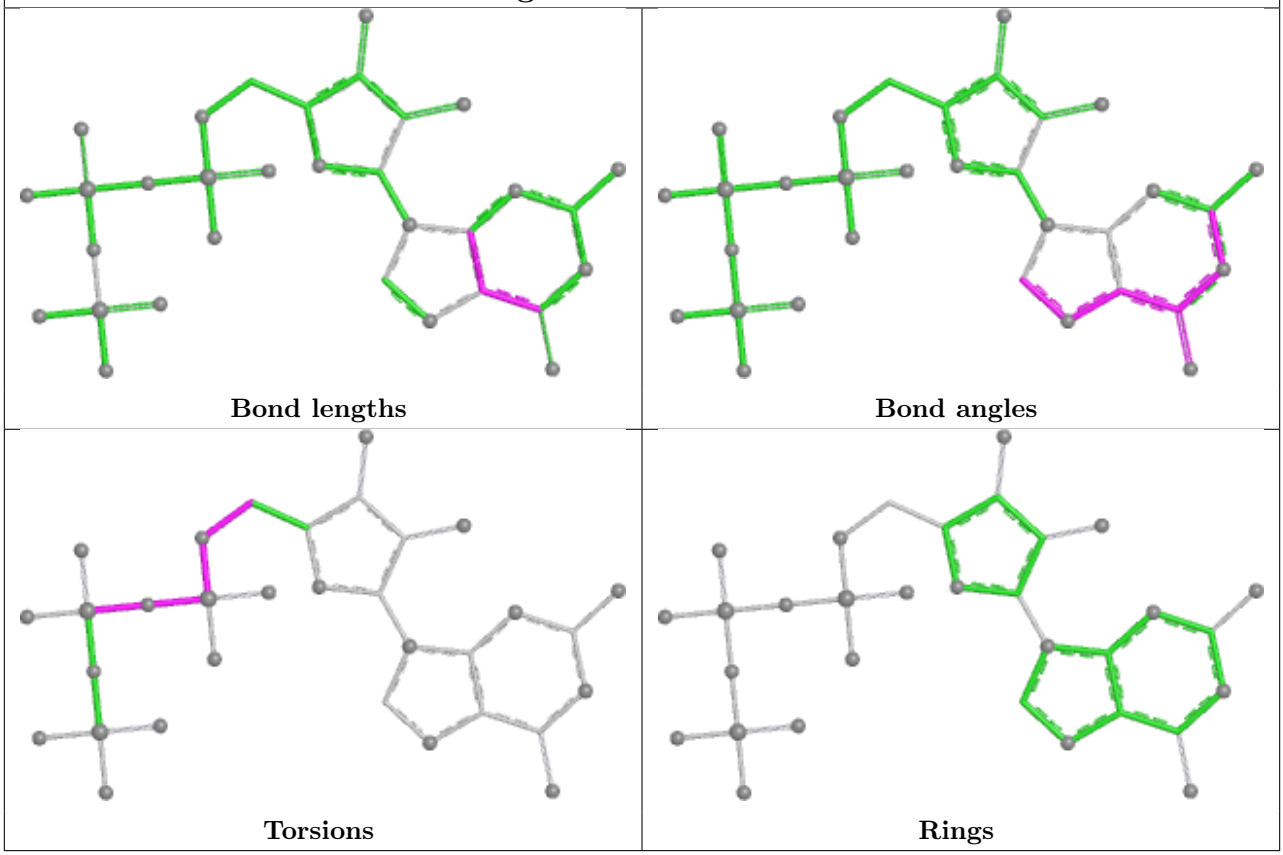
Ligand GTP O4 501



Ligand GDP C4 501



Ligand GTP L6 501



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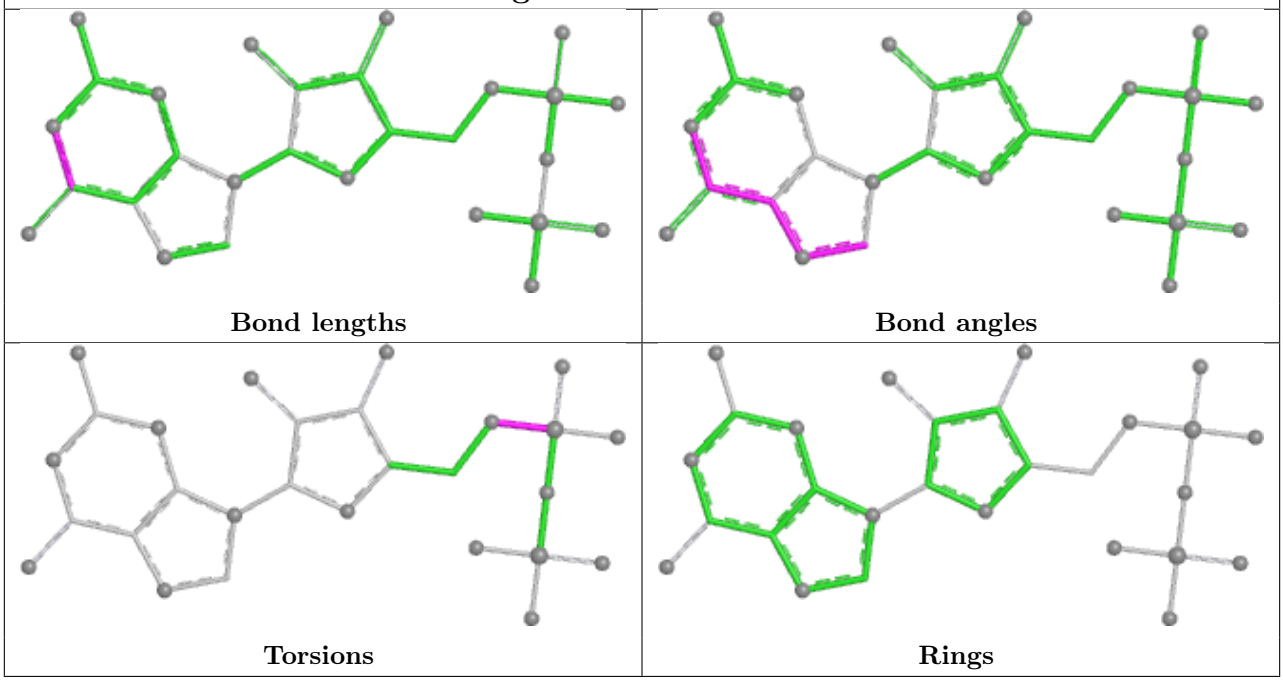

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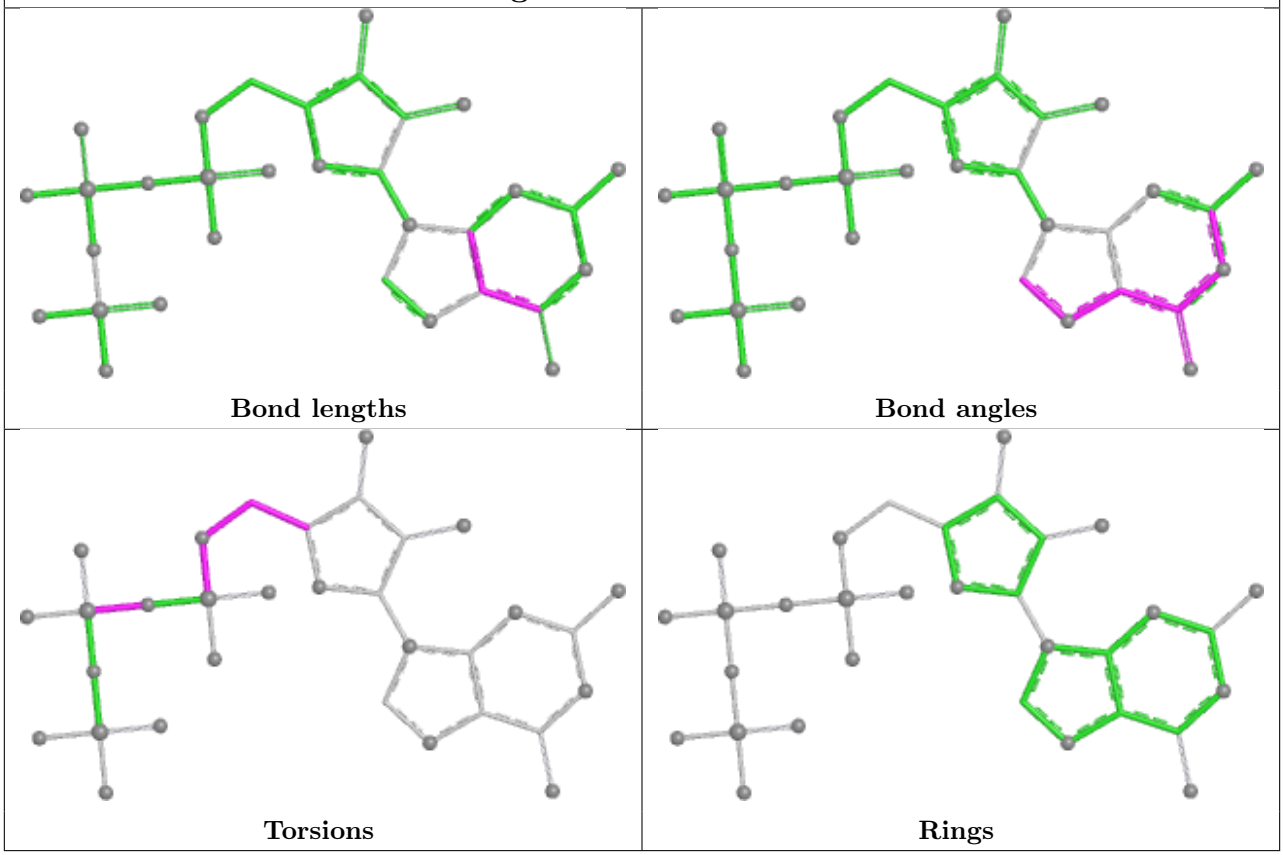
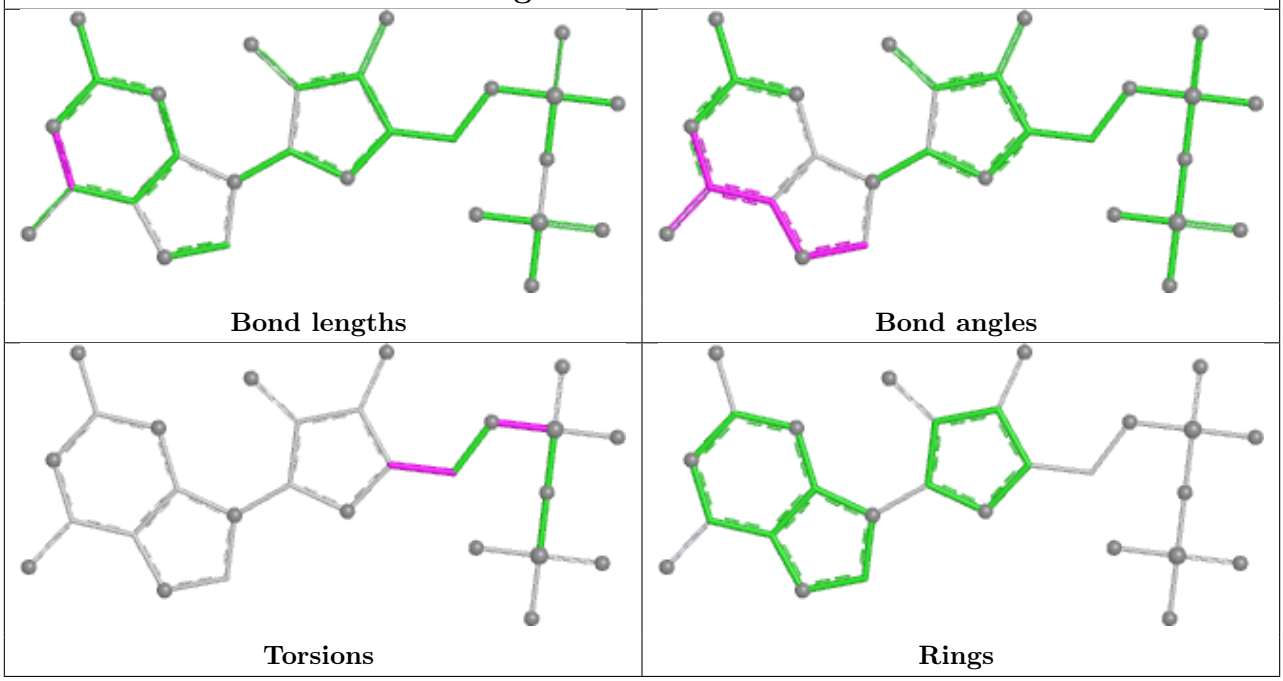
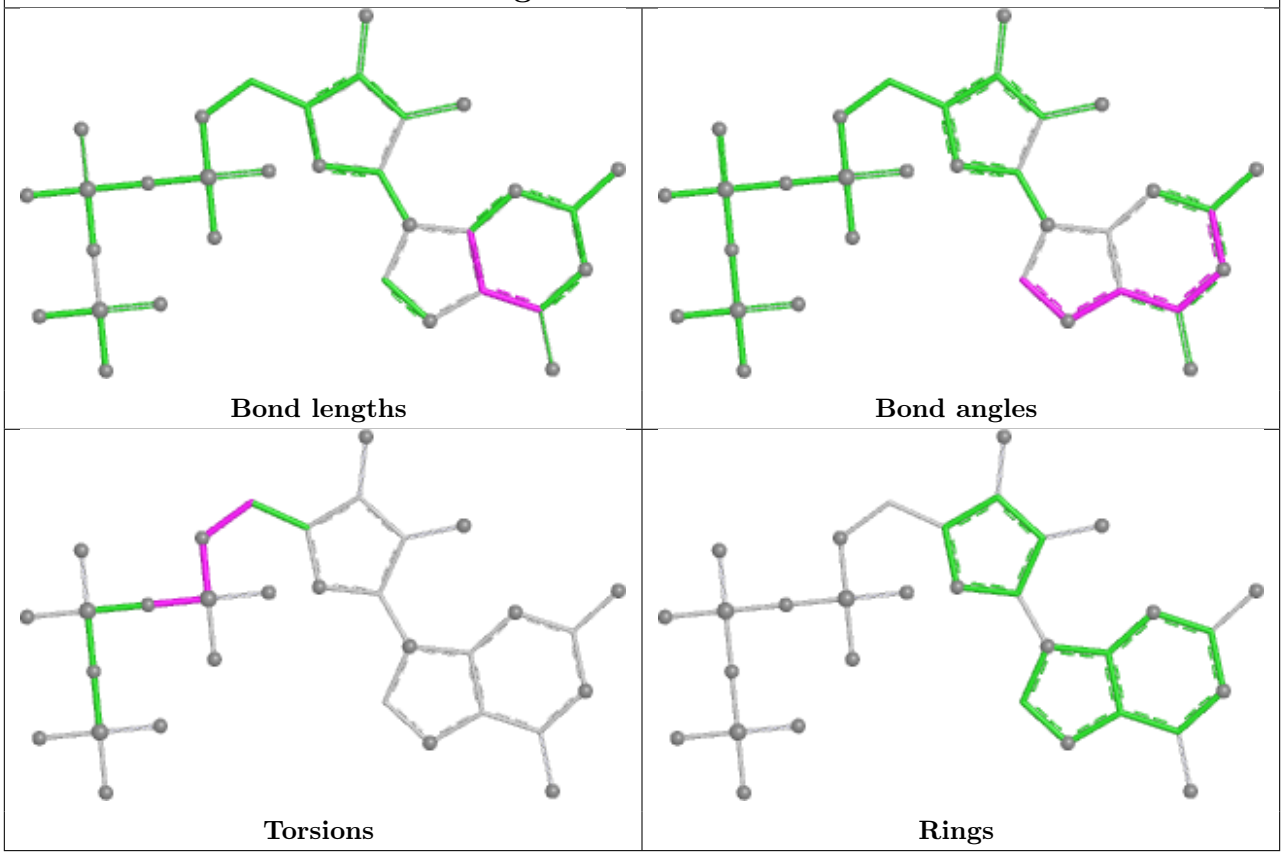


Ligand GDP T4 502



Ligand GTP D3 501



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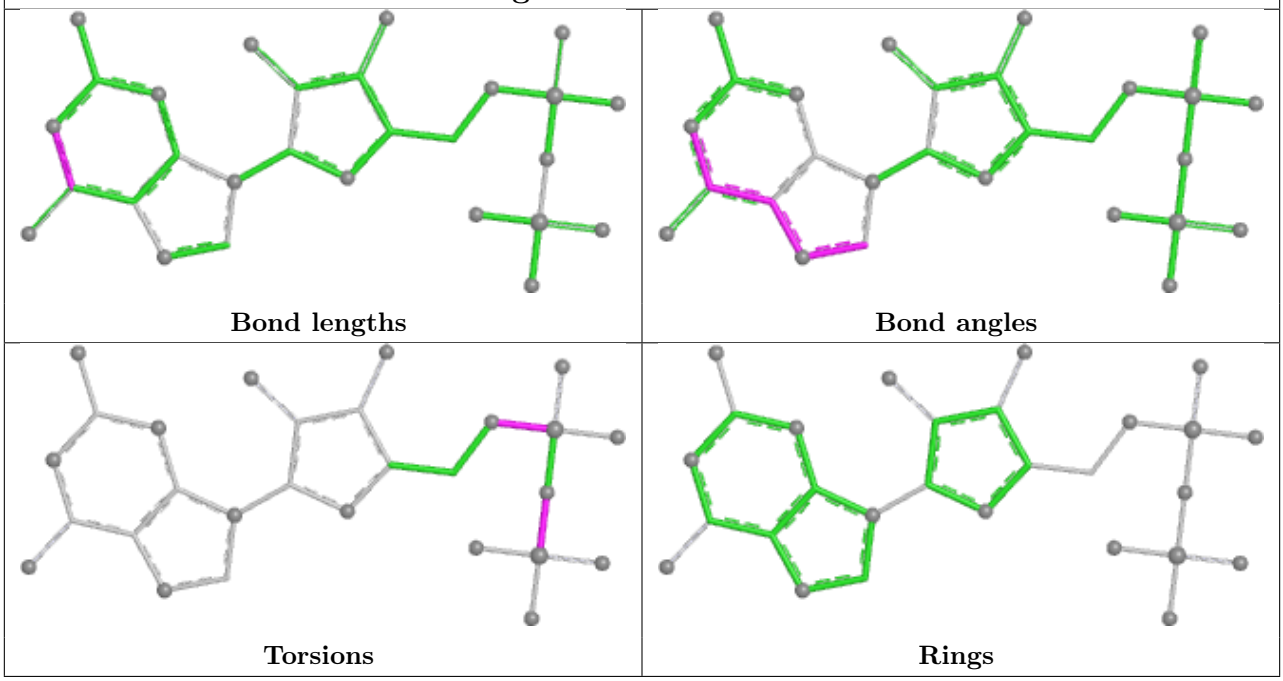
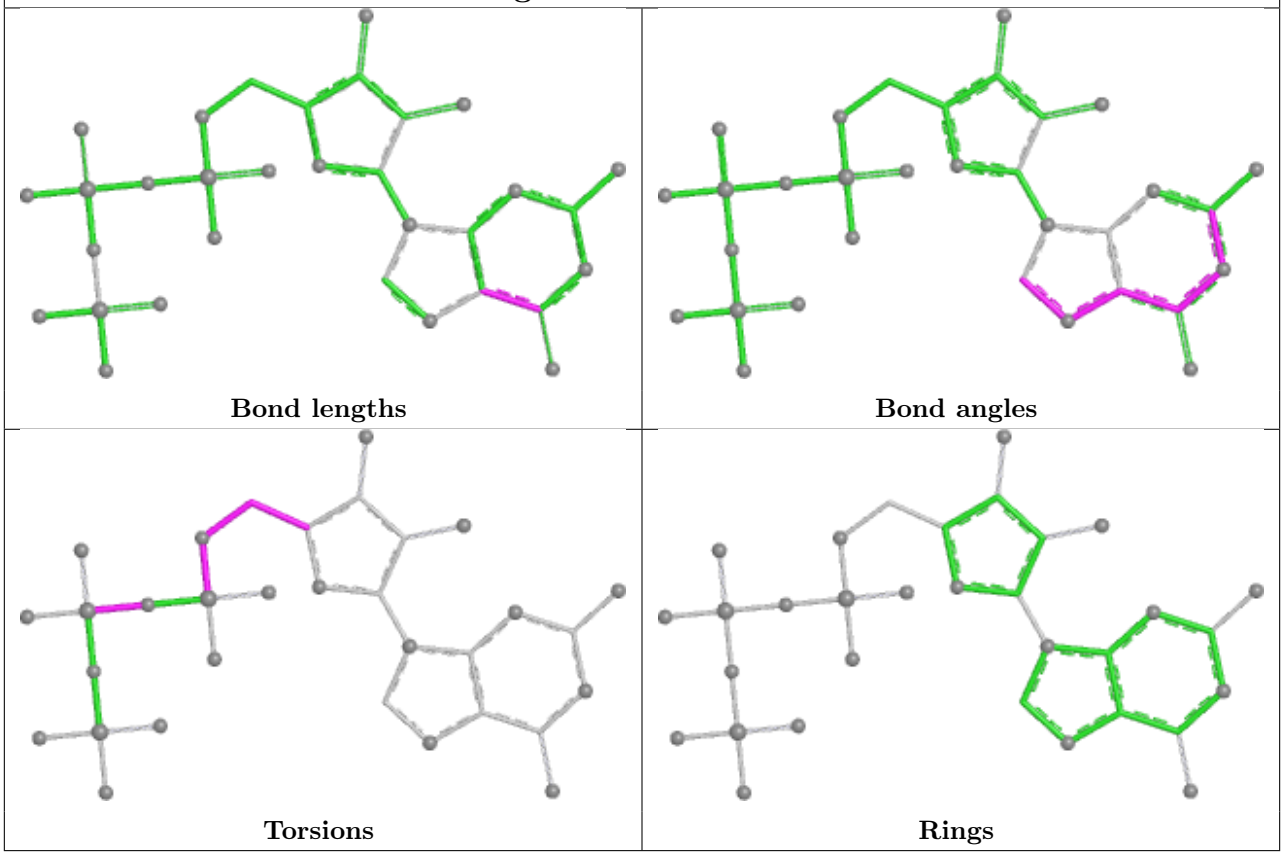
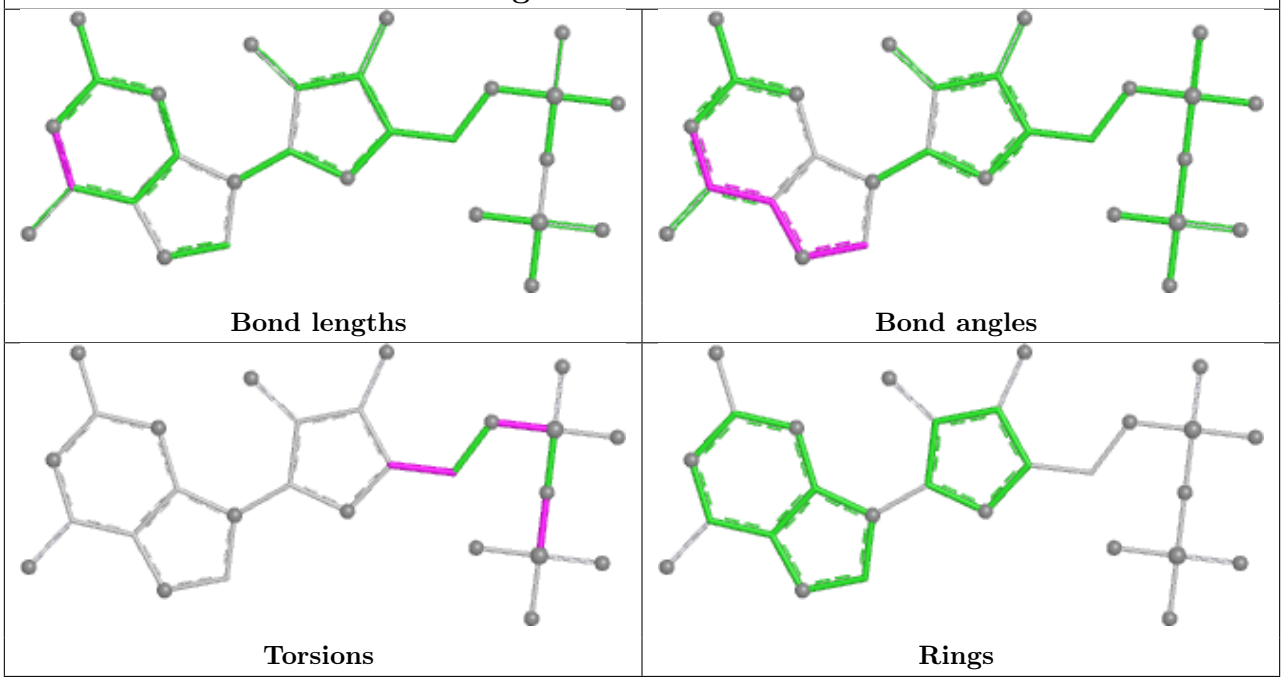


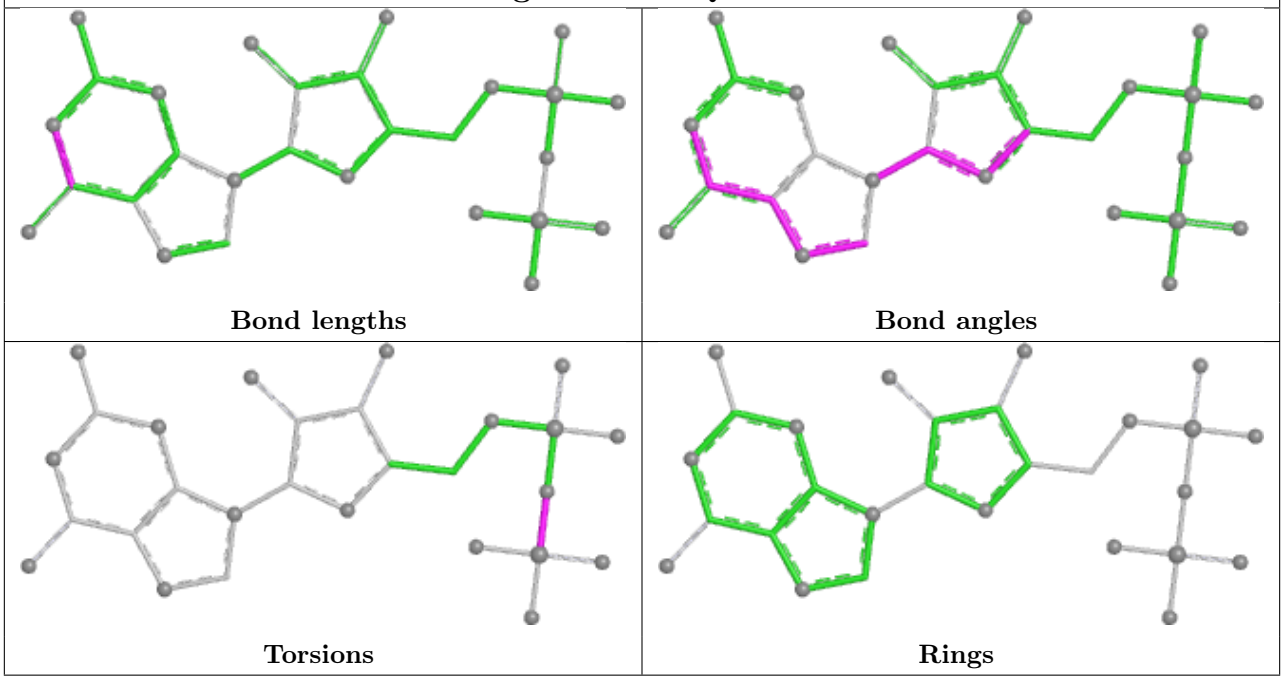
Ligand GTP 2A 501



Ligand GDP G6 501



Ligand GDP Q8 501



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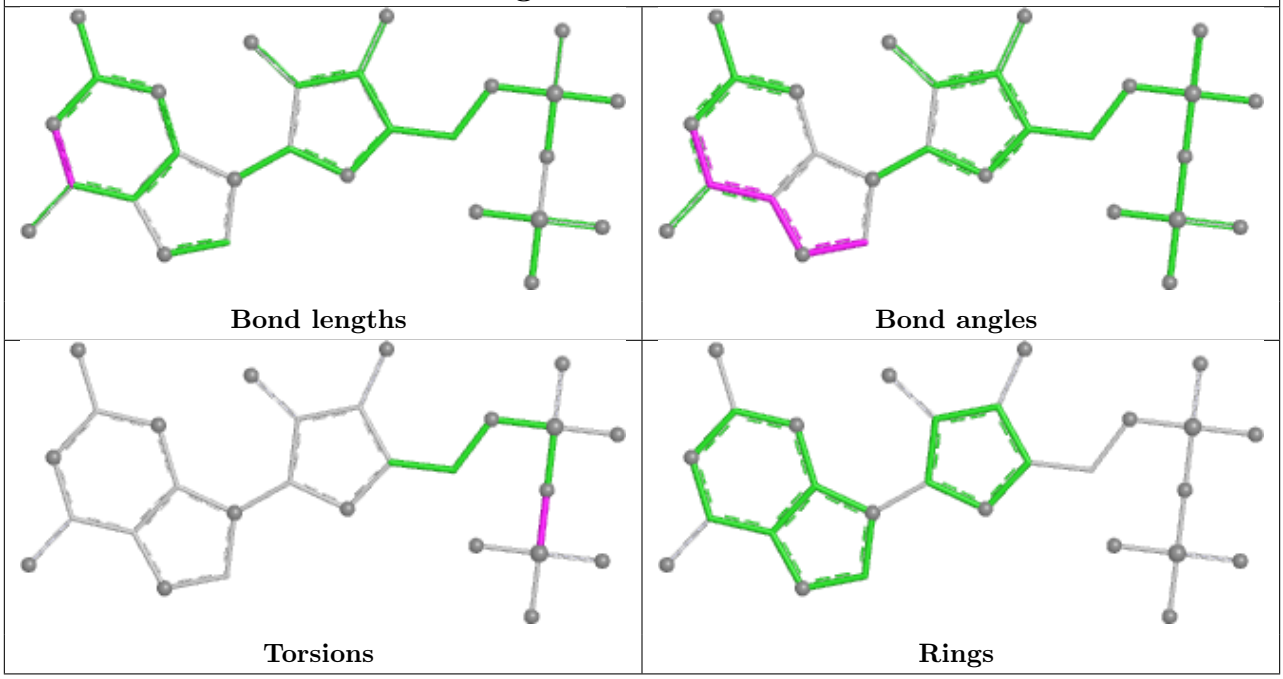
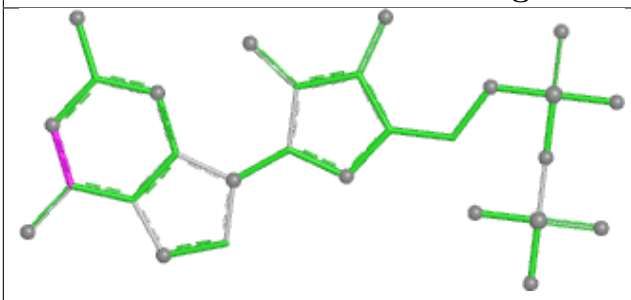
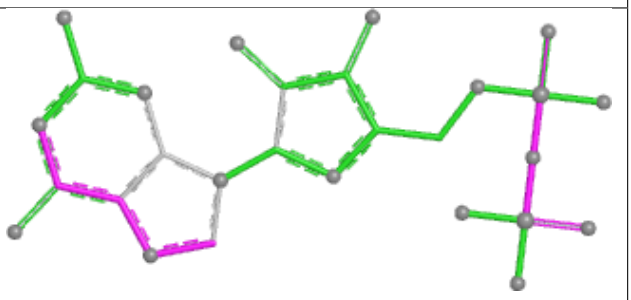


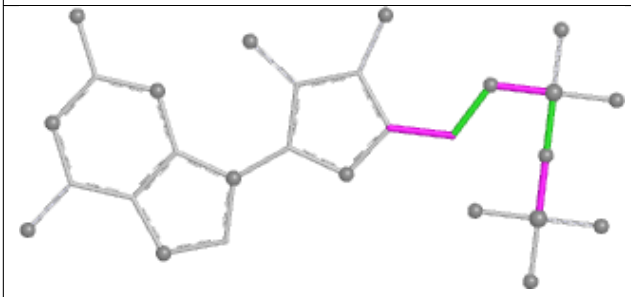
Ligand GDP A3 501



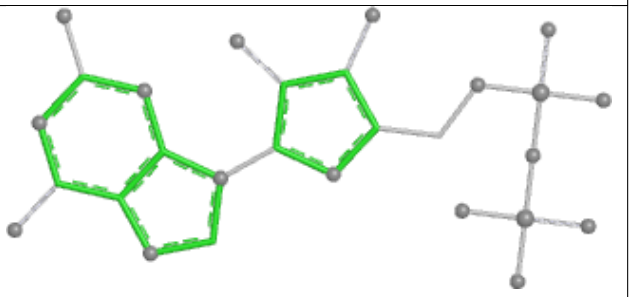
Bond lengths



Bond angles

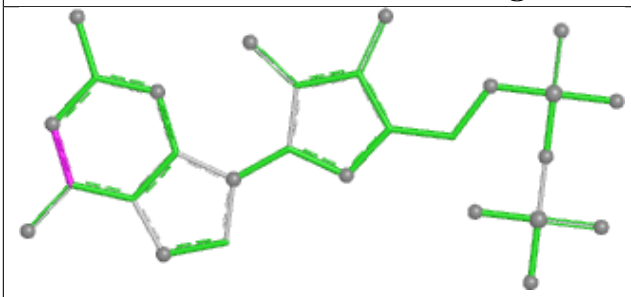


Torsions



Rings

Ligand GDP 2M 501



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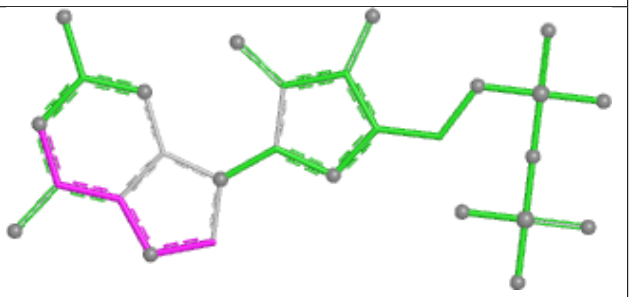
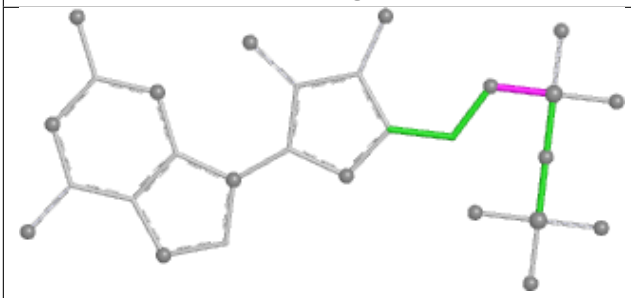


Bond angles



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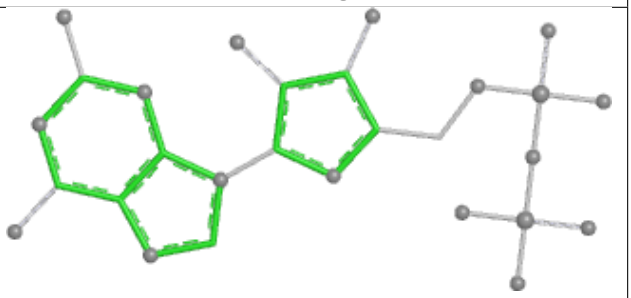
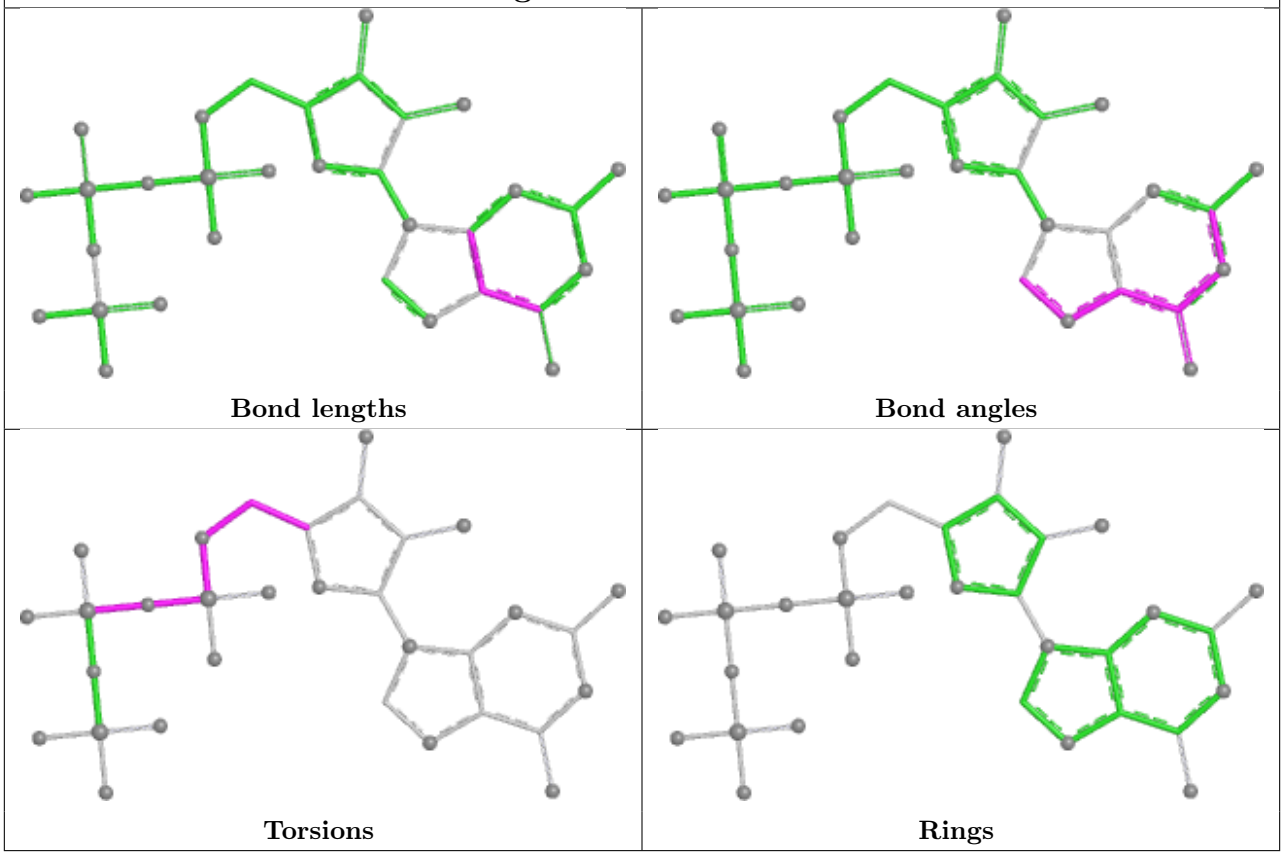
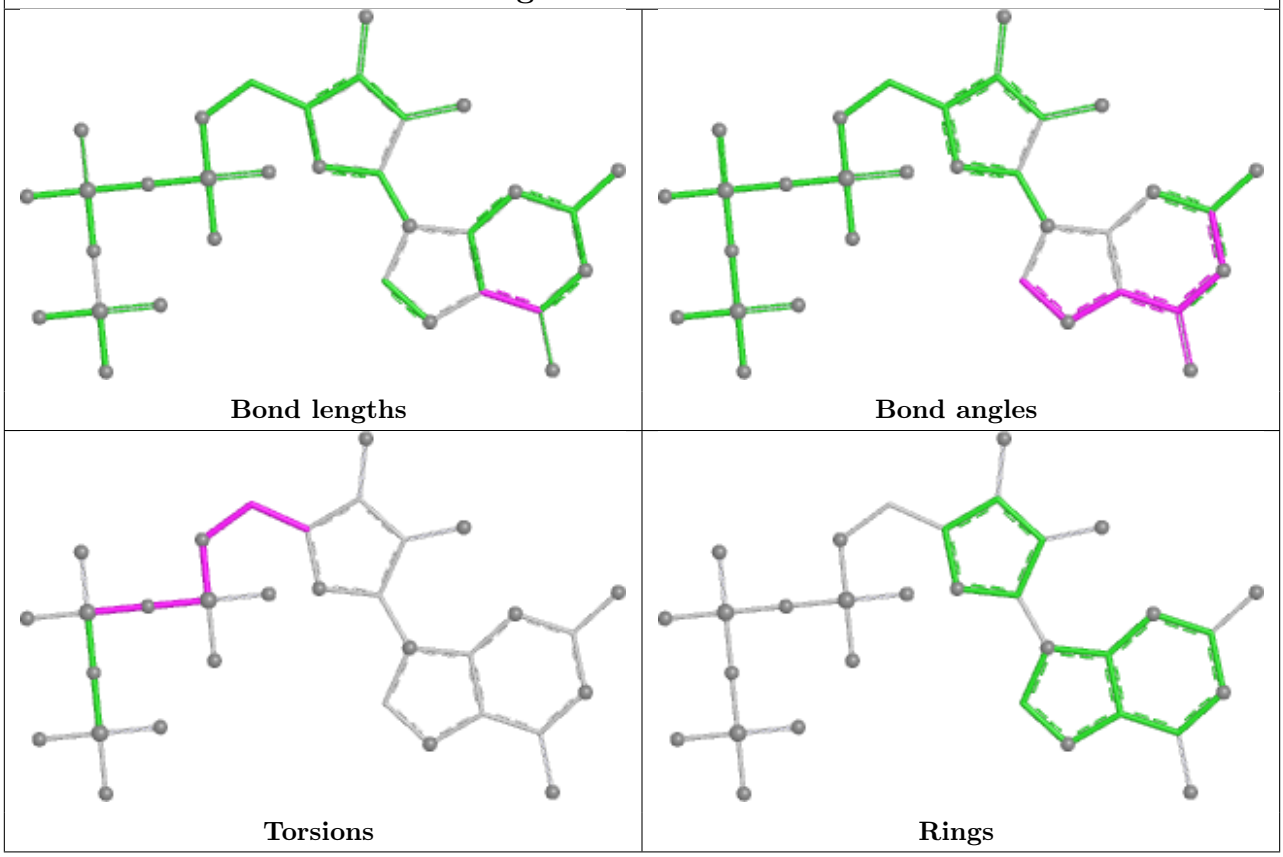


Rings

Ligand GTP Y4 501



Ligand GTP Z3 501



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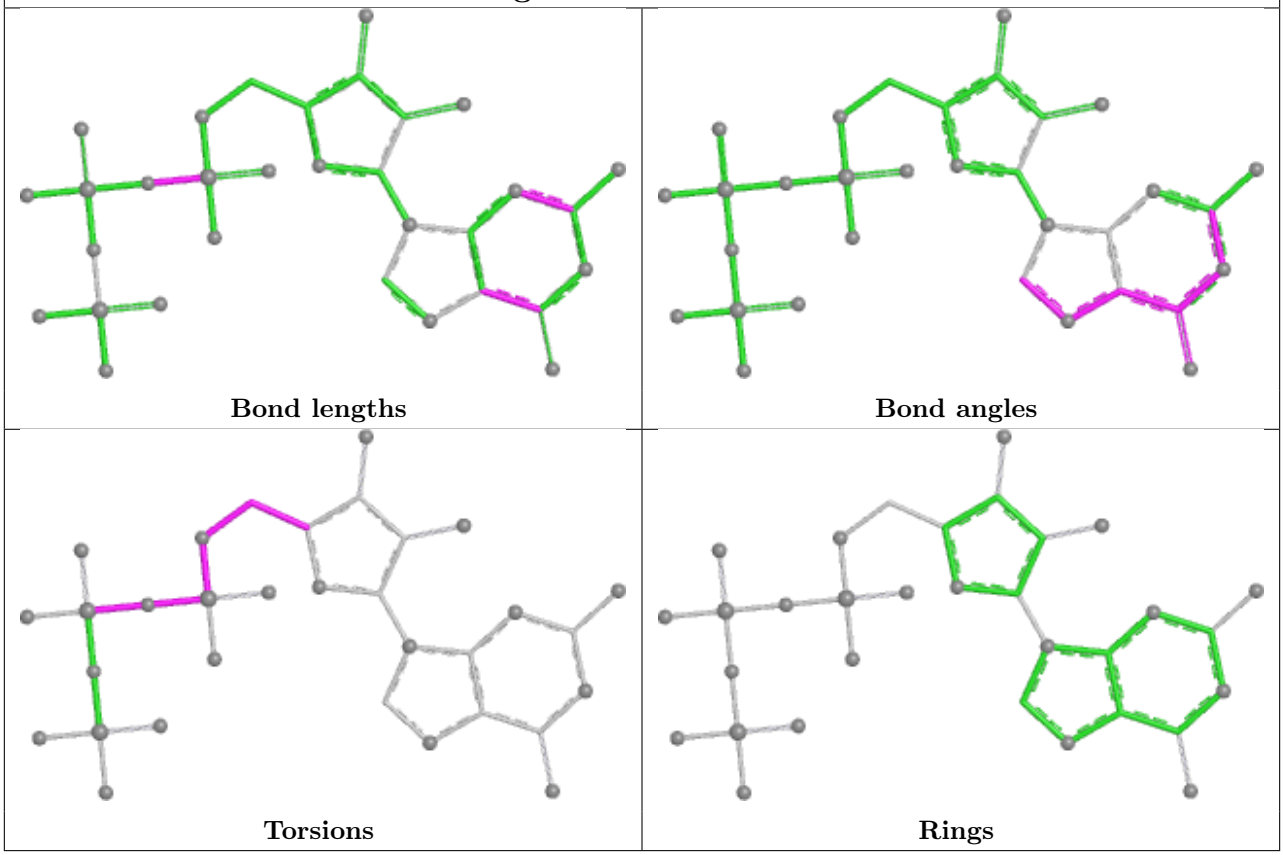

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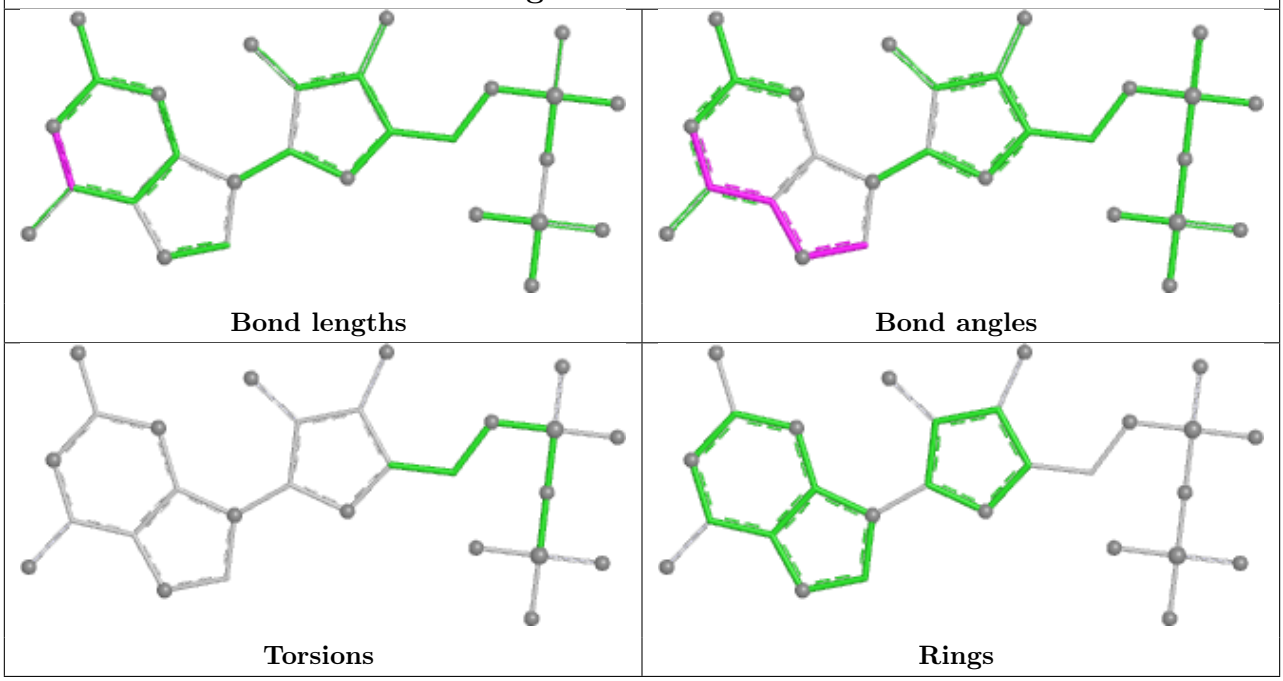

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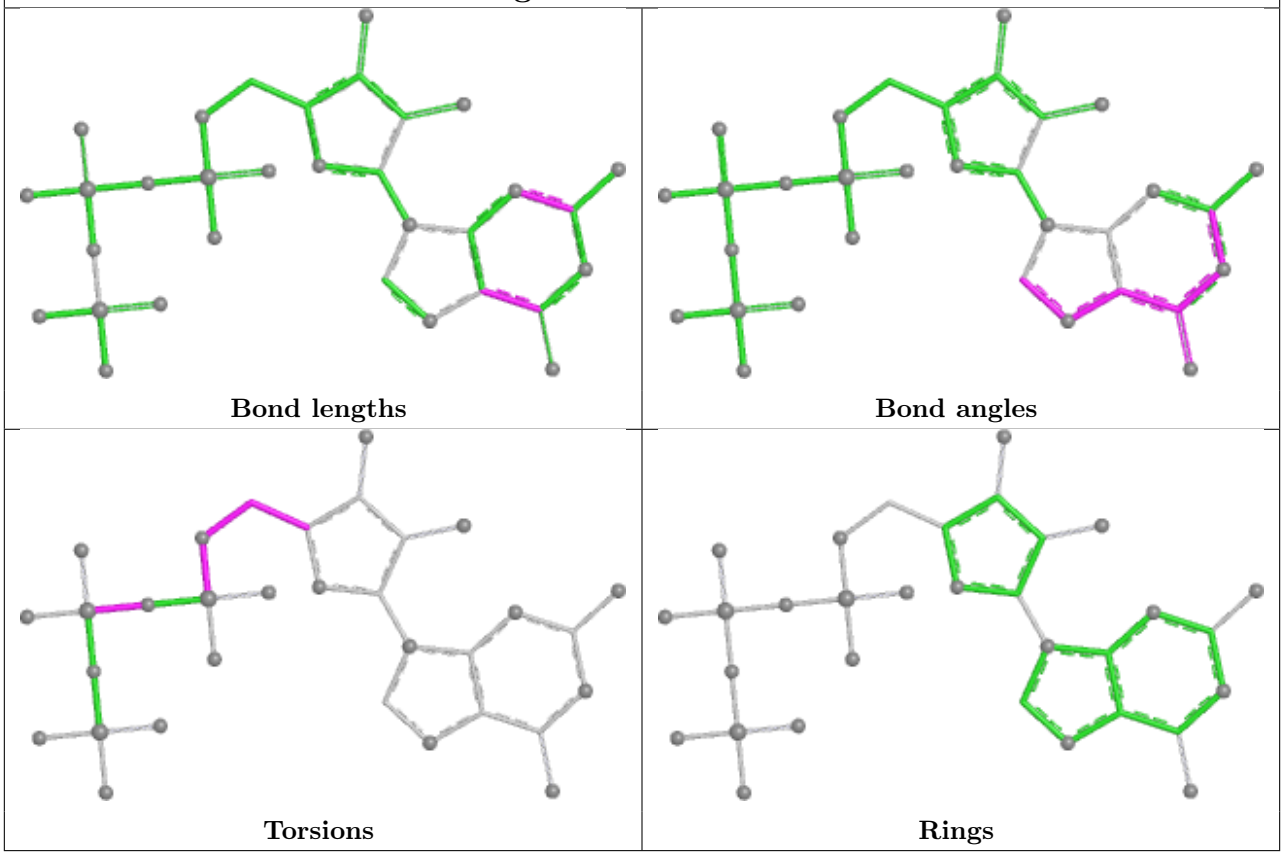

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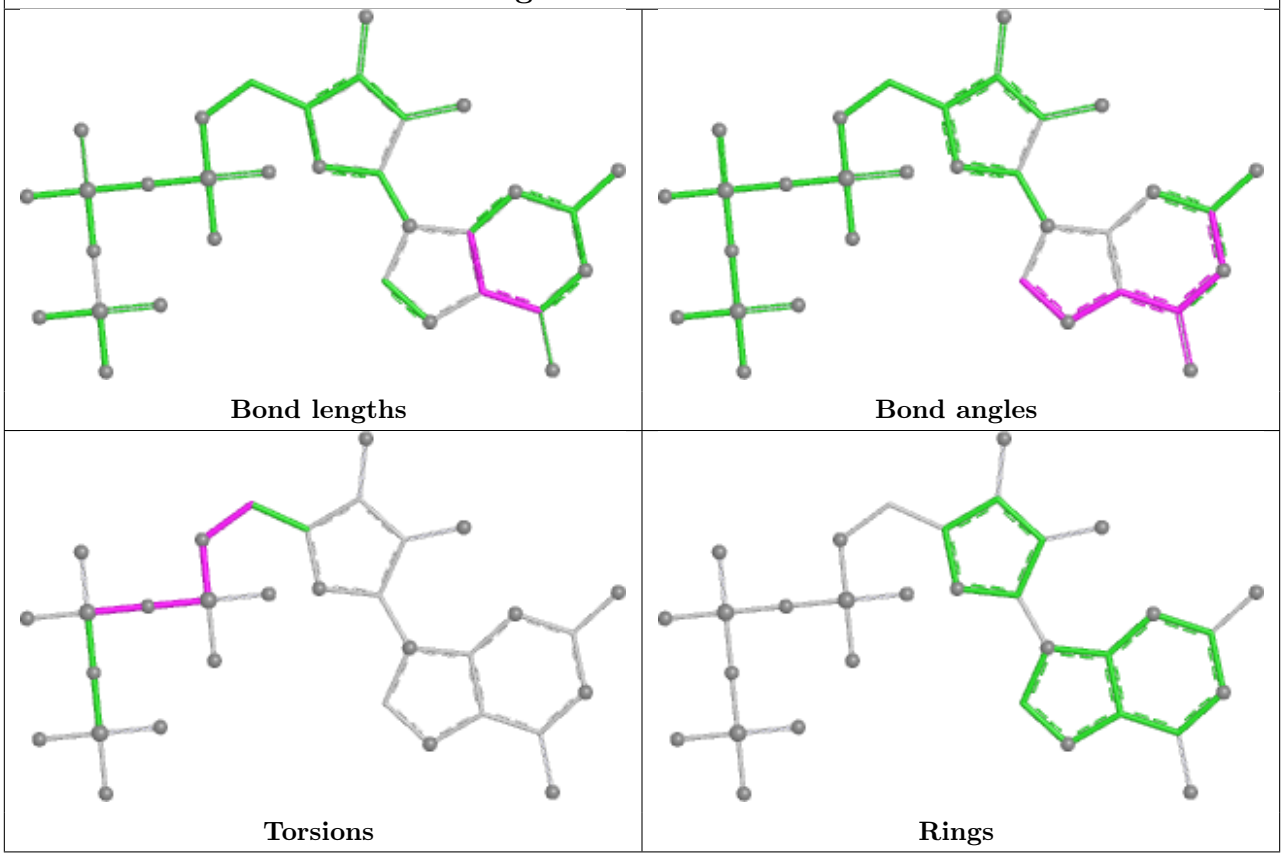

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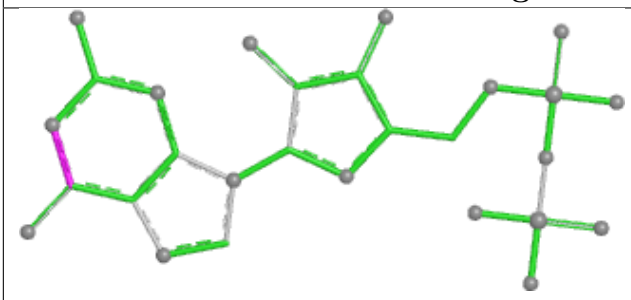
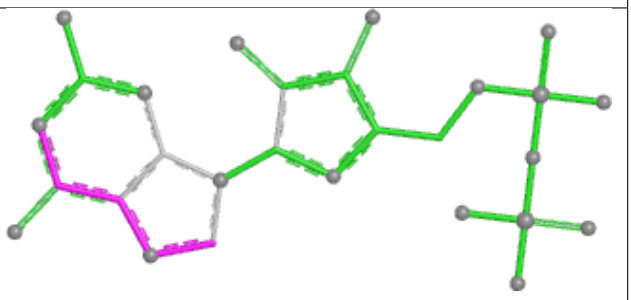
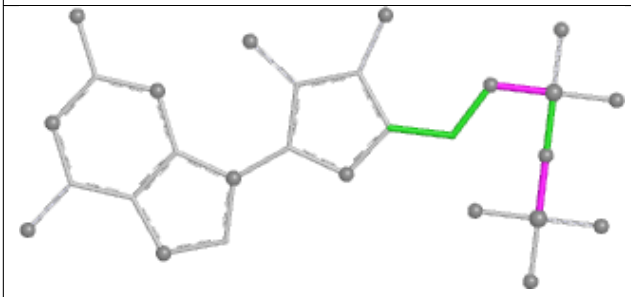
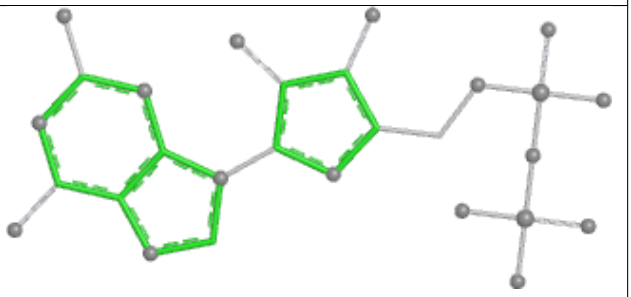
 Bond lengths	 Bond angles
 Torsions	 Rings

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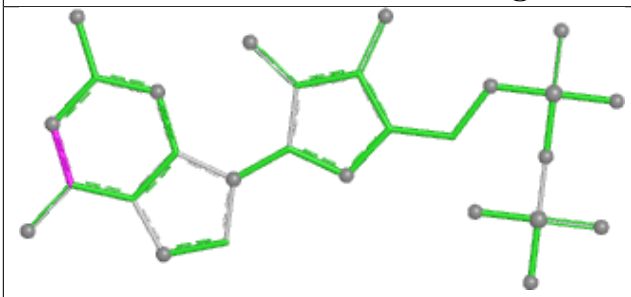
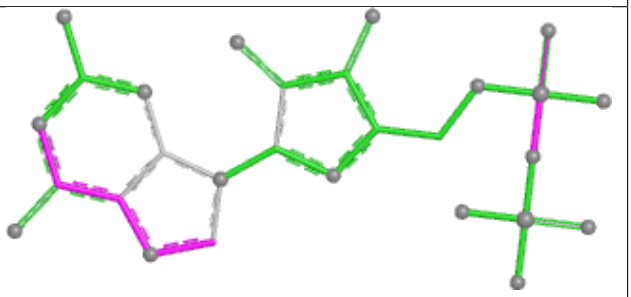
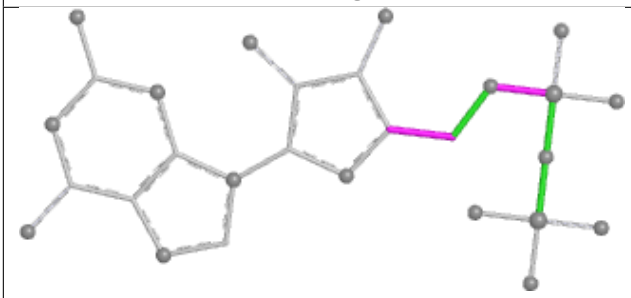
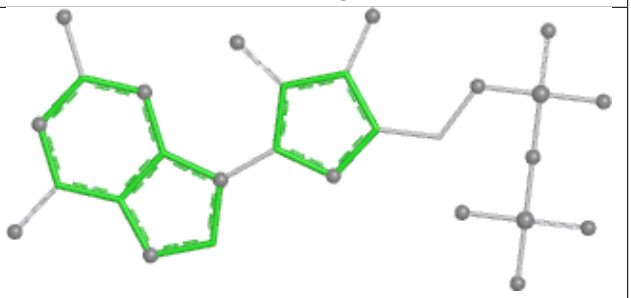
 Bond lengths	 Bond angles
 Torsions	 Rings

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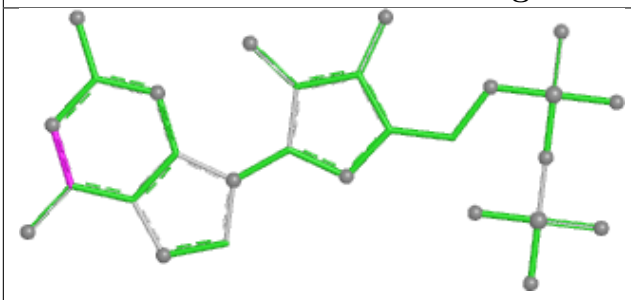
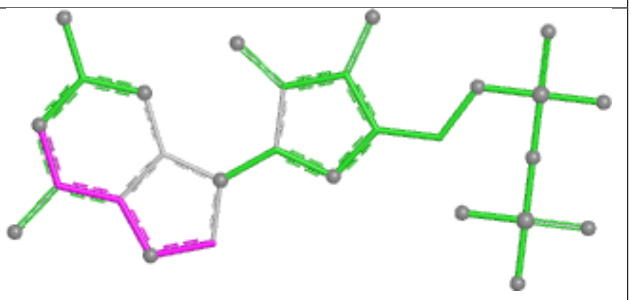
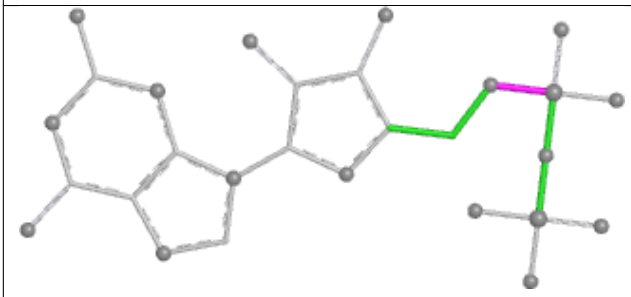
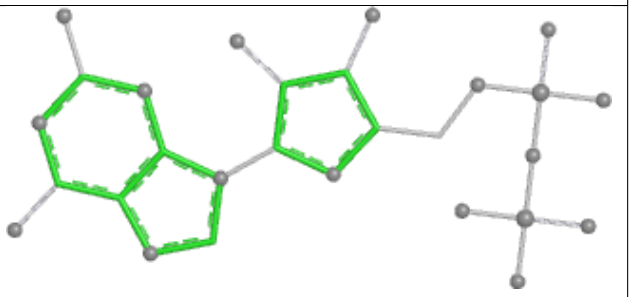
 Bond lengths	 Bond angles
 Torsions	 Rings

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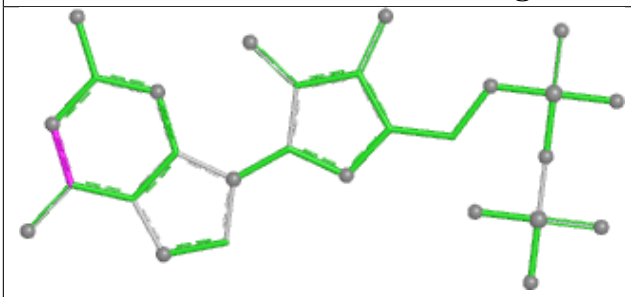
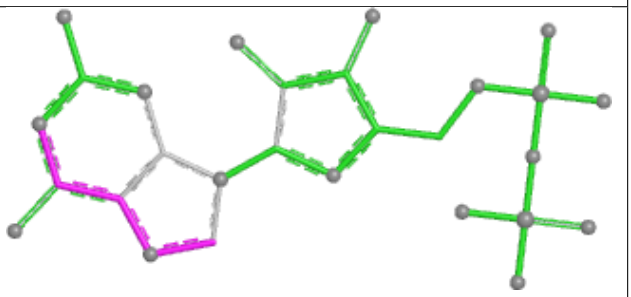
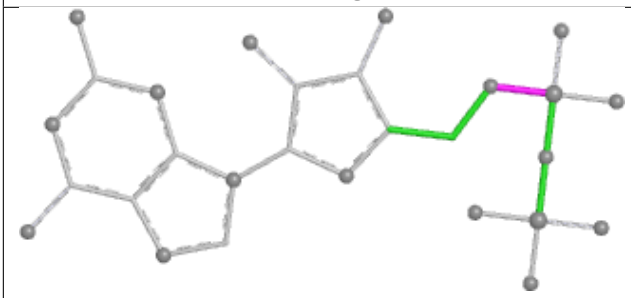
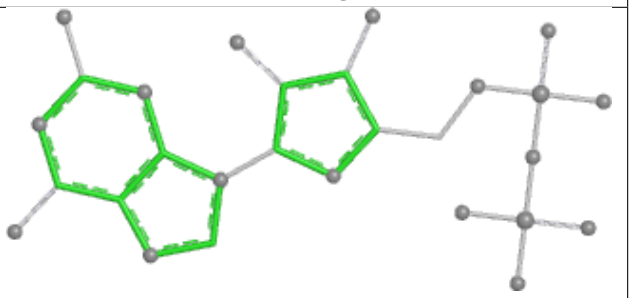
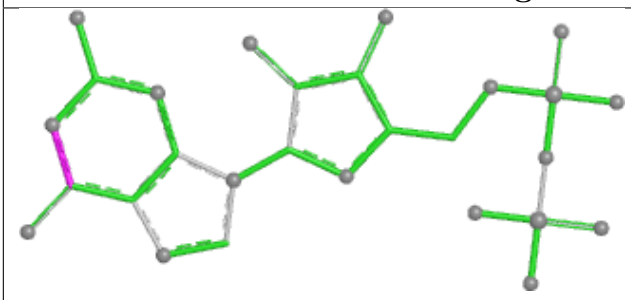
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP L2 502



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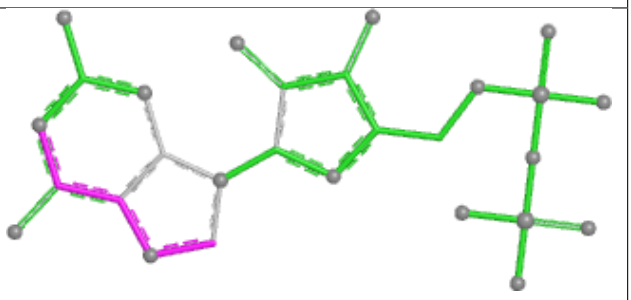

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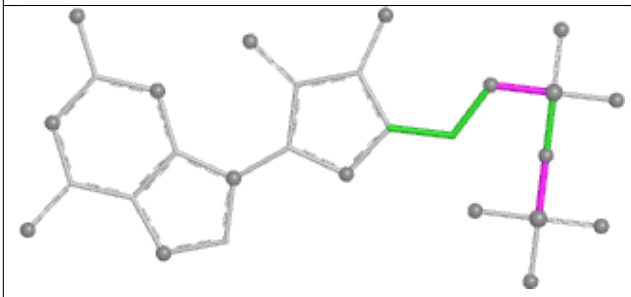

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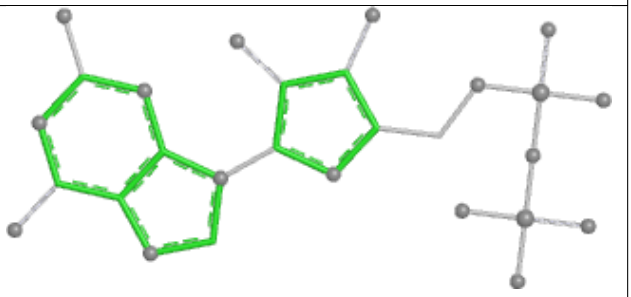

Rings

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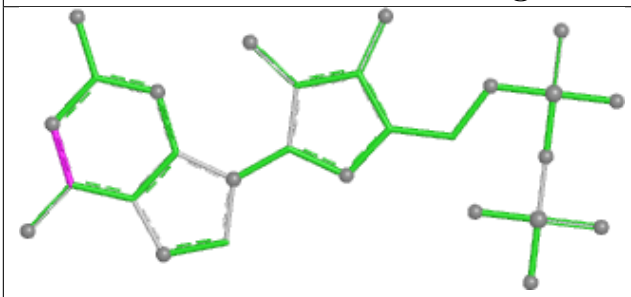

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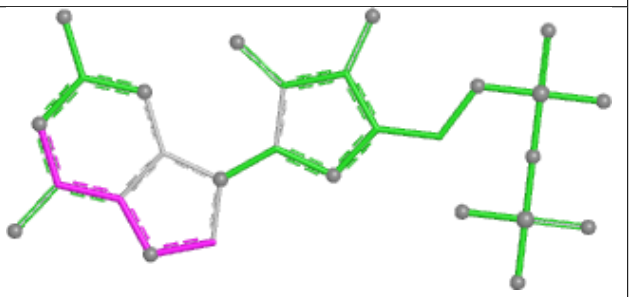

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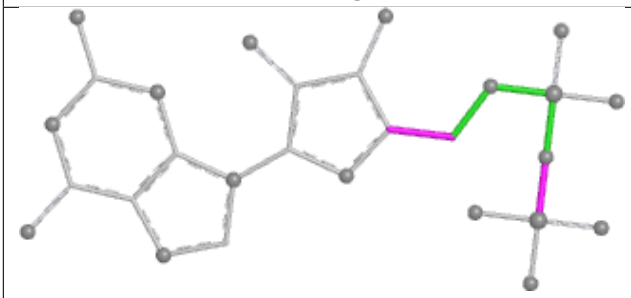

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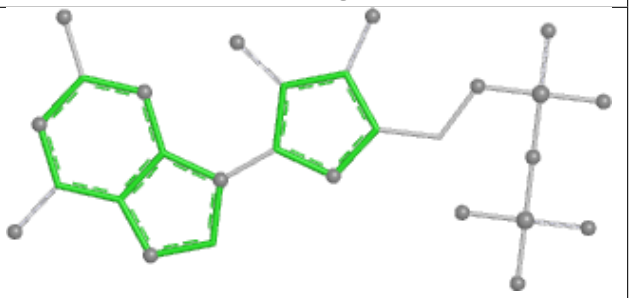

Rings

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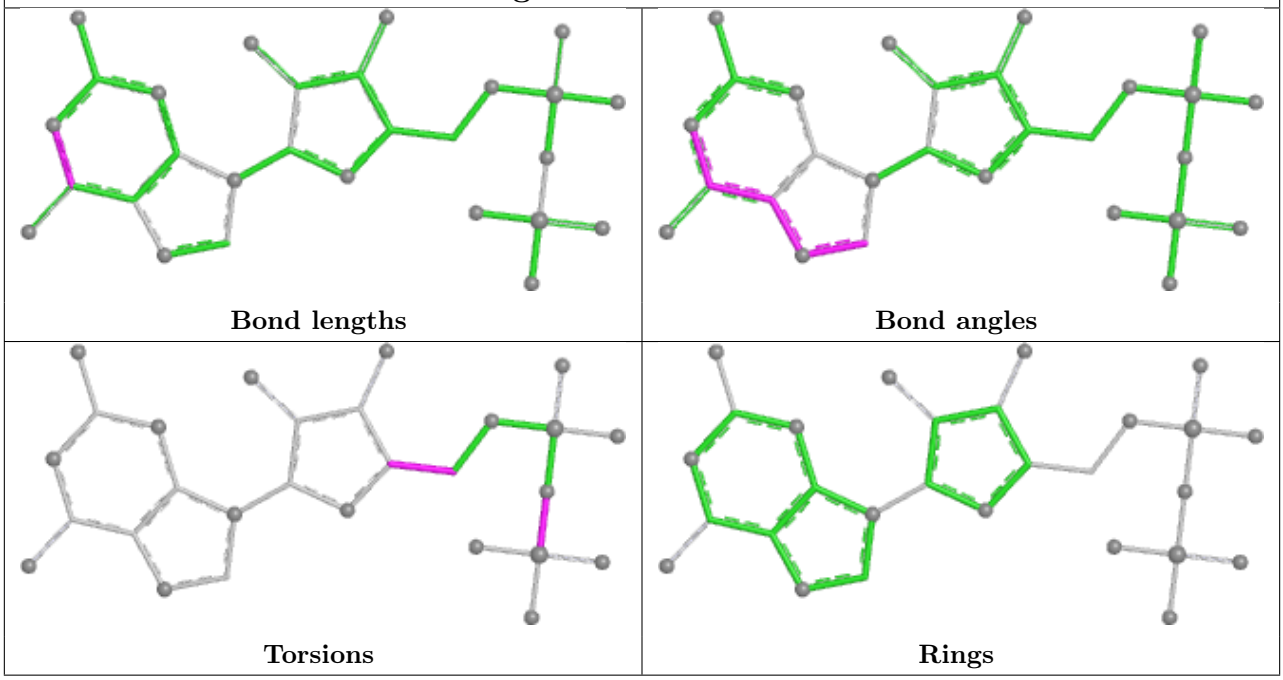

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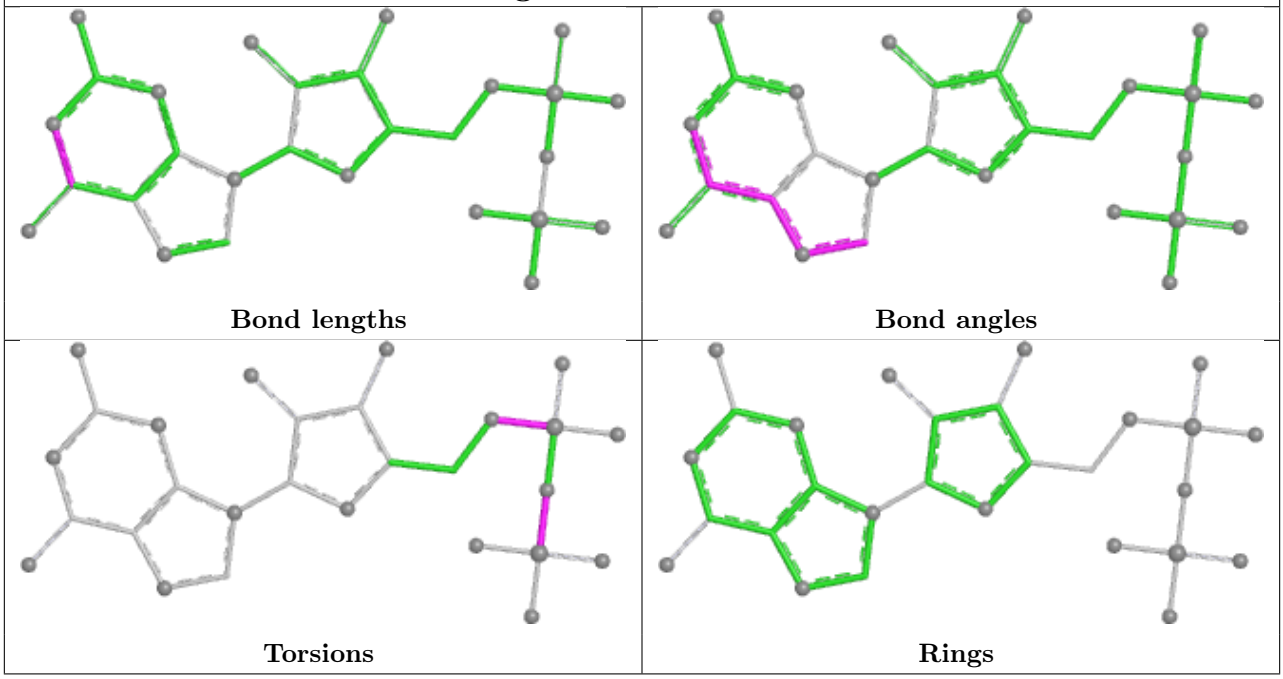

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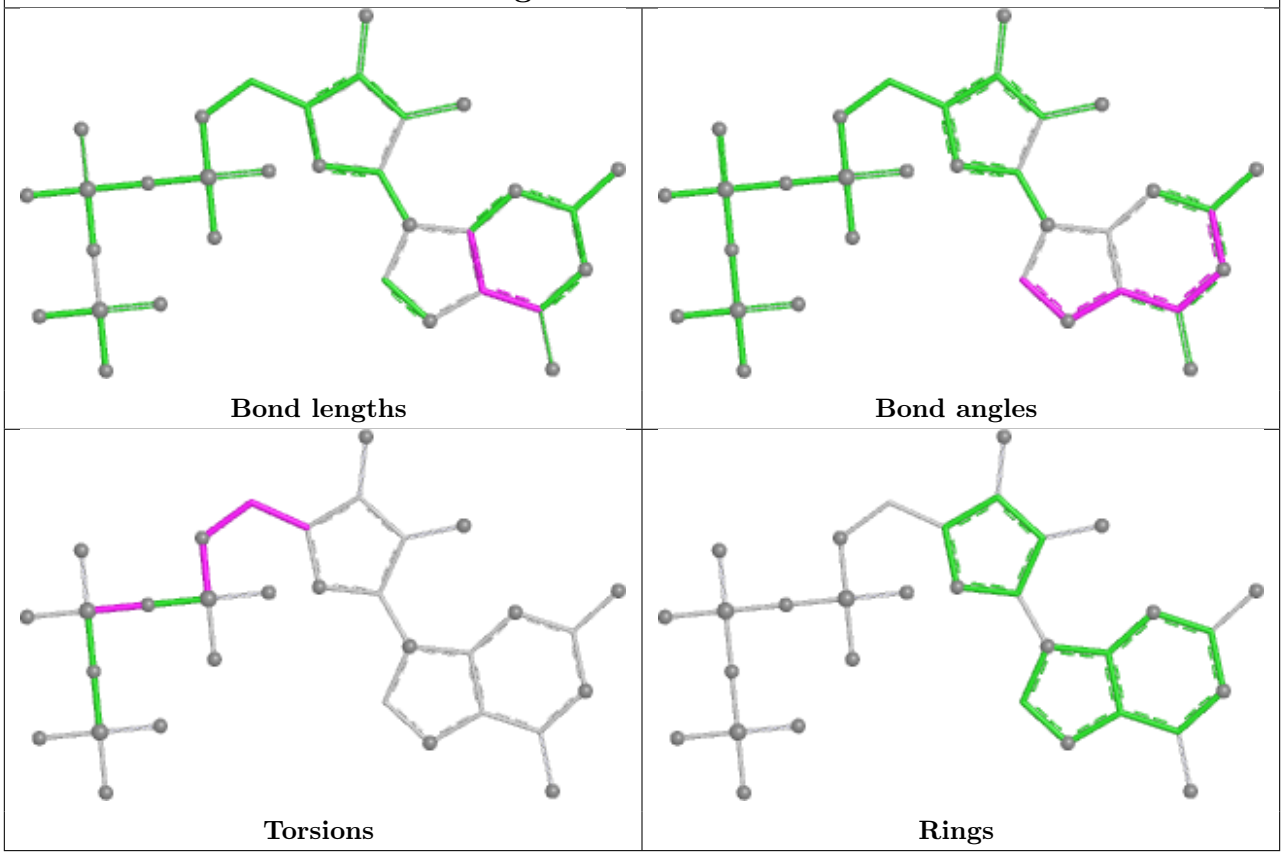

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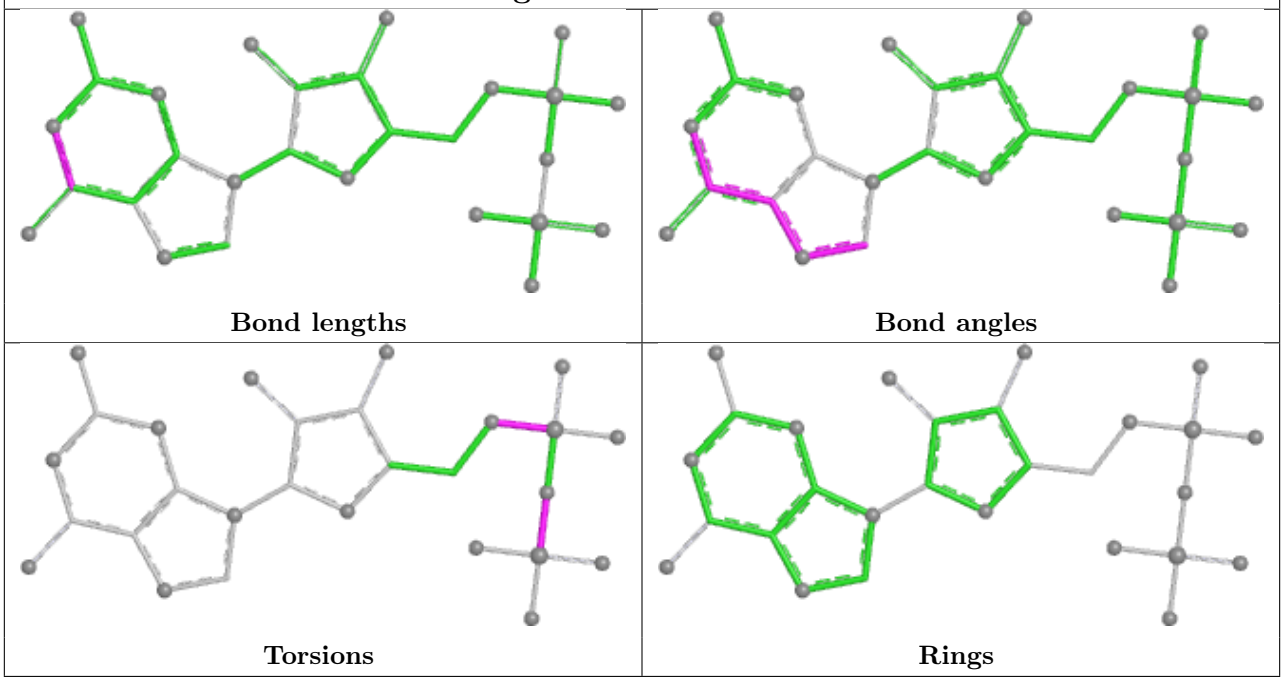

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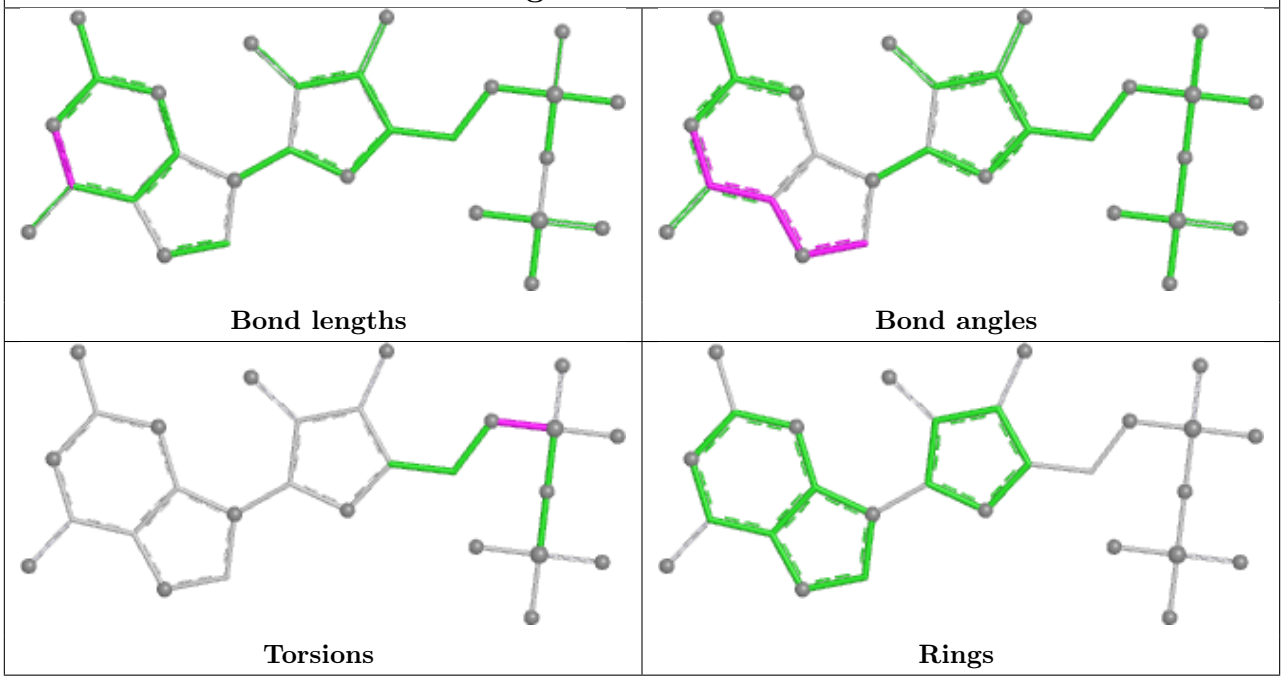

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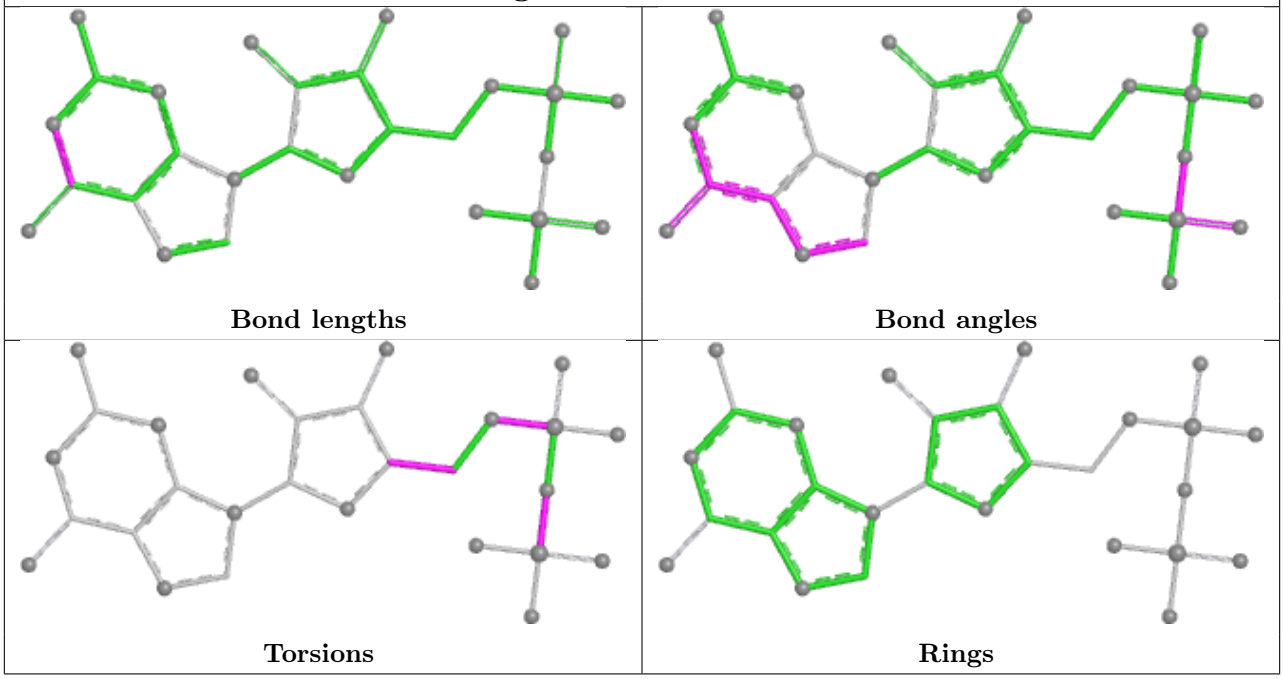

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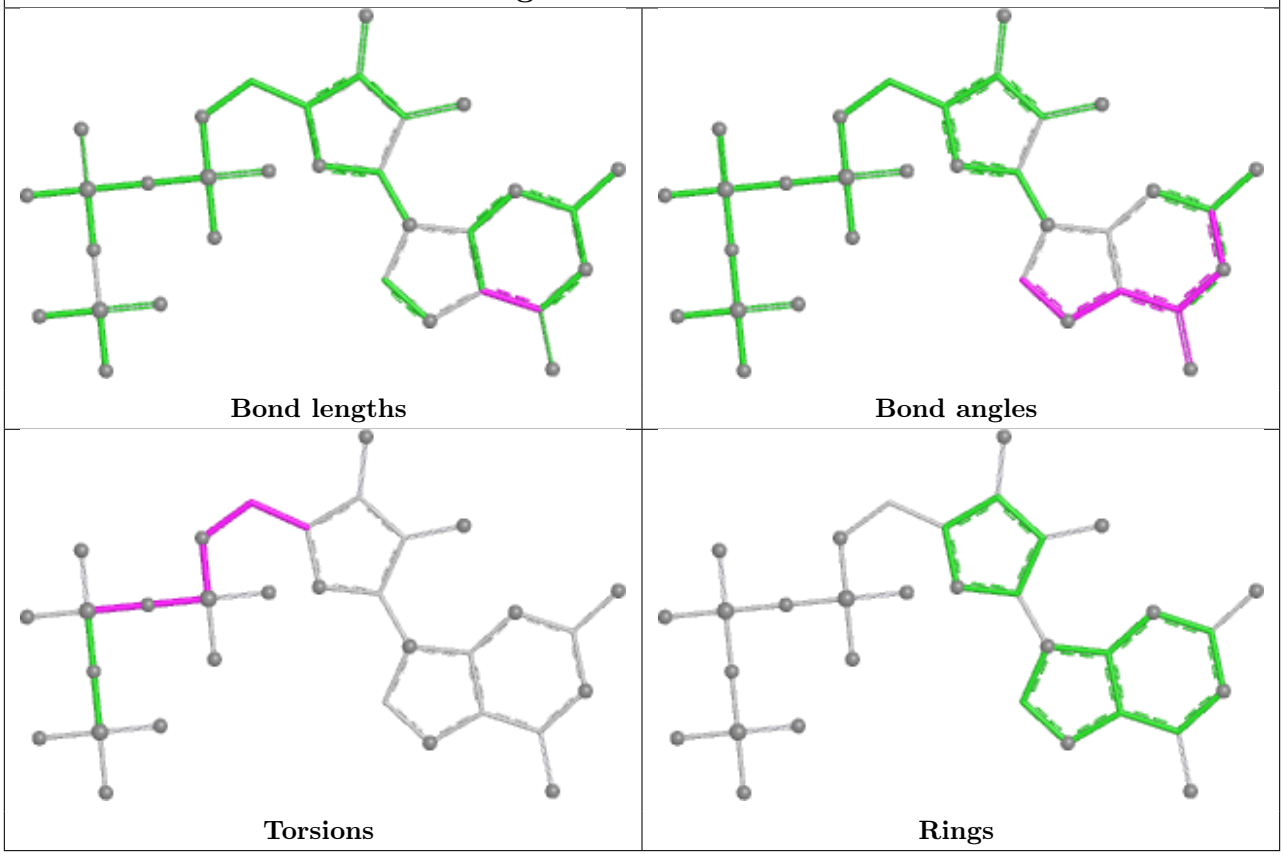

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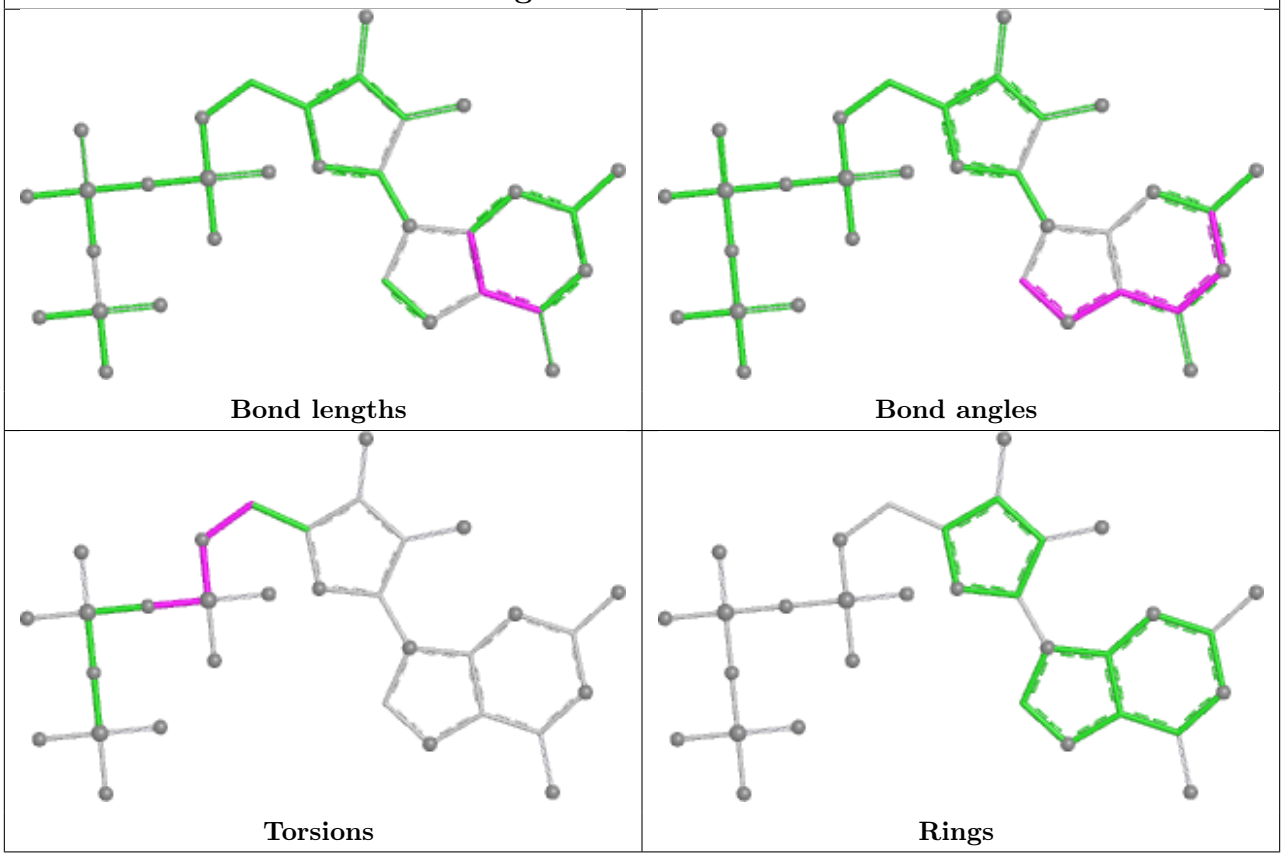

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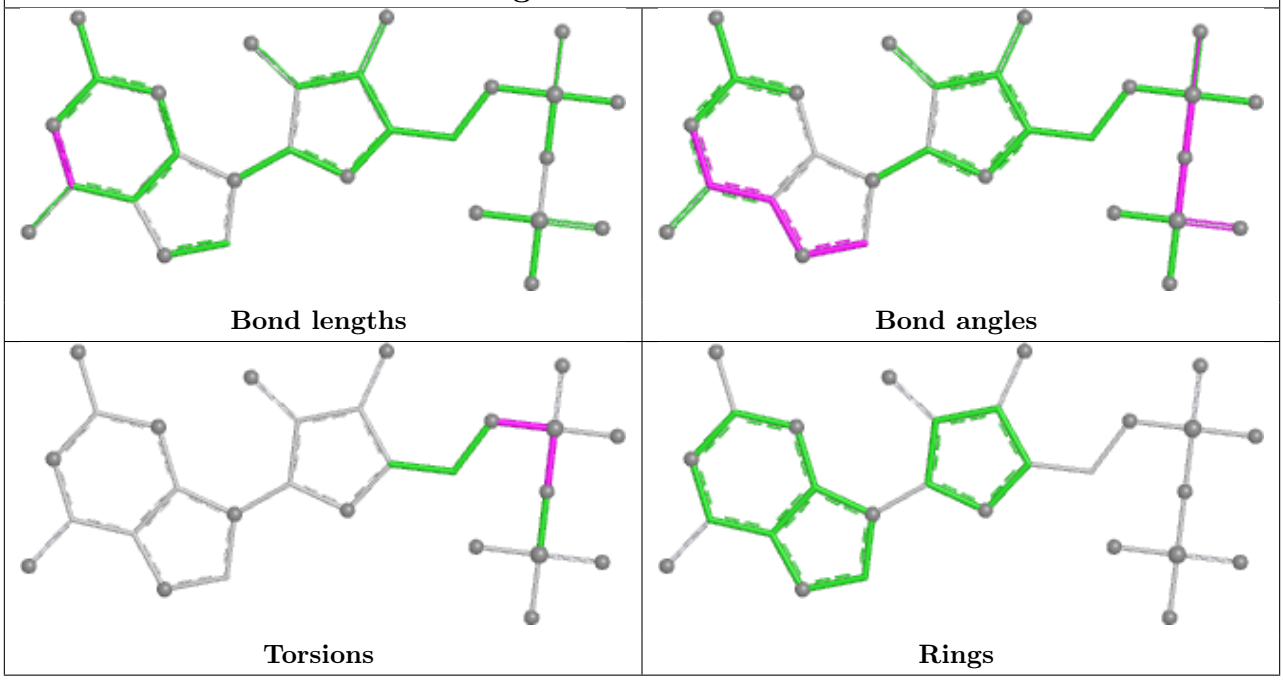

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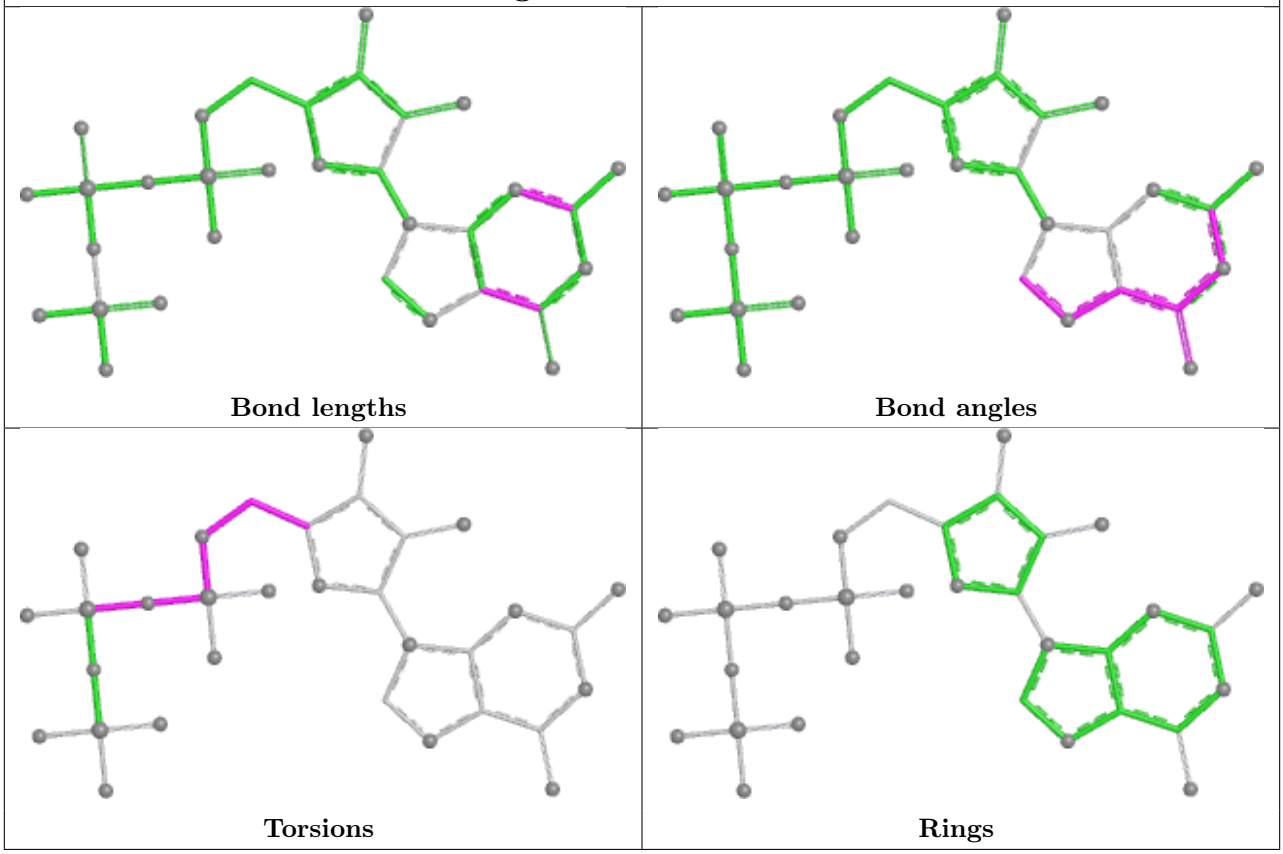

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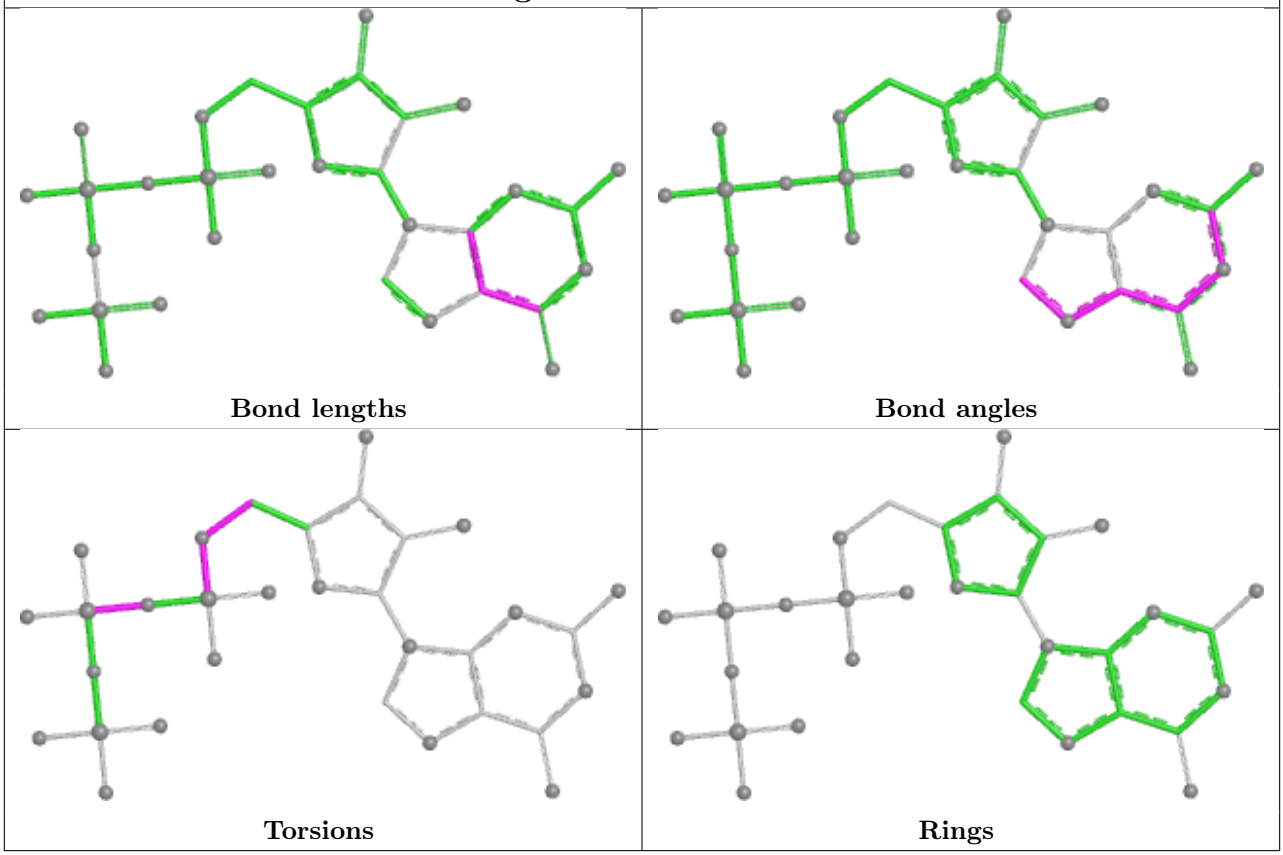

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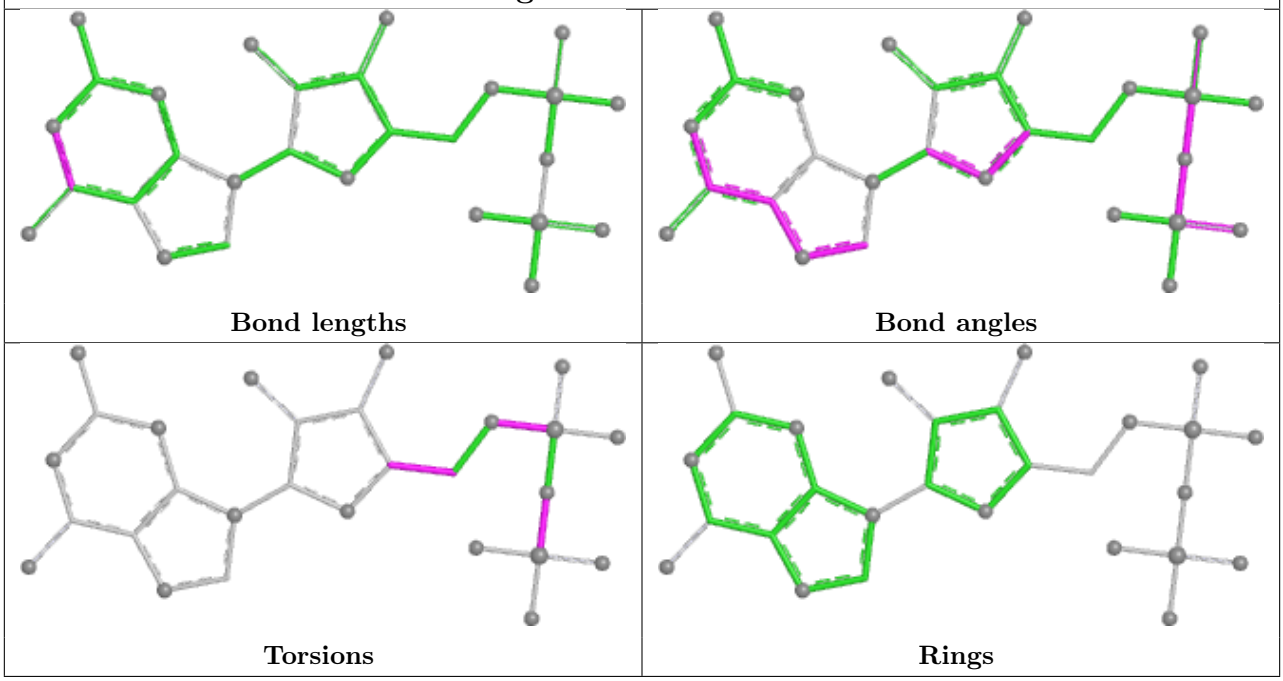

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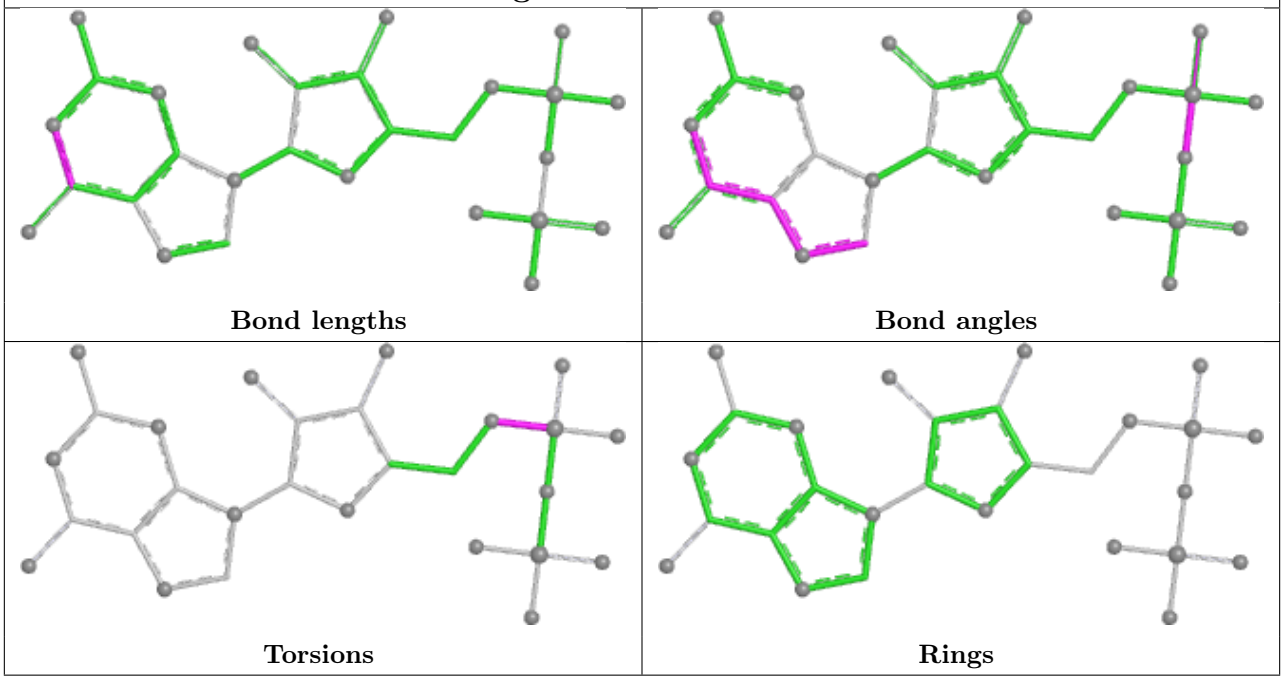

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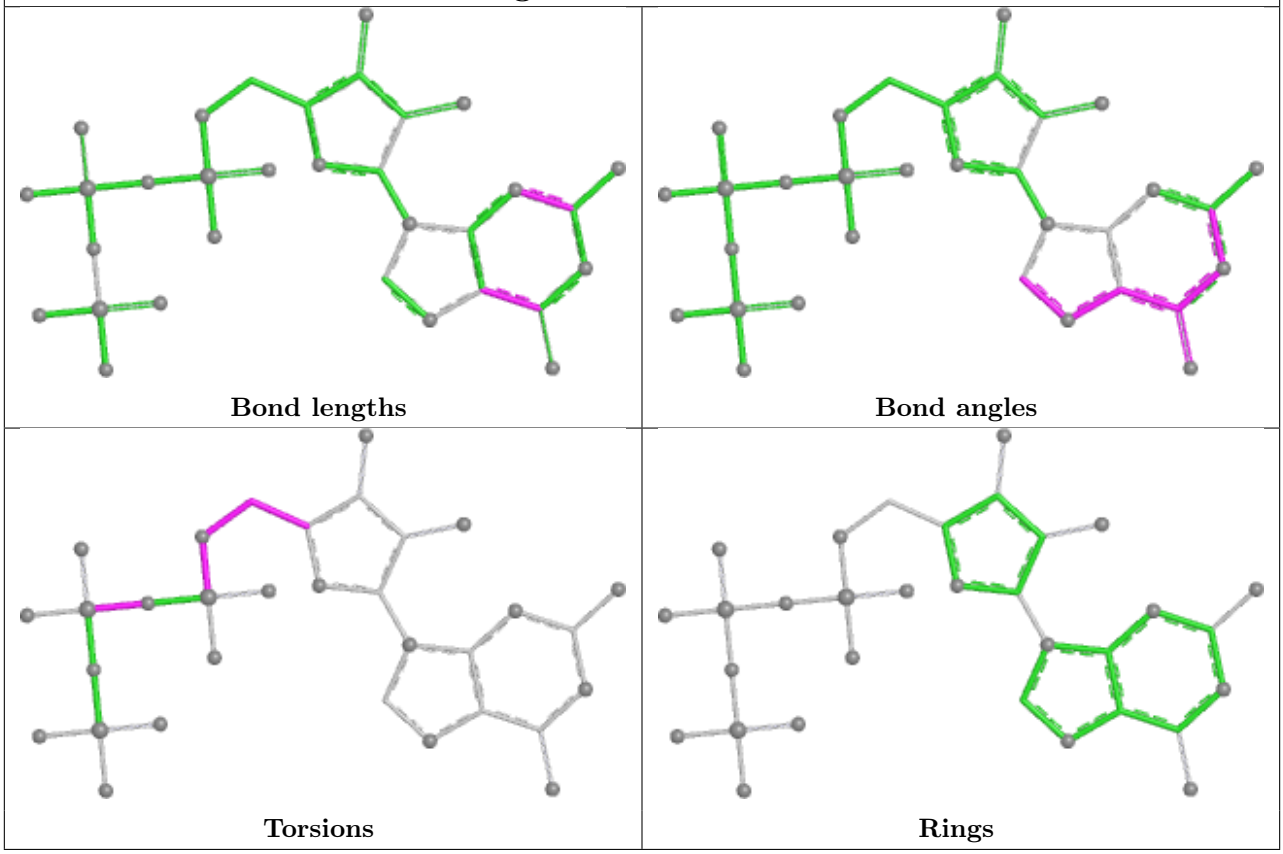

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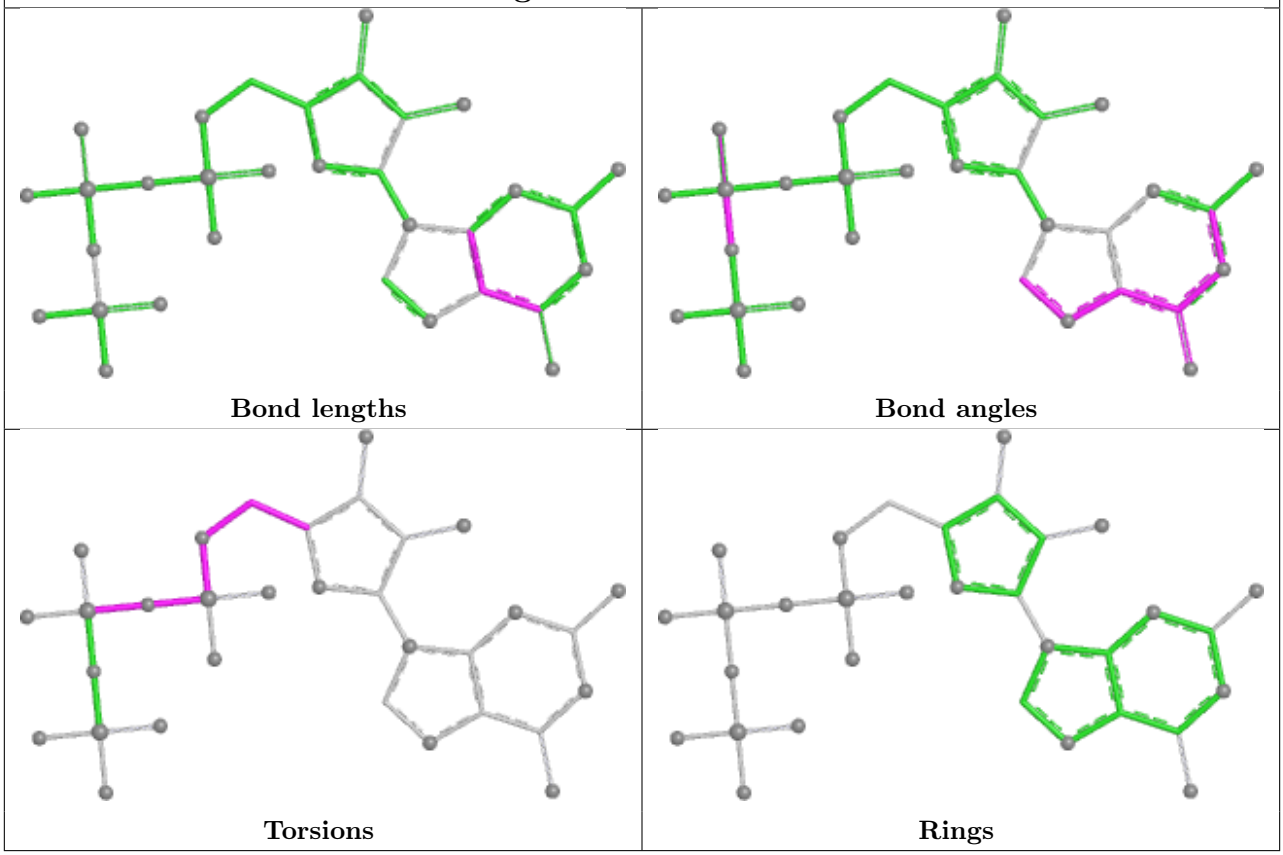

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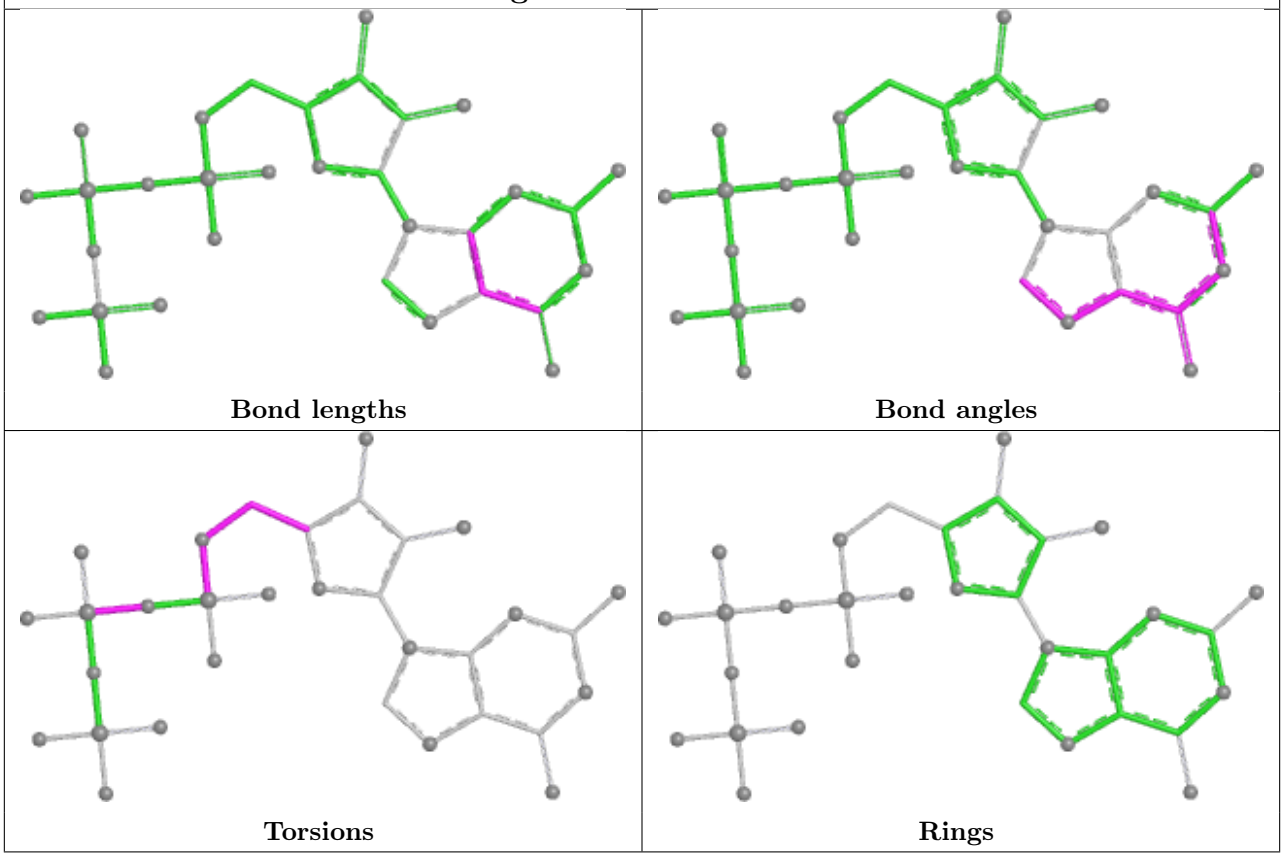
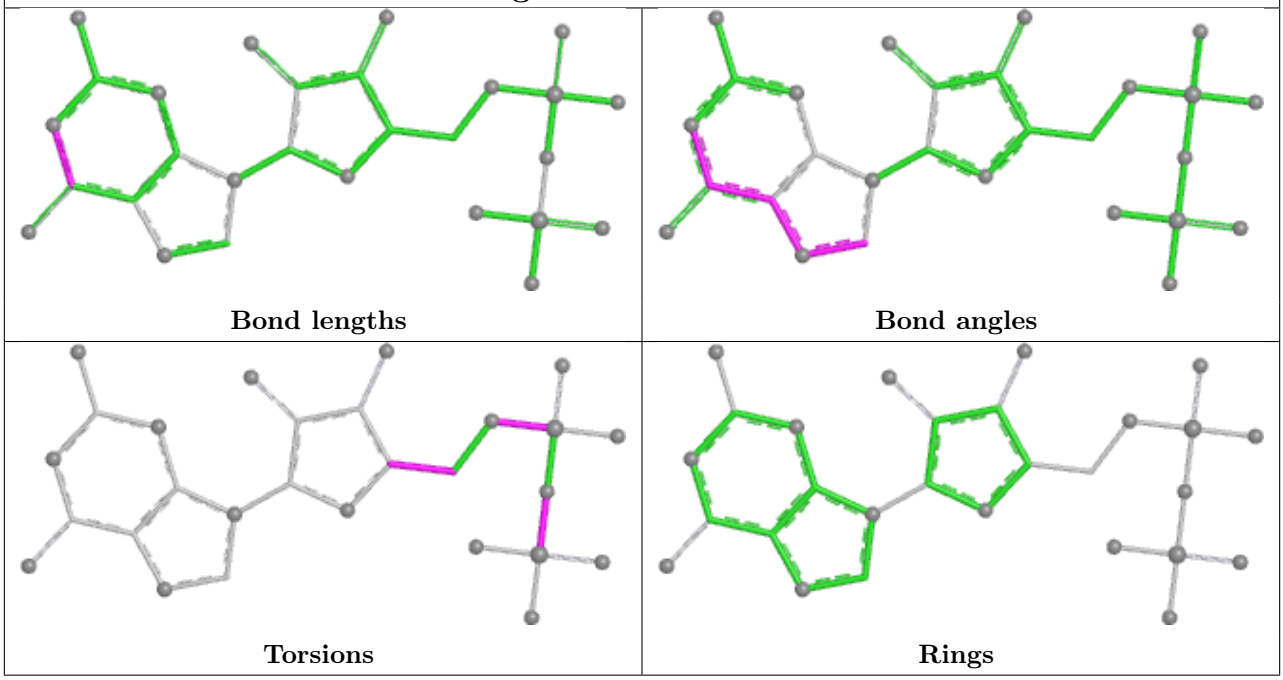


Ligand GDP N6 503



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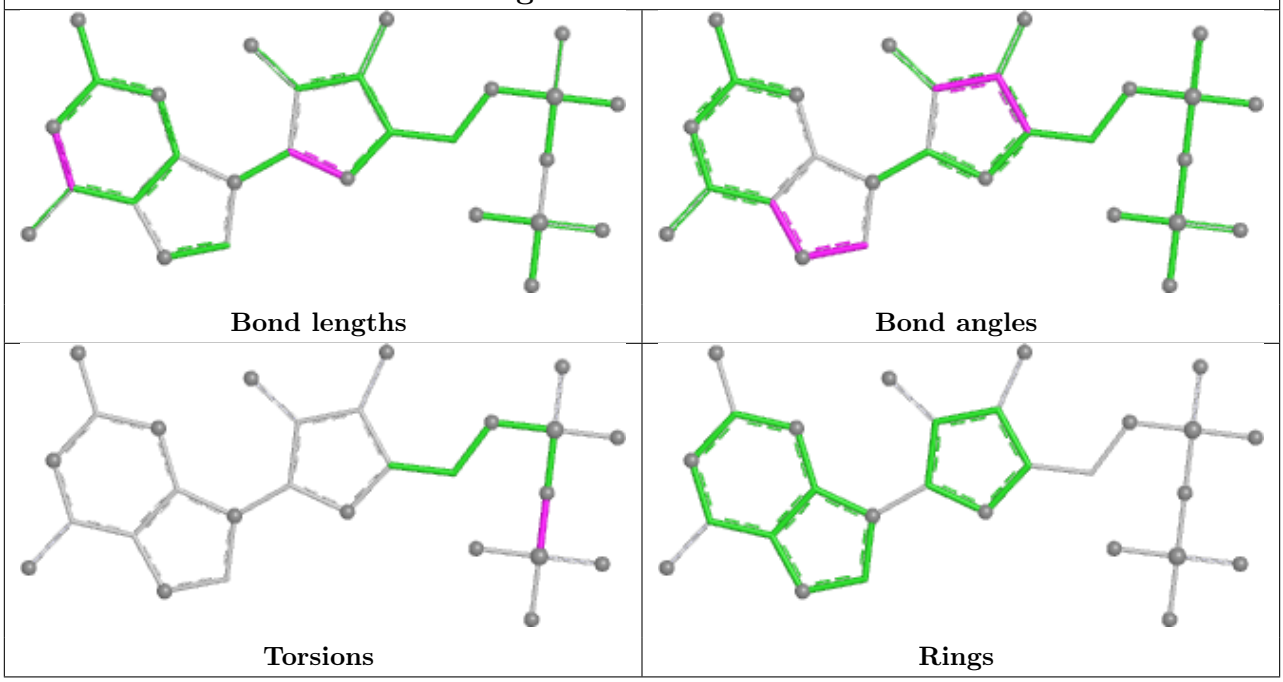

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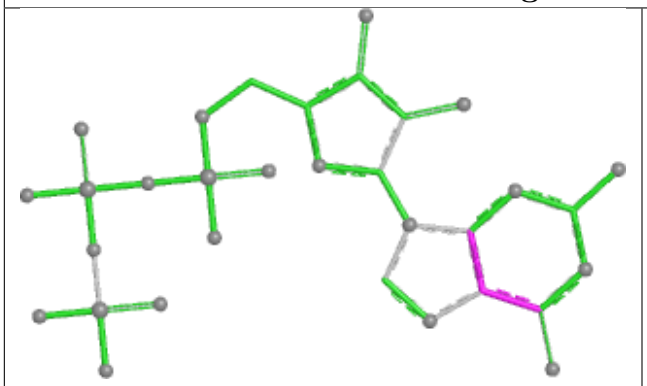
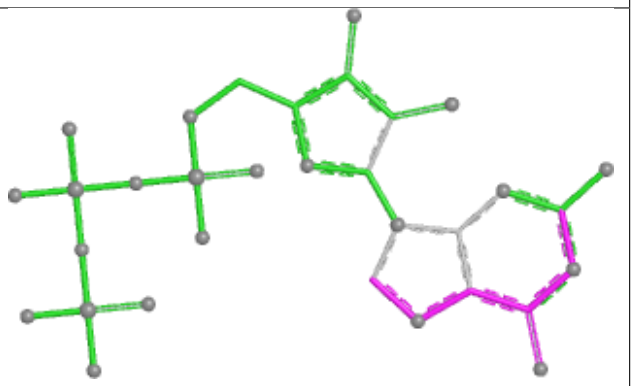
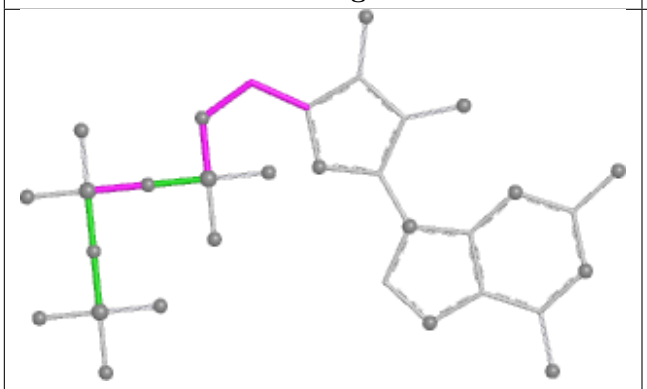


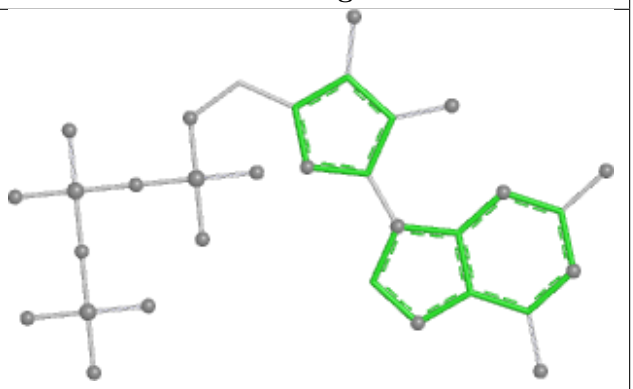
Bond lengths



Bond angles

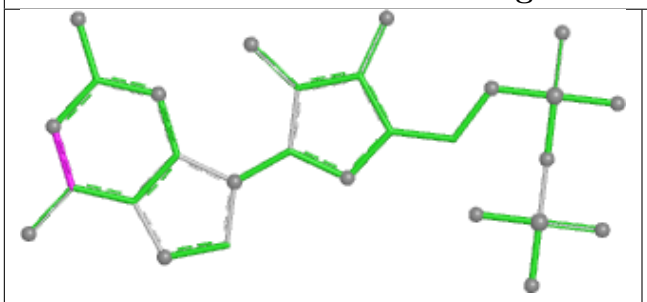


Torsions



Rings

Ligand GDP L6 502



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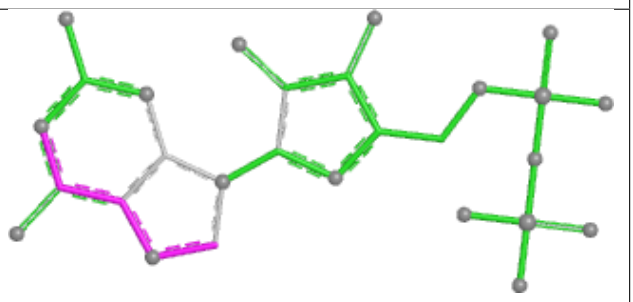
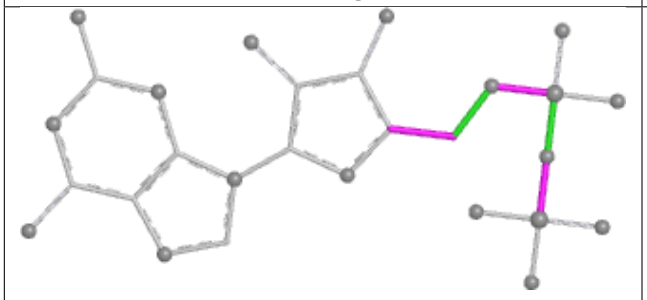
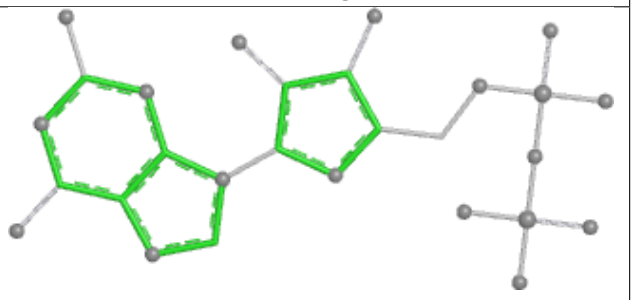


Bond angles



Torsions



Rings

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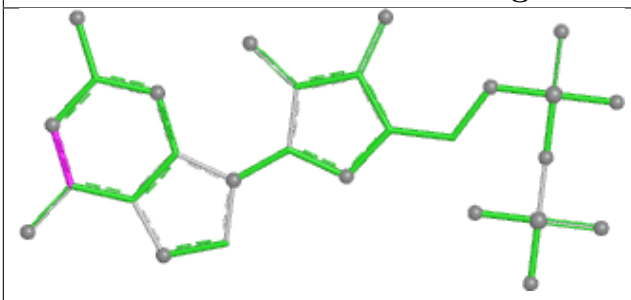
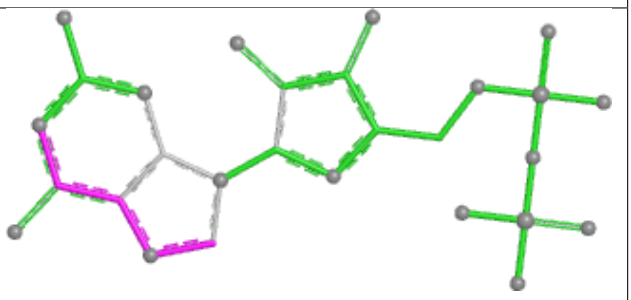
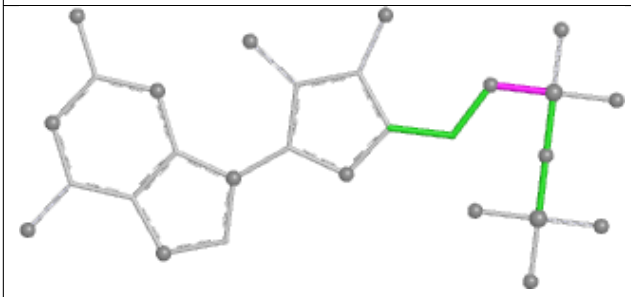
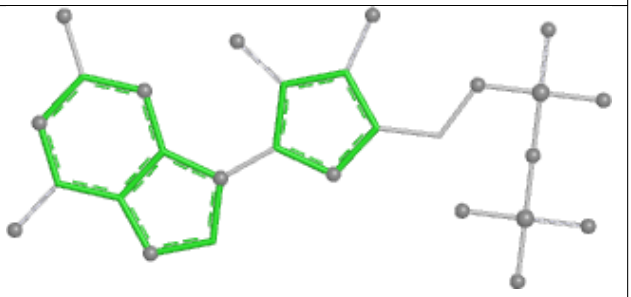
 Bond lengths	 Bond angles
 Torsions	 Rings

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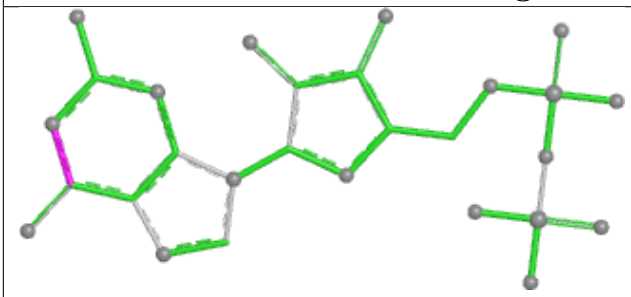
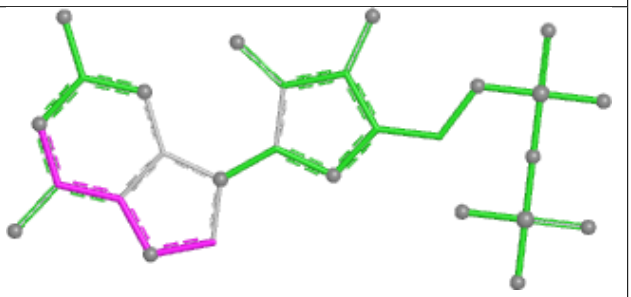
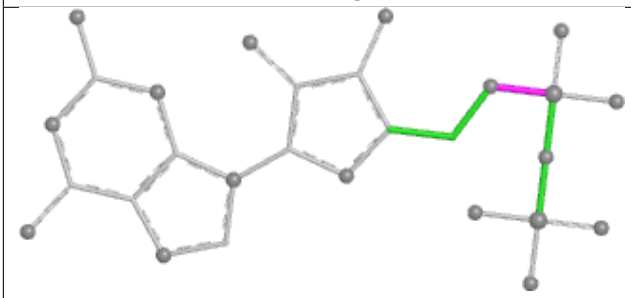
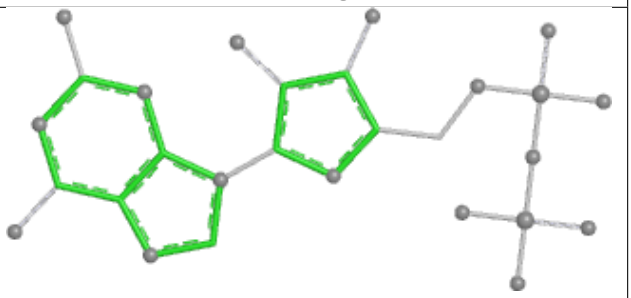
 Bond lengths	 Bond angles
 Torsions	 Rings

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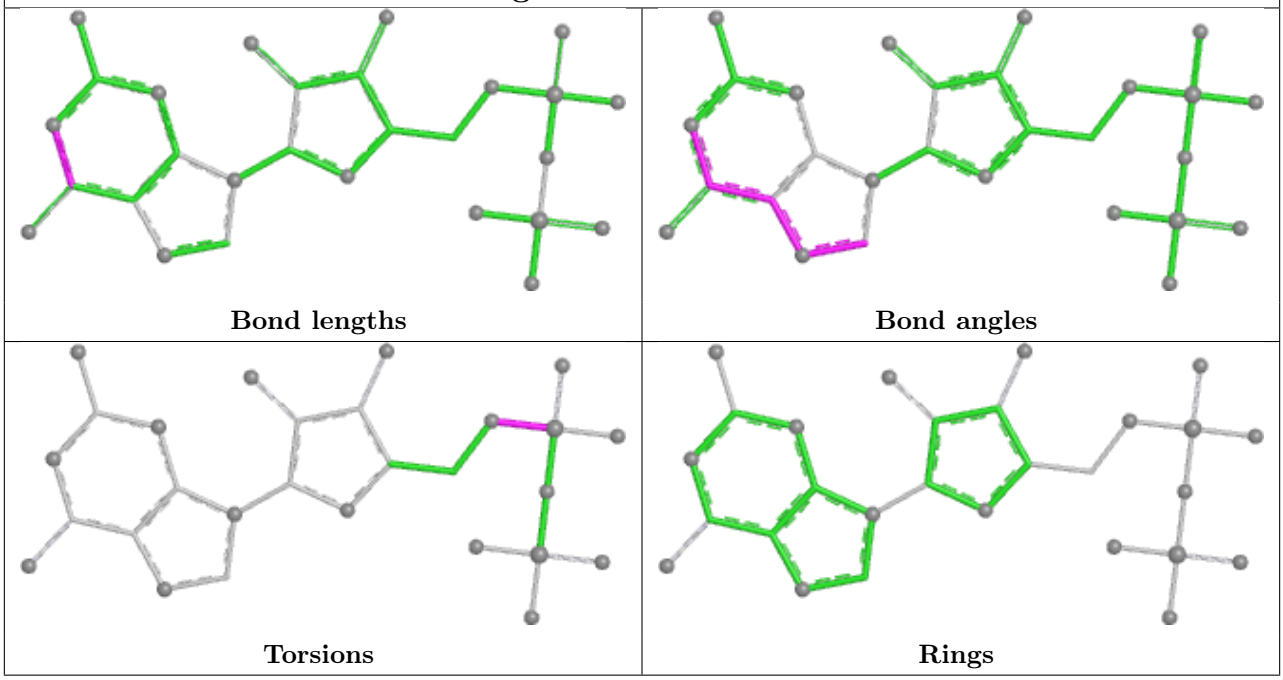

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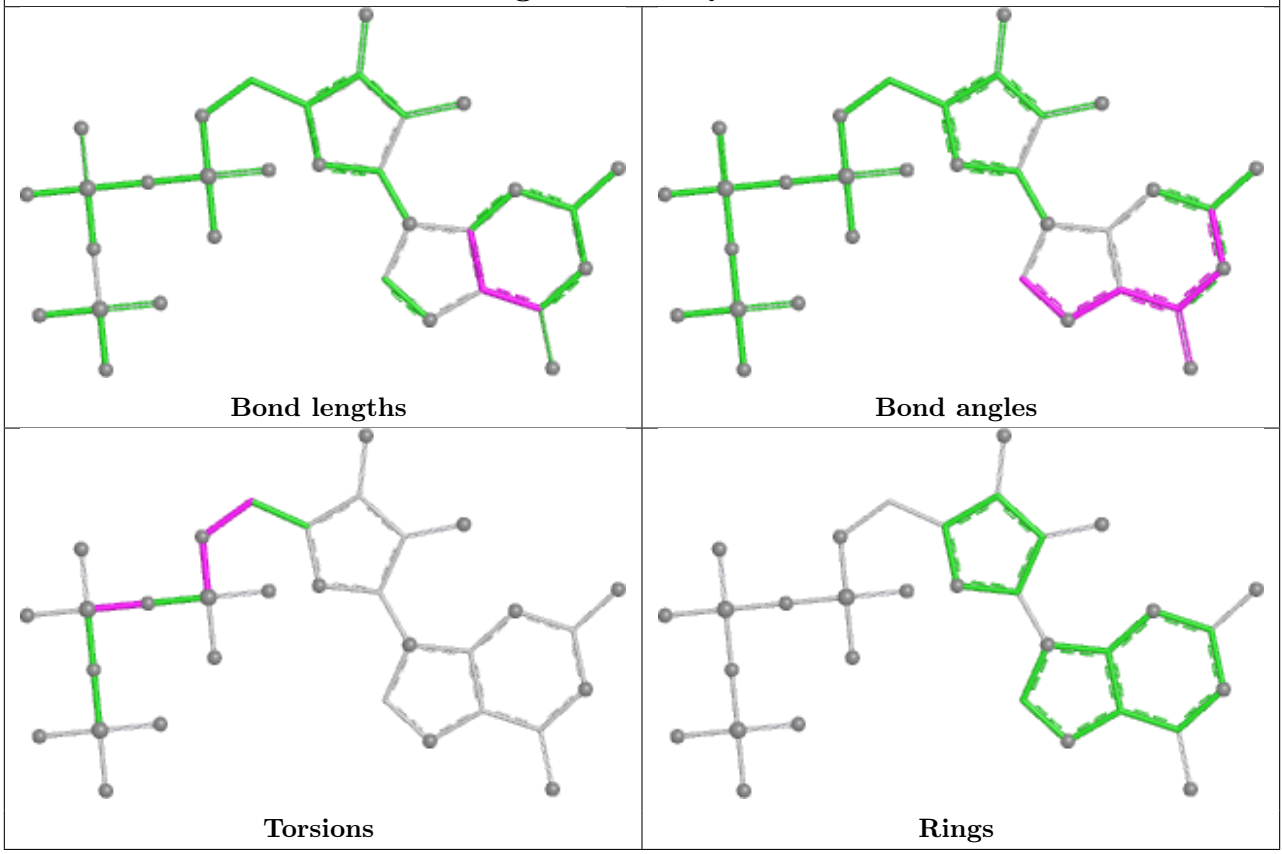

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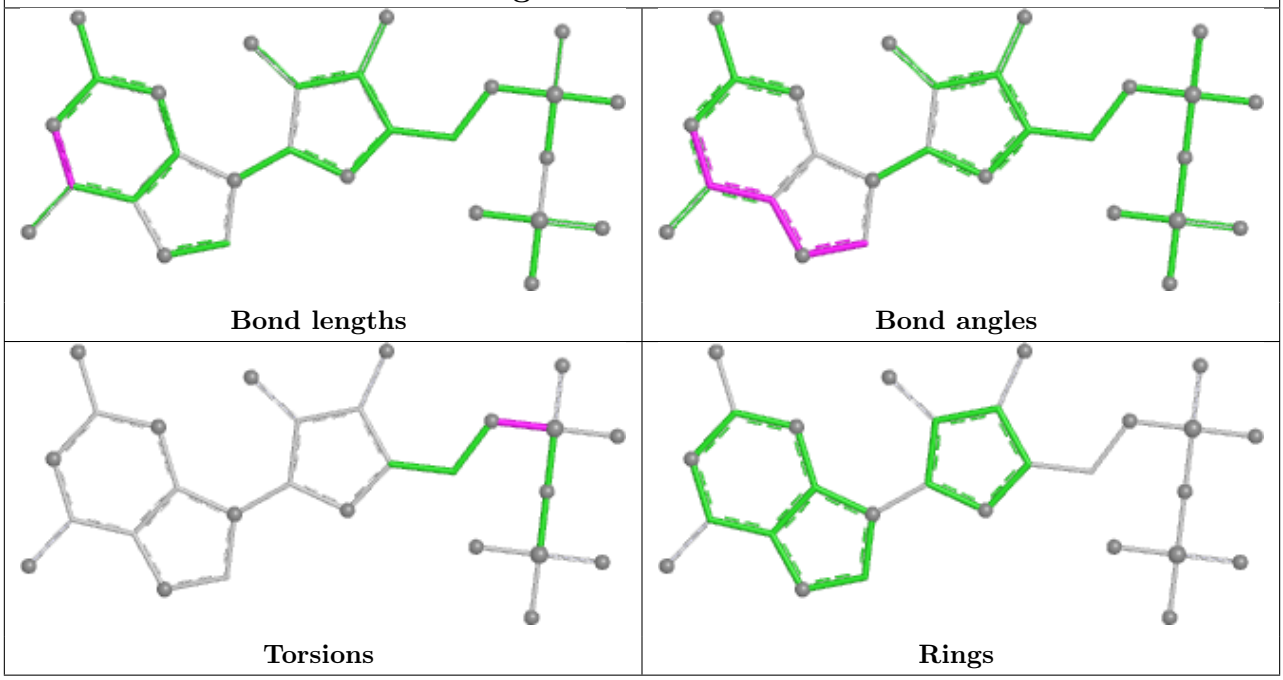

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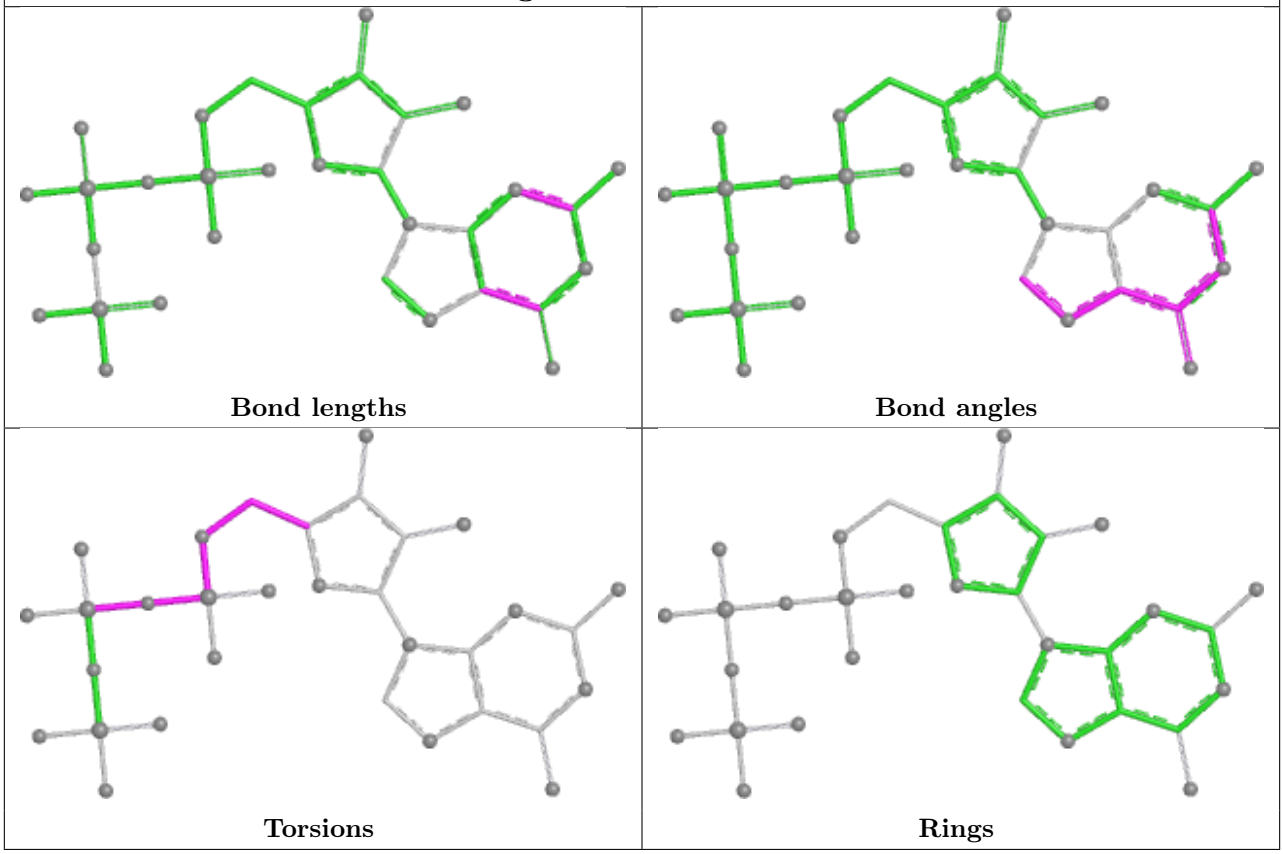

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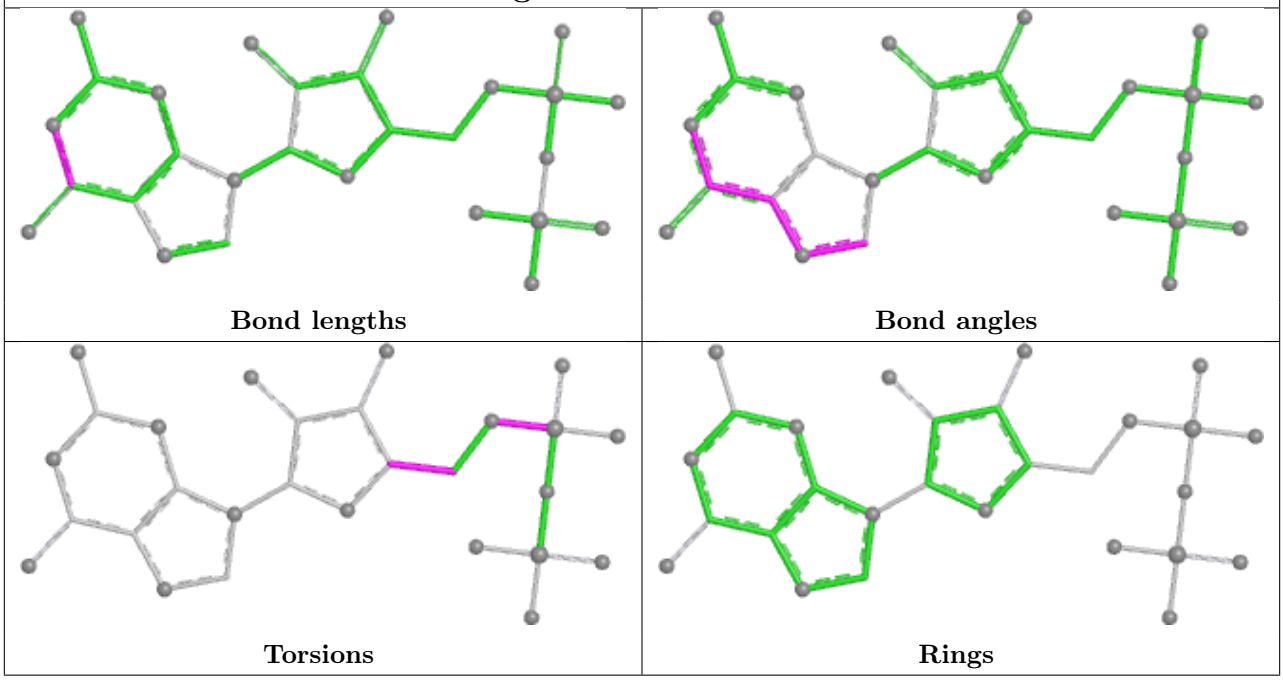

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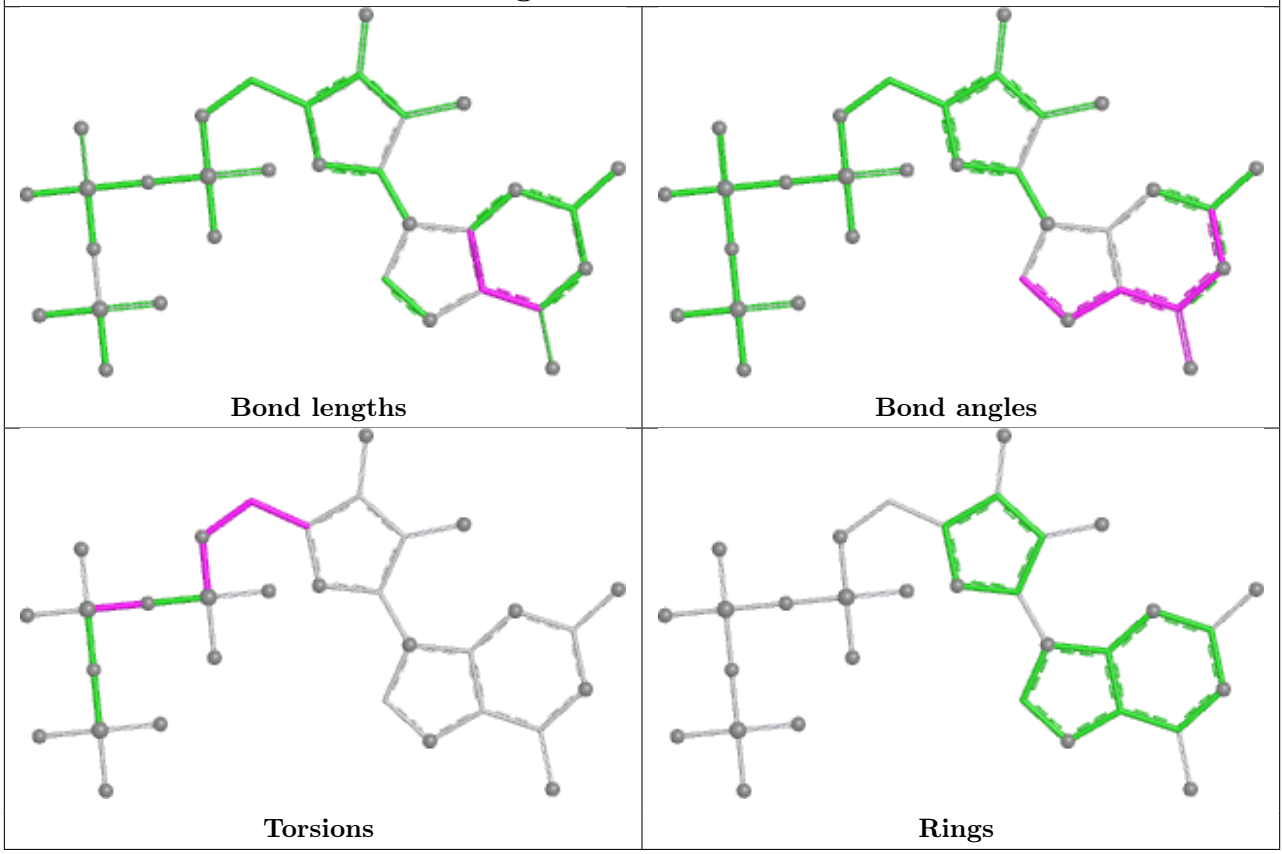

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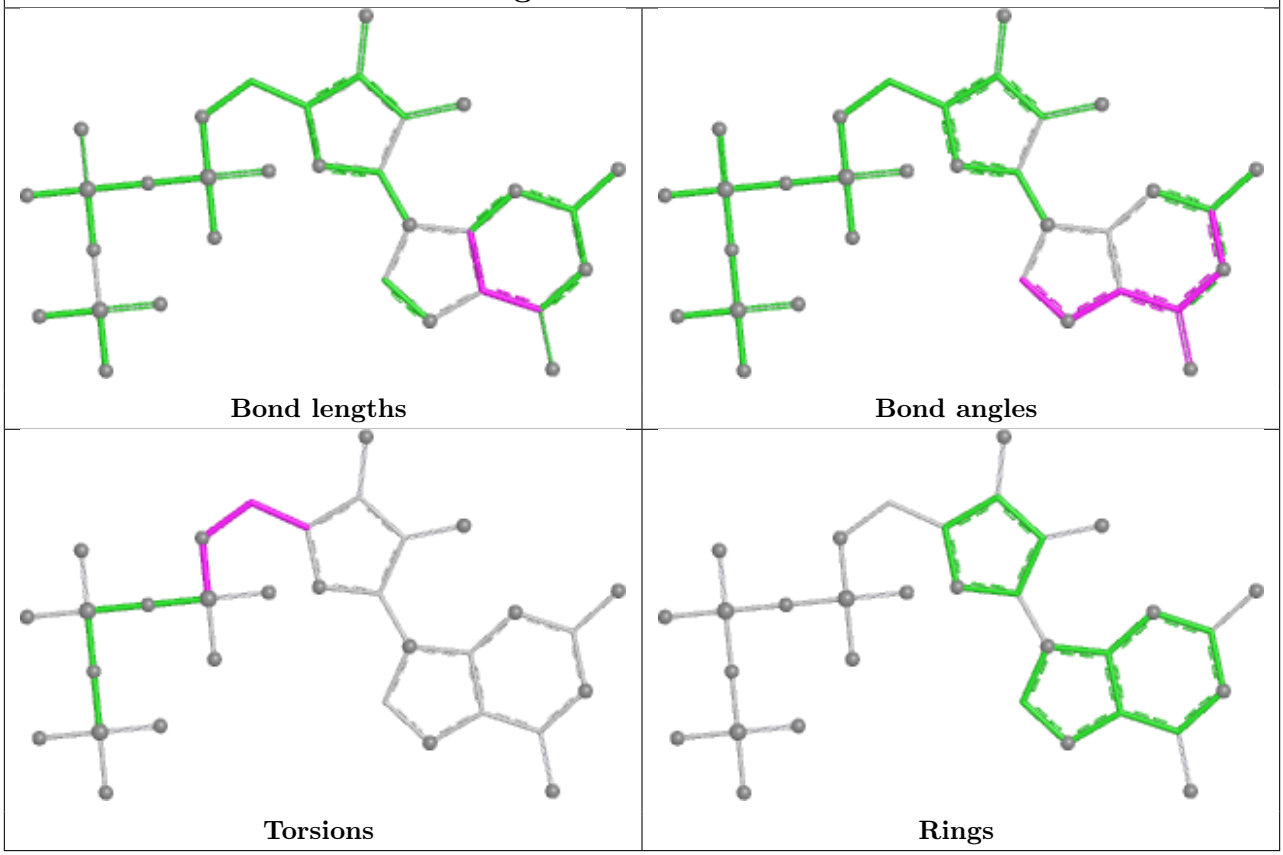

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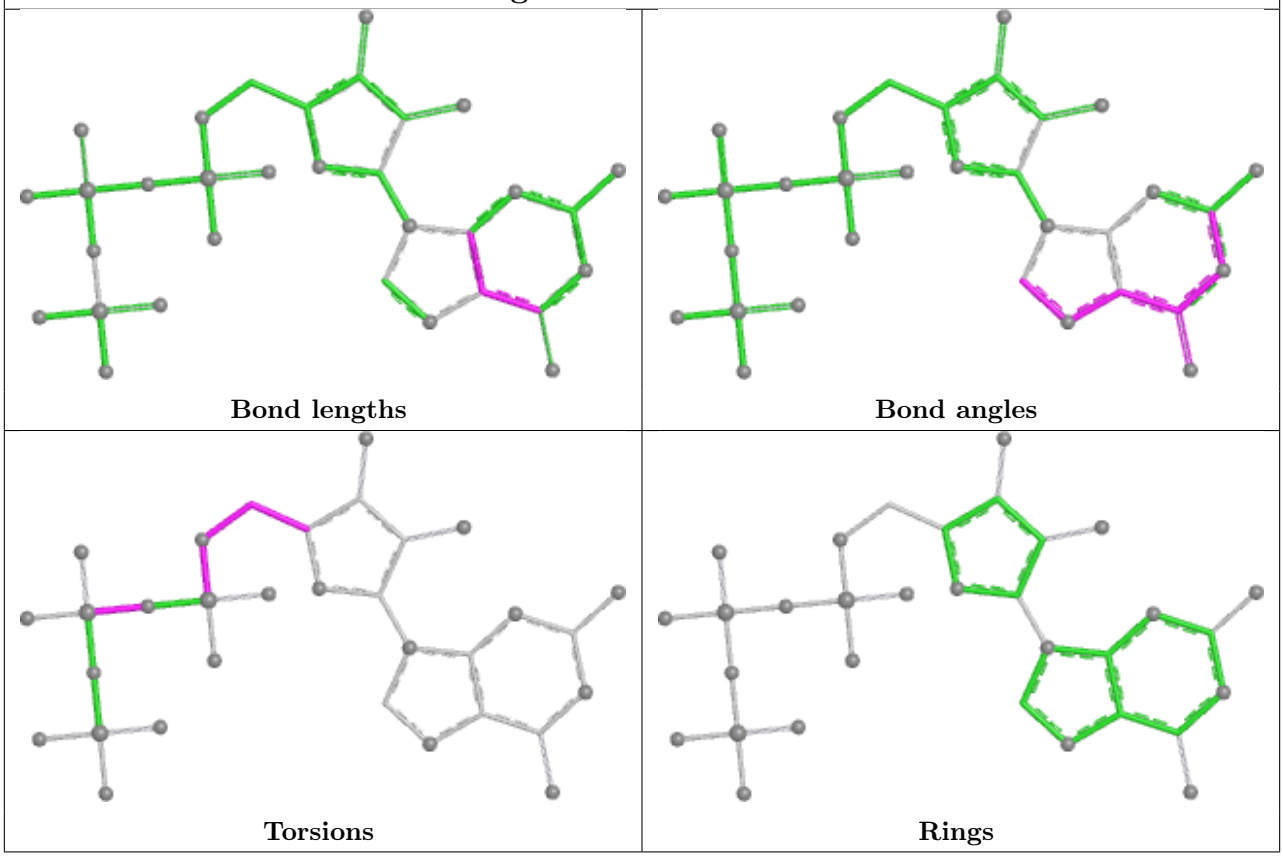

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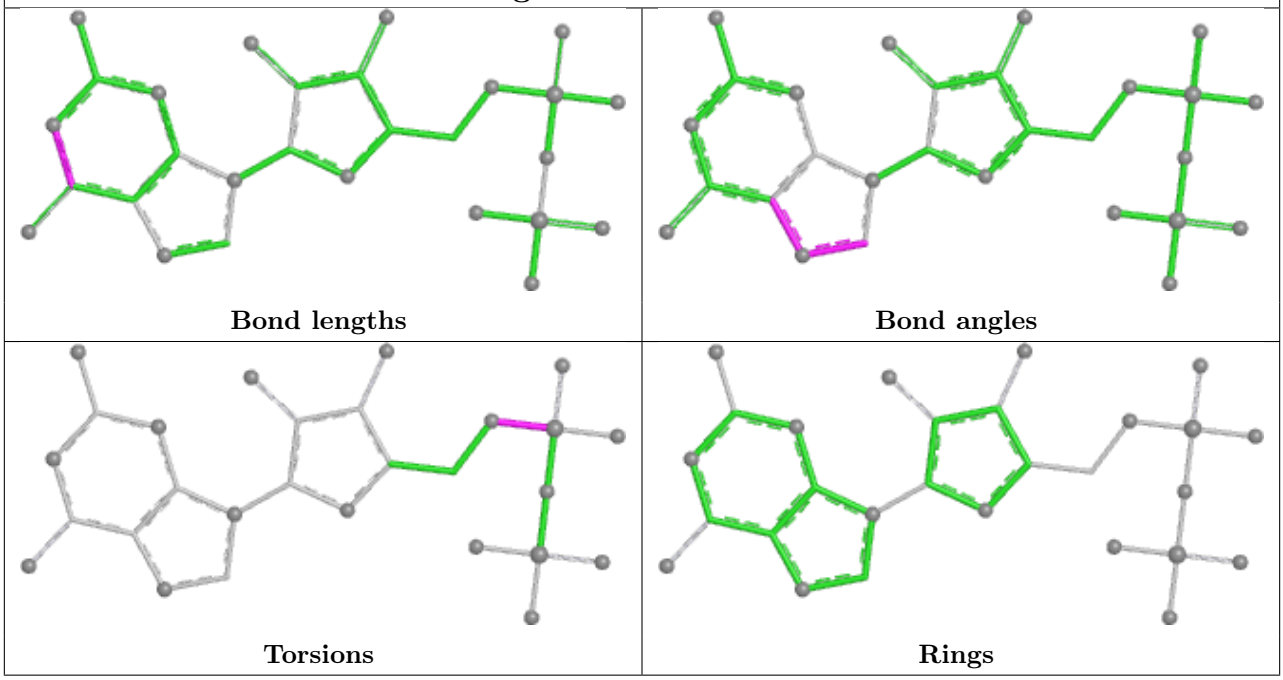

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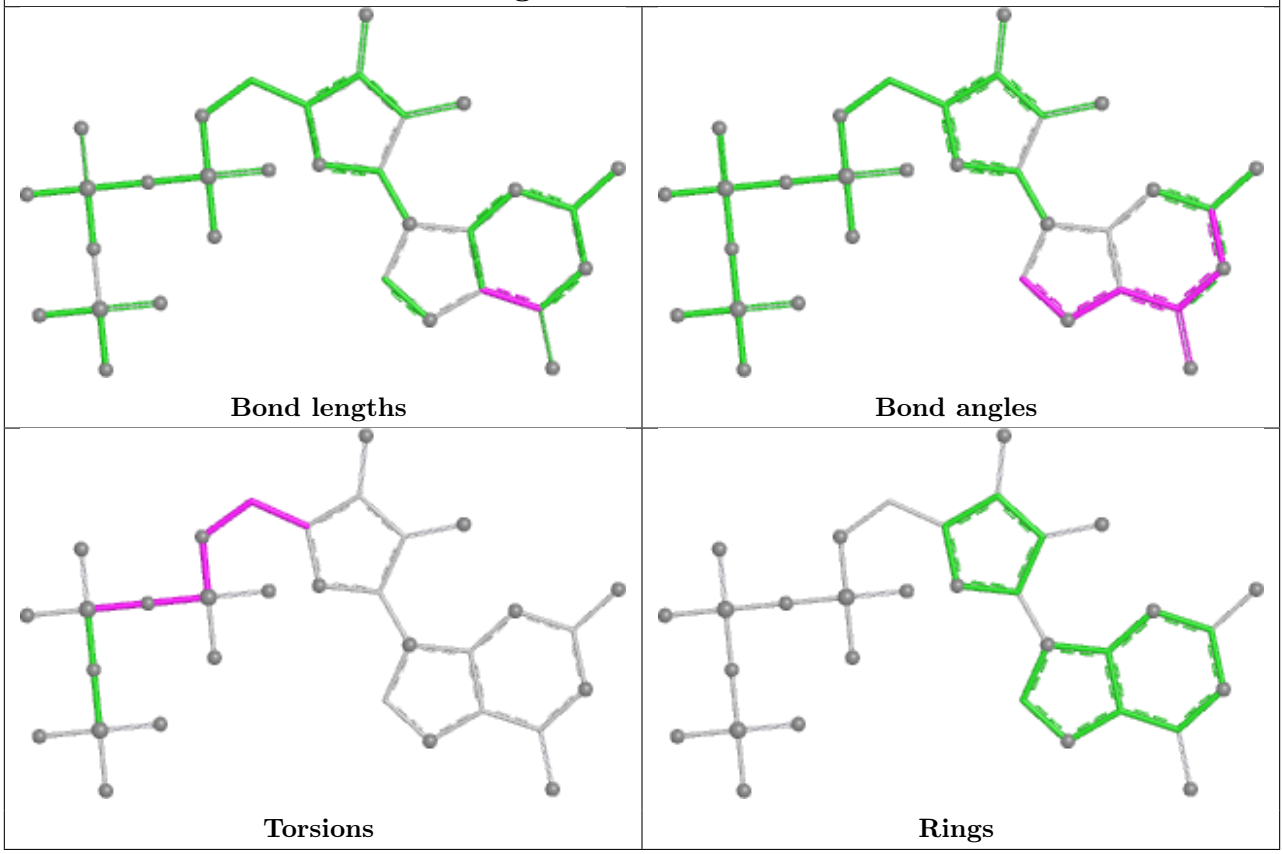

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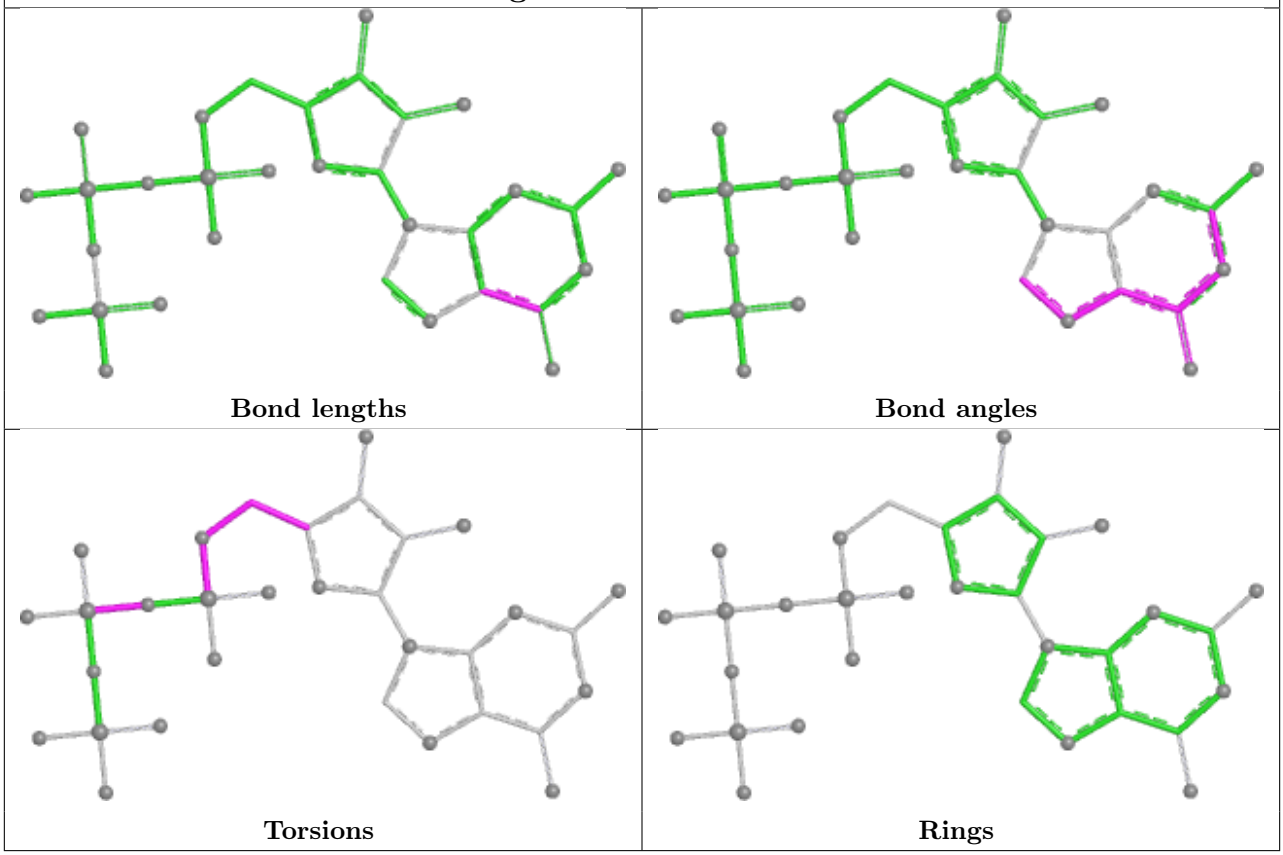

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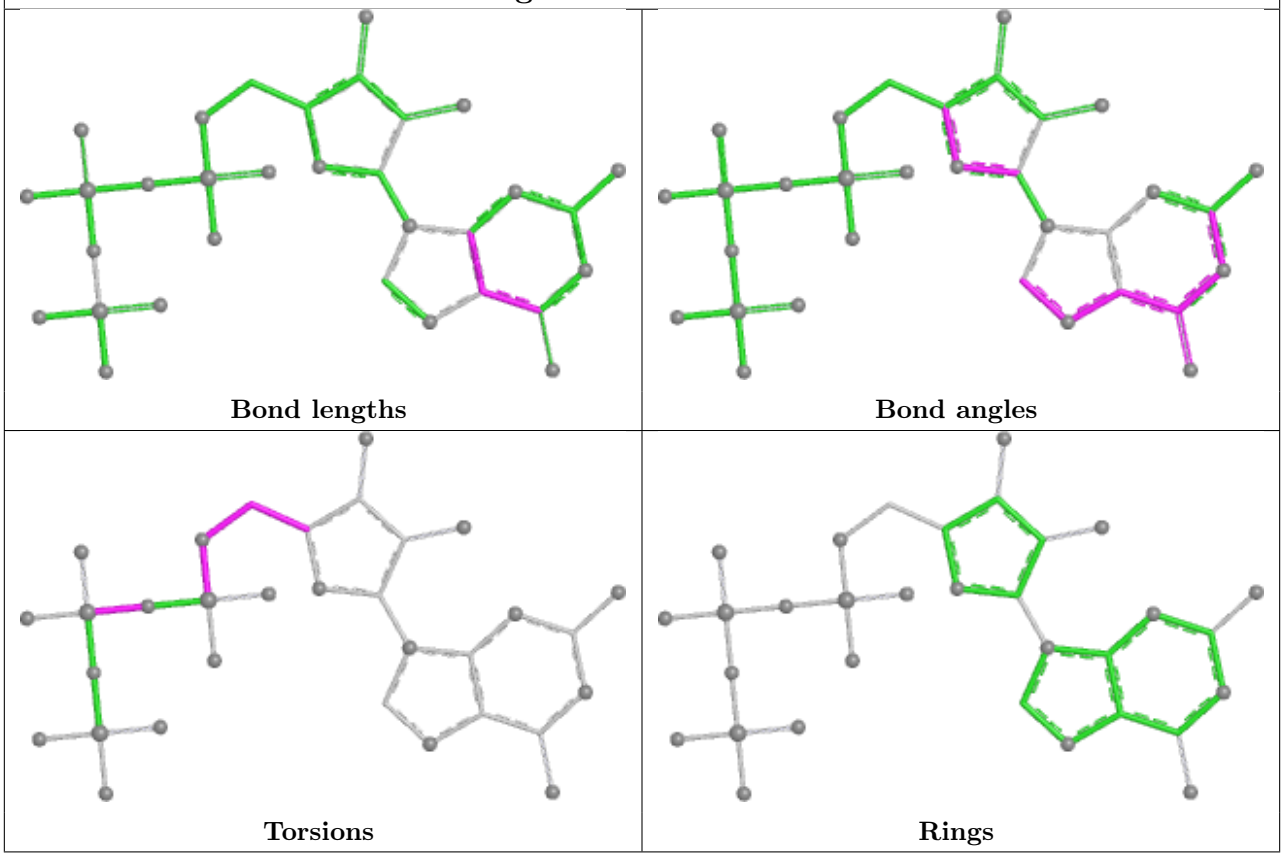

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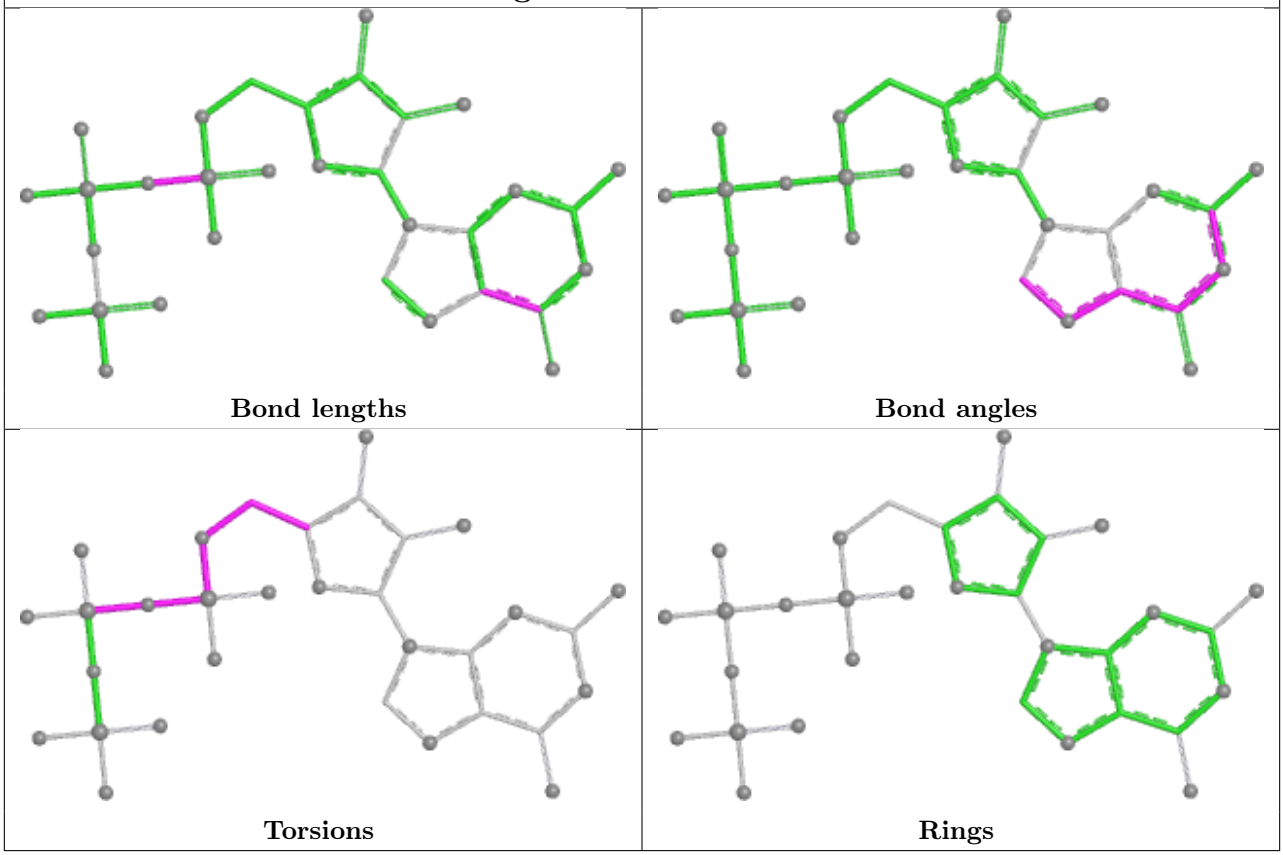

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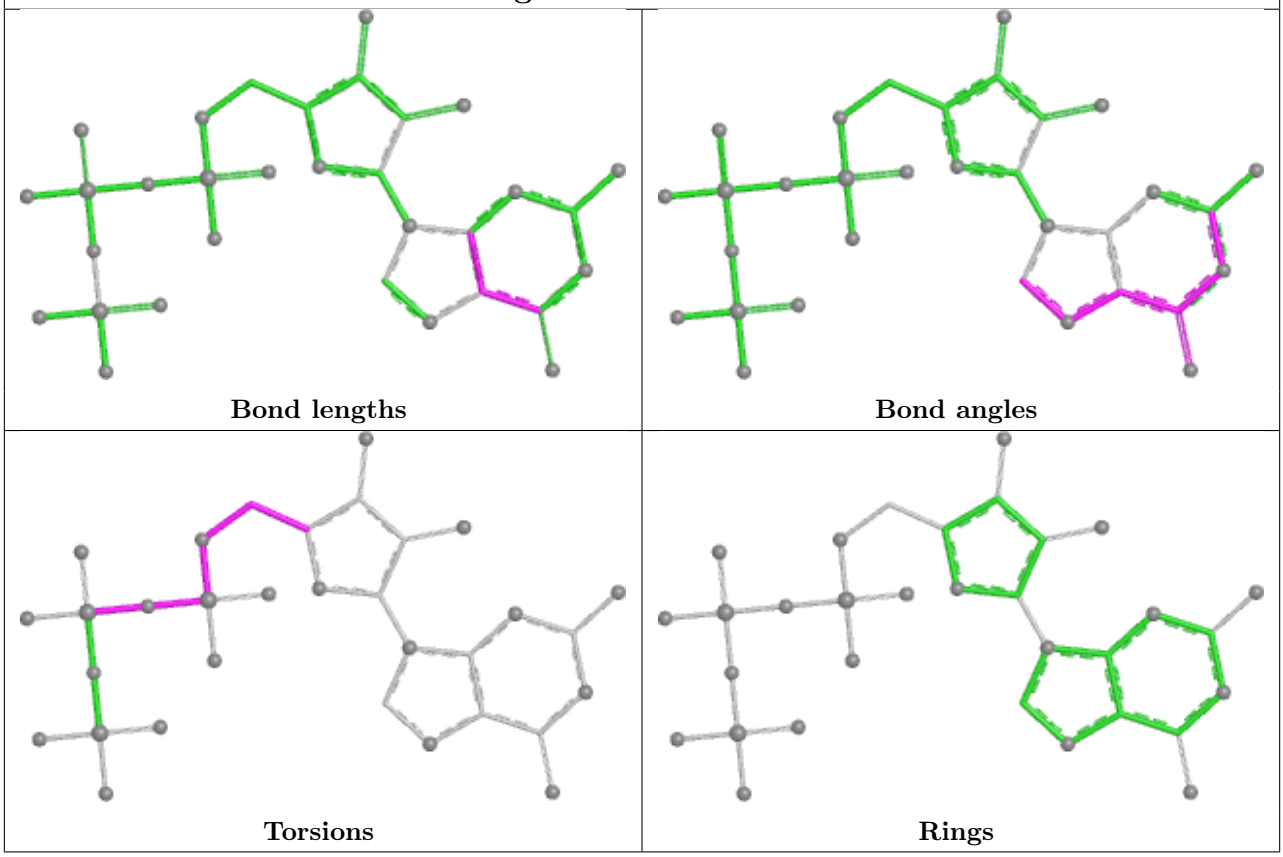

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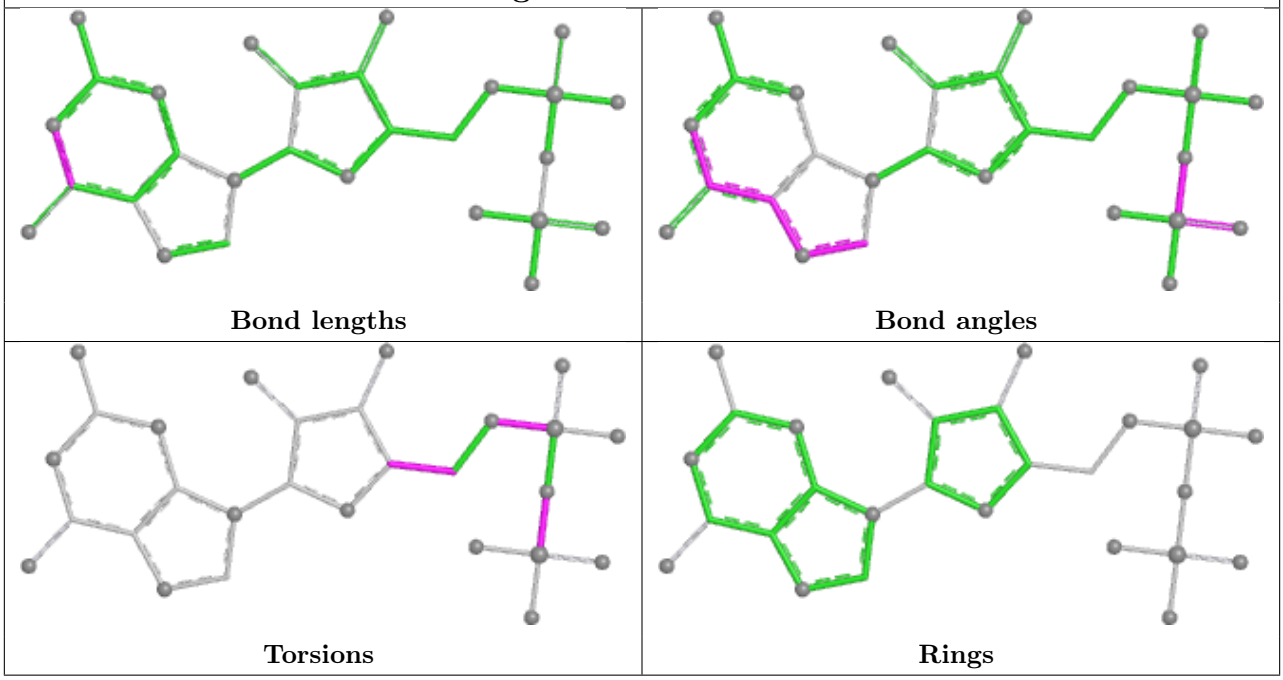

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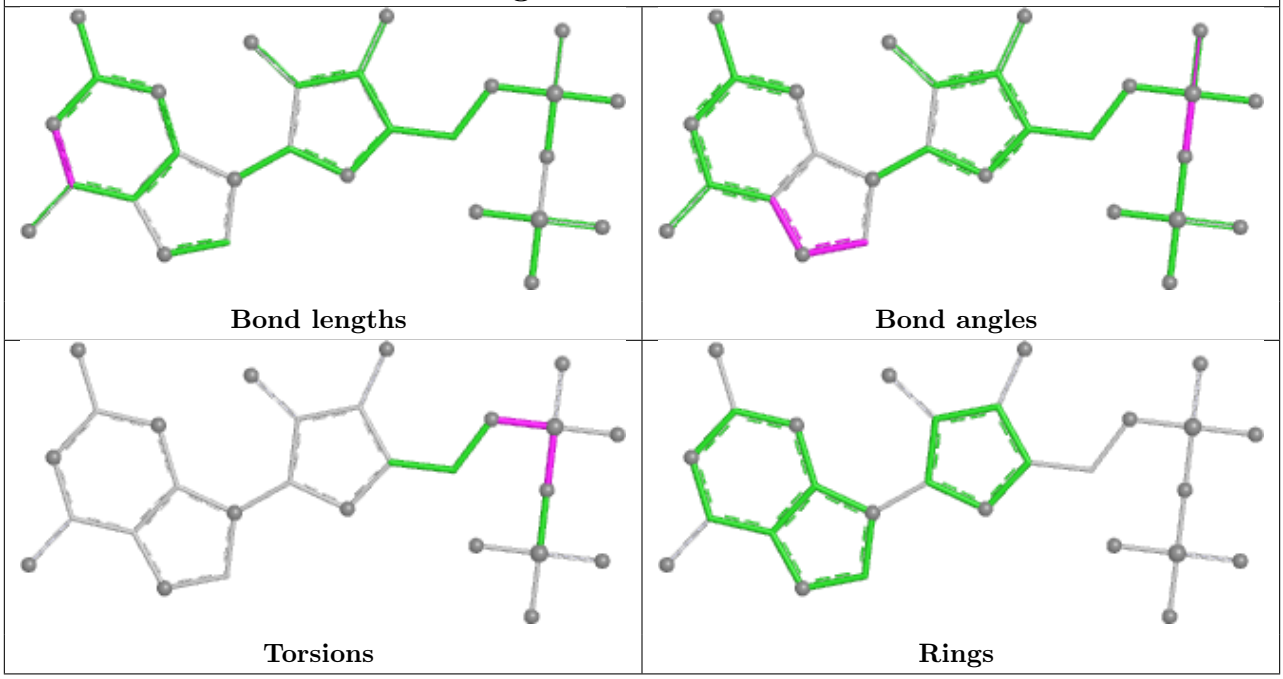

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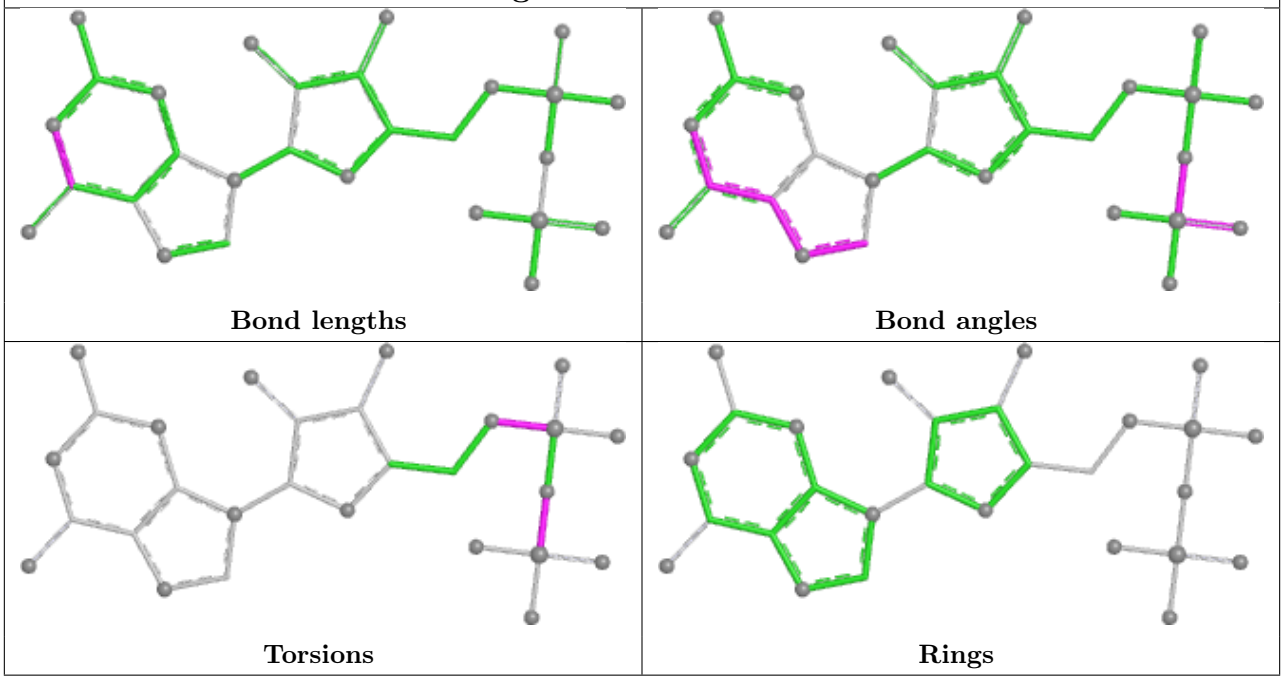

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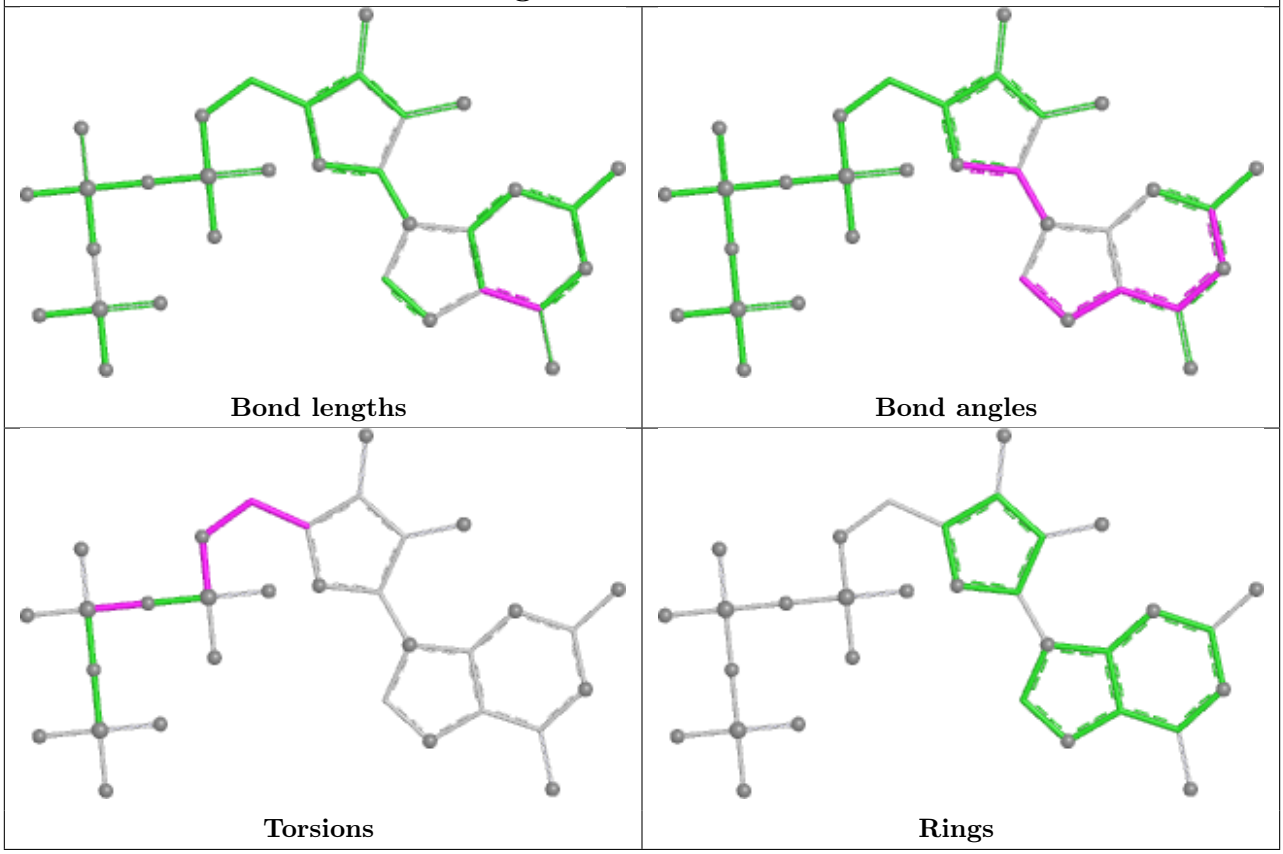

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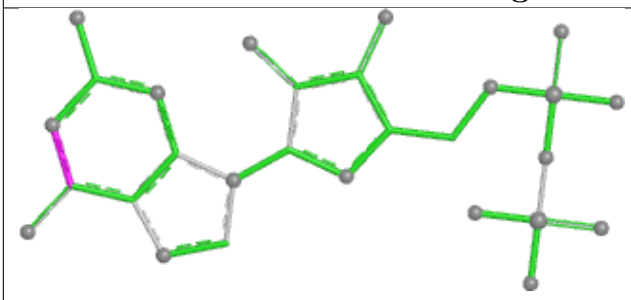
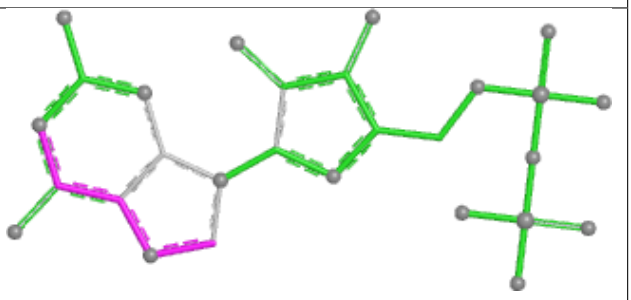
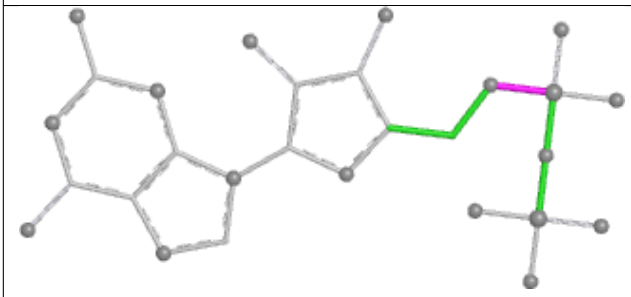
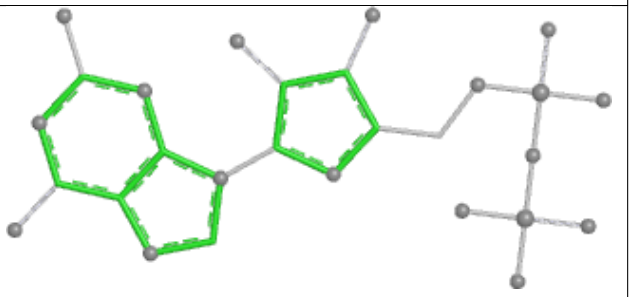
 Bond lengths	 Bond angles
 Torsions	 Rings

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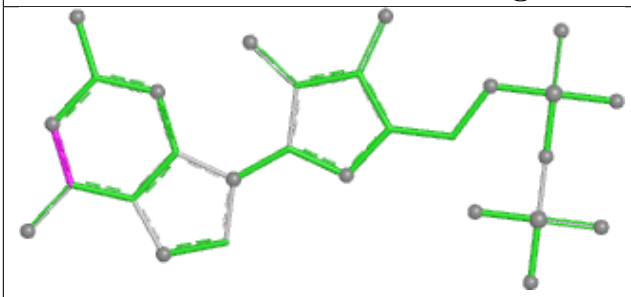
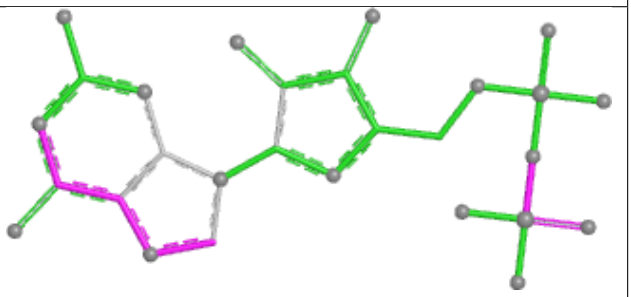
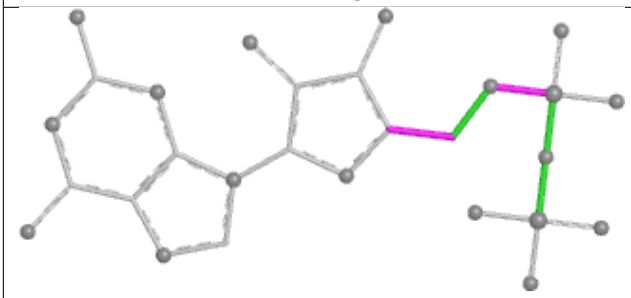
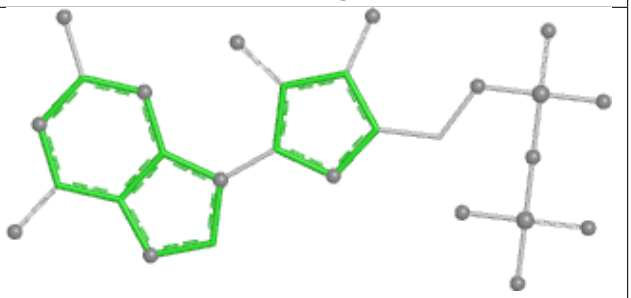
 Bond lengths	 Bond angles
 Torsions	 Rings

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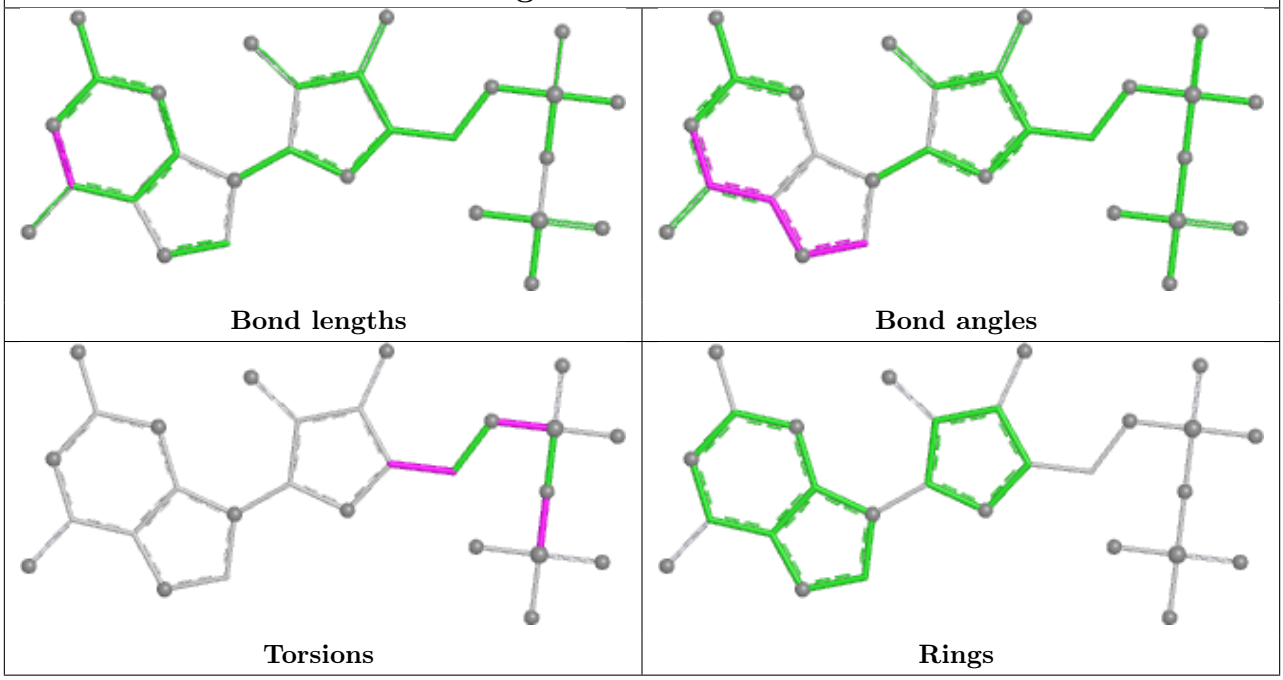

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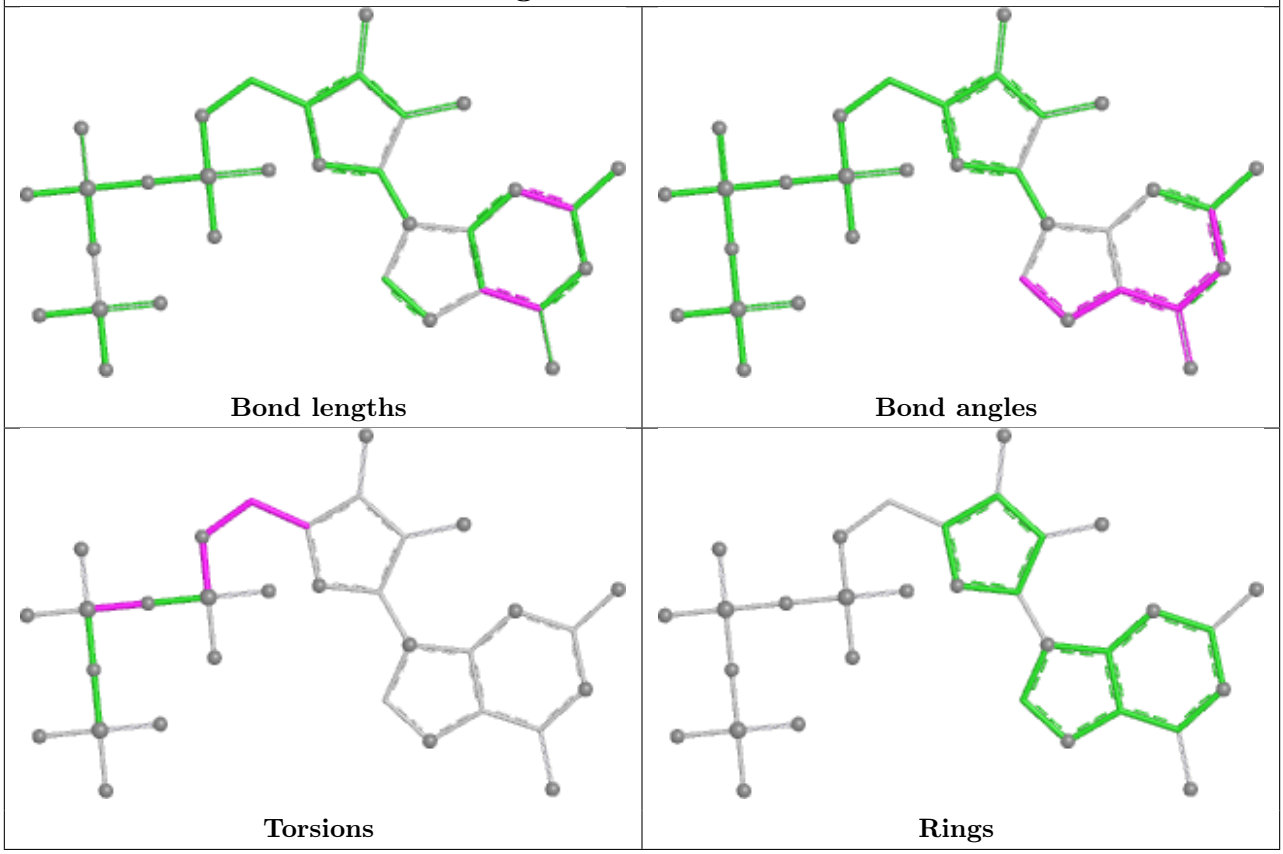

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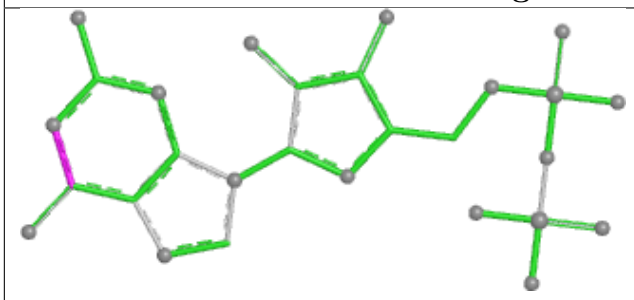
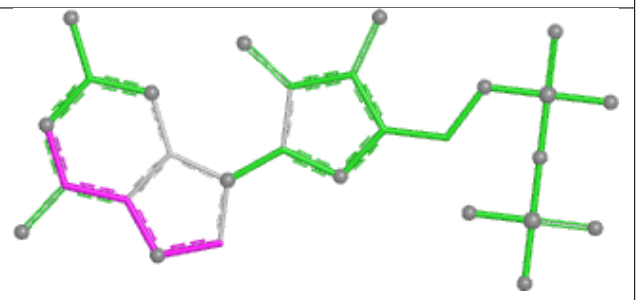
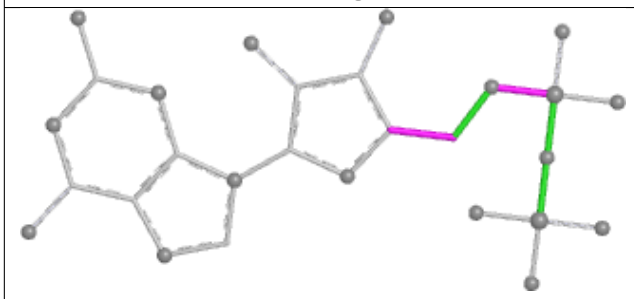


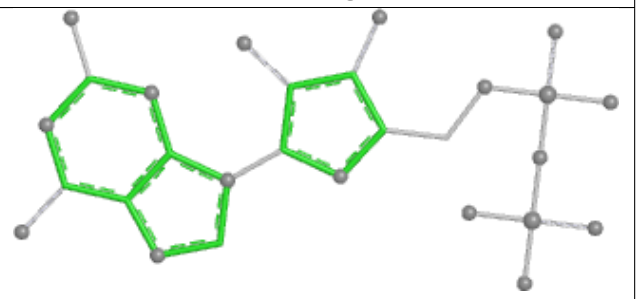
Bond lengths



Bond angles



Torsions



Rings

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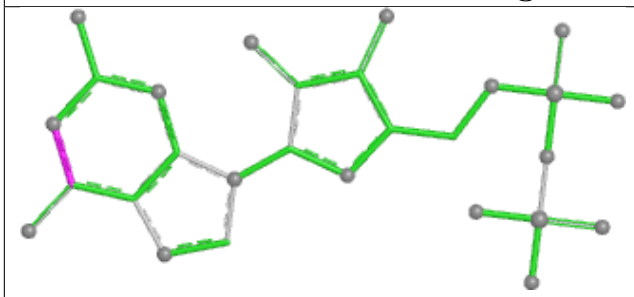

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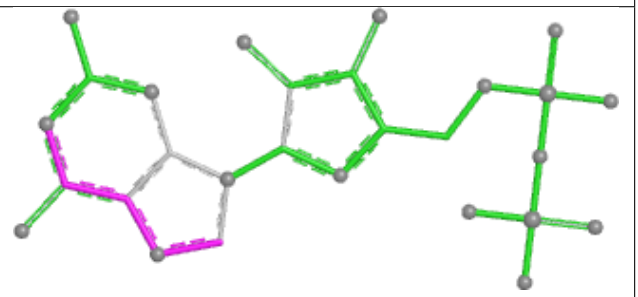

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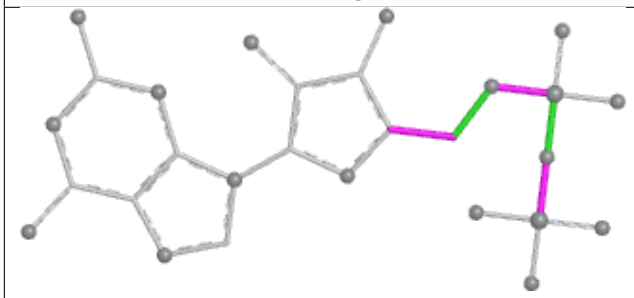

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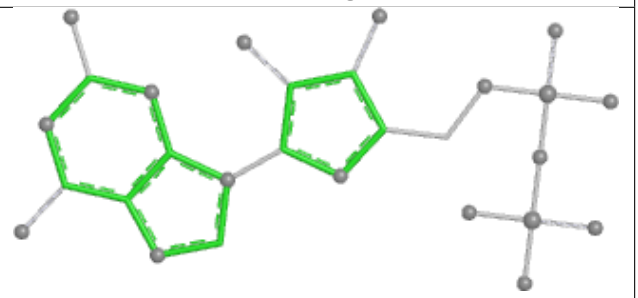

Rings

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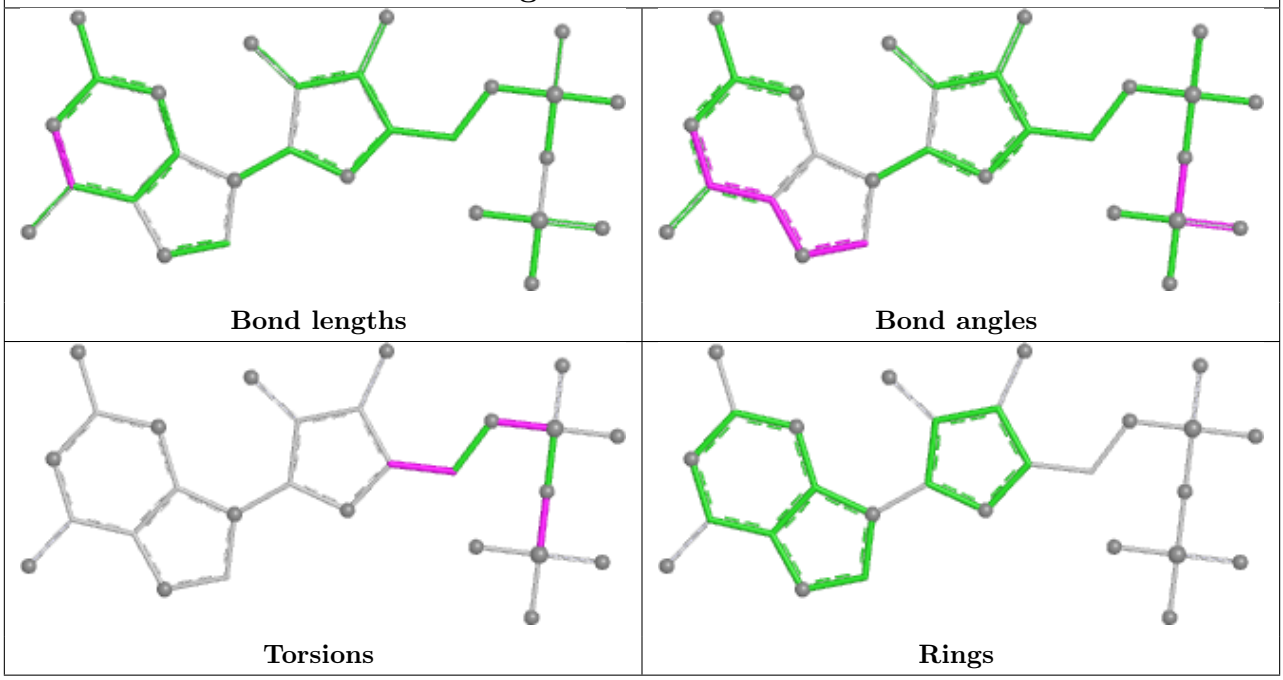

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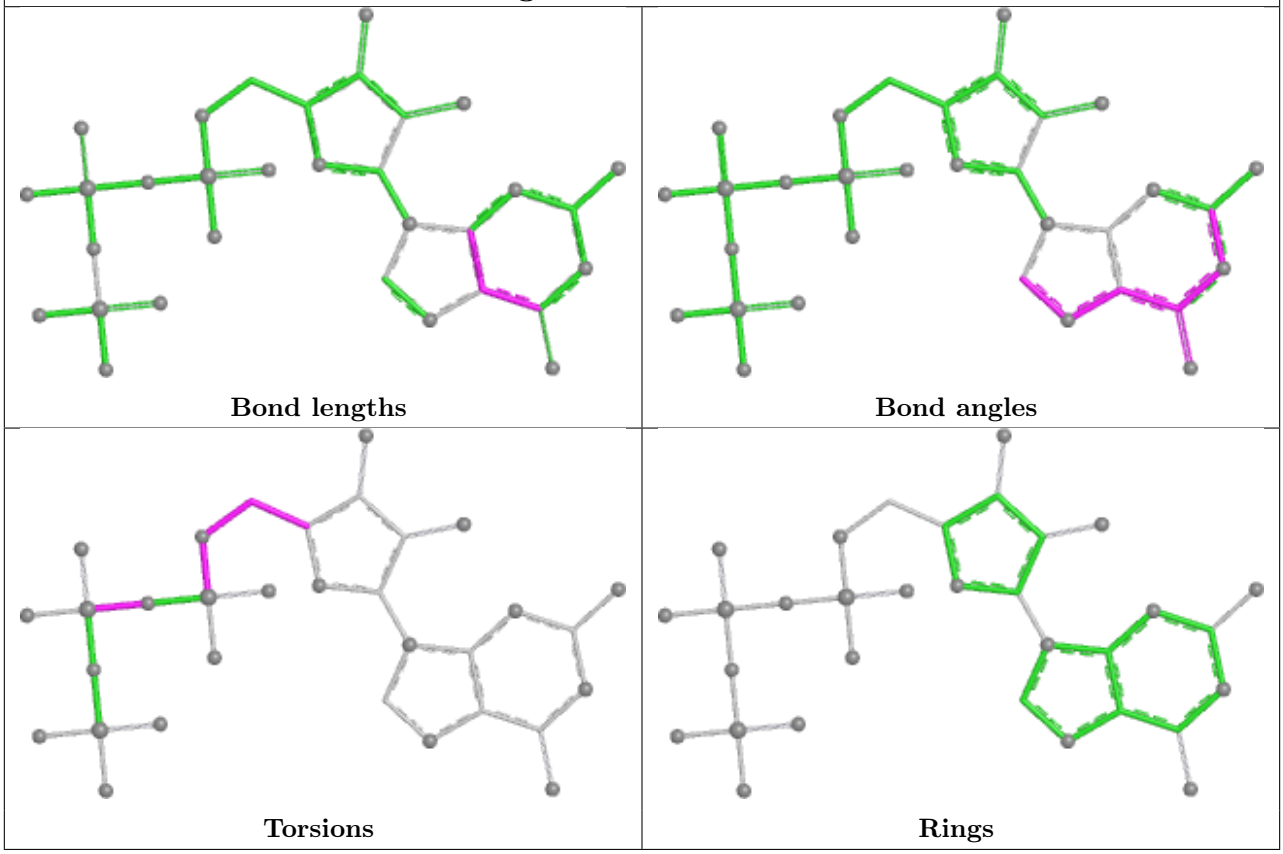

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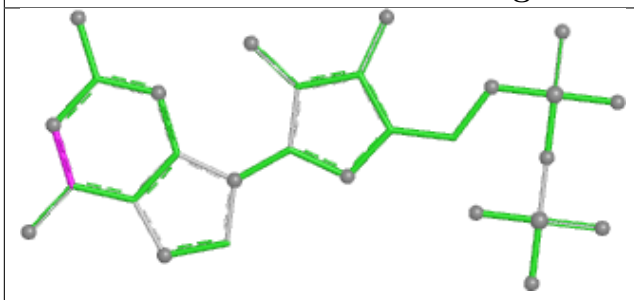

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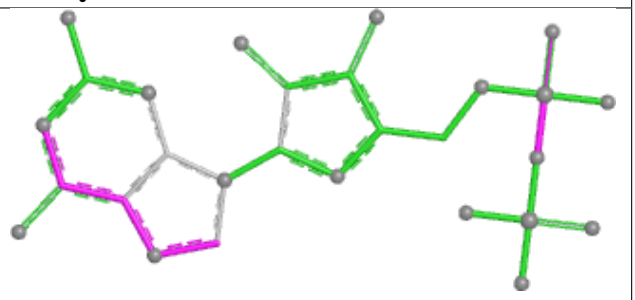

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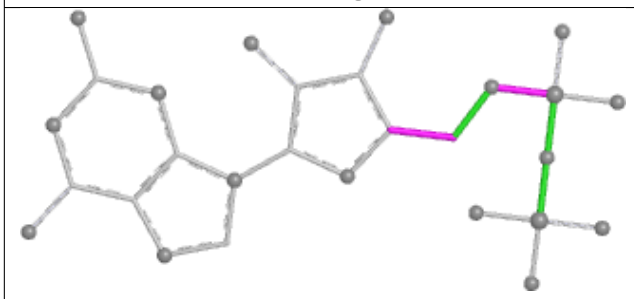

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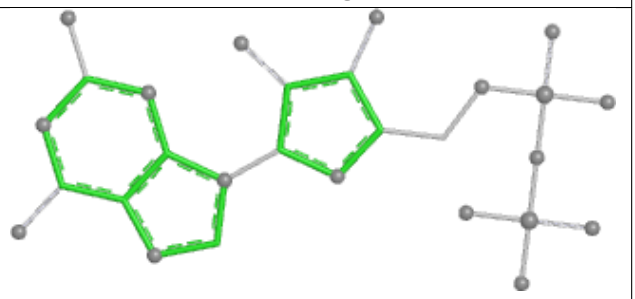

Rings

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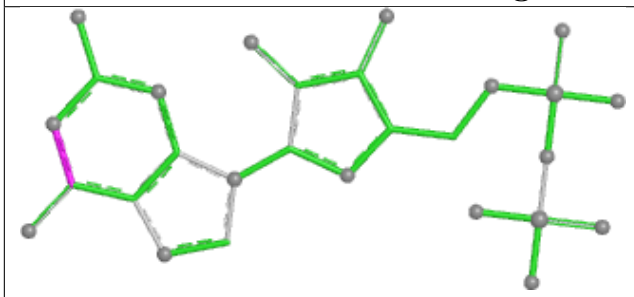

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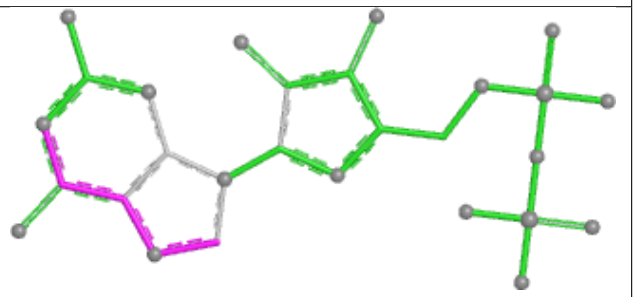

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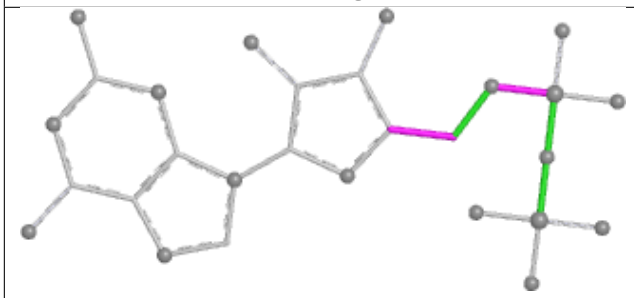
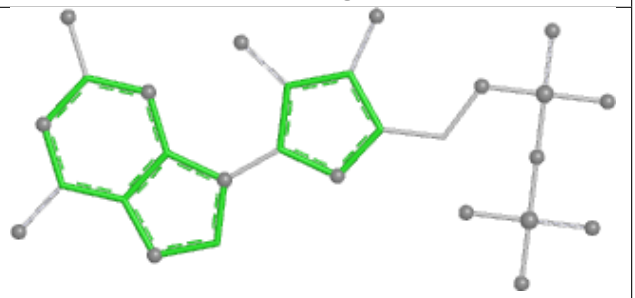
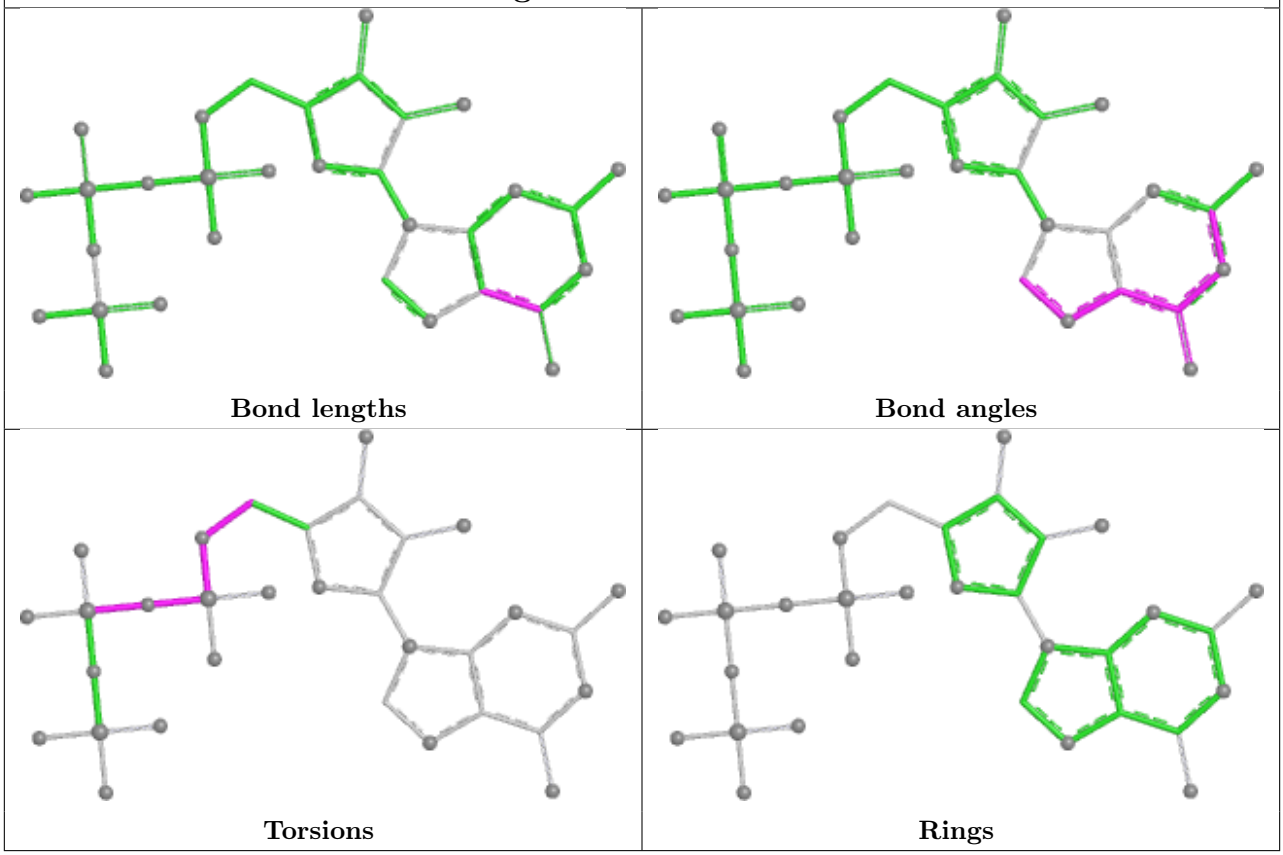


Torsions

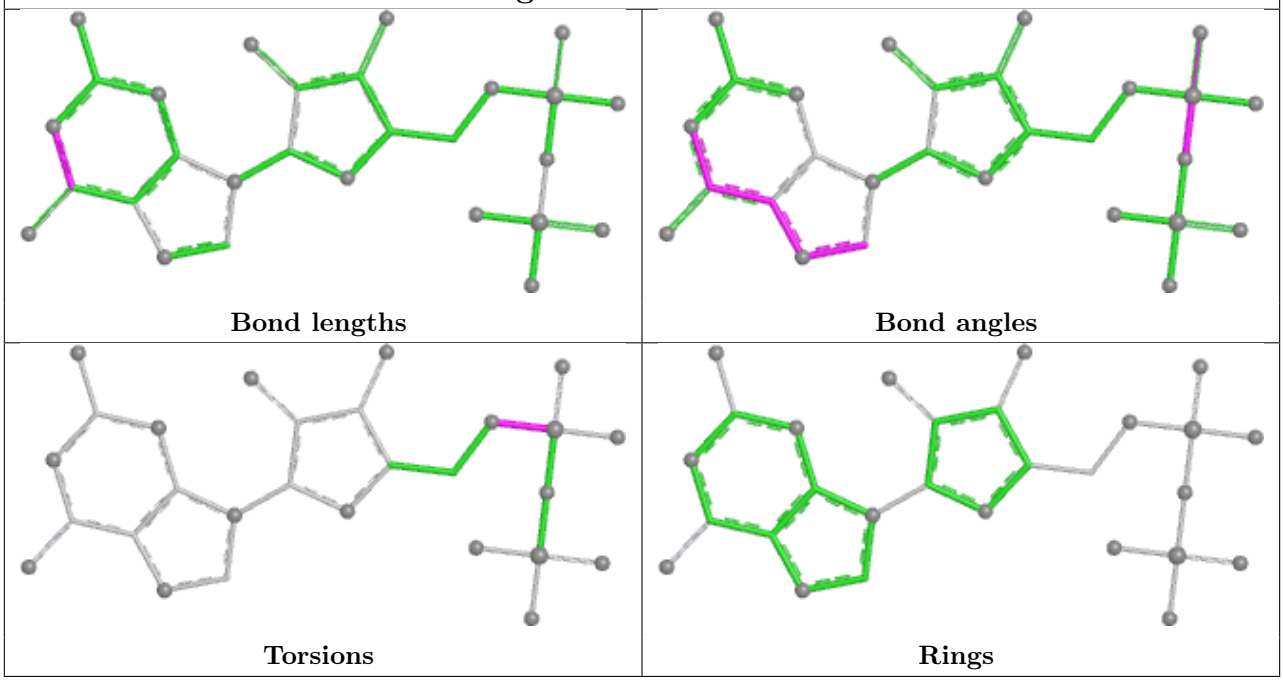


Rings

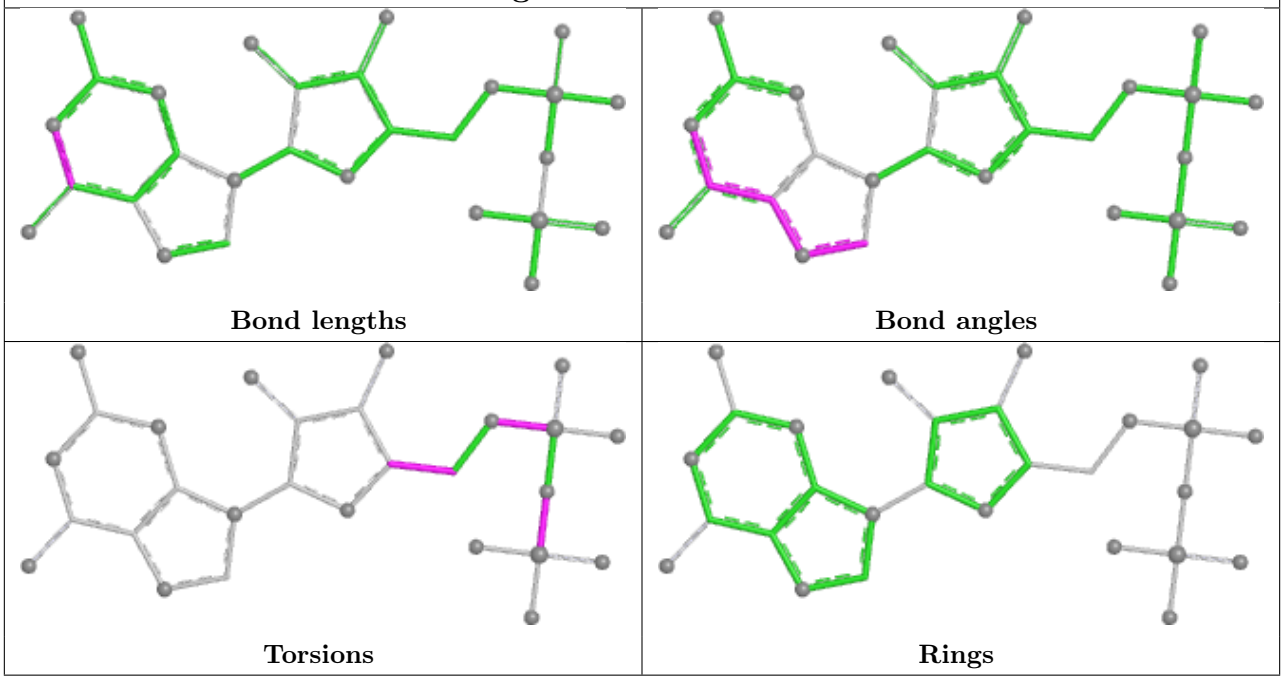
Ligand GTP G7 501



Ligand GDP S4 501



Ligand GDP K8 501



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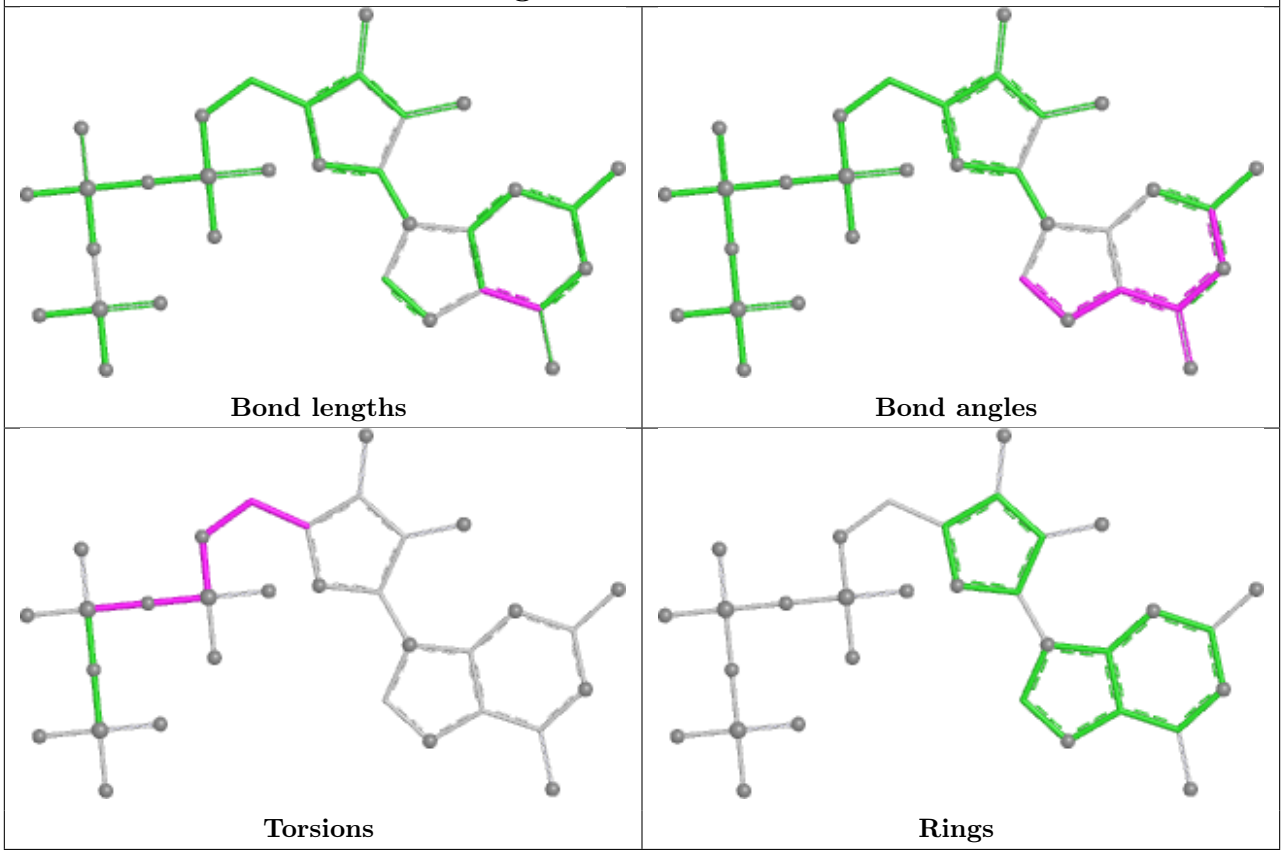

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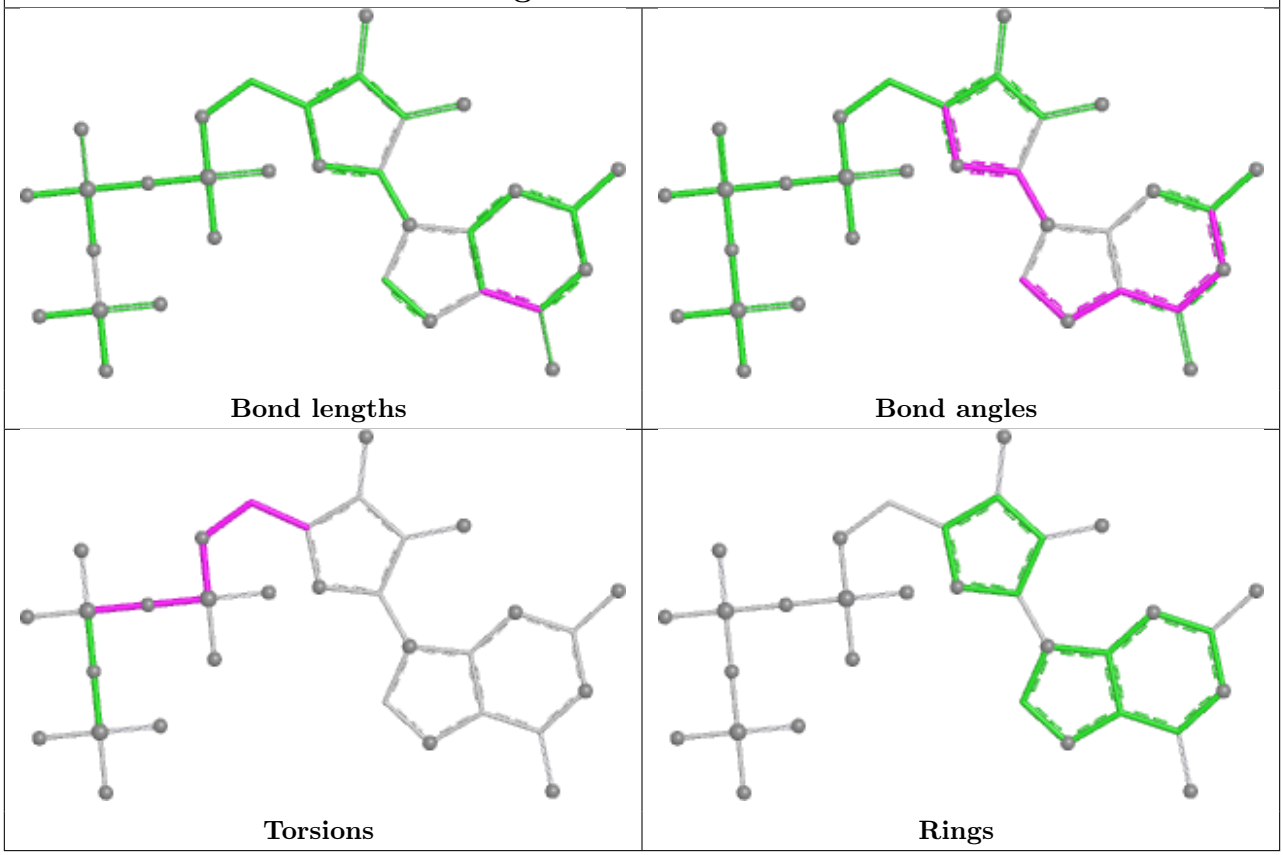
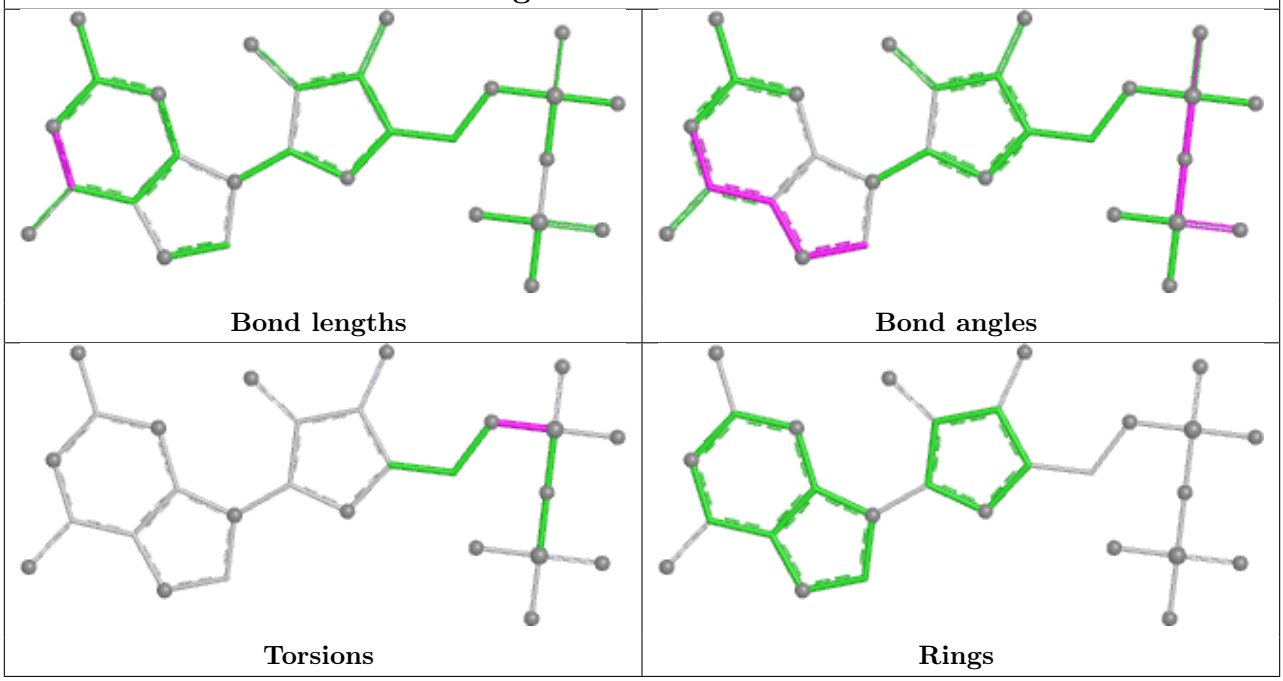


Ligand GDP 0O 502



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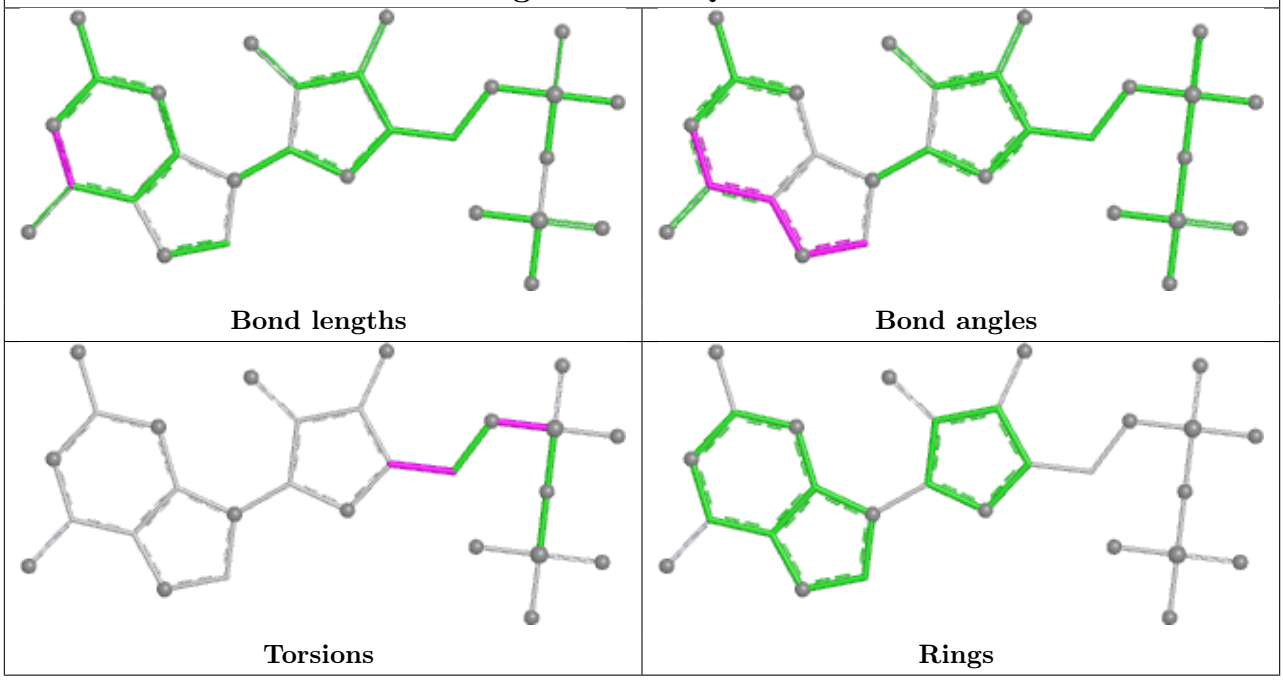

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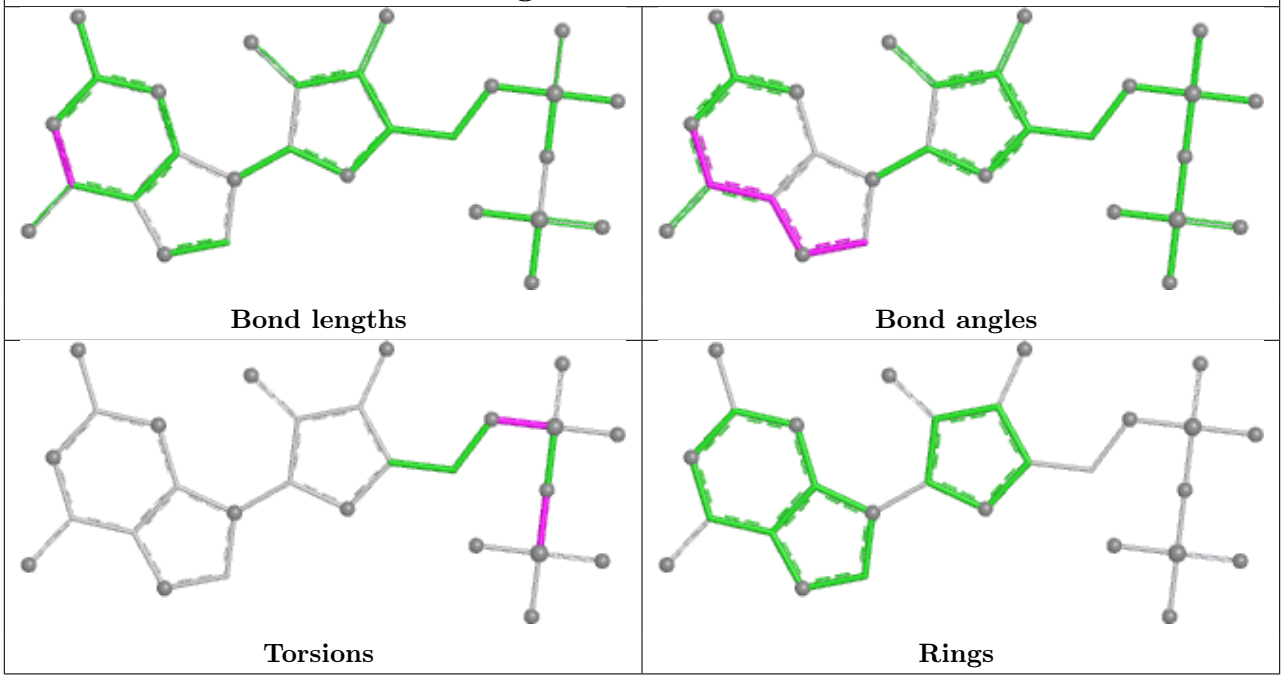

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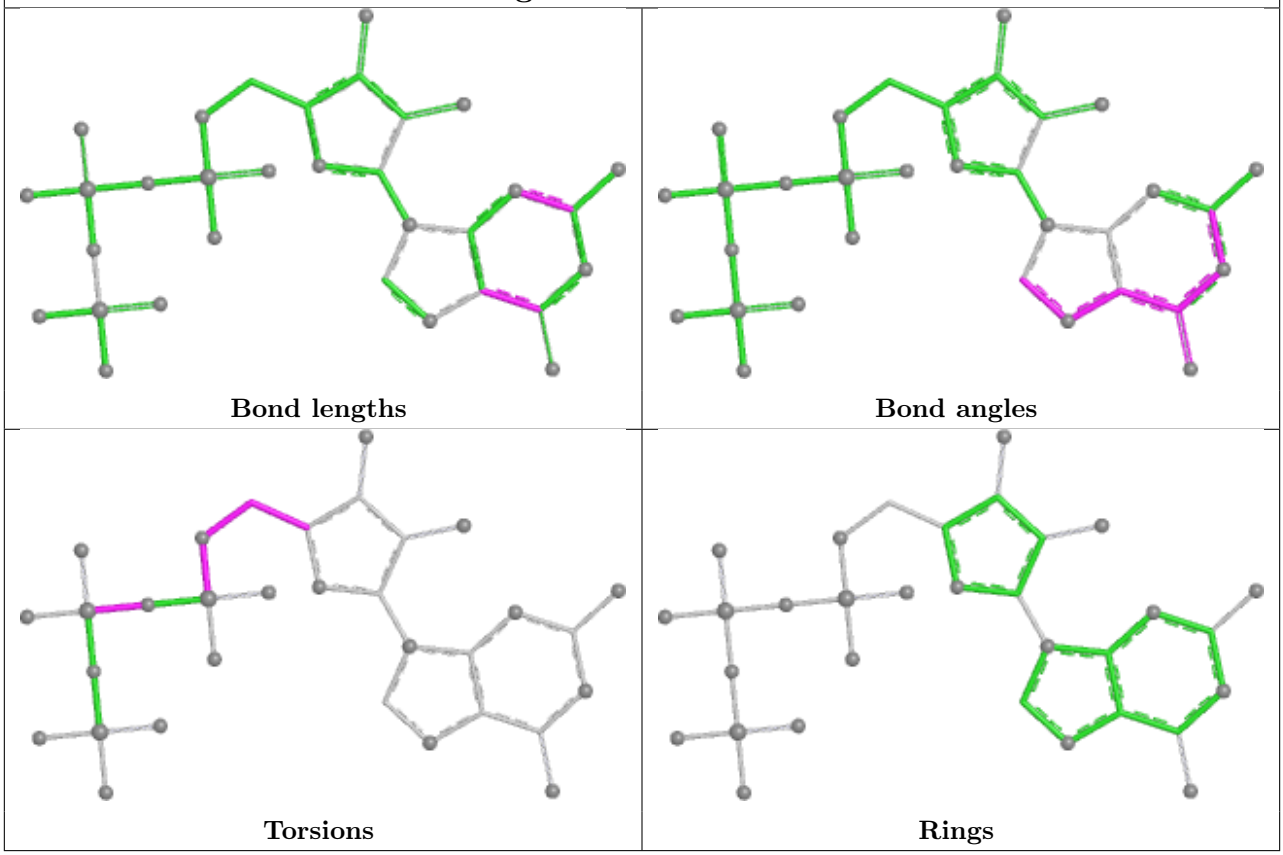

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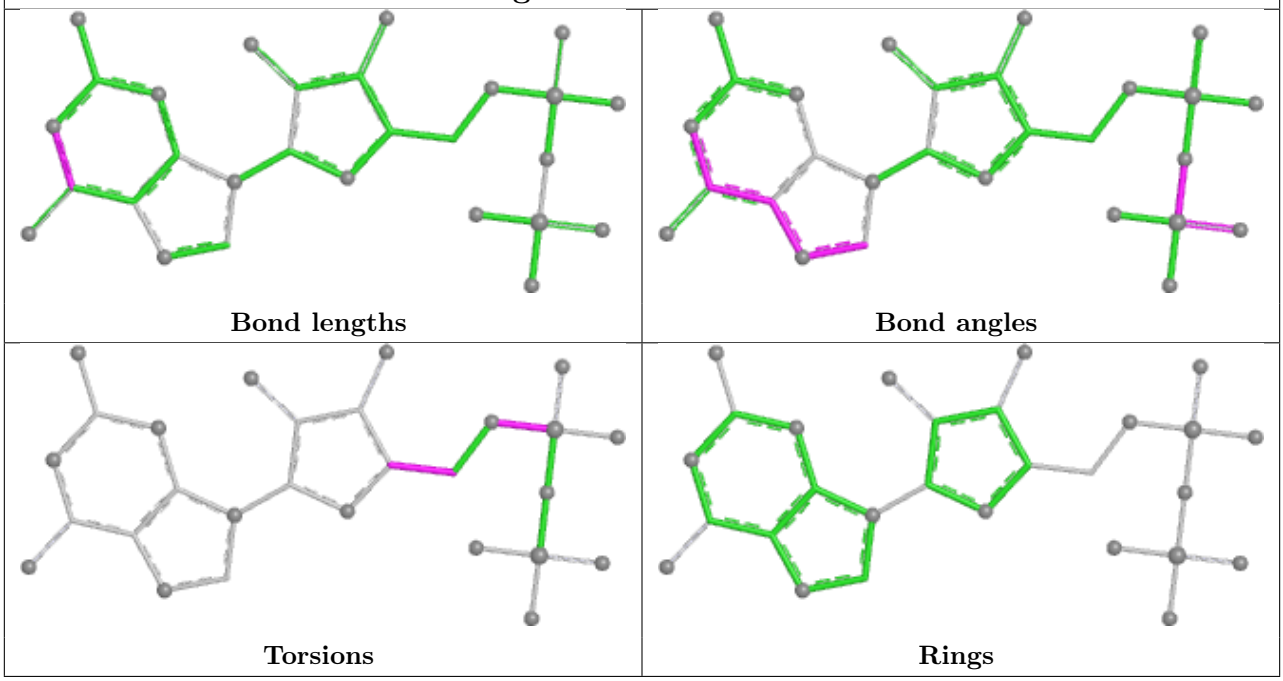

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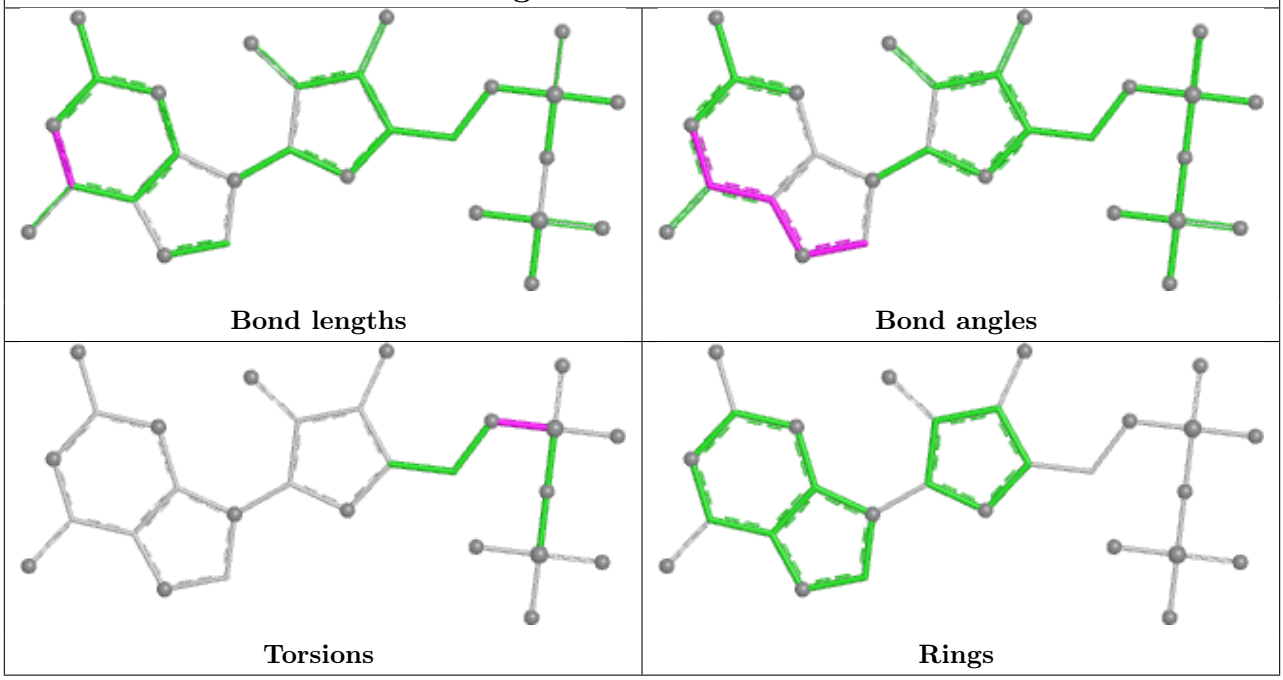

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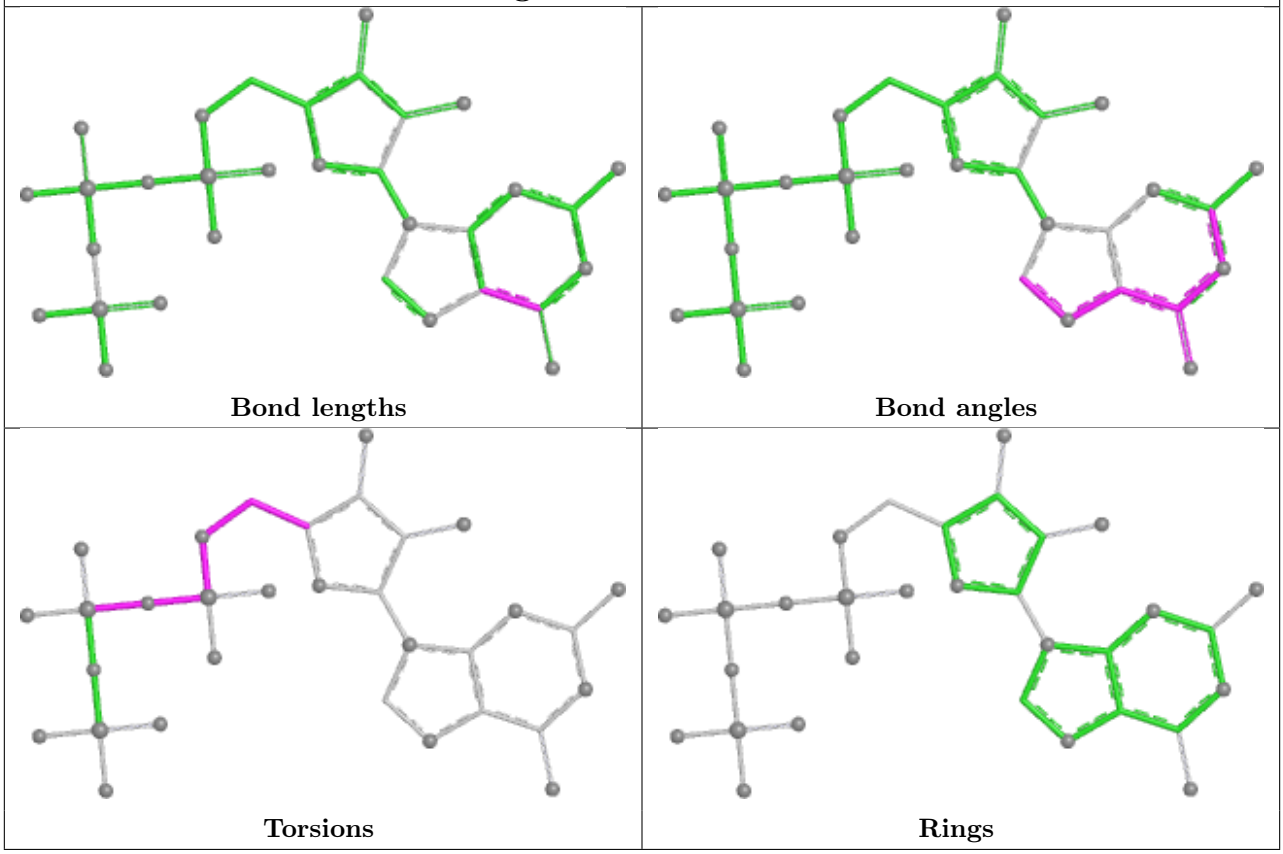

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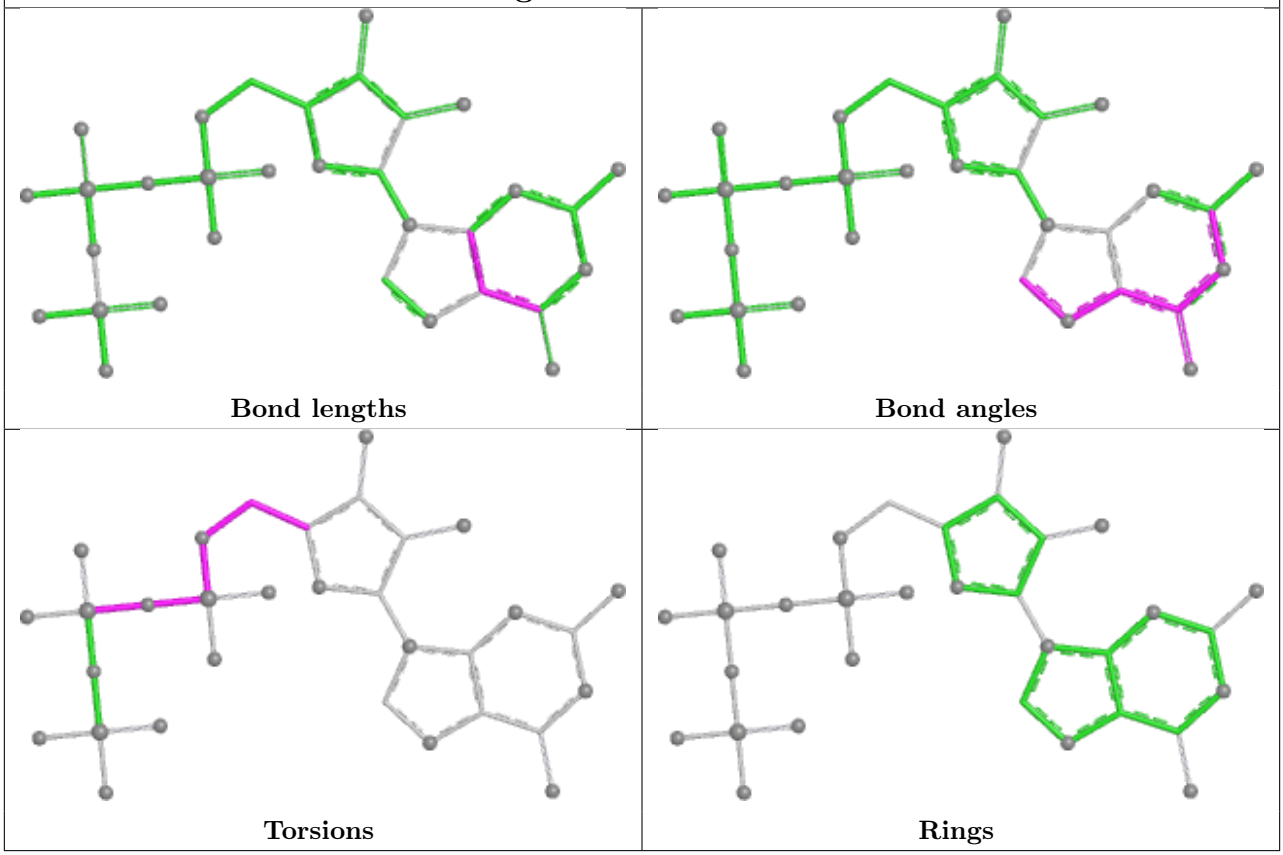
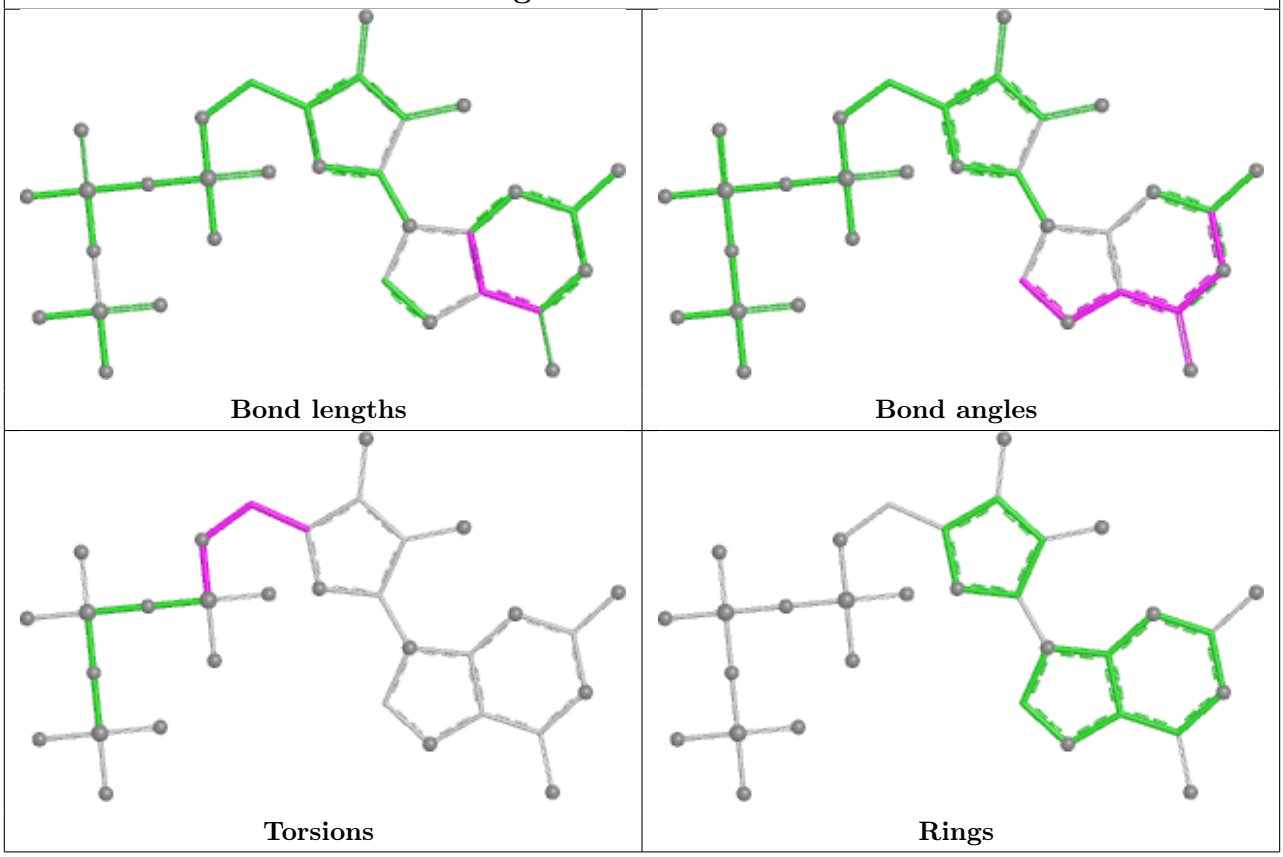


Ligand GTP K6 501



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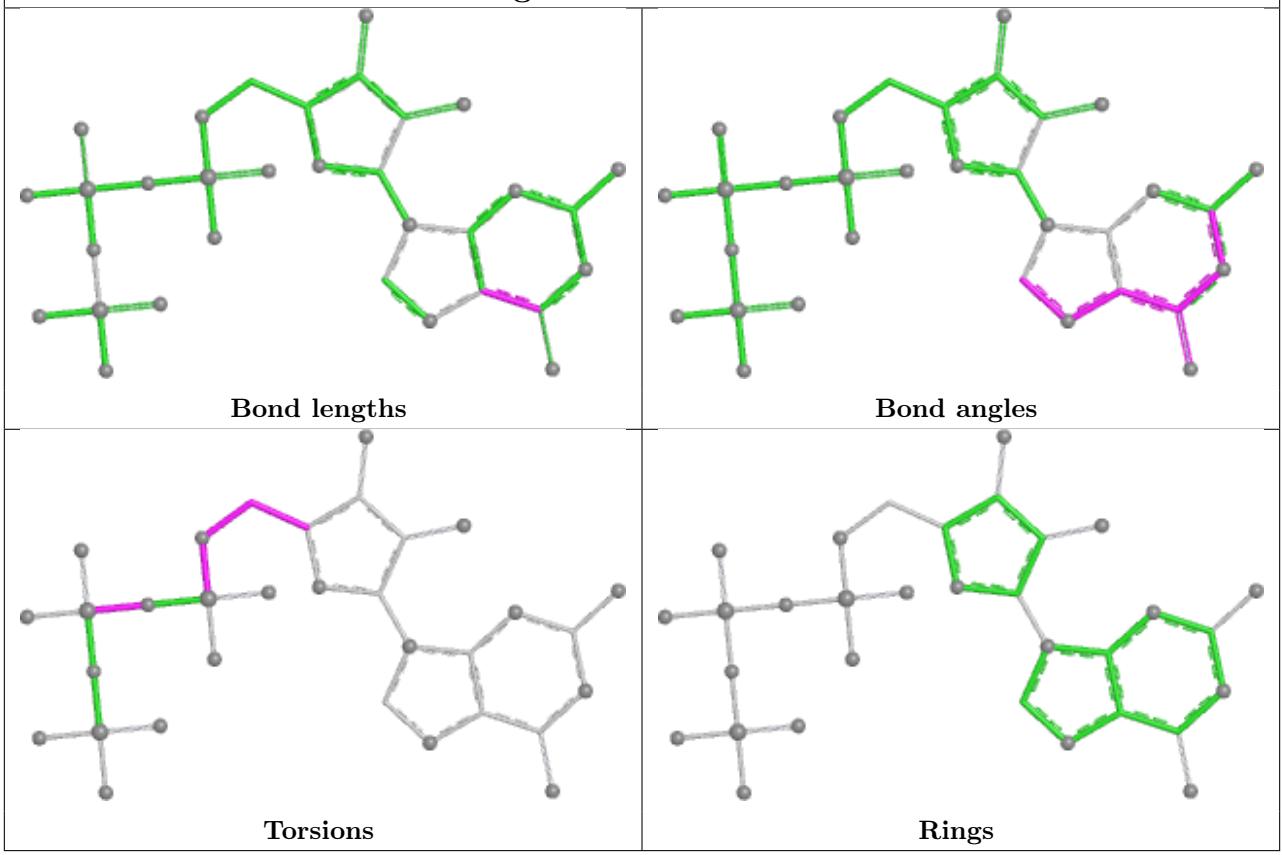
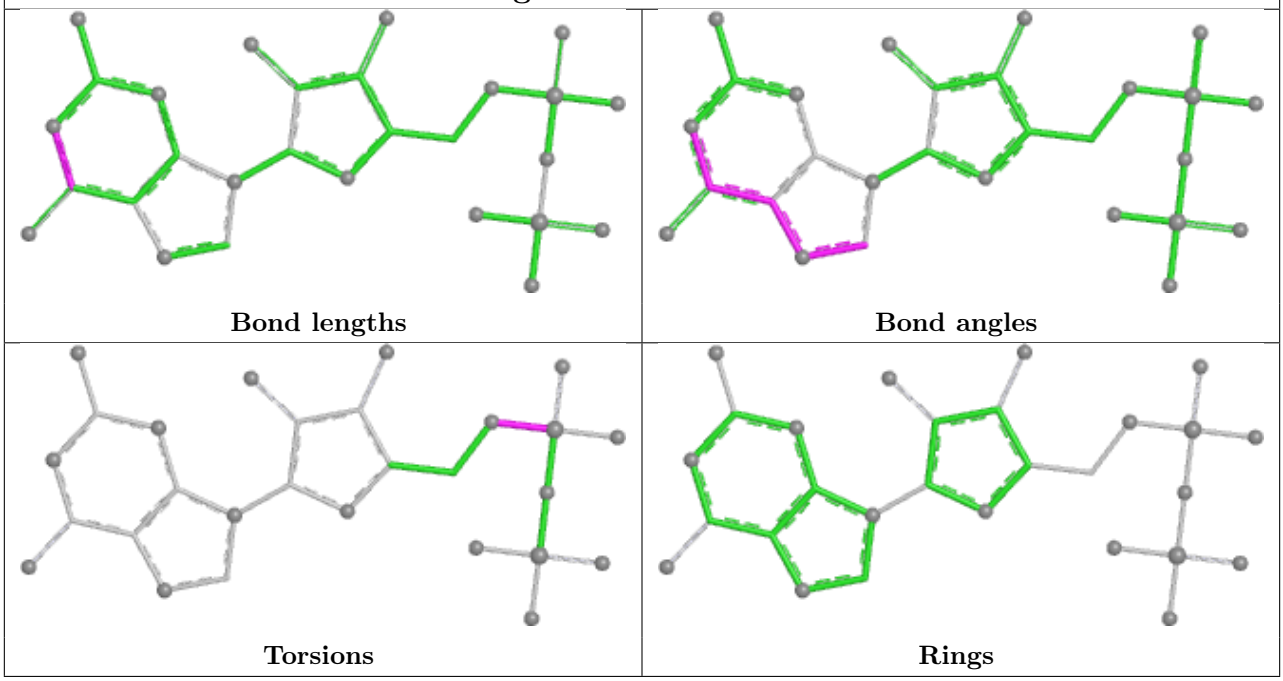


Ligand GDP 2C 502



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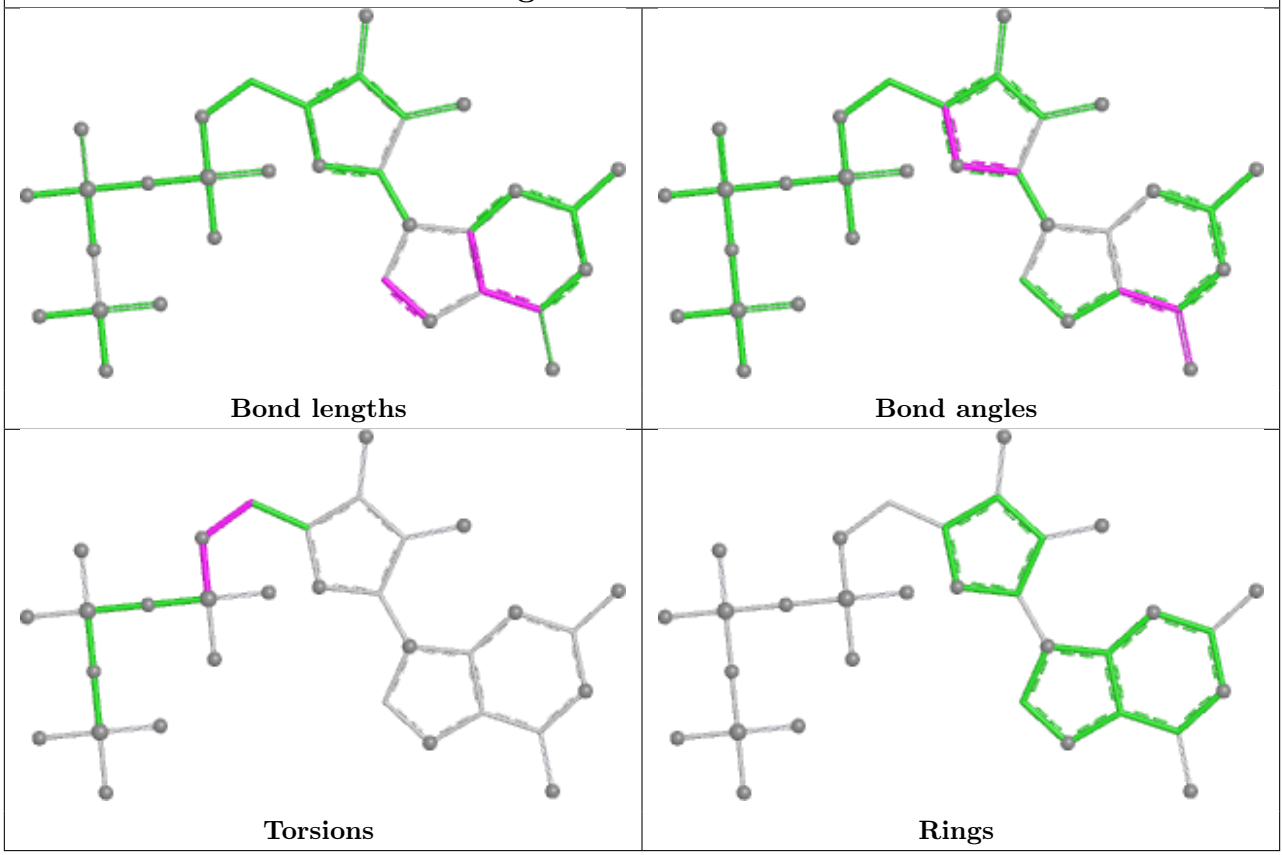

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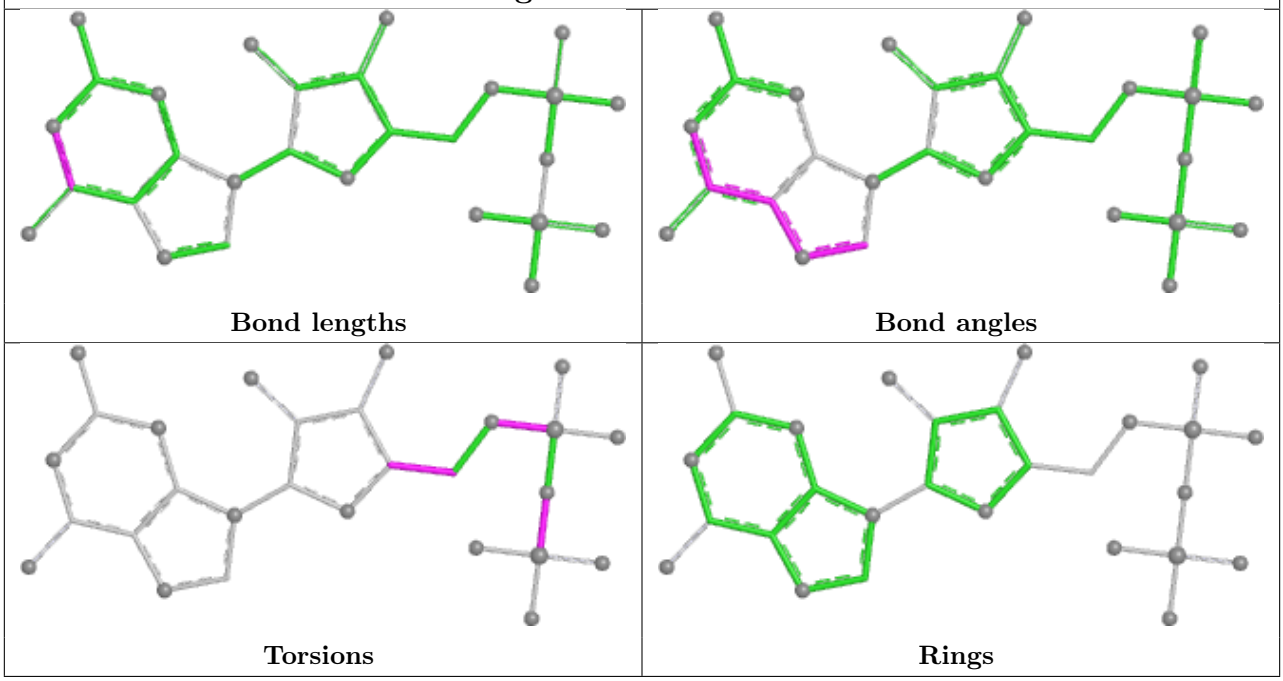
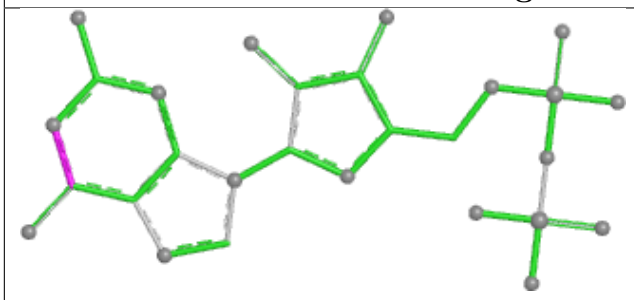
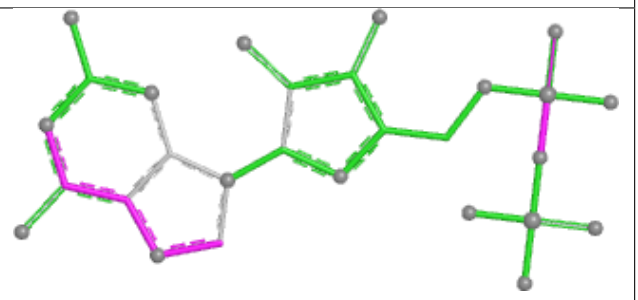


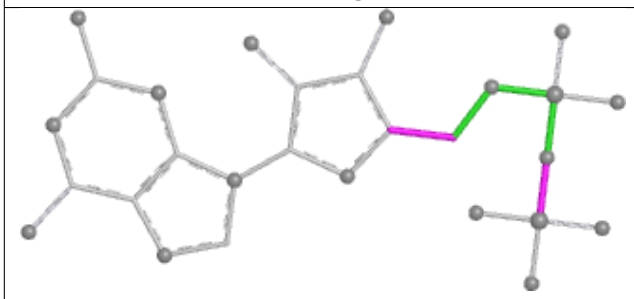
Ligand GDP Z0 502



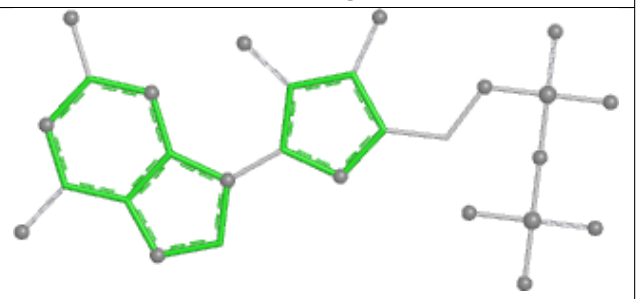
Bond lengths



Bond angles

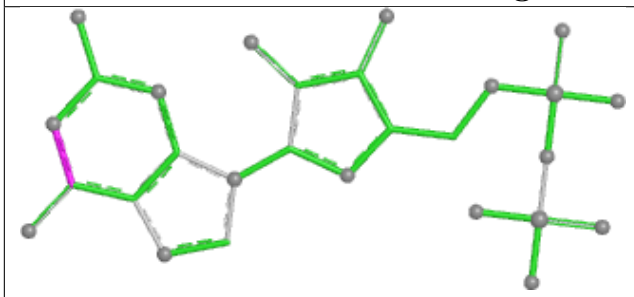


Torsions



Rings

Ligand GDP C2 501



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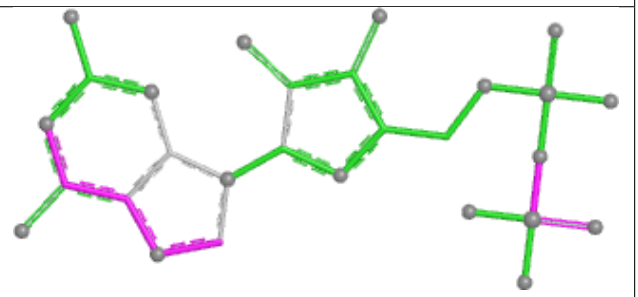
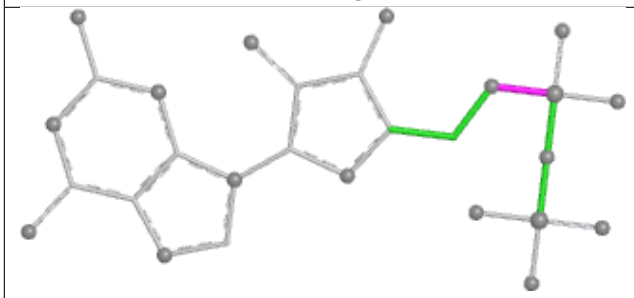
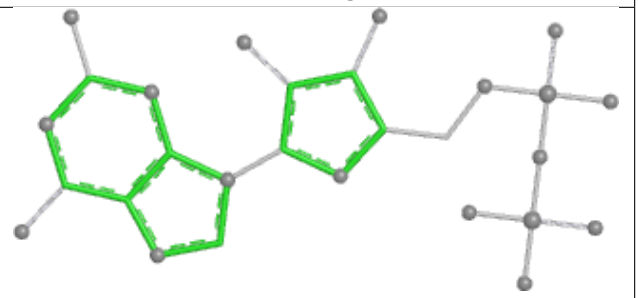


Bond angles

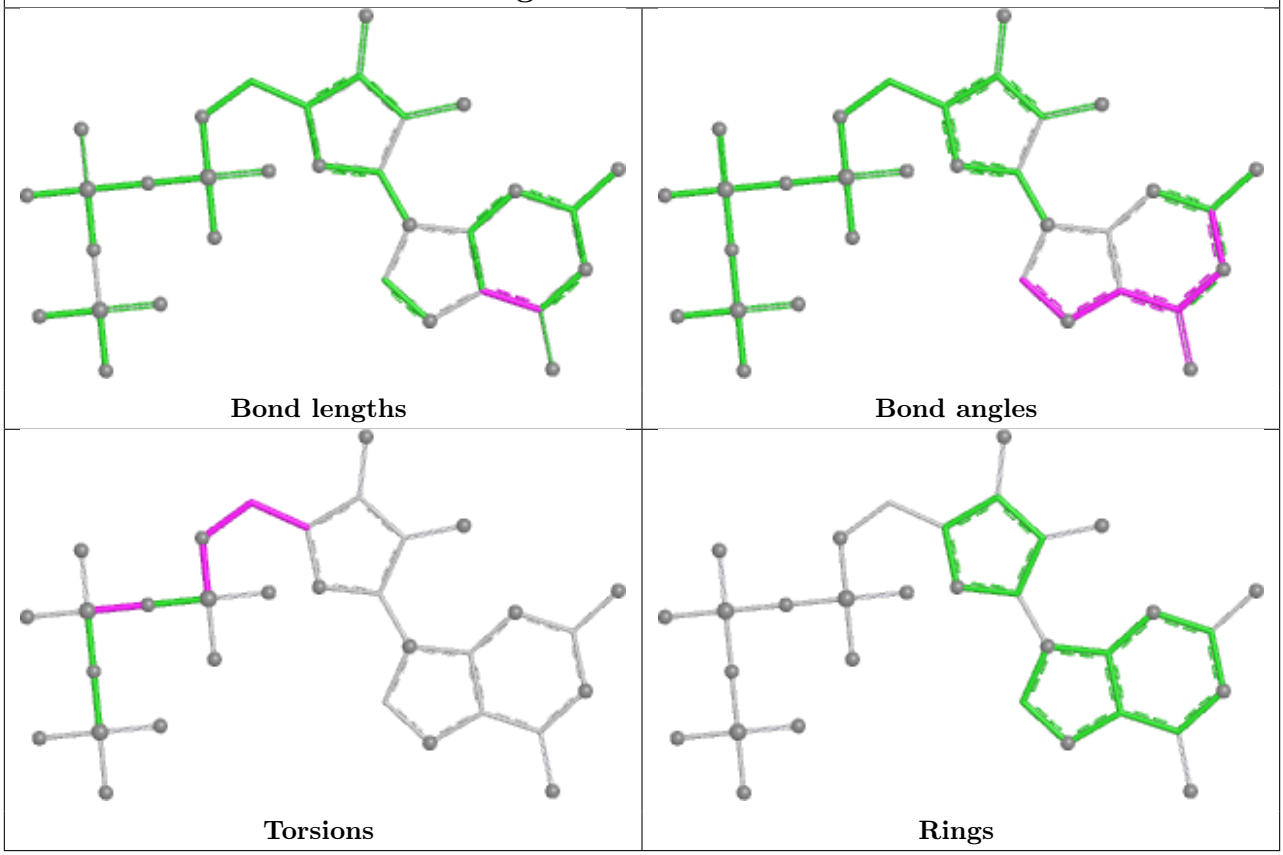


Torsions

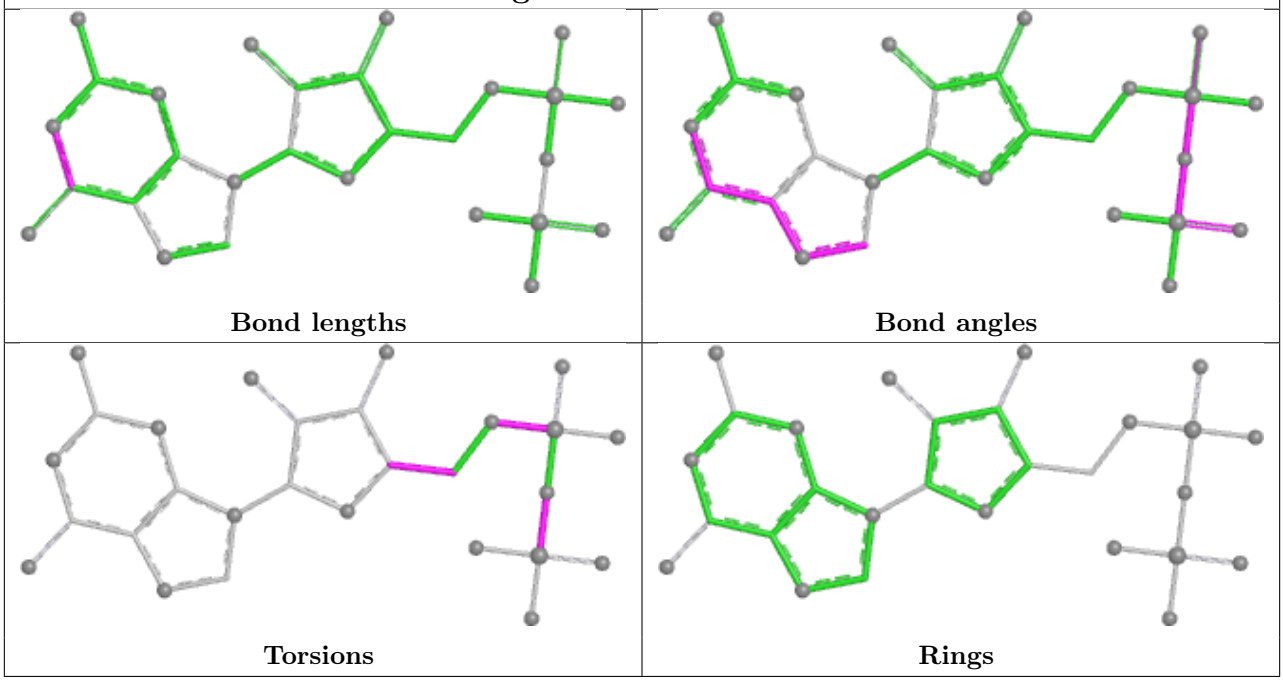


Rings

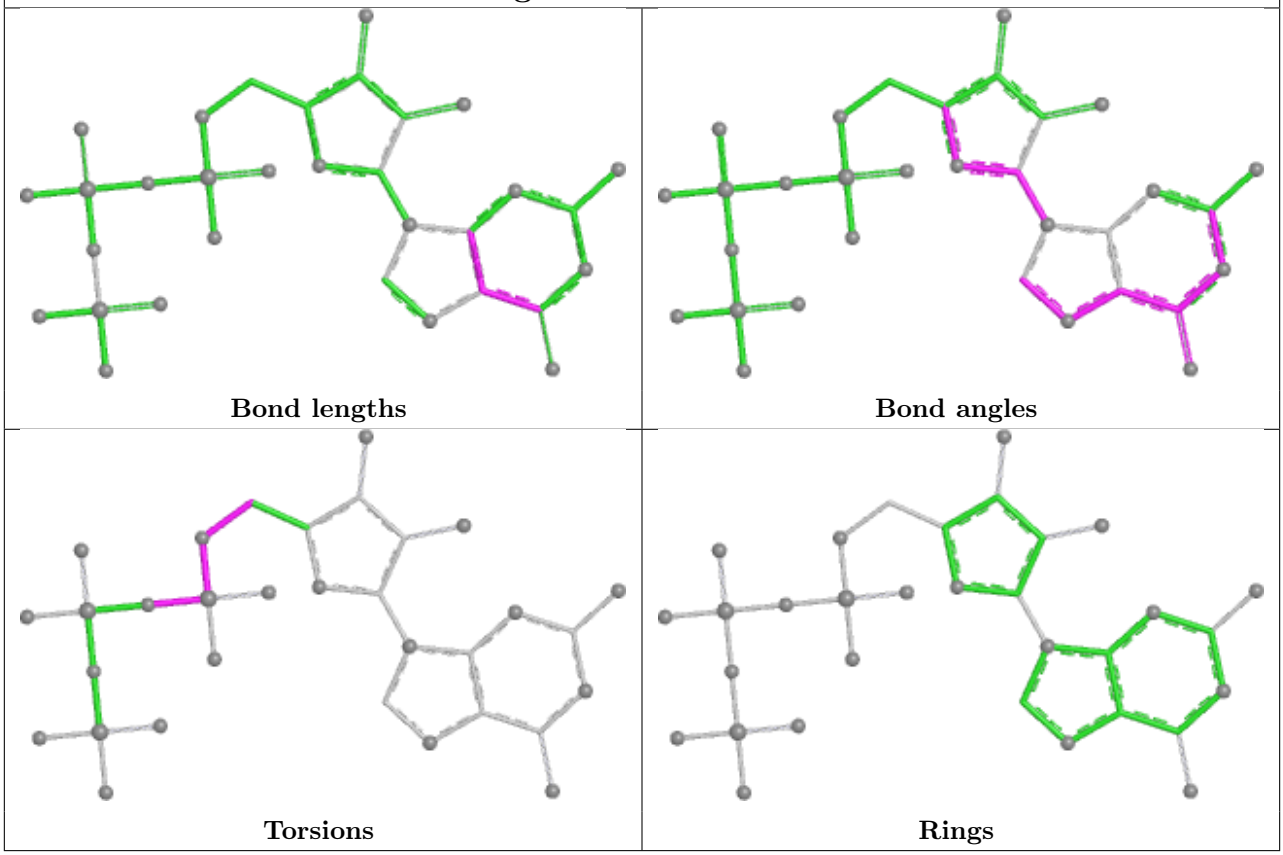
Ligand GTP F1 501



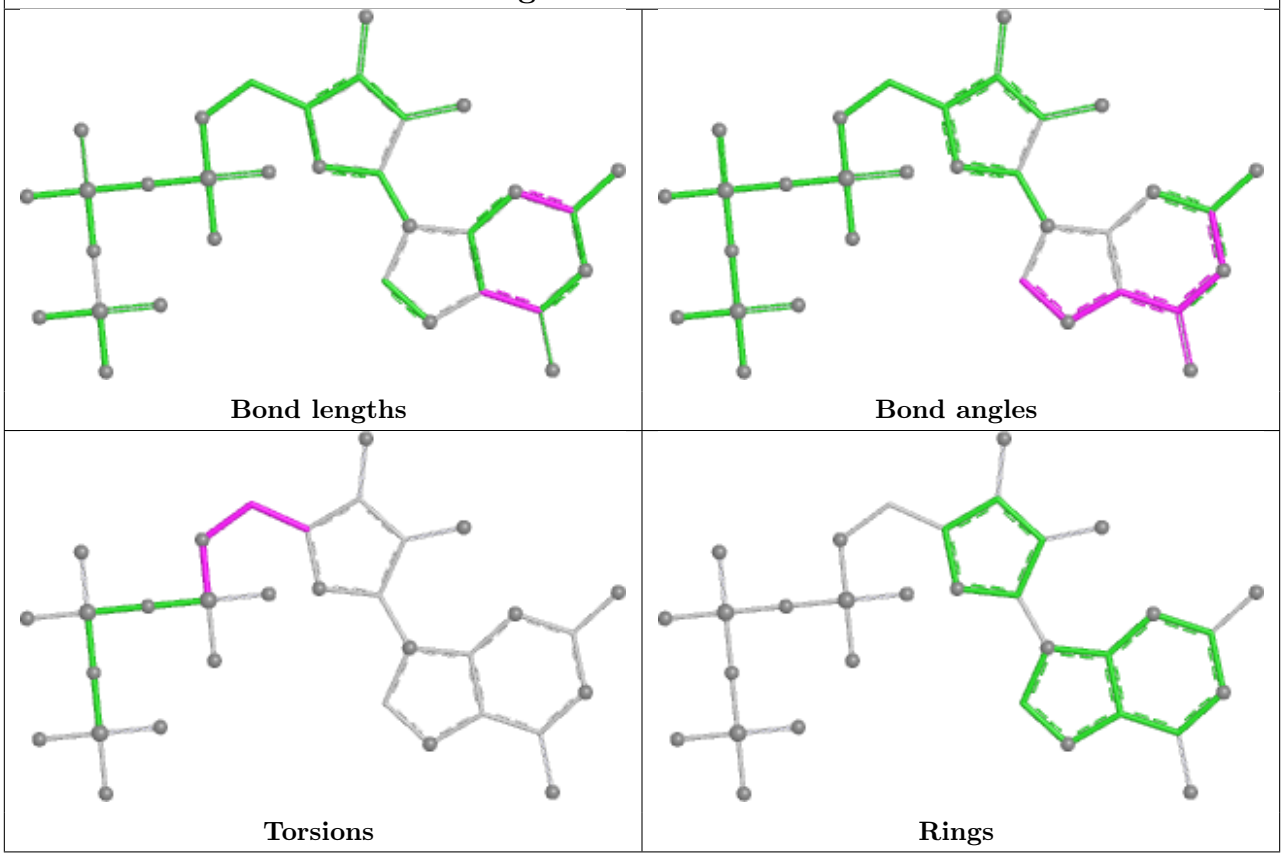
Ligand GDP K0 502



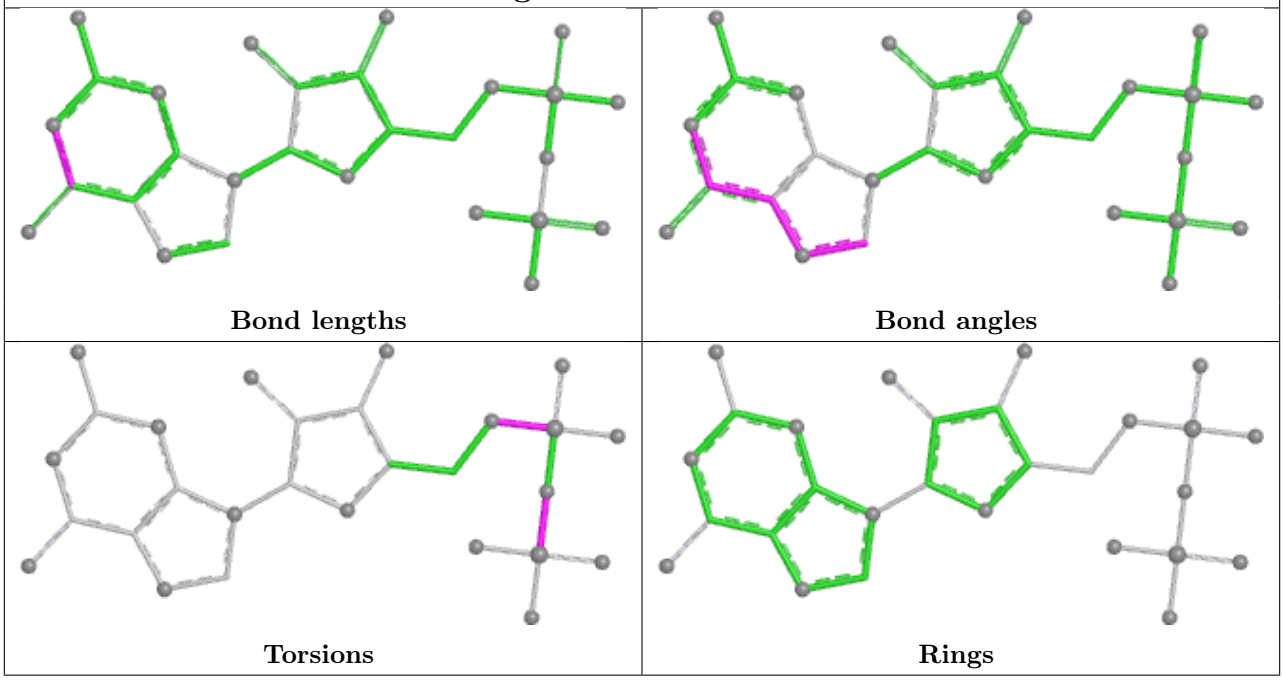
Ligand GTP D1 501



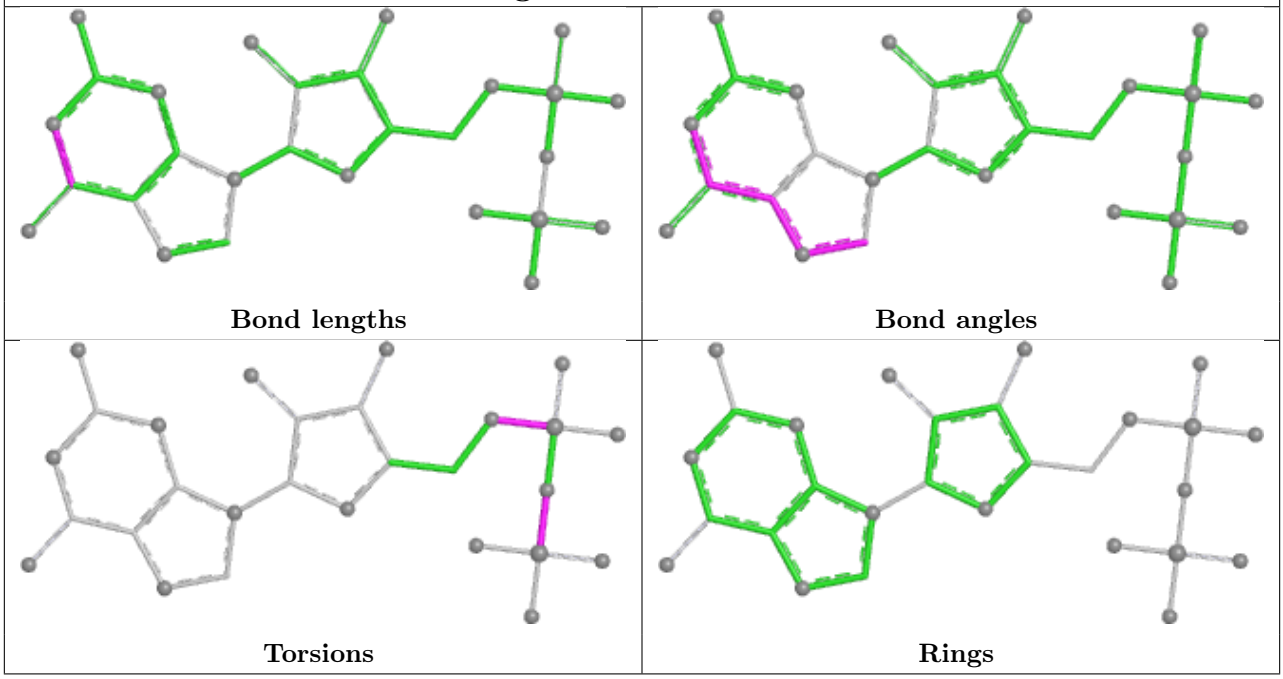
Ligand GTP J8 501



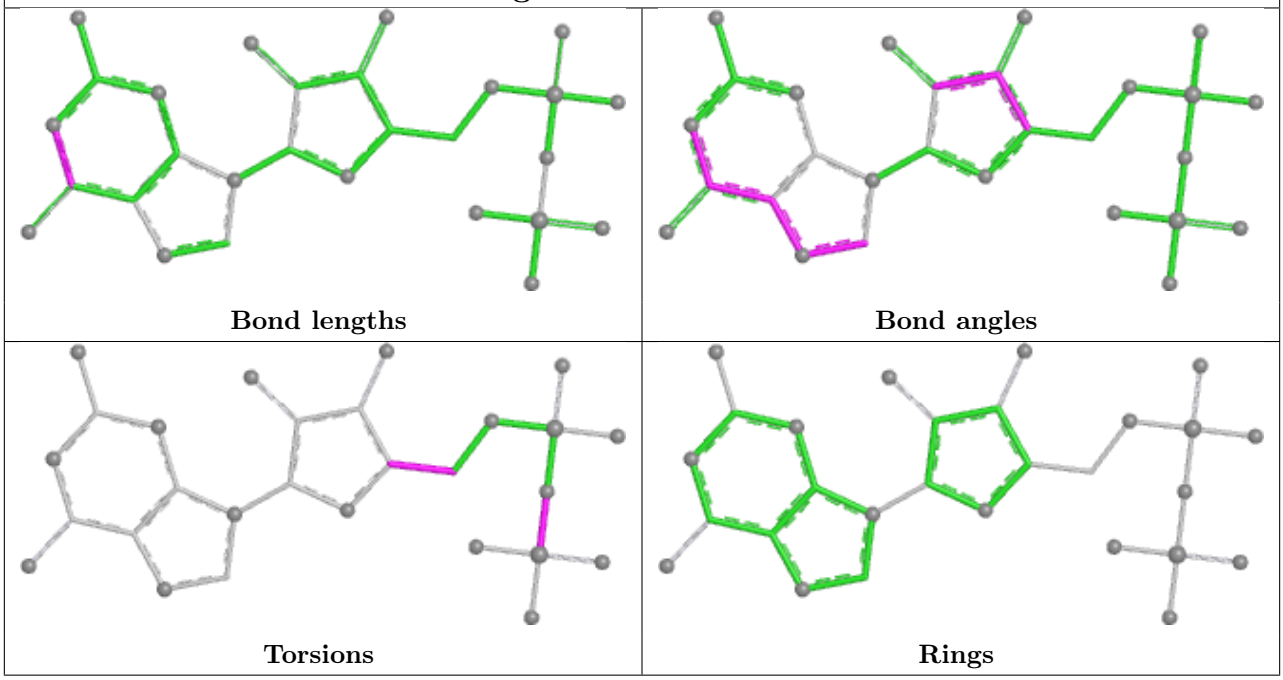
Ligand GDP B5 502



Ligand GDP T2 502



Ligand GDP X4 502



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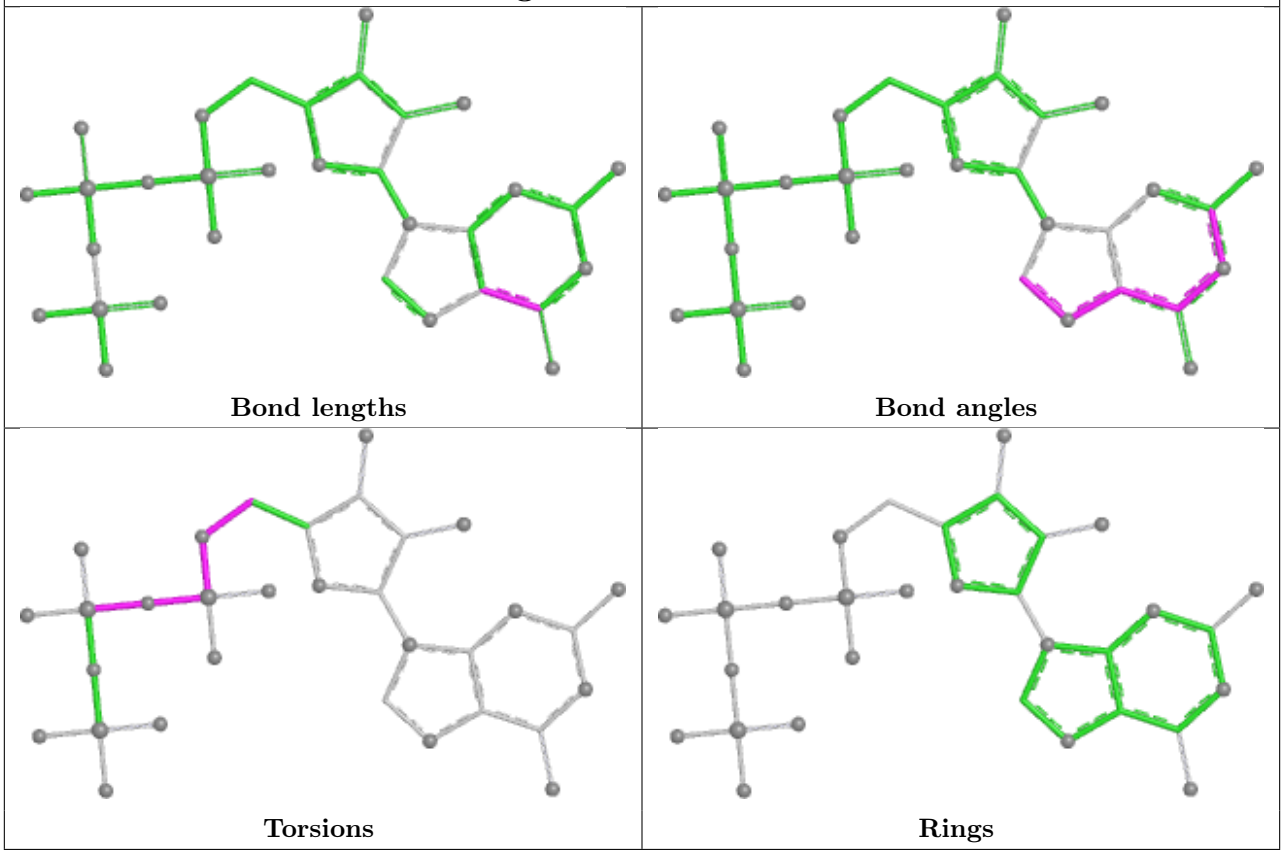
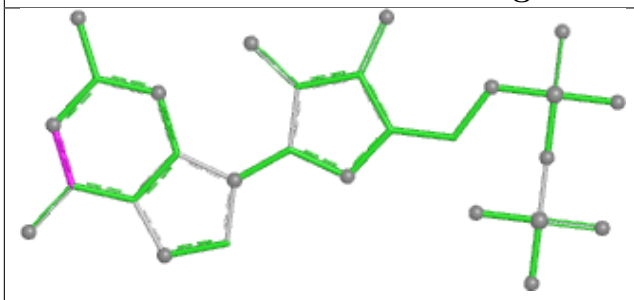
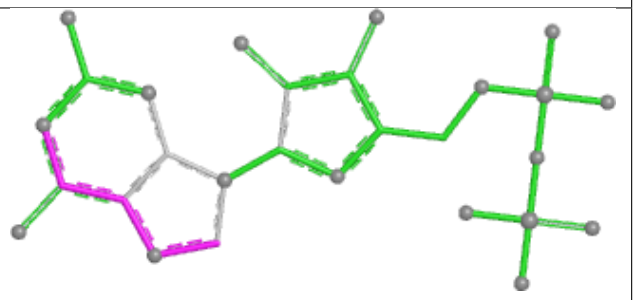


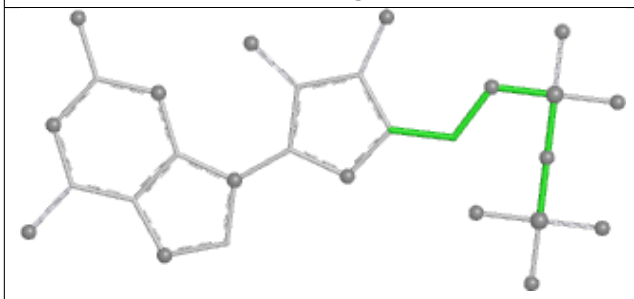
Ligand GDP A5 501



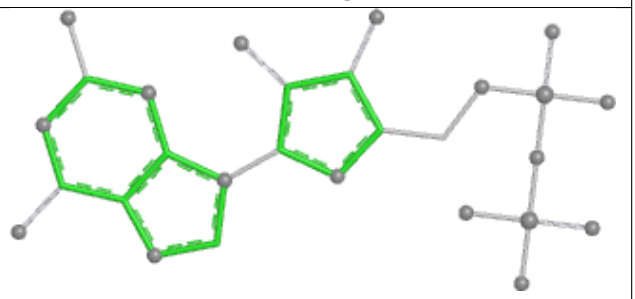
Bond lengths



Bond angles

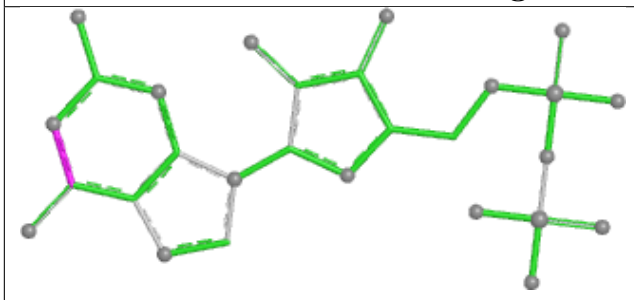


Torsions



Rings

Ligand GDP M2 502



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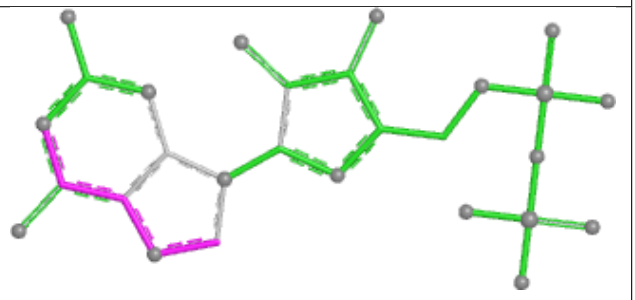
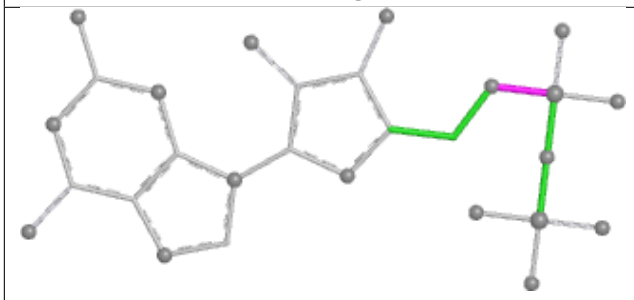
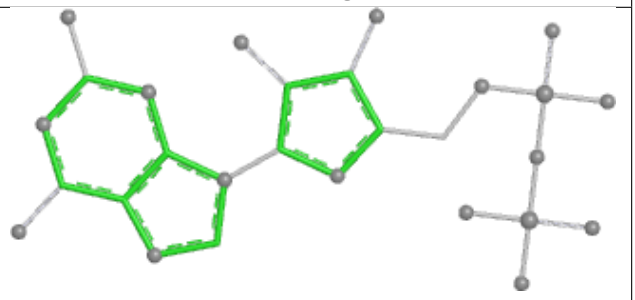


Bond angles

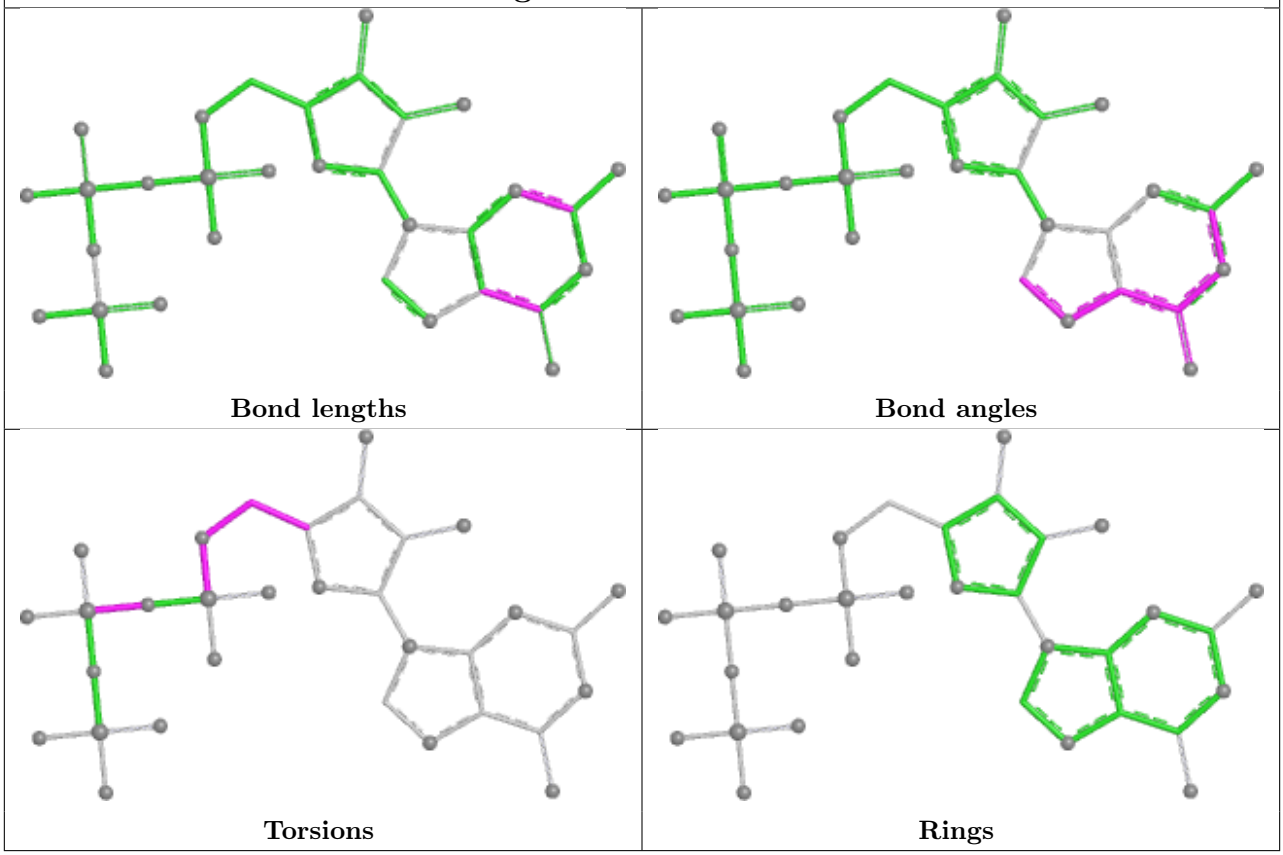


Torsions

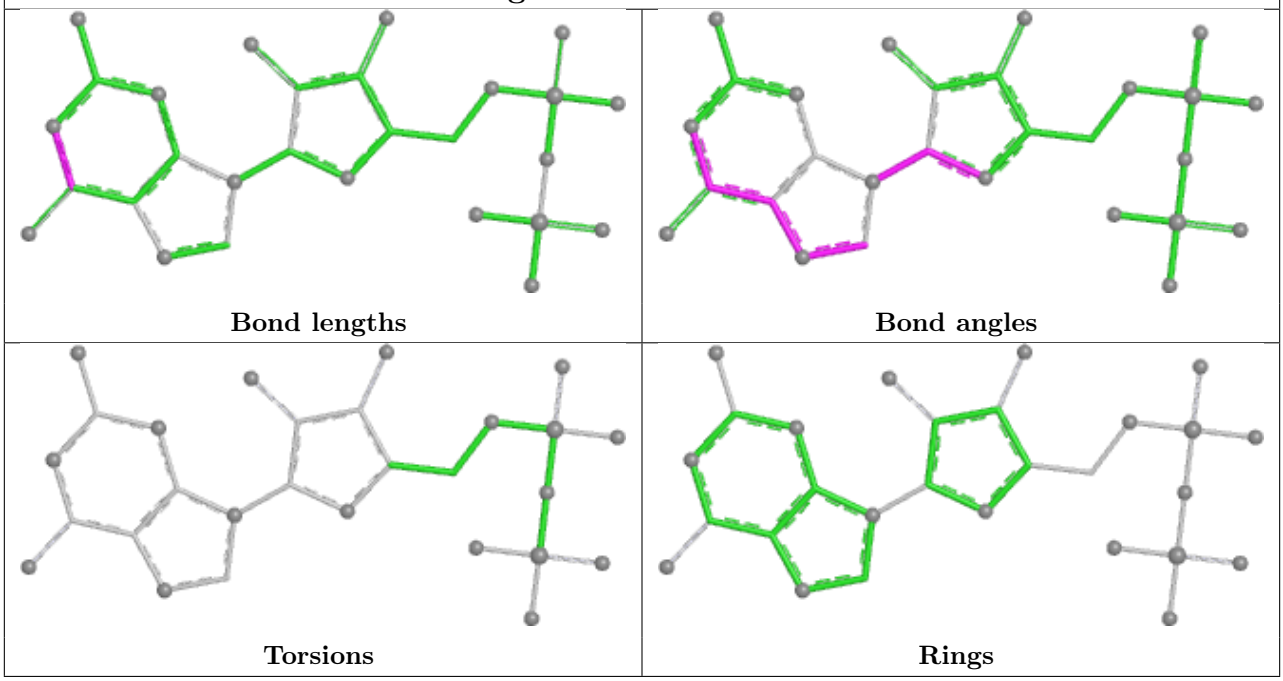


Rings

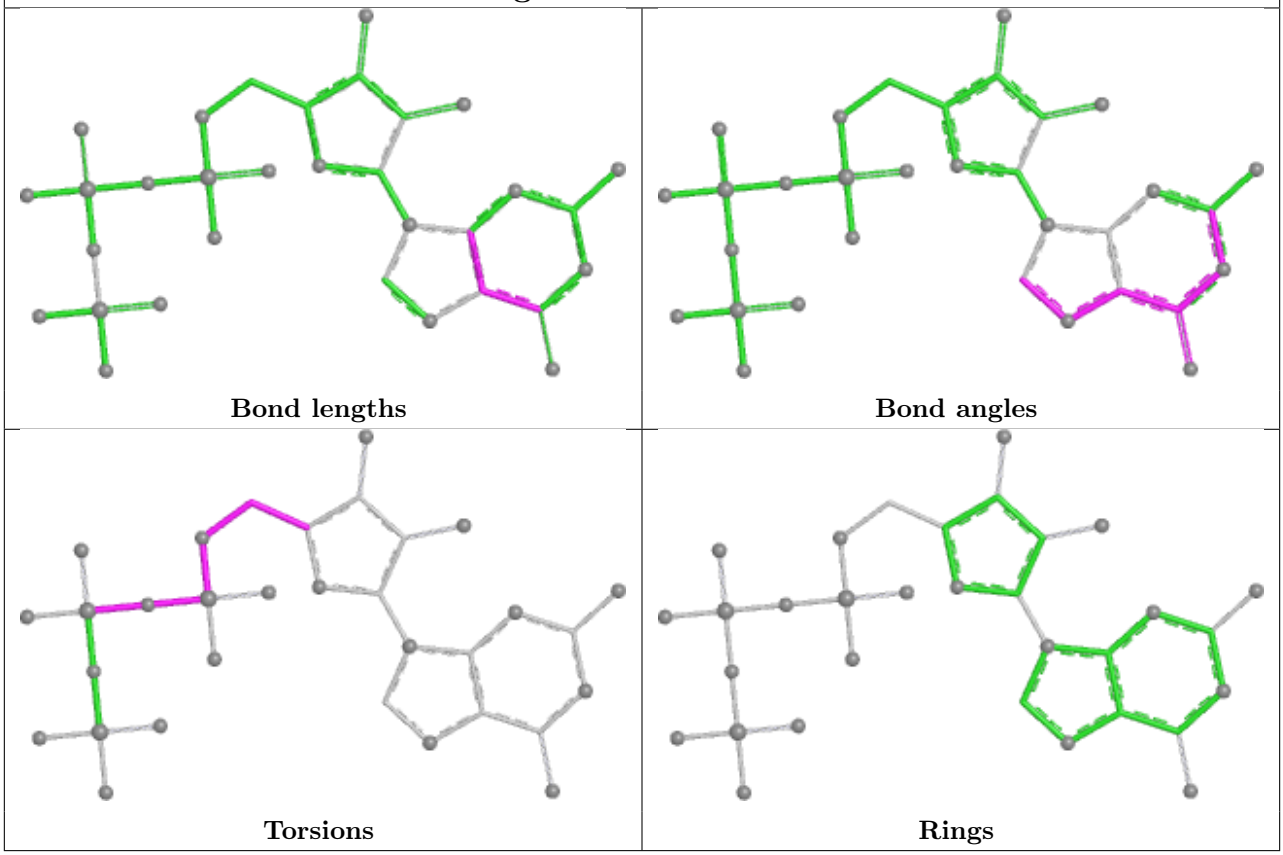
Ligand GTP U7 501



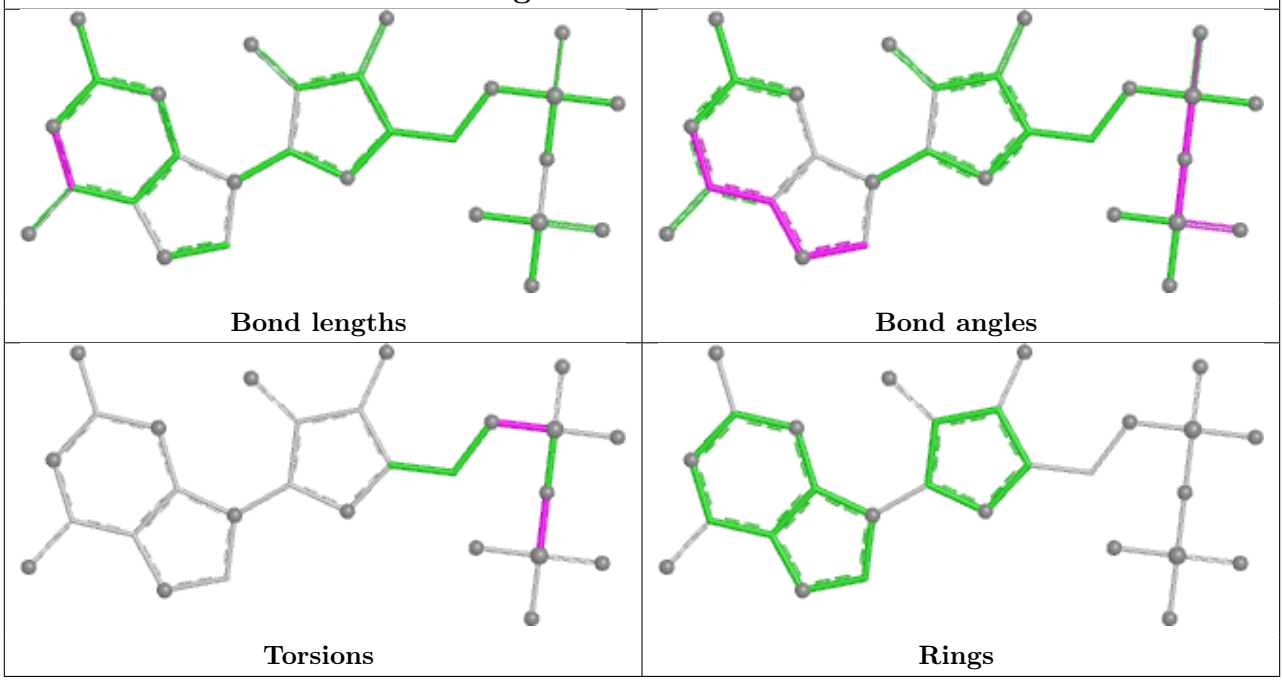
Ligand GDP W6 501



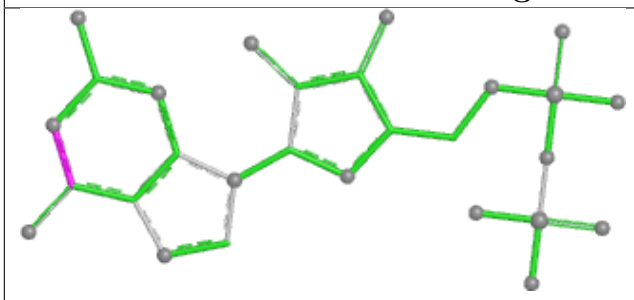
Ligand GTP H8 501



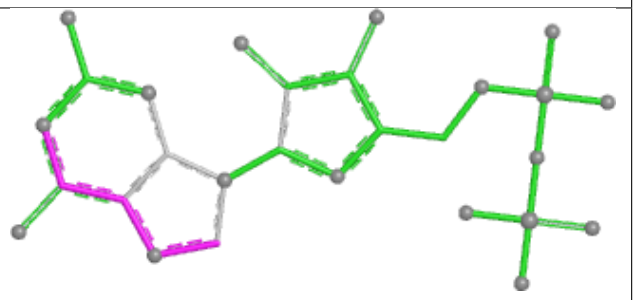
Ligand GDP 3C 502



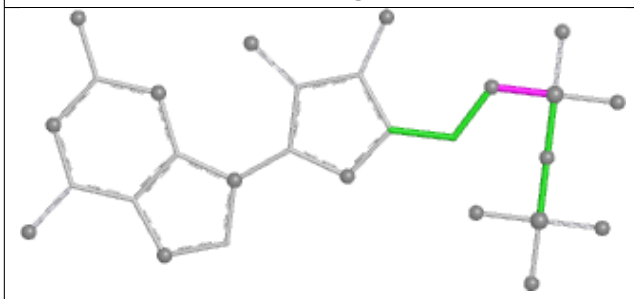
Ligand GDP 1C 502



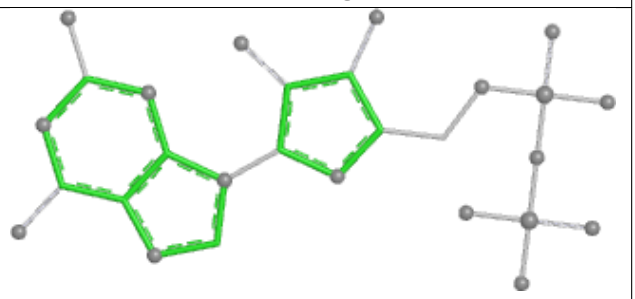
Bond lengths



Bond angles

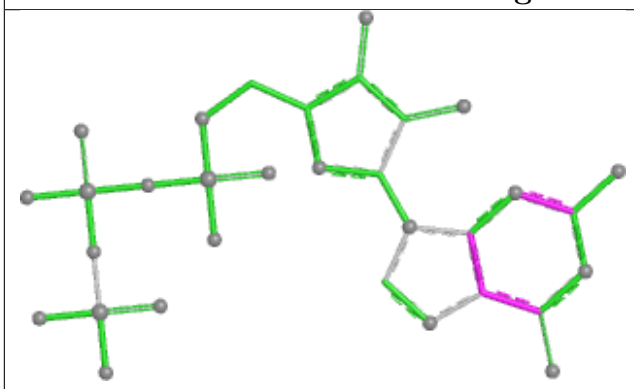


Torsions



Rings

Ligand GTP 3O 501



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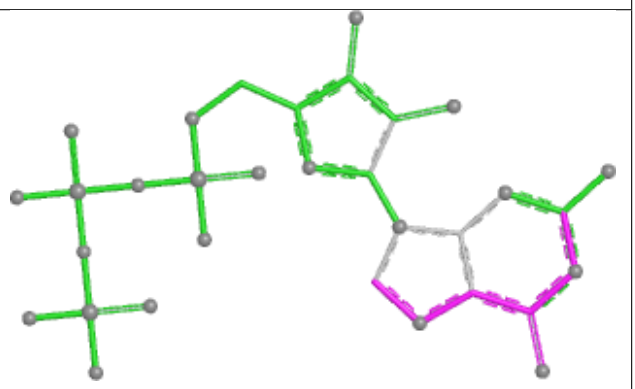
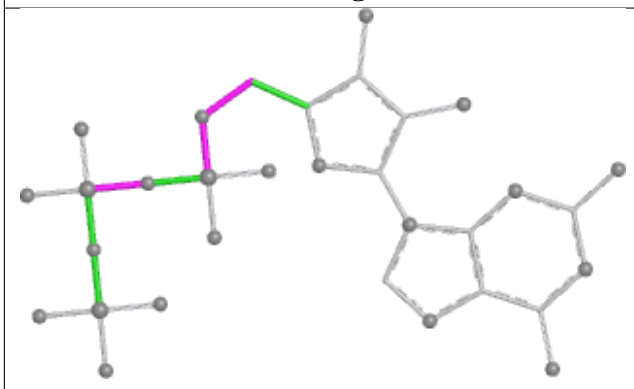
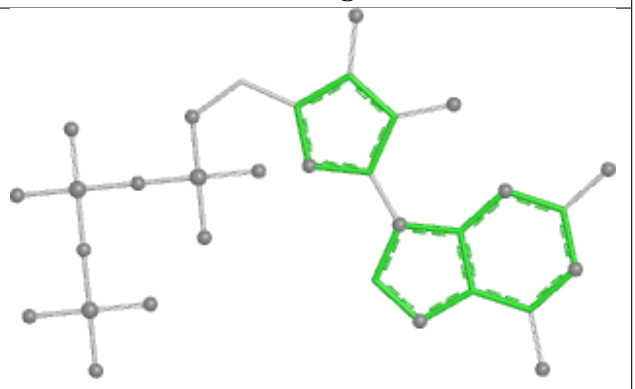


Bond angles

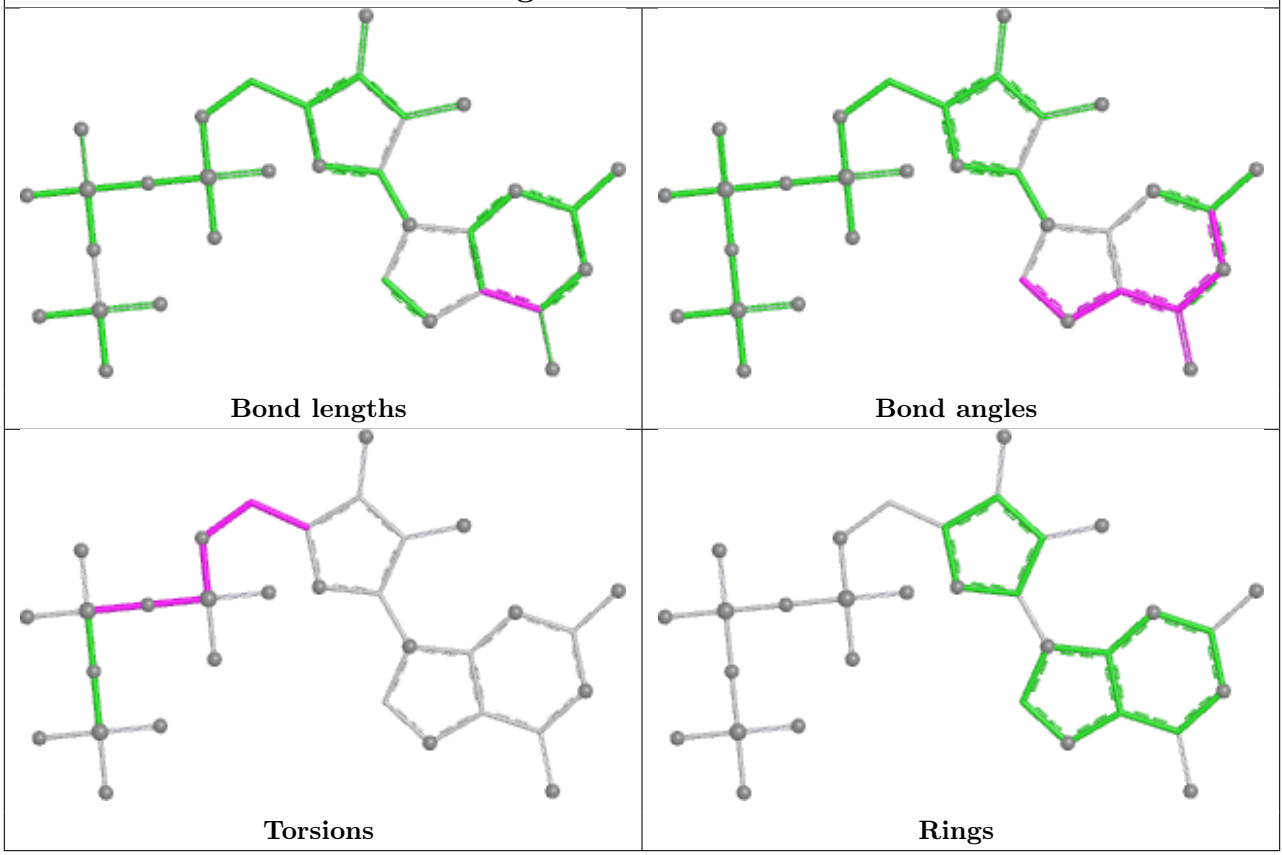


Torsions



Rings

Ligand GTP Z6 501



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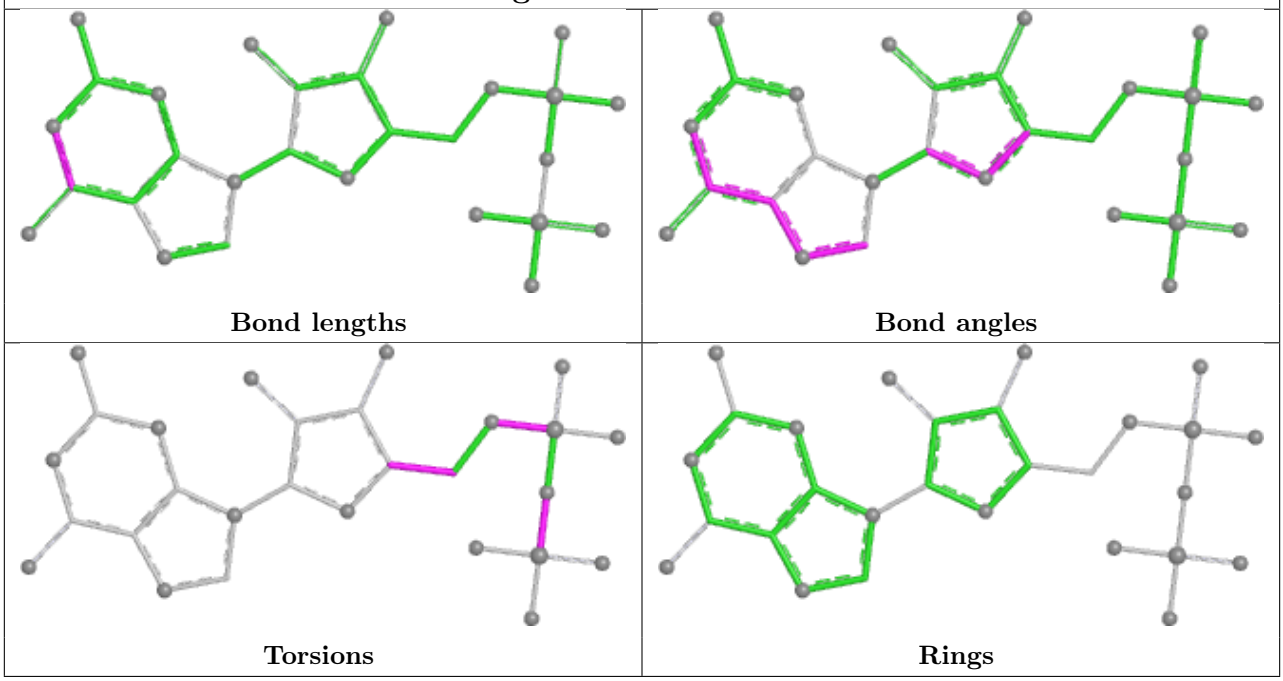

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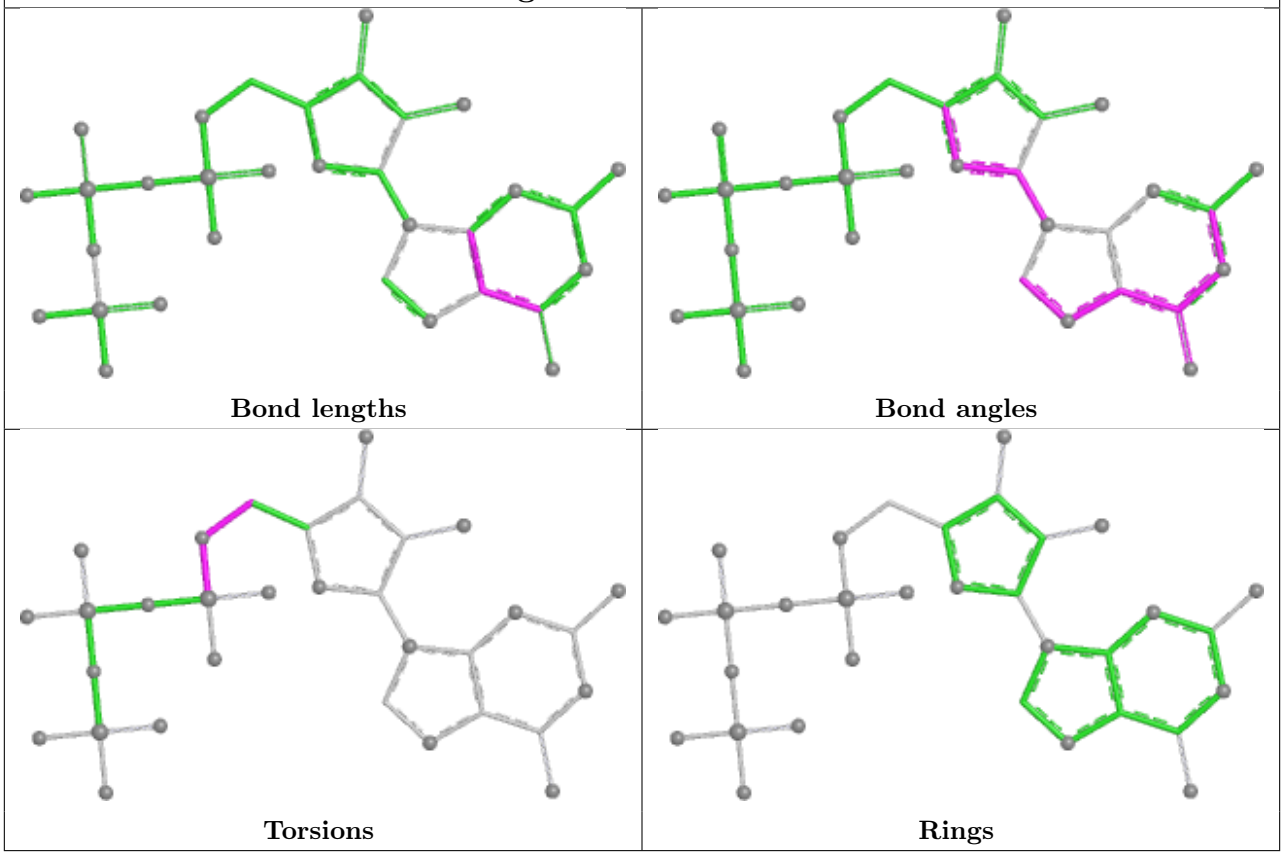

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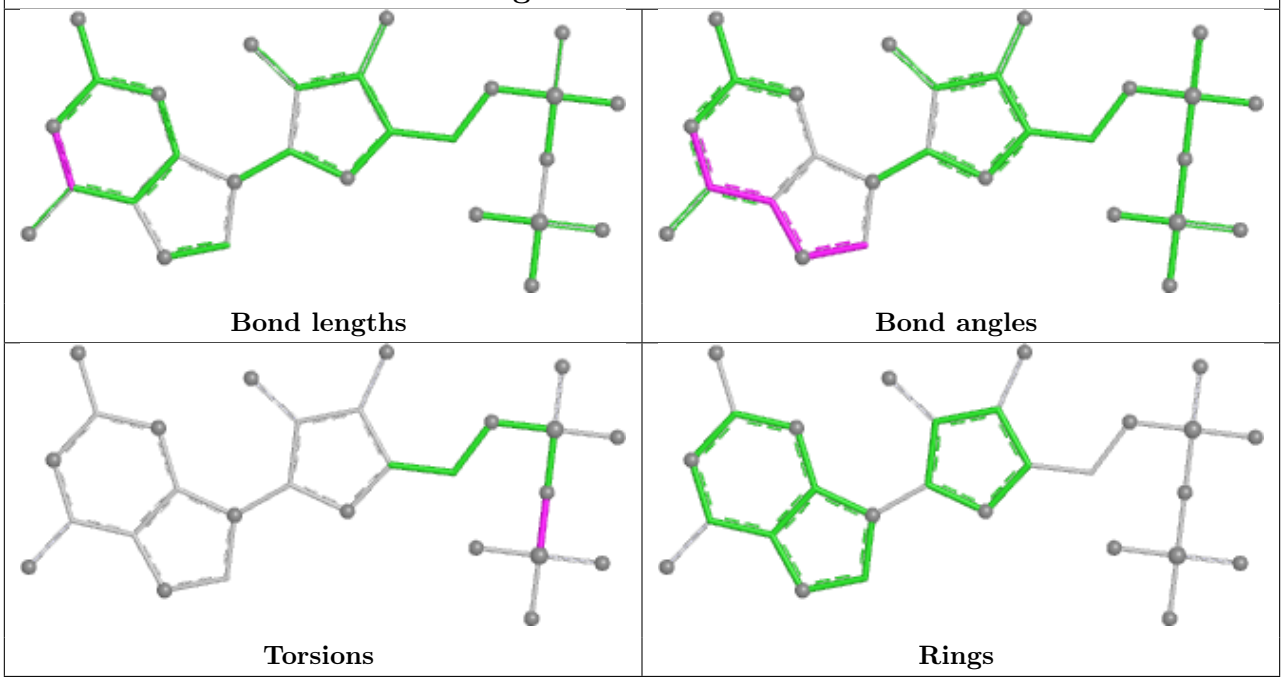

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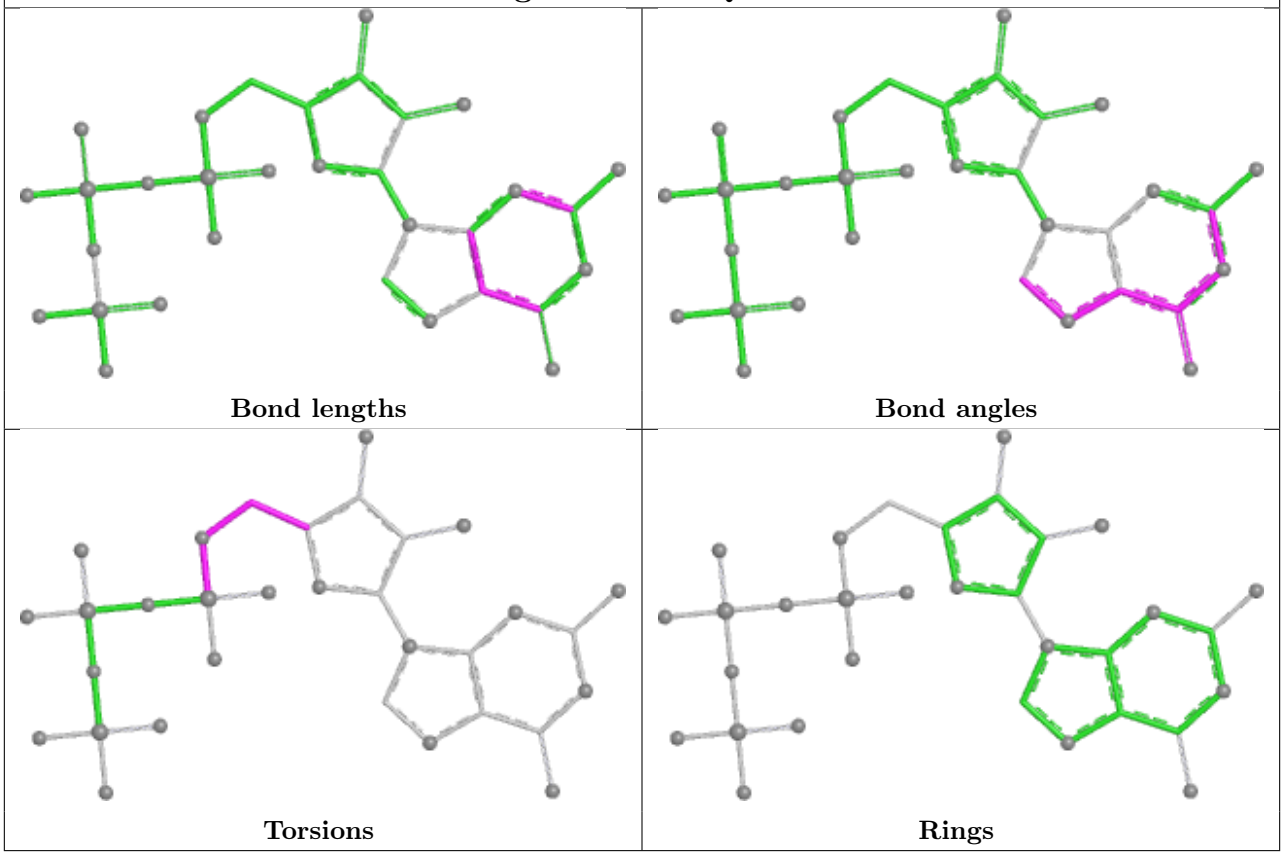

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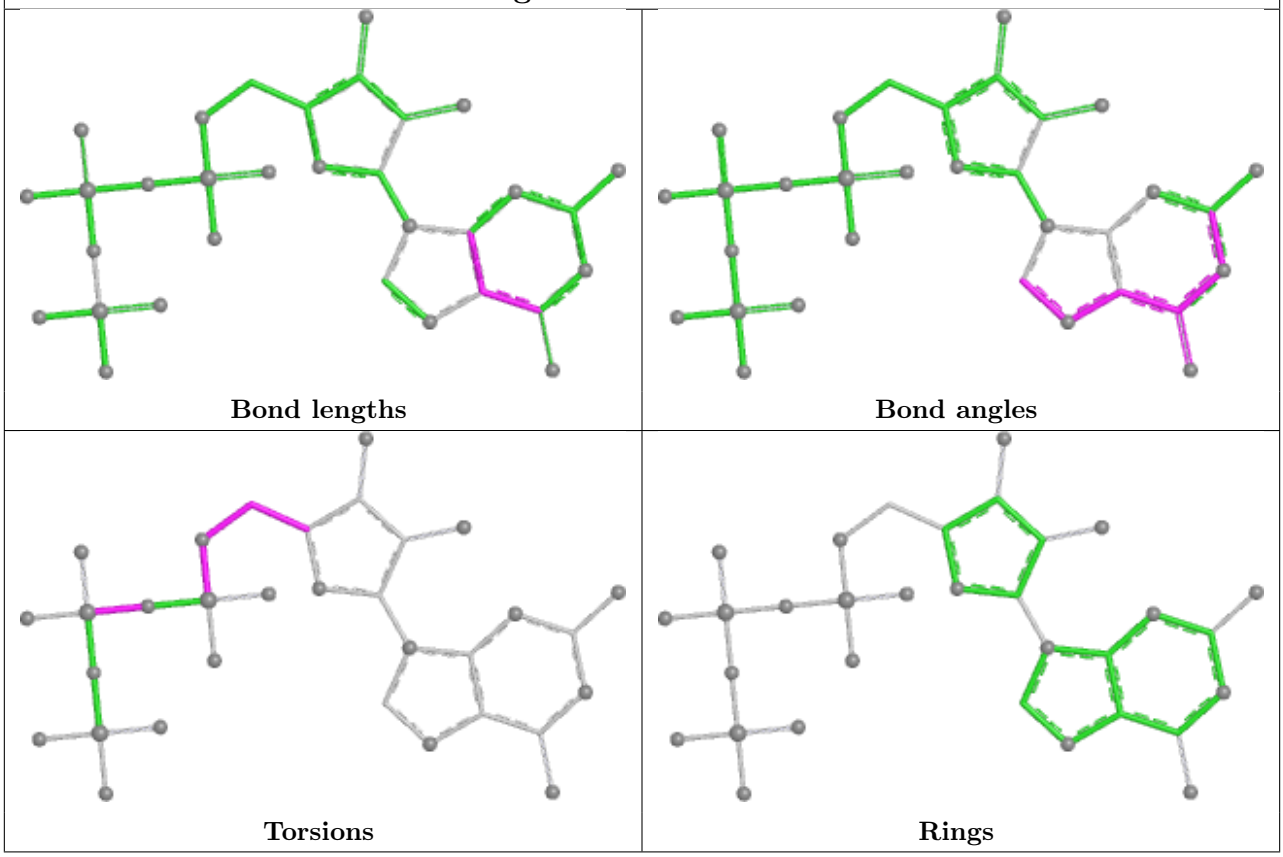

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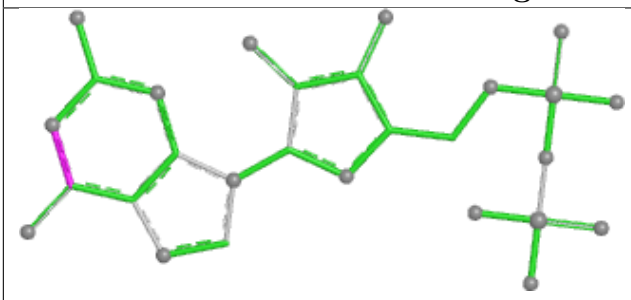
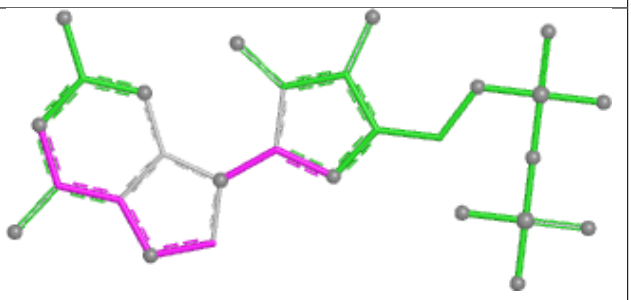
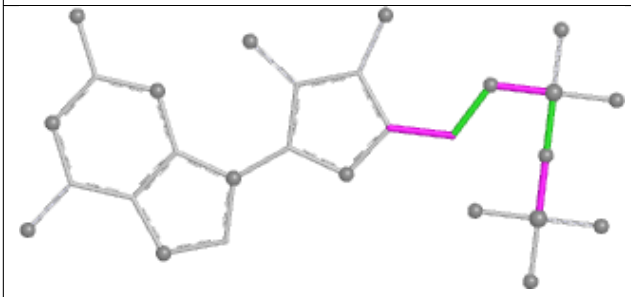
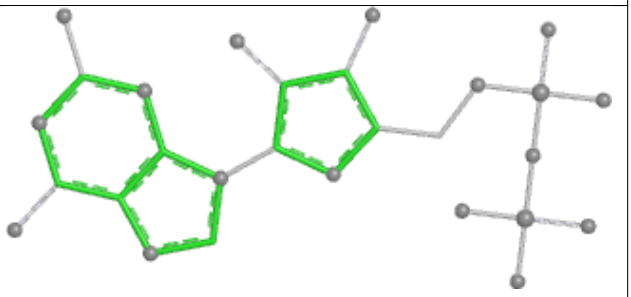
 Bond lengths	 Bond angles
 Torsions	 Rings

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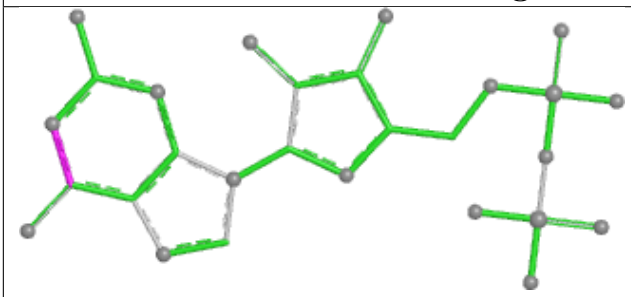
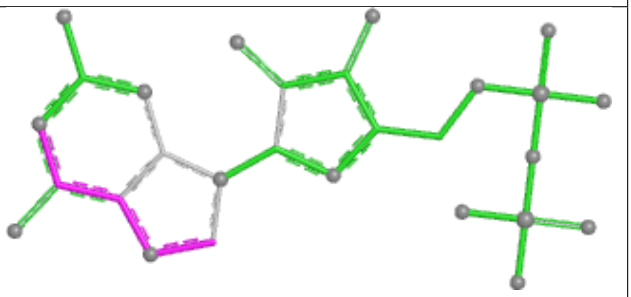
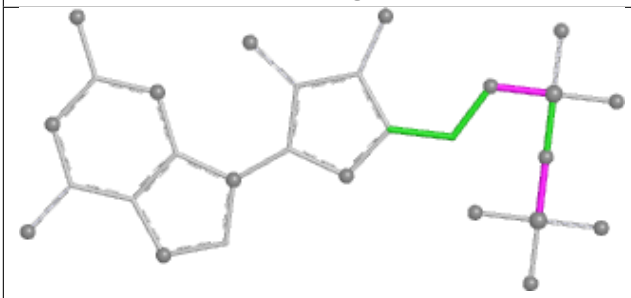
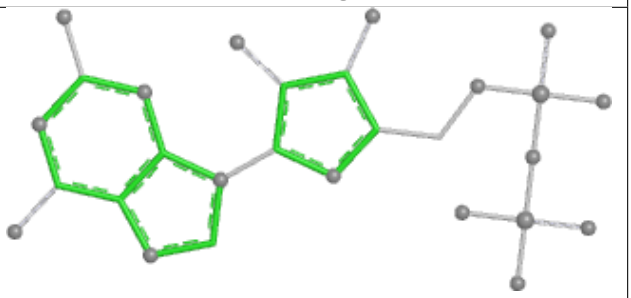
 Bond lengths	 Bond angles
 Torsions	 Rings

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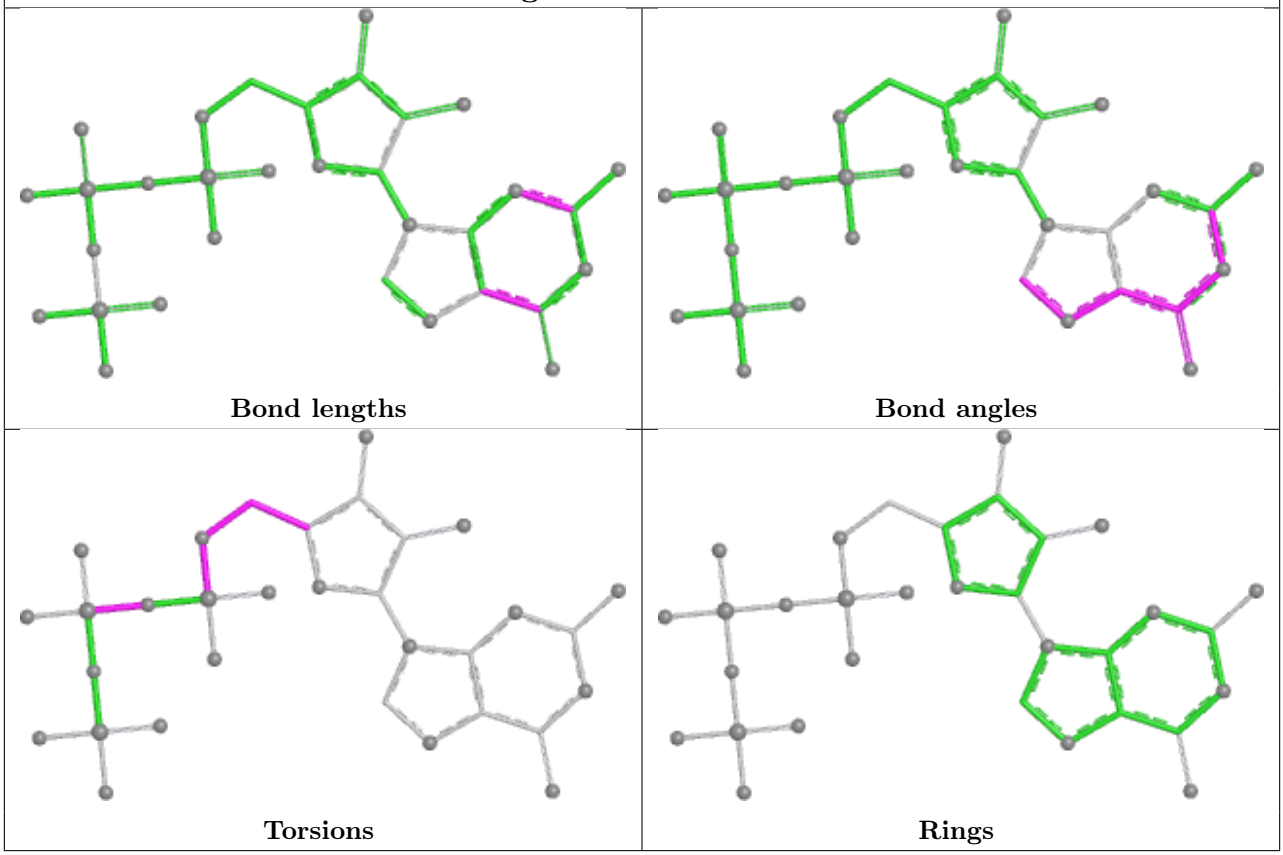

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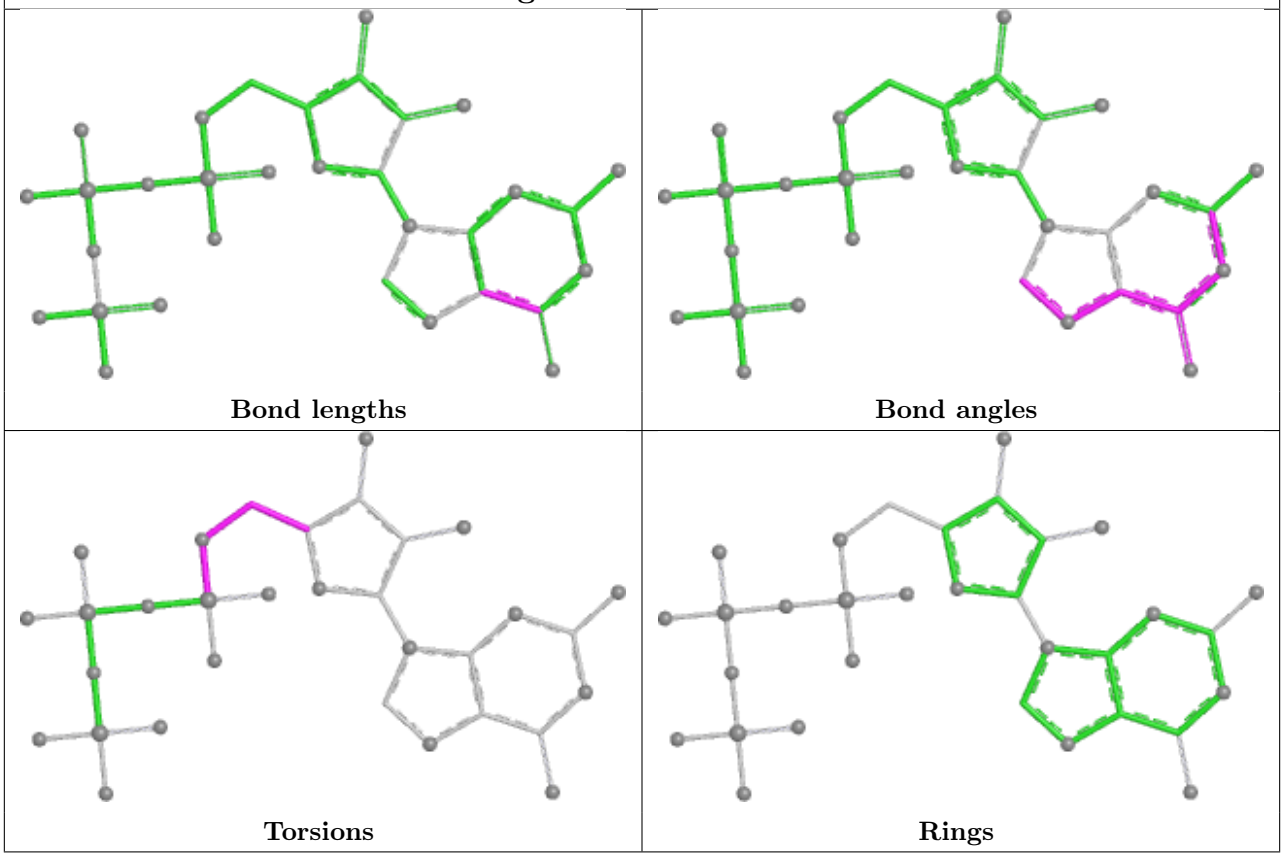

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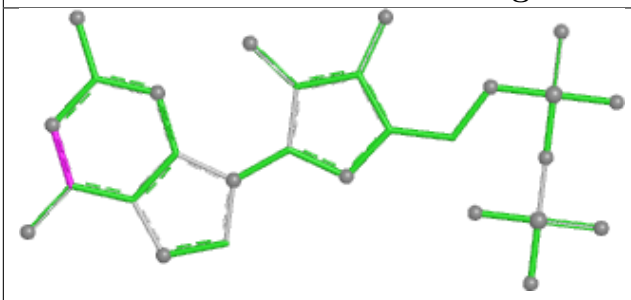
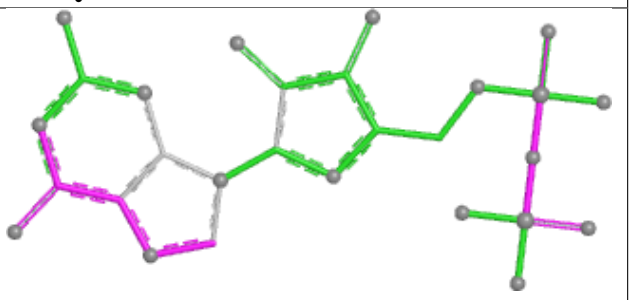
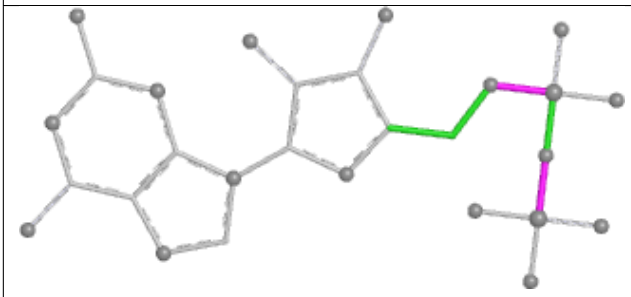


Bond lengths



Bond angles



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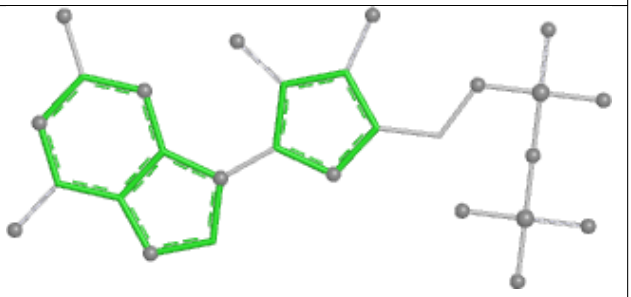
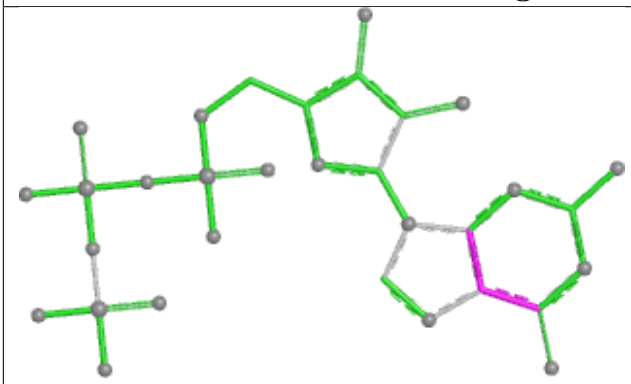


Rings

Ligand GTP T8 501



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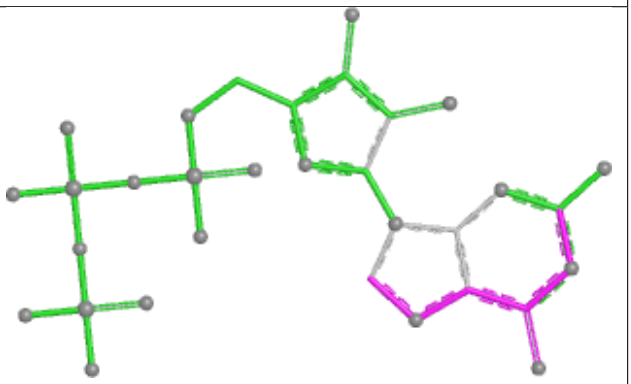

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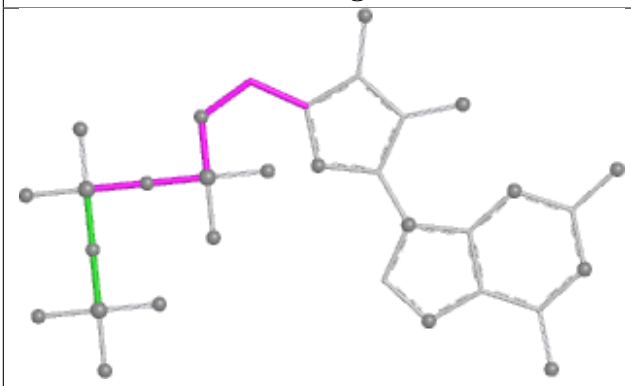

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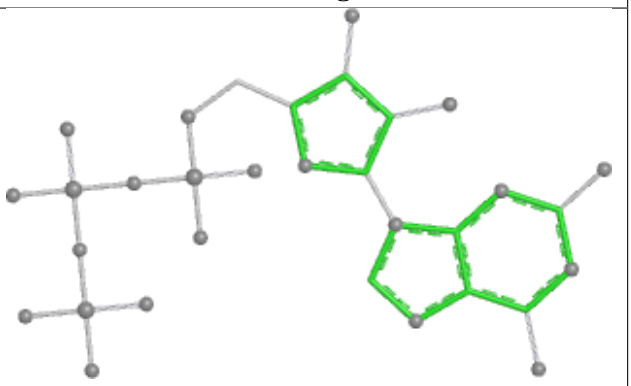

Rings

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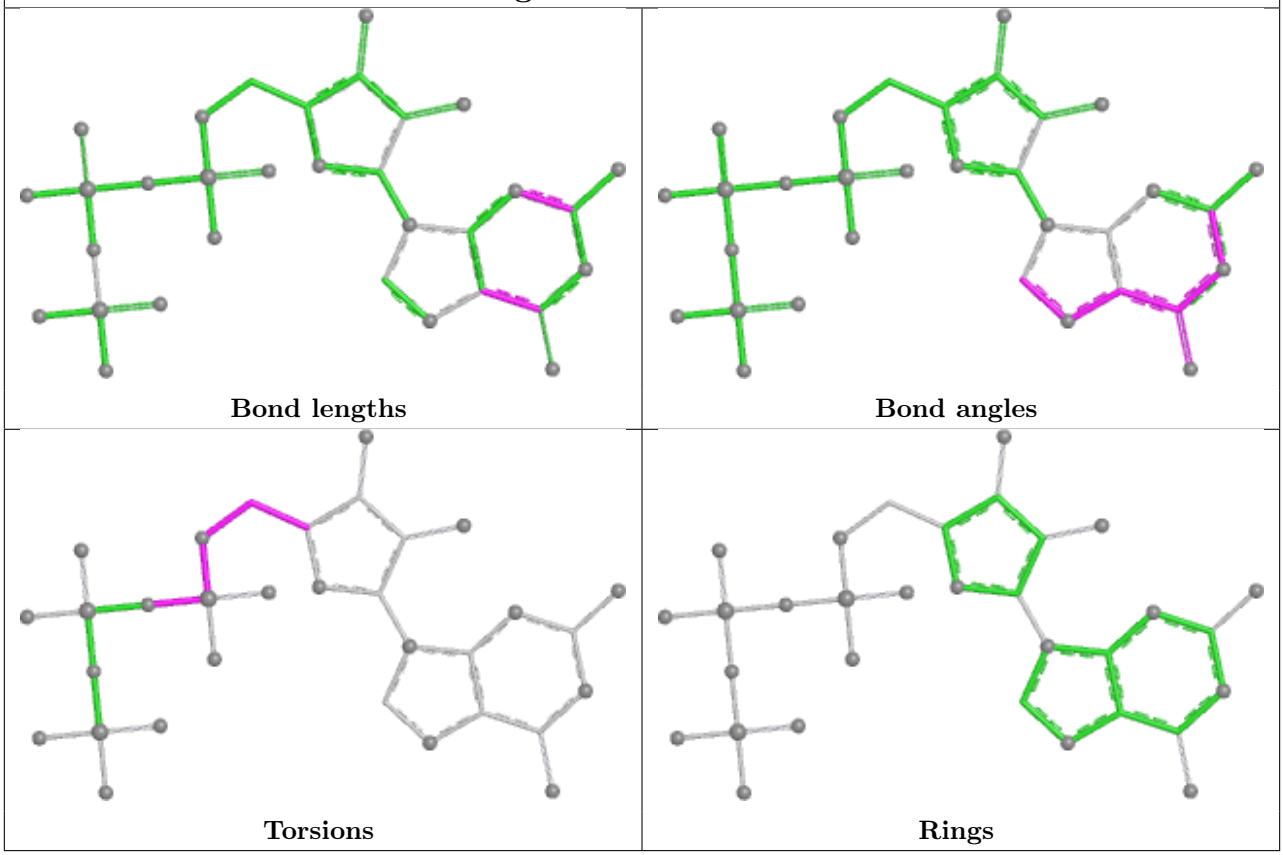

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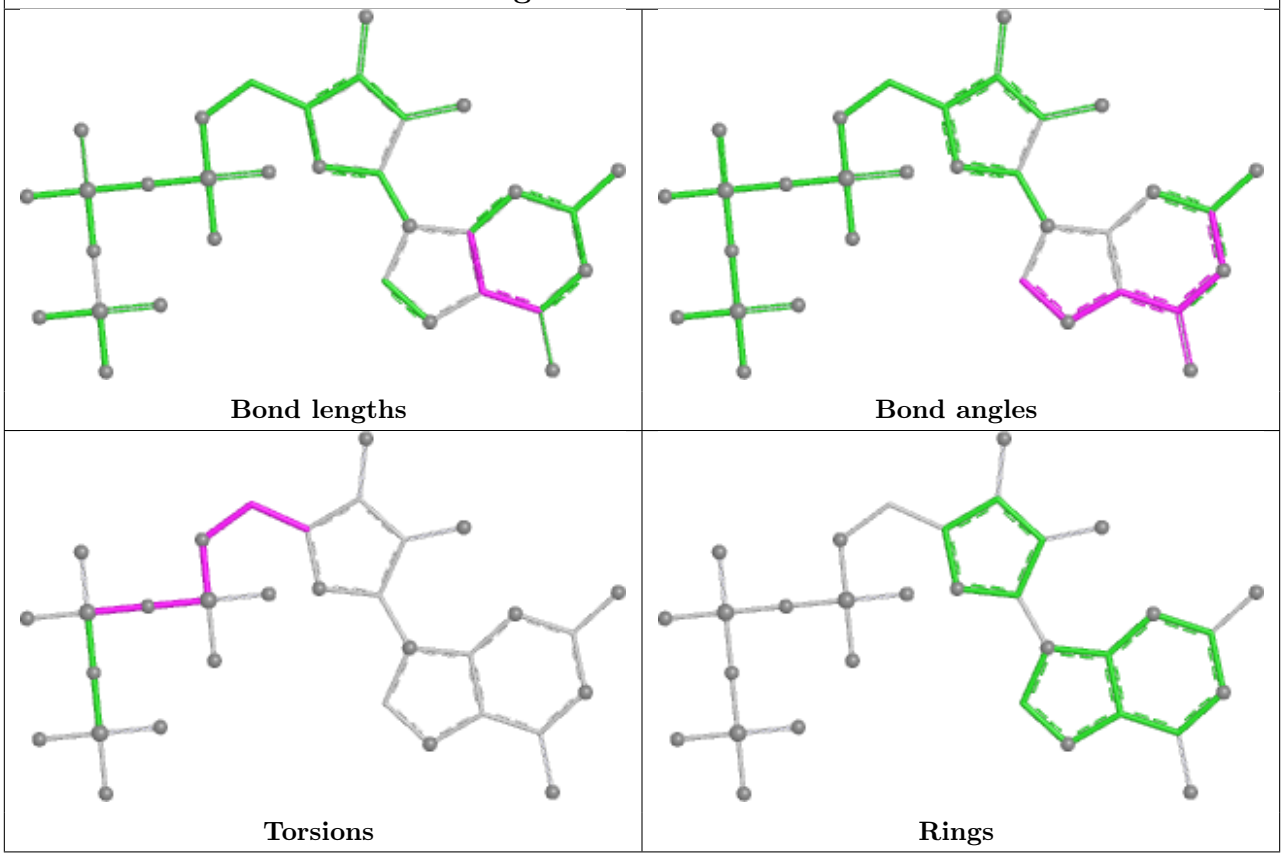

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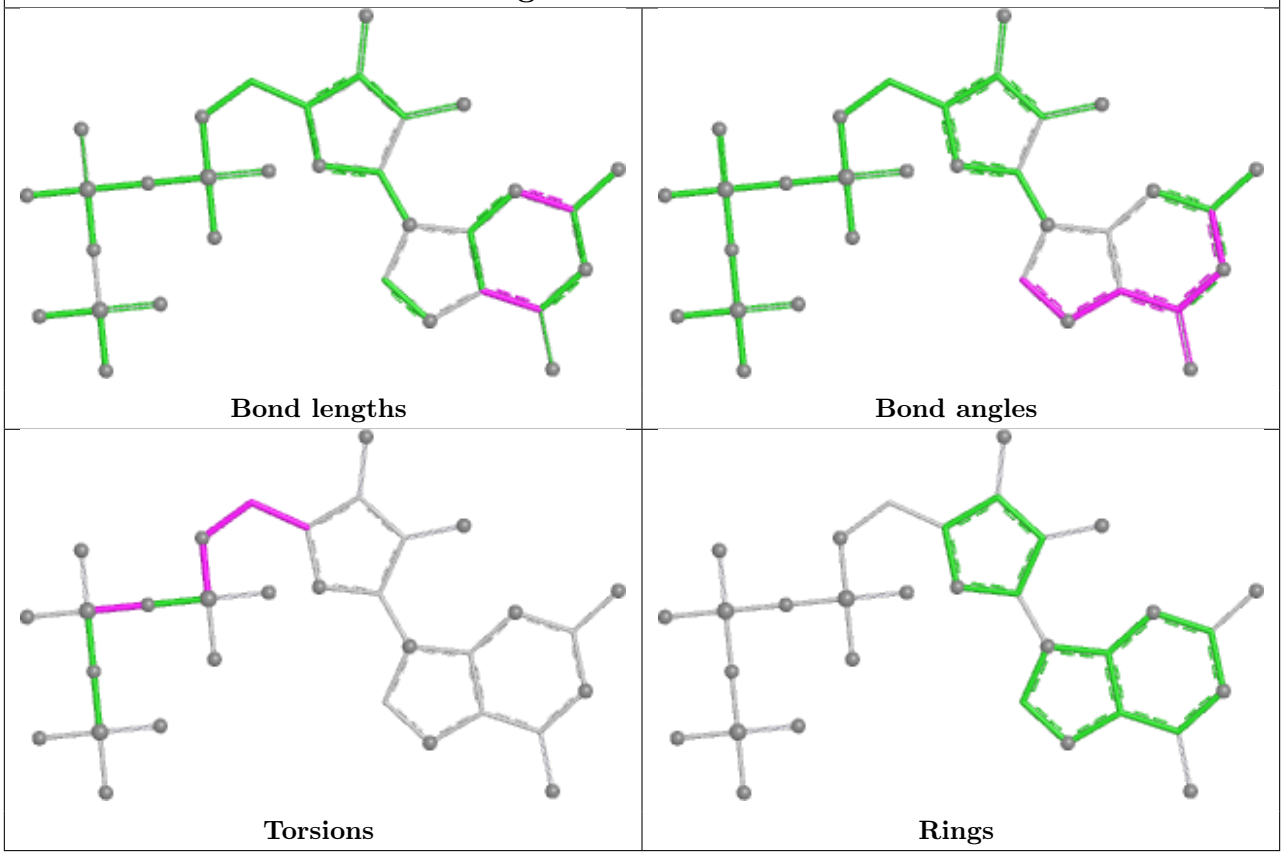

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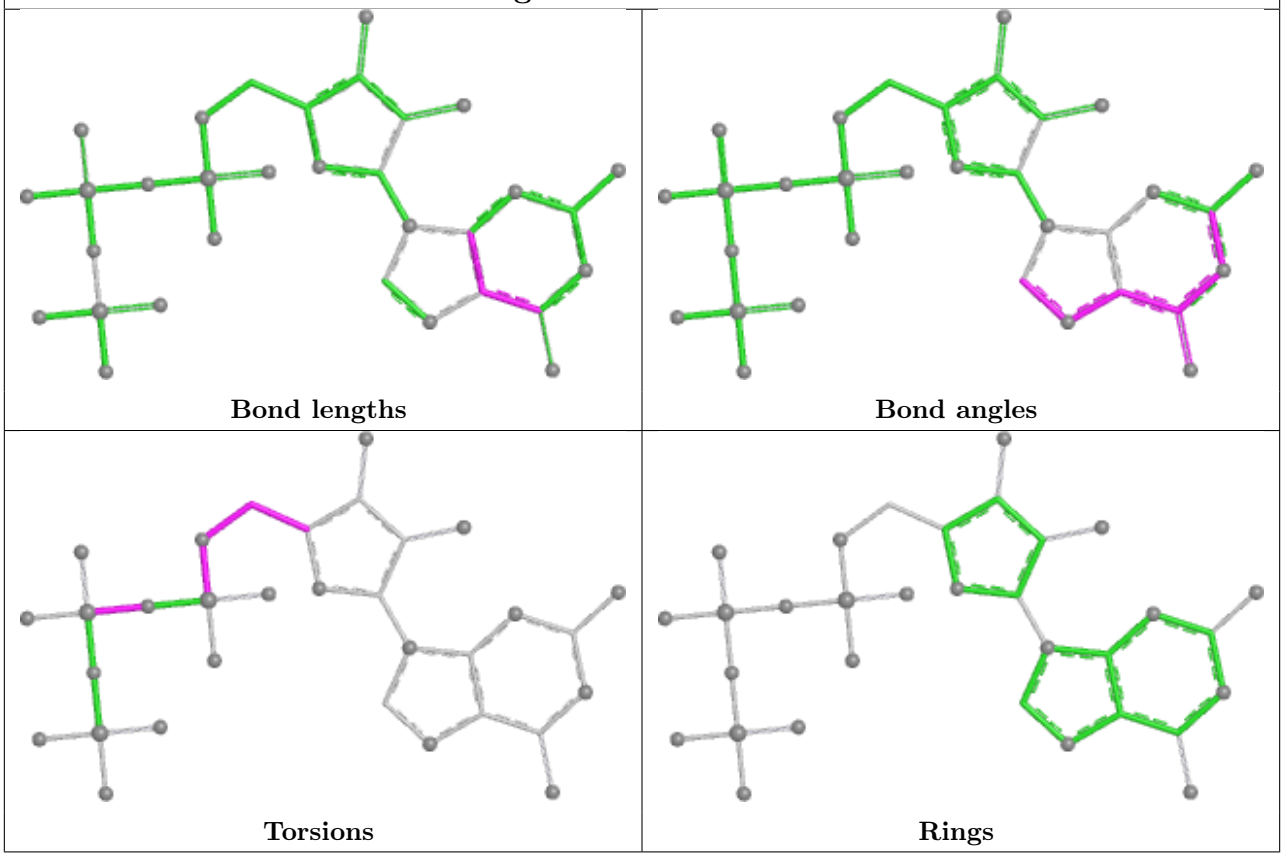

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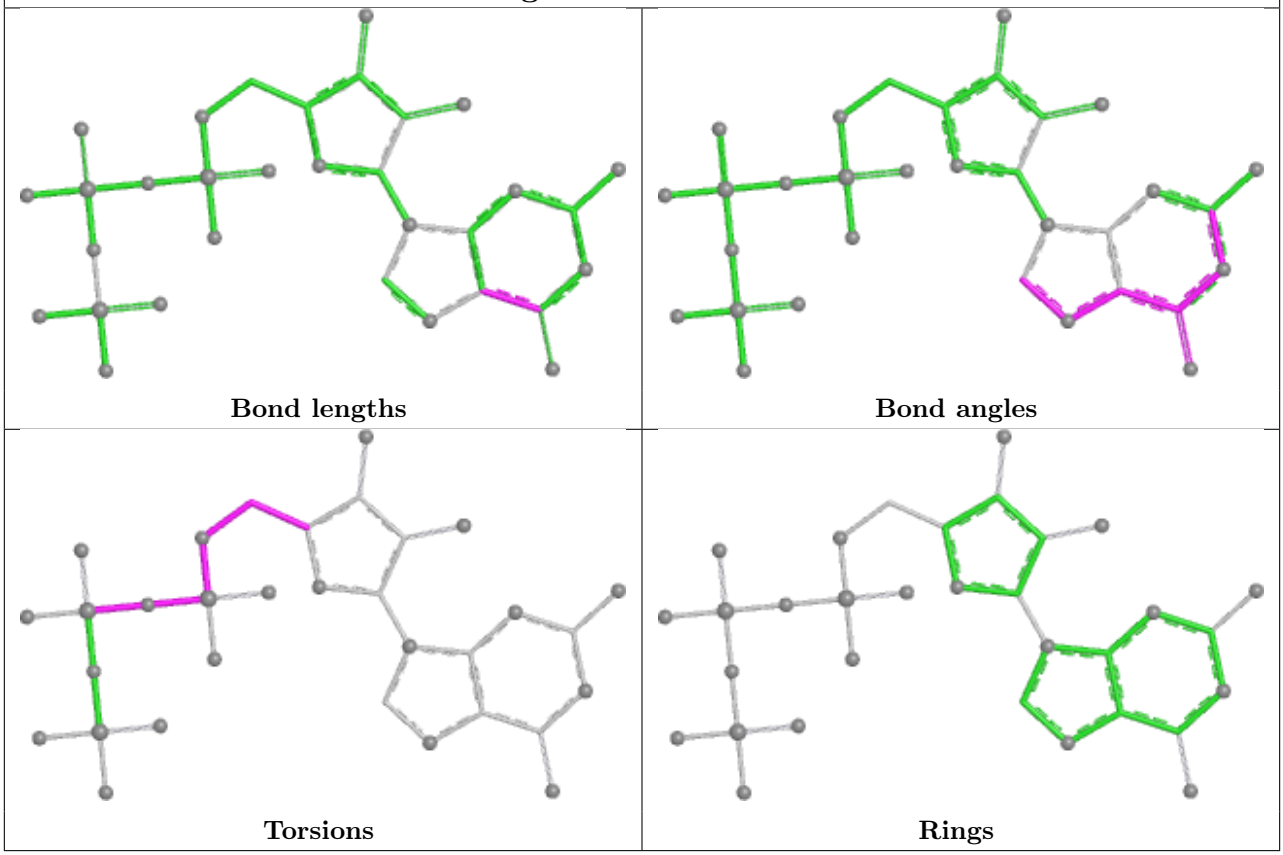

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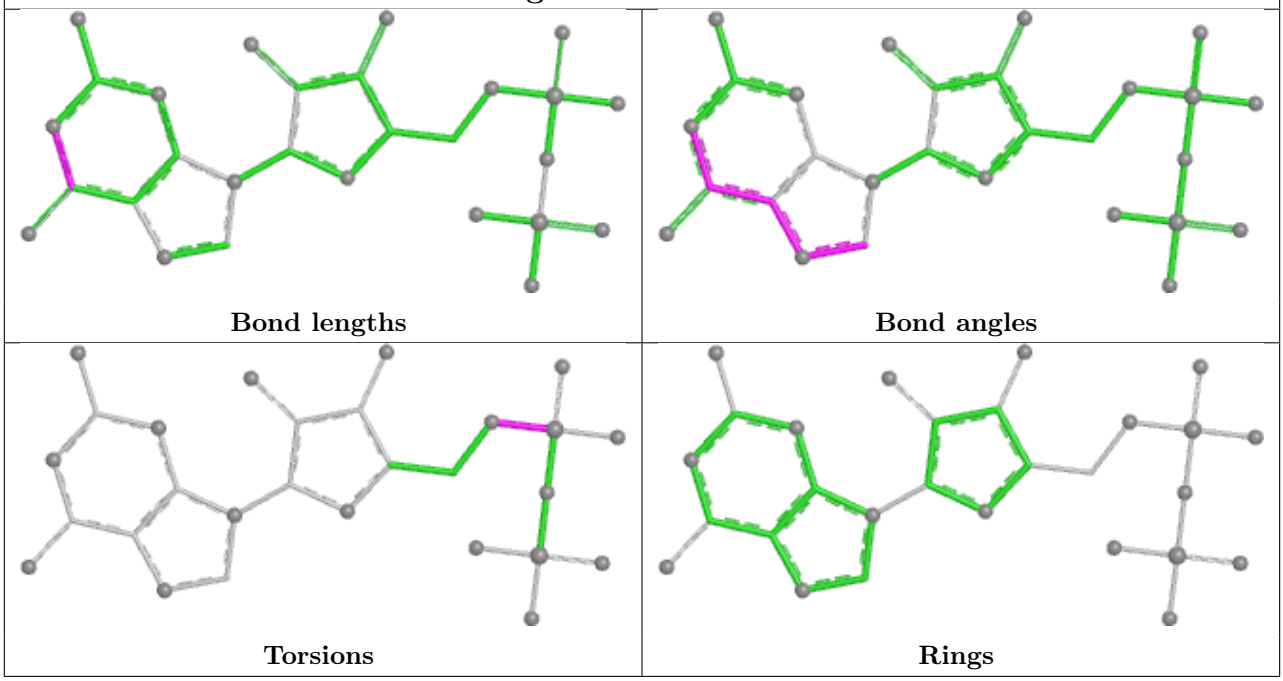

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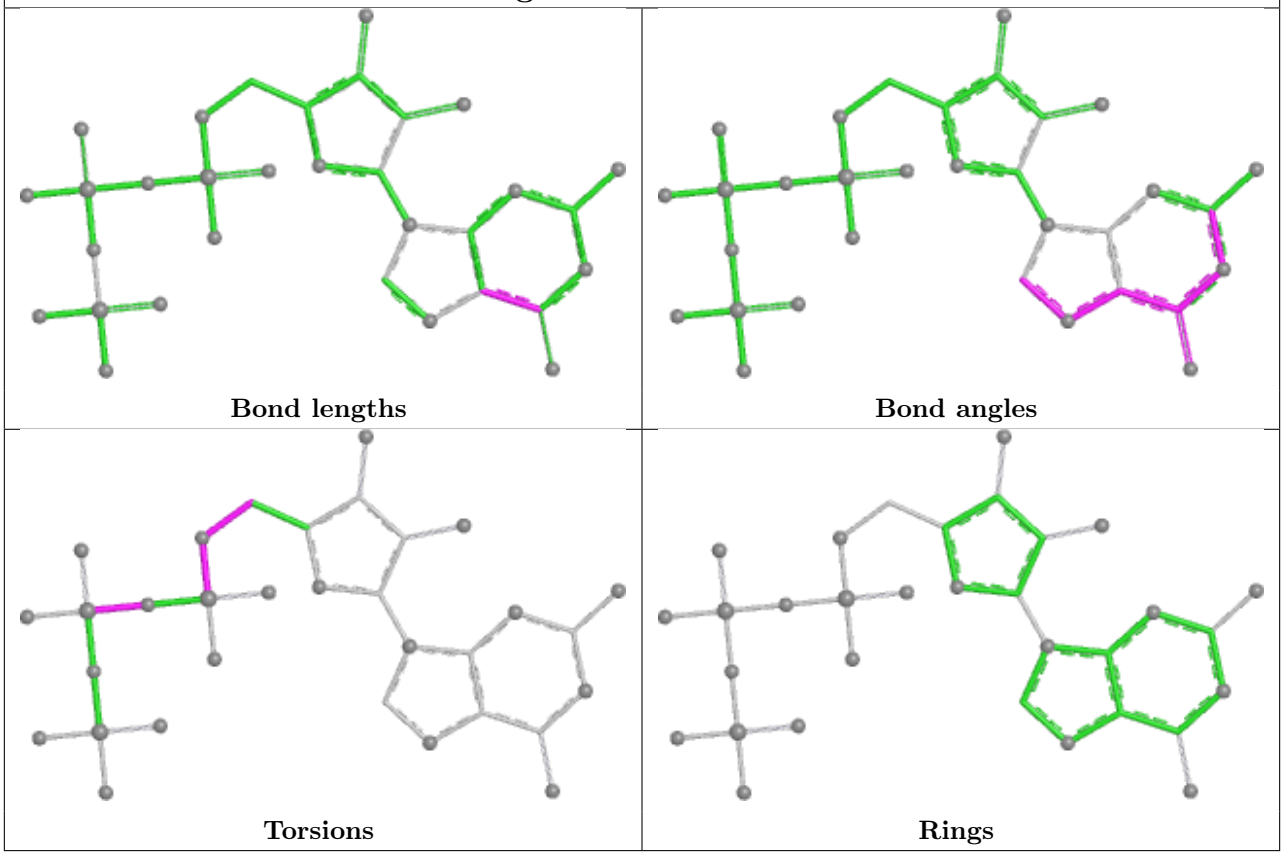

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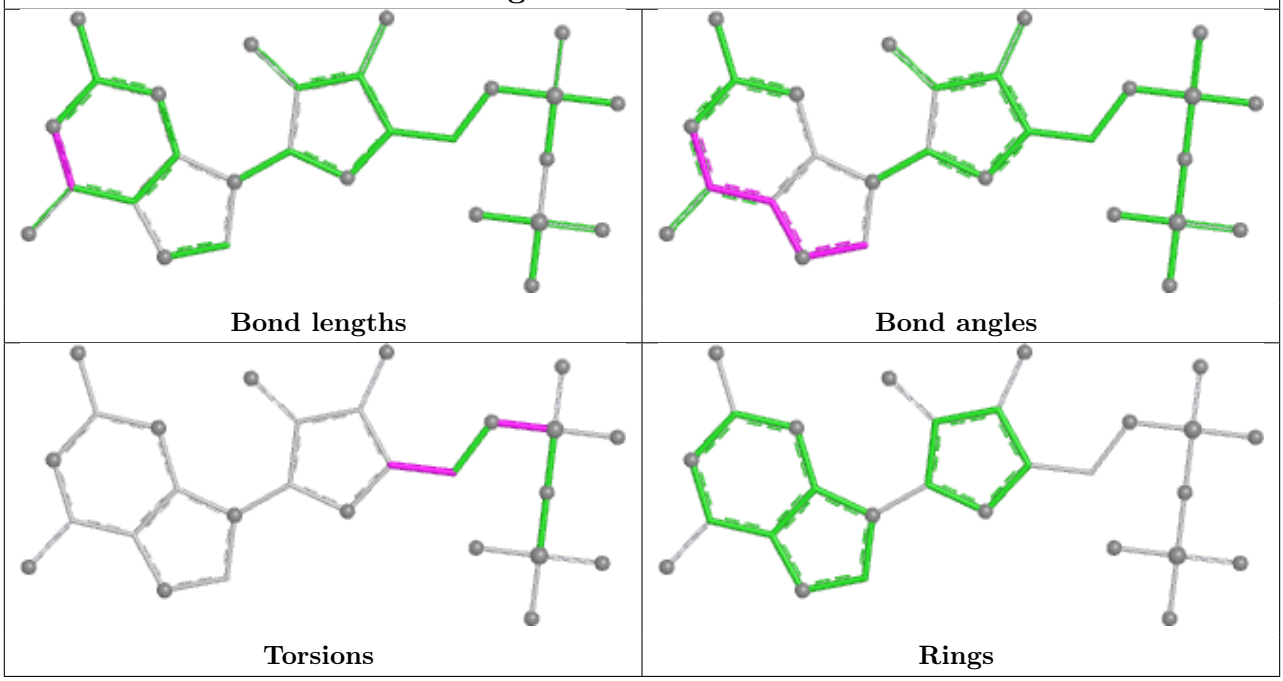

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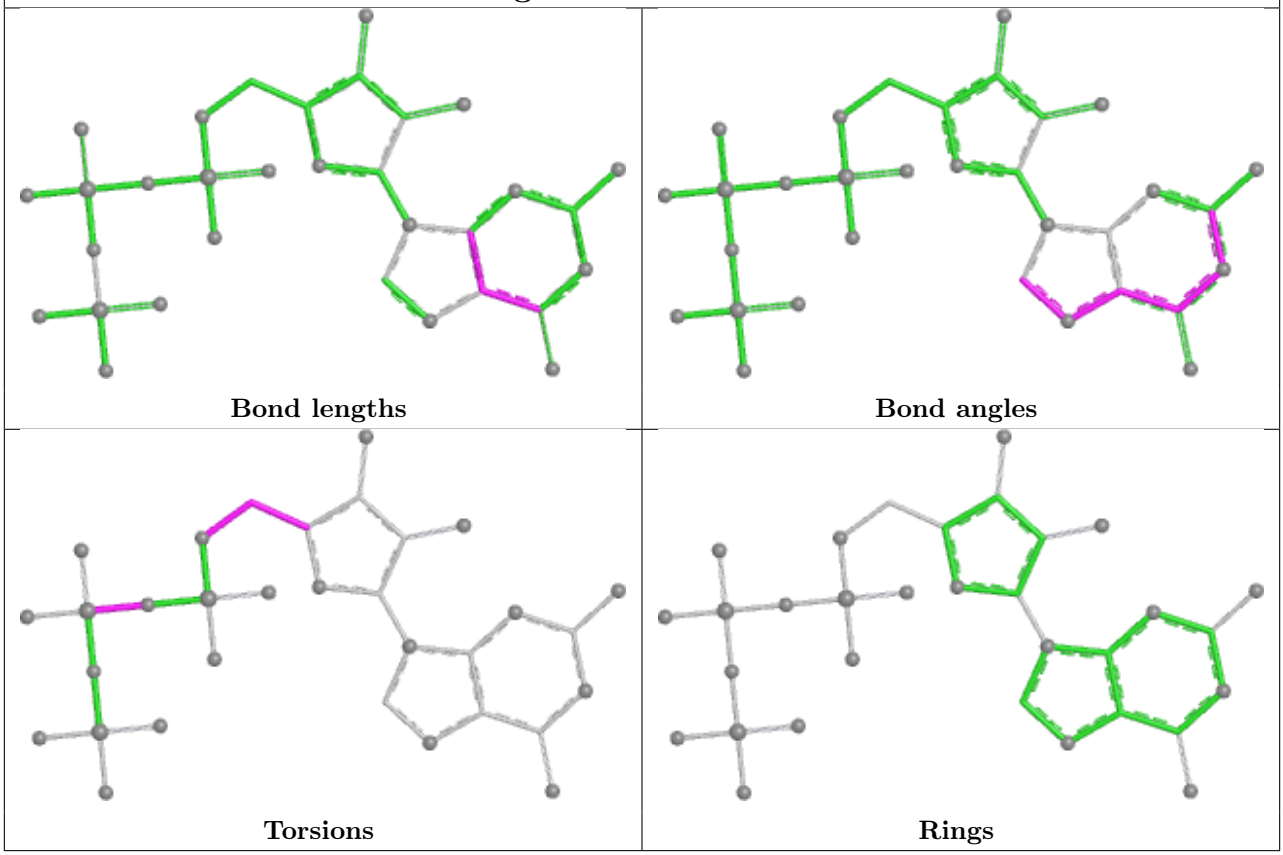

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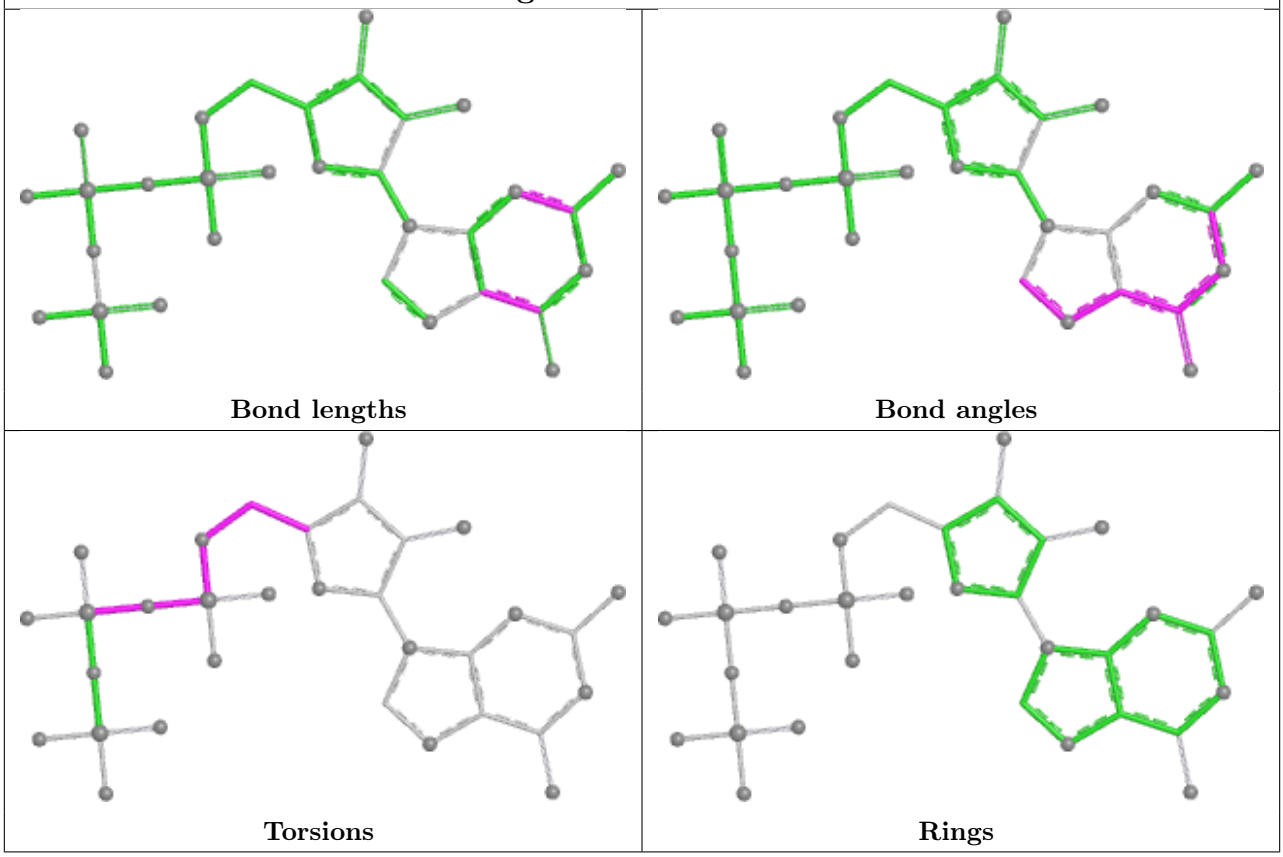

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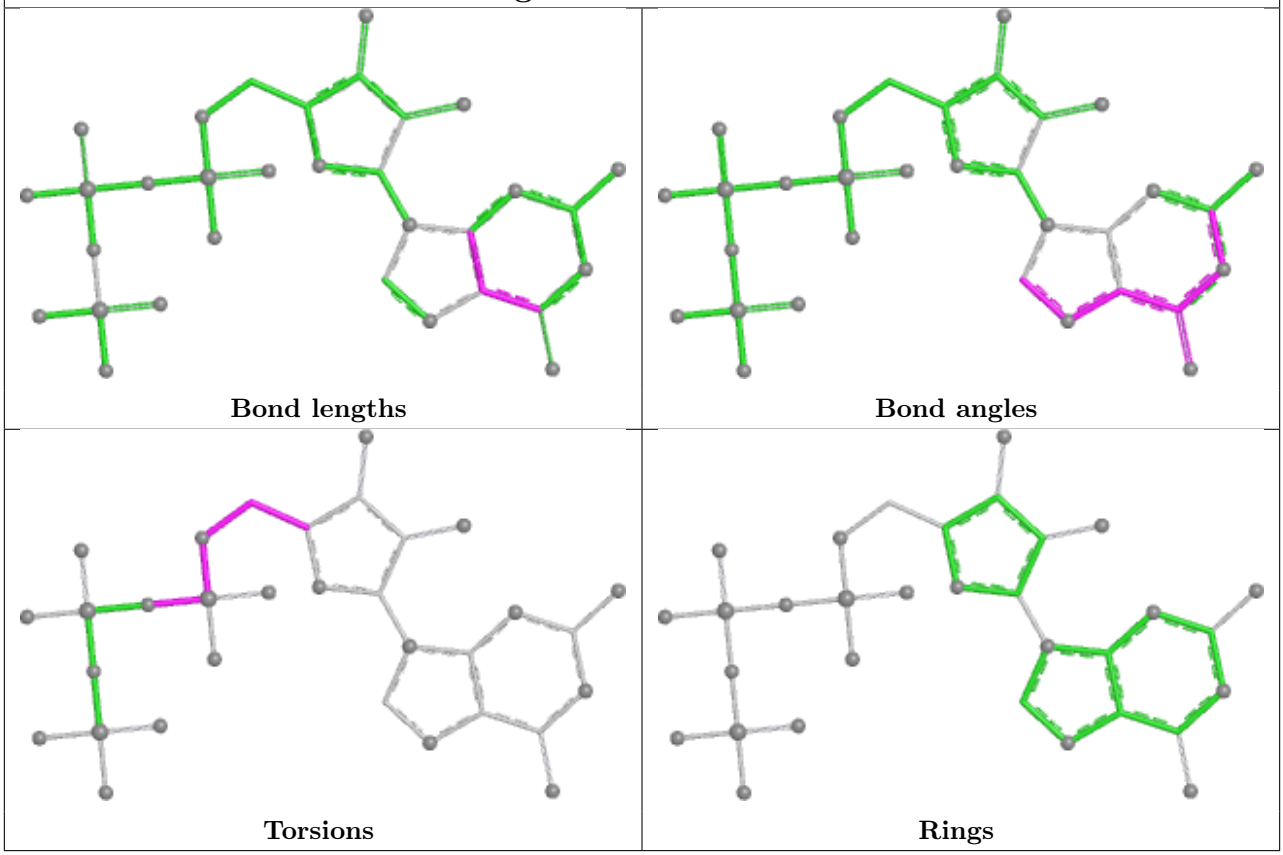

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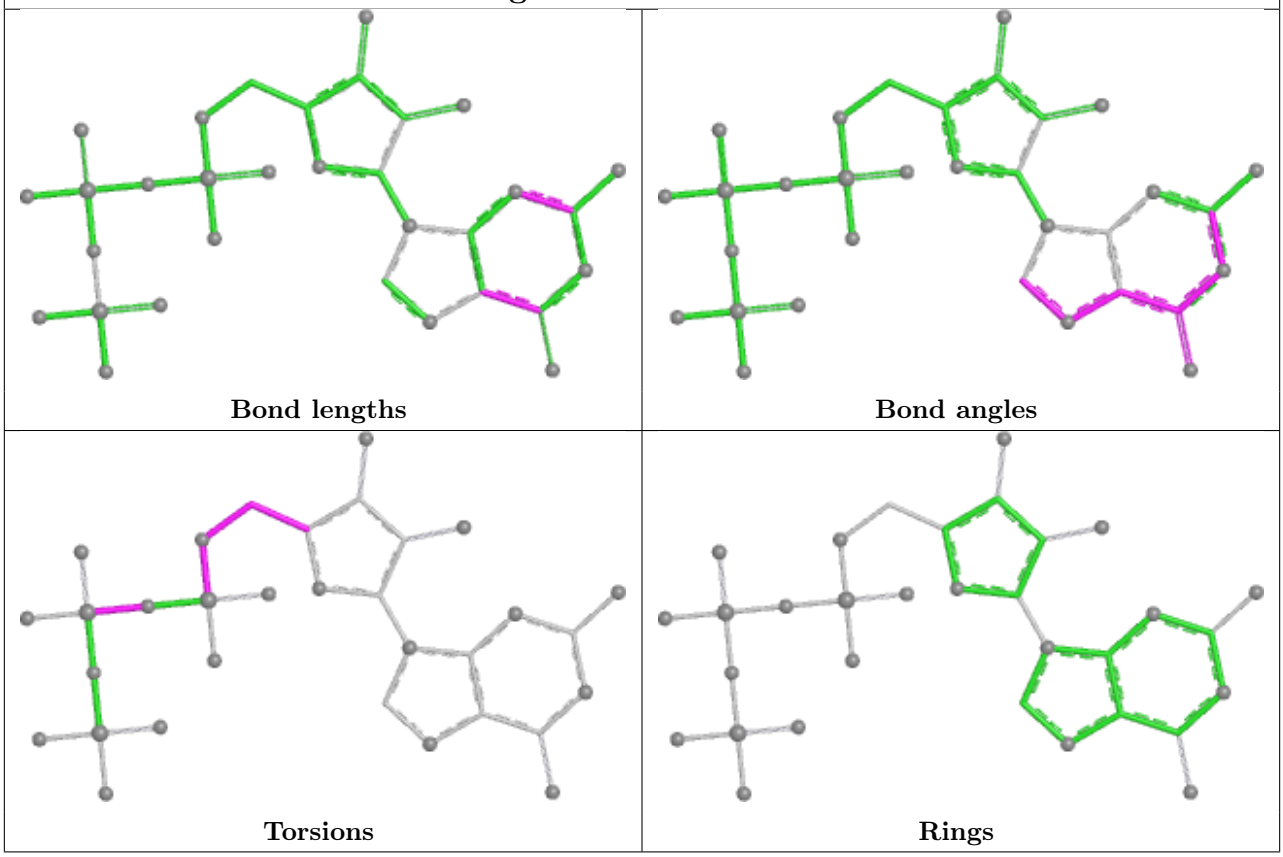

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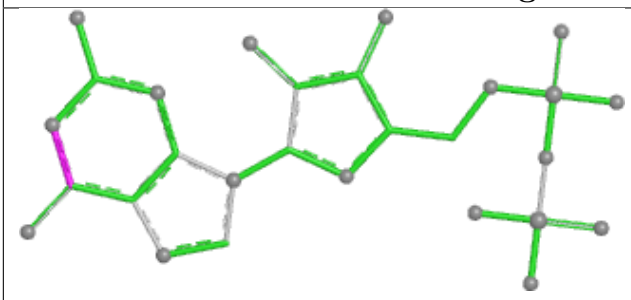
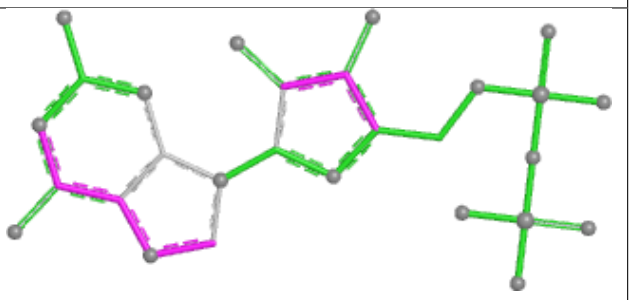
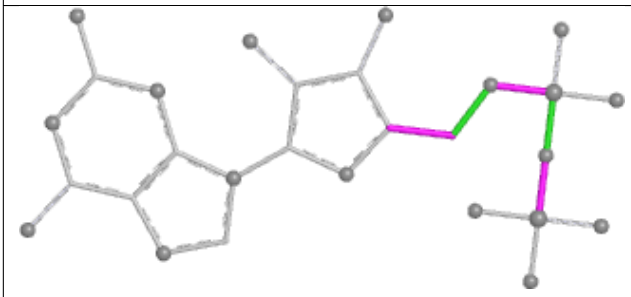


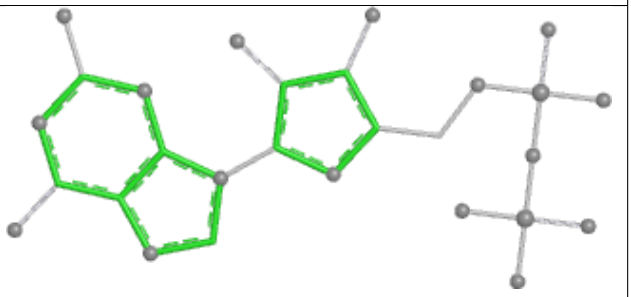
Bond lengths



Bond angles

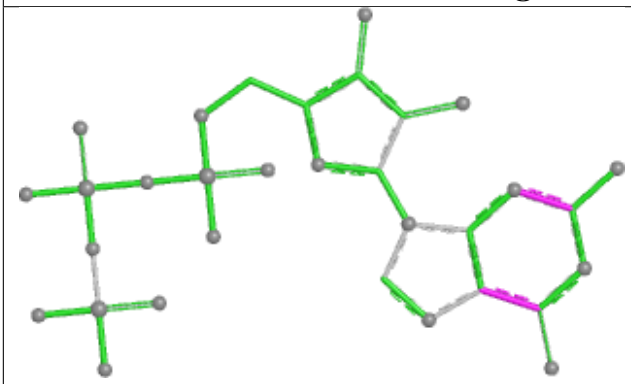


Torsions



Rings

Ligand GTP 3T 501



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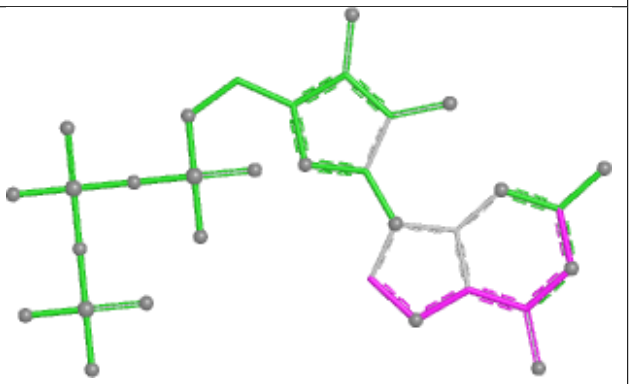

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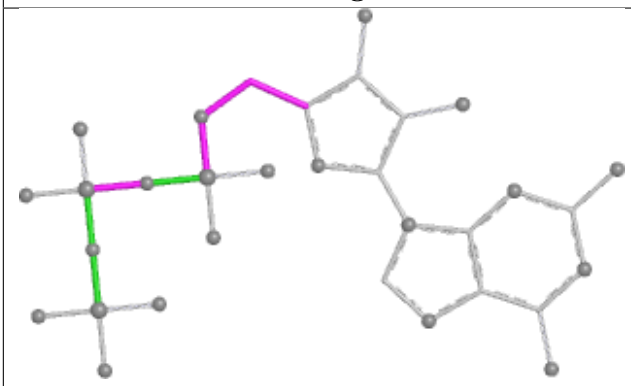

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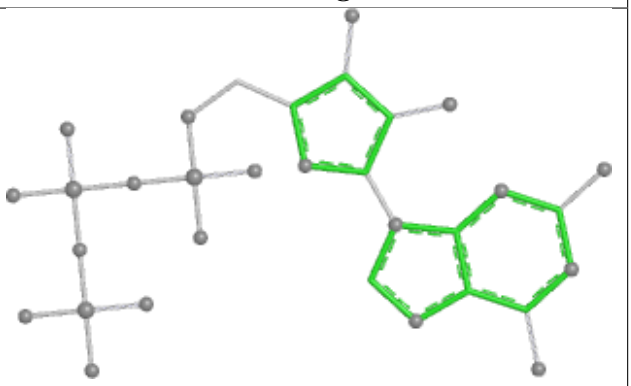
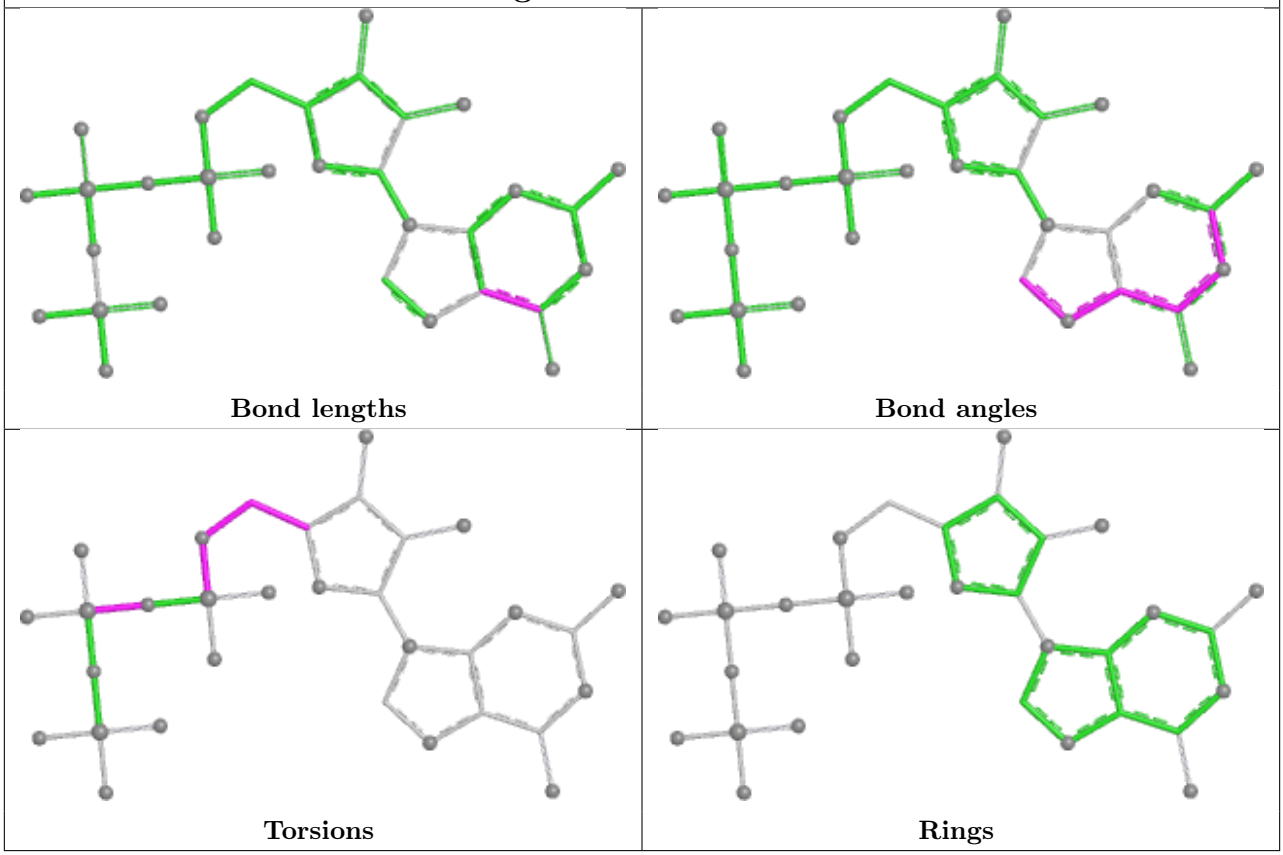


Rings

Ligand GTP Y6 501



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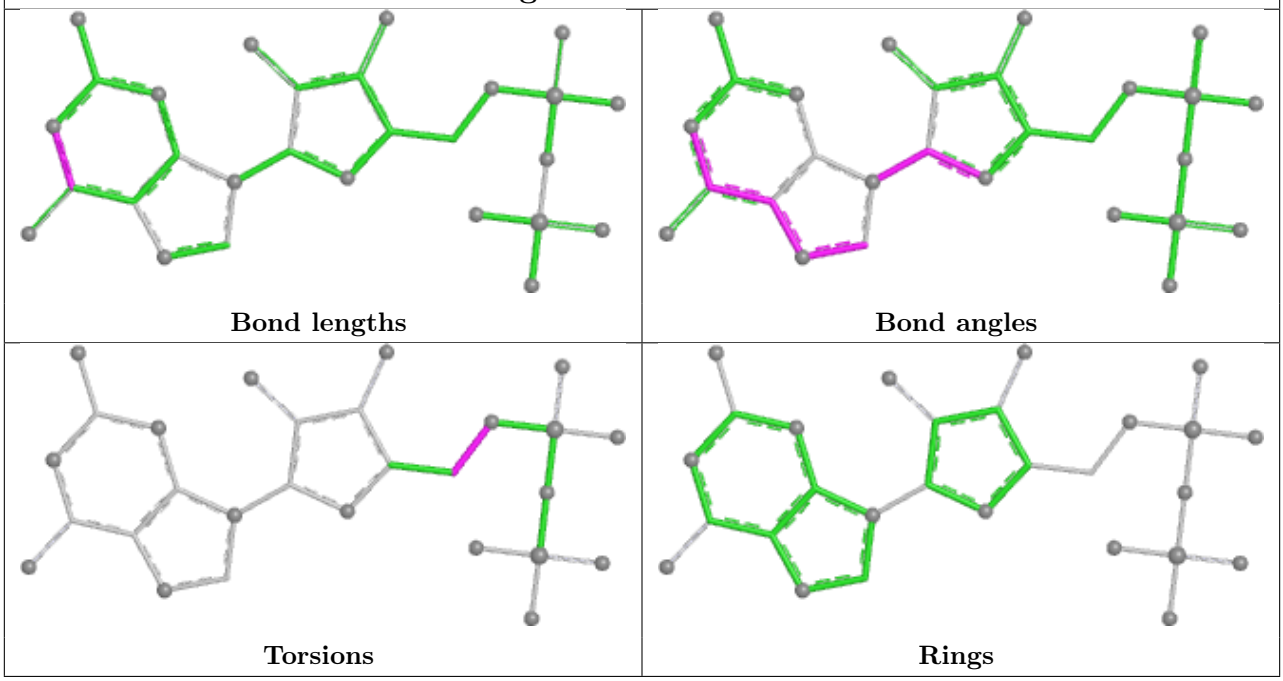
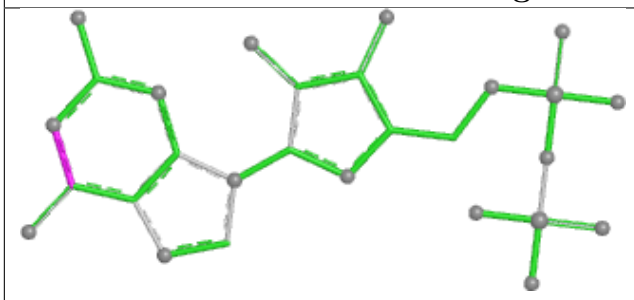


Ligand GDP Q0 501



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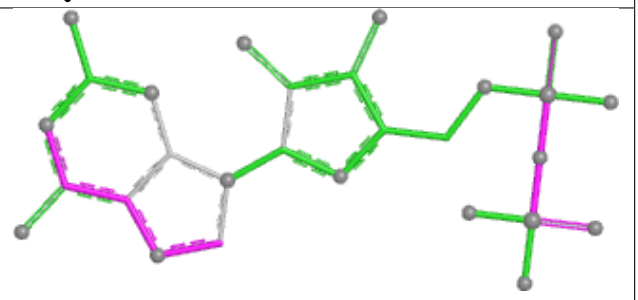
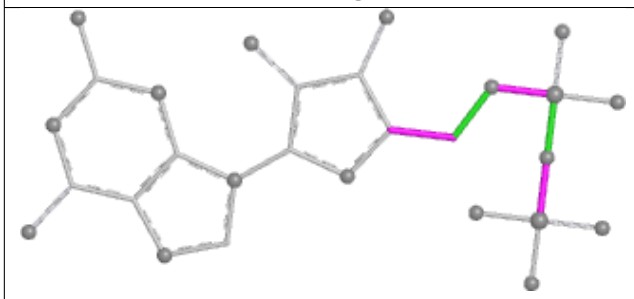


Bond angles



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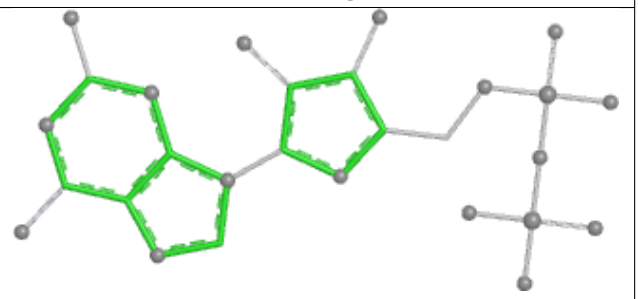
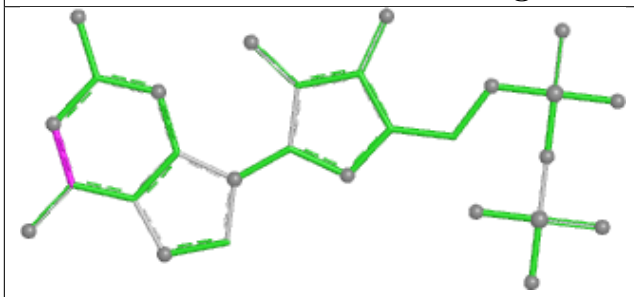


Rings

Ligand GDP Y4 502



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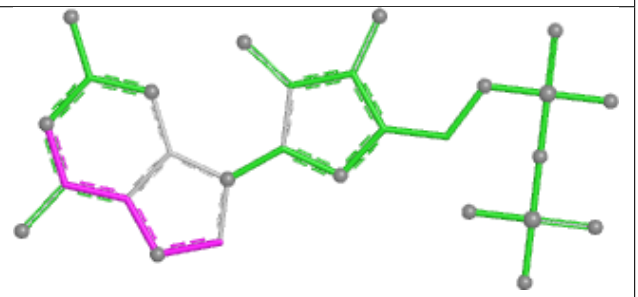

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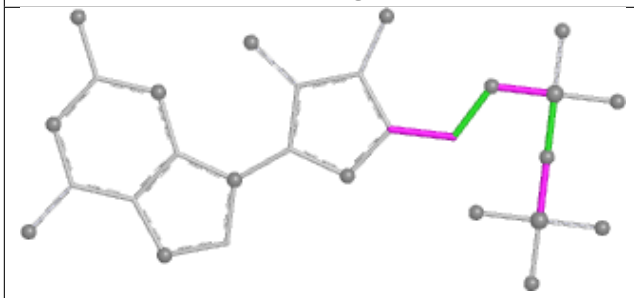
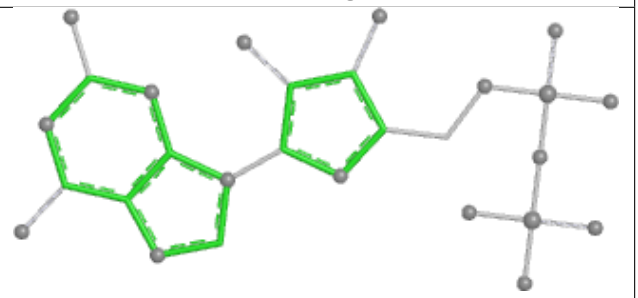
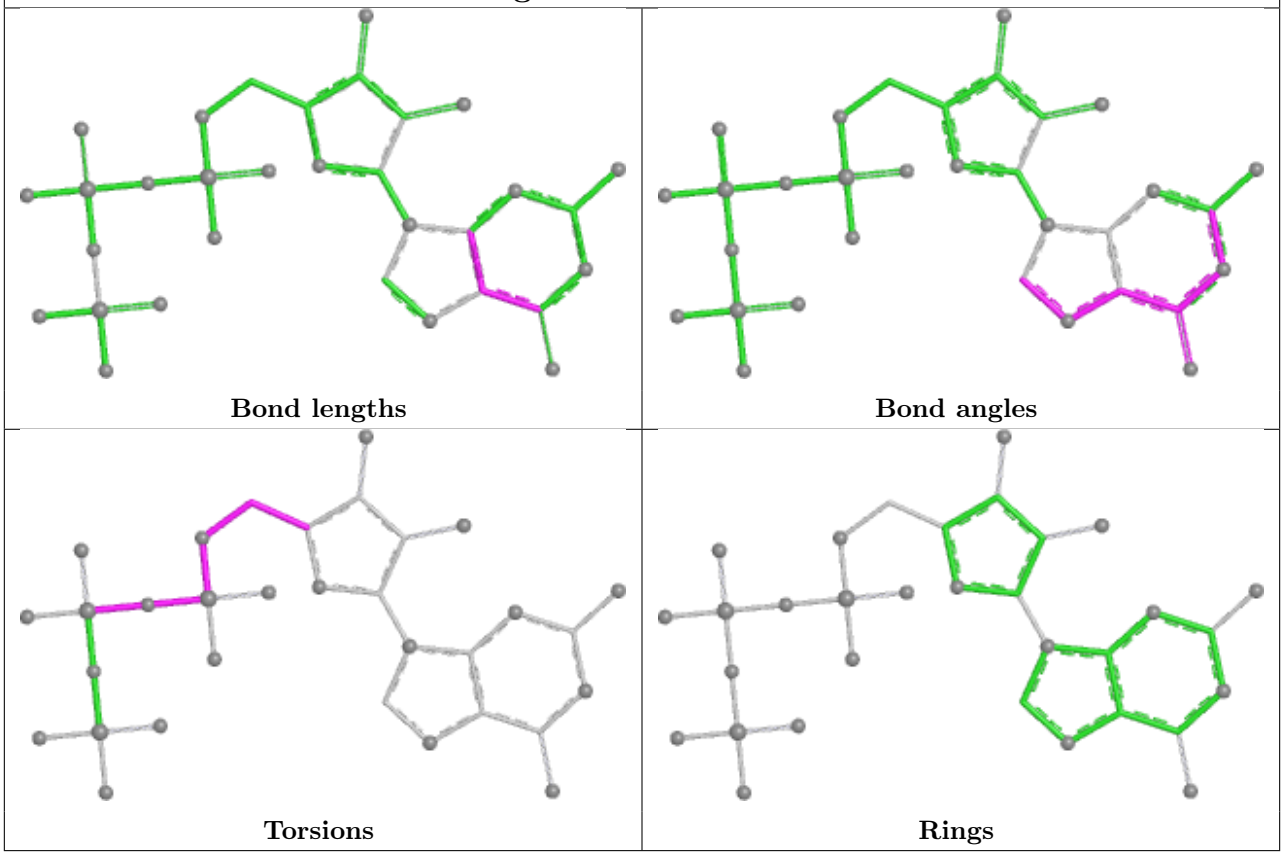


Torsions

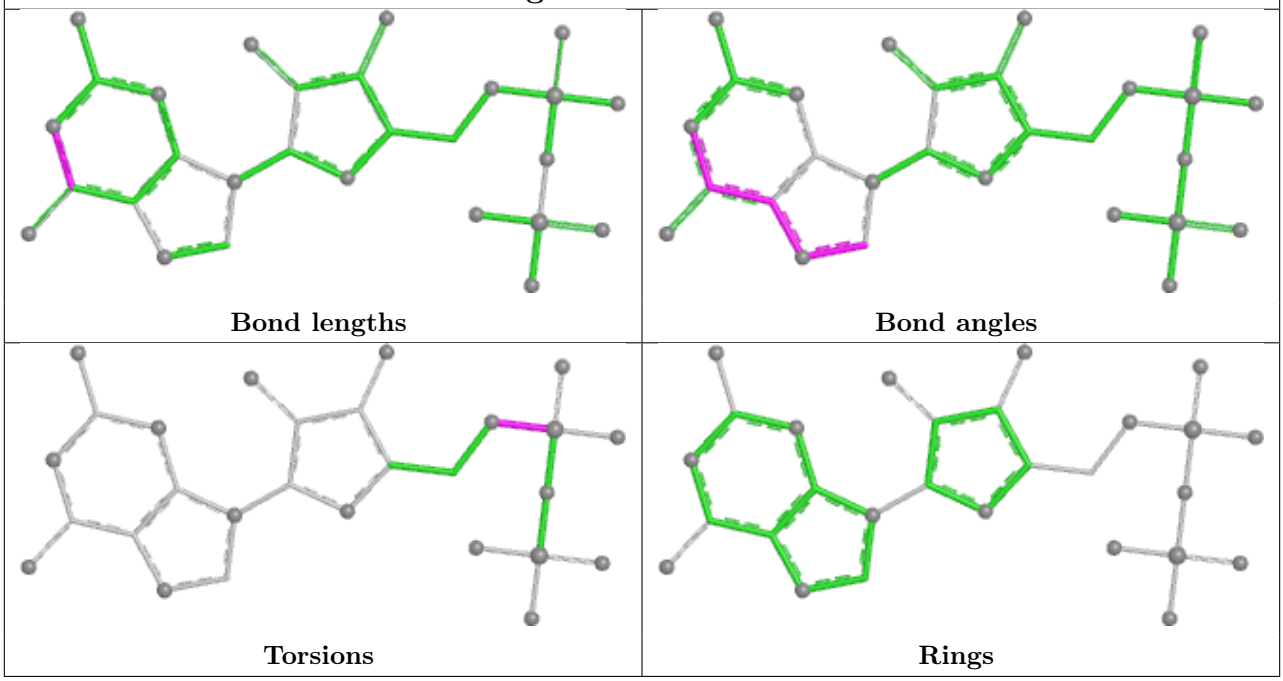


Rings

Ligand GTP N6 501



Ligand GDP 3 502



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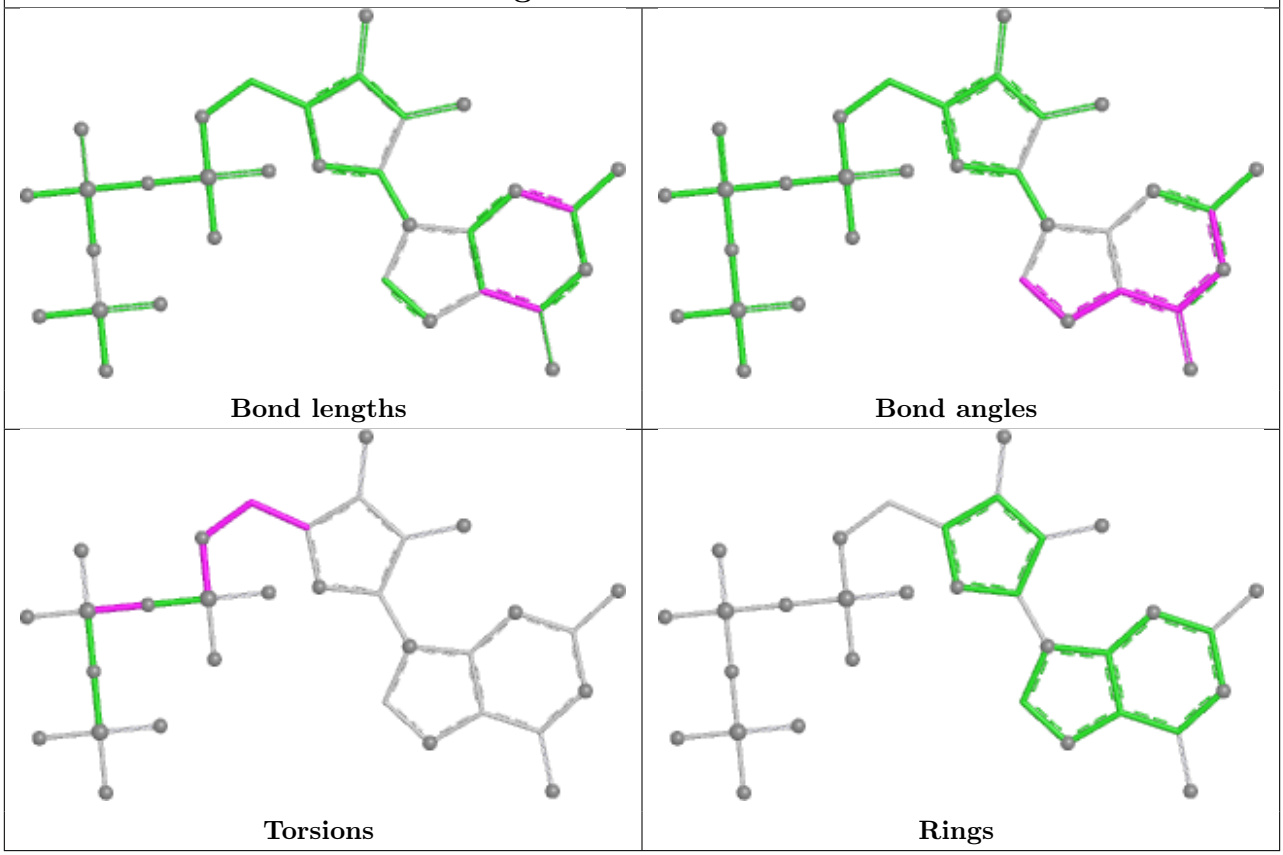
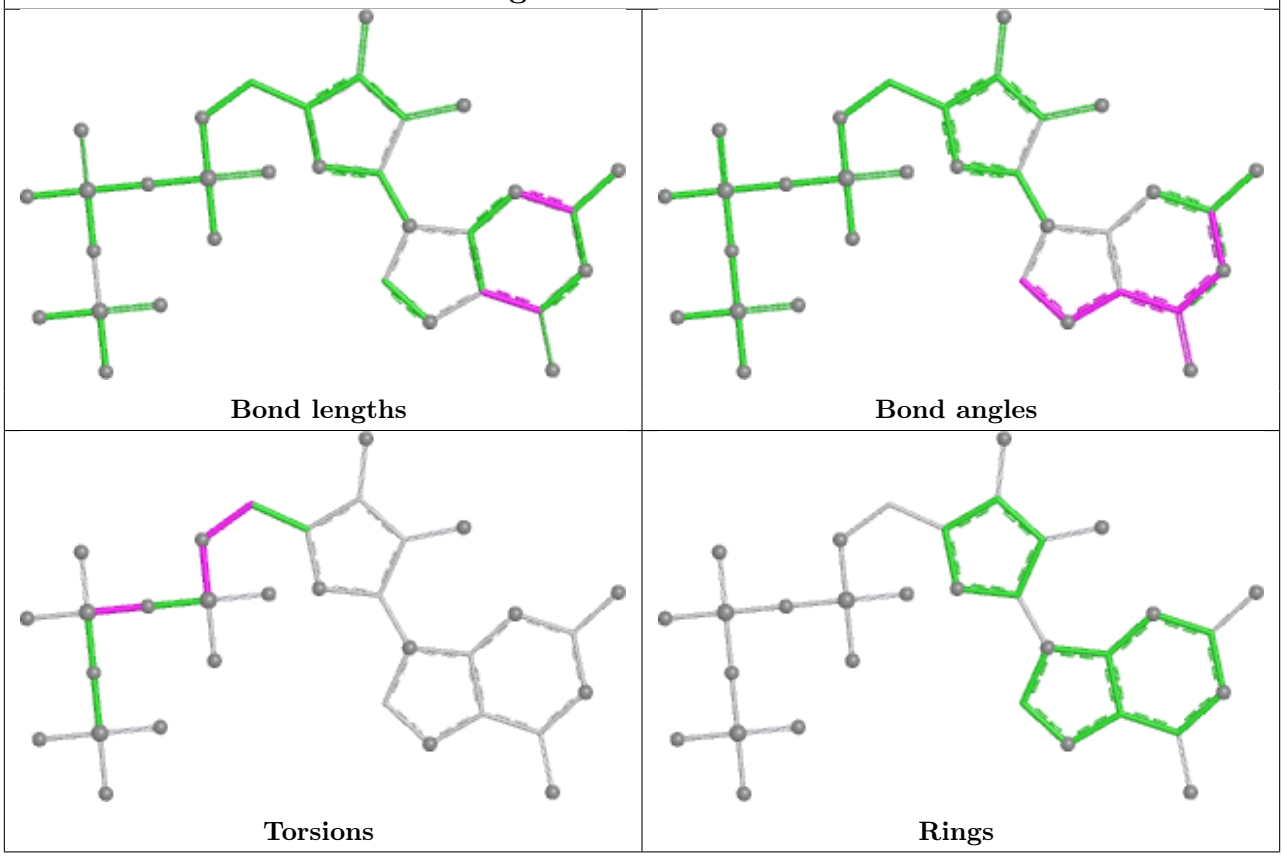


Ligand GTP W5 501



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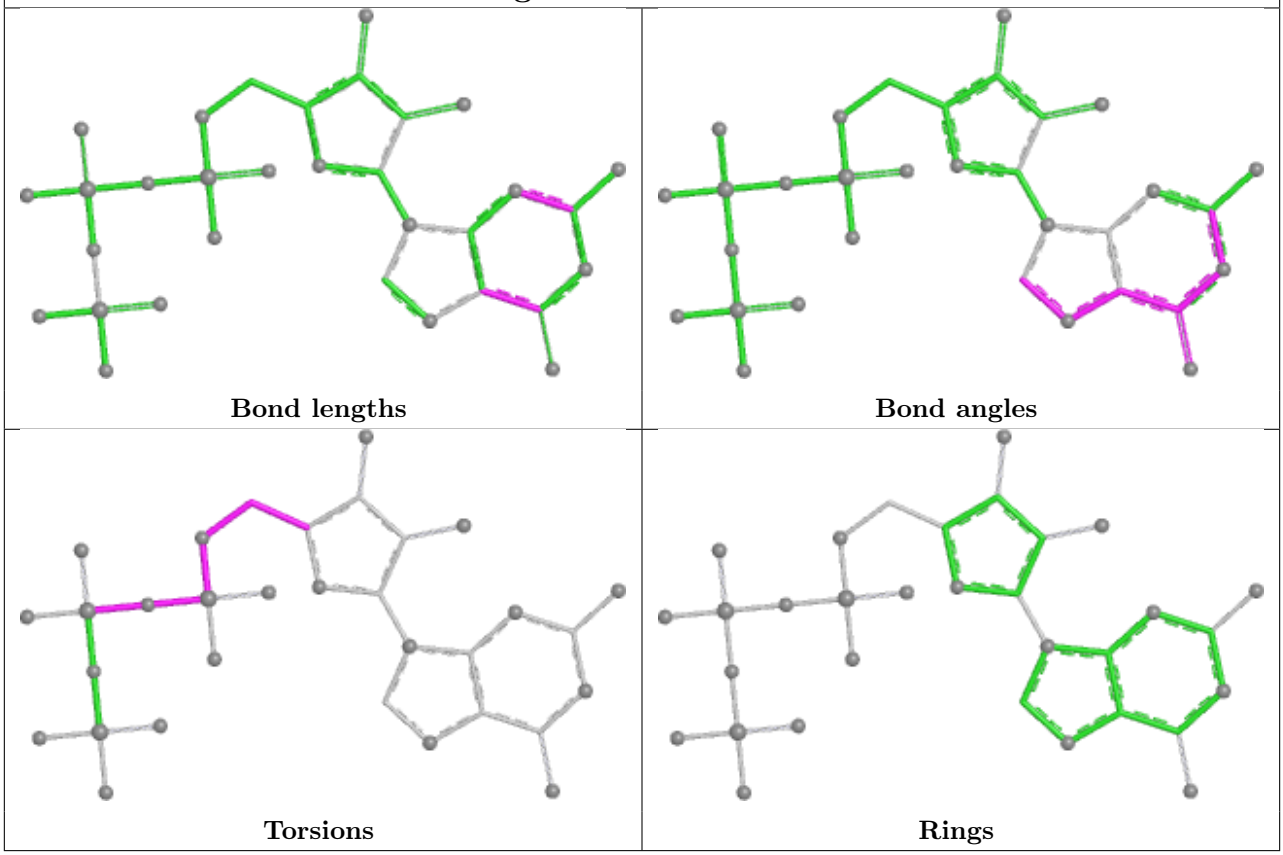

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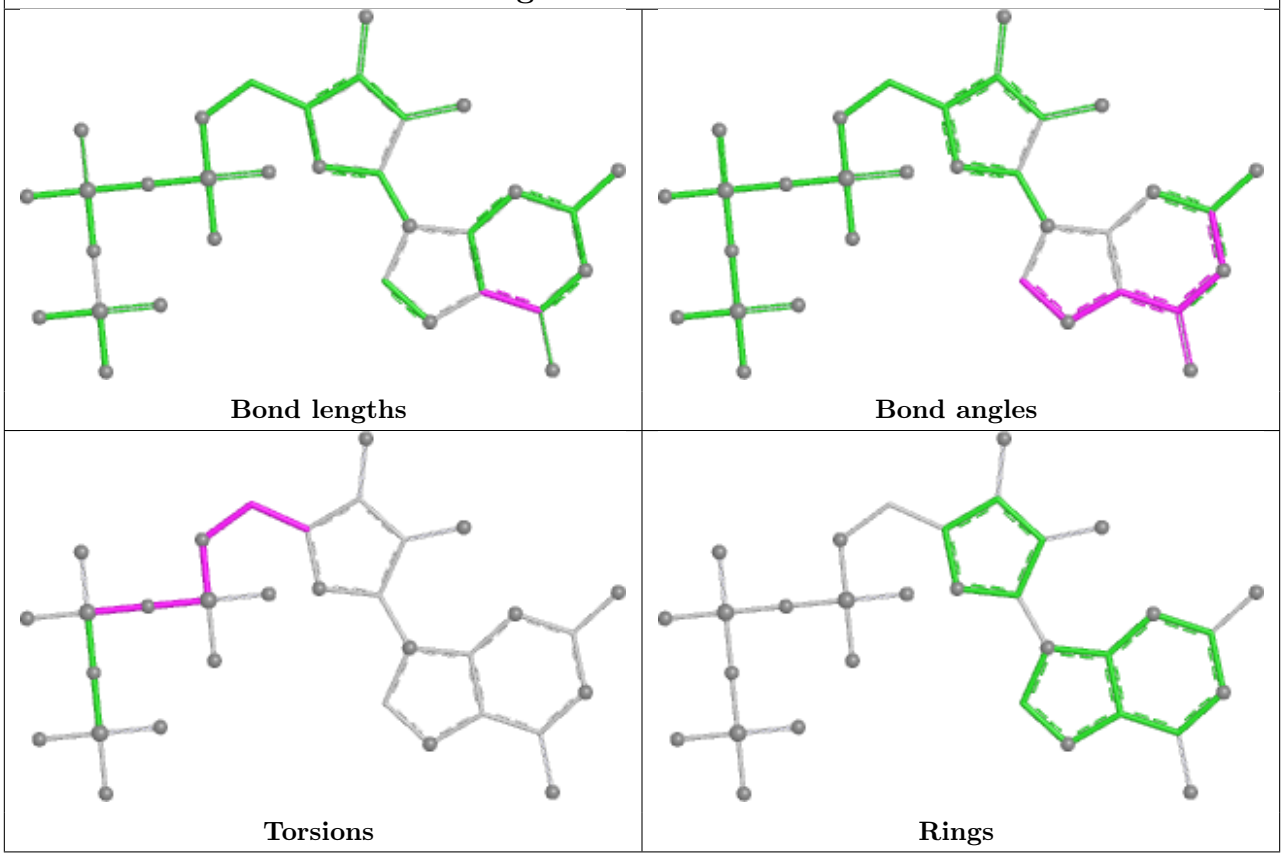

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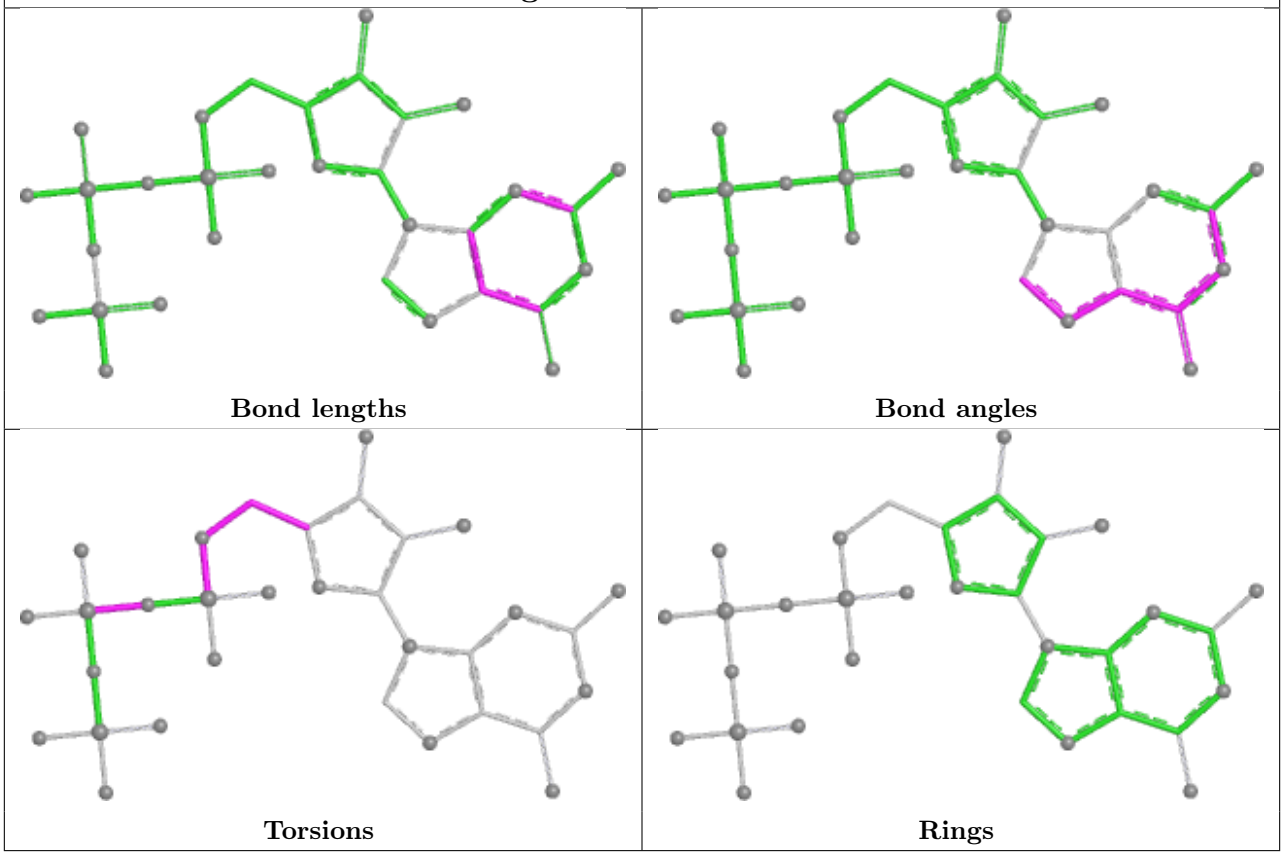
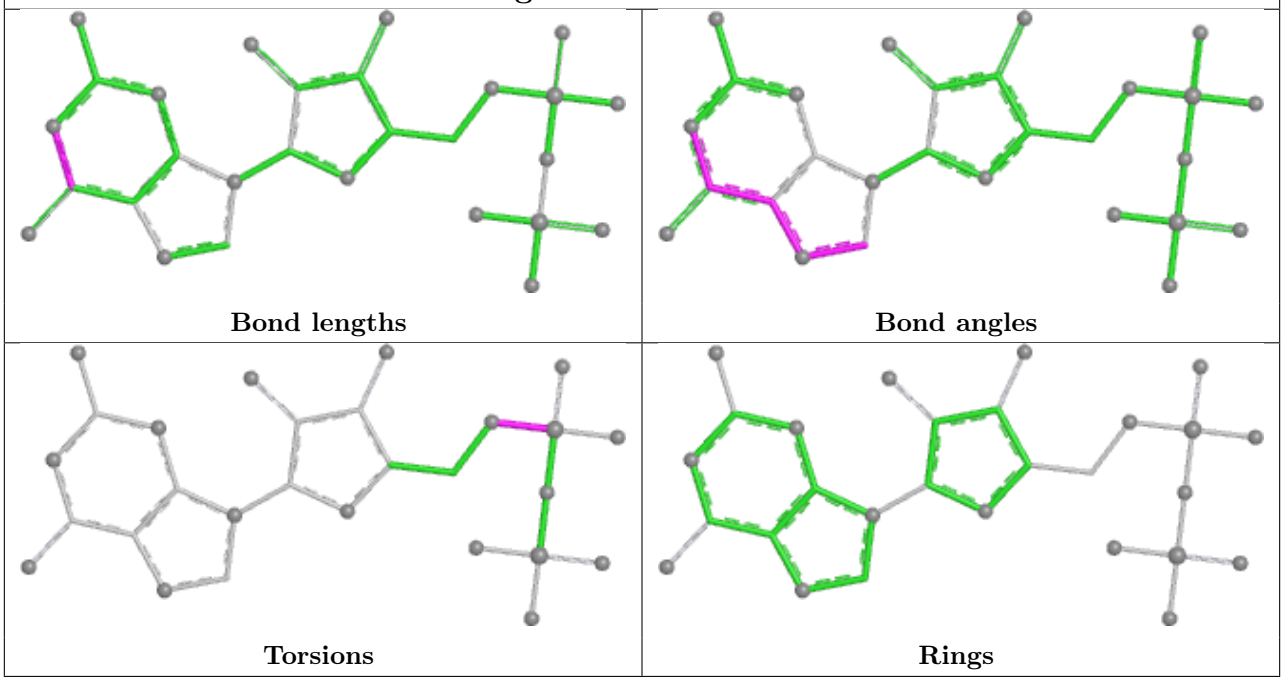


Ligand GDP F8 502



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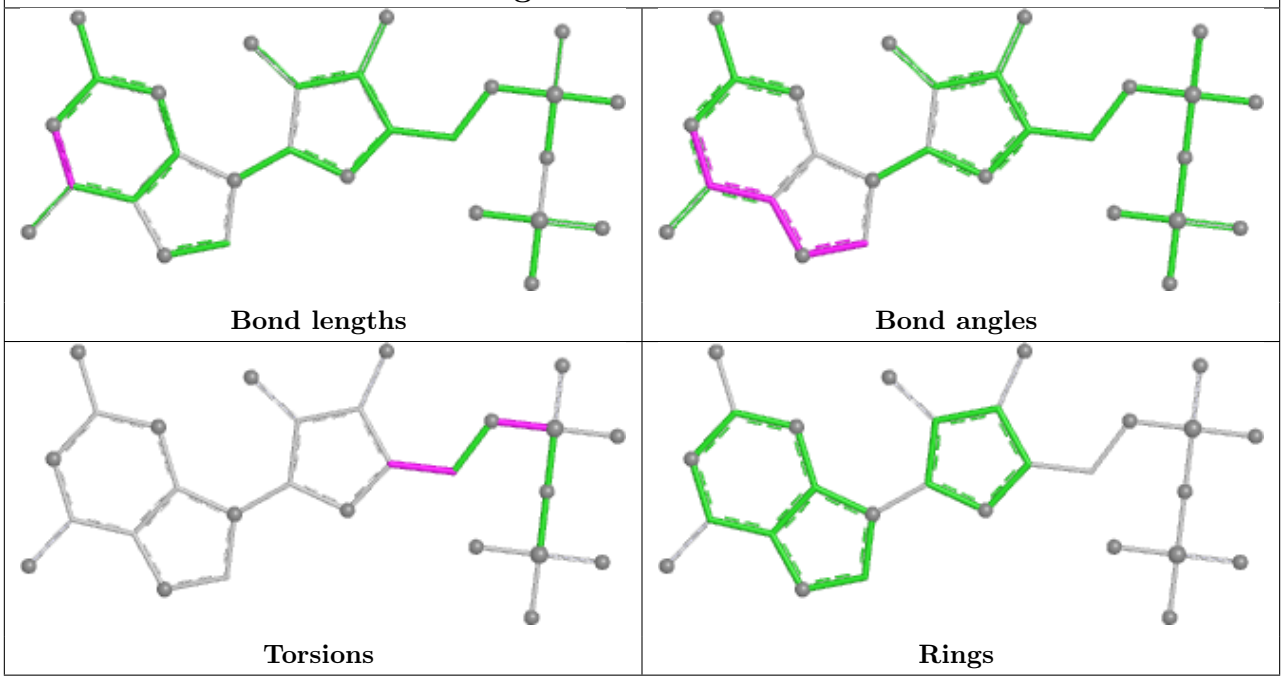

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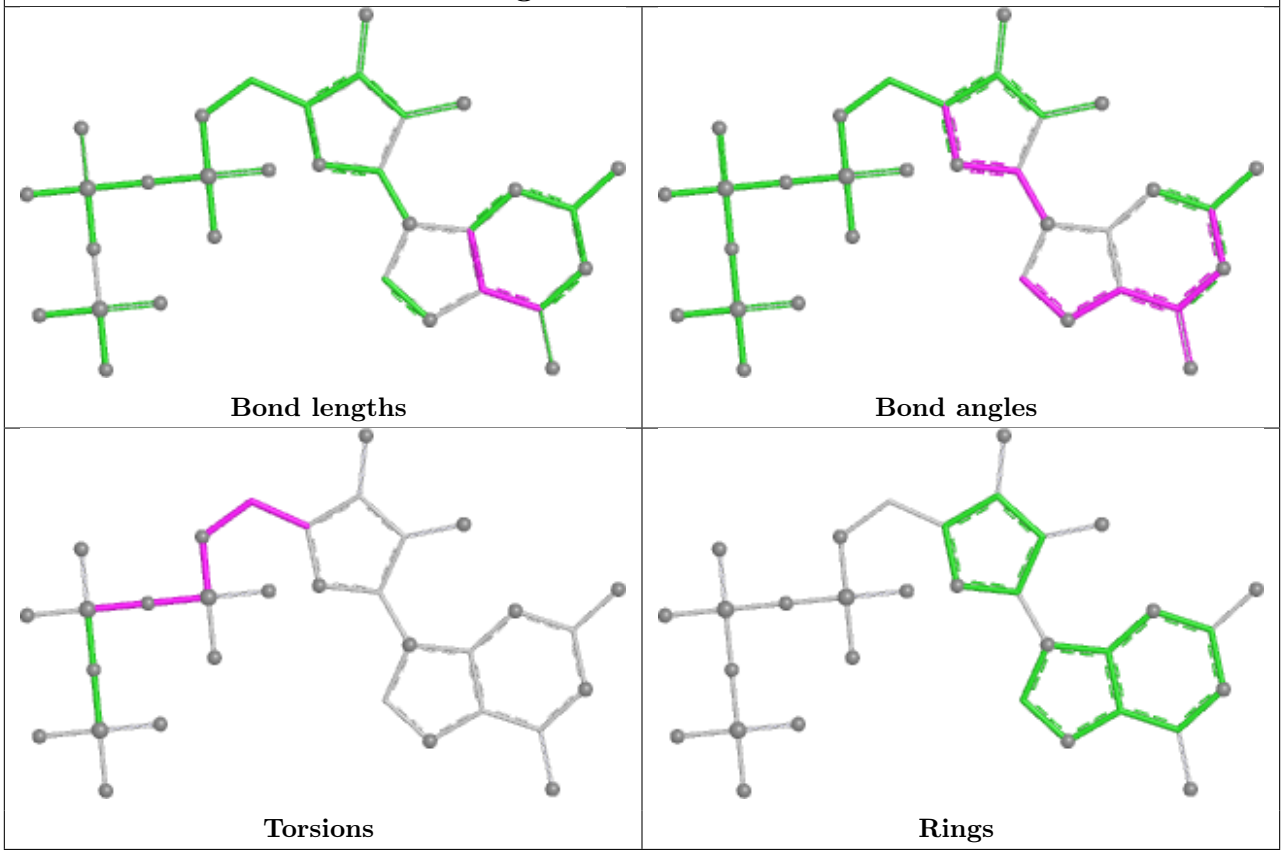
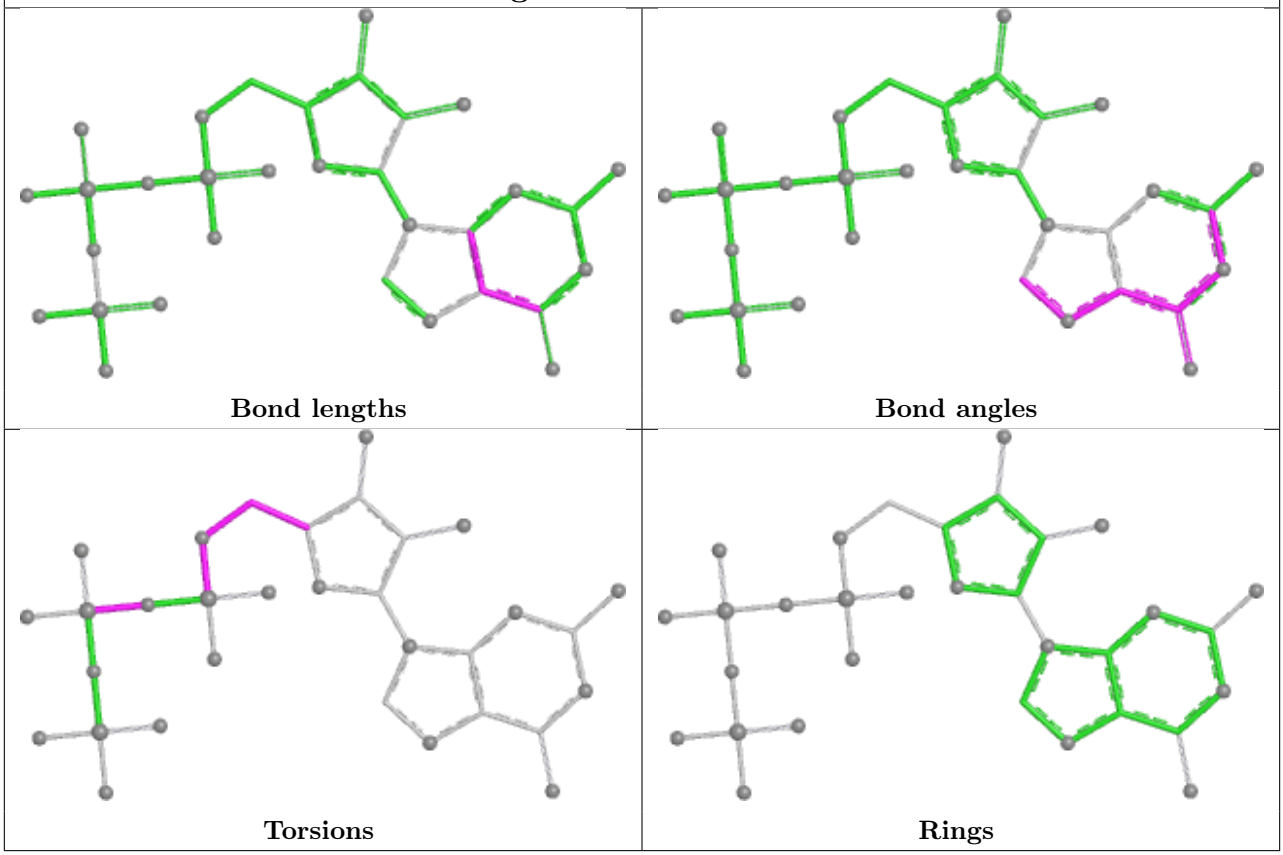


Ligand GTP M6 501



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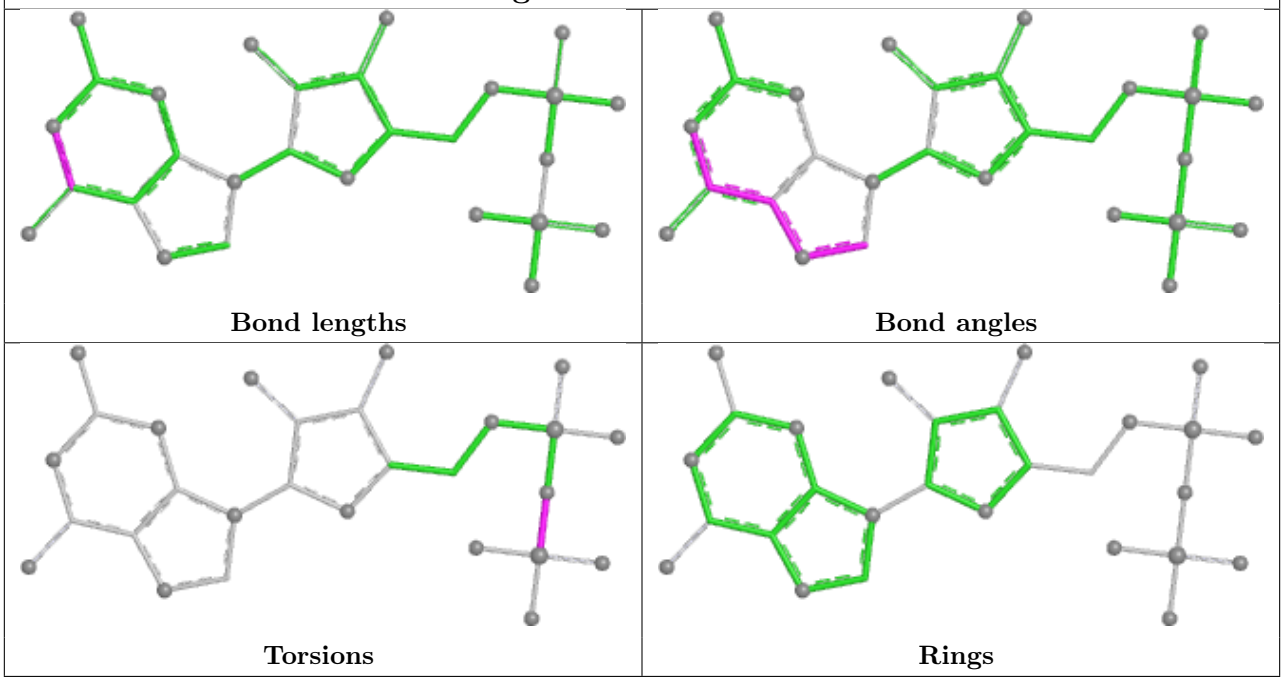

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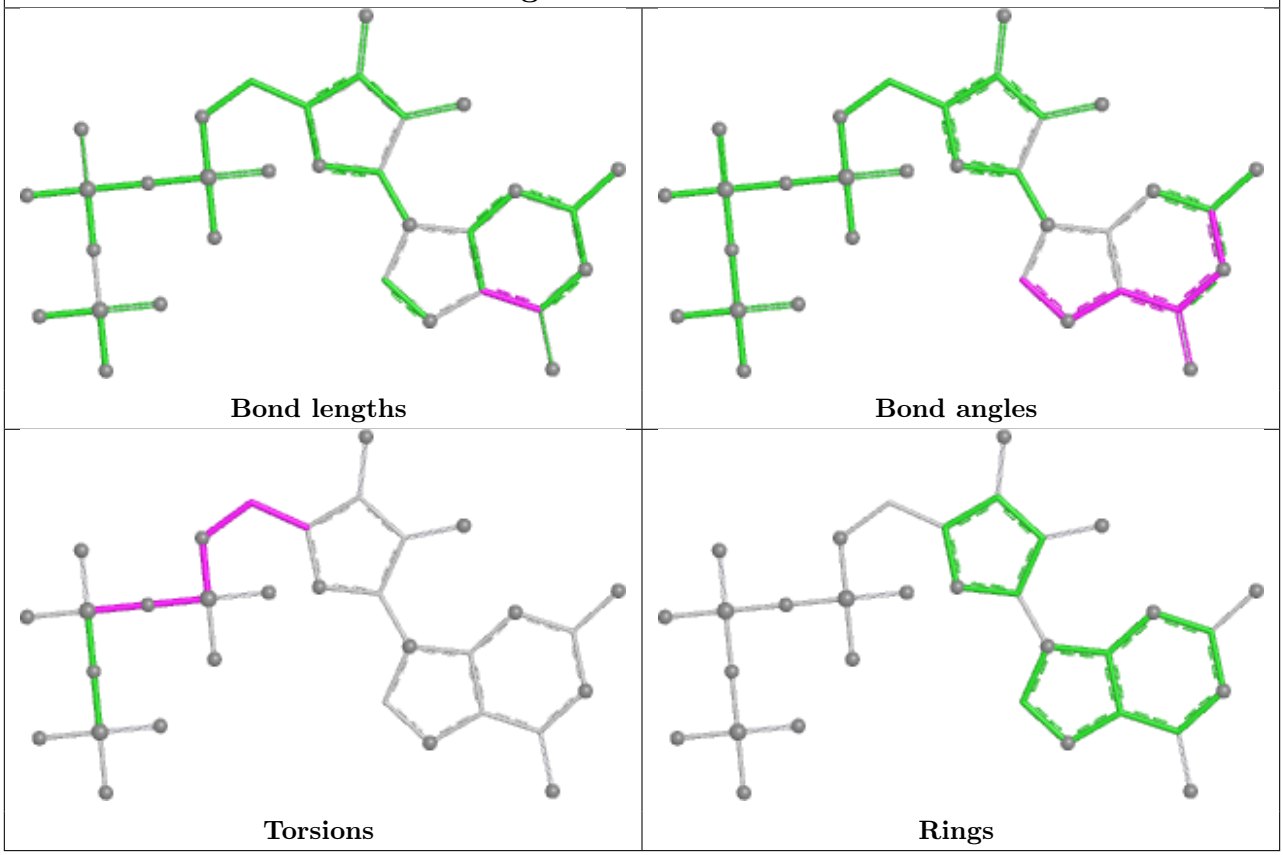

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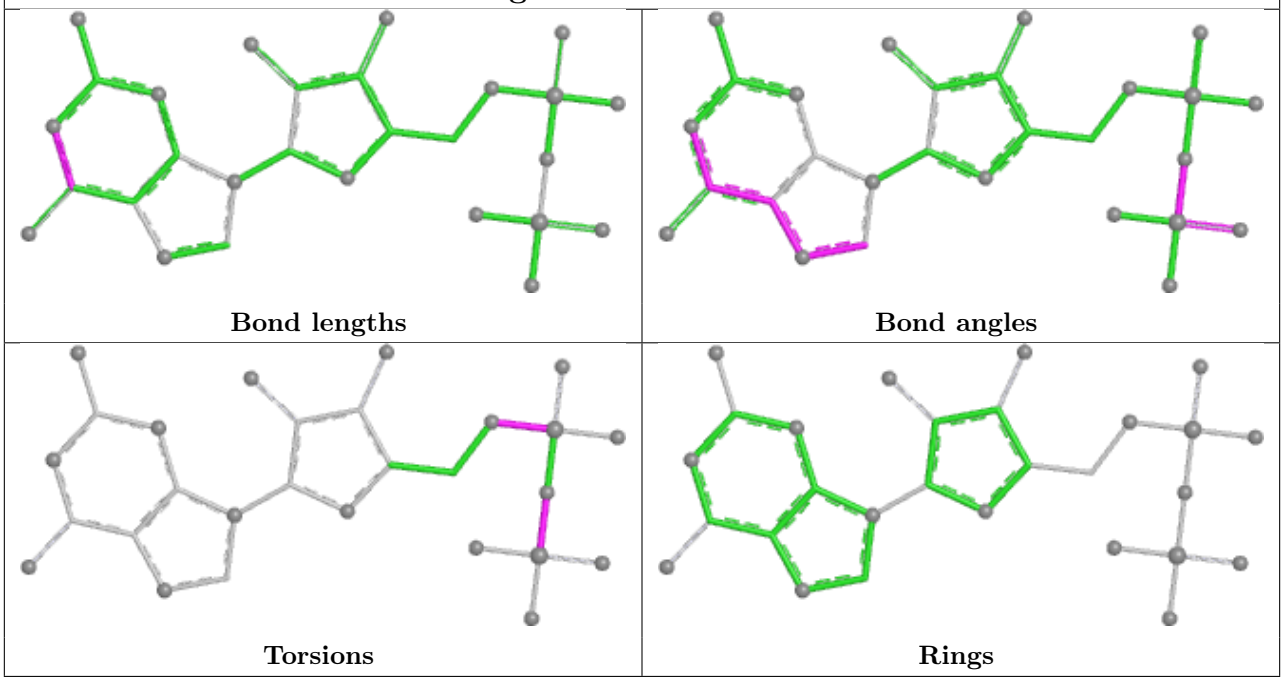

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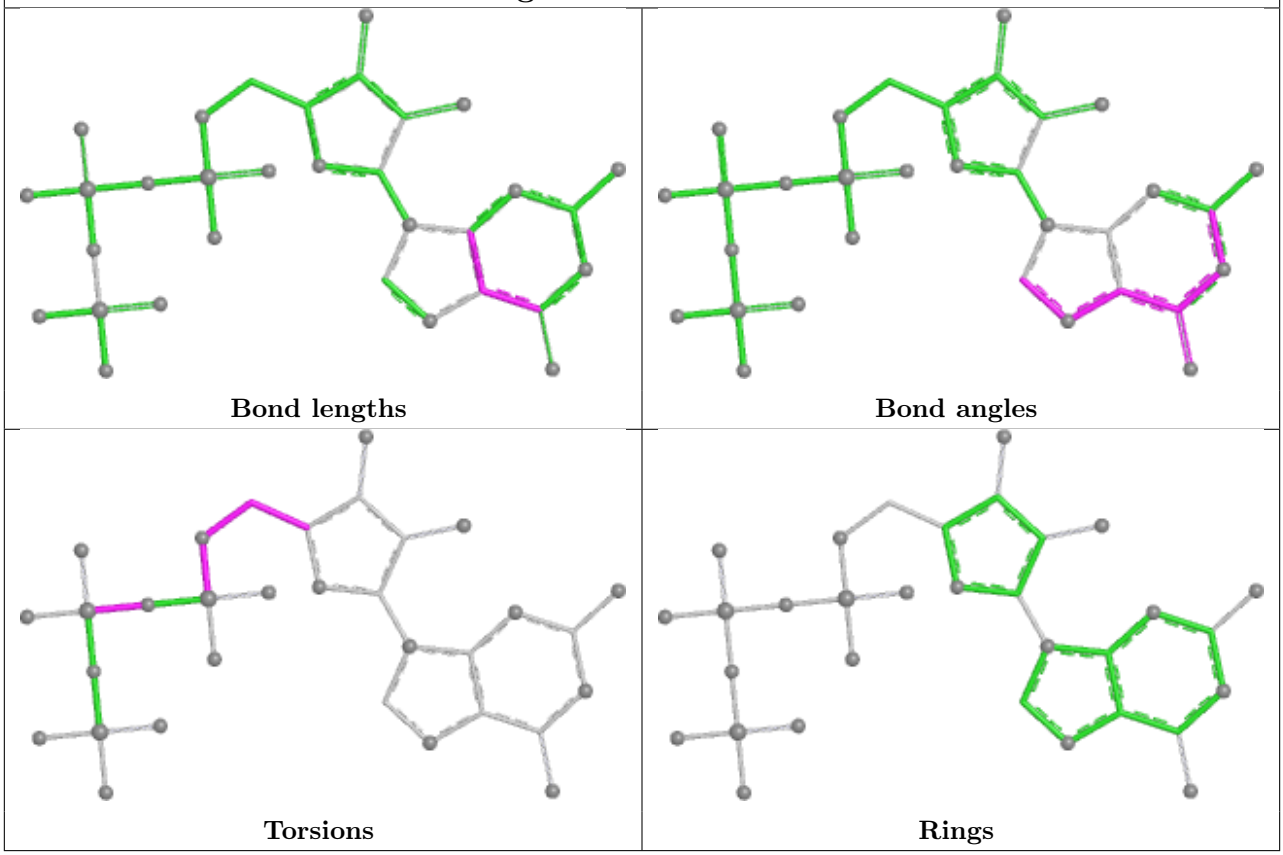

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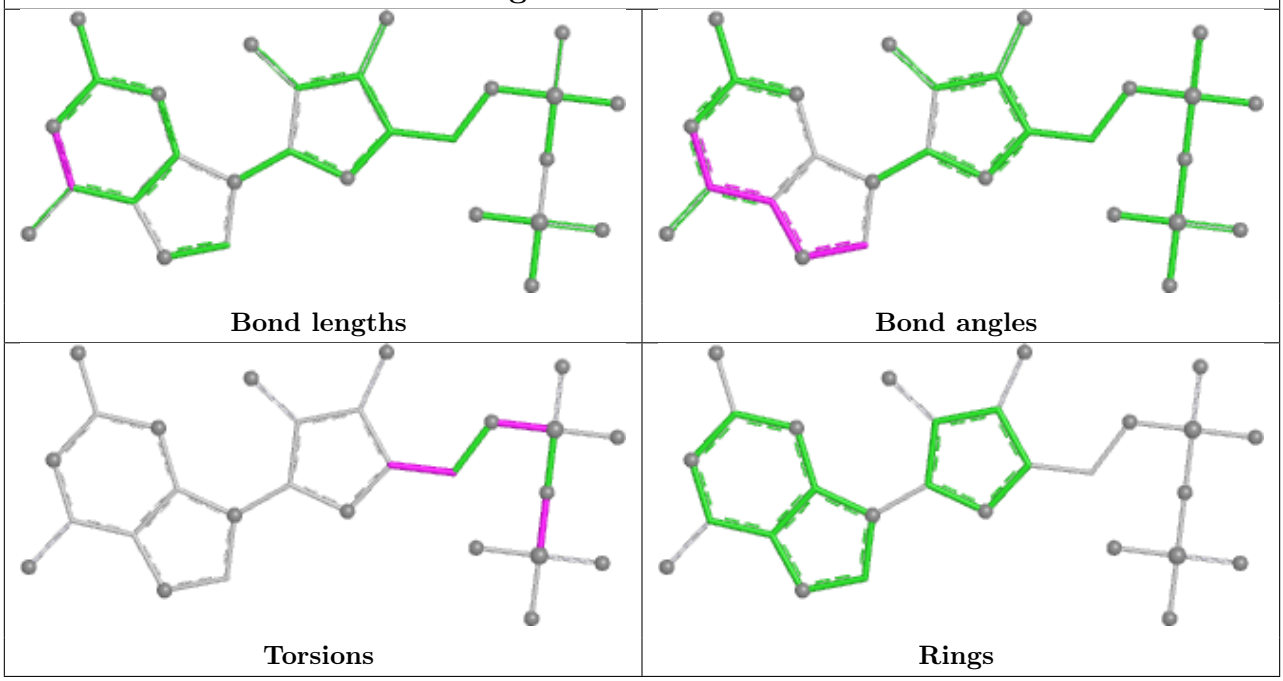

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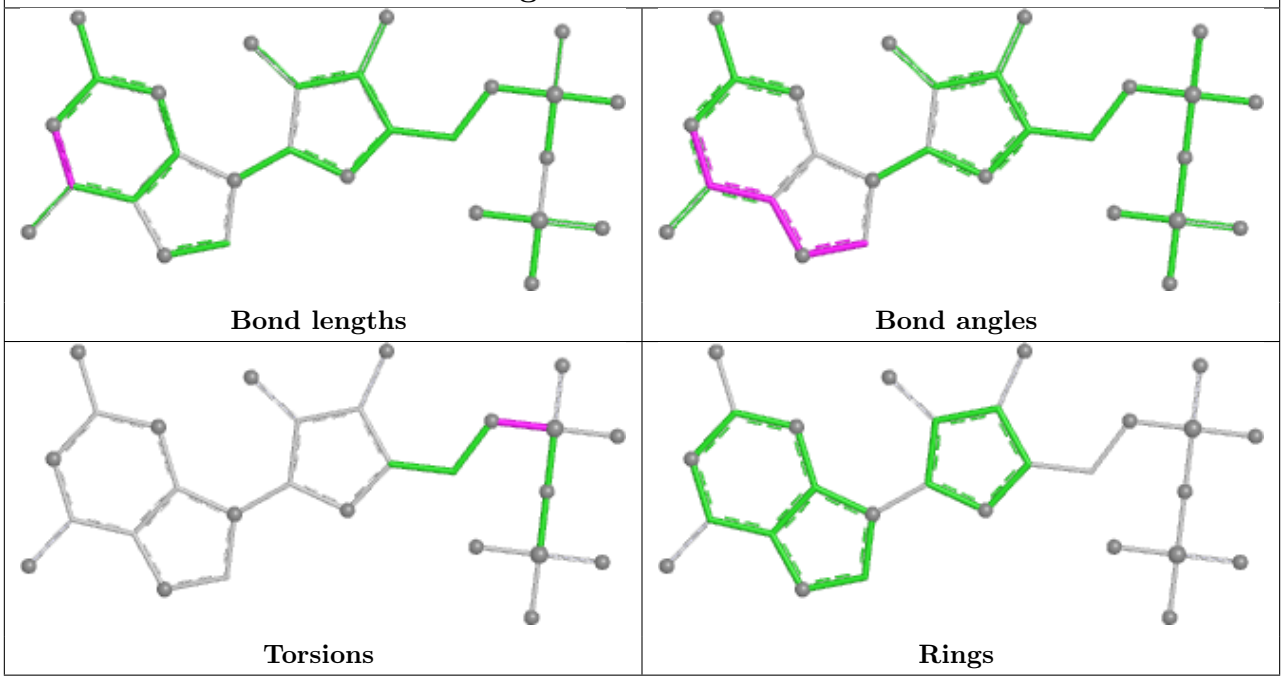

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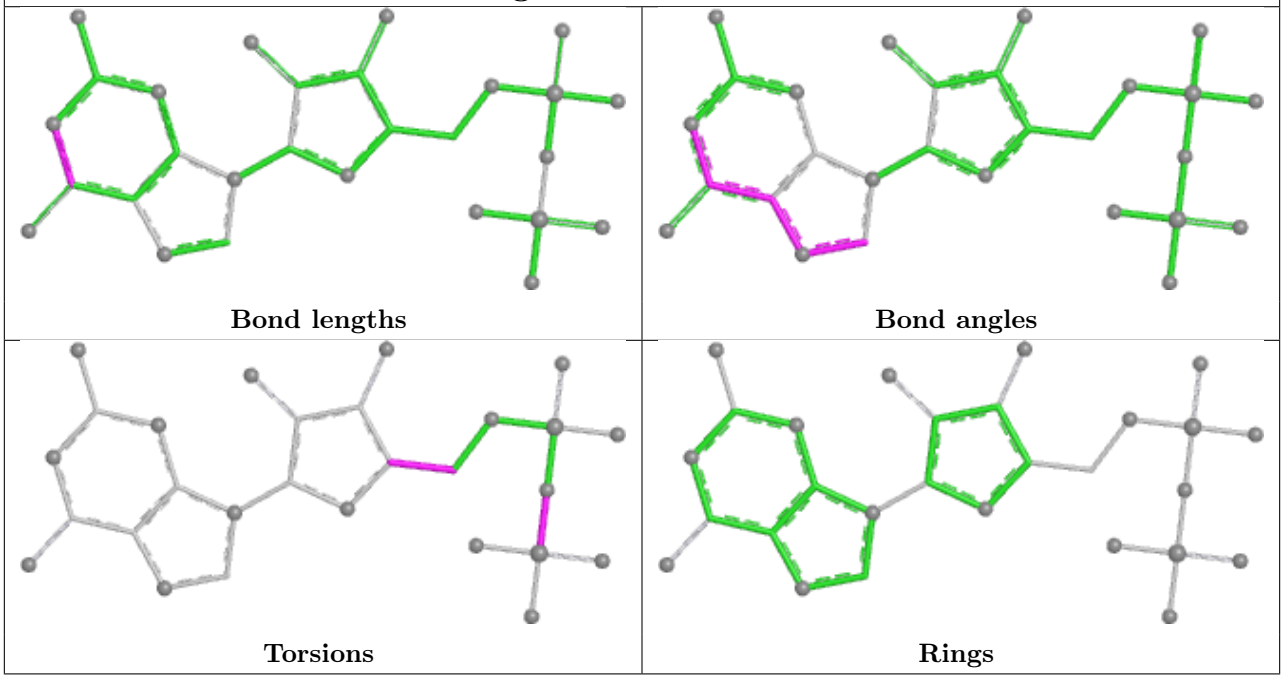

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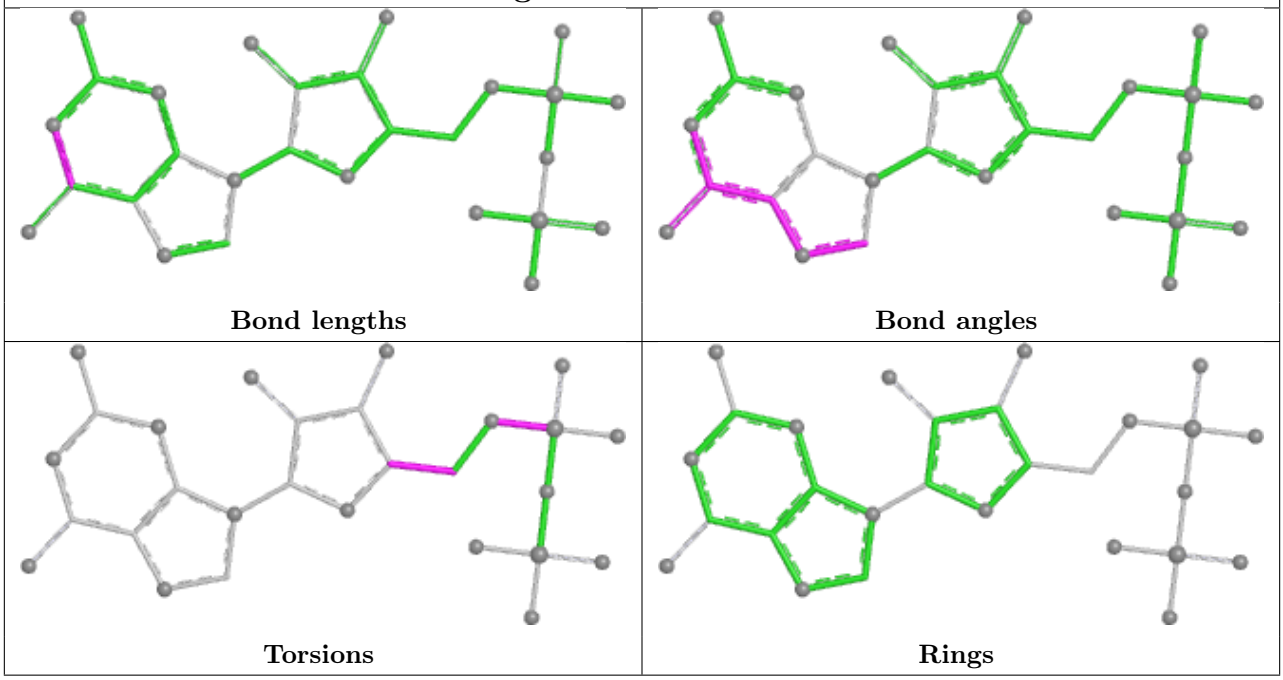

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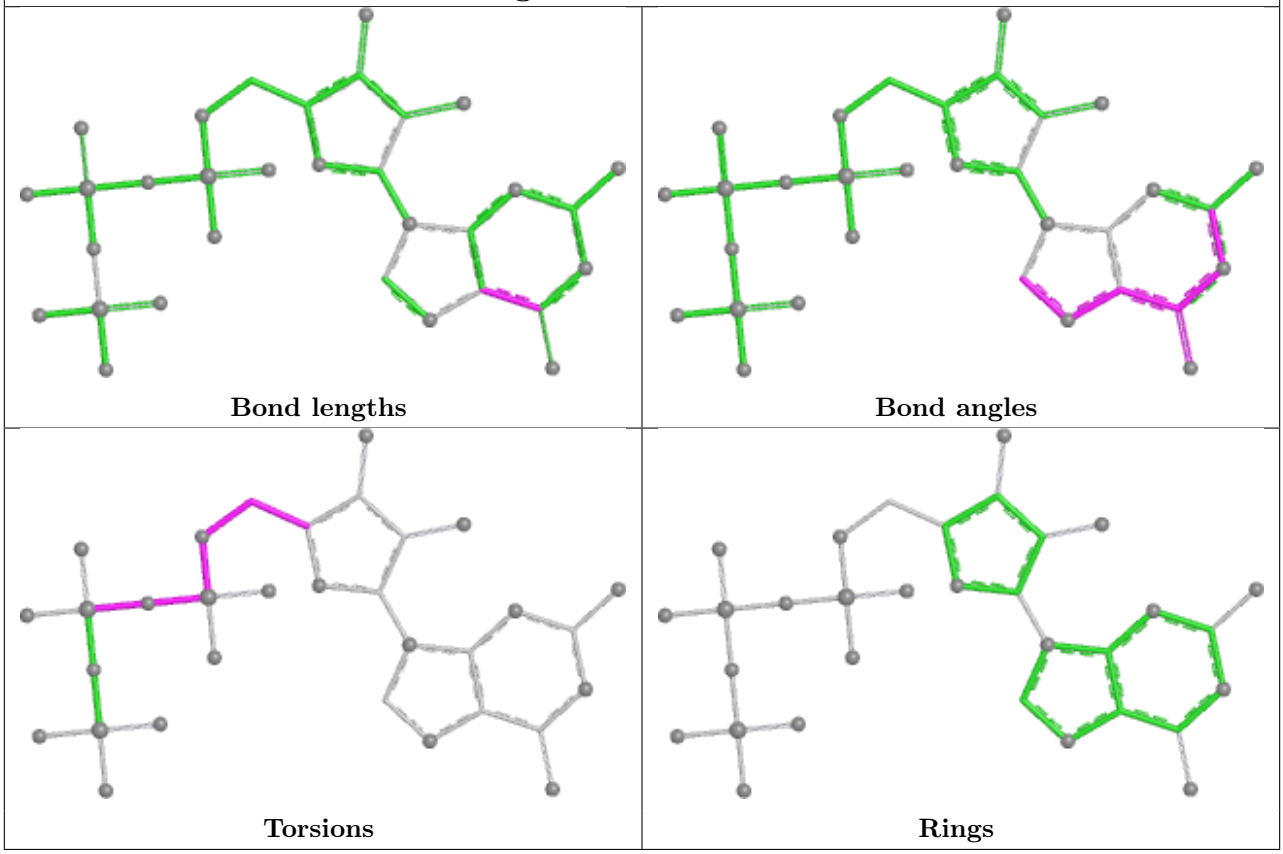

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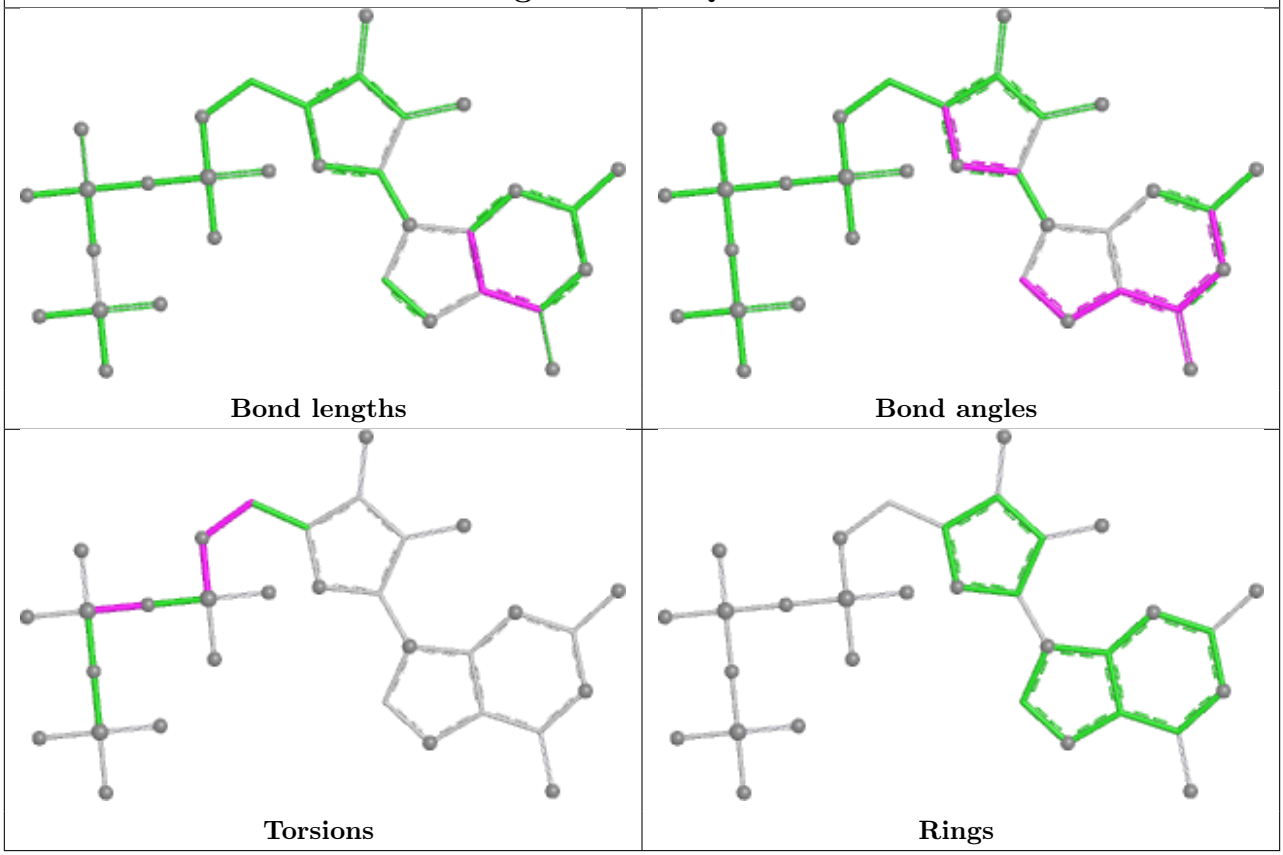
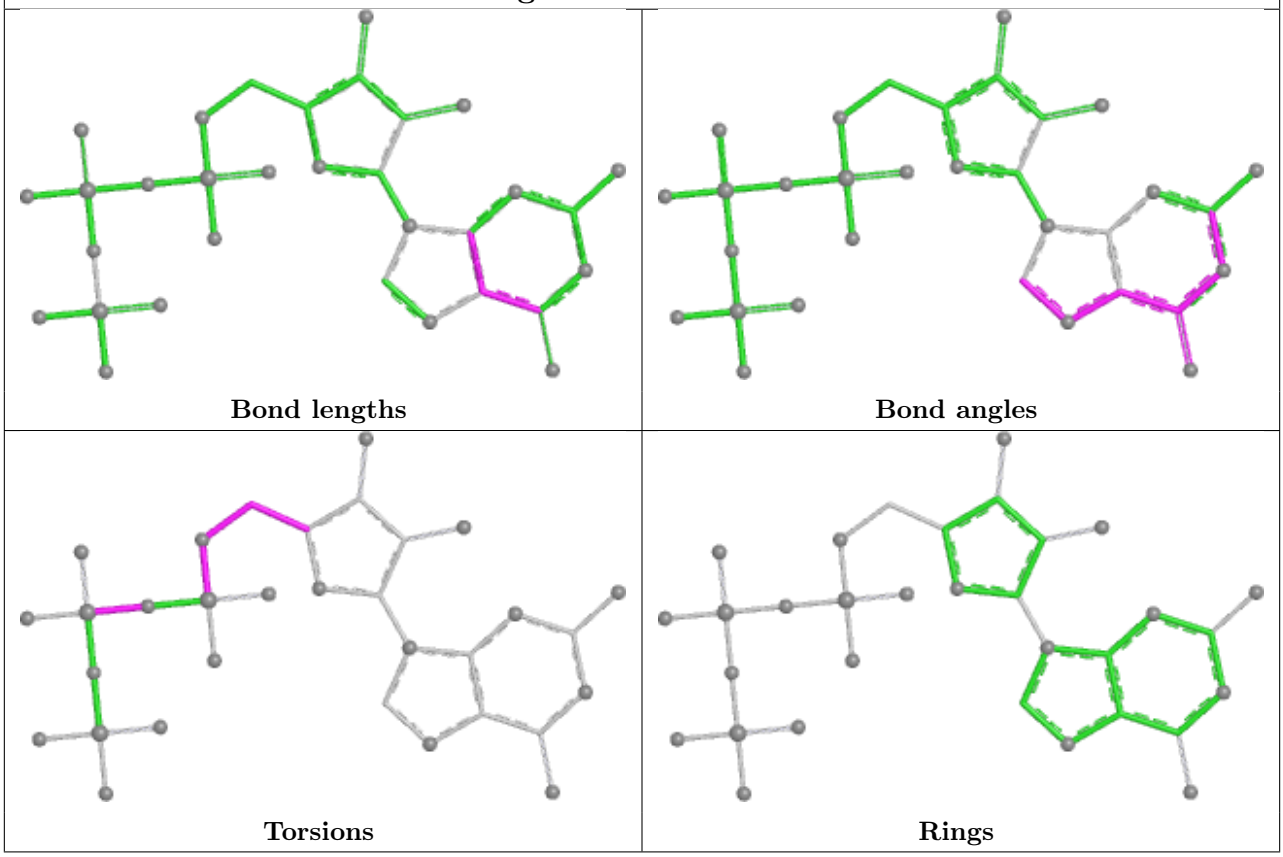


Ligand GTP S8 501



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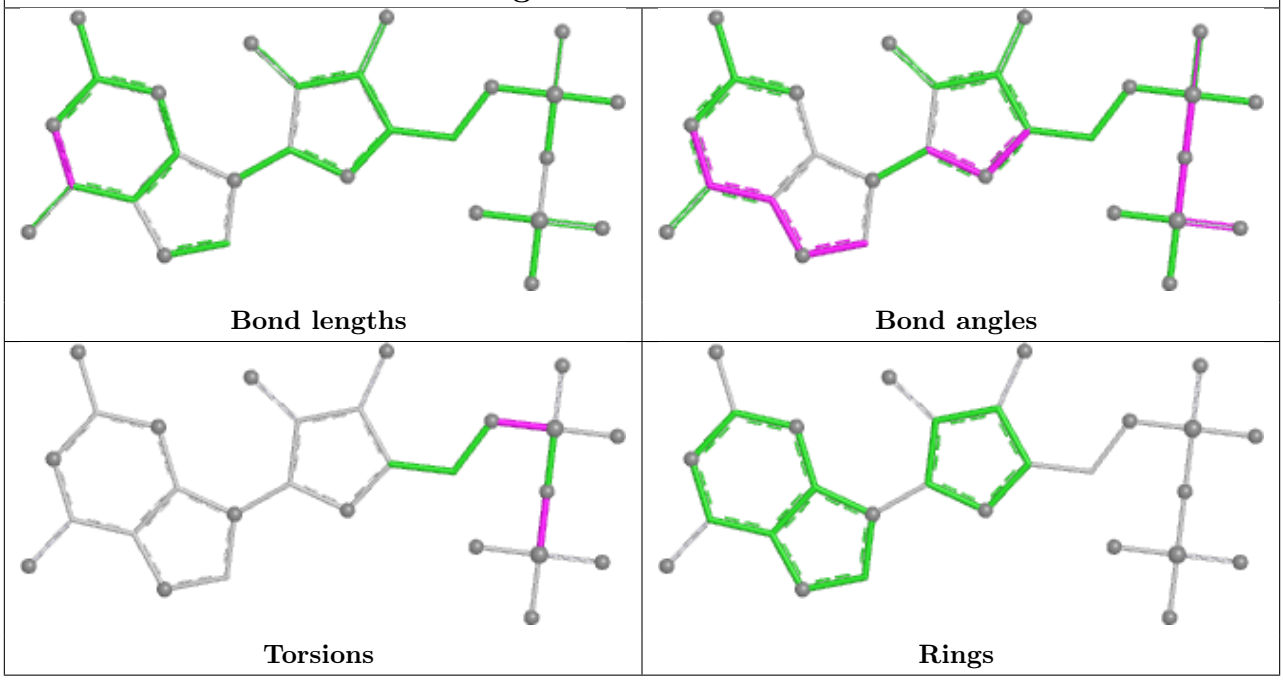

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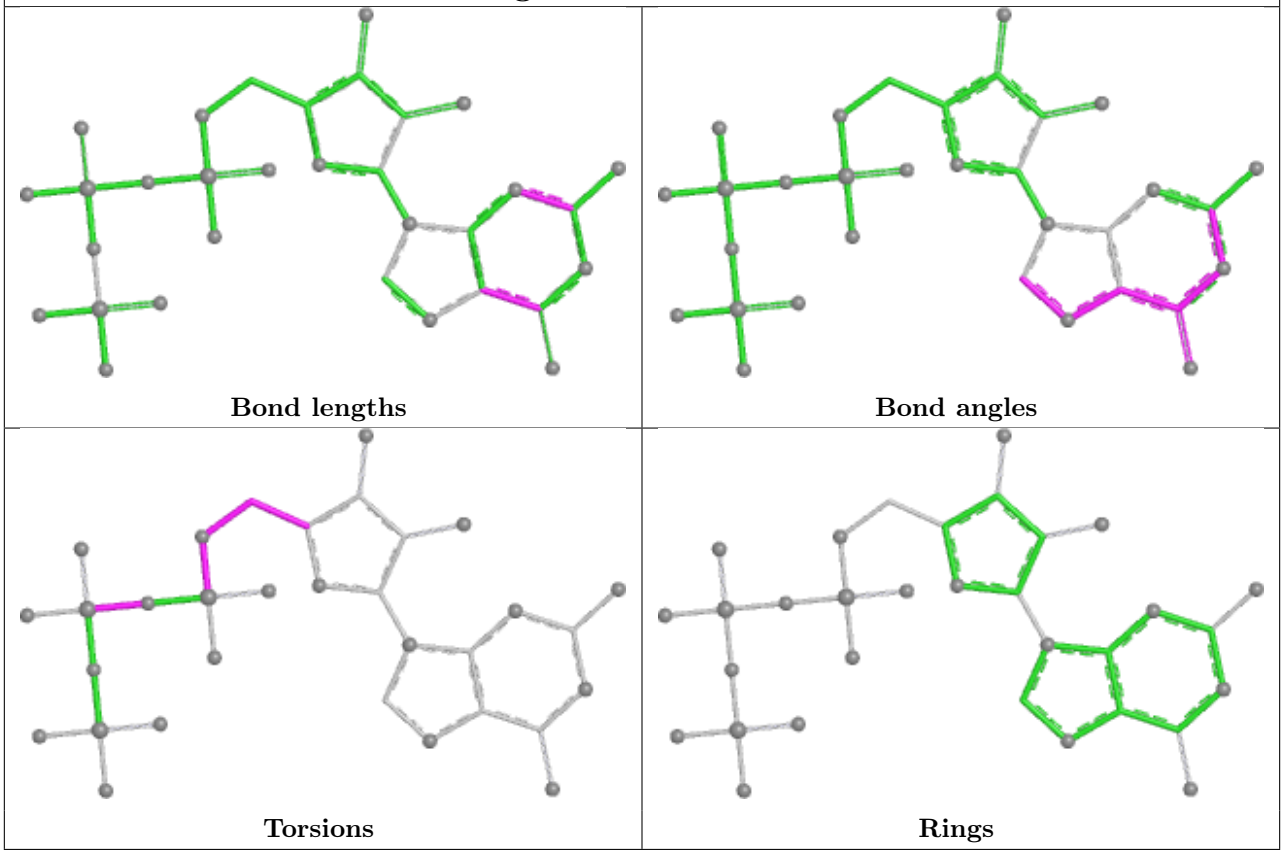

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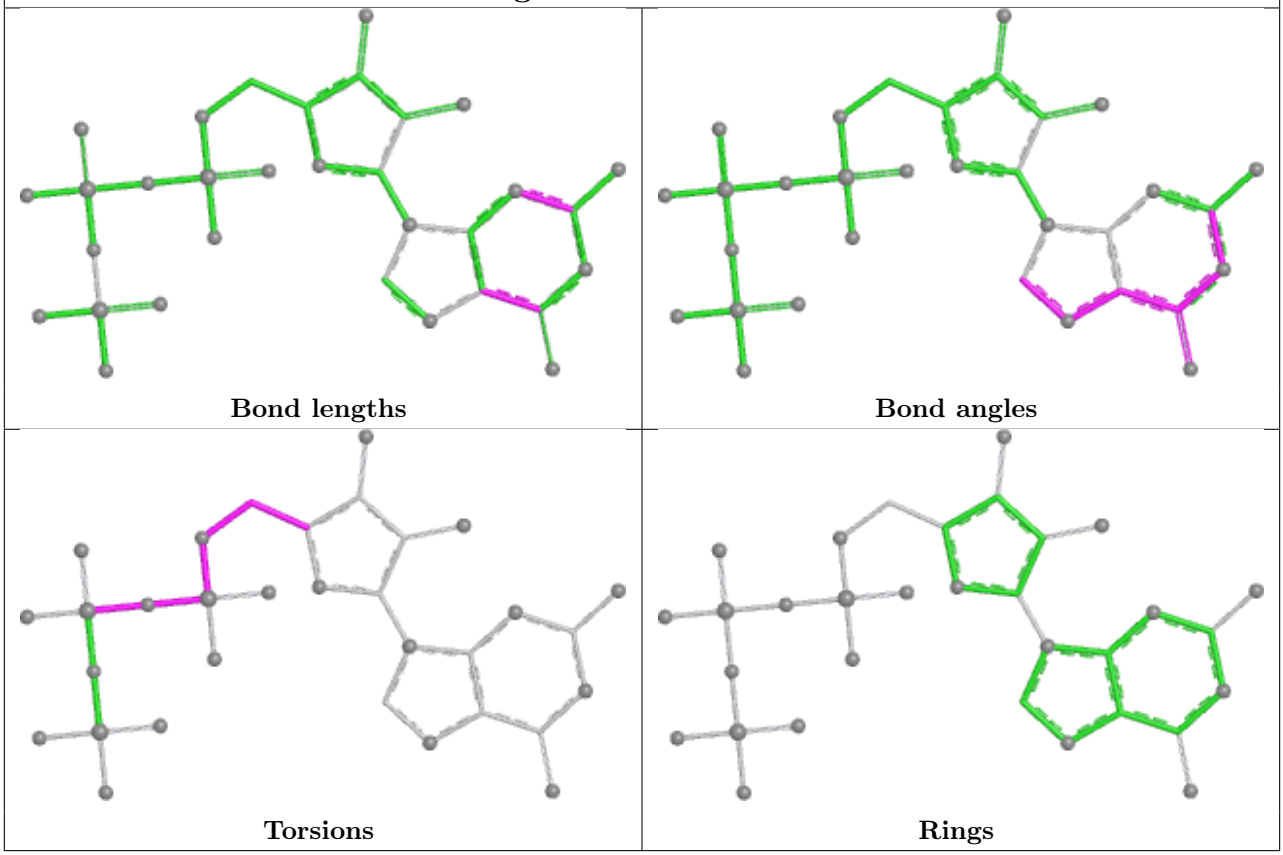

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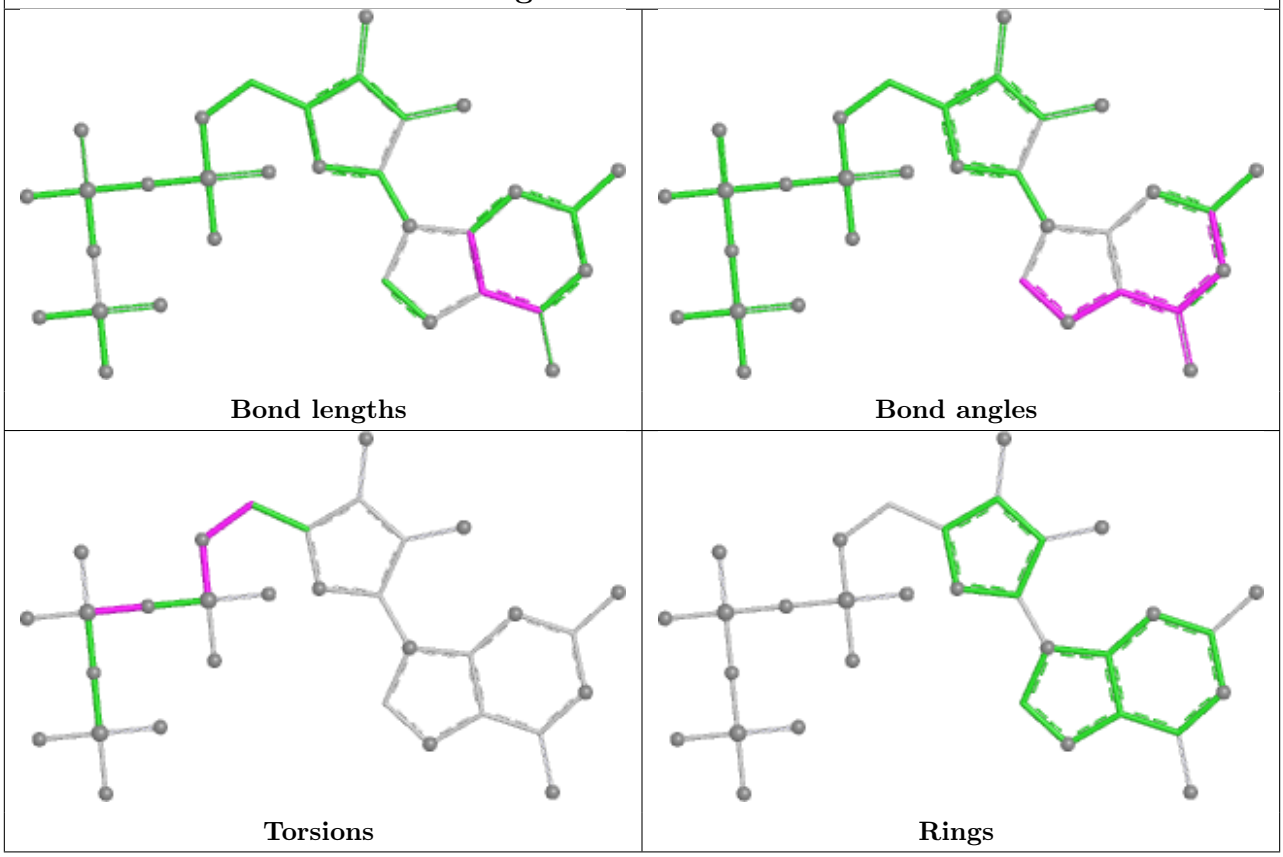

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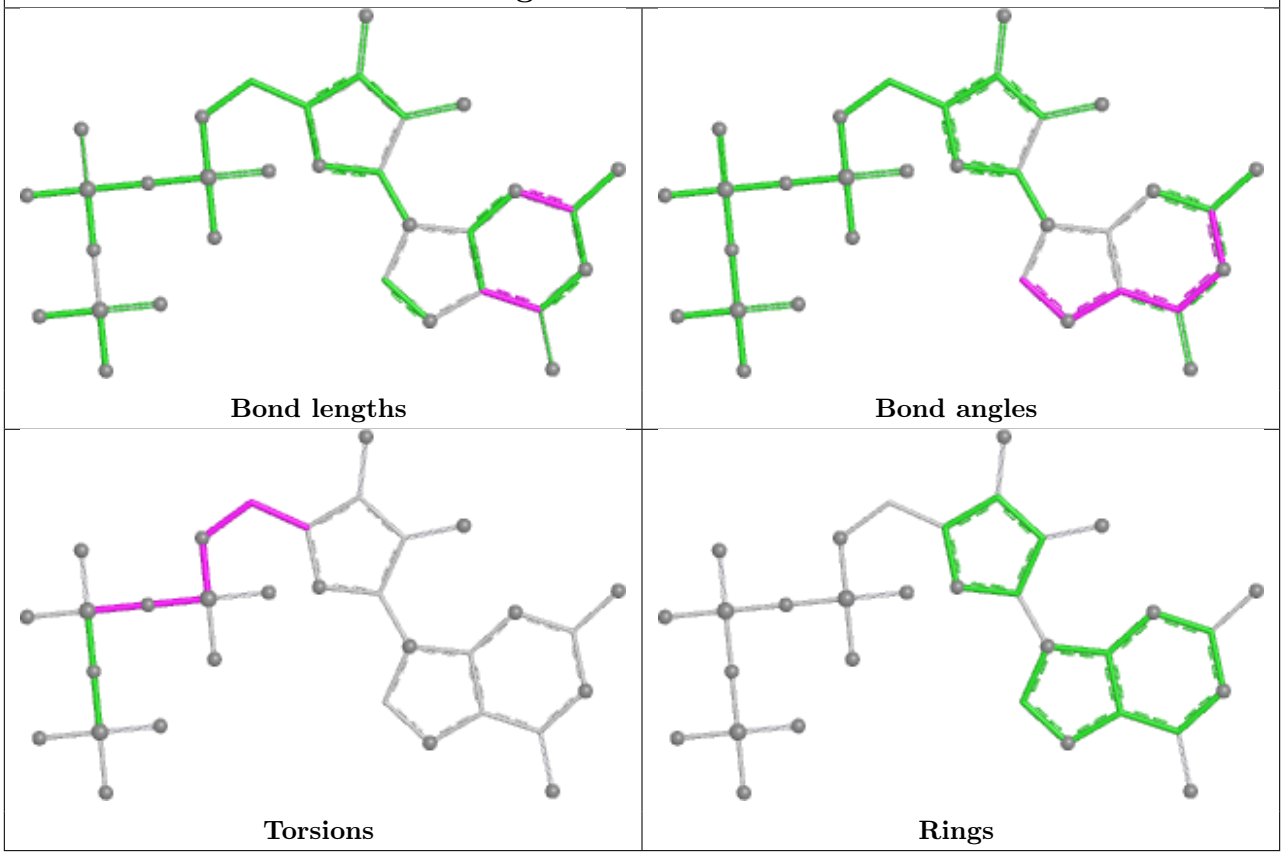

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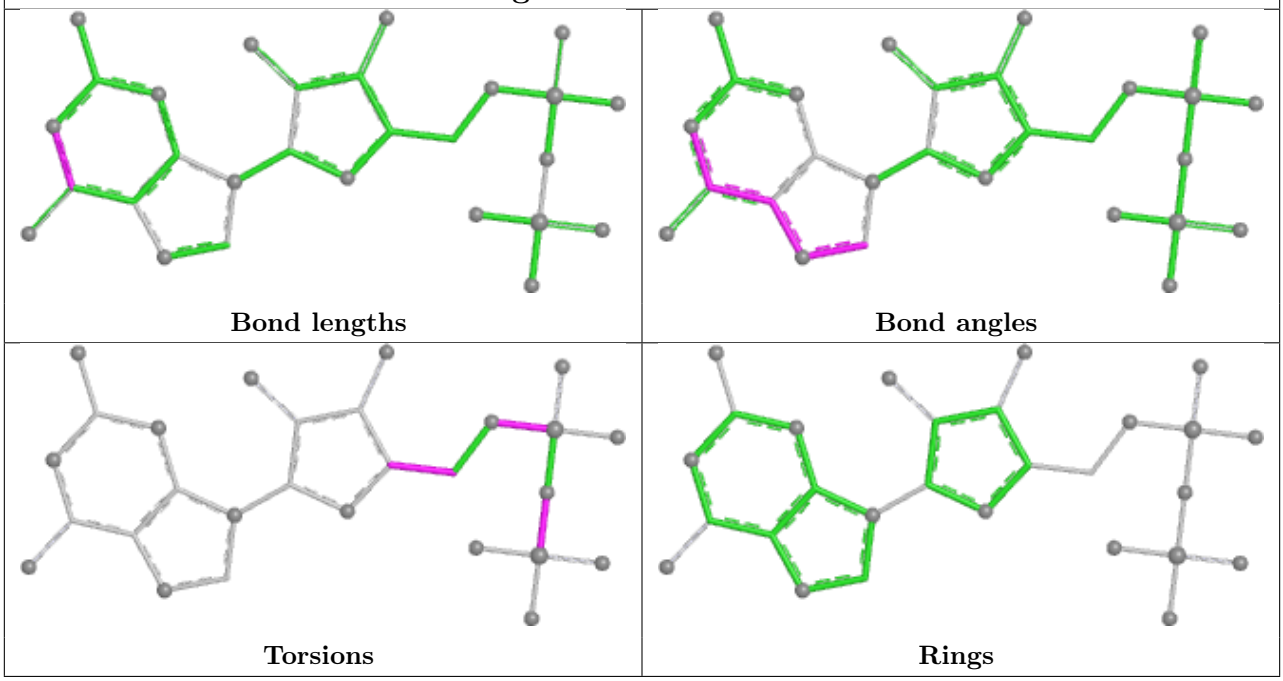

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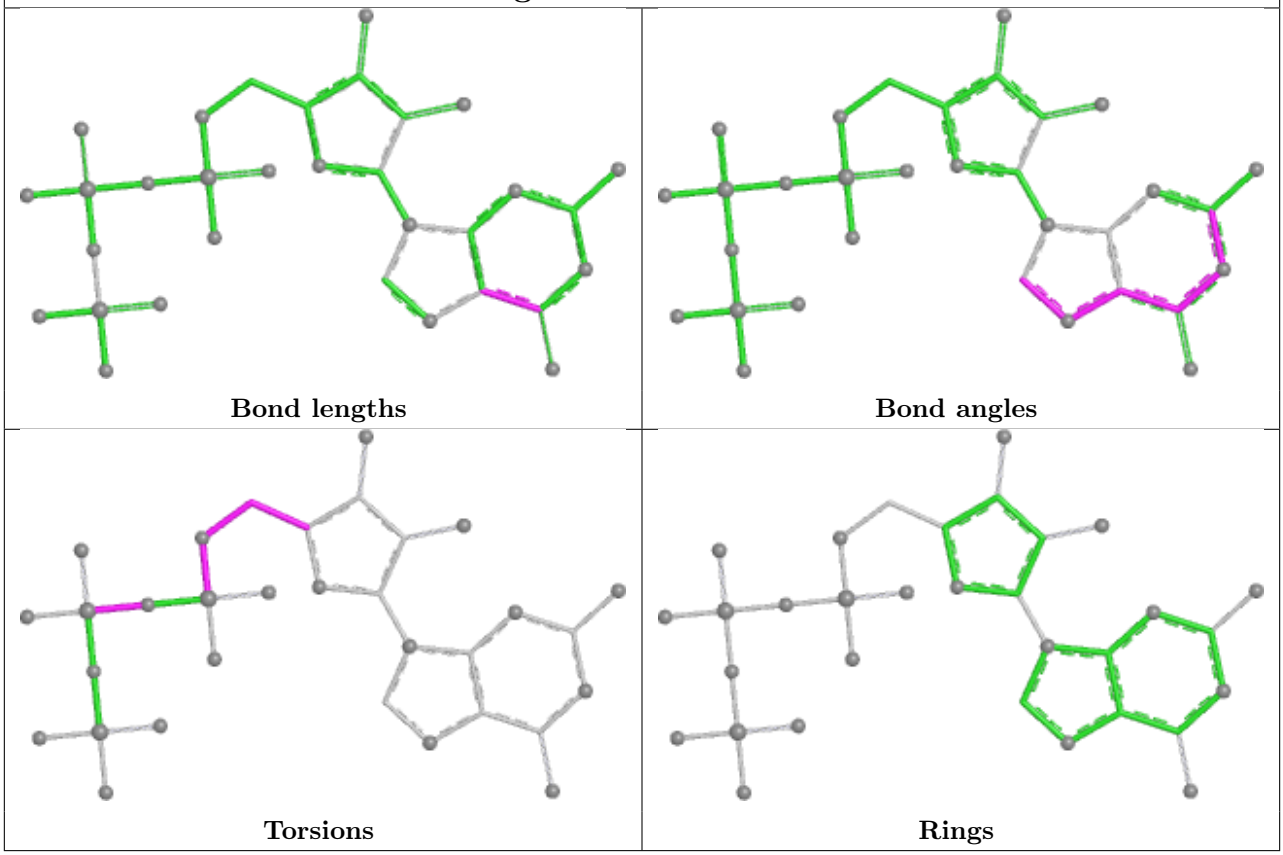

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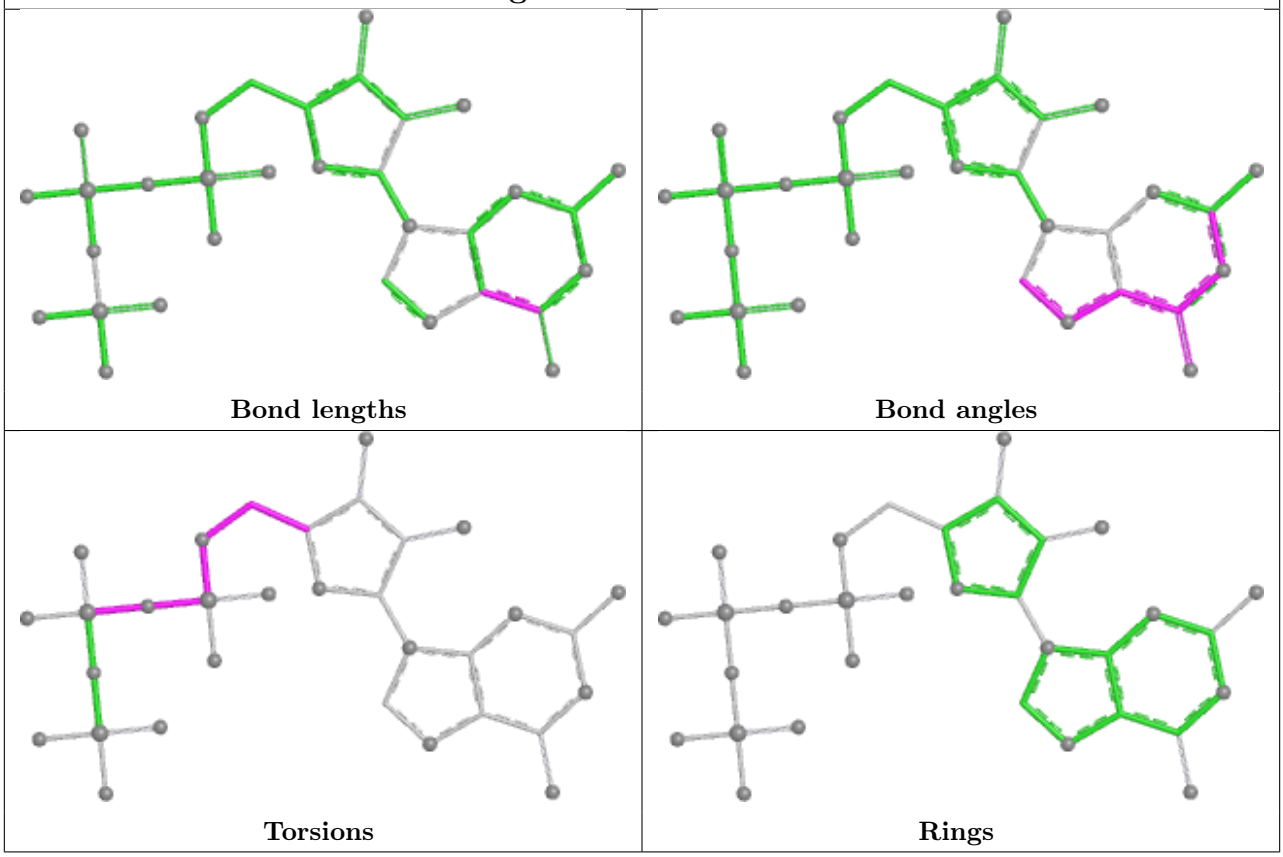

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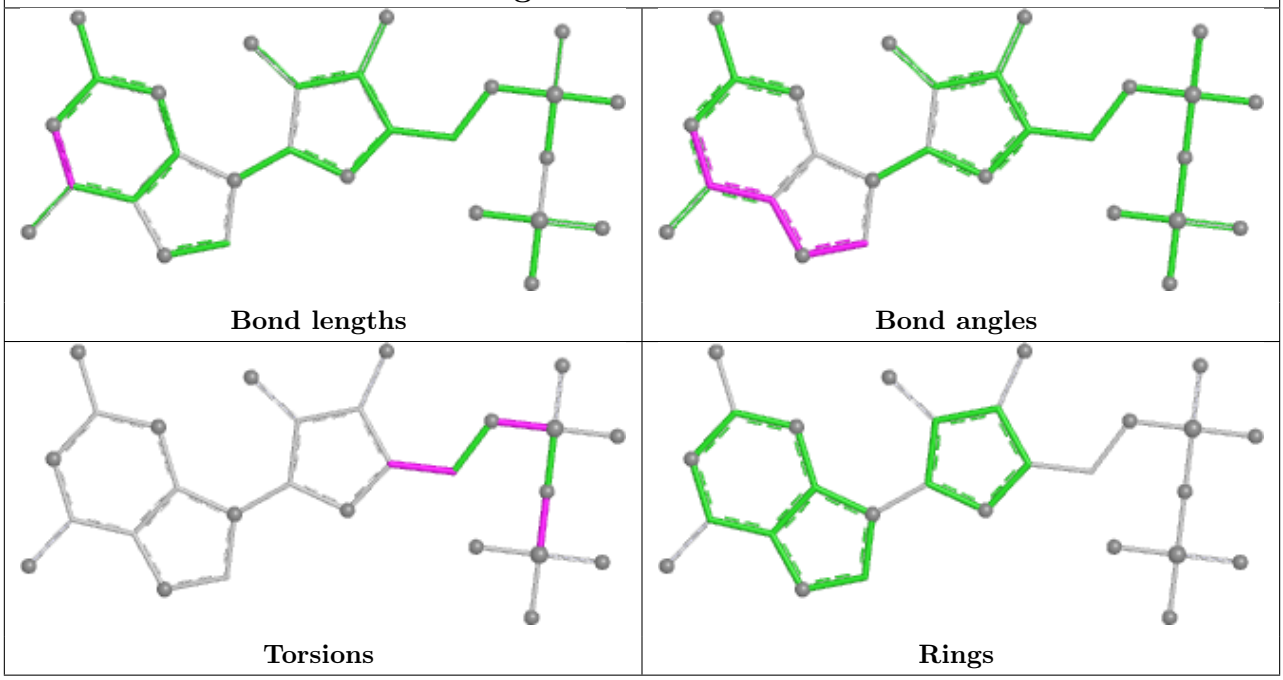

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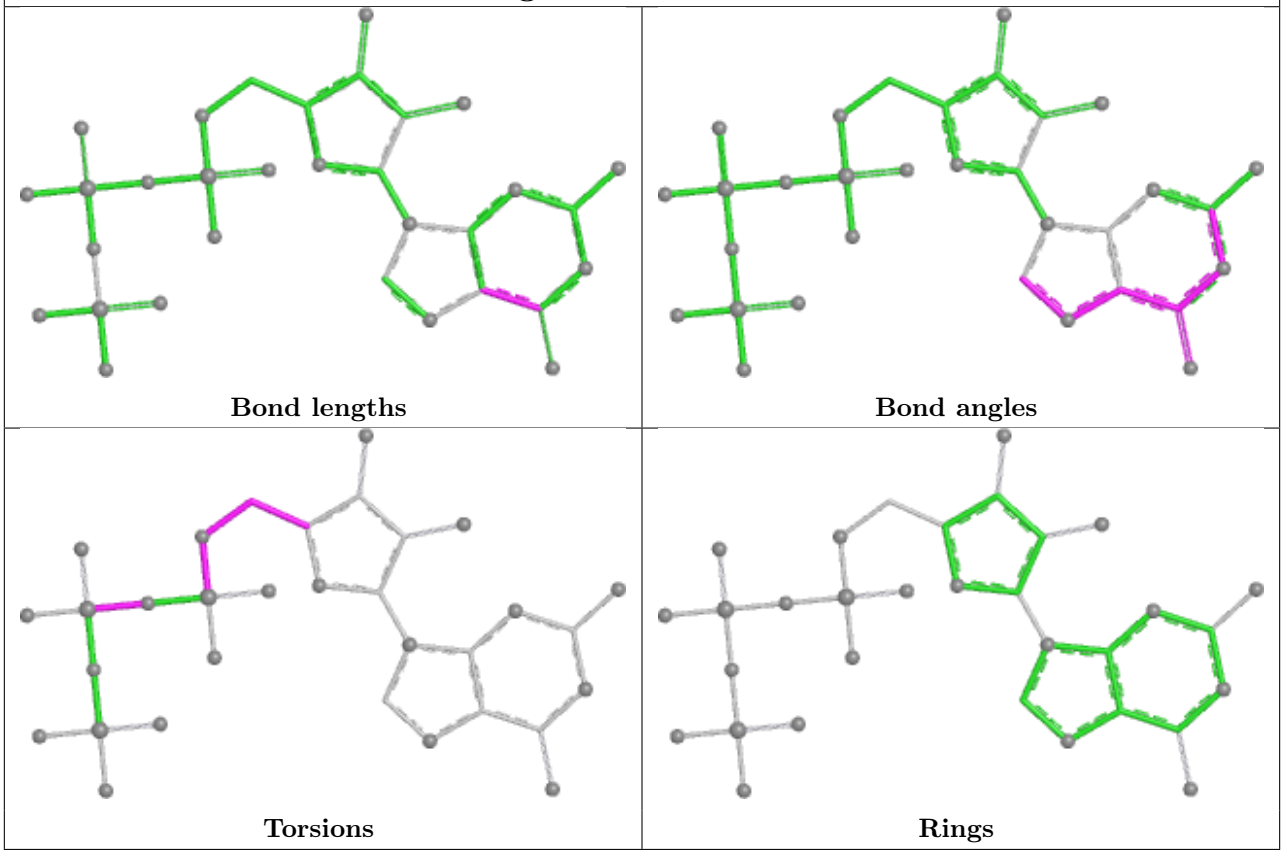

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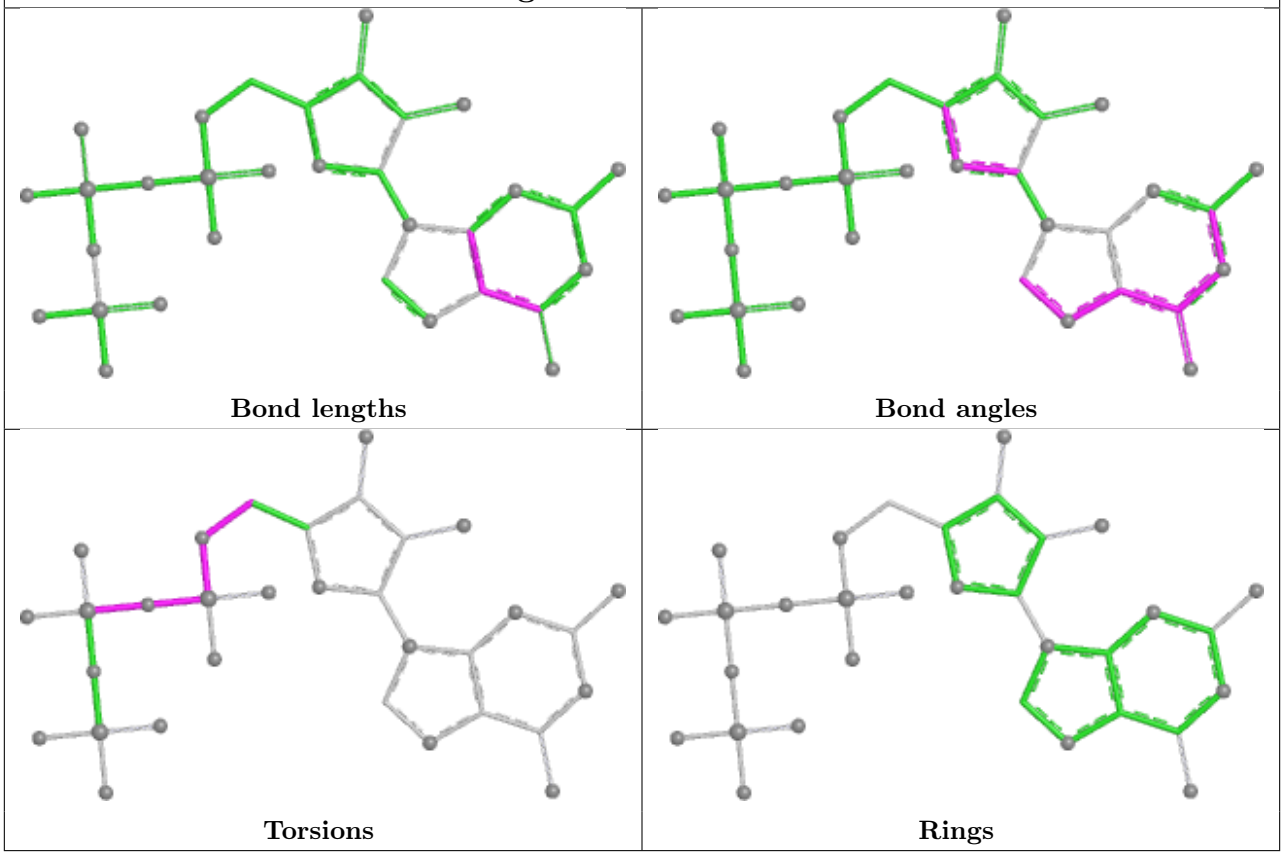

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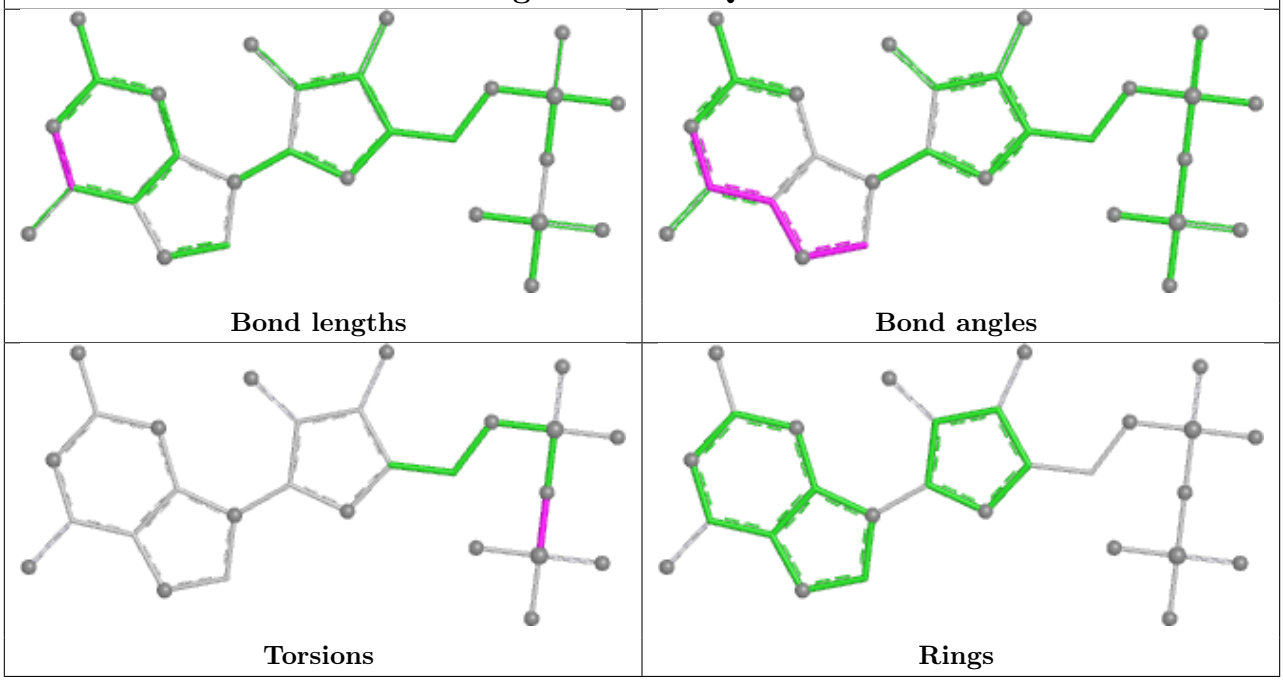

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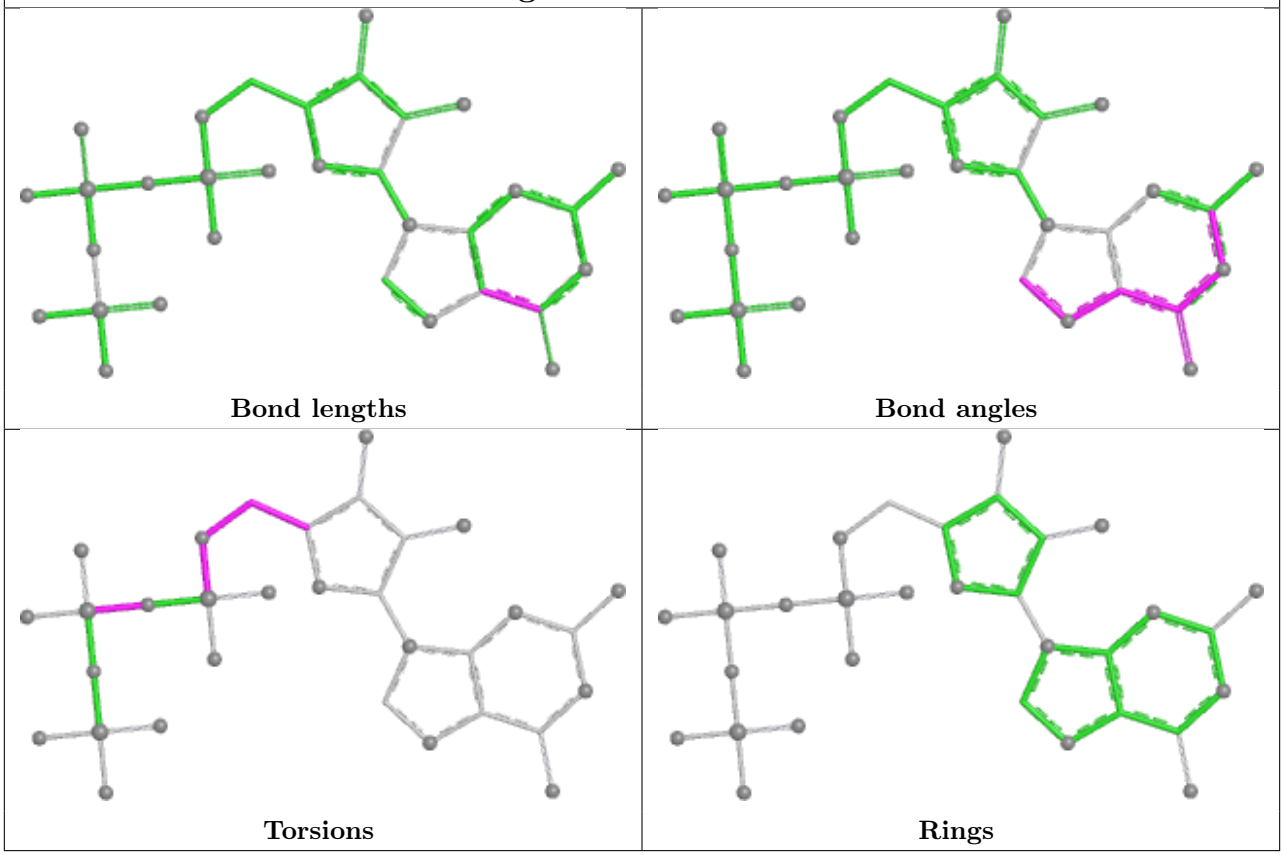

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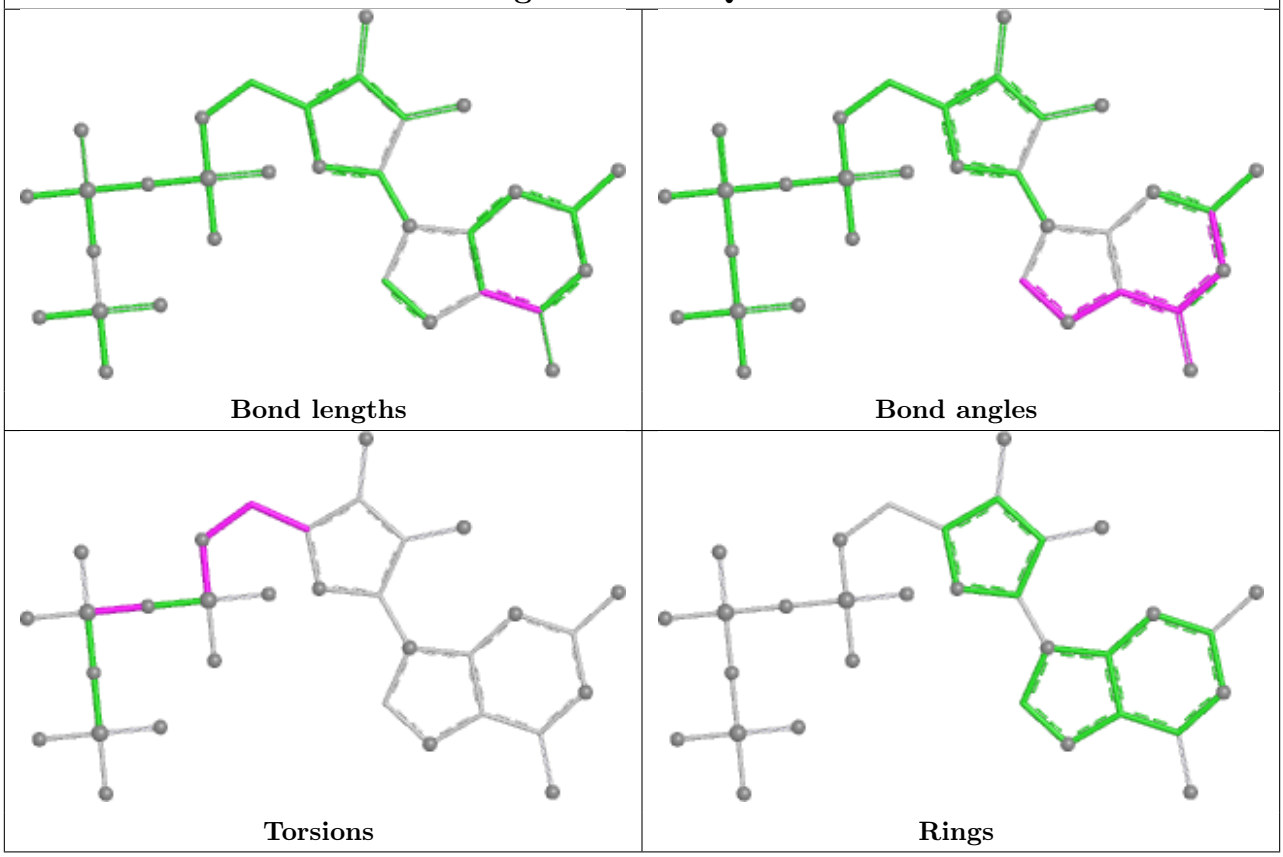

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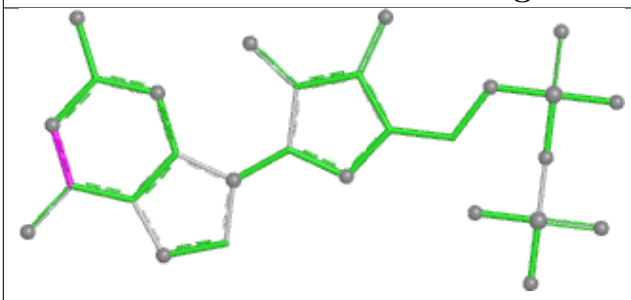
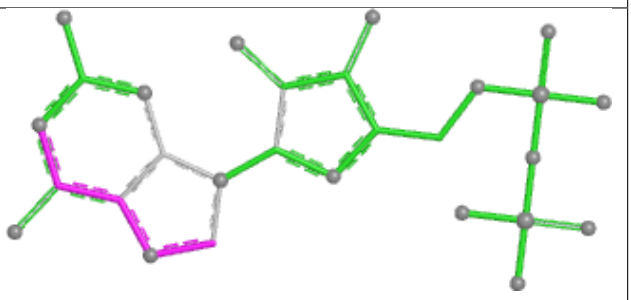


Bond lengths



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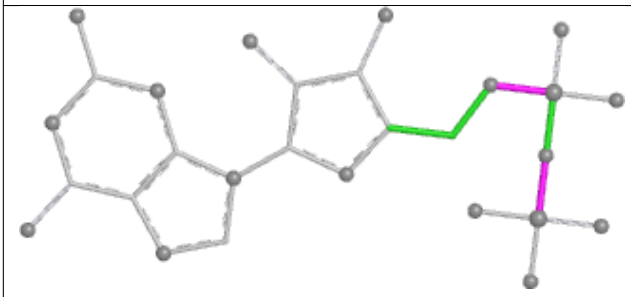
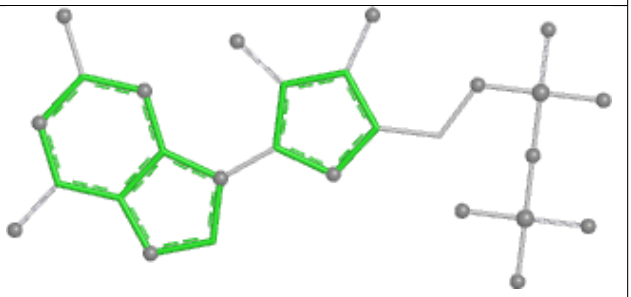
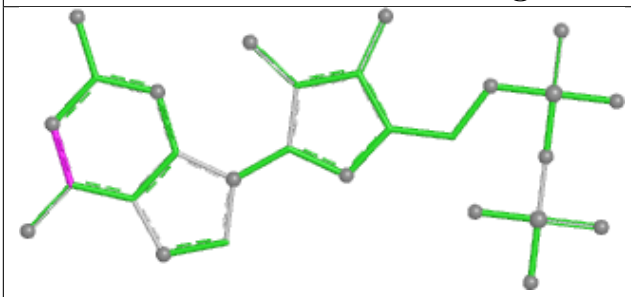


Torsions



Rings

Ligand GDP 2U 502



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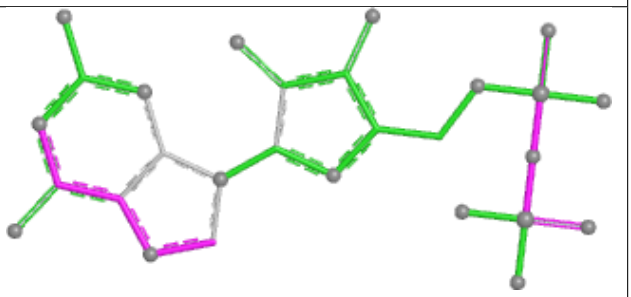

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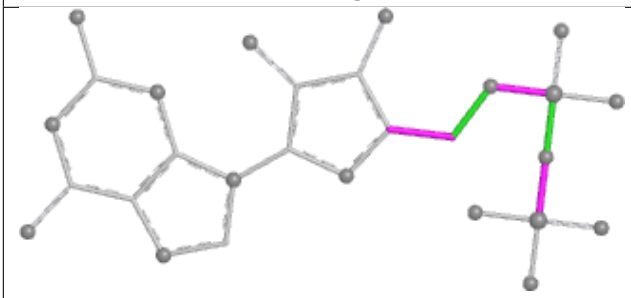

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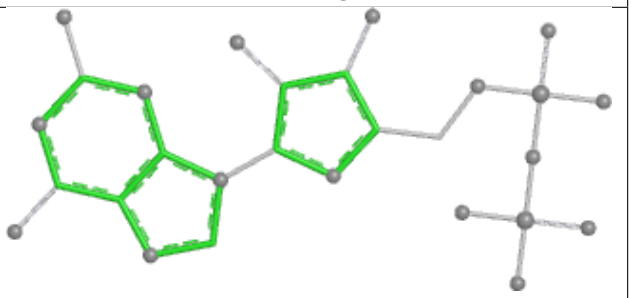
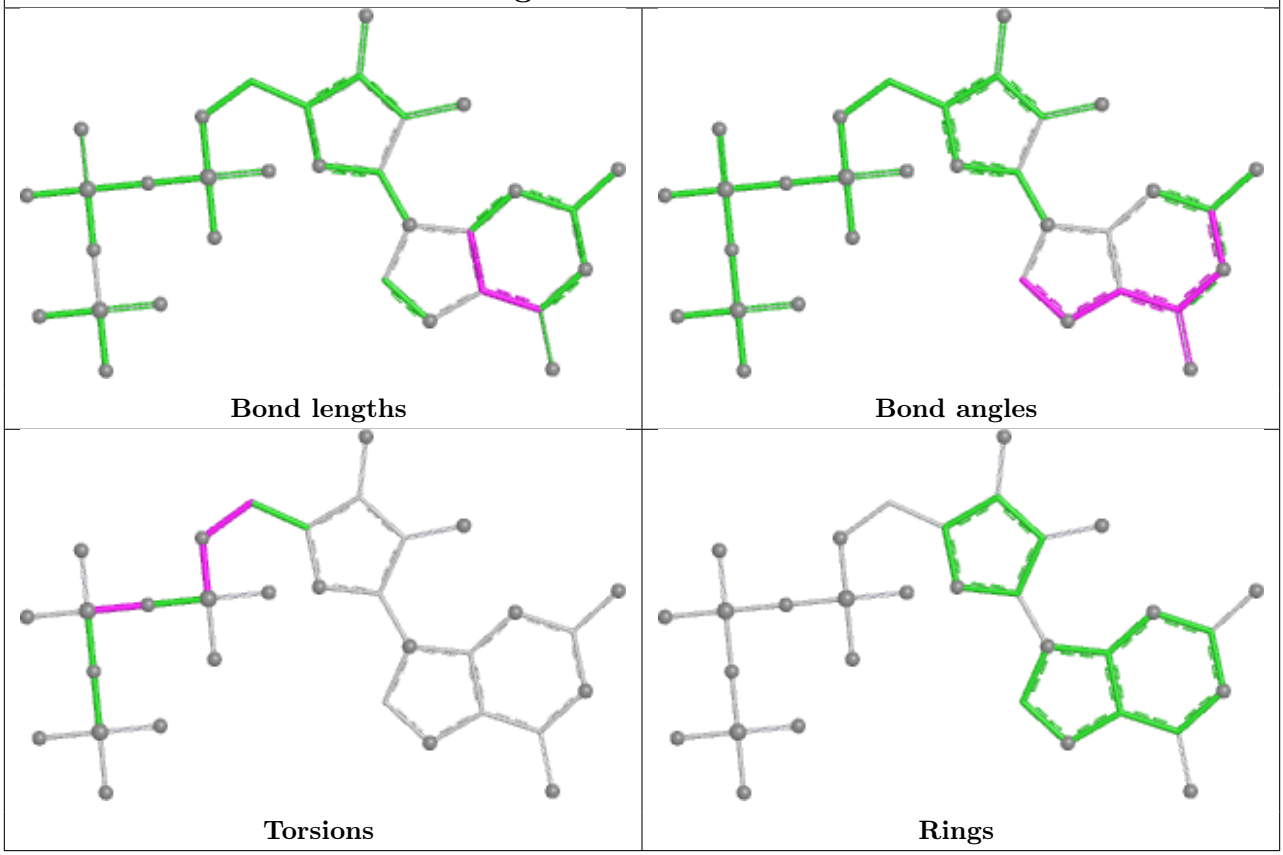


Rings

Ligand GTP R8 501



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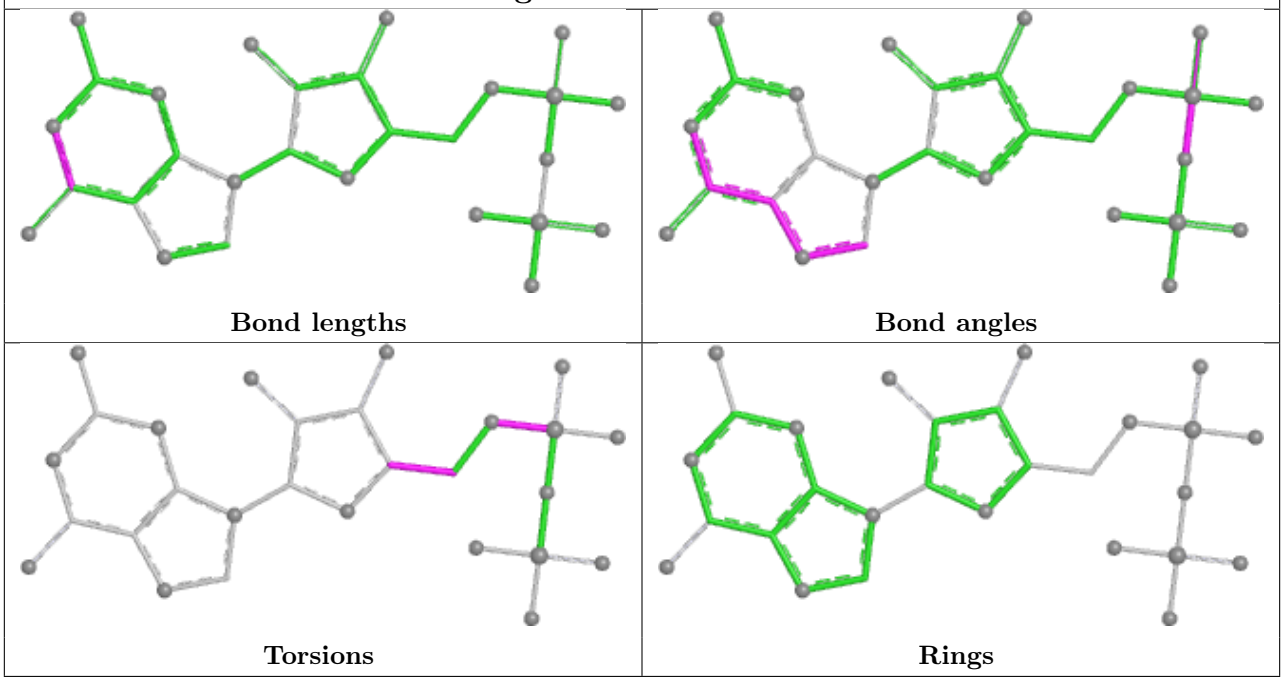

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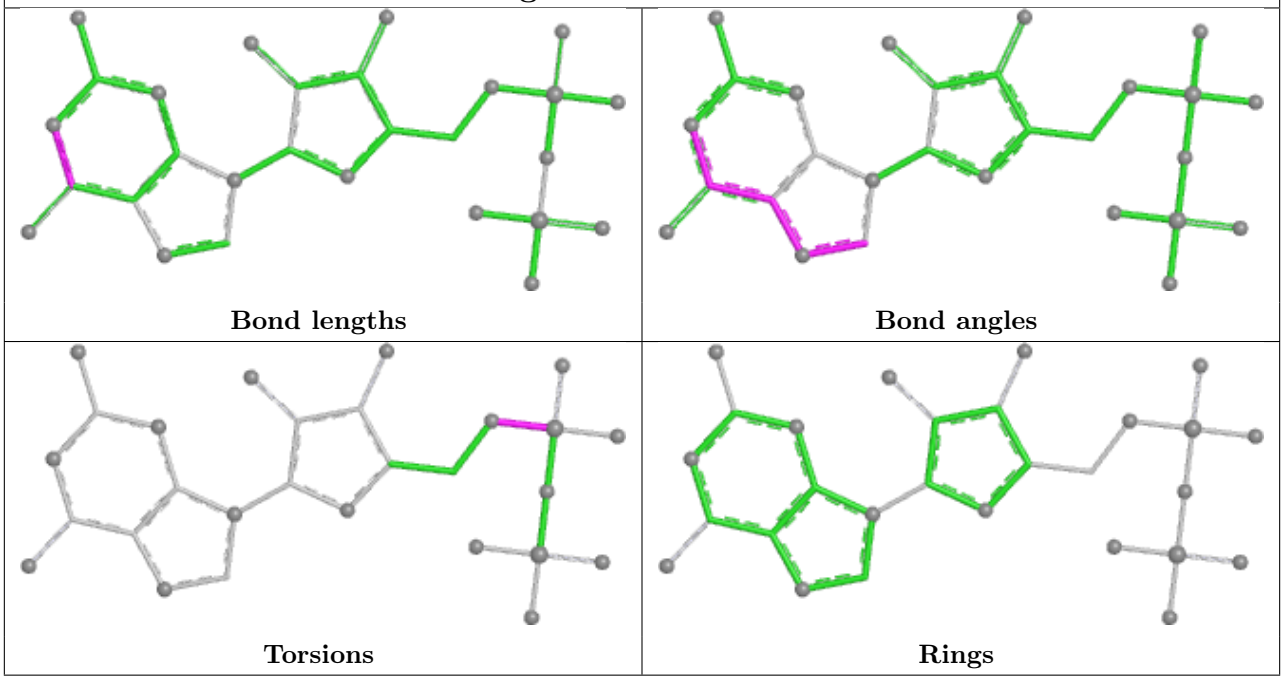

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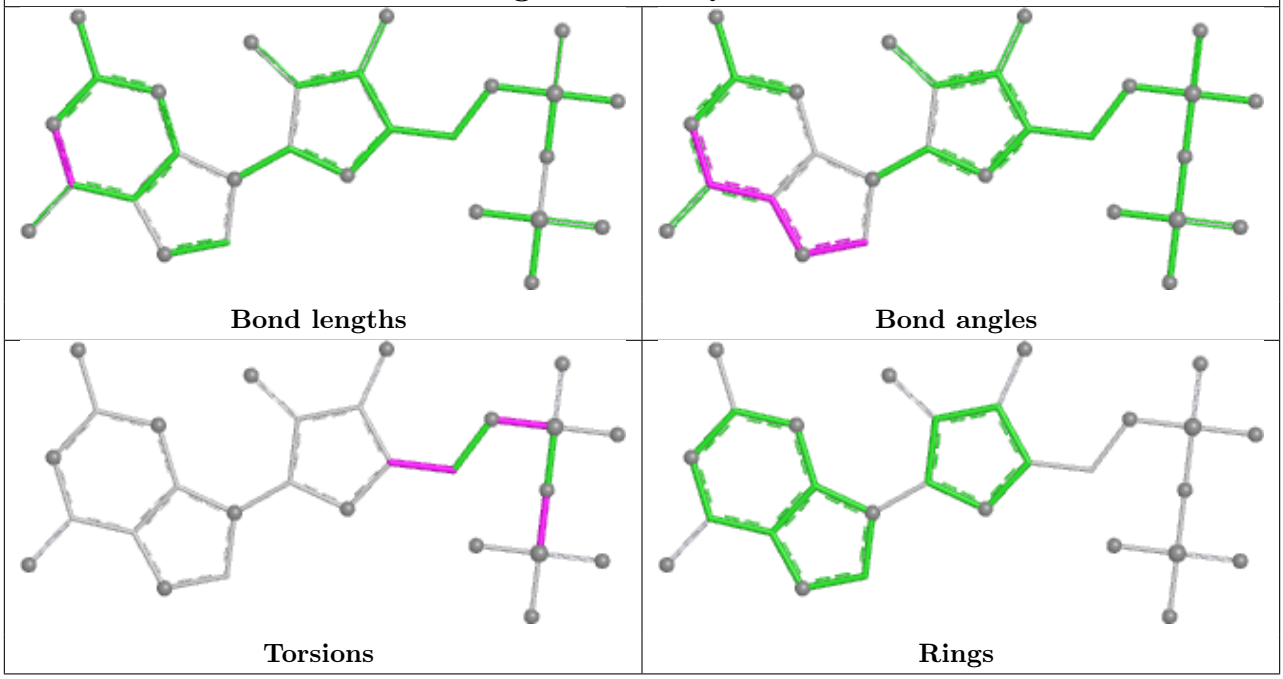

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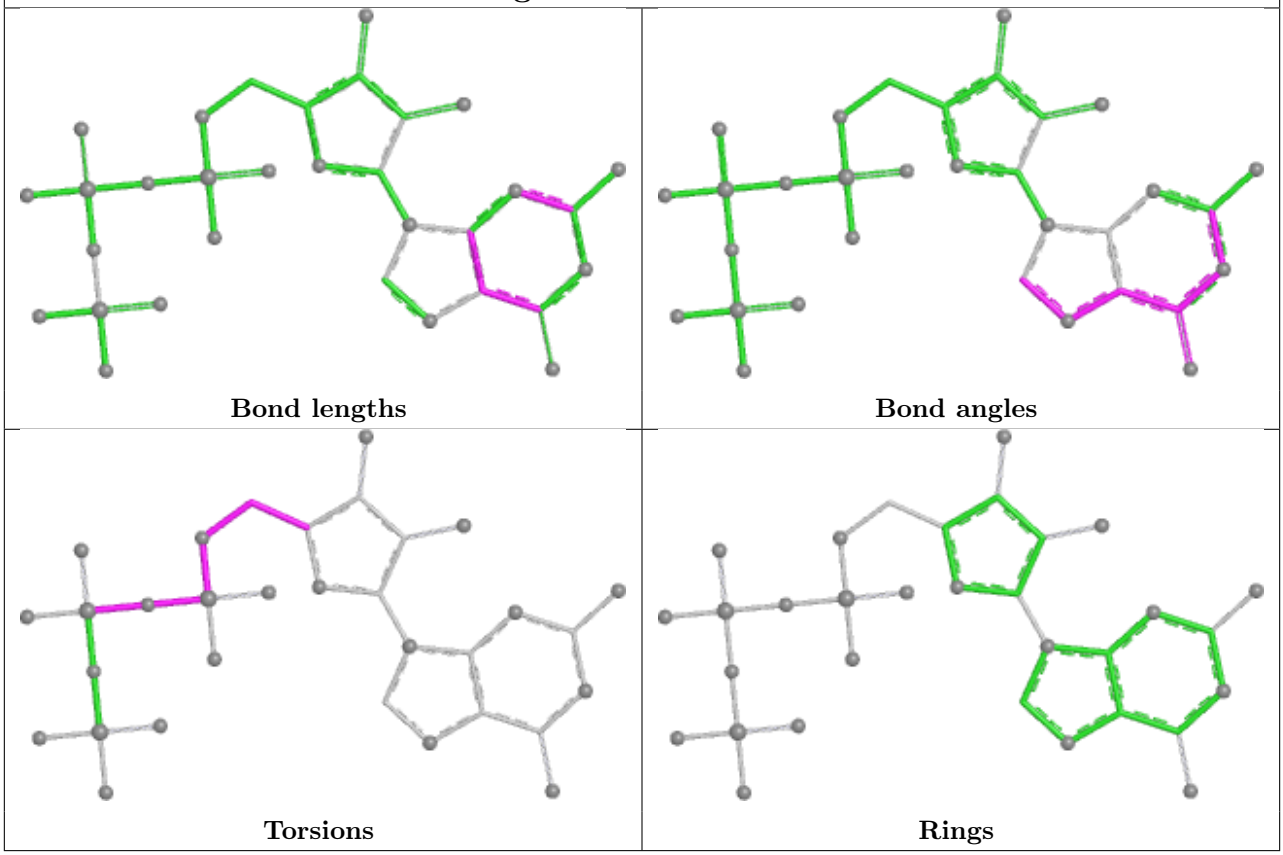

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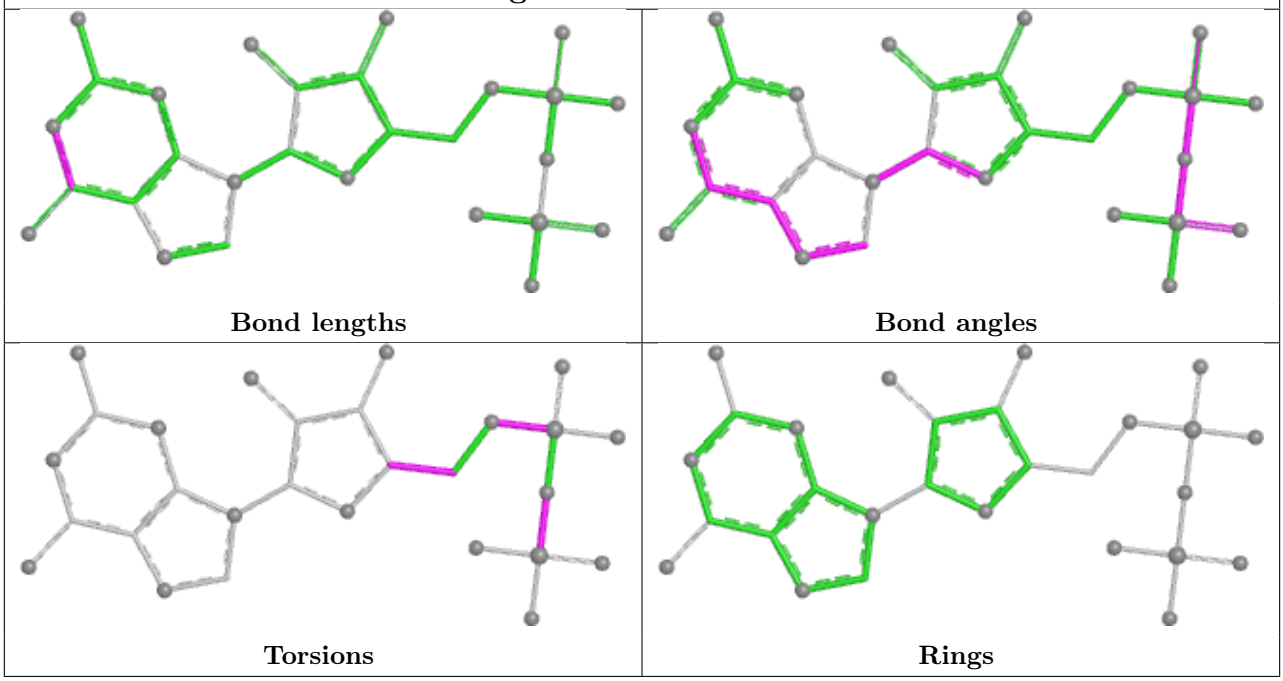

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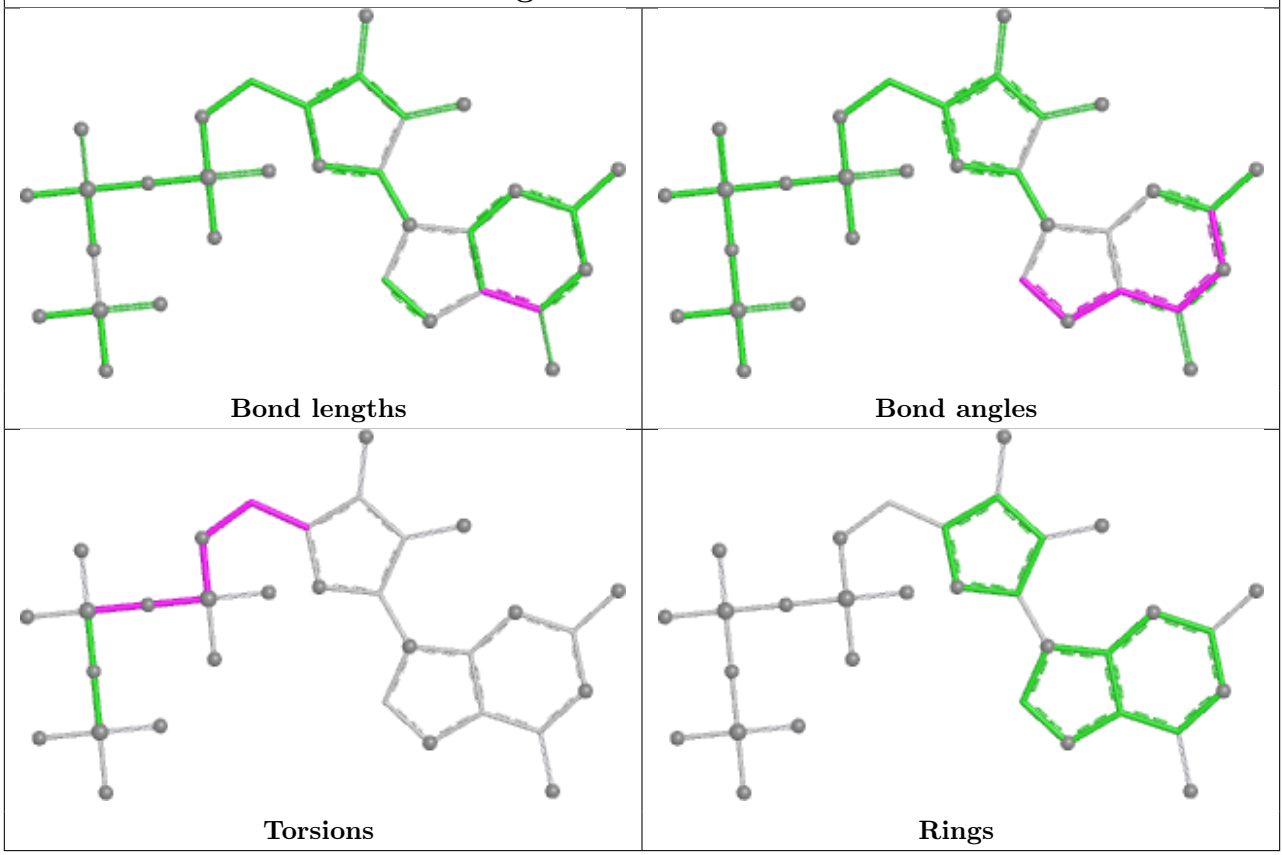

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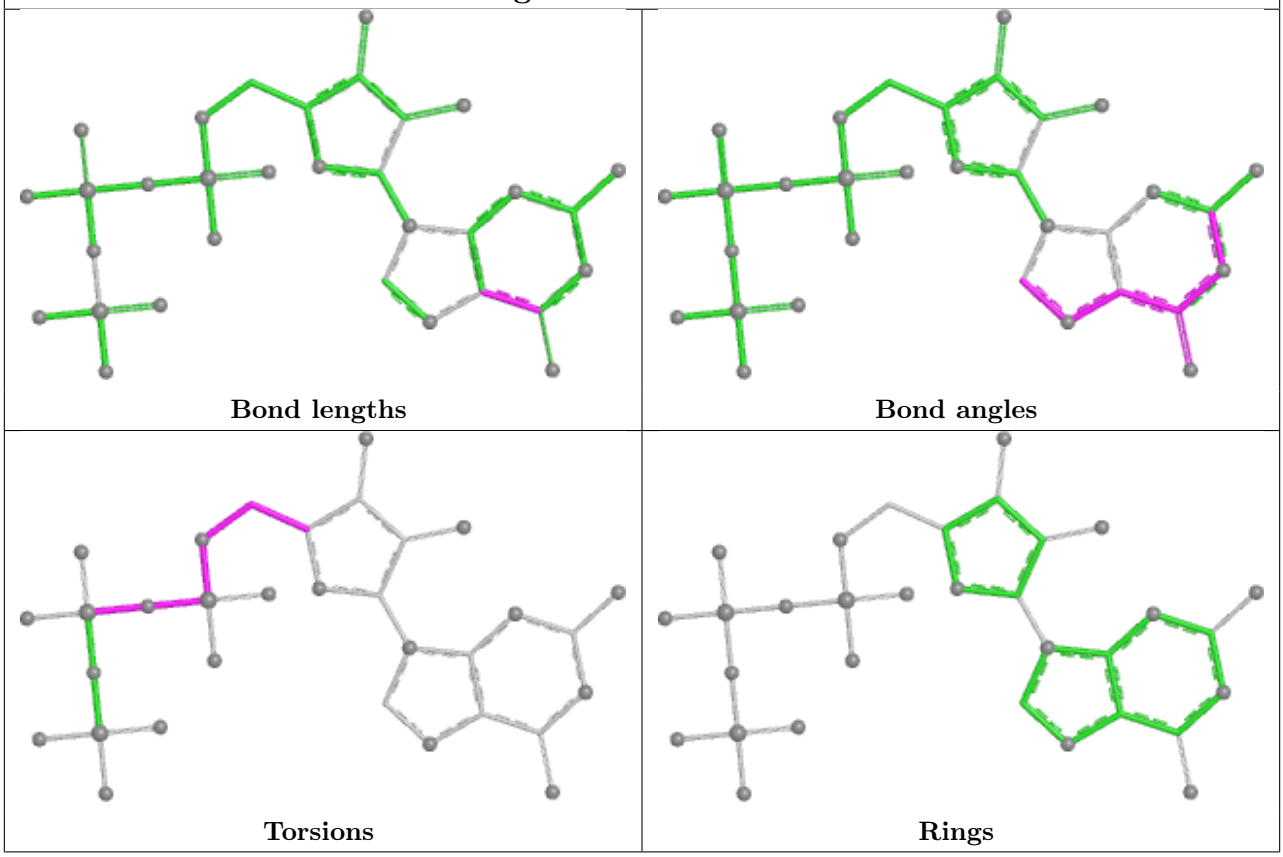
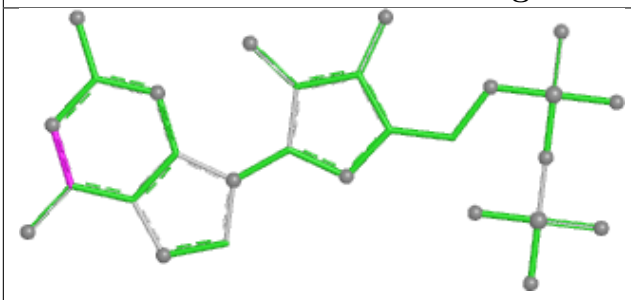
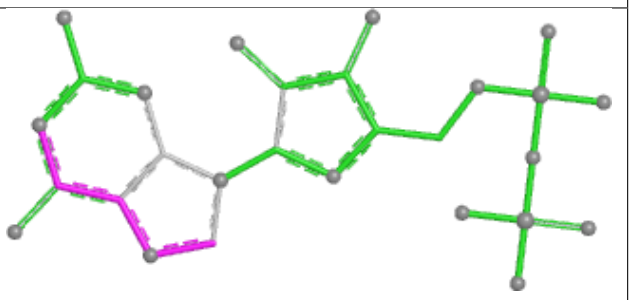


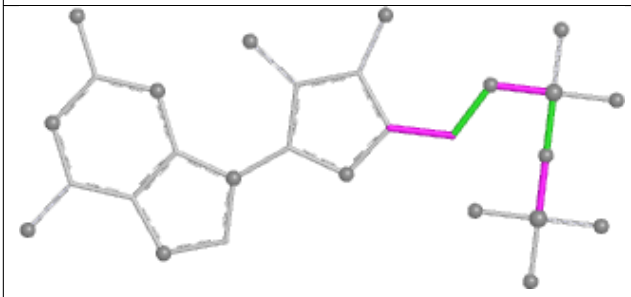
Ligand GDP Y6 502



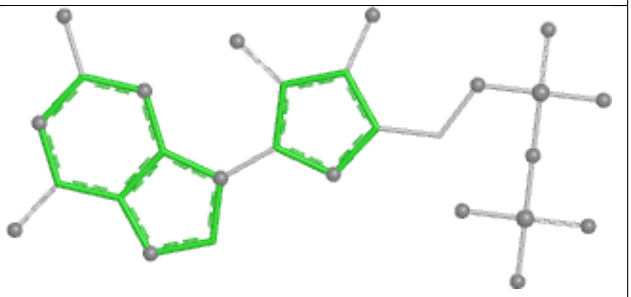
Bond lengths



Bond angles

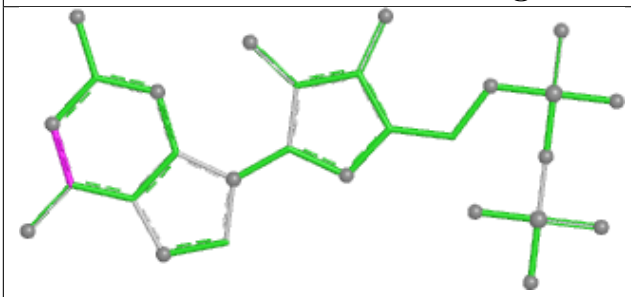


Torsions



Rings

Ligand GDP C6 501



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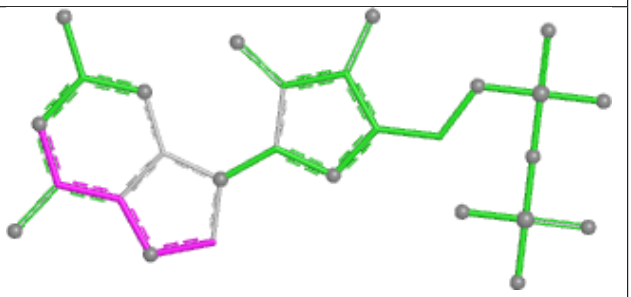

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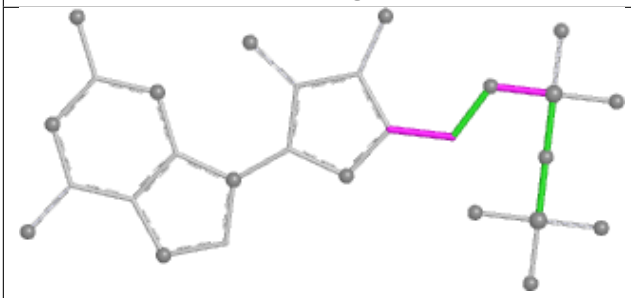

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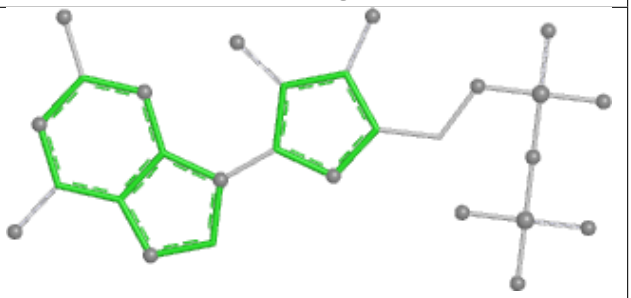
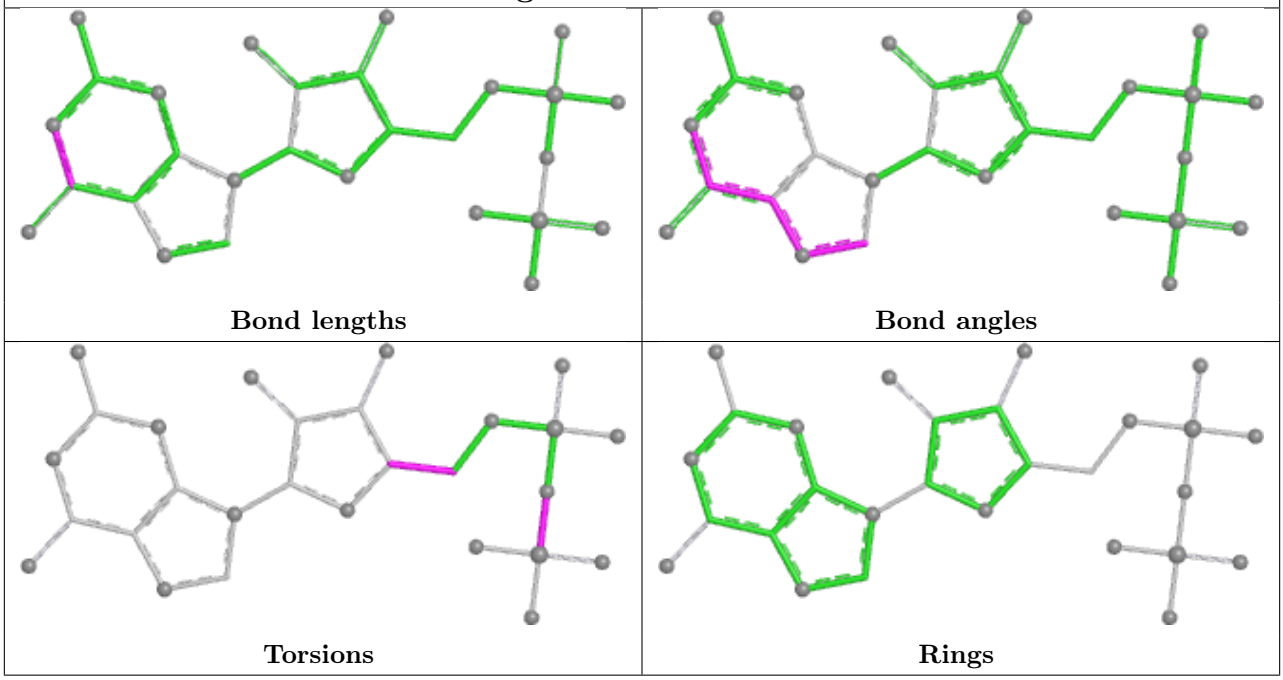
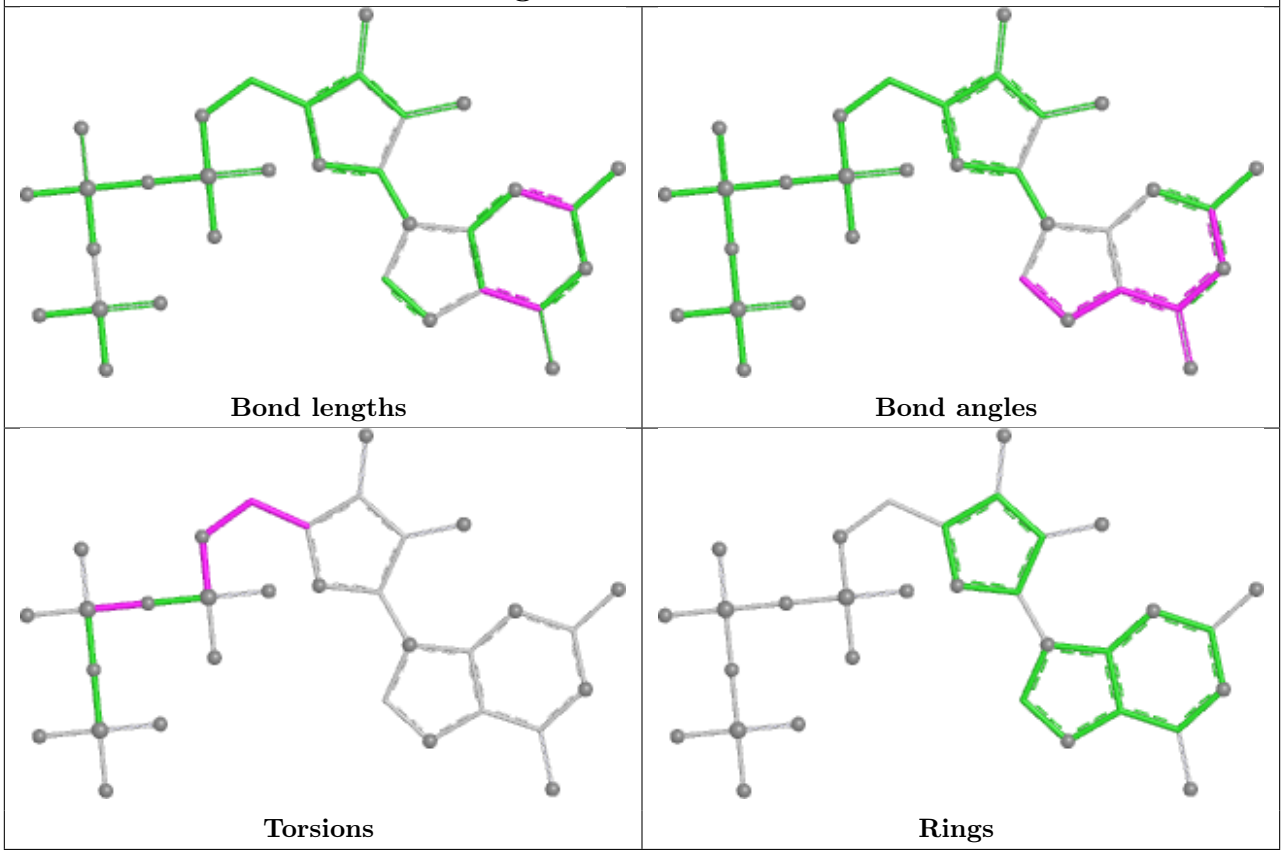


Rings

Ligand GDP 3S 502



Ligand GTP U4 501



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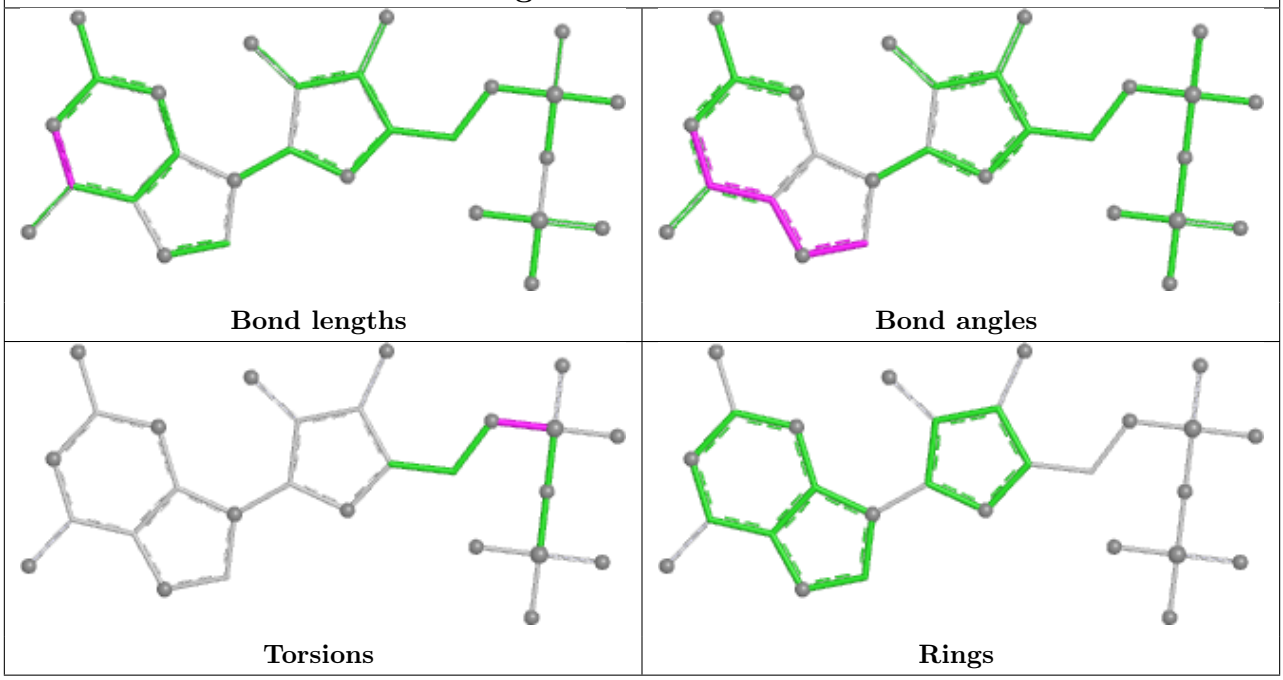

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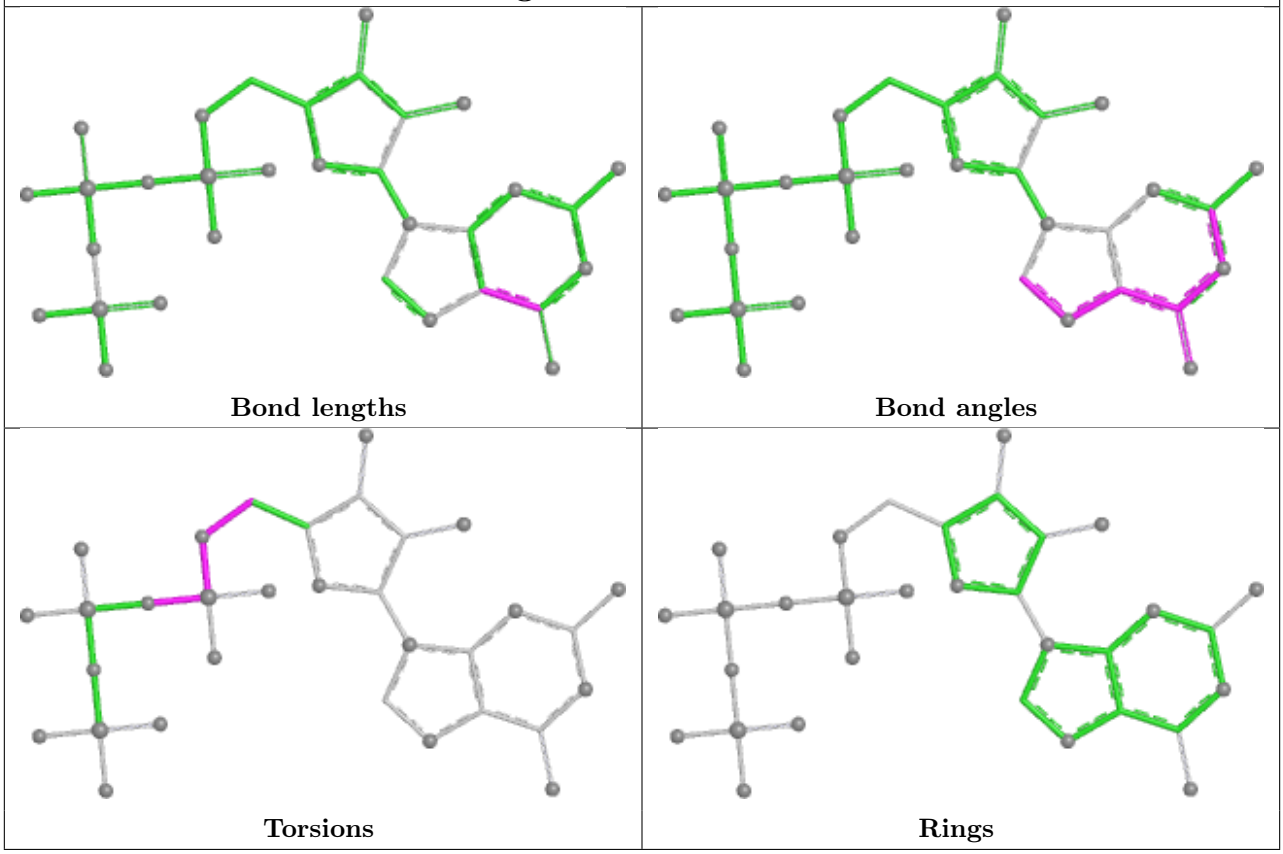

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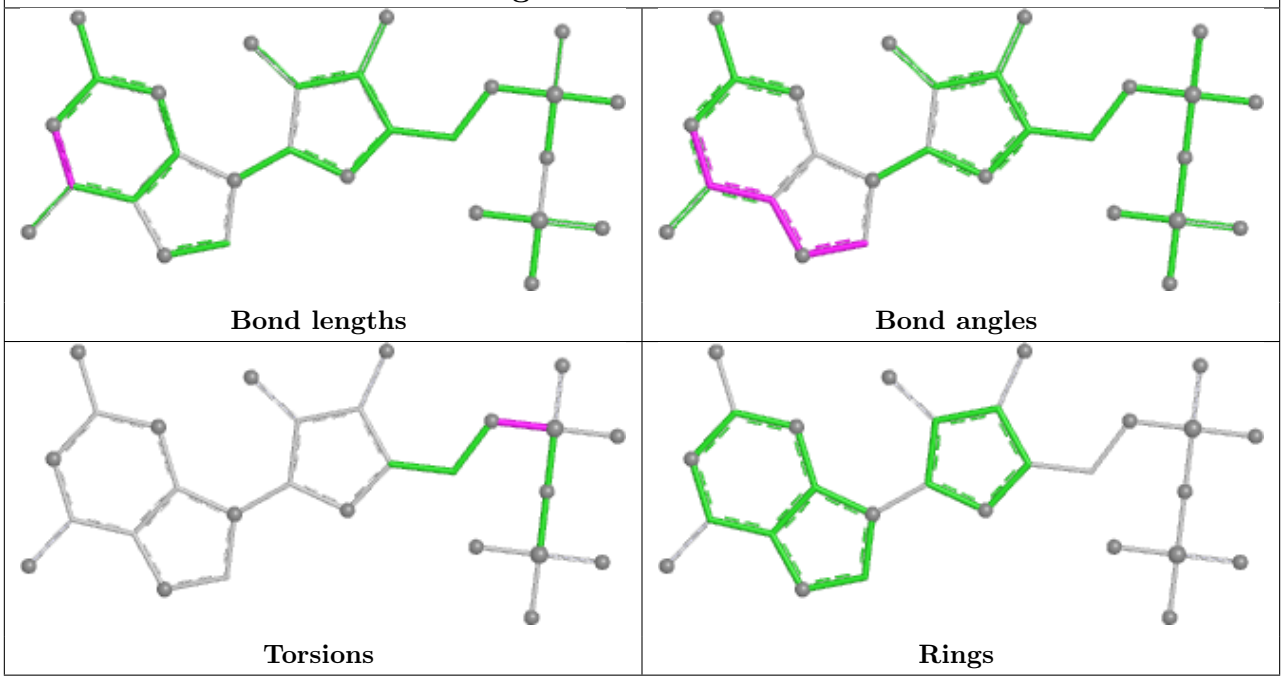
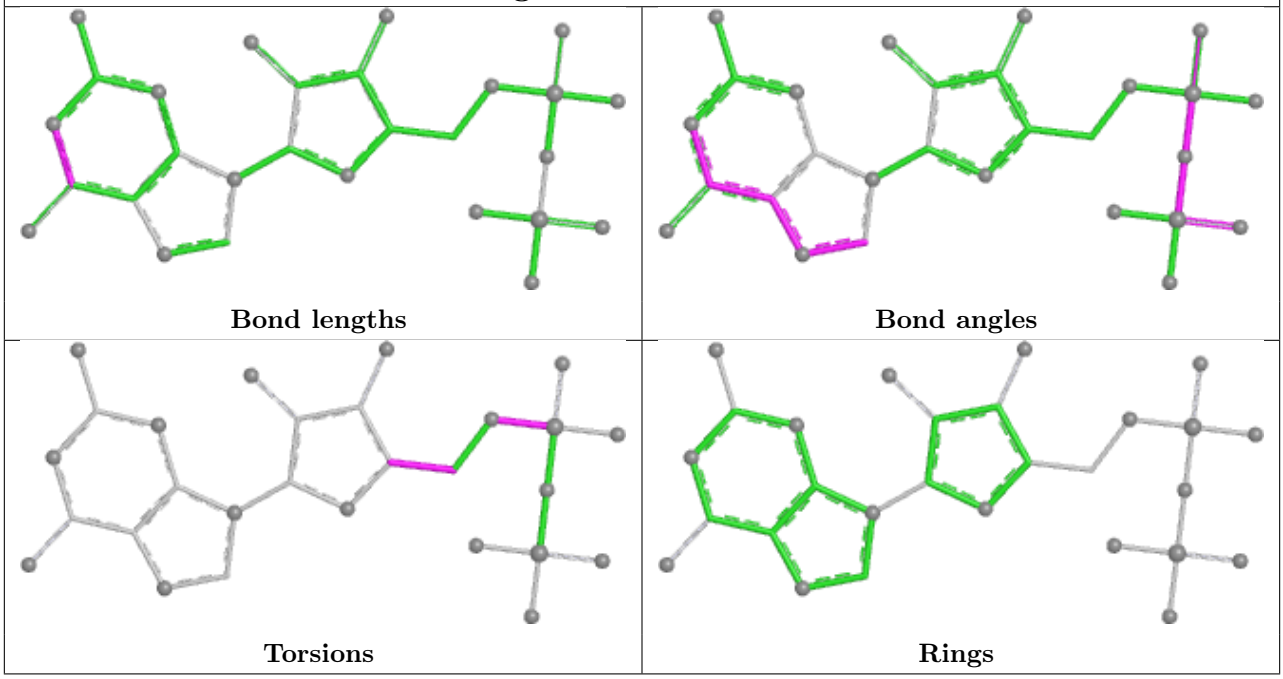


Ligand GDP R8 502



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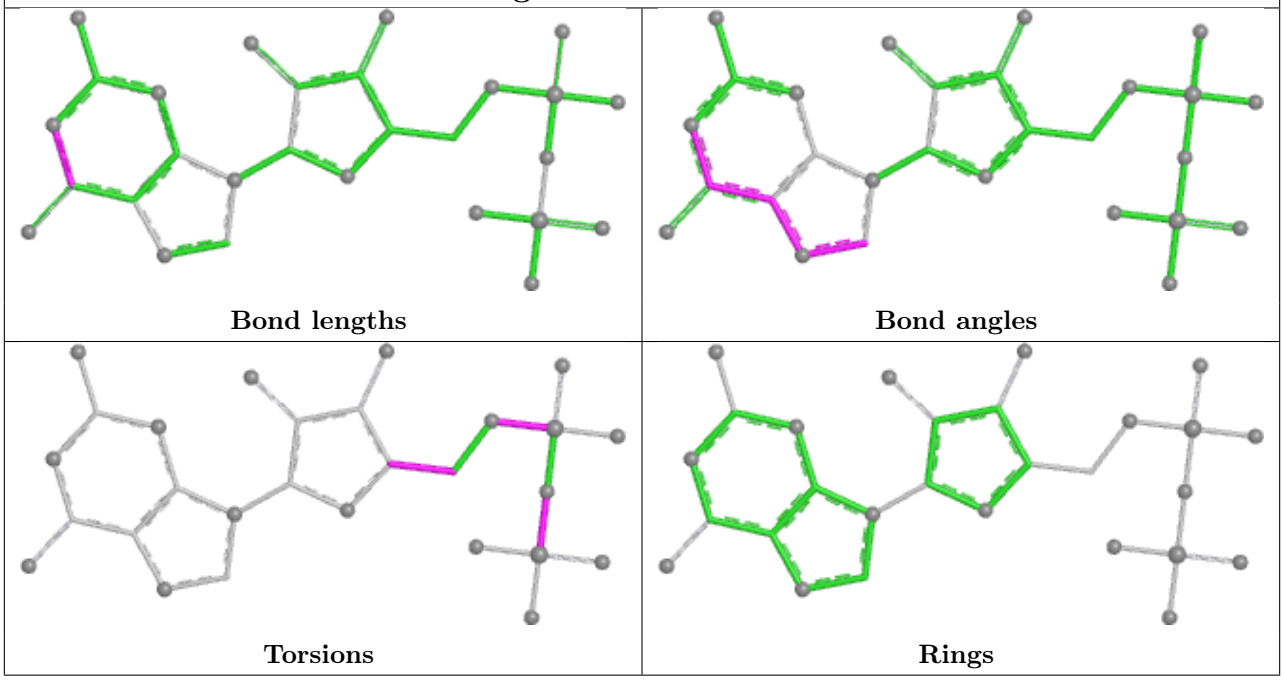

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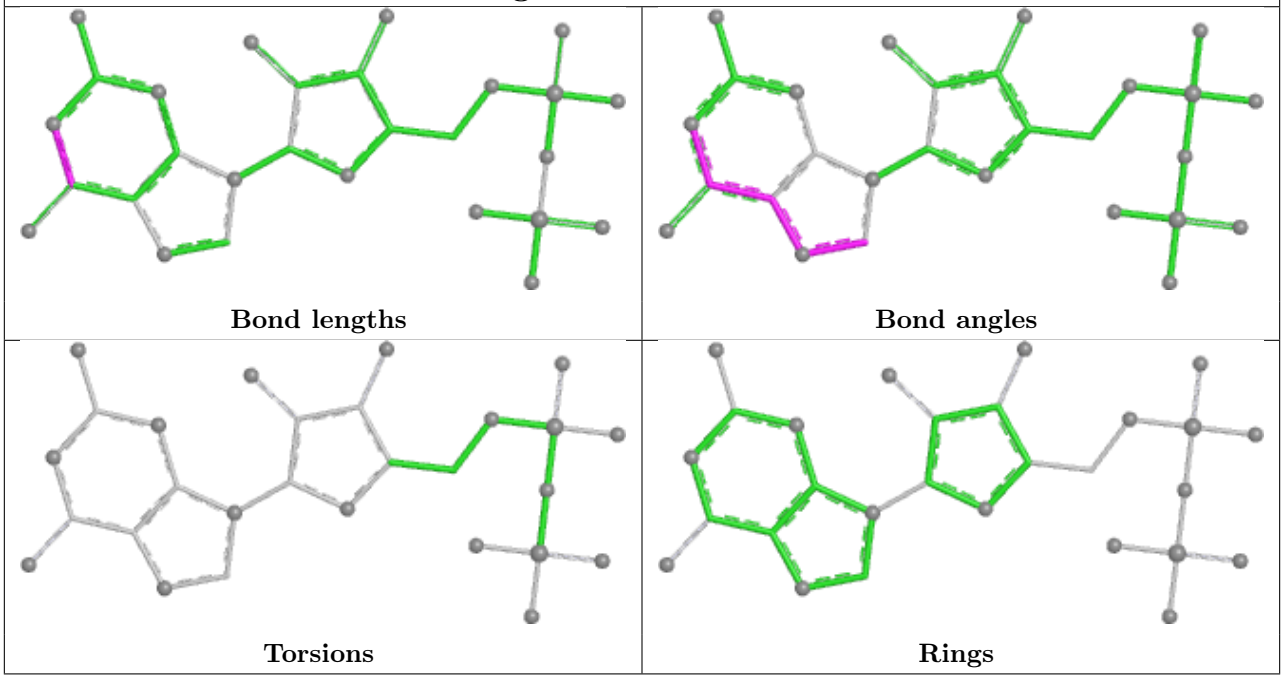
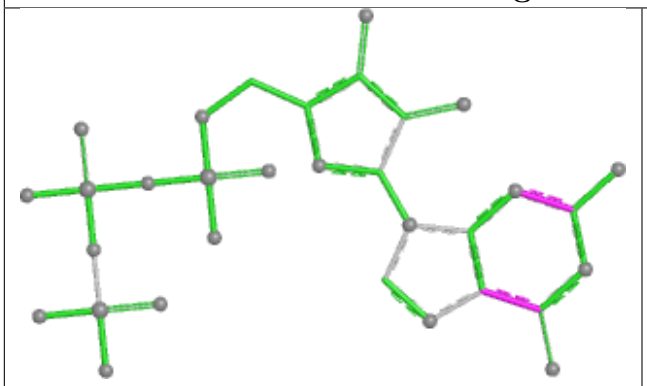
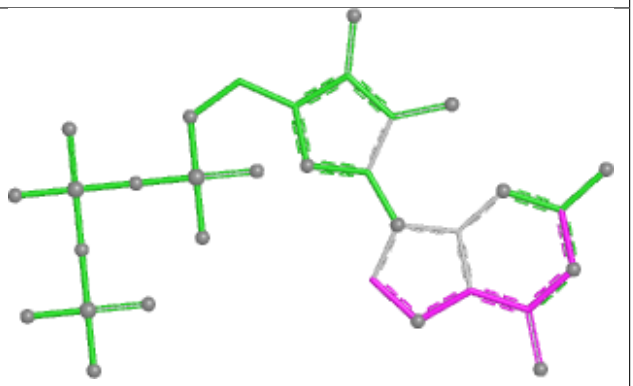


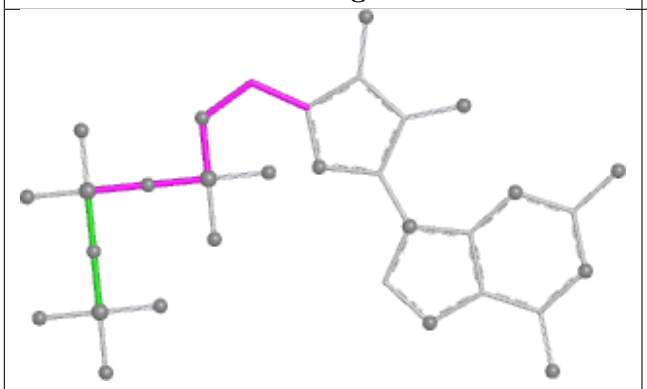
Ligand GTP K7 501



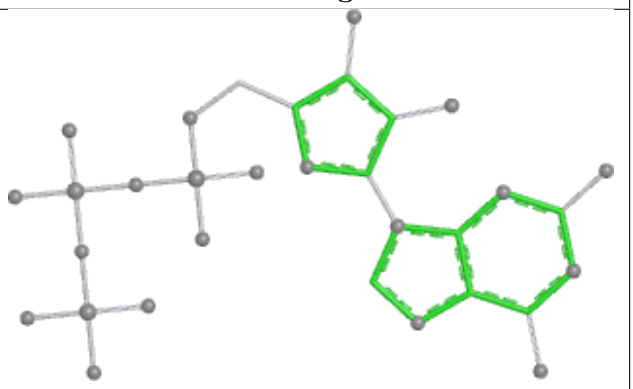
Bond lengths



Bond angles



Torsions



Rings

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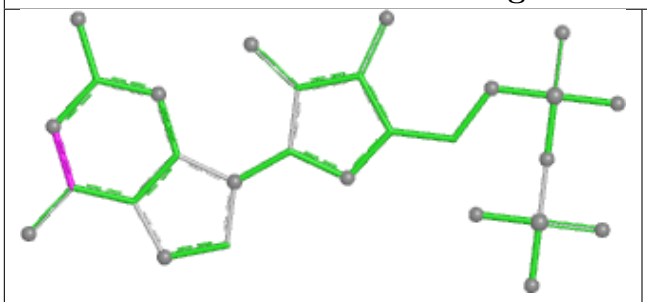

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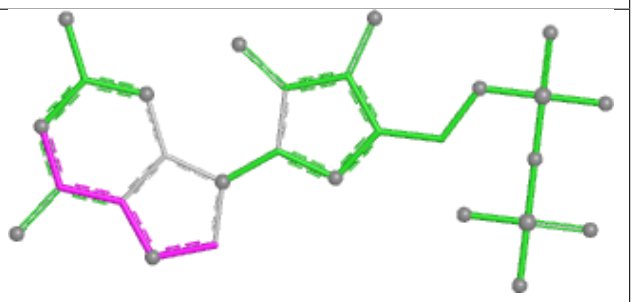

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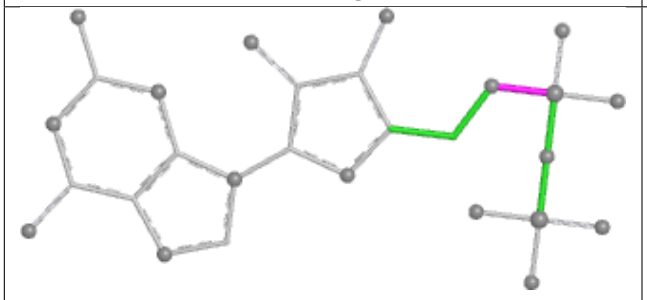

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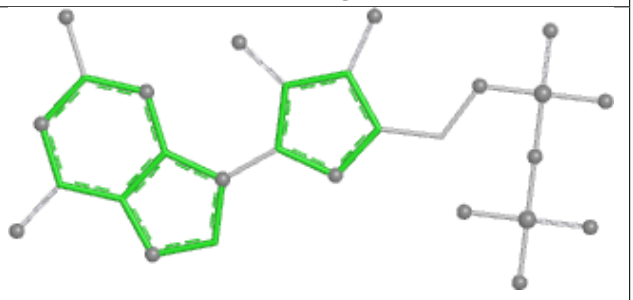
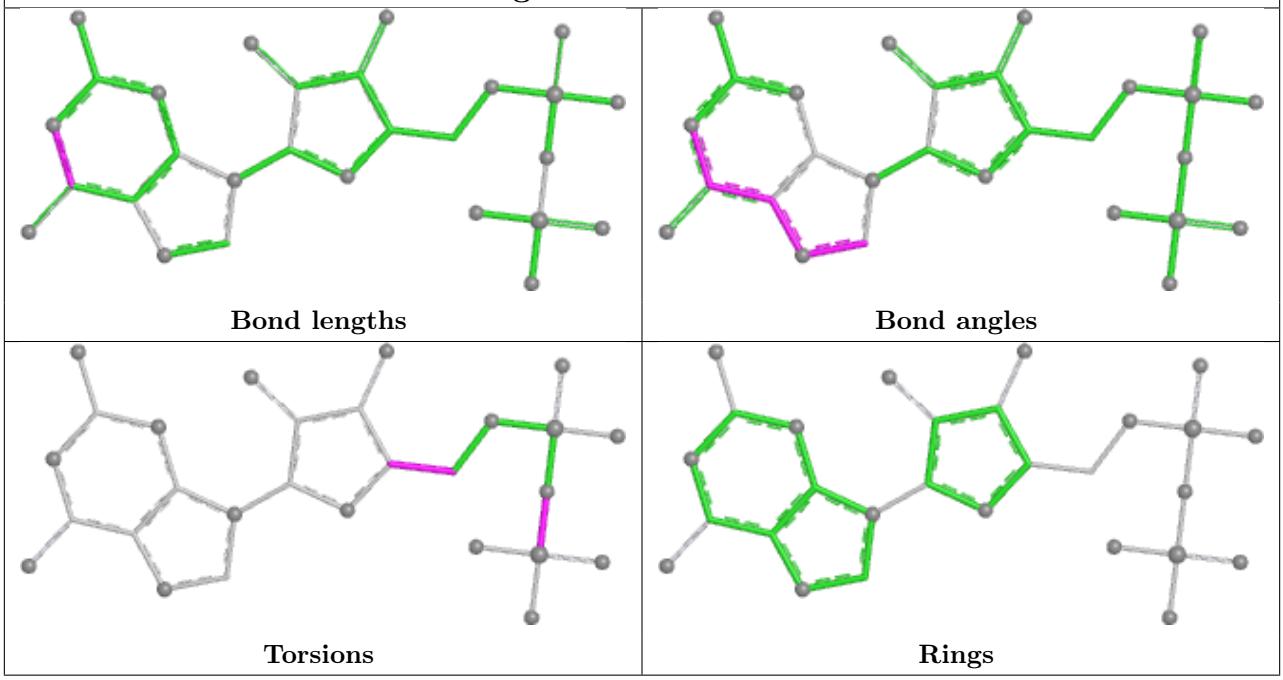


Rings

Ligand GDP X8 501



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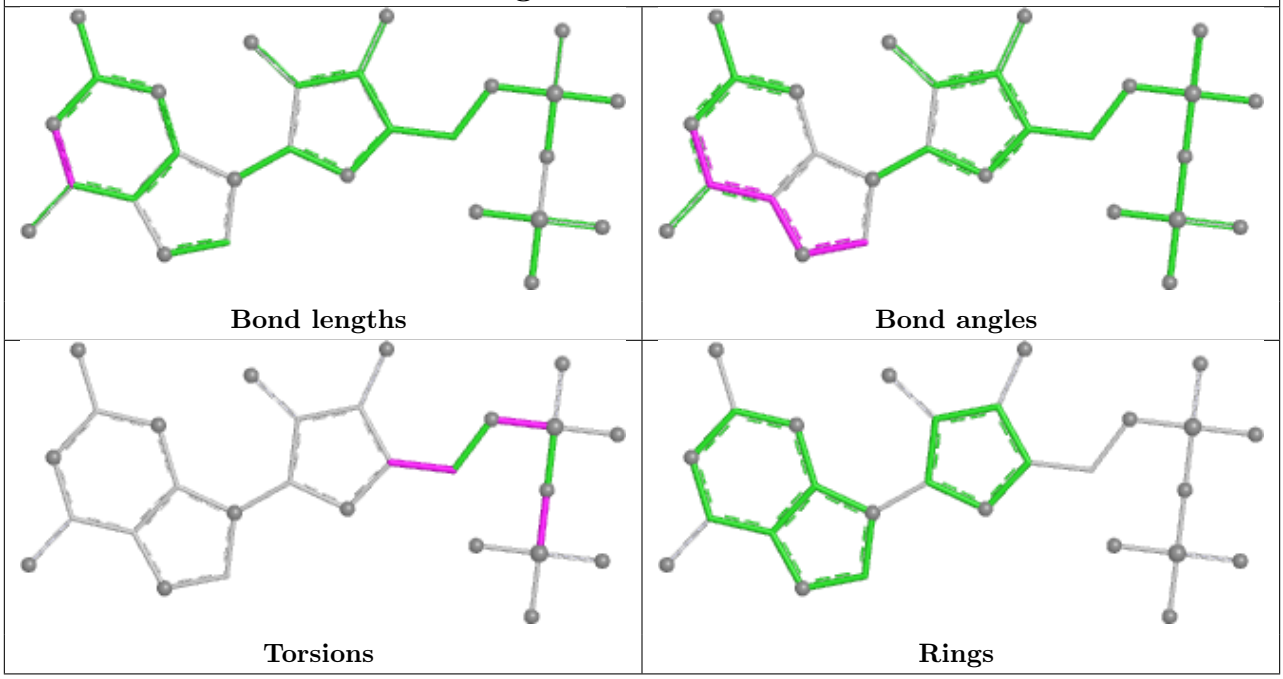

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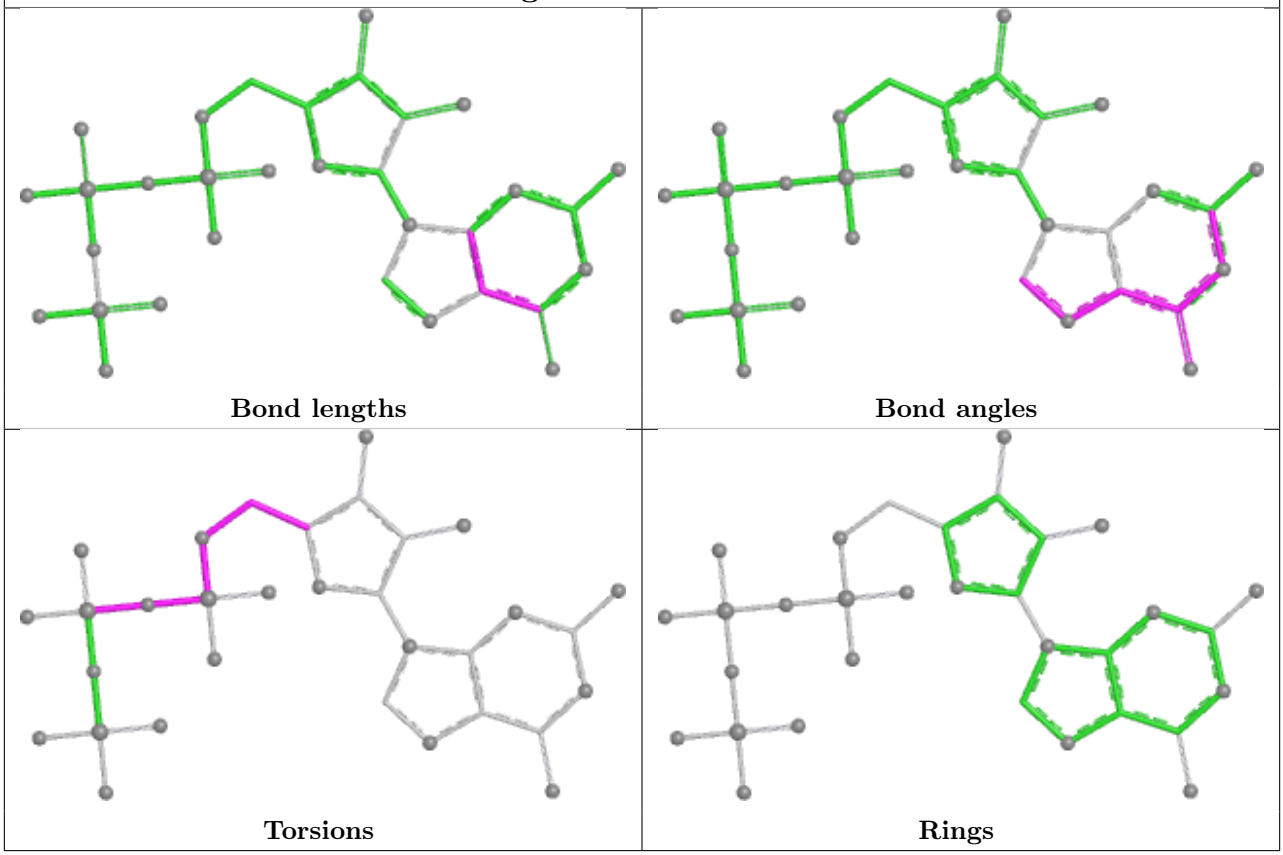

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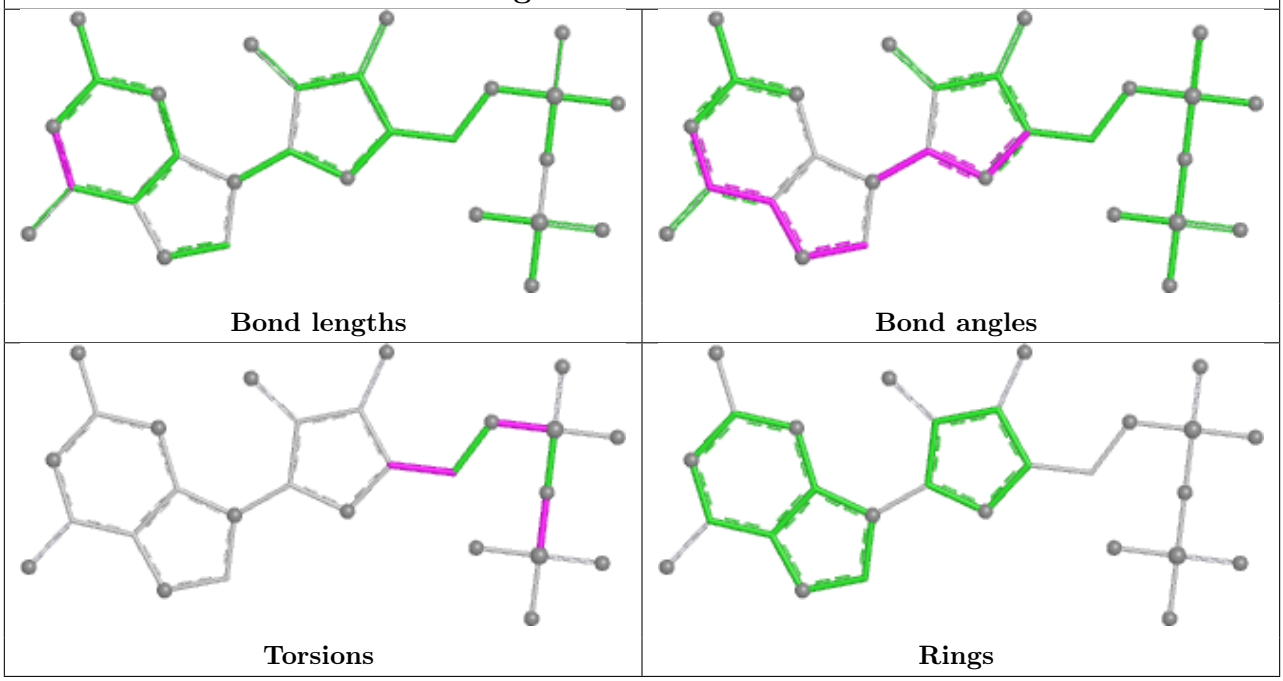

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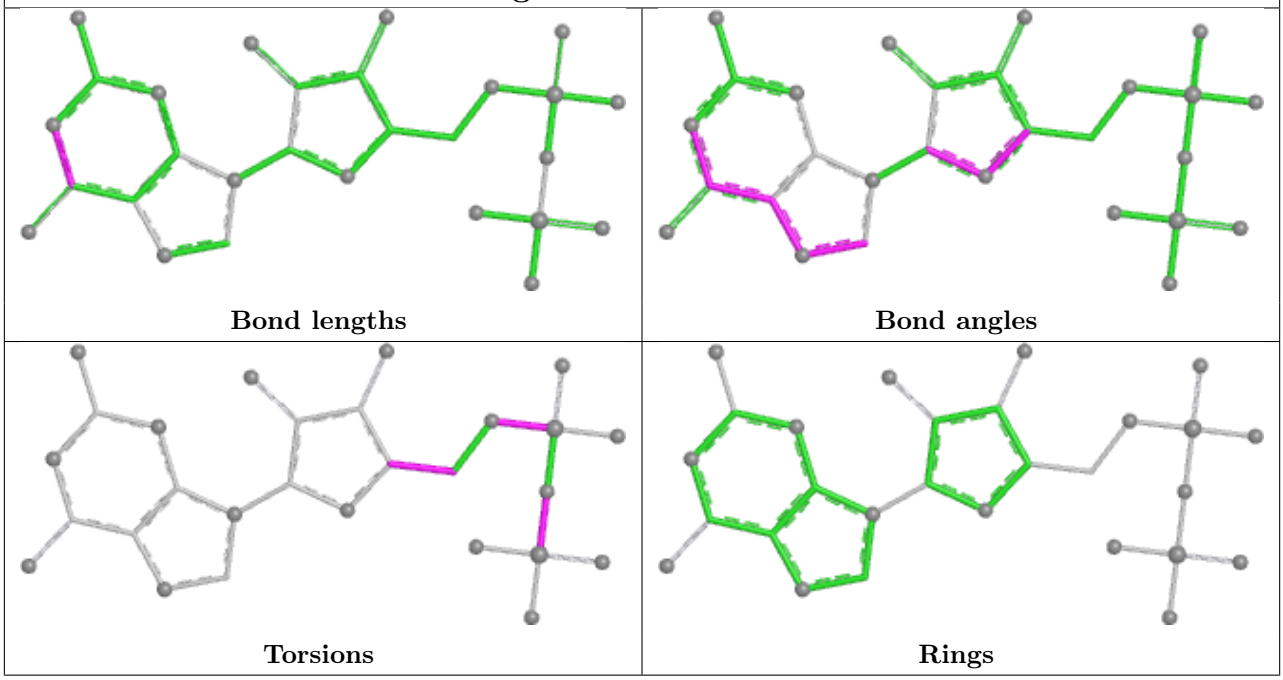

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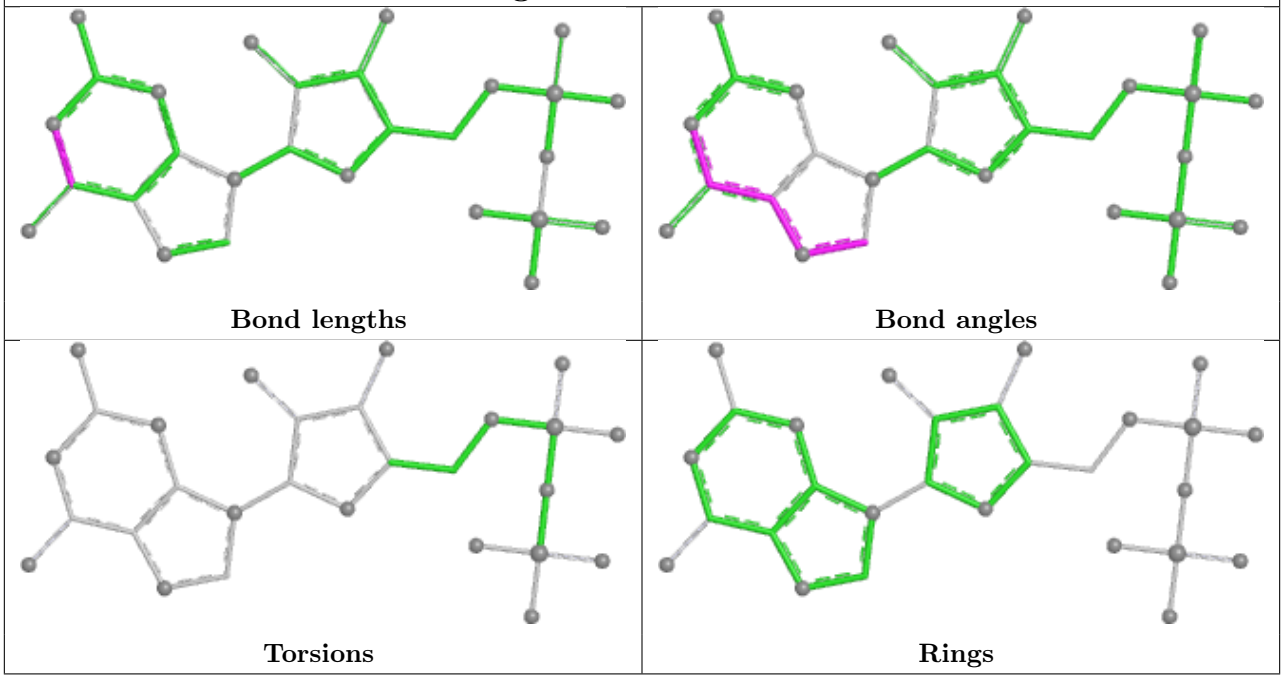

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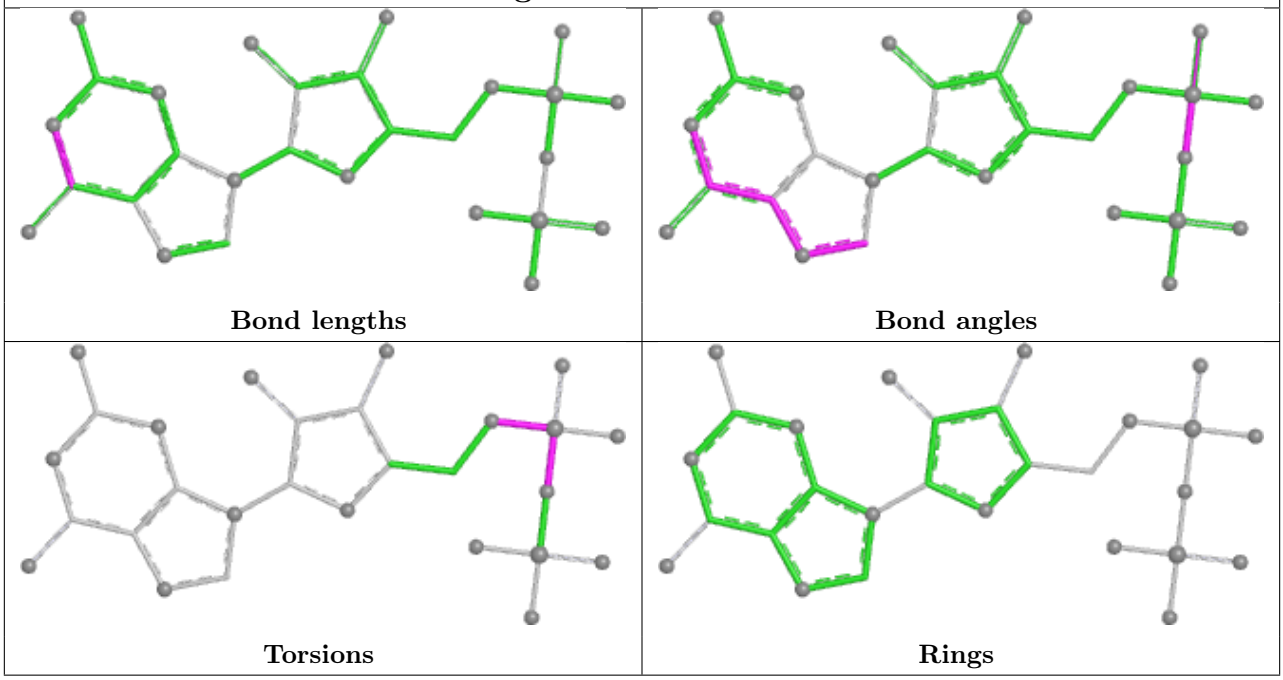

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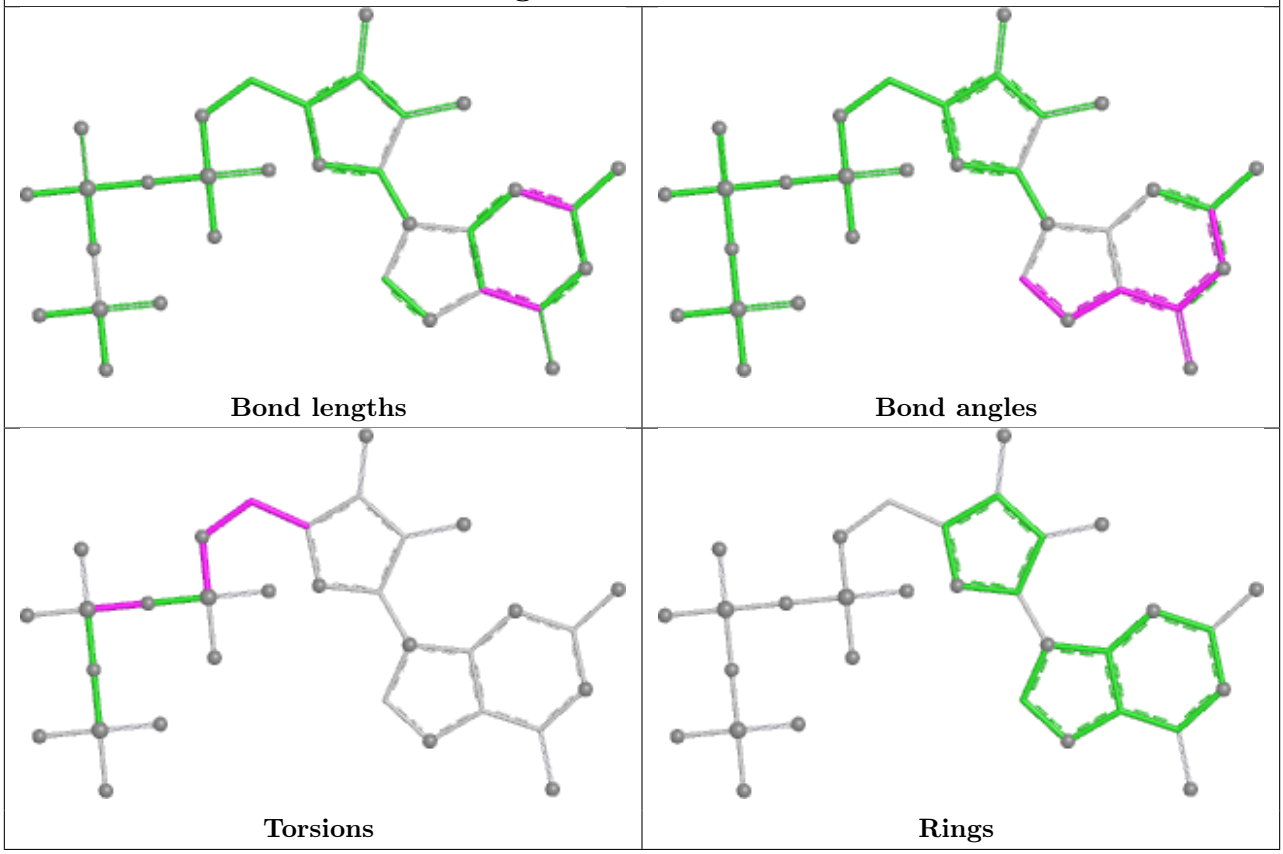

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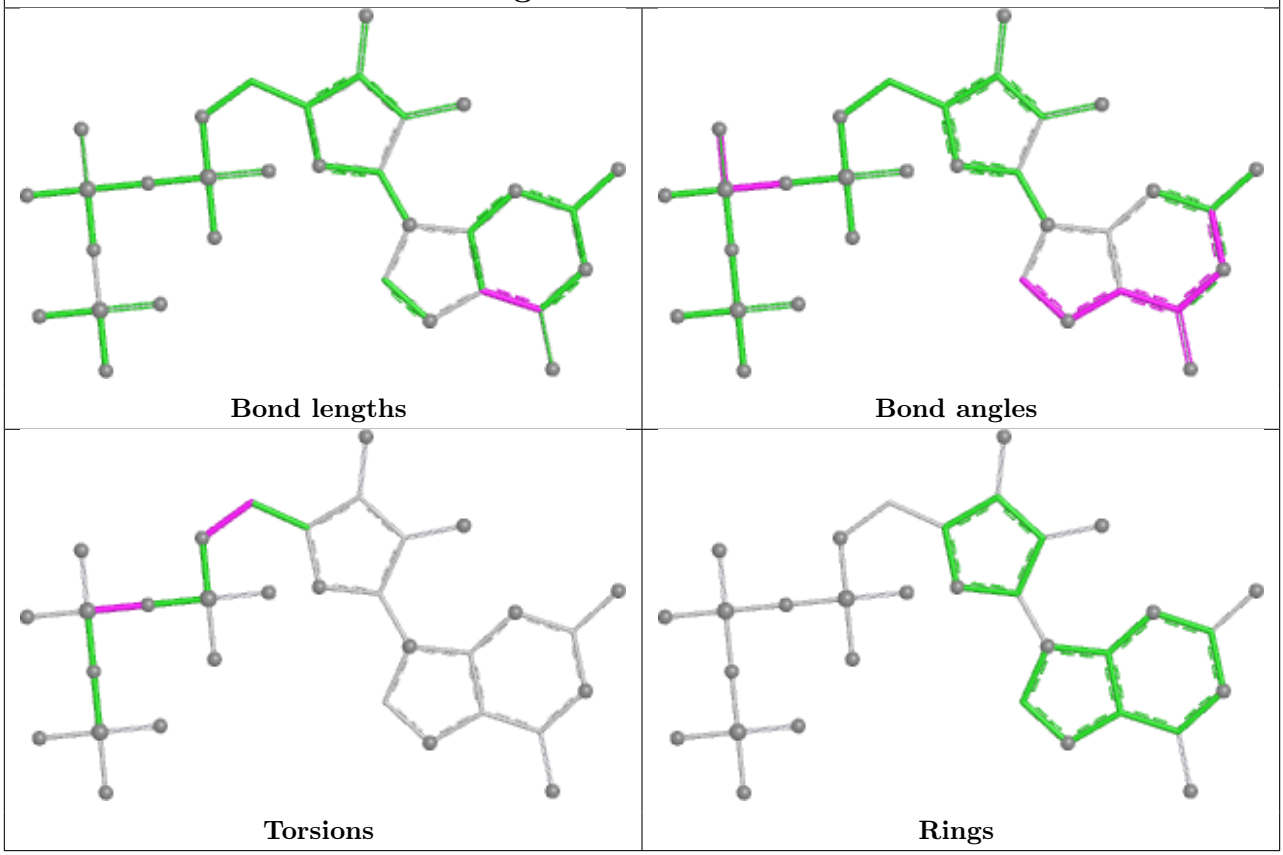
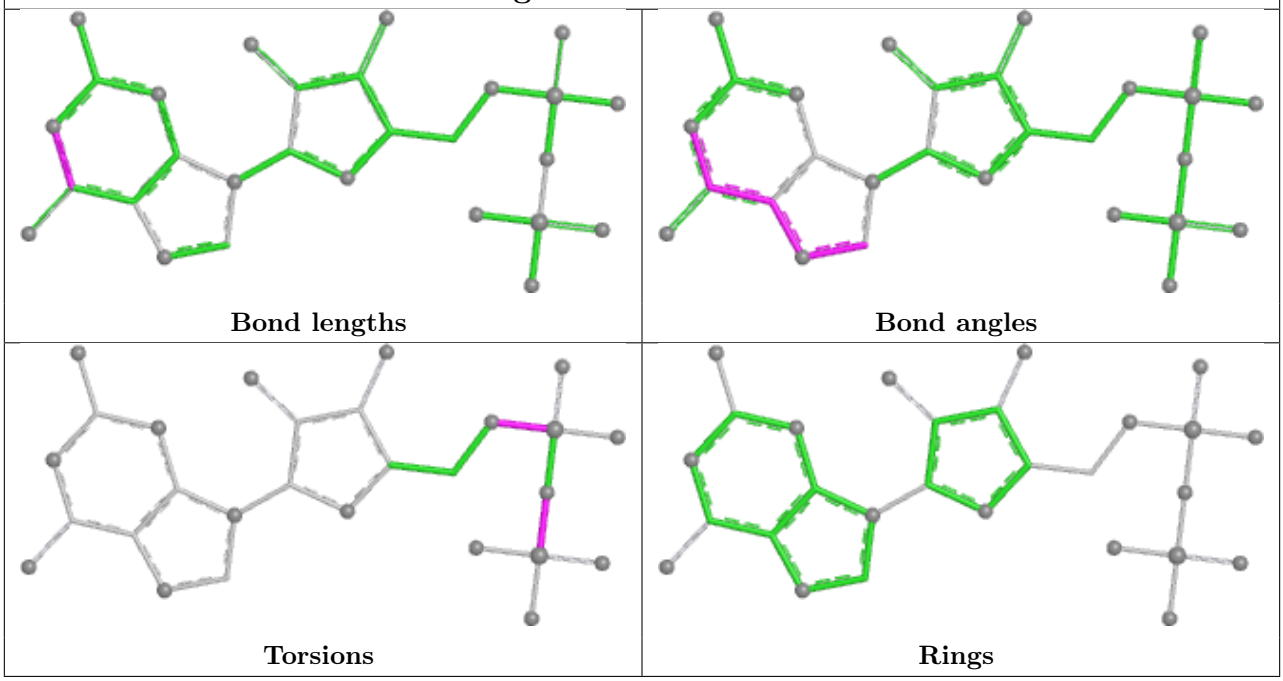
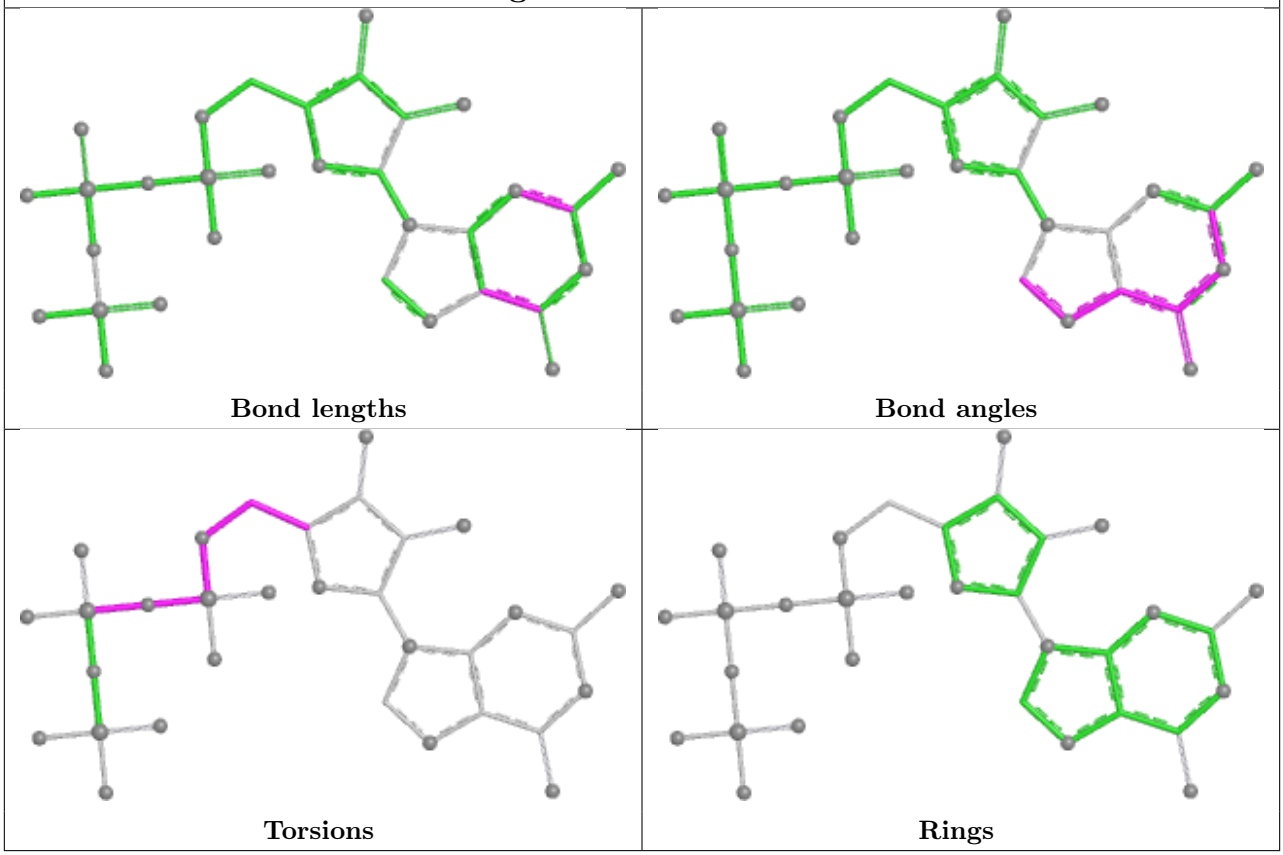


Ligand GDP B1 501



Ligand GTP W0 501



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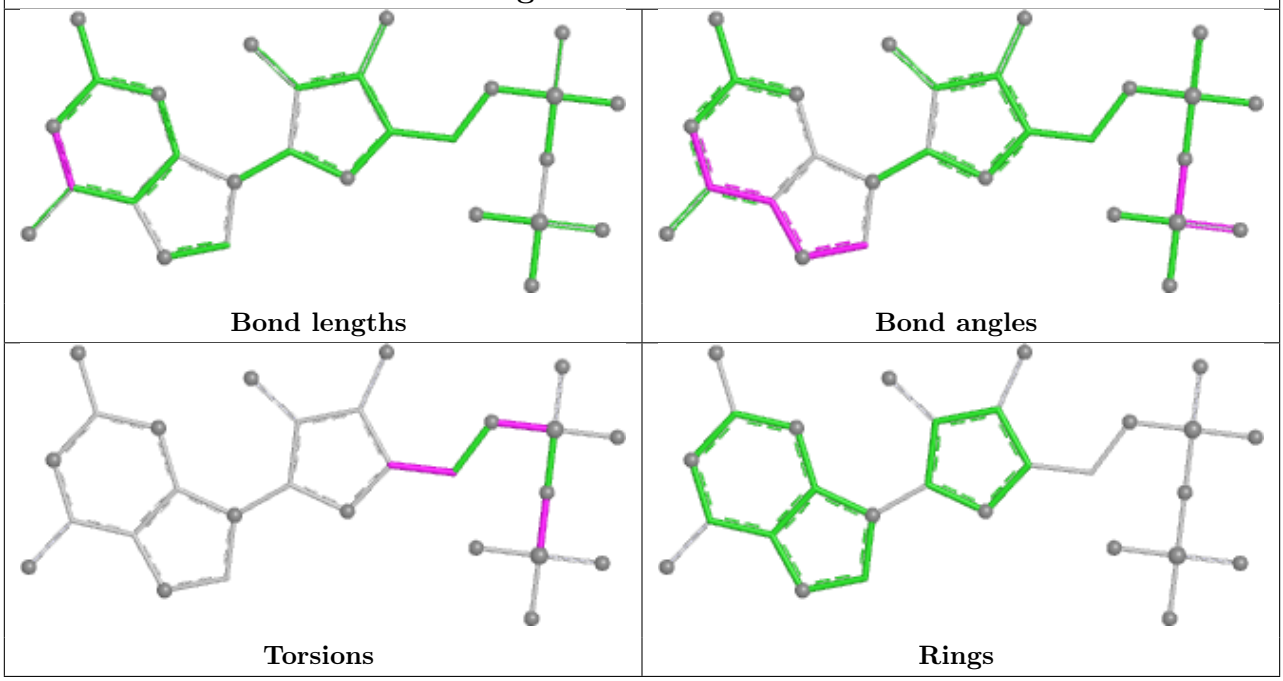
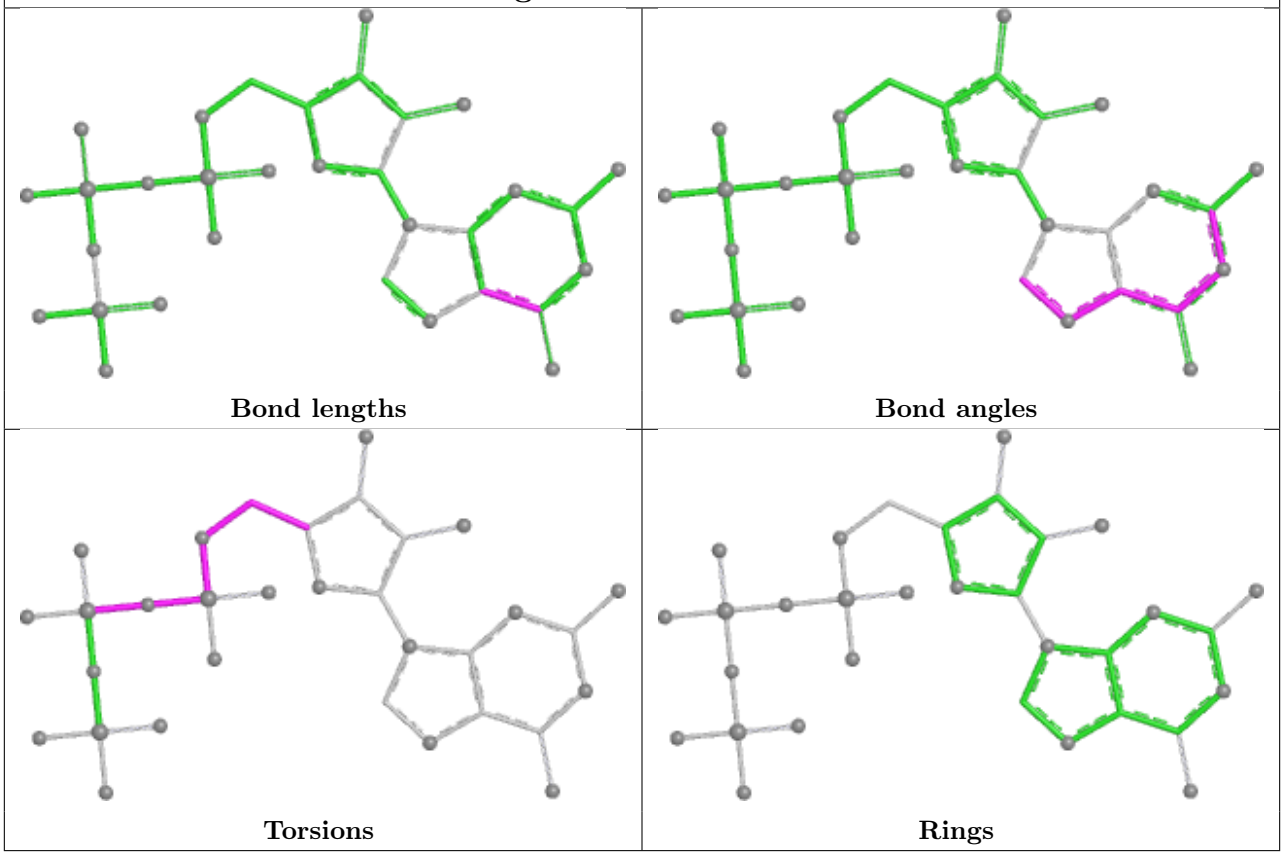


Ligand GTP 2C 501



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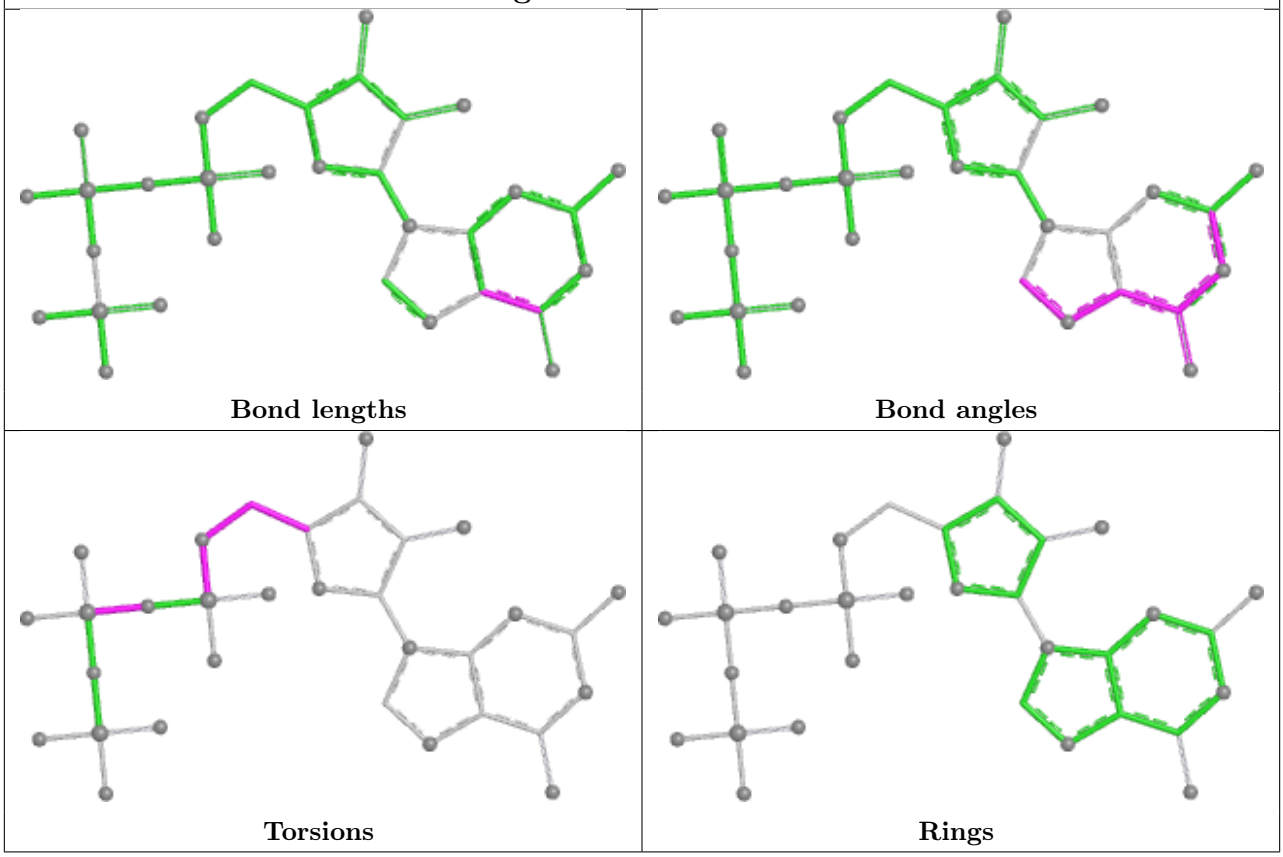

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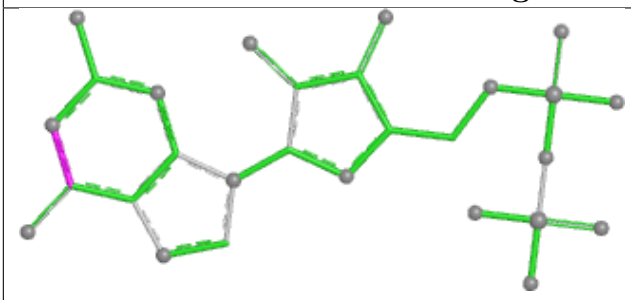
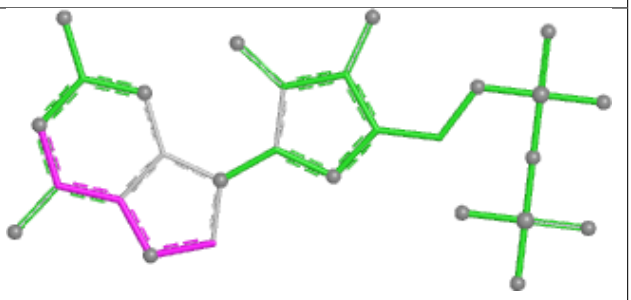
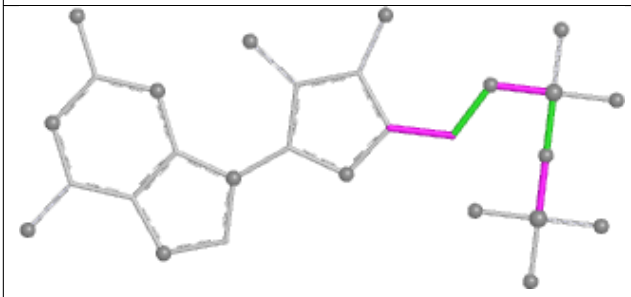
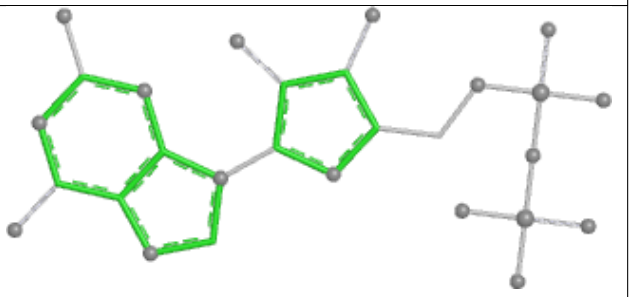
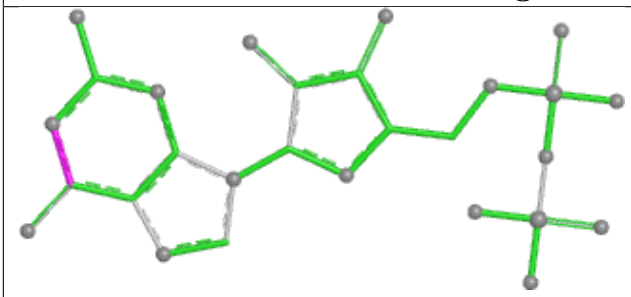
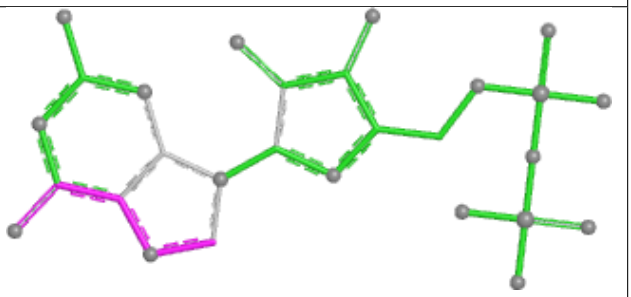
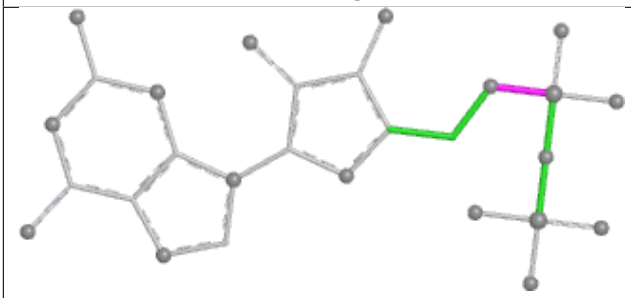
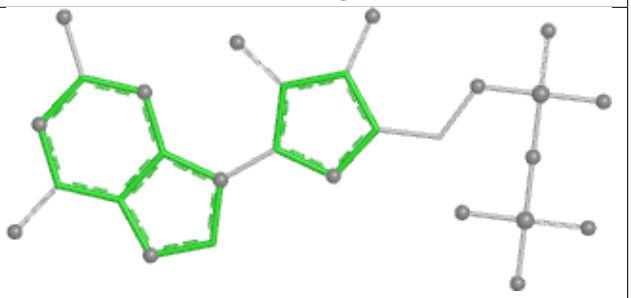
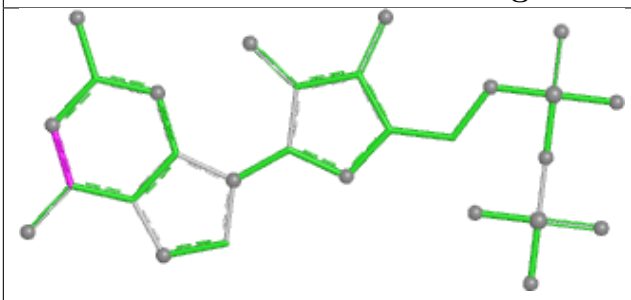
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP Z4 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP H8 503



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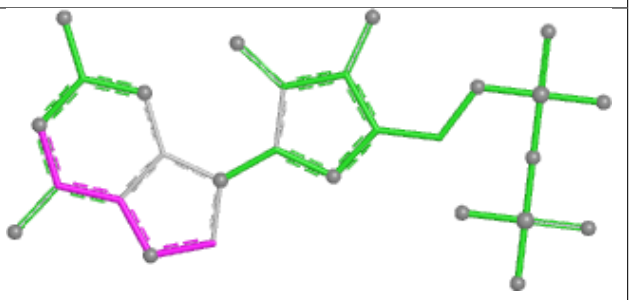

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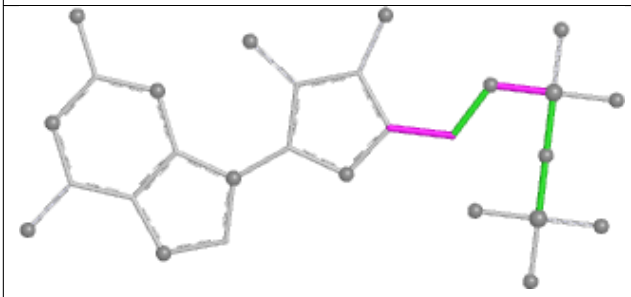

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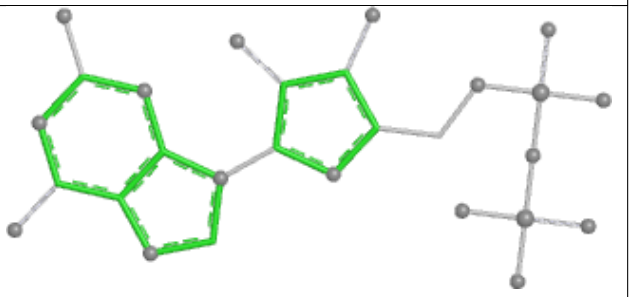
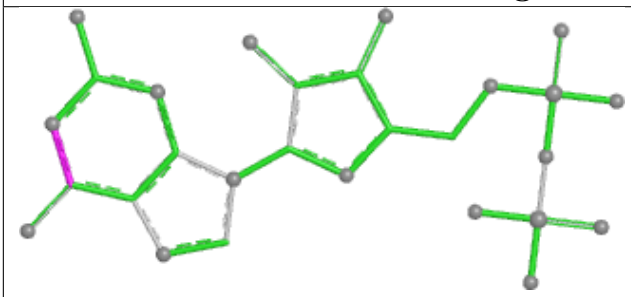


Rings

Ligand GDP E4 502



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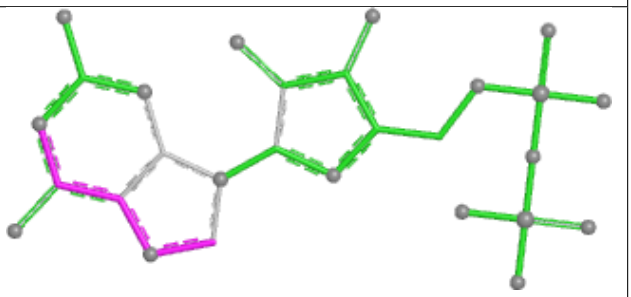

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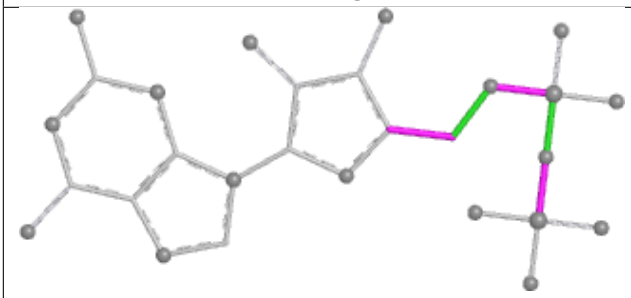

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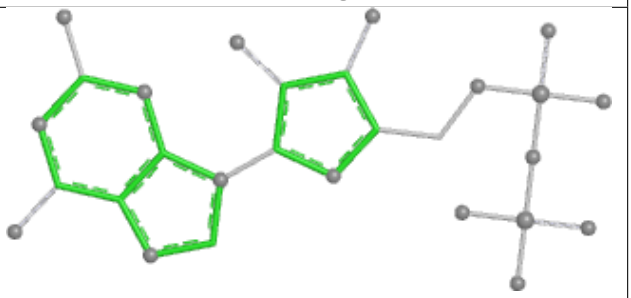
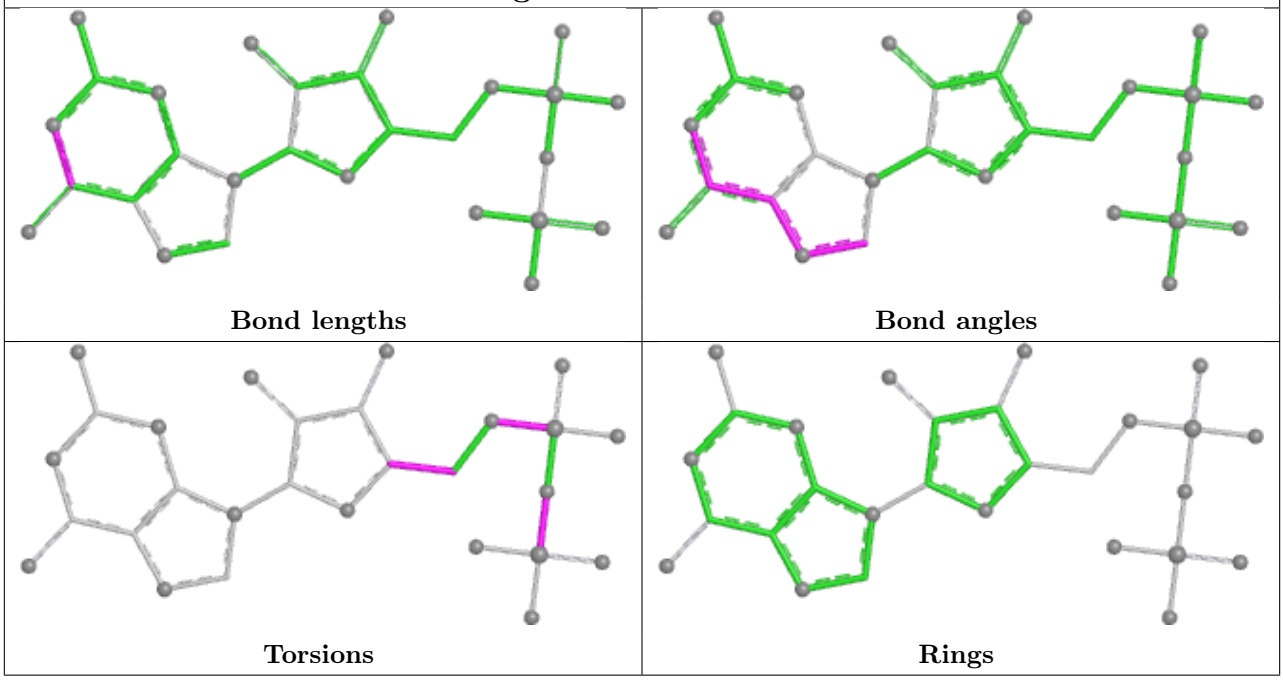
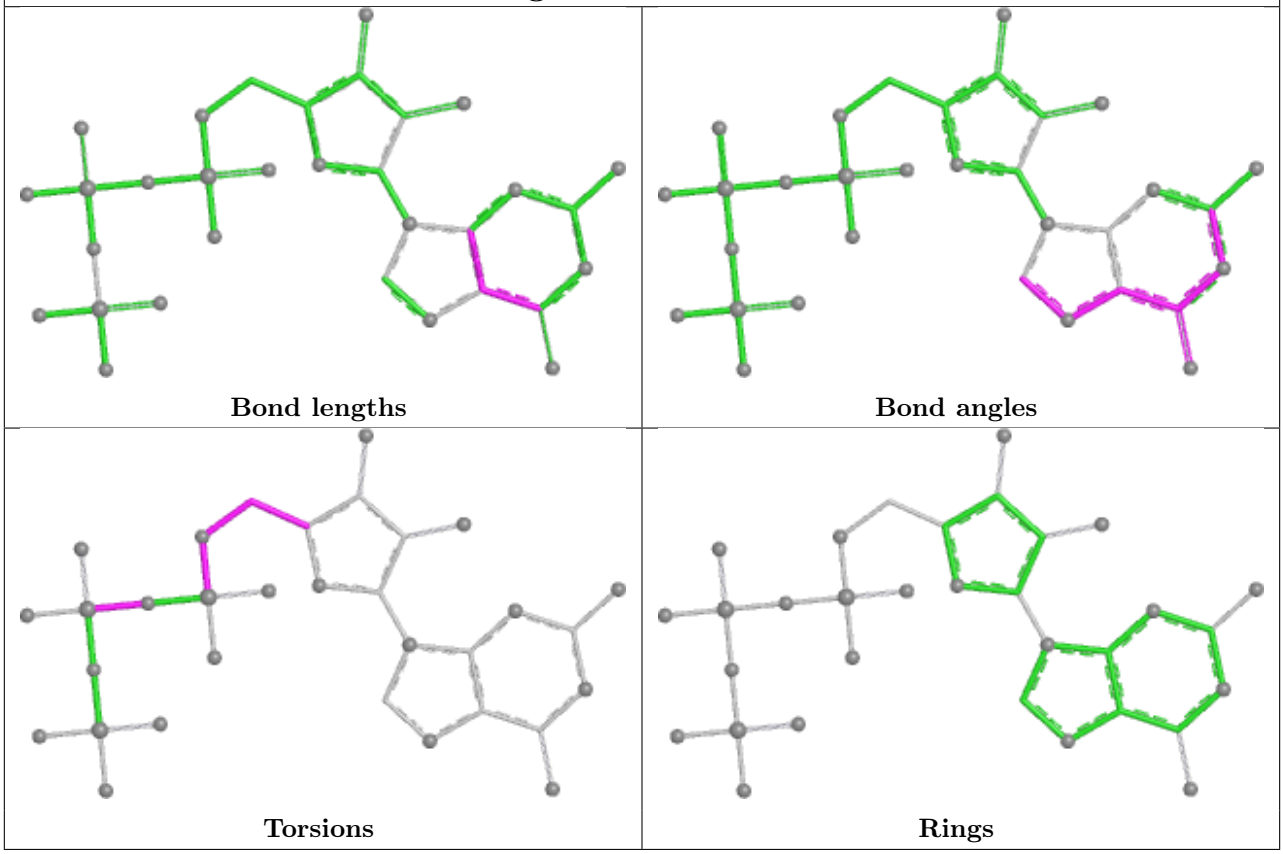


Rings

Ligand GDP O4 502



Ligand GTP 7 501



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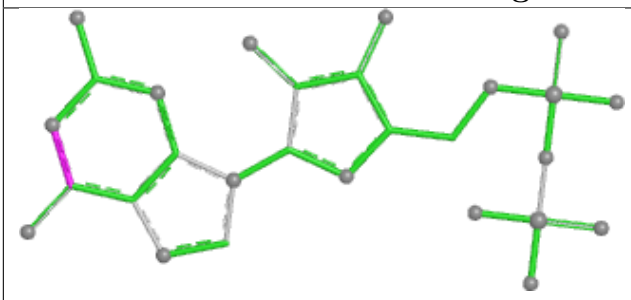
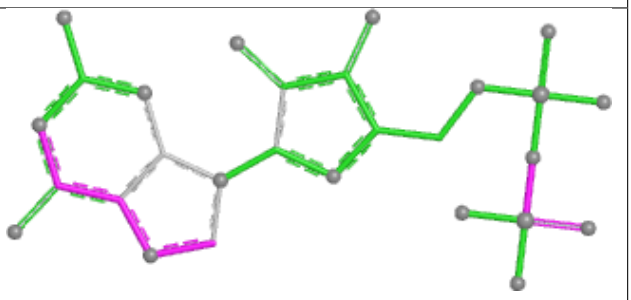
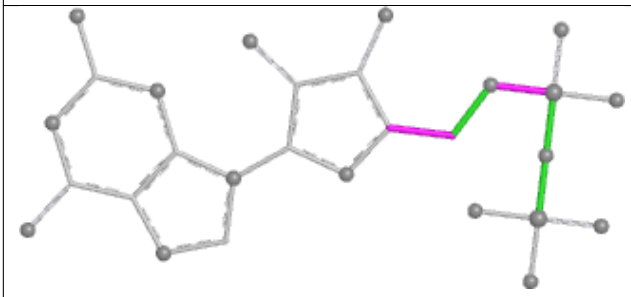
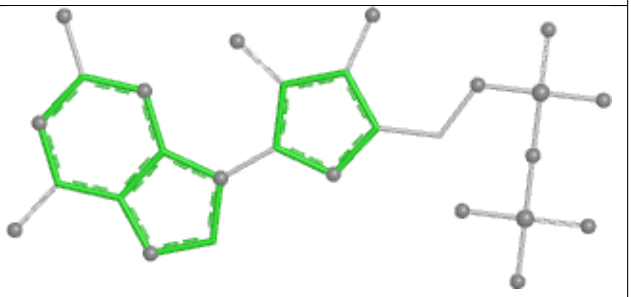
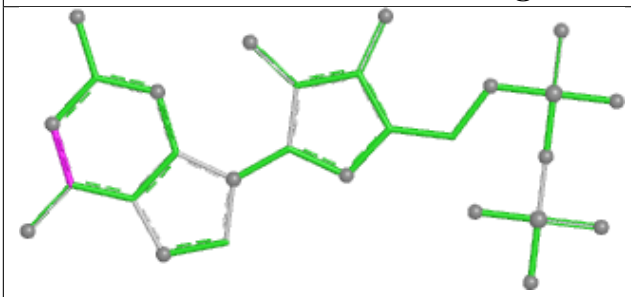
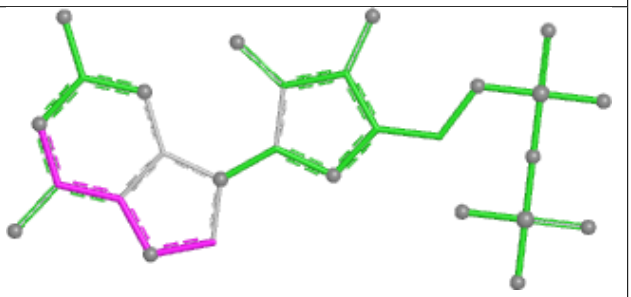
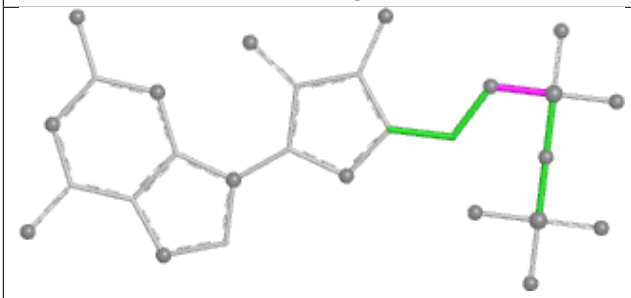
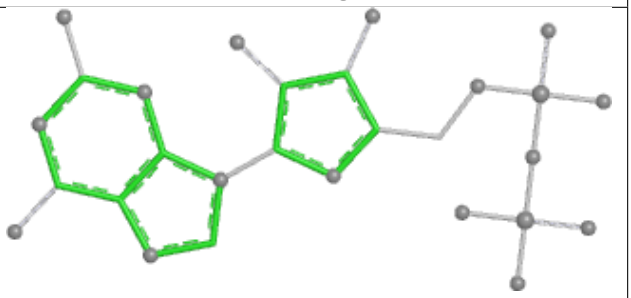
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP Z8 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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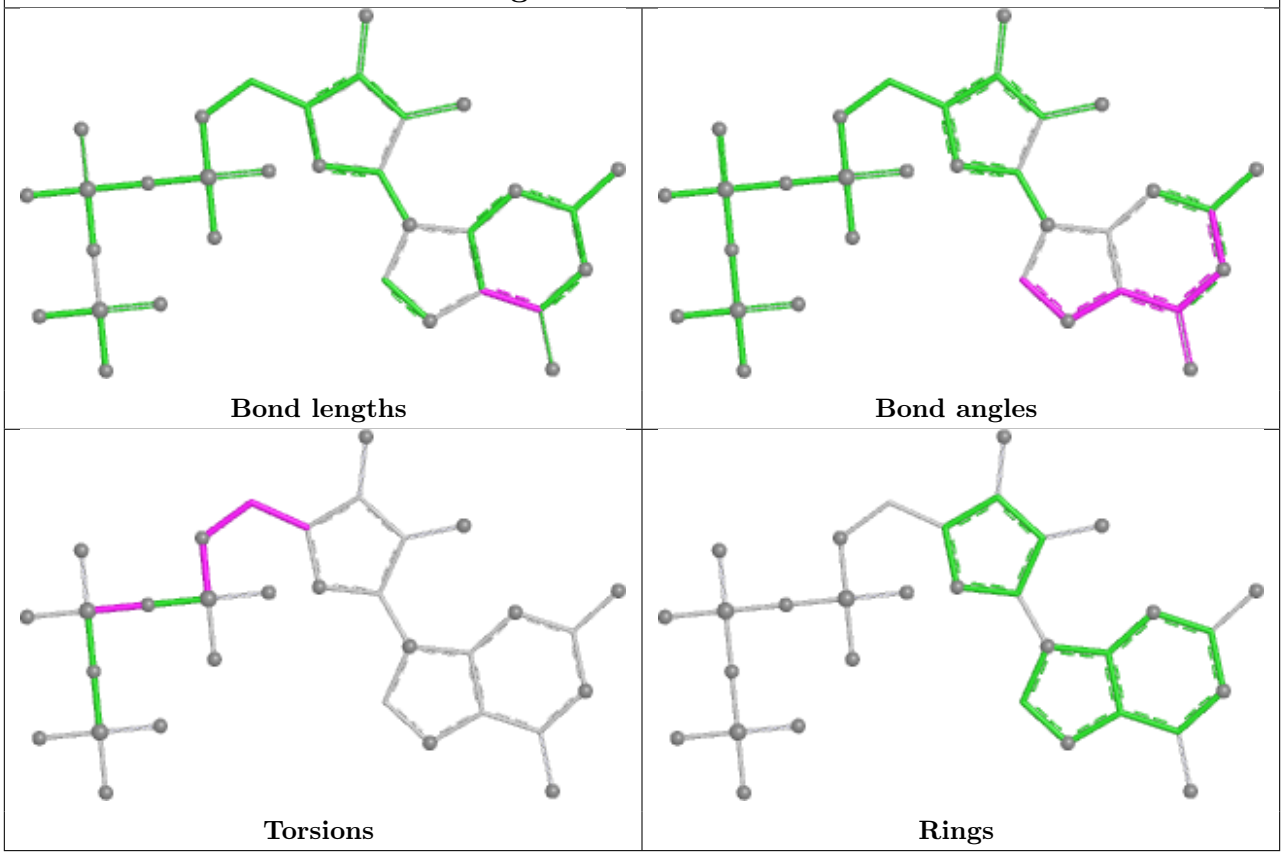

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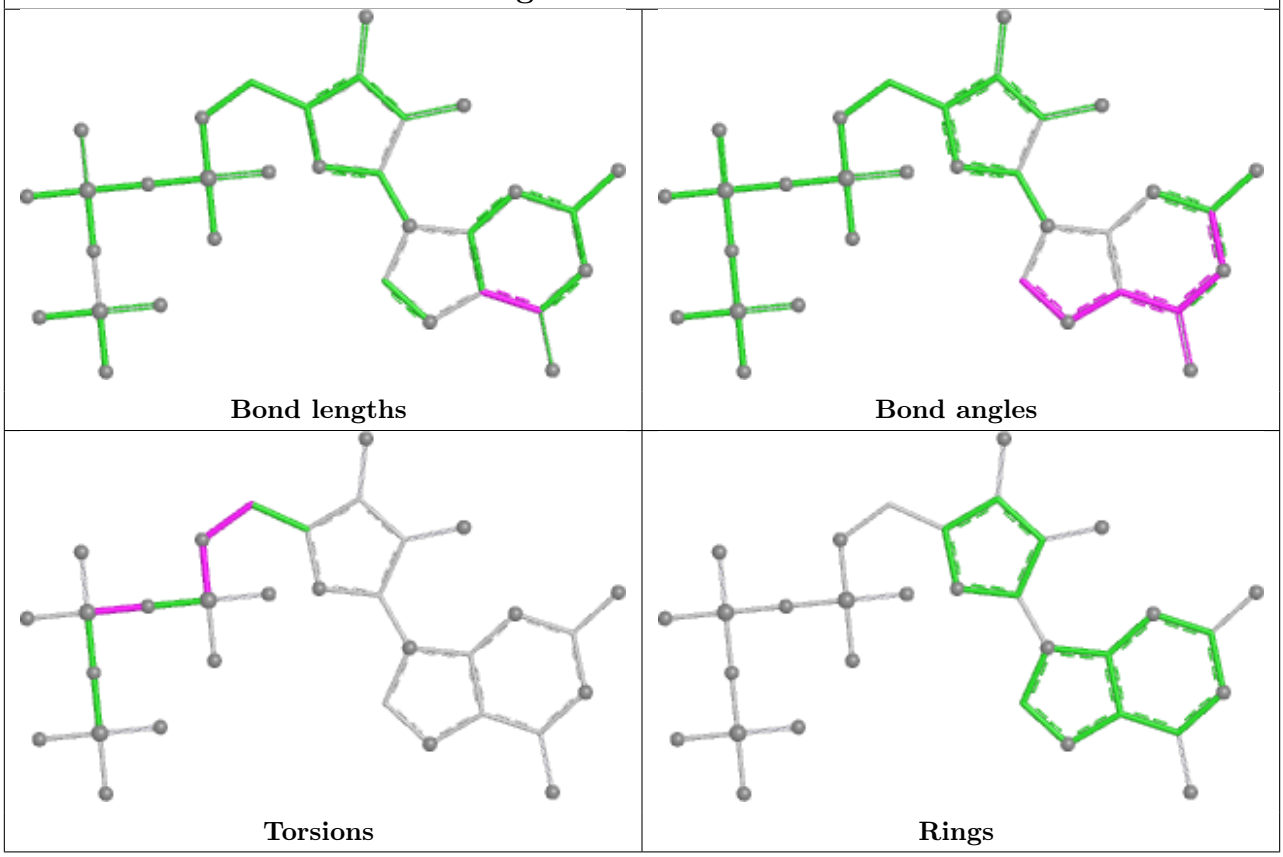
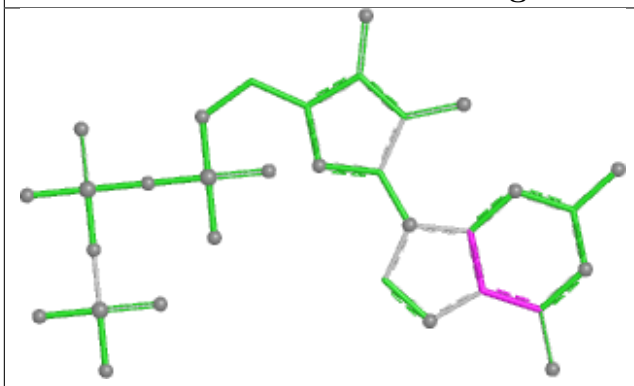
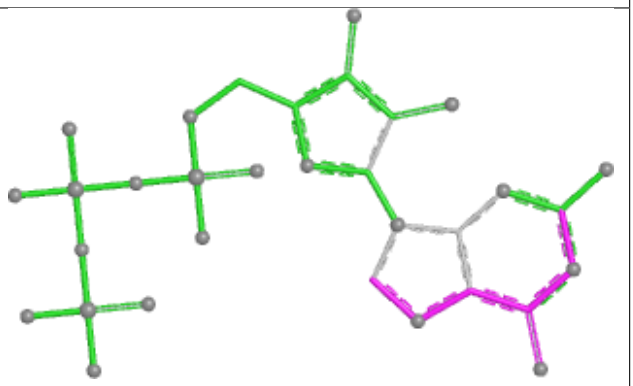


Ligand GTP 2W 501



Bond lengths



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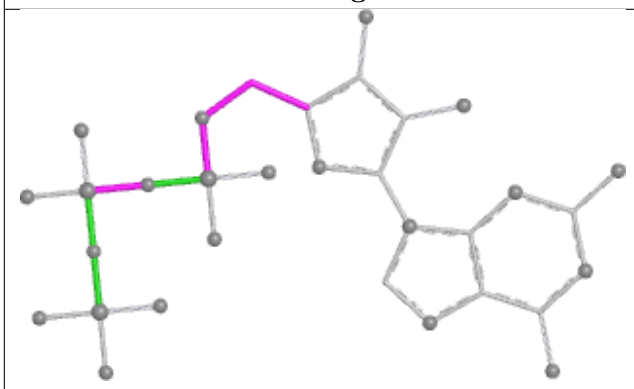

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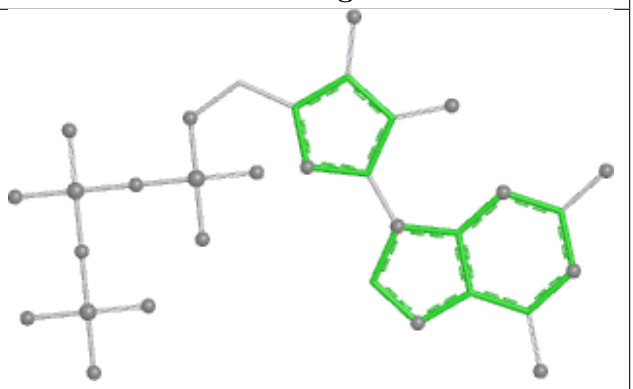

Rings

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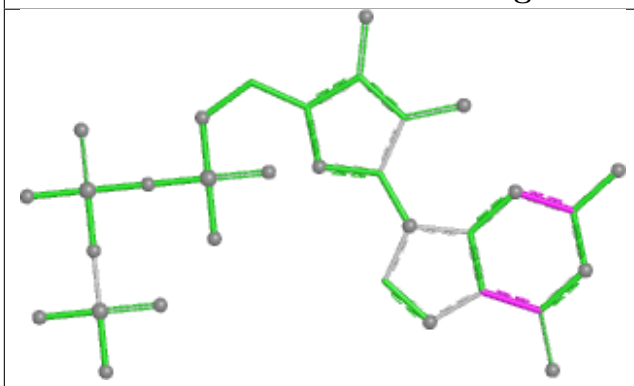

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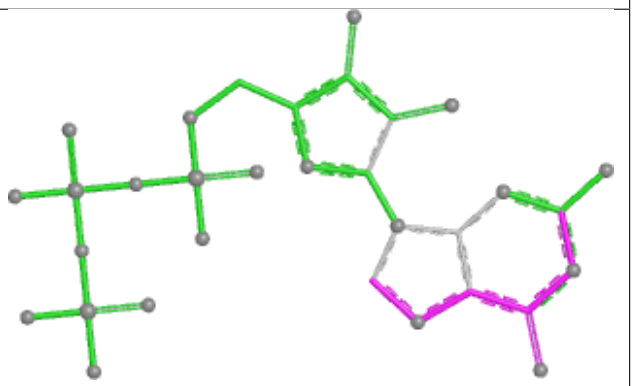

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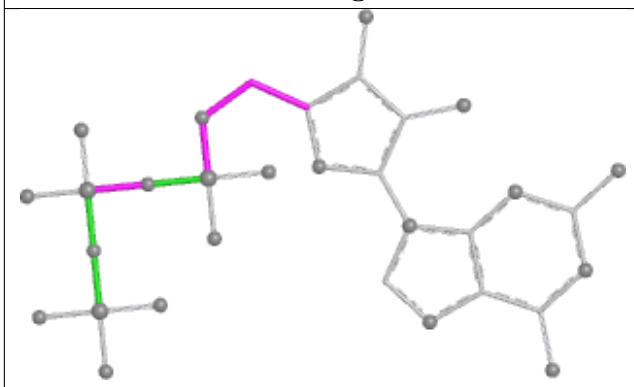

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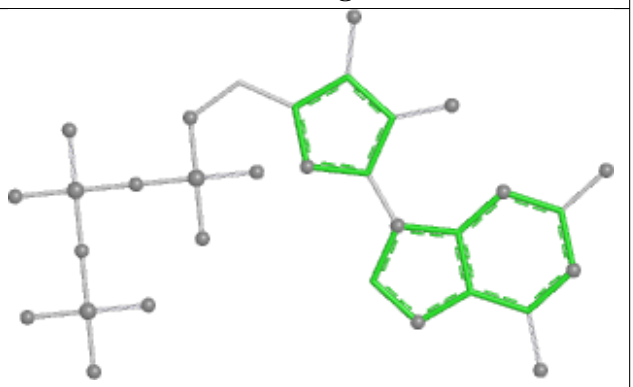

Rings

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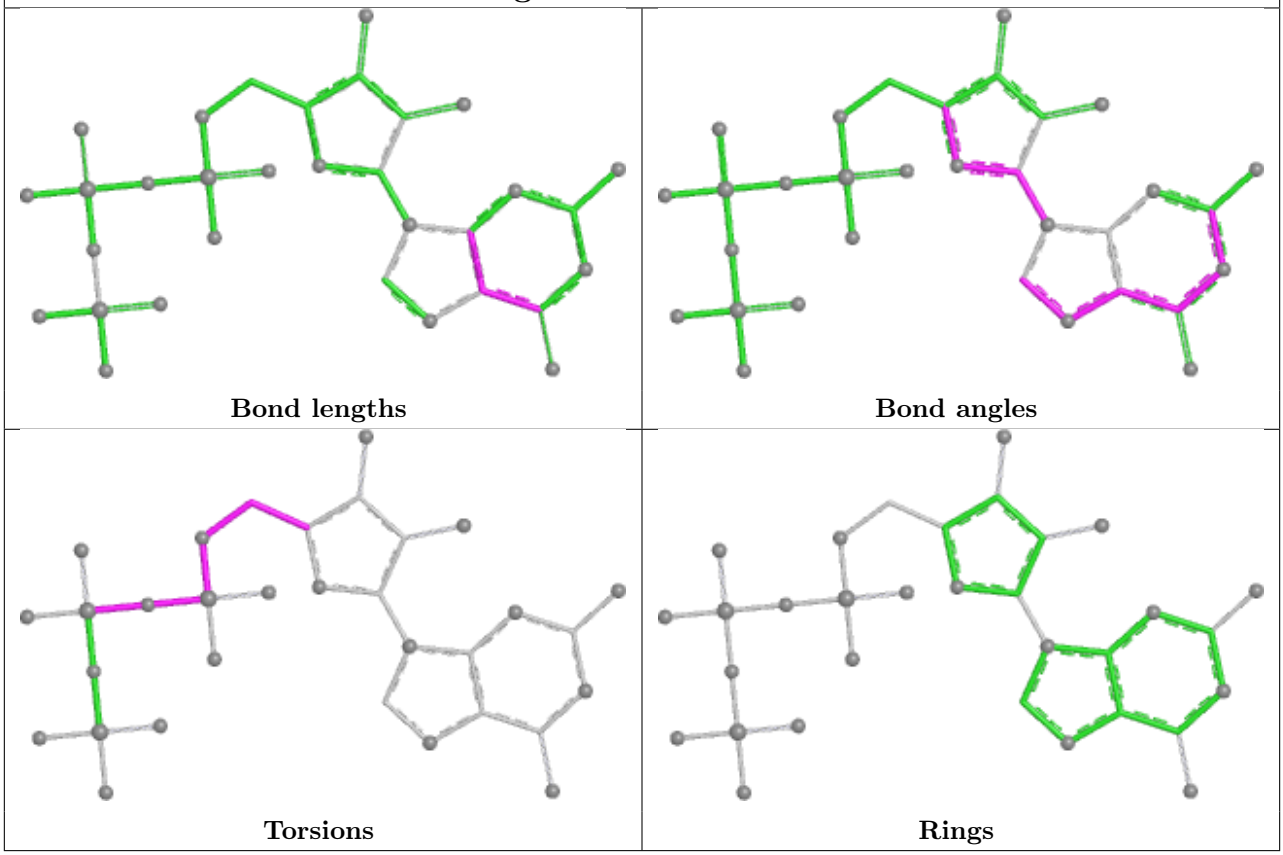

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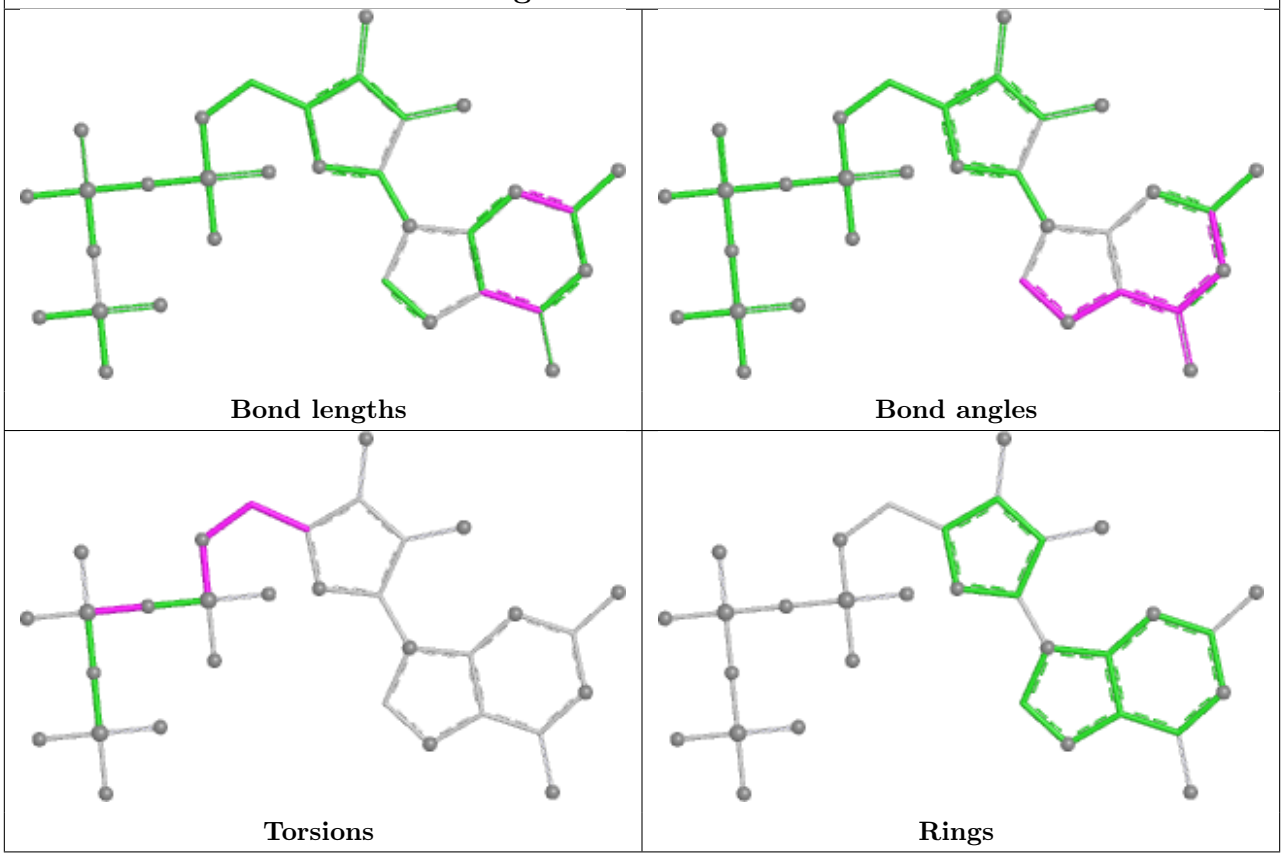

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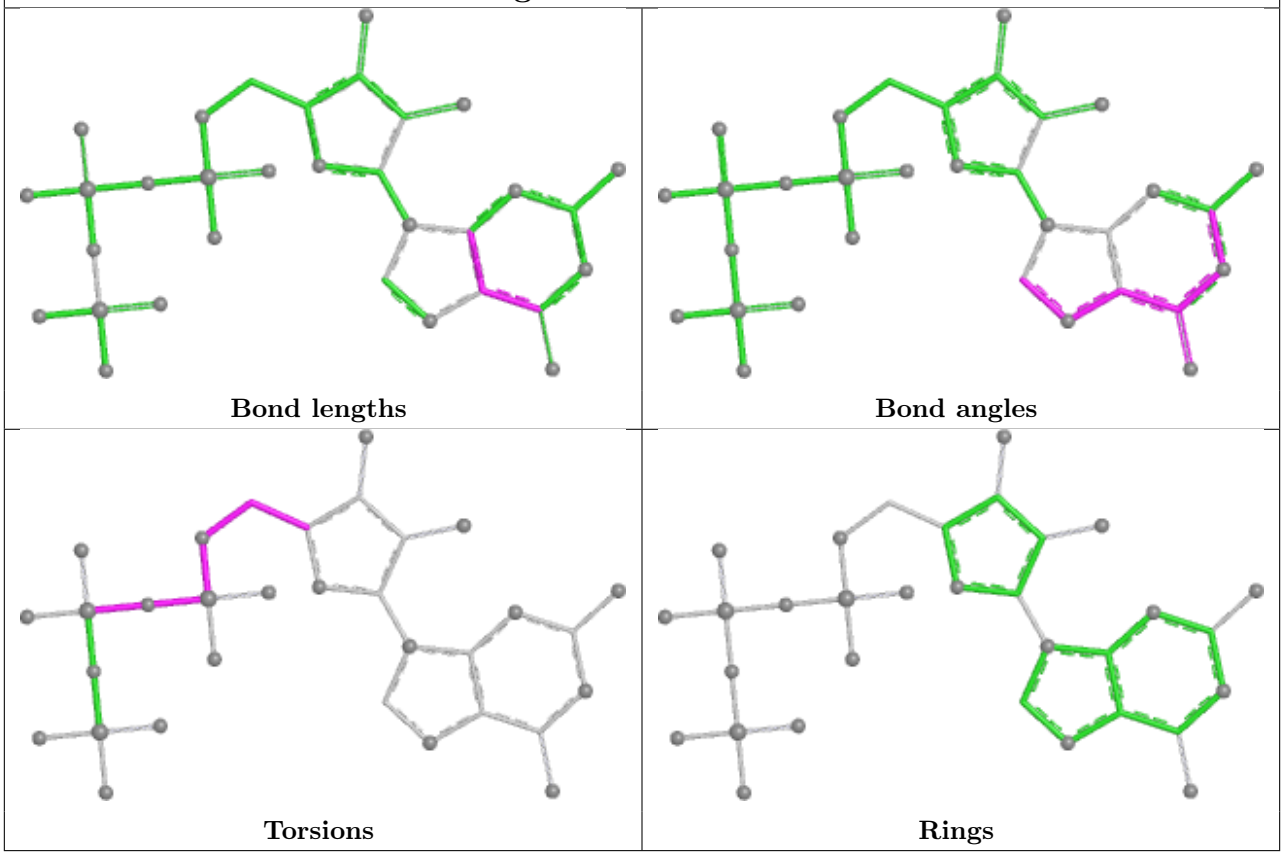

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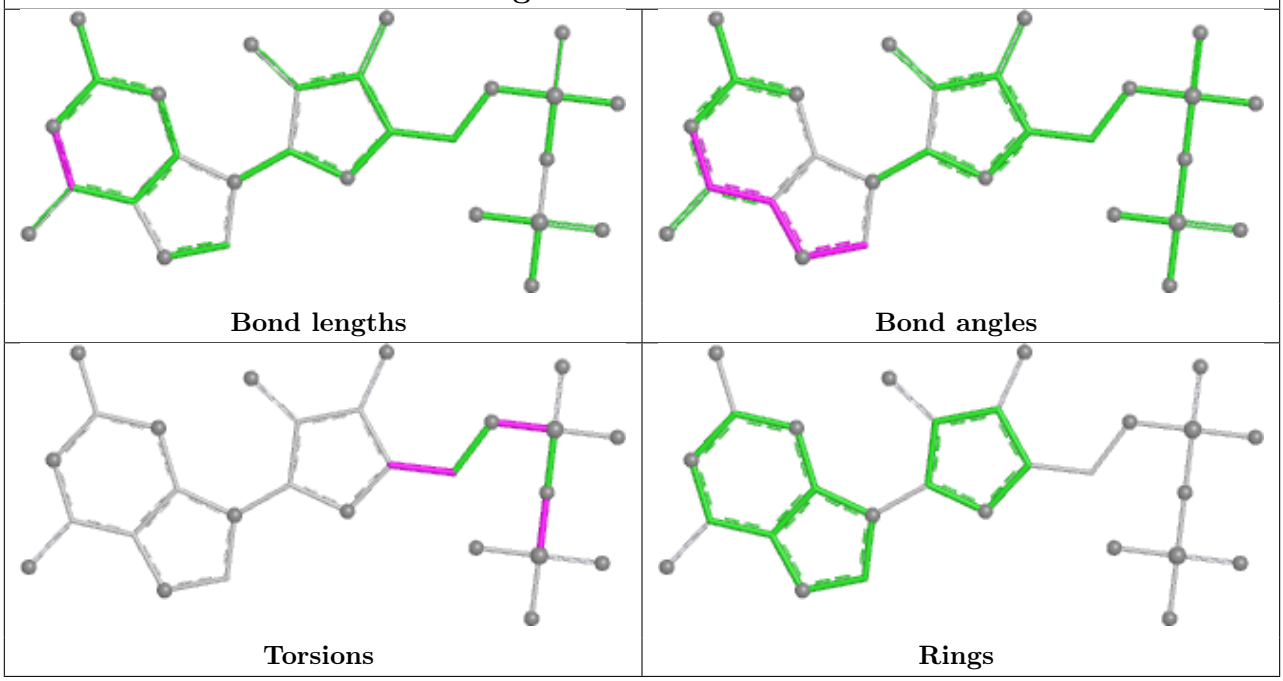

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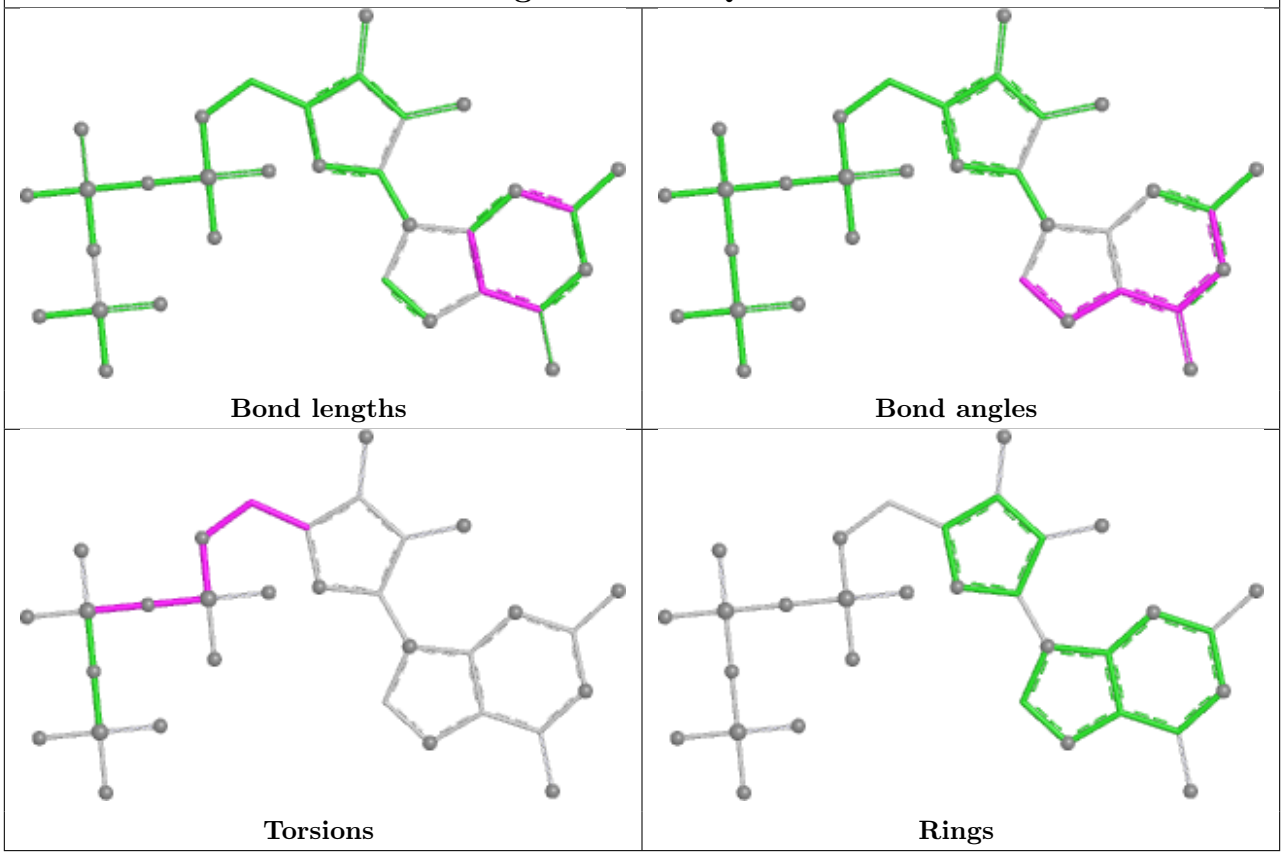

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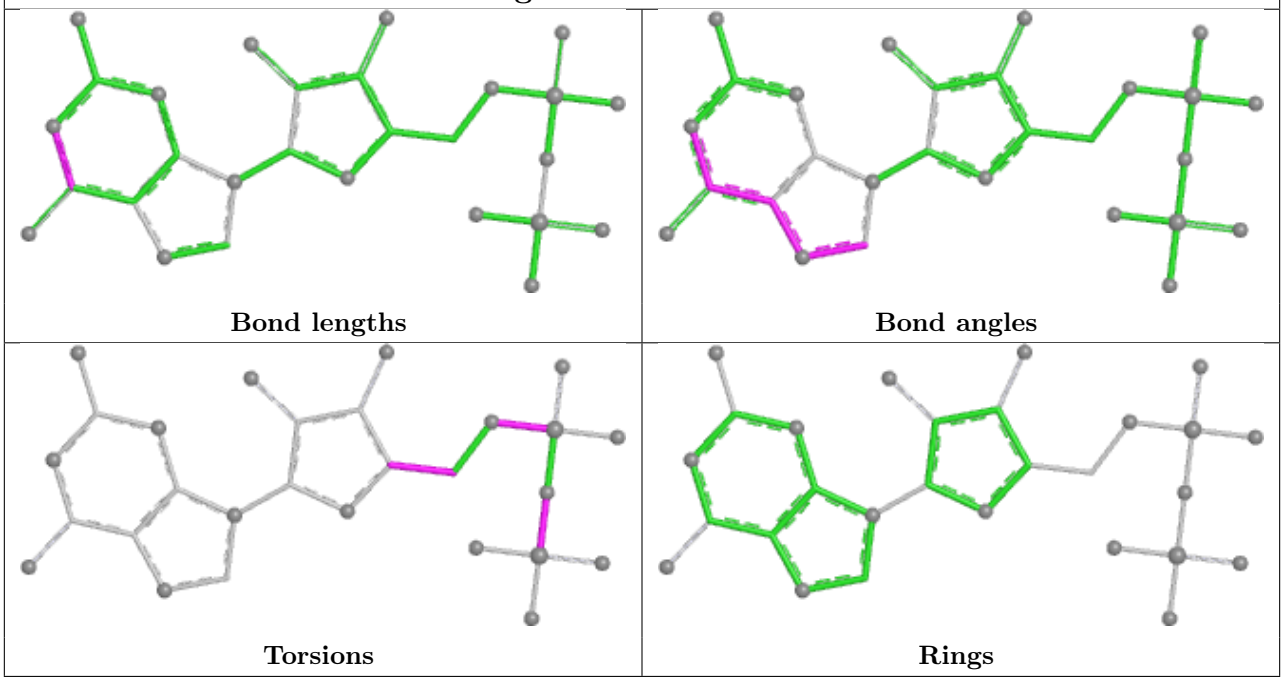

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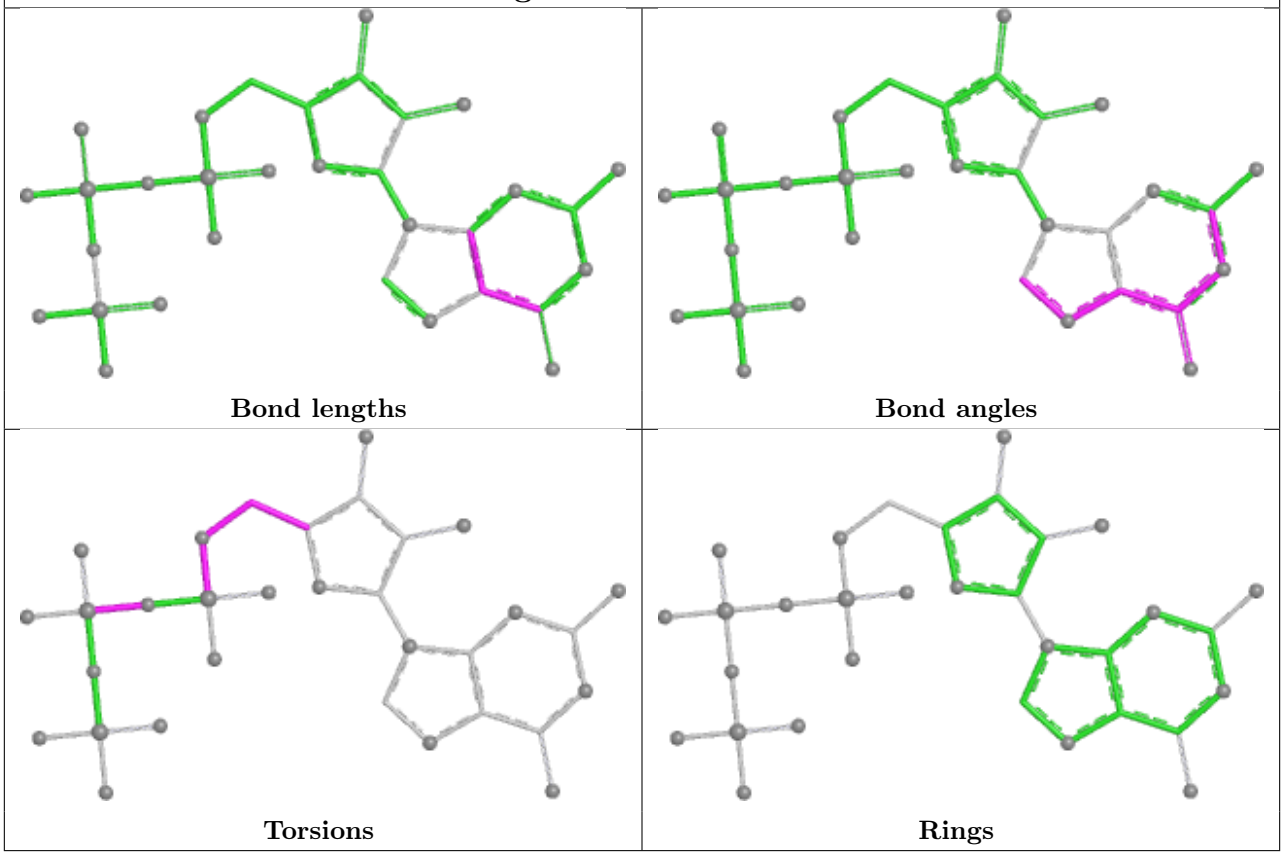

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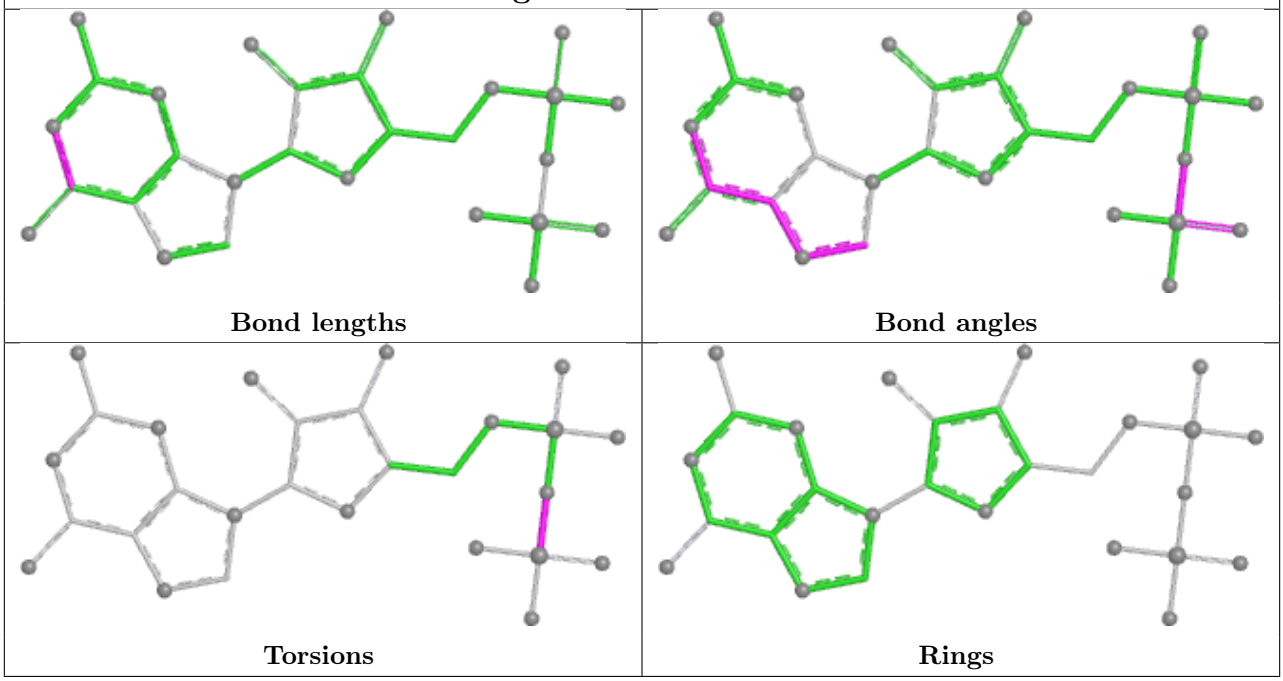

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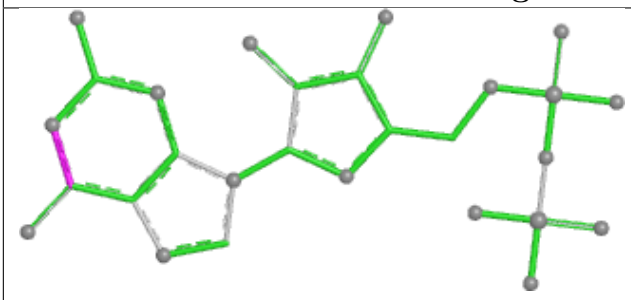
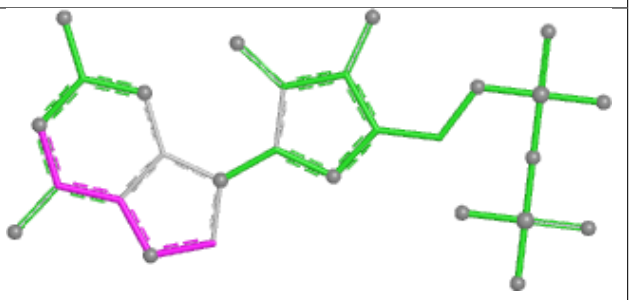
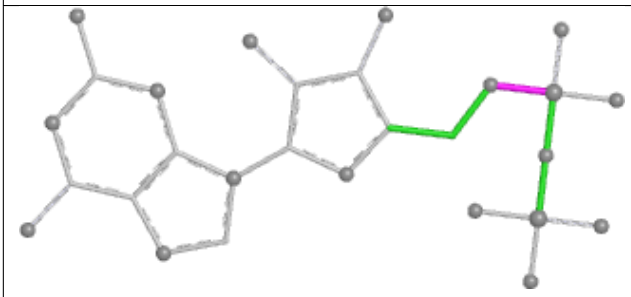
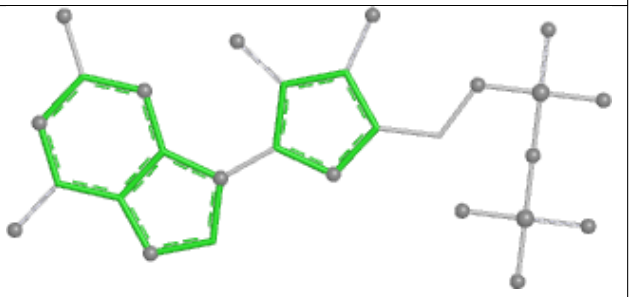
 Bond lengths	 Bond angles
 Torsions	 Rings

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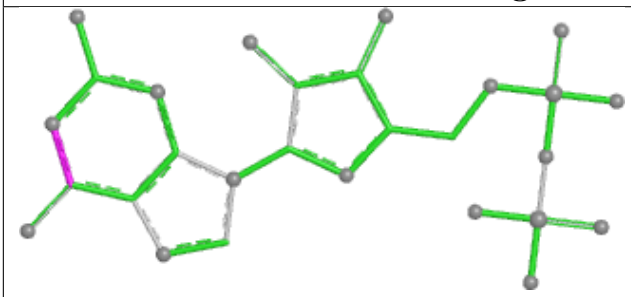
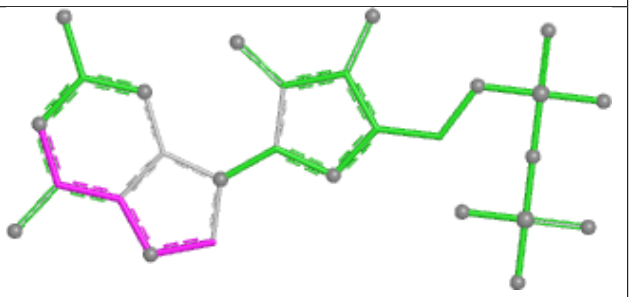
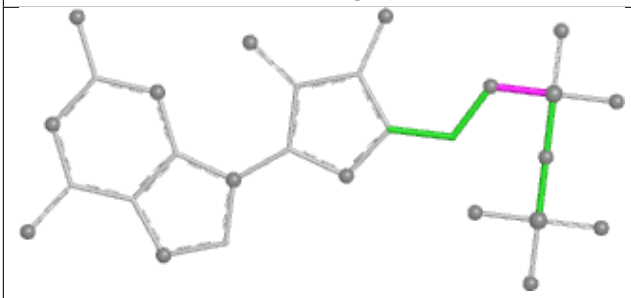
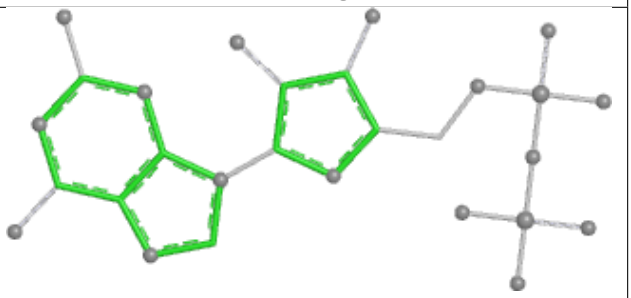
 Bond lengths	 Bond angles
 Torsions	 Rings

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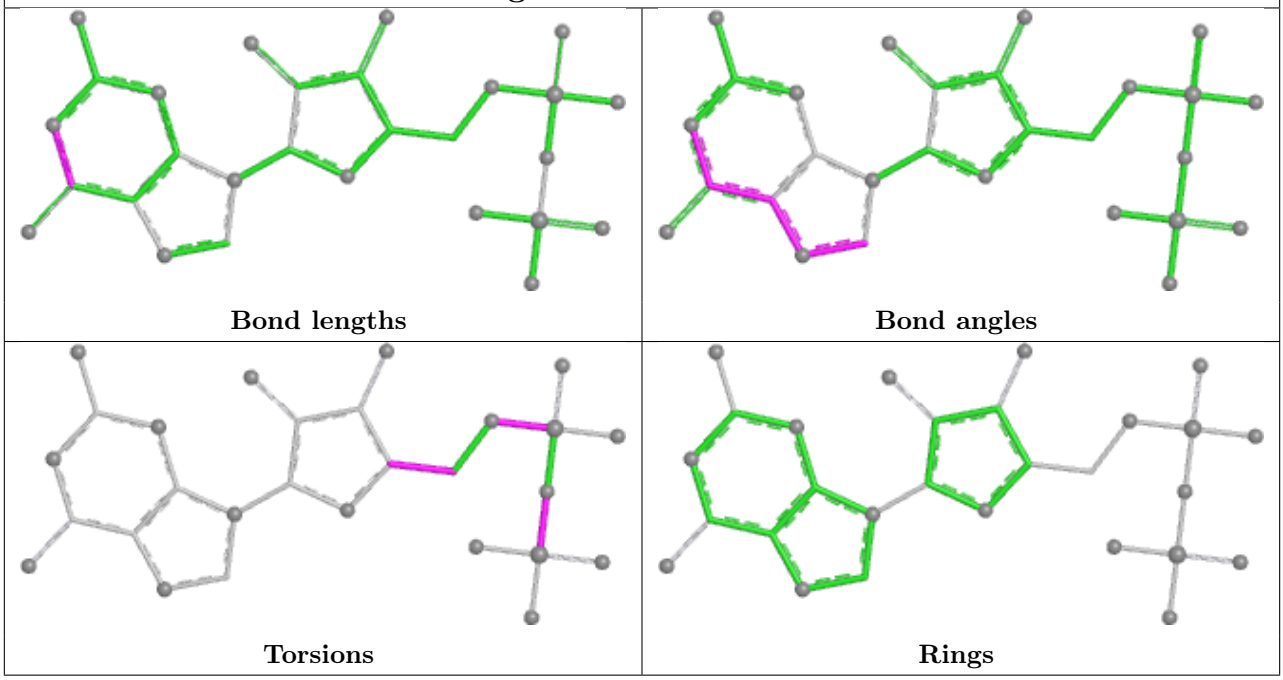

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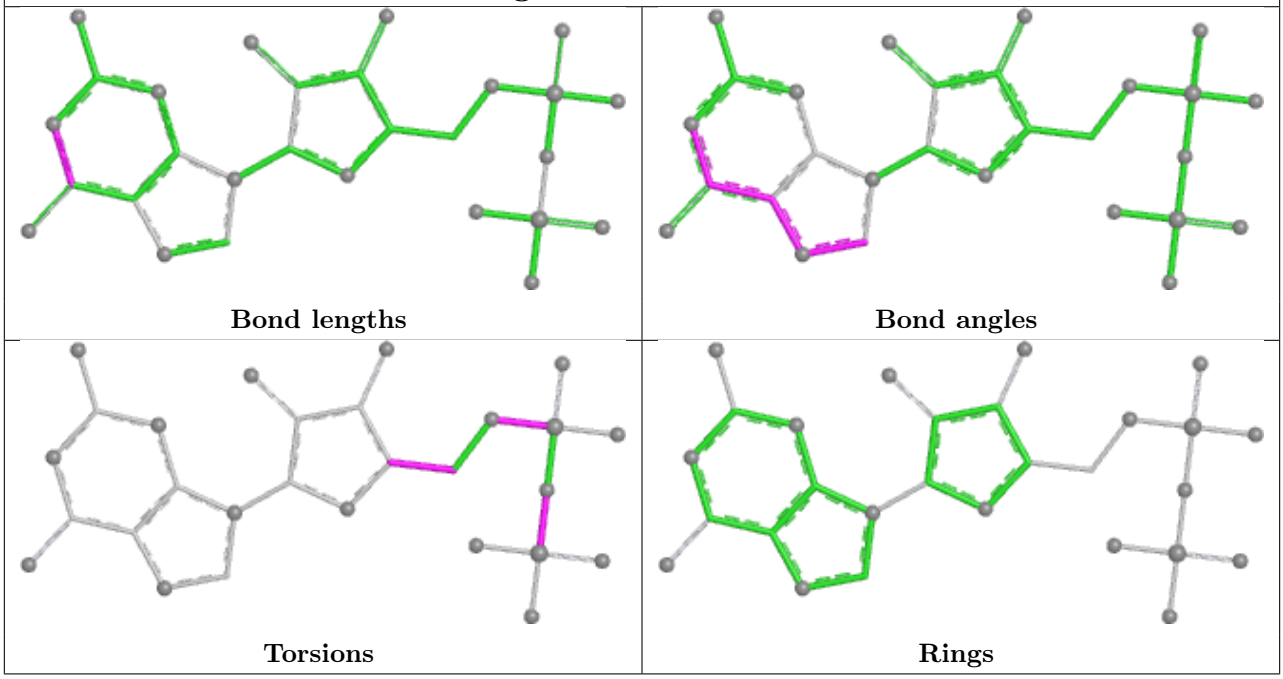

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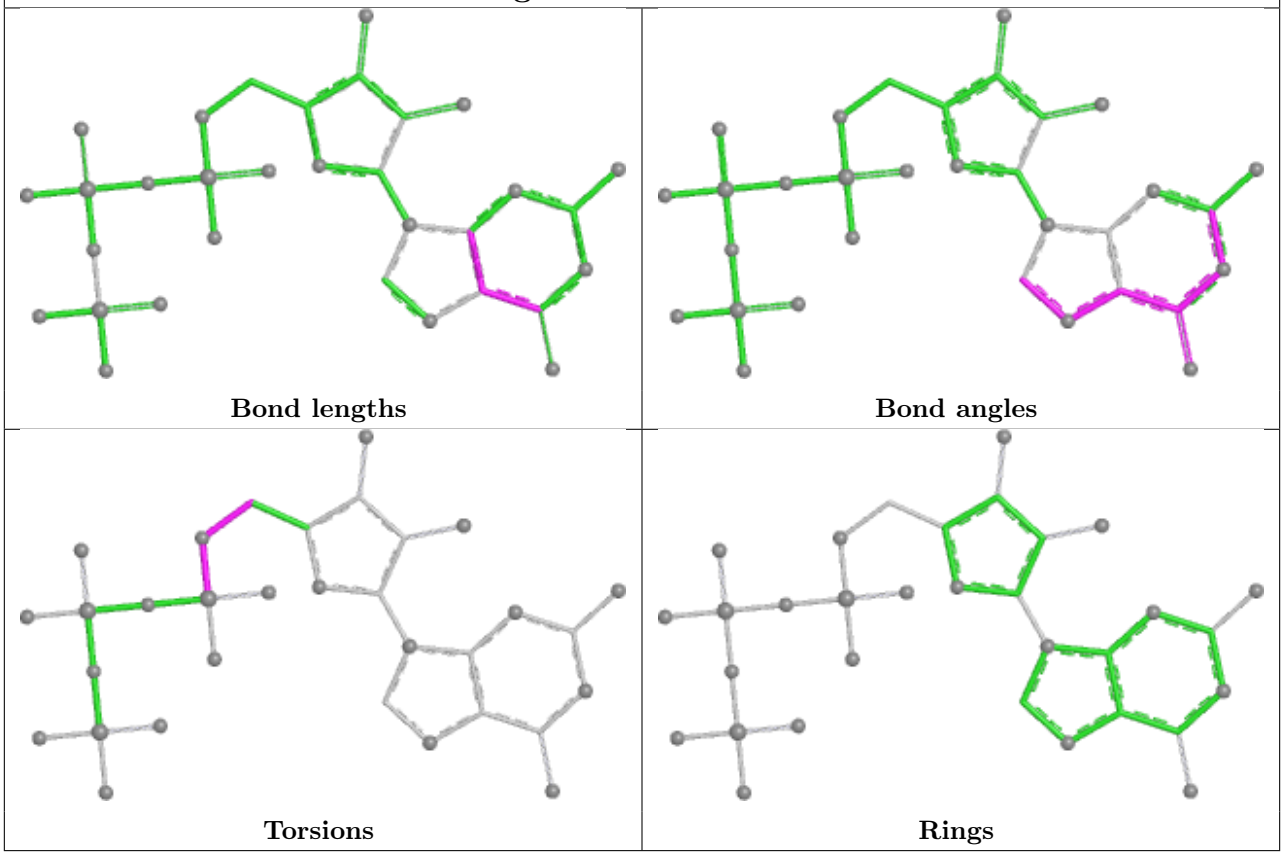

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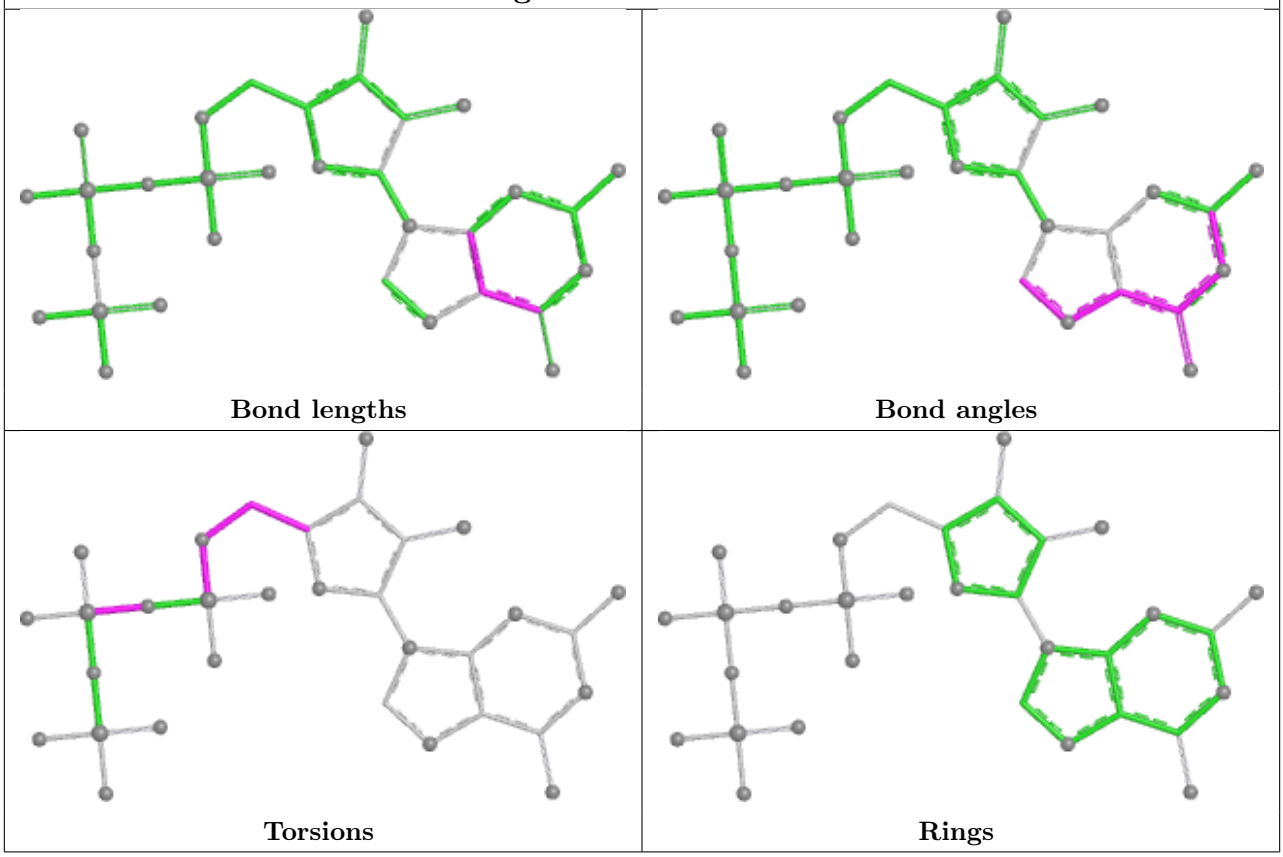

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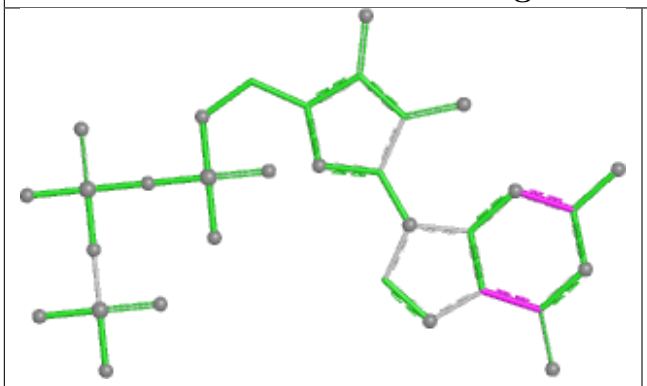
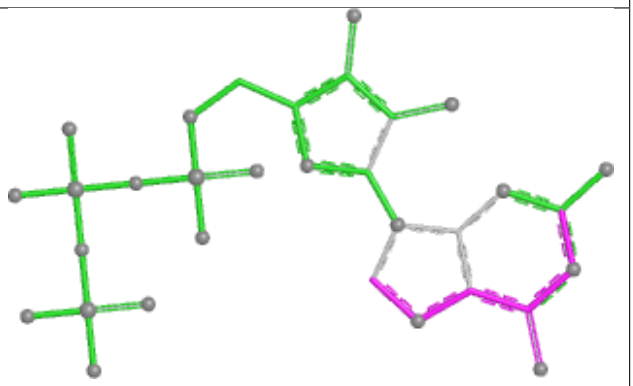
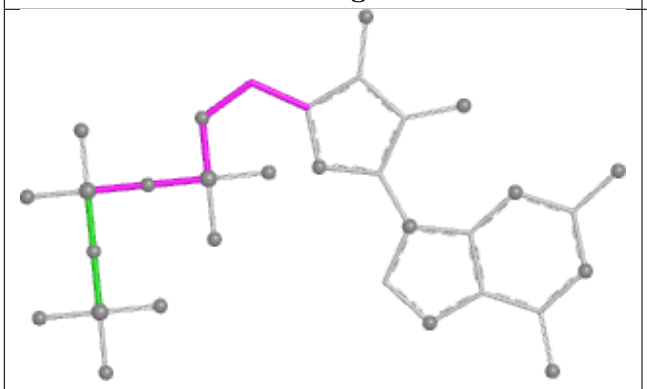


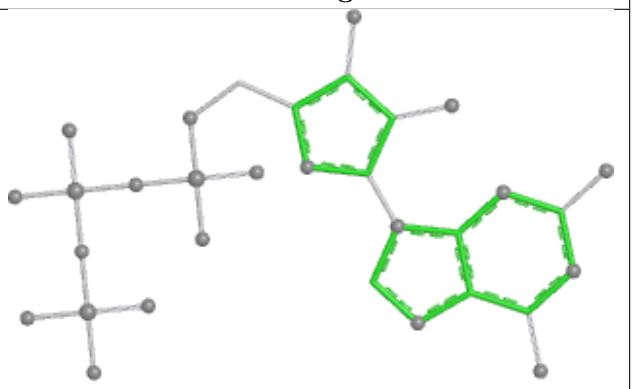
Bond lengths



Bond angles

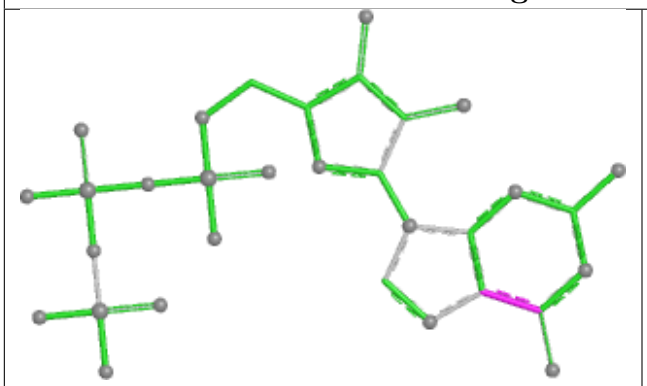


Torsions



Rings

Ligand GTP M0 501



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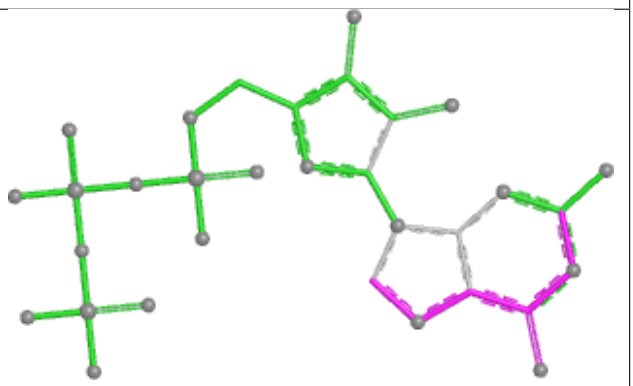

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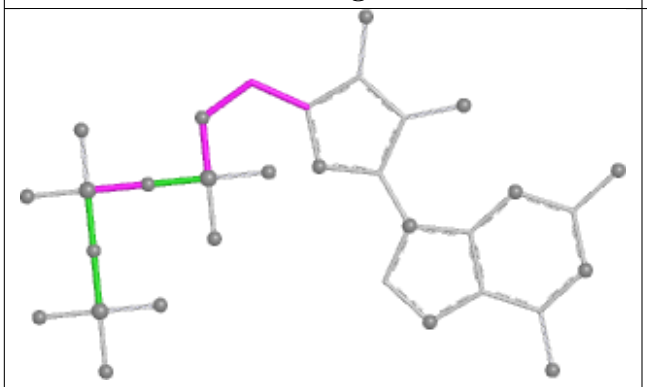
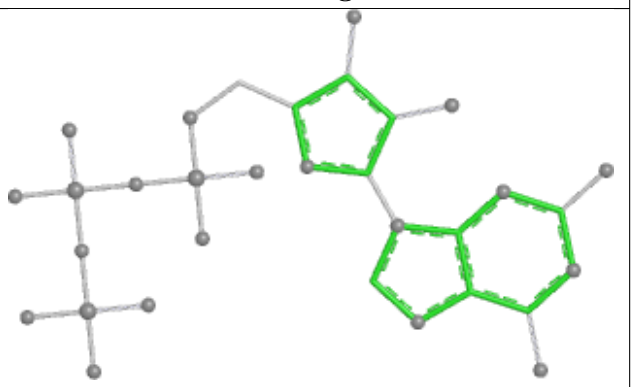
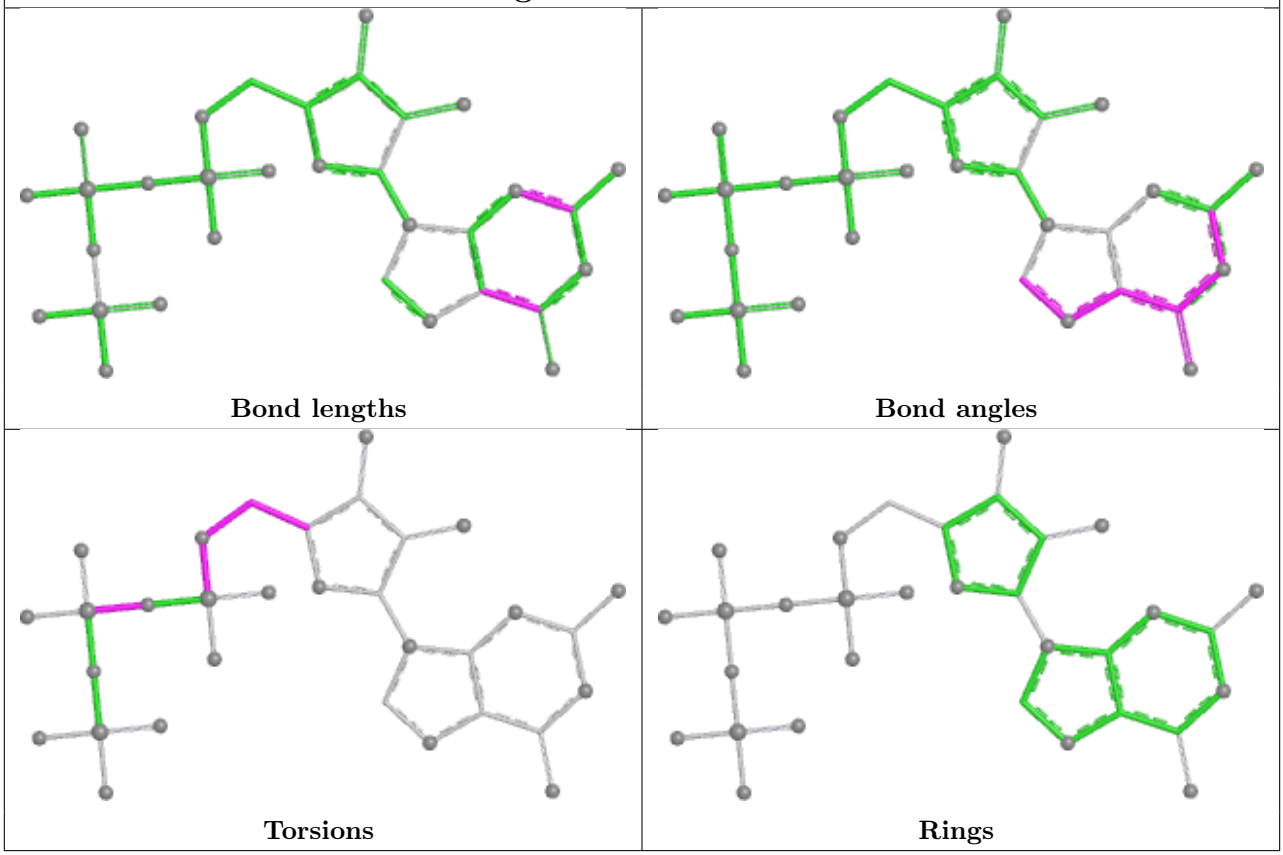


Torsions

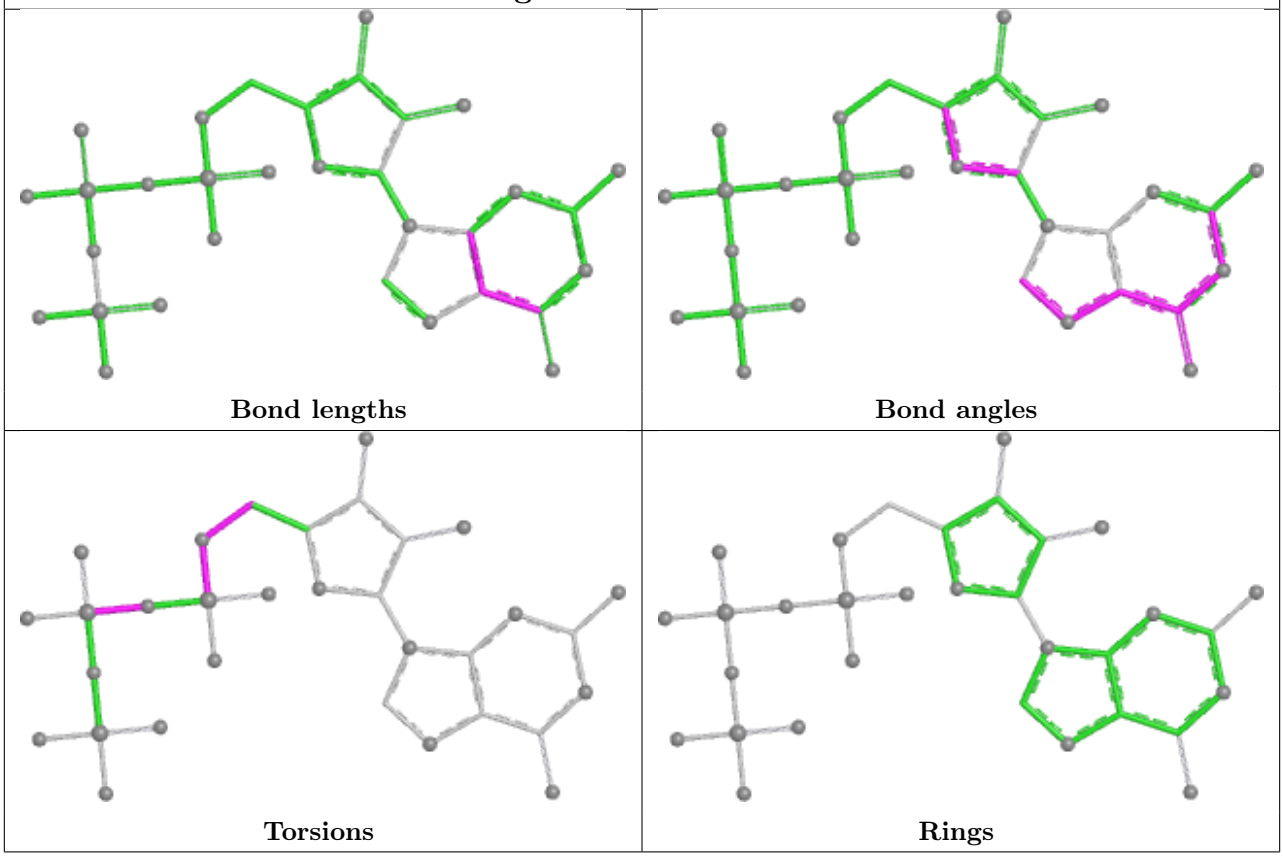


Rings

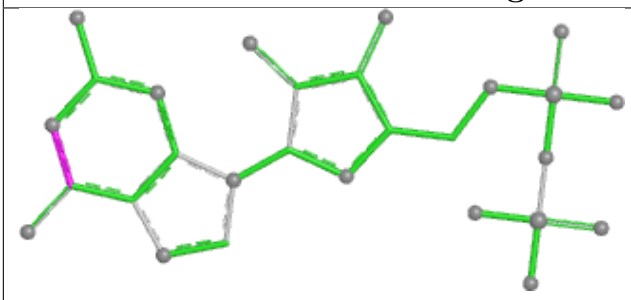
Ligand GTP C0 501



Ligand GTP R6 501



Ligand GDP W2 503



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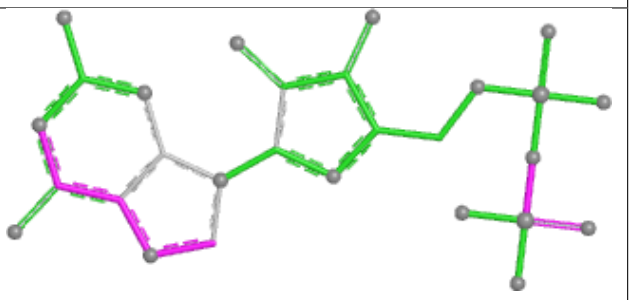
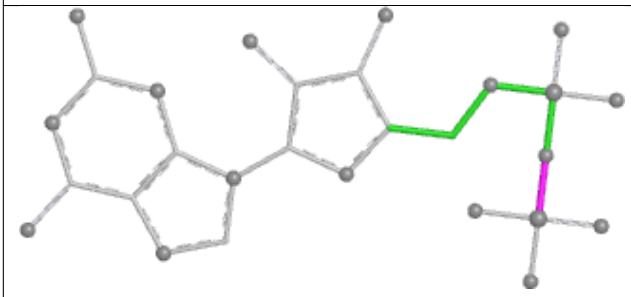


Bond angles



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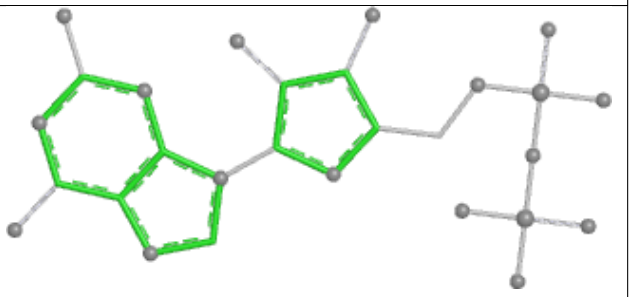
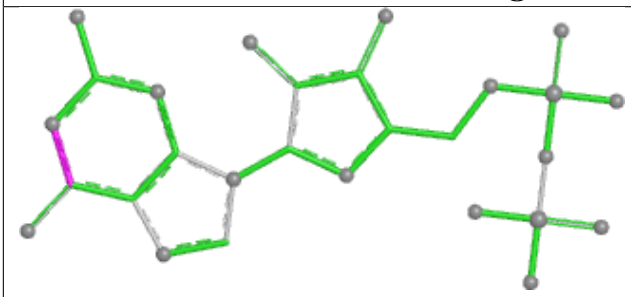
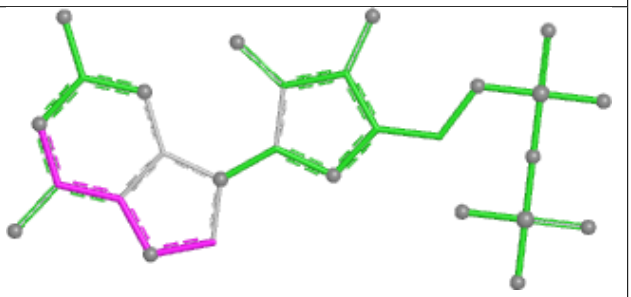


Rings

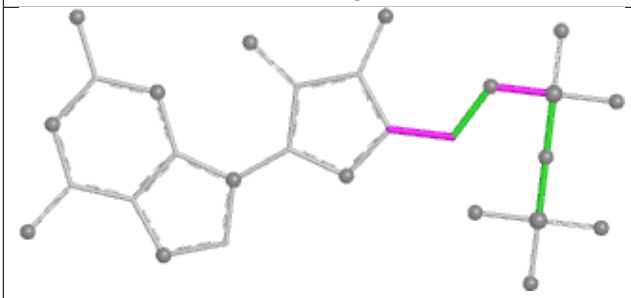
Ligand GDP M4 502



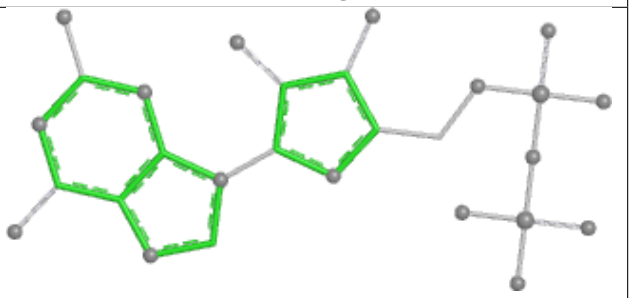
Bond lengths



Bond angles

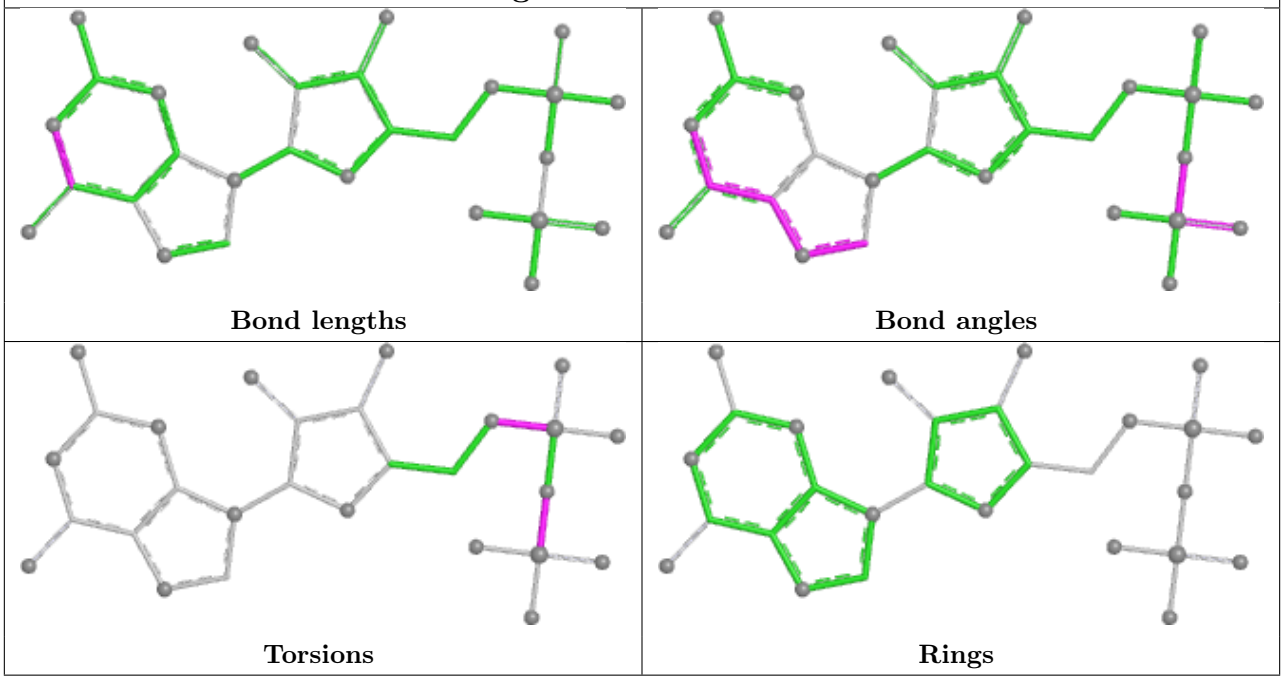


Torsions

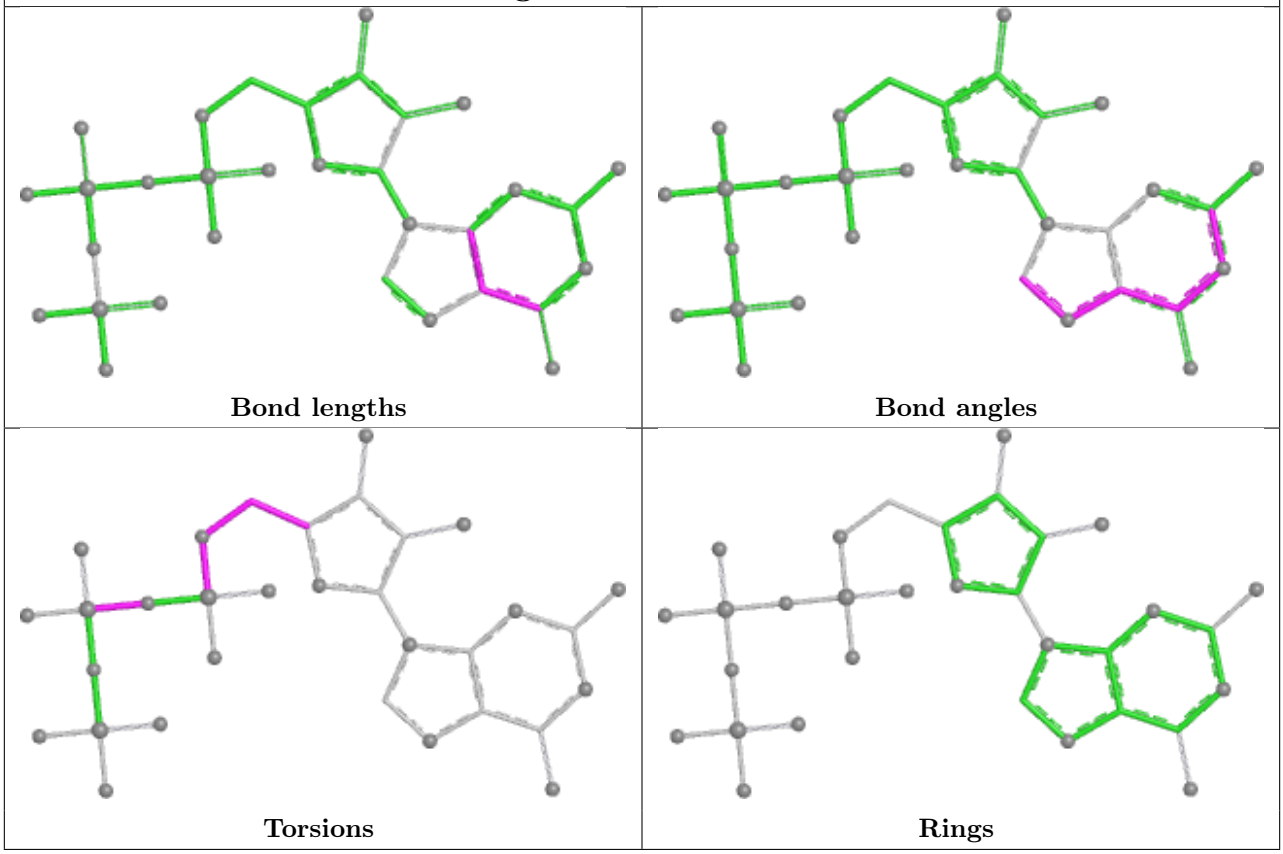


Rings

Ligand GDP 3G 502



Ligand GTP O6 501



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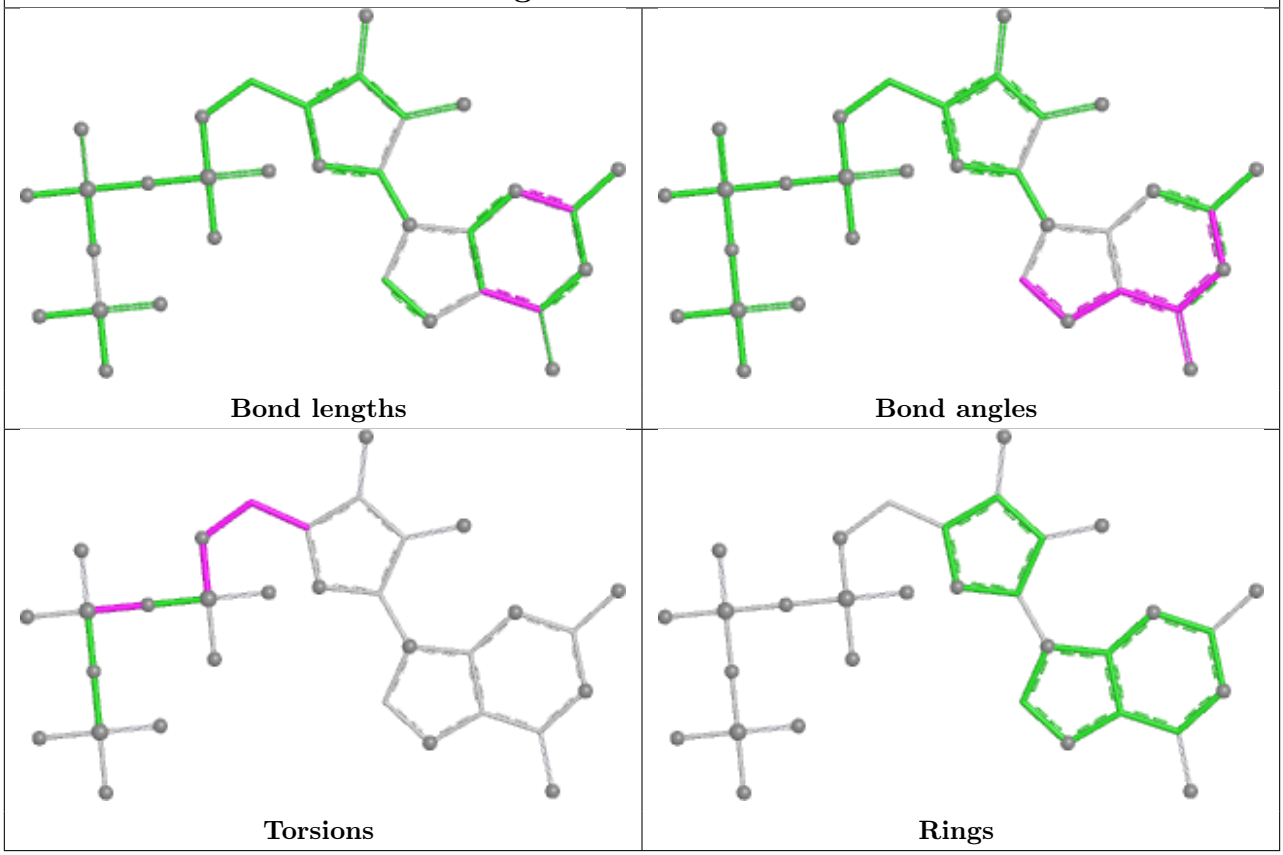
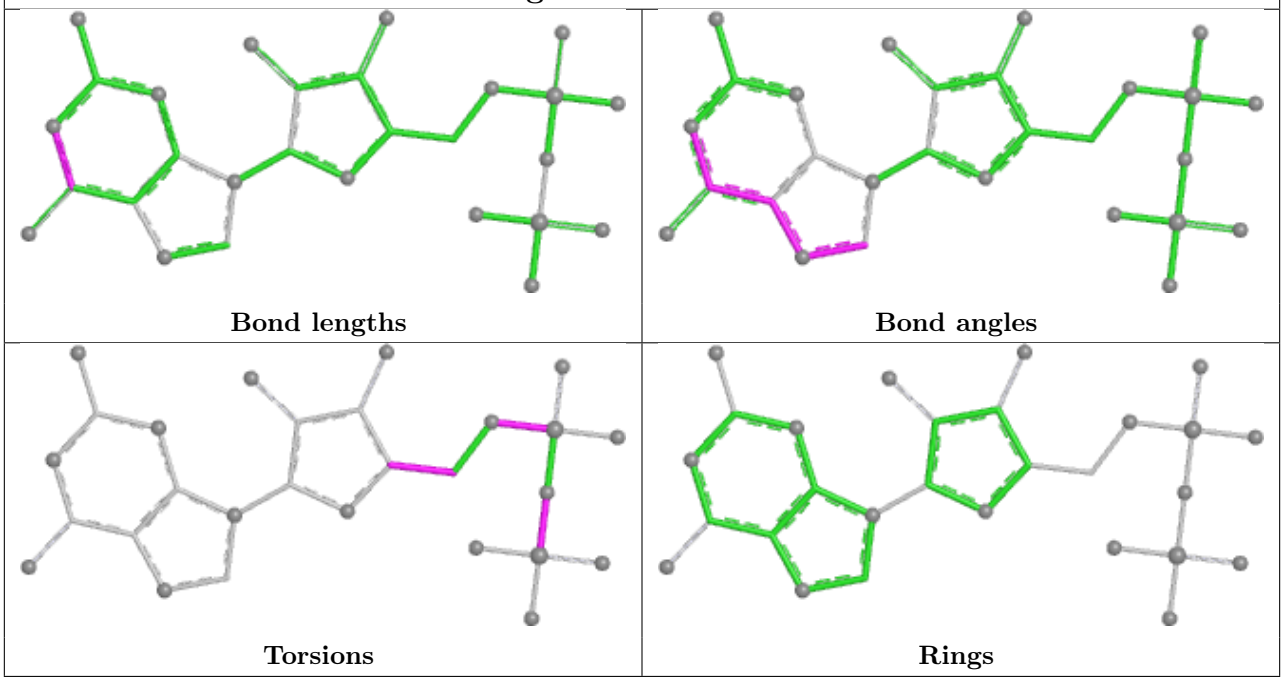
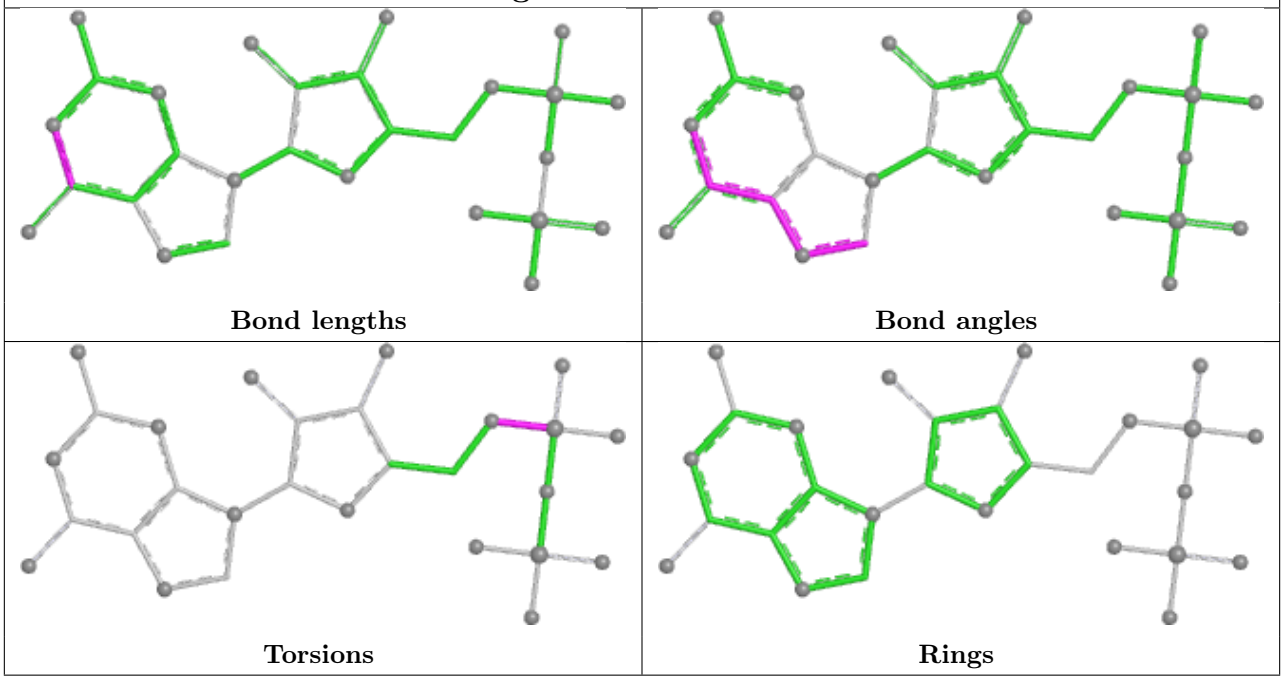


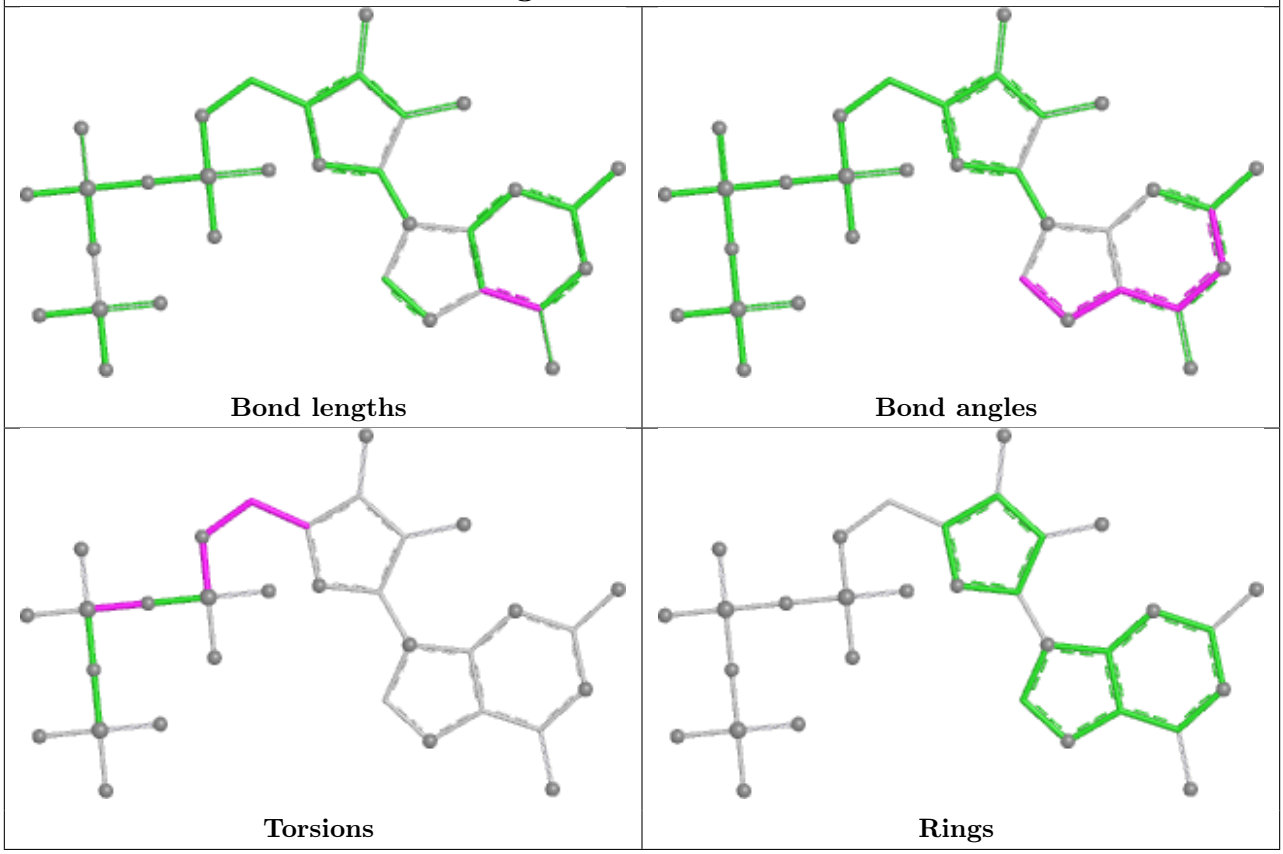
Ligand GDP 2 501



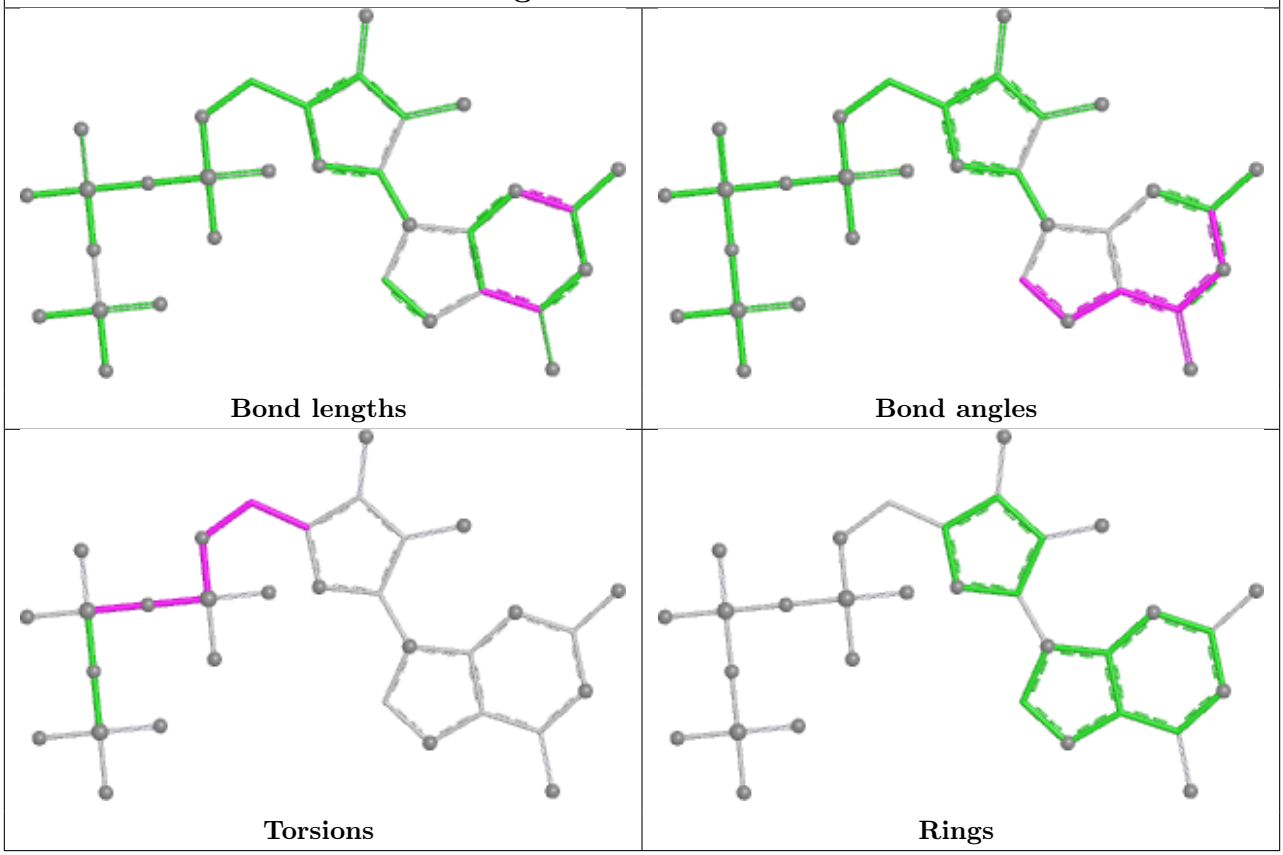
Ligand GDP G0 502



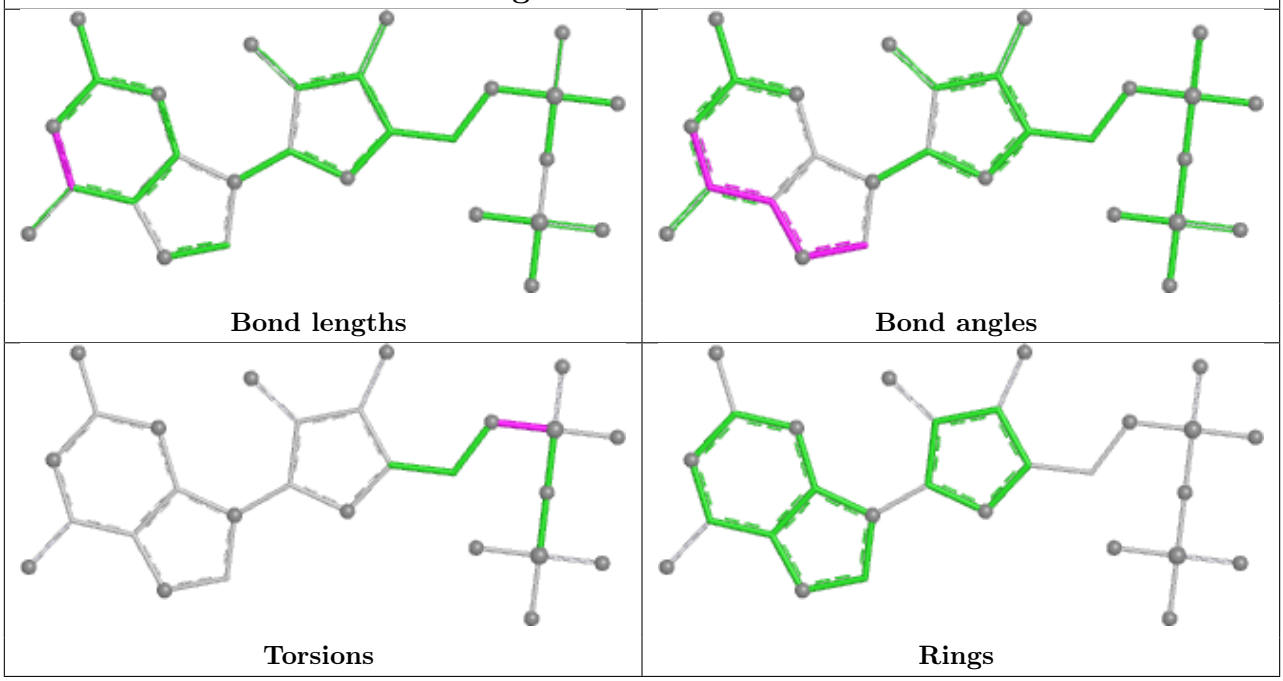
Ligand GTP E6 501



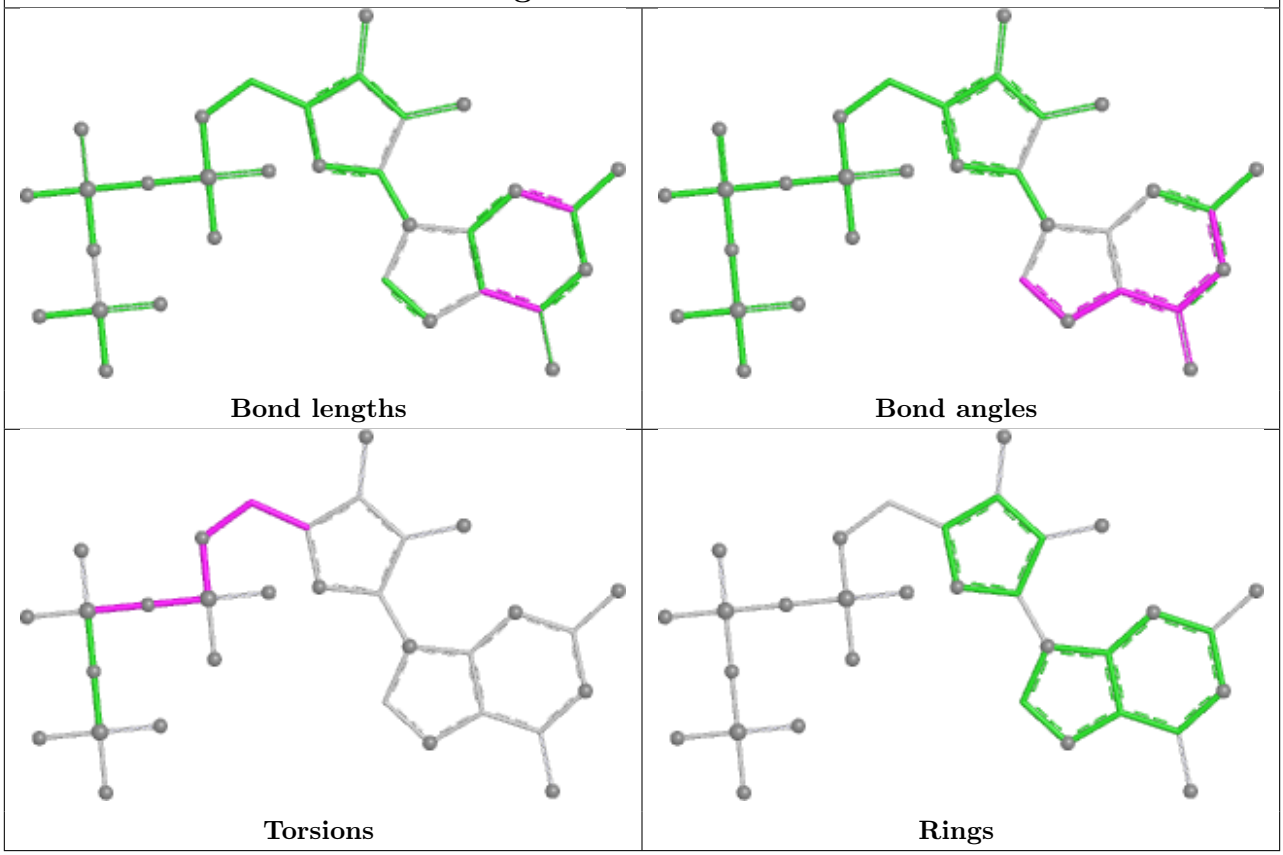
Ligand GTP 1D 501



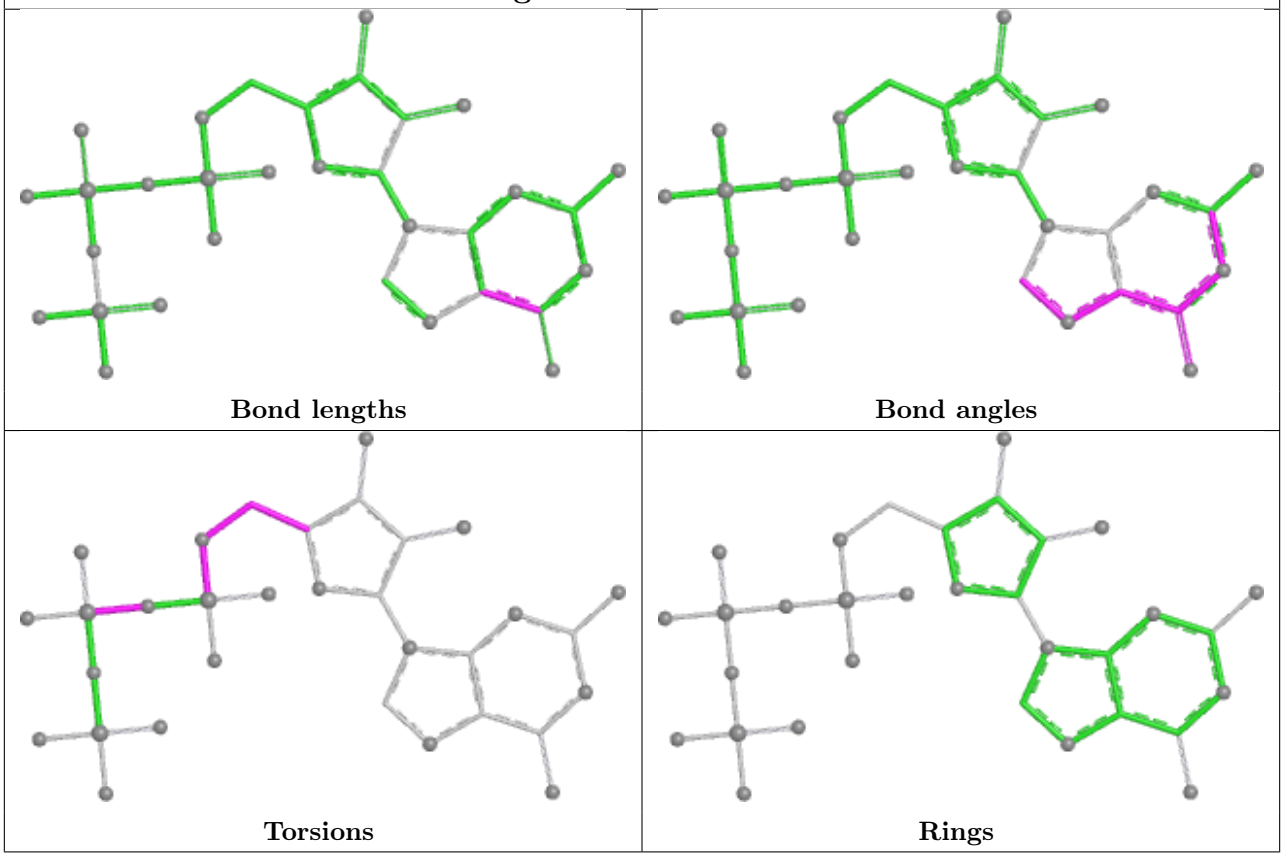
Ligand GDP G8 501



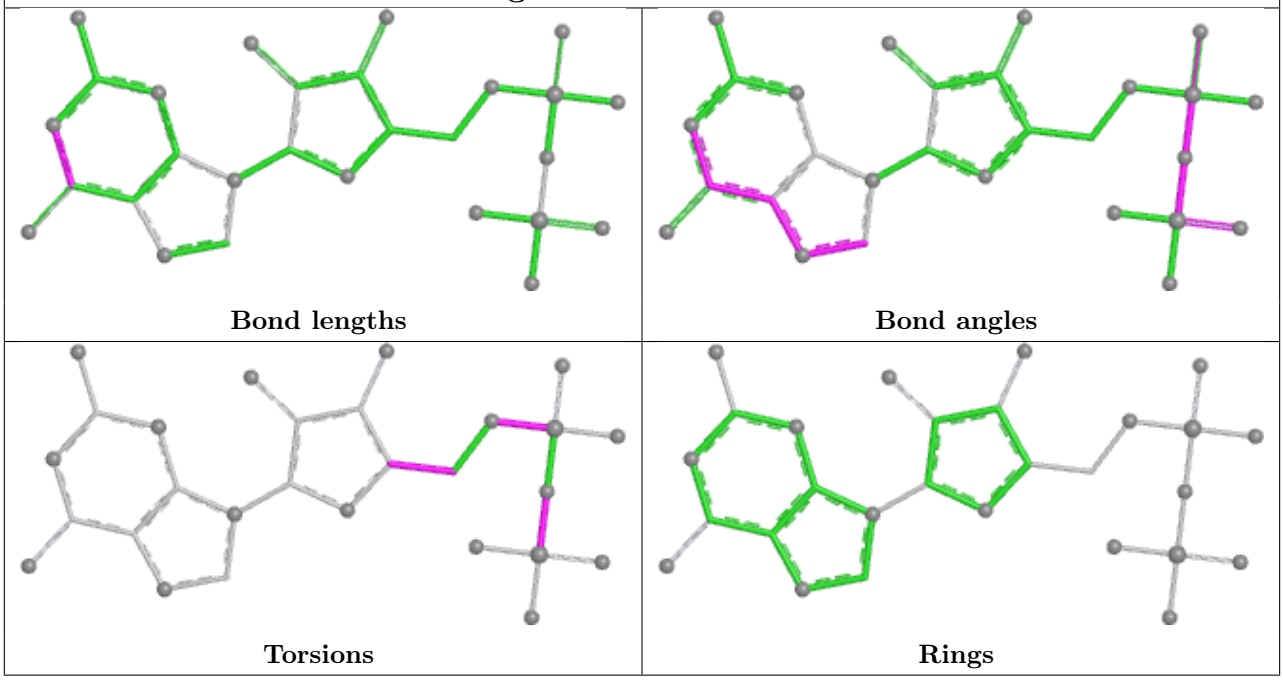
Ligand GTP 0V 501



Ligand GTP 0K 501



Ligand GDP 2W 502



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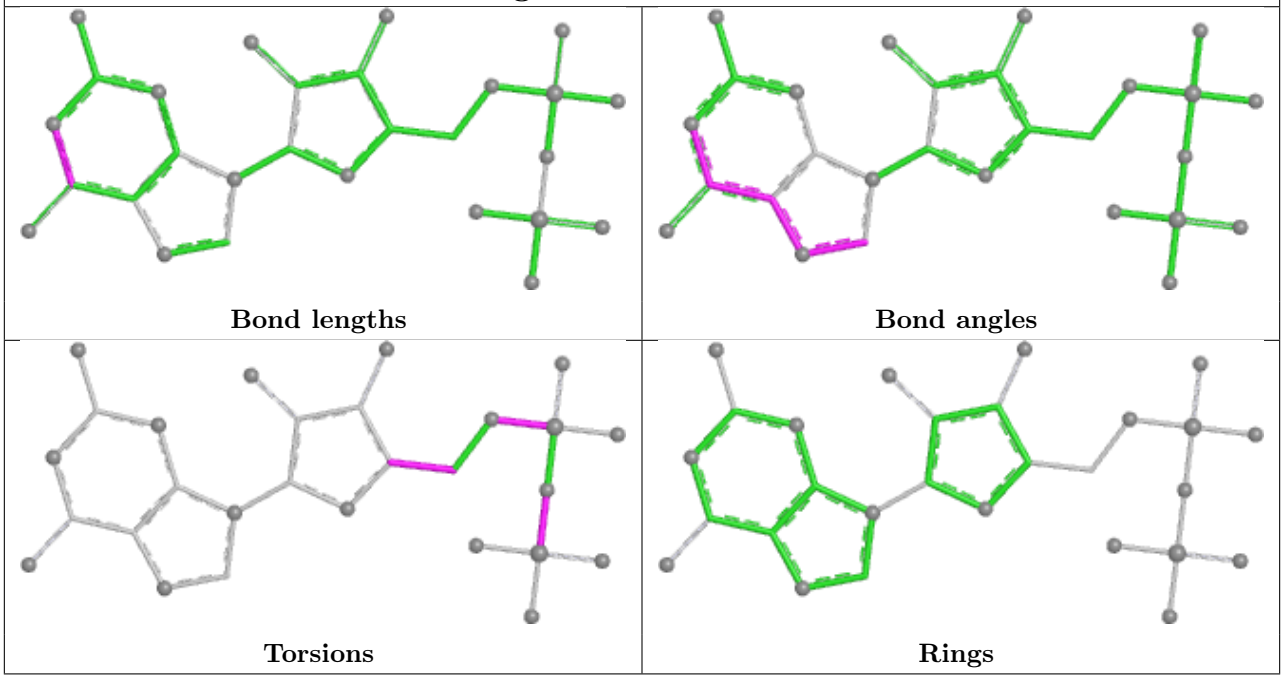
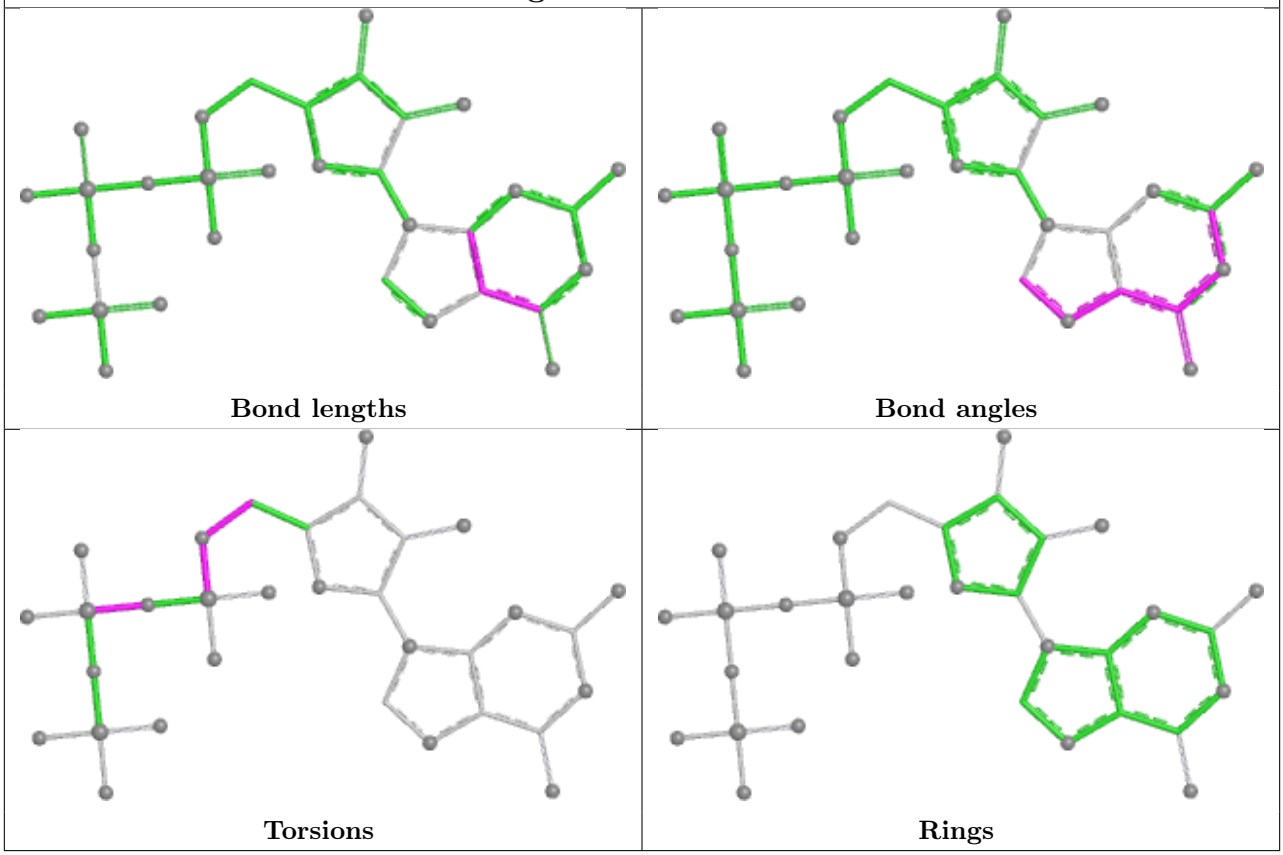
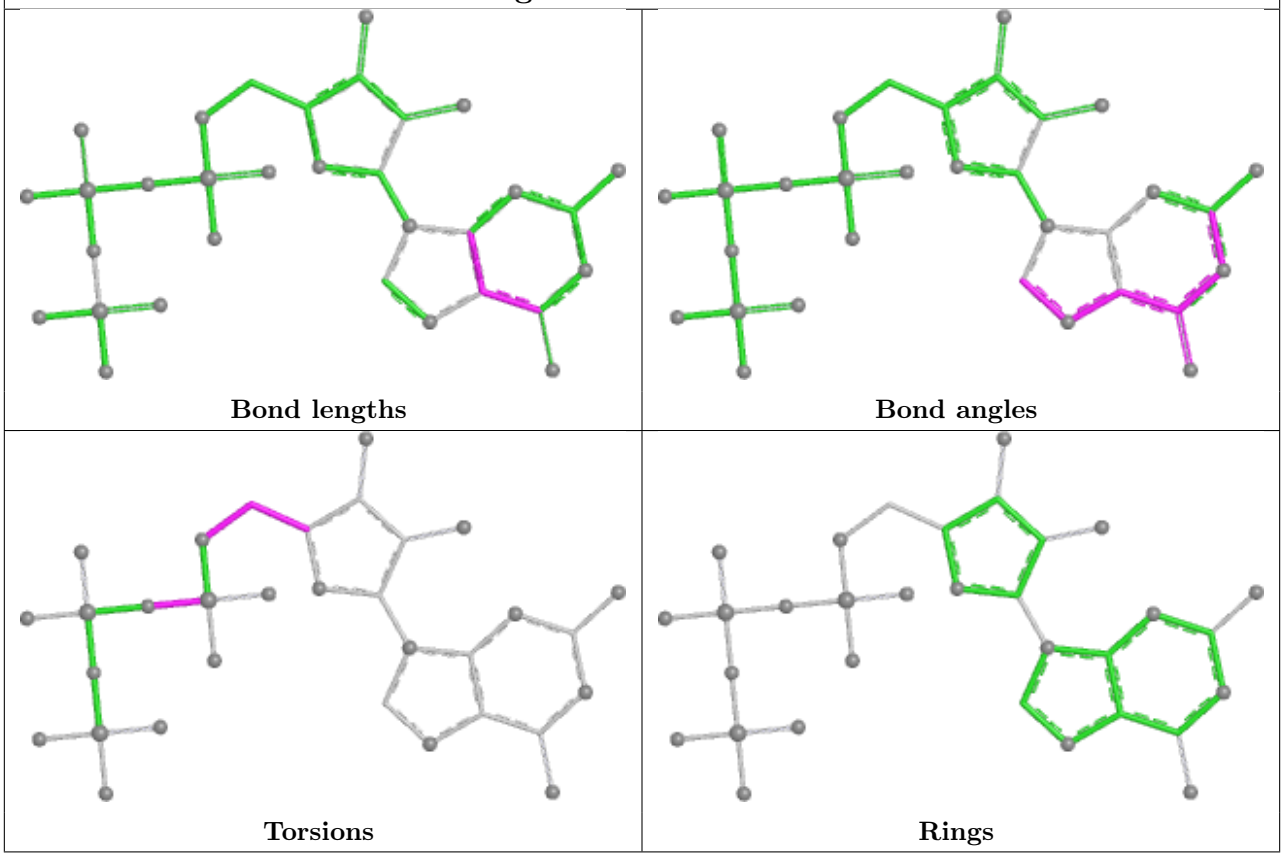


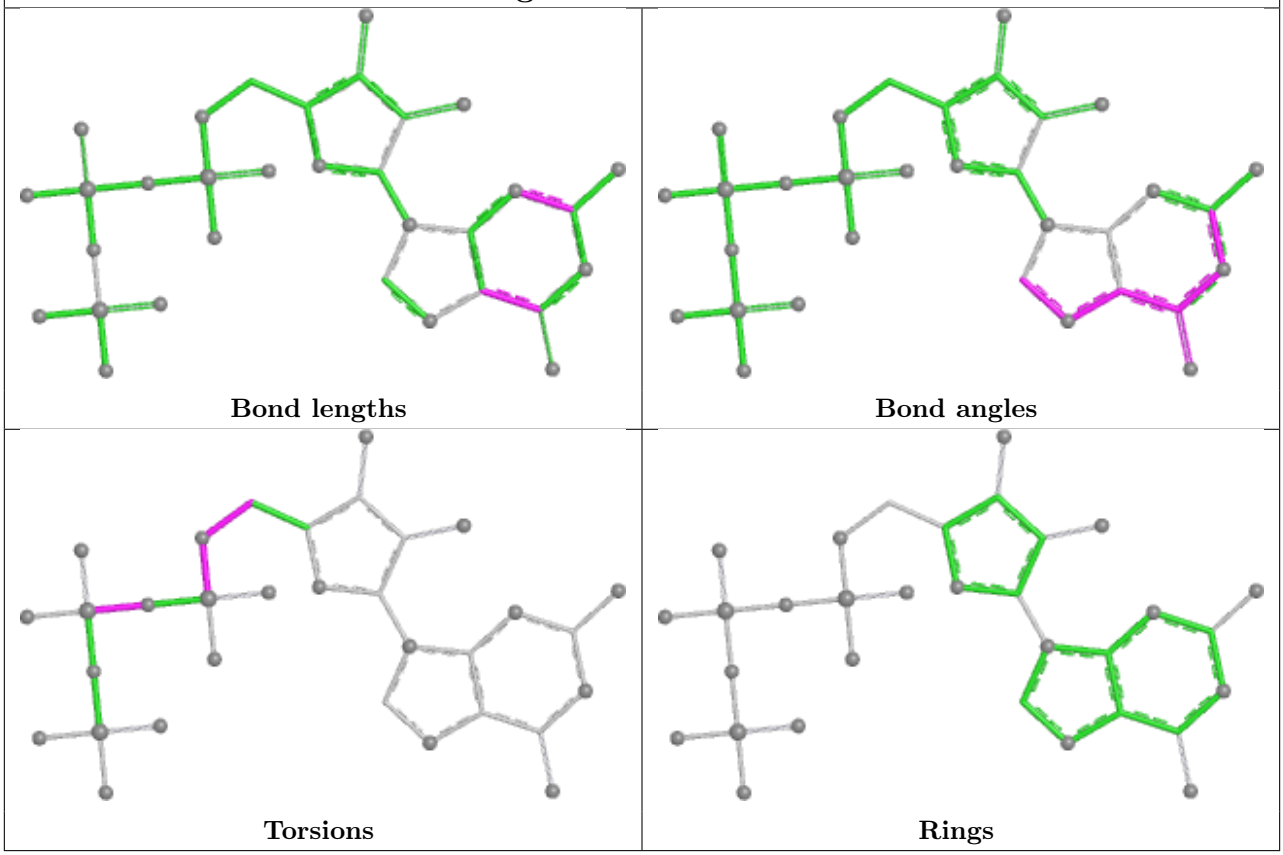
Ligand GTP 3 501



Ligand GTP B2 501



Ligand GTP F3 501



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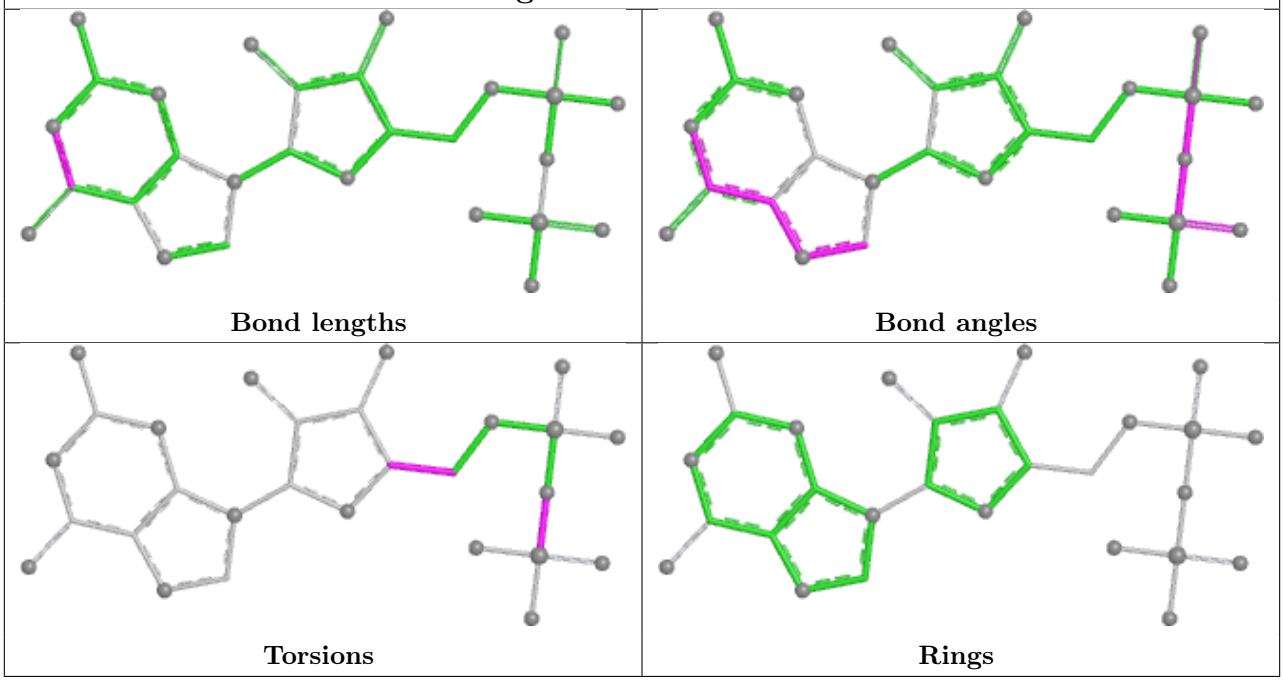

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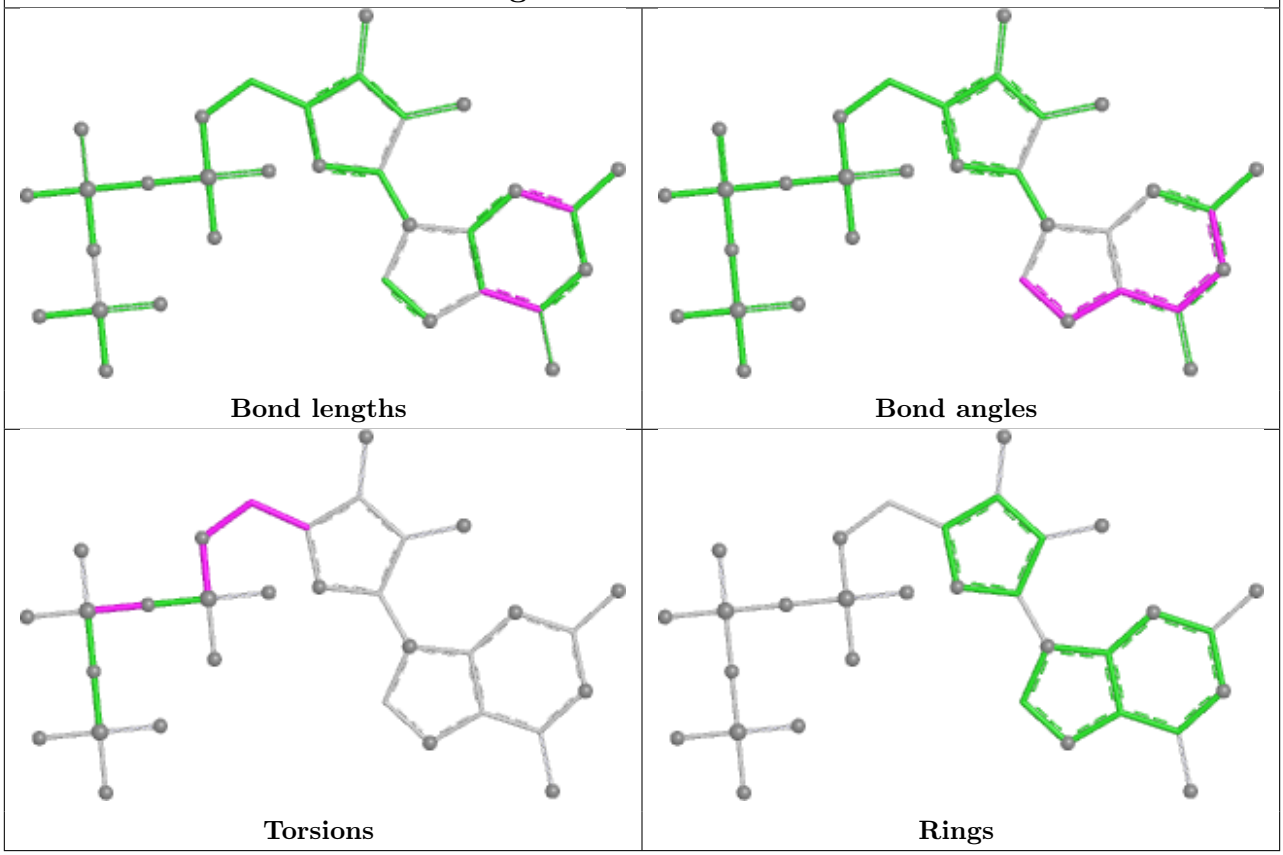
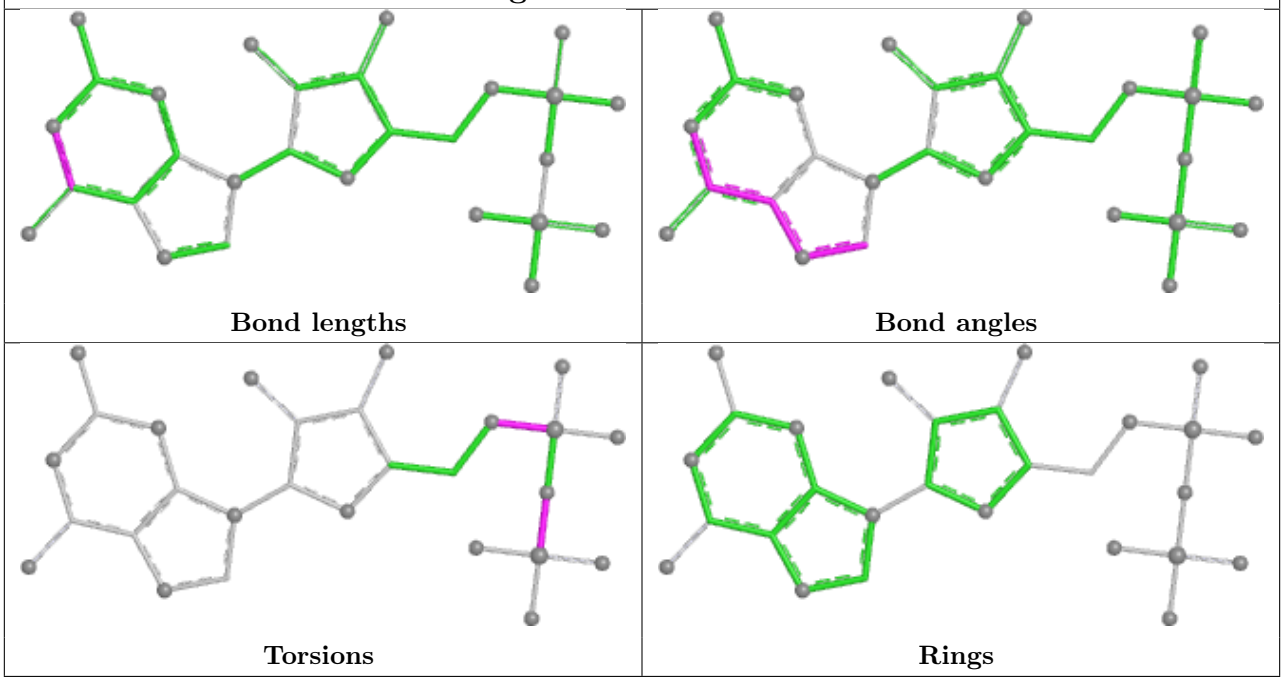
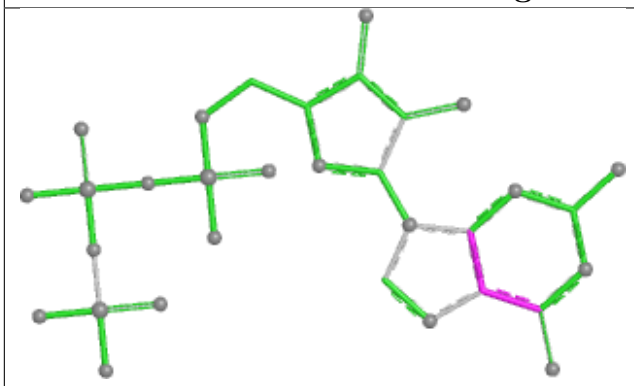


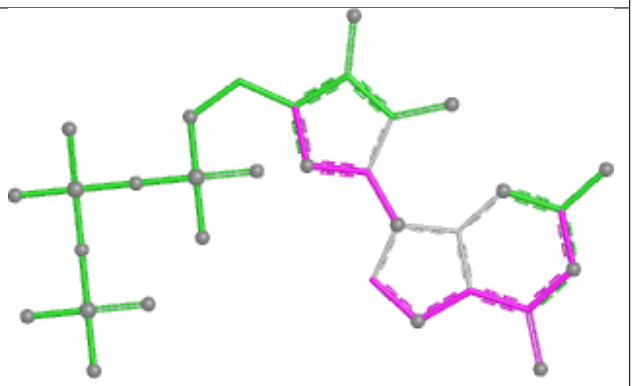
Ligand GDP M8 501



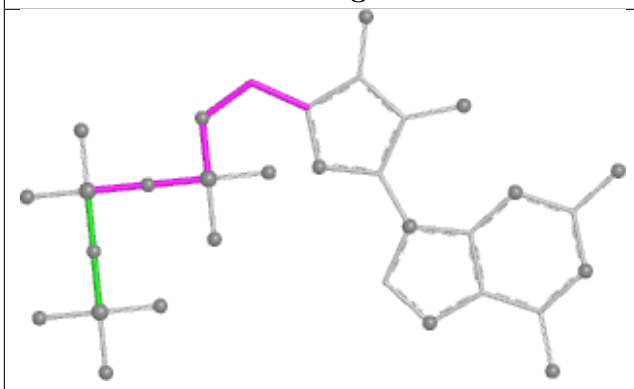
Ligand GTP O2 501



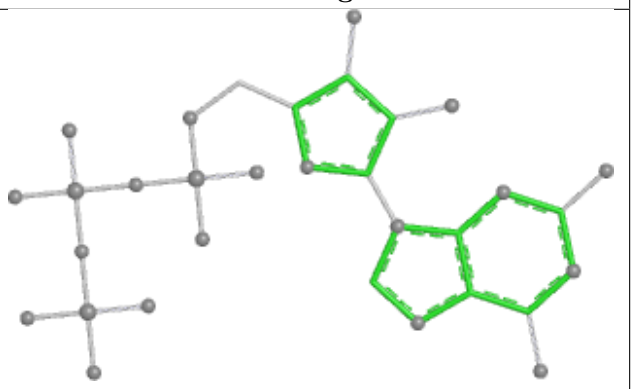
Bond lengths



Bond angles

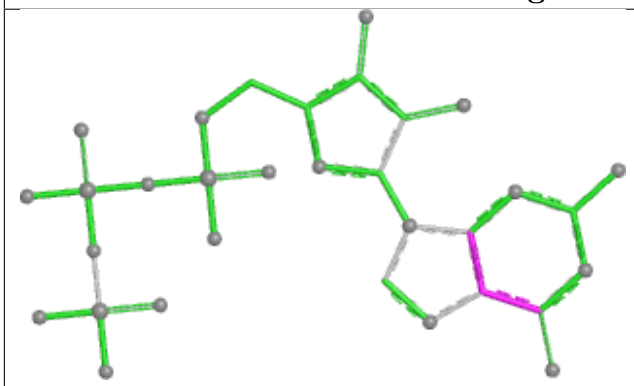


Torsions



Rings

Ligand GTP 4 501



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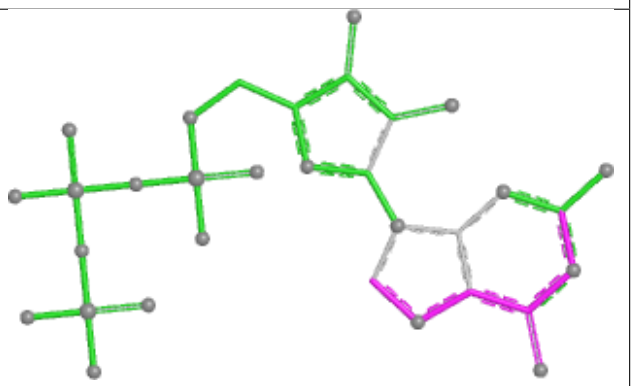

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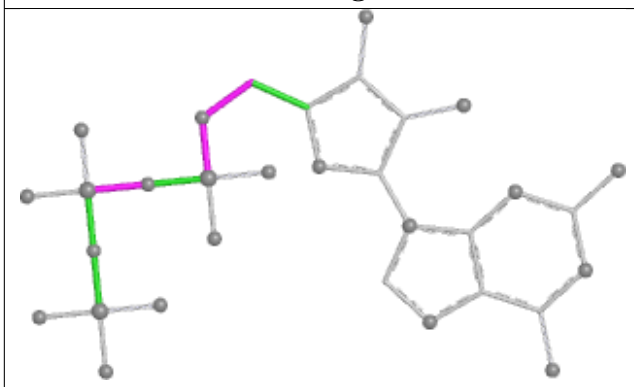

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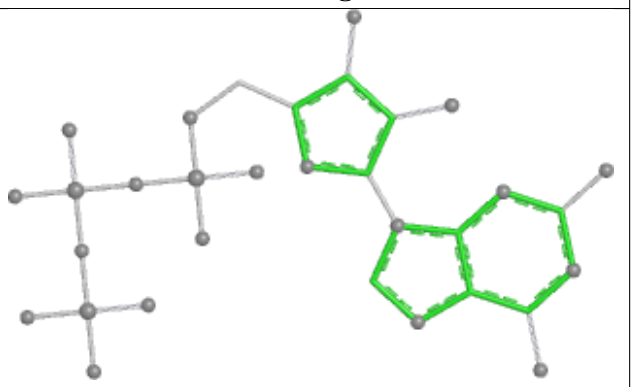
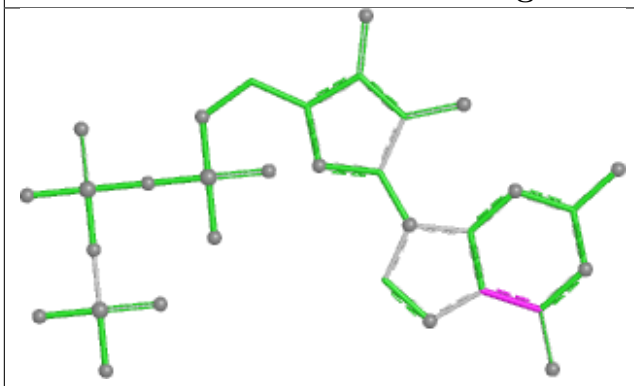


Rings

Ligand GTP Z7 501



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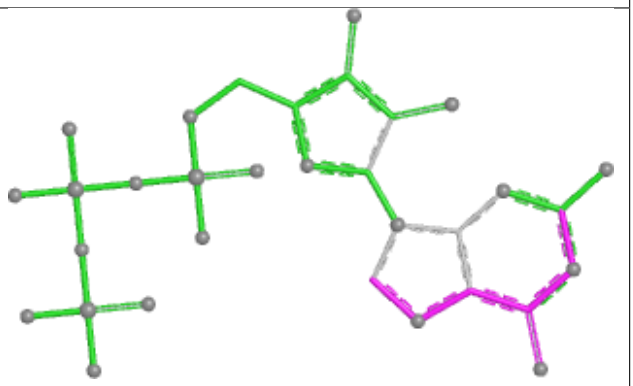
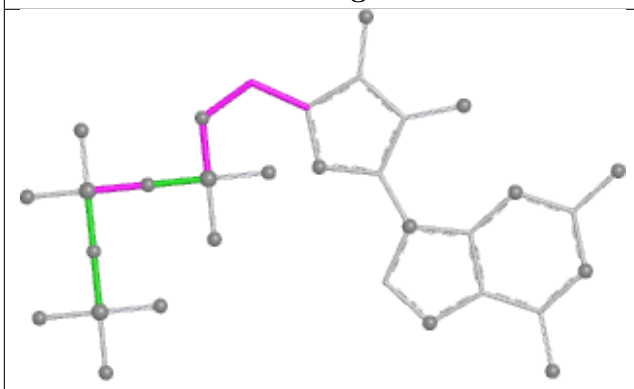
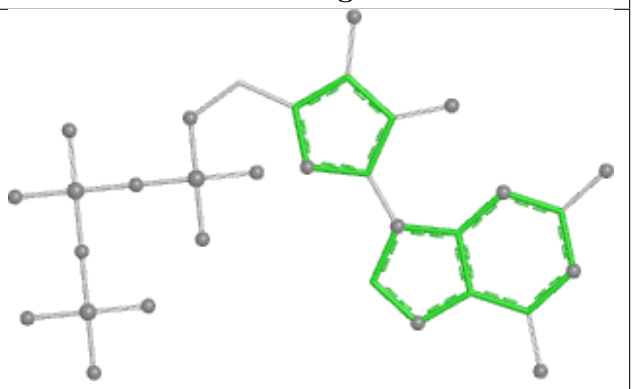


Bond angles

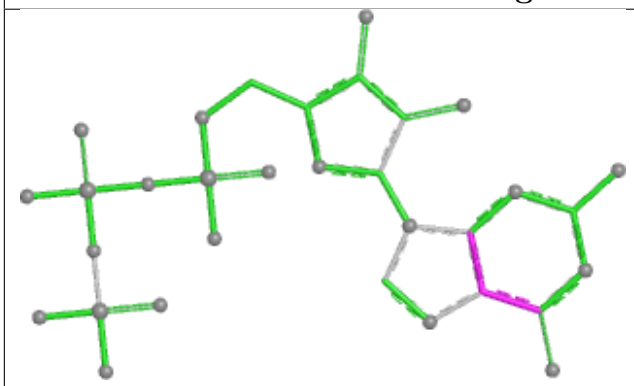


Torsions

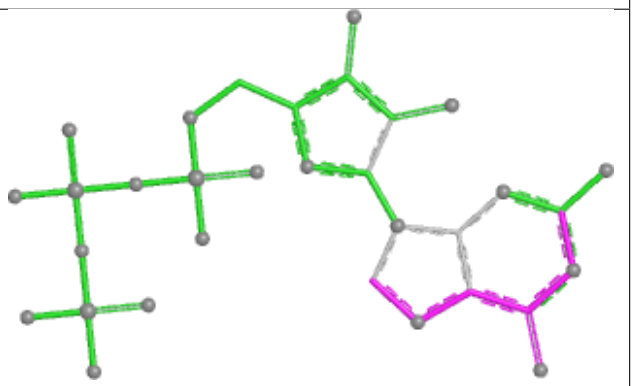


Rings

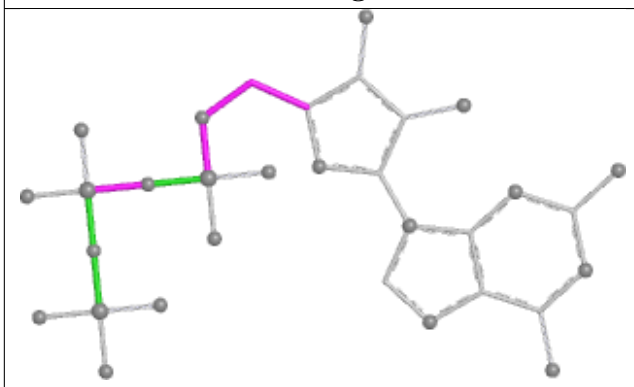
Ligand GTP T2 501



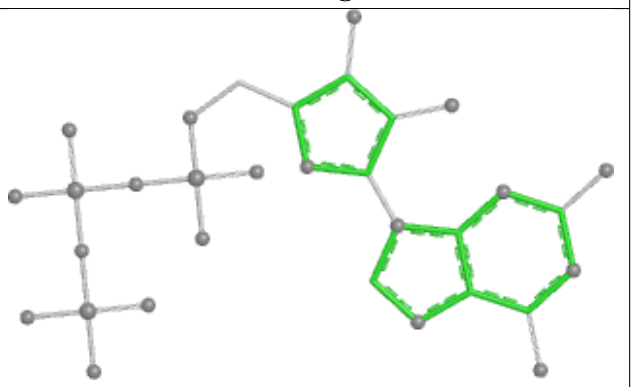
Bond lengths



Bond angles

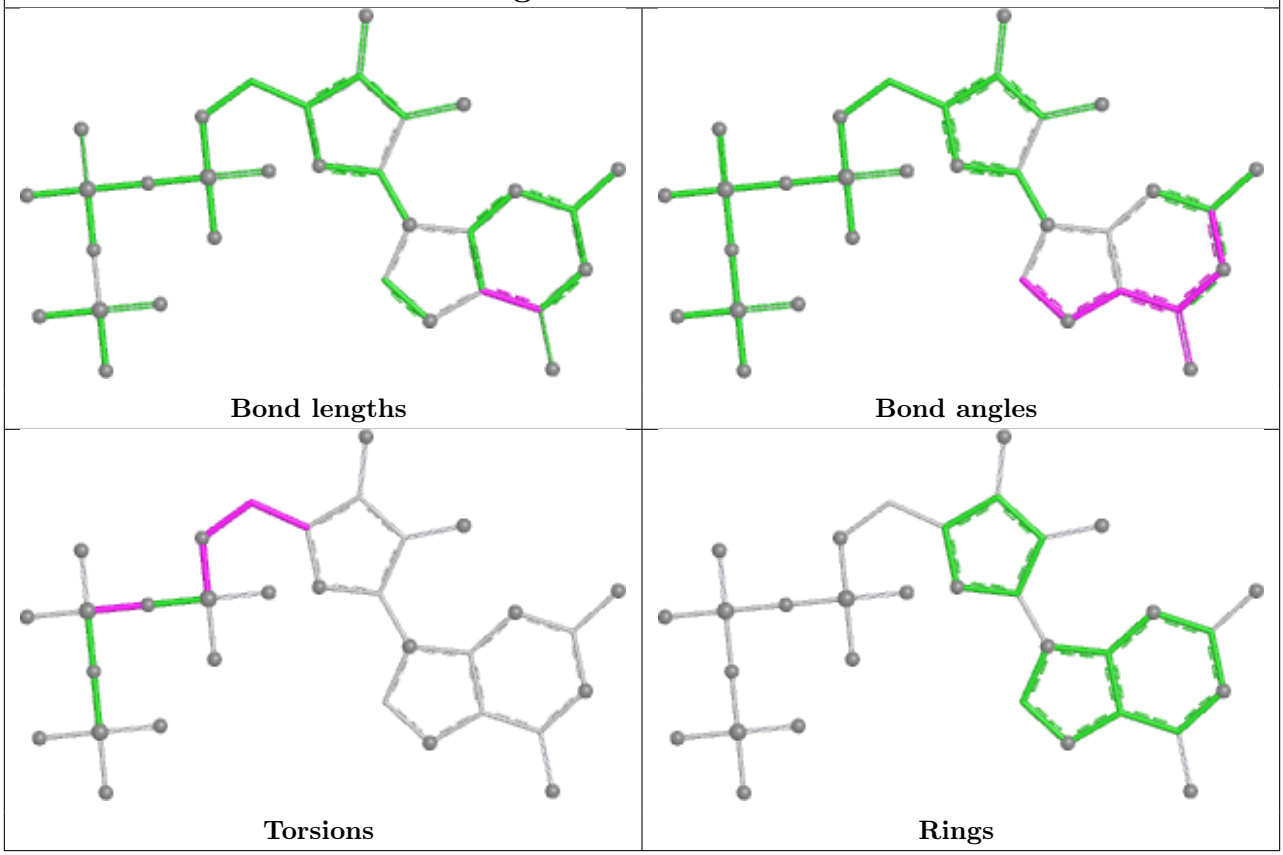


Torsions

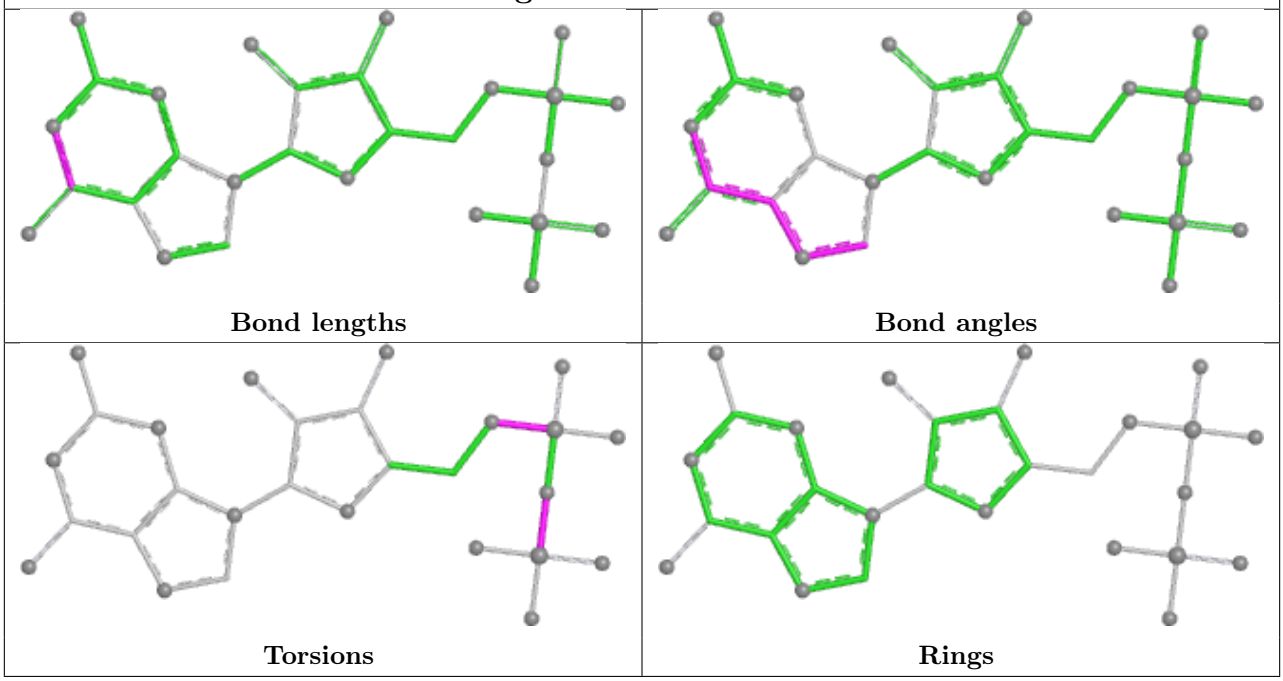


Rings

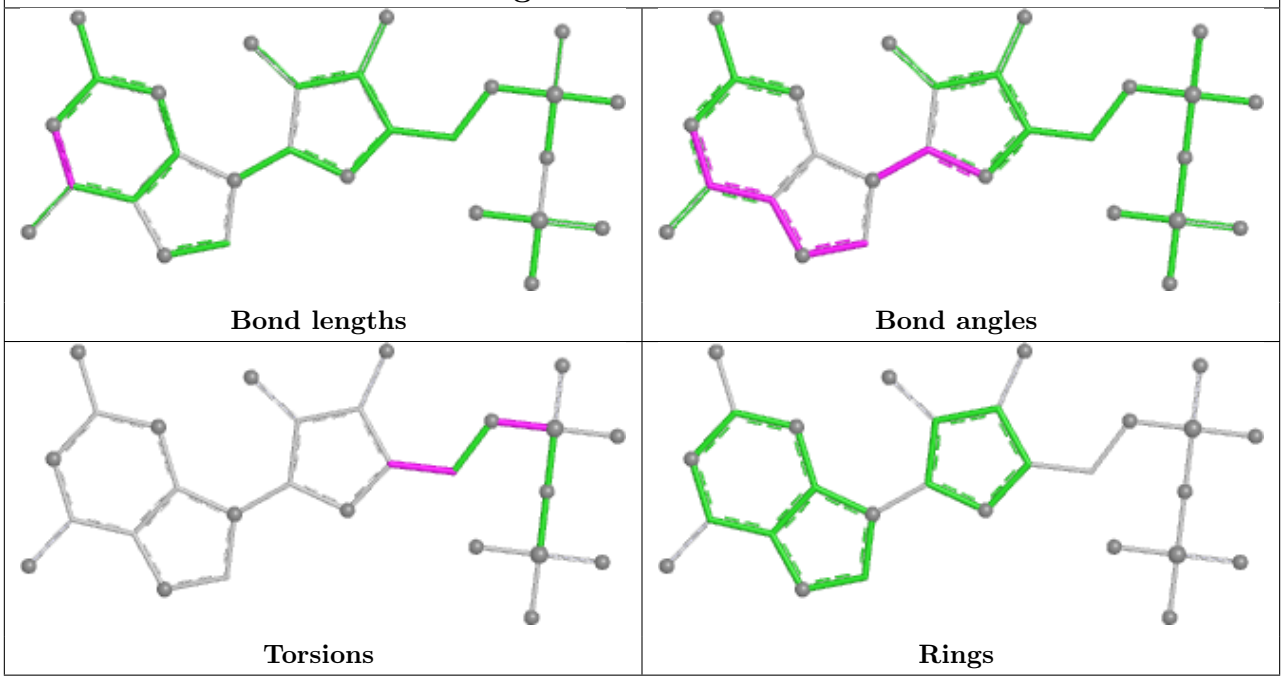
Ligand GTP 2K 501



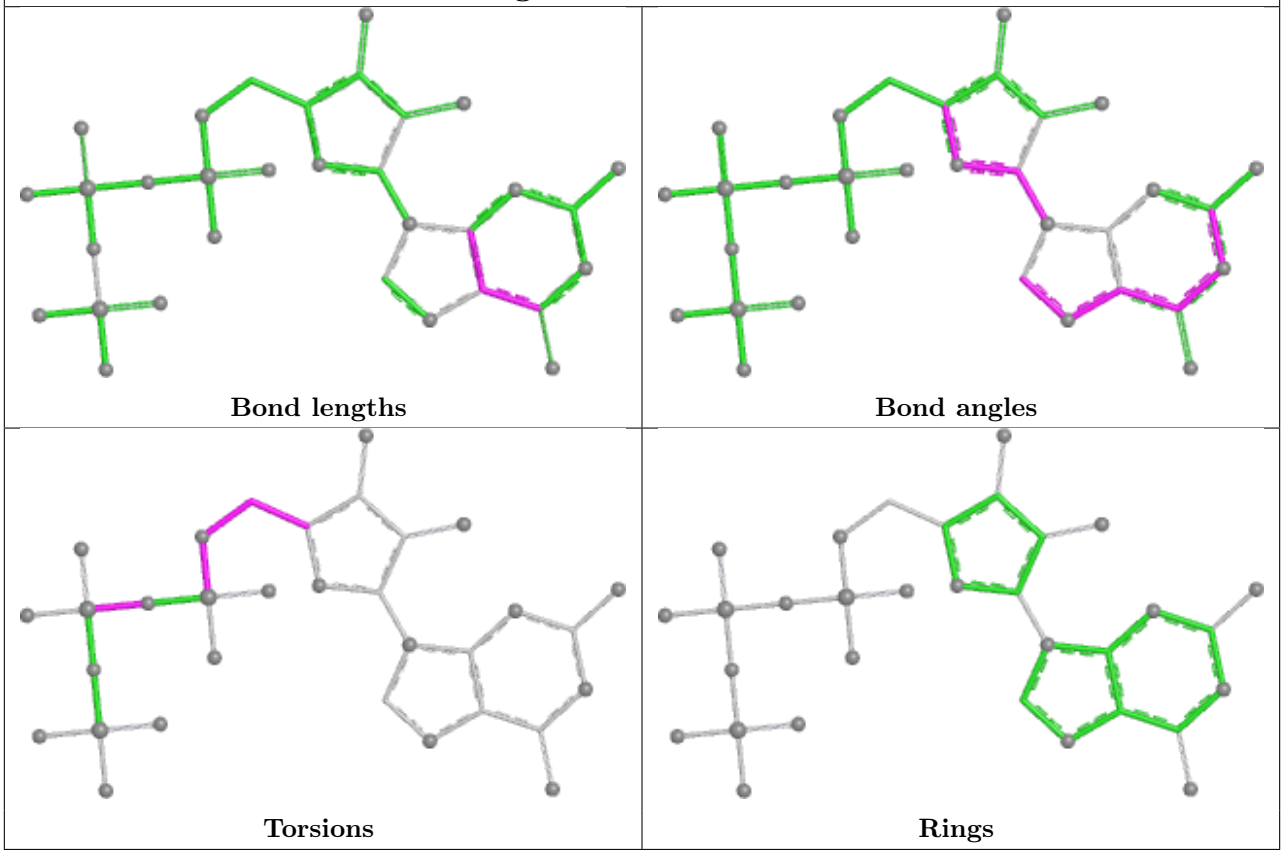
Ligand GDP F2 501



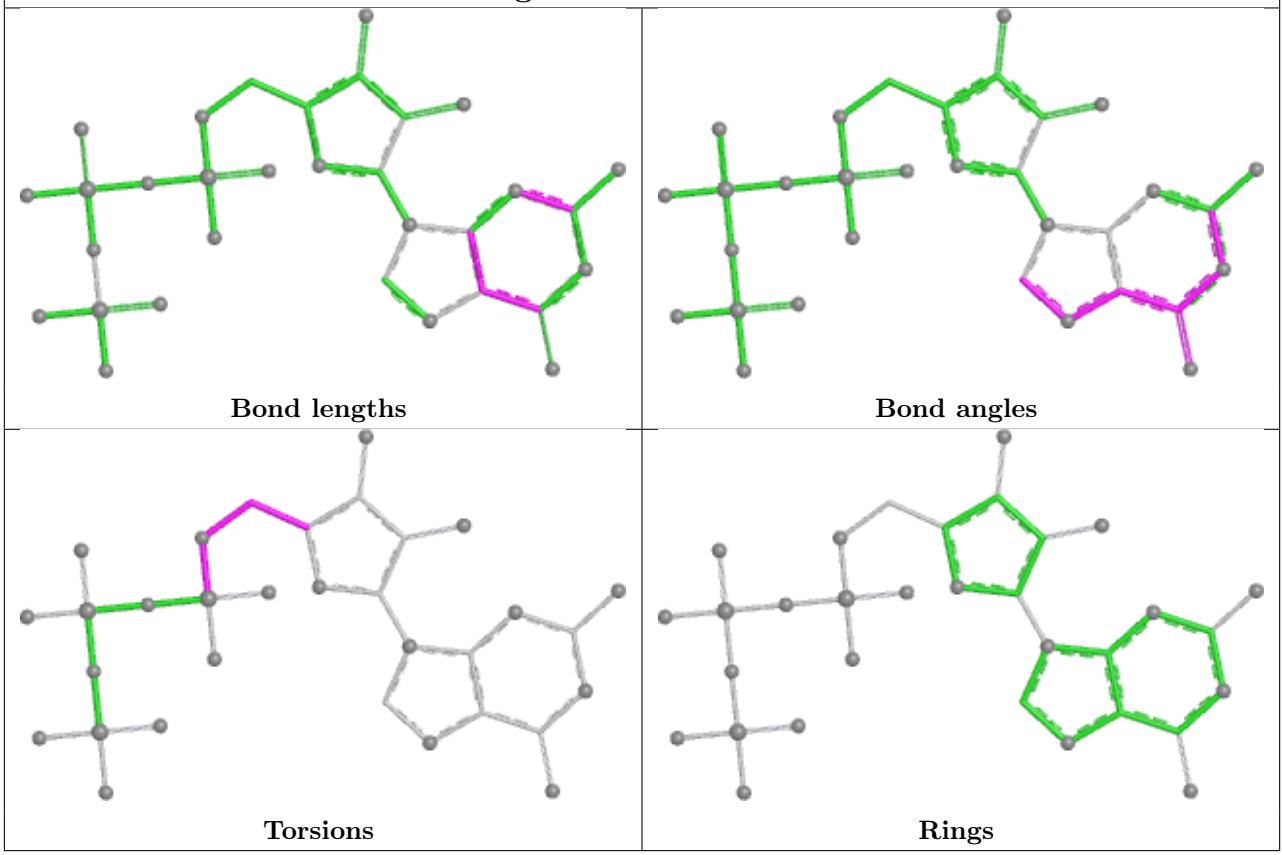
Ligand GDP B3 501



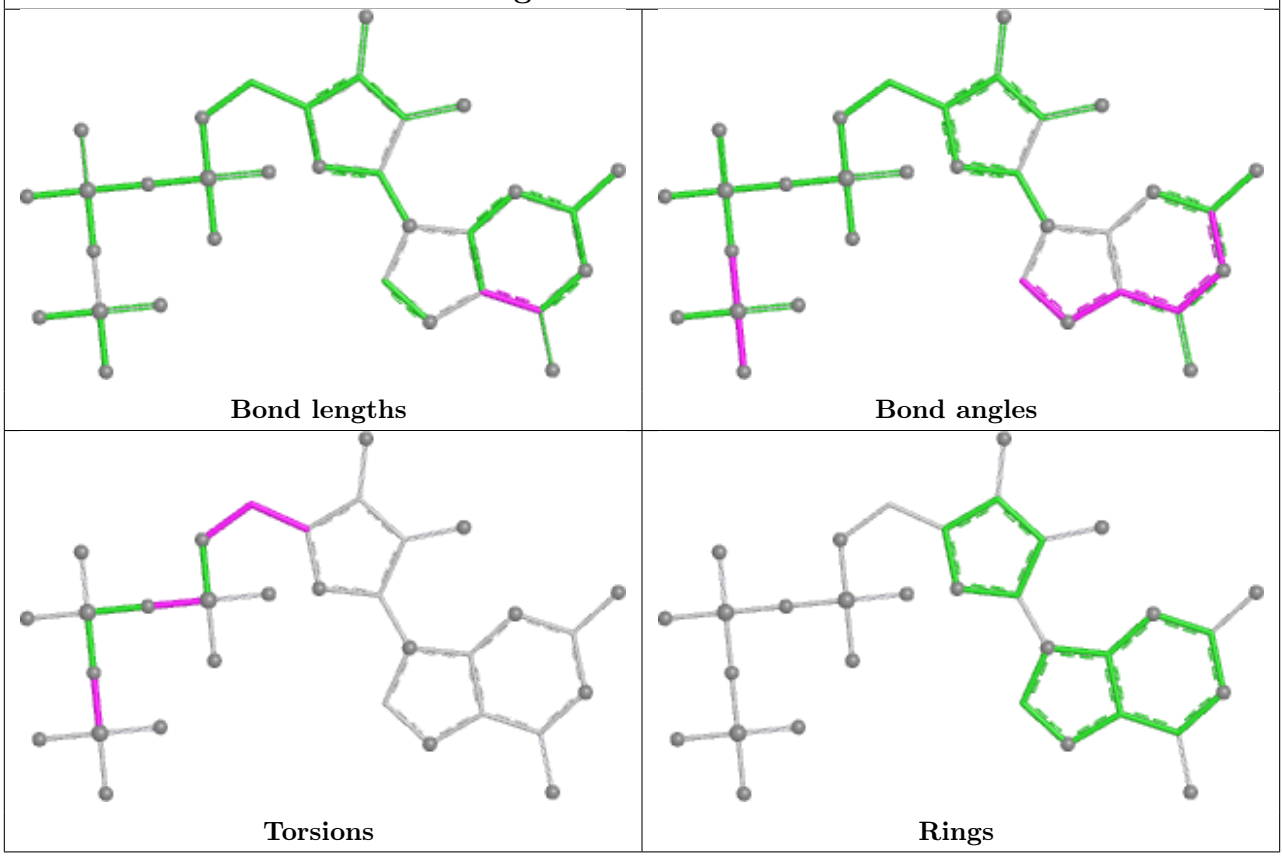
Ligand GTP X6 501



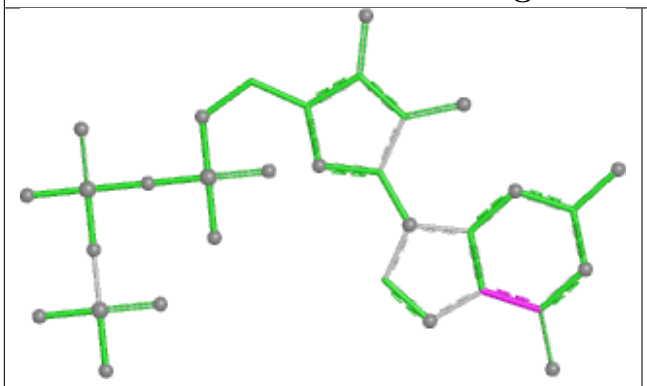
Ligand GTP 3C 501



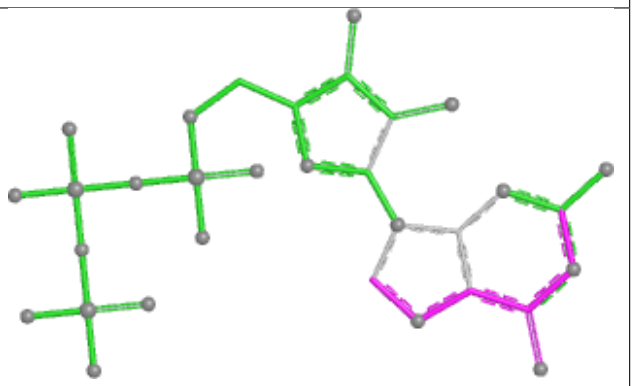
Ligand GTP X0 501



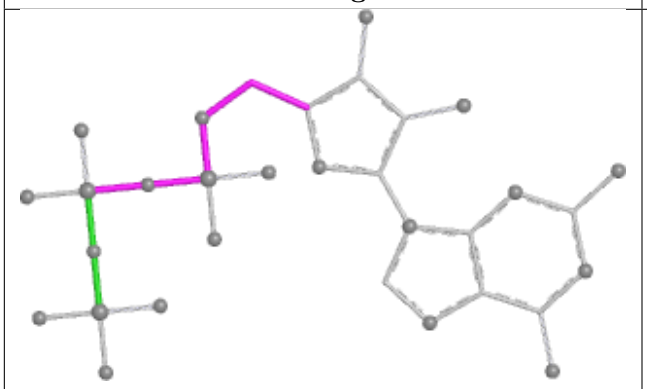
Ligand GTP 0A 501



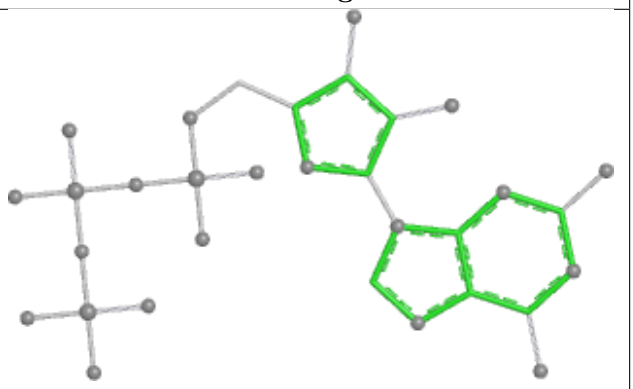
Bond lengths



Bond angles

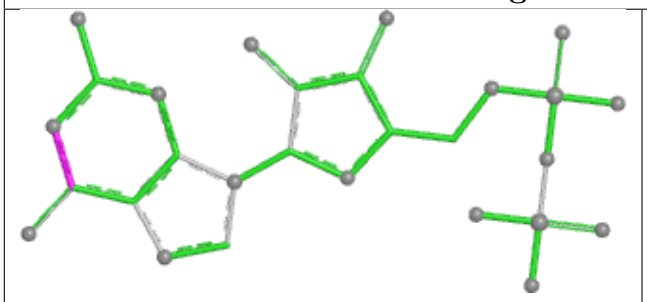


Torsions



Rings

Ligand GDP 0M 502



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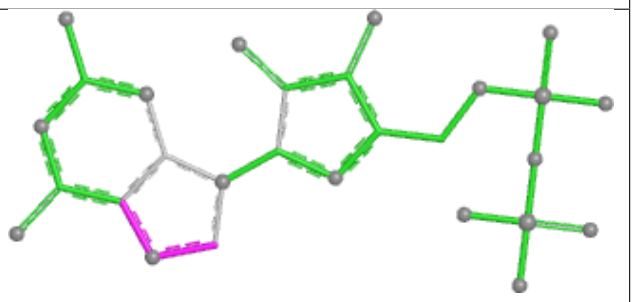
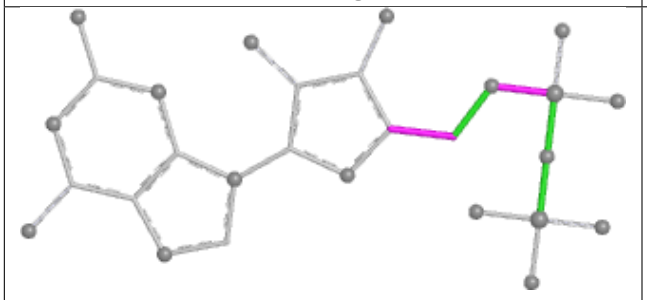


Bond angles



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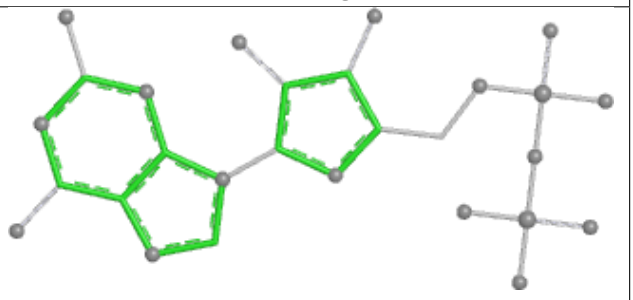
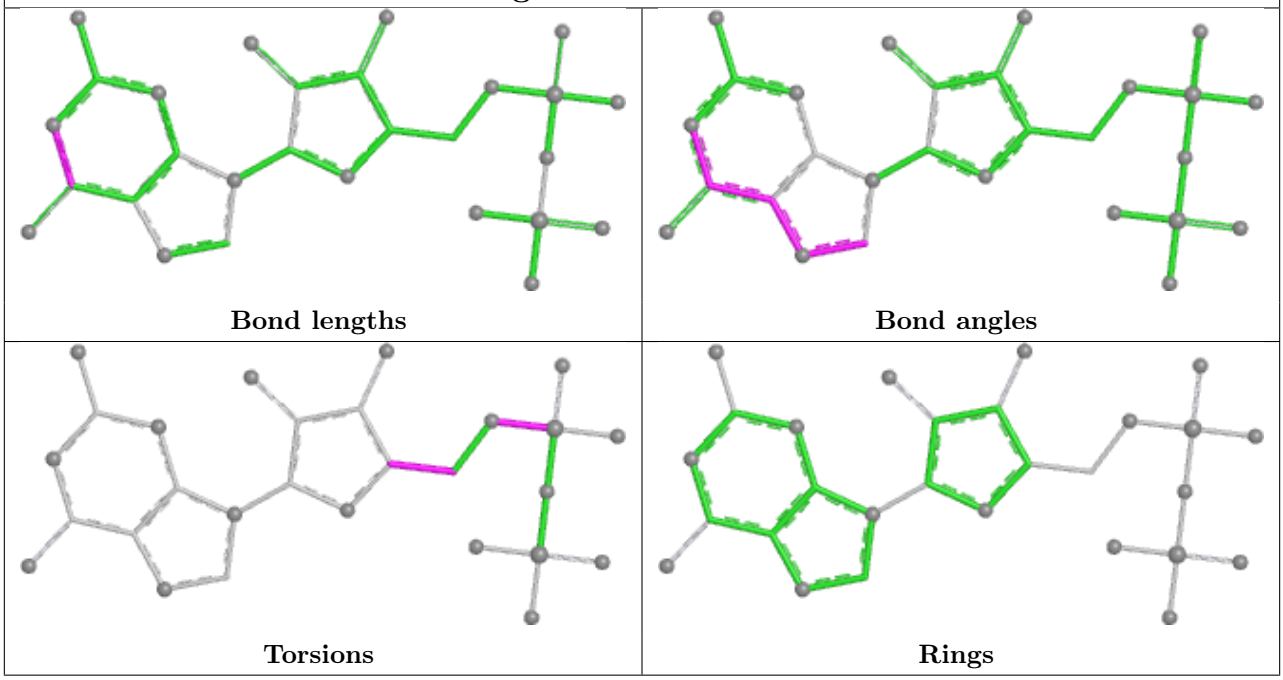
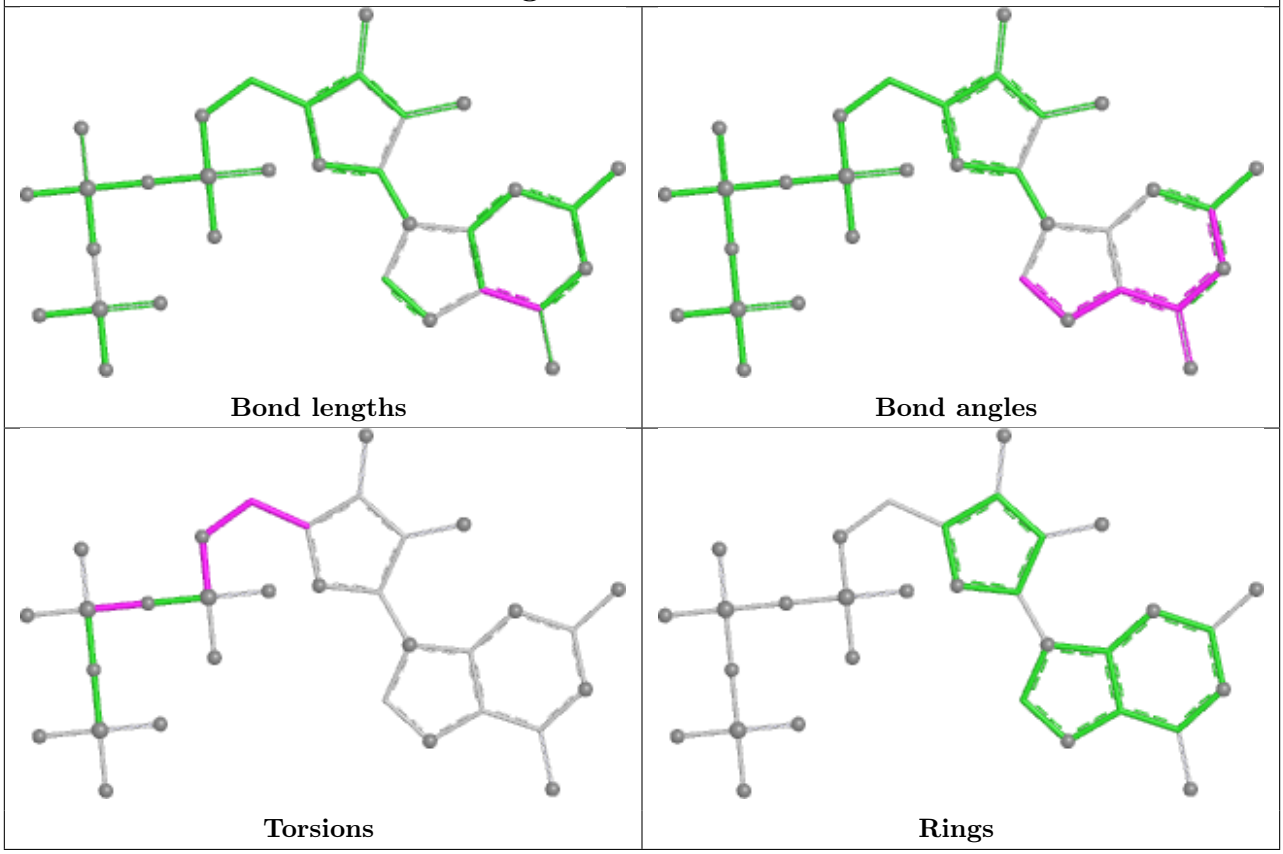


Rings

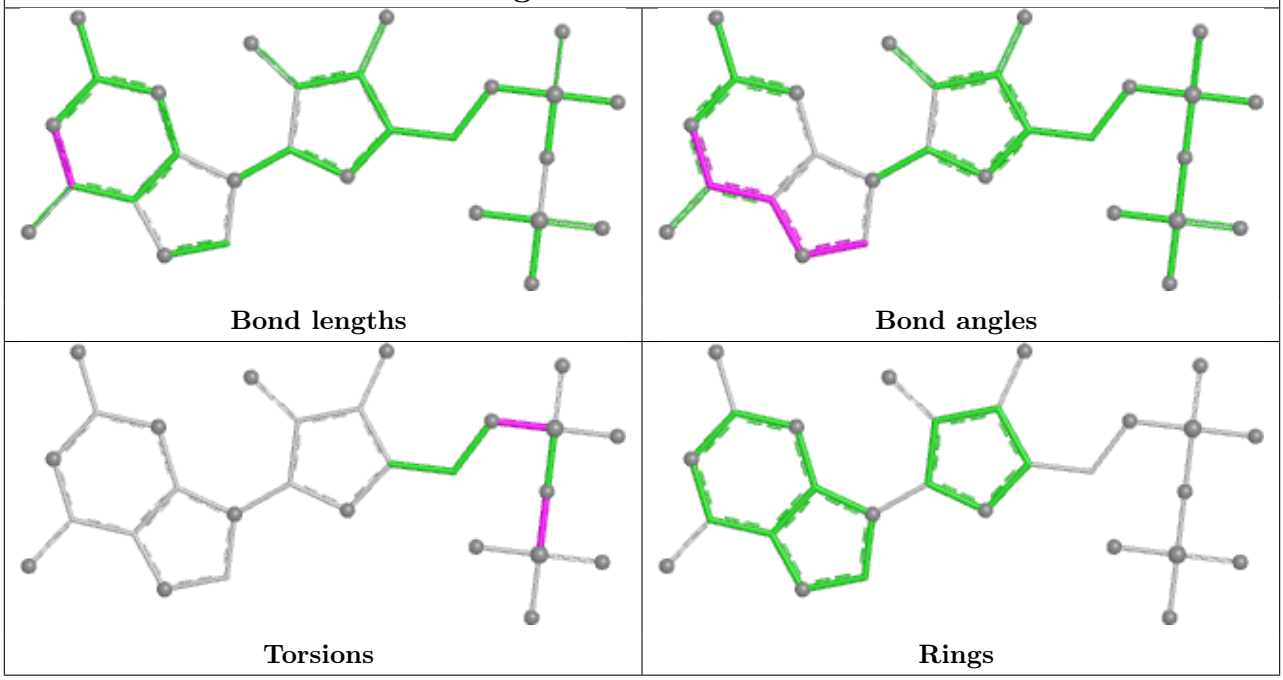
Ligand GDP U8 501



Ligand GTP 2I 501



Ligand GDP C0 502



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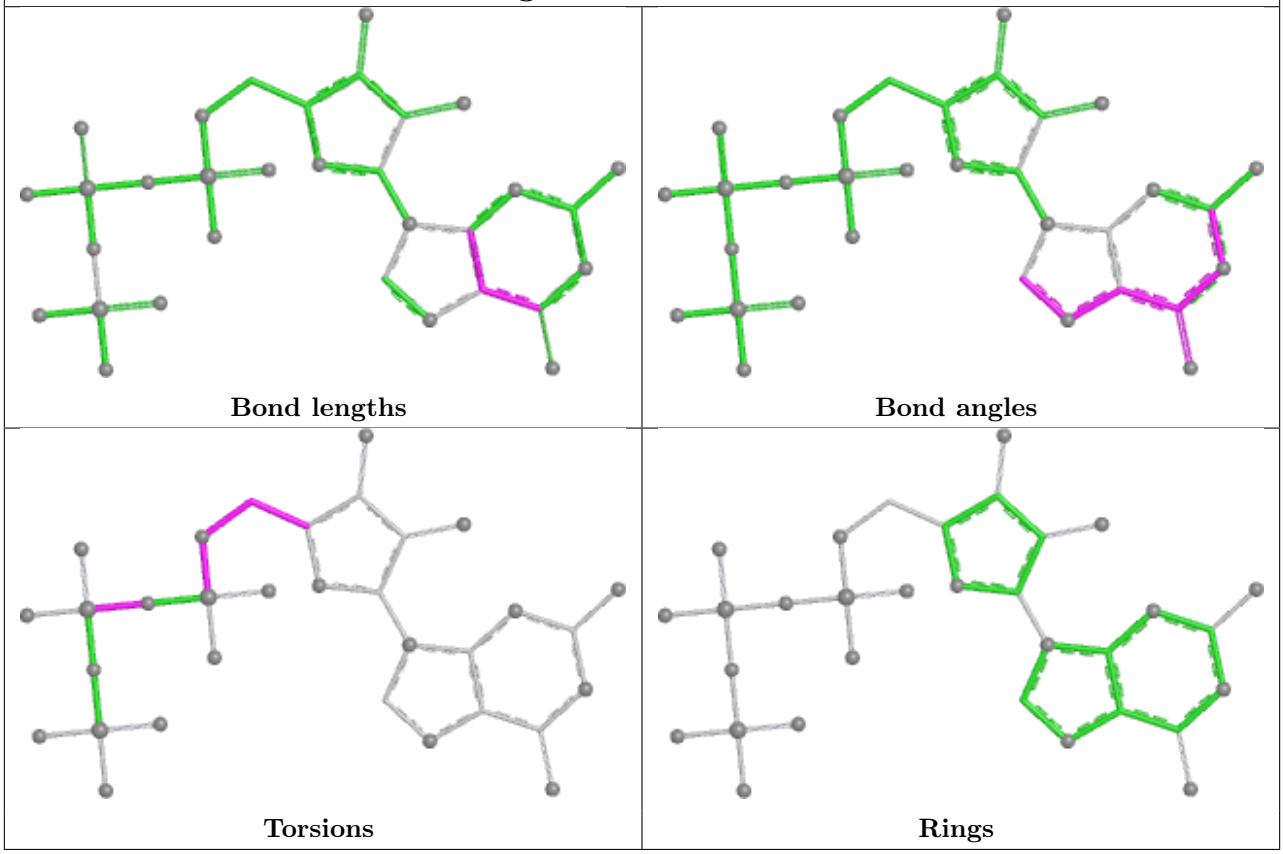

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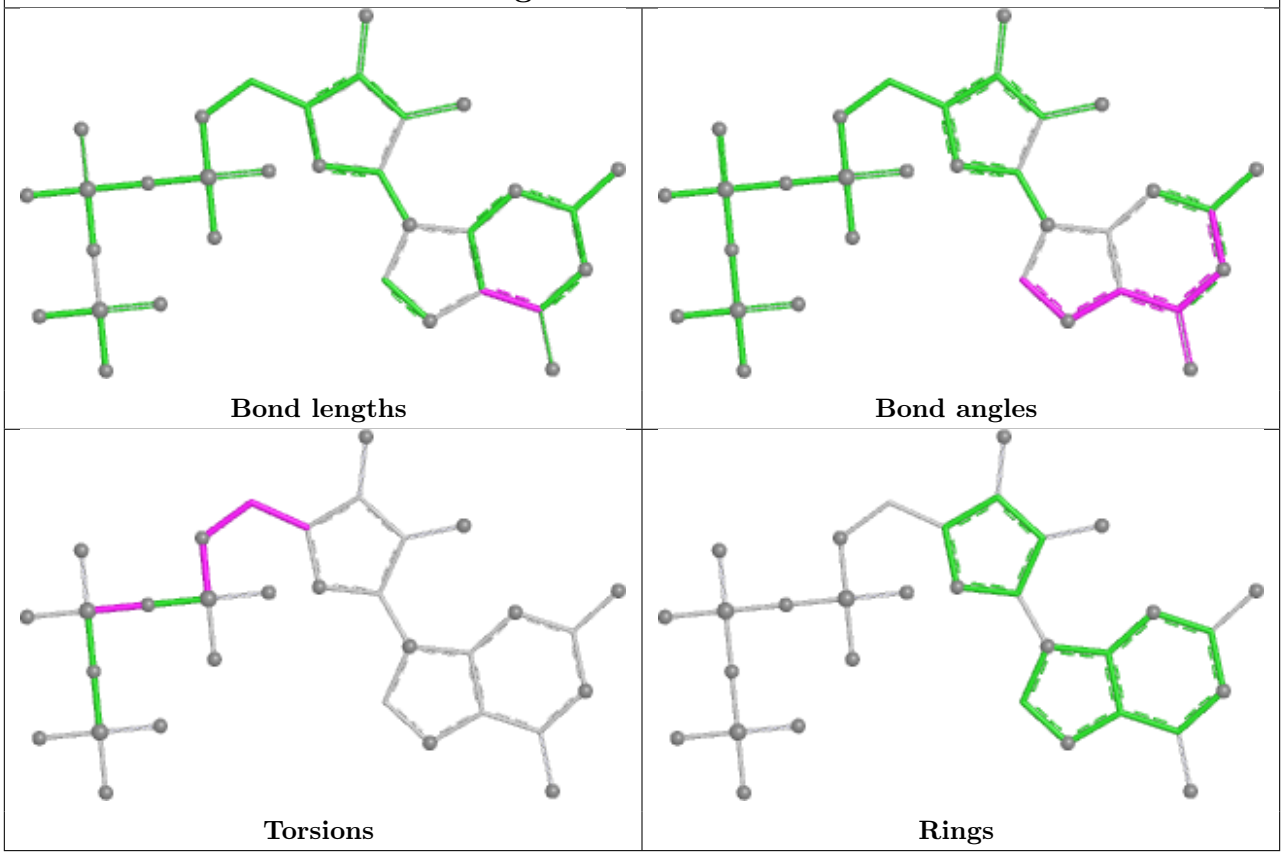
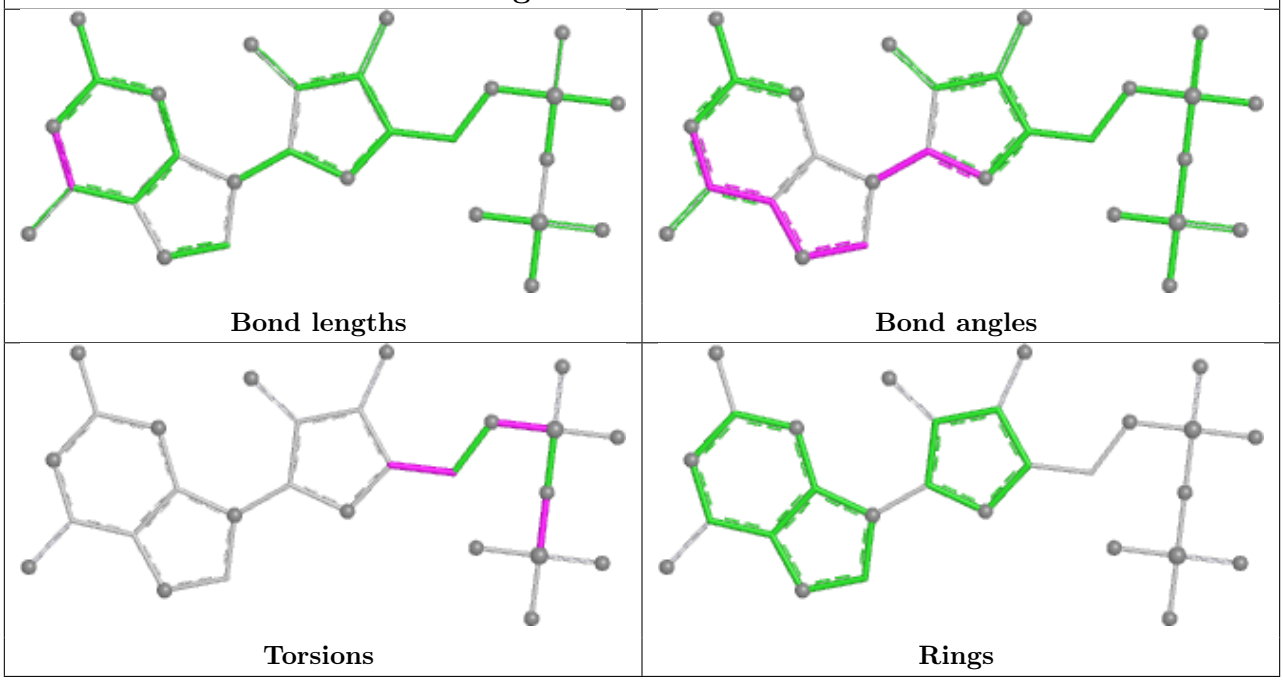
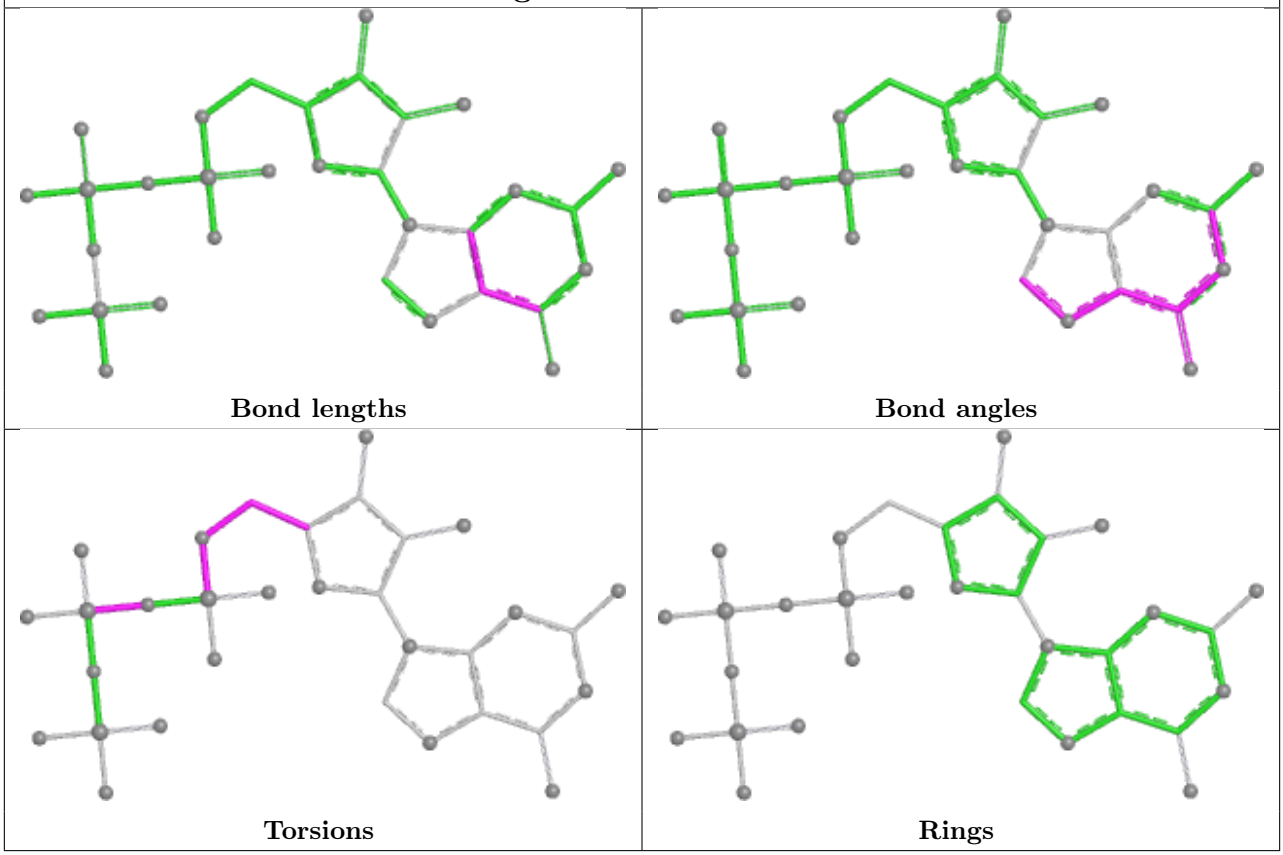


Ligand GDP O6 502



Ligand GTP N1 501



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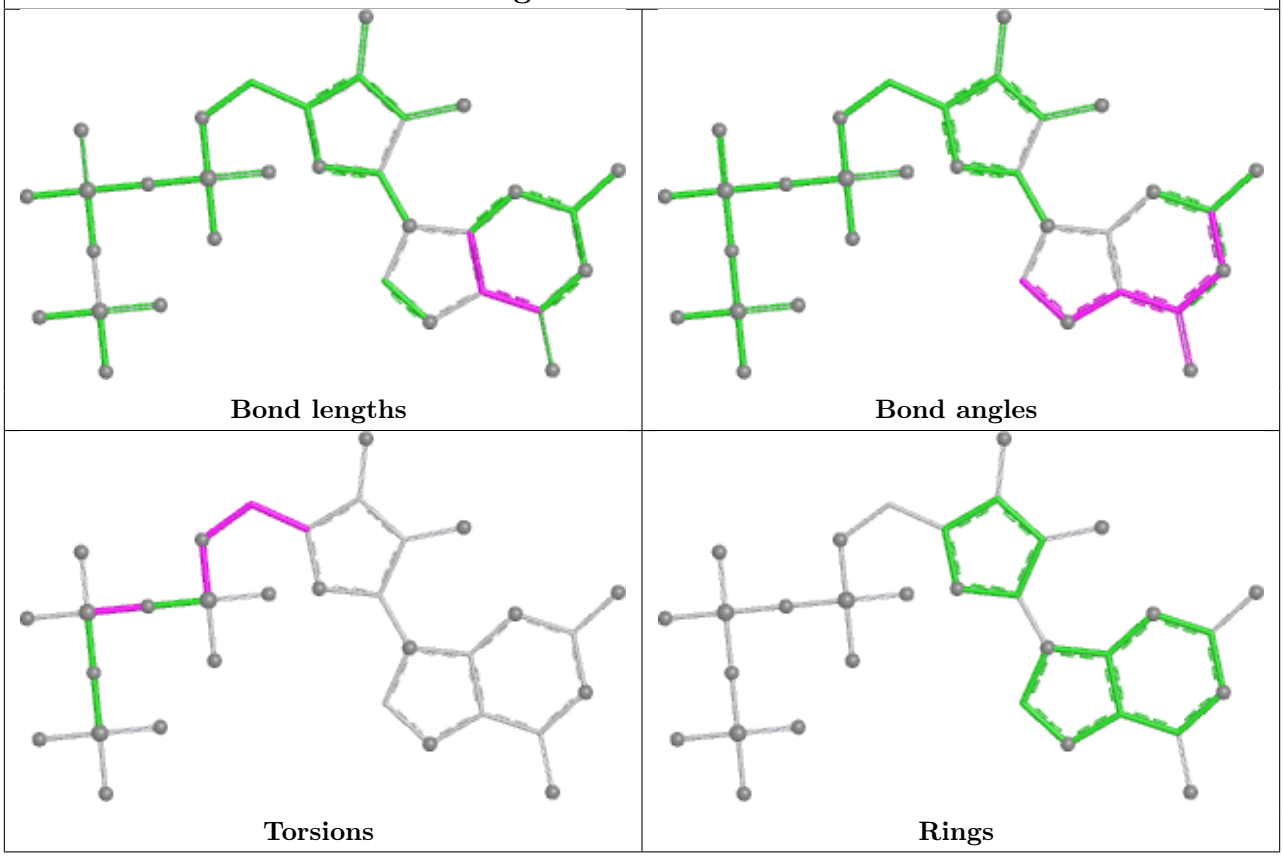

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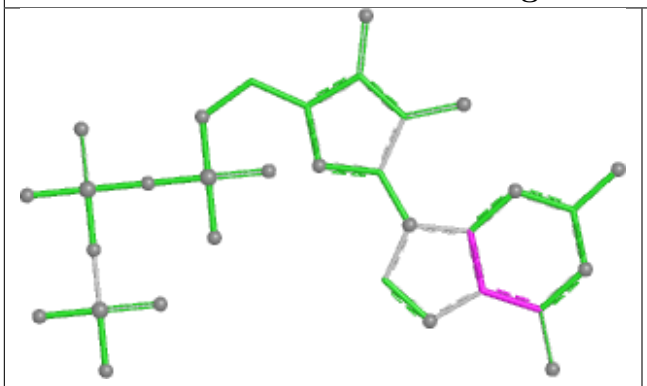

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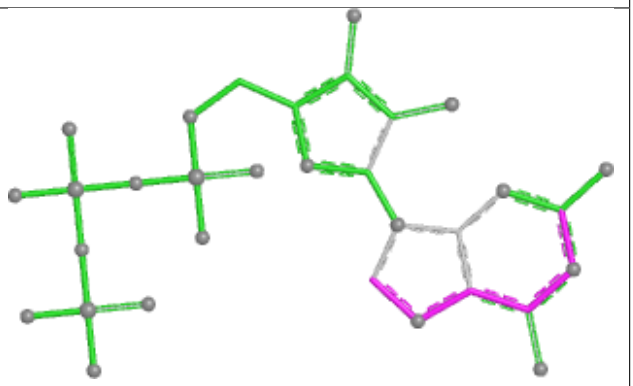
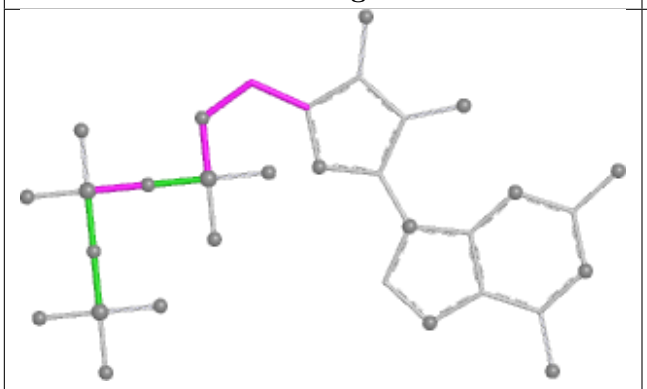
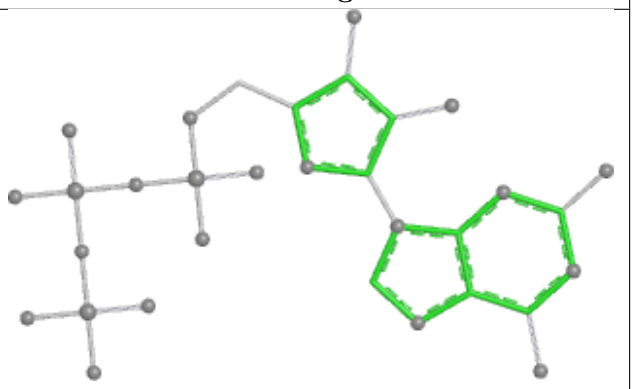


Bond angles

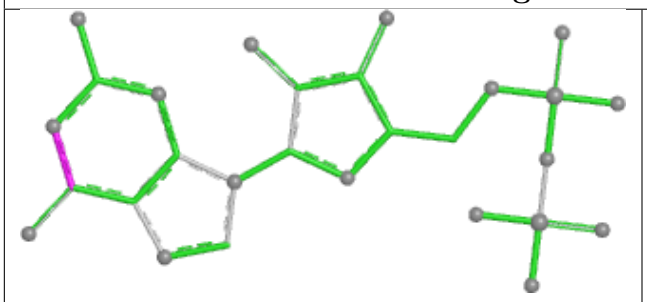


Torsions



Rings

Ligand GDP R4 502



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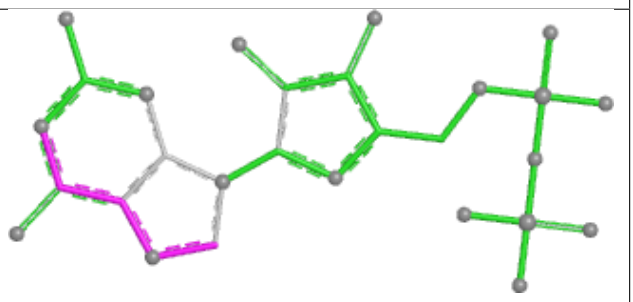

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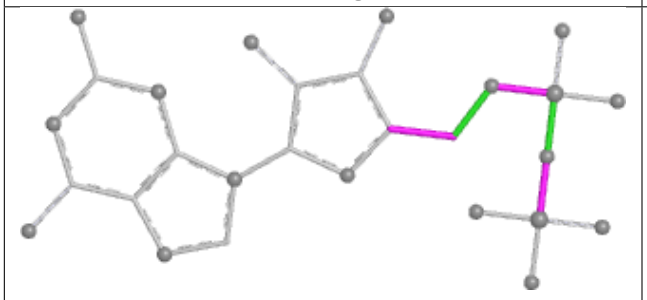

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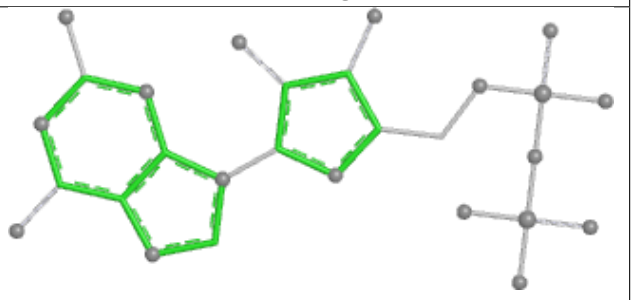
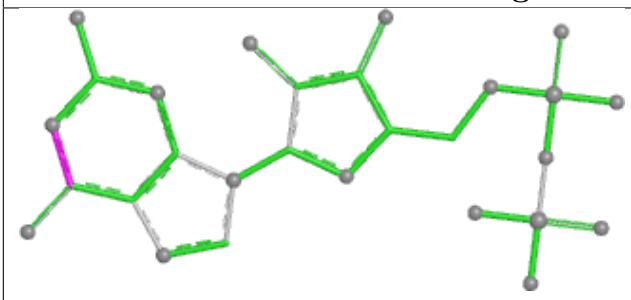
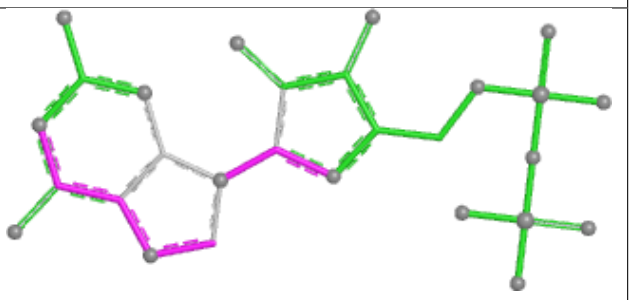
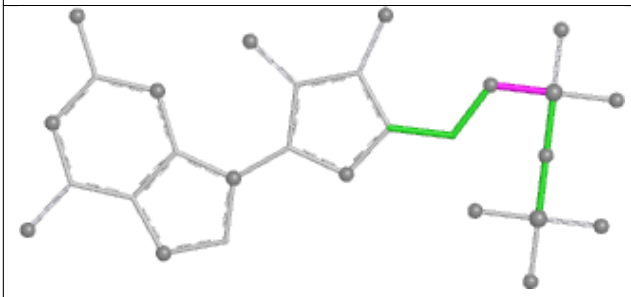
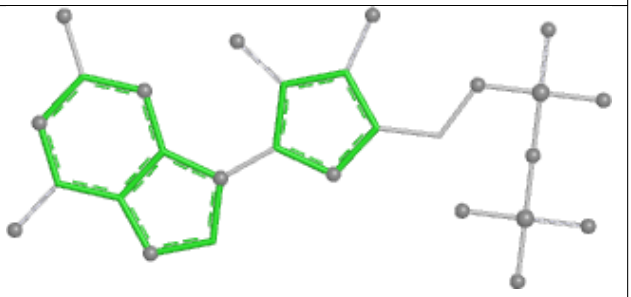
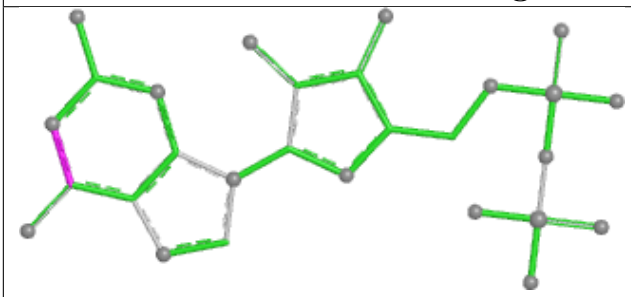
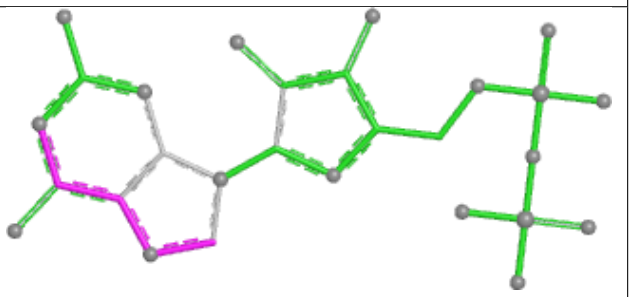
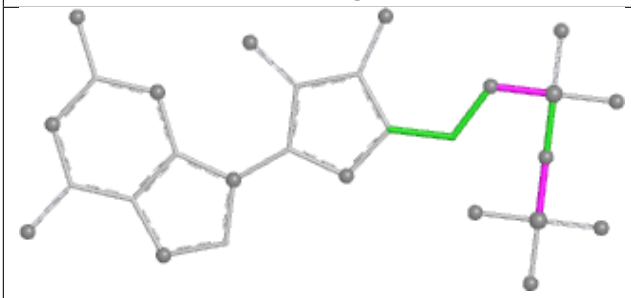
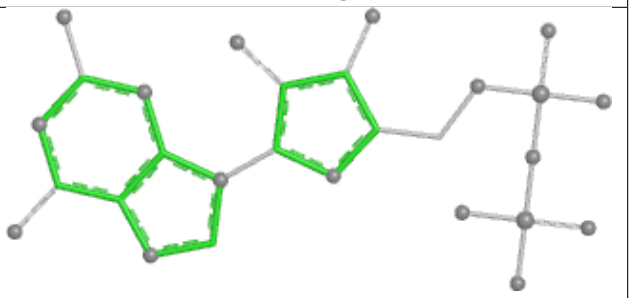
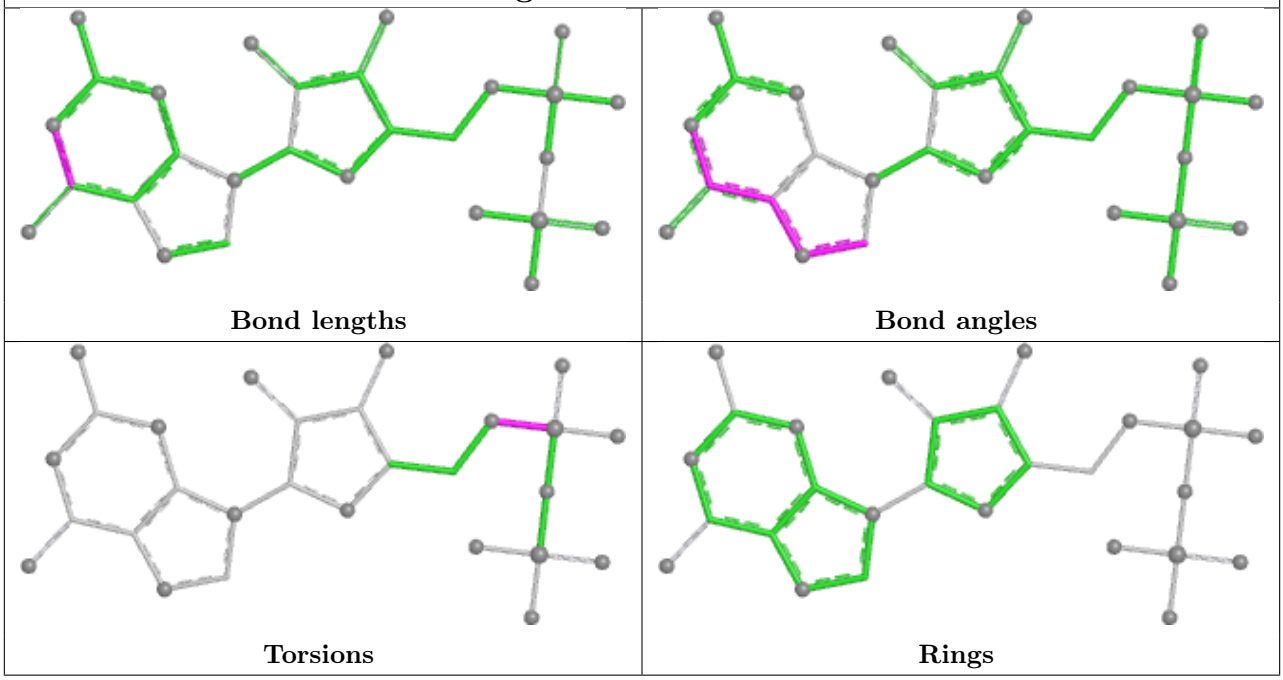


Rings

Ligand GDP O8 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP D2 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP L0 501



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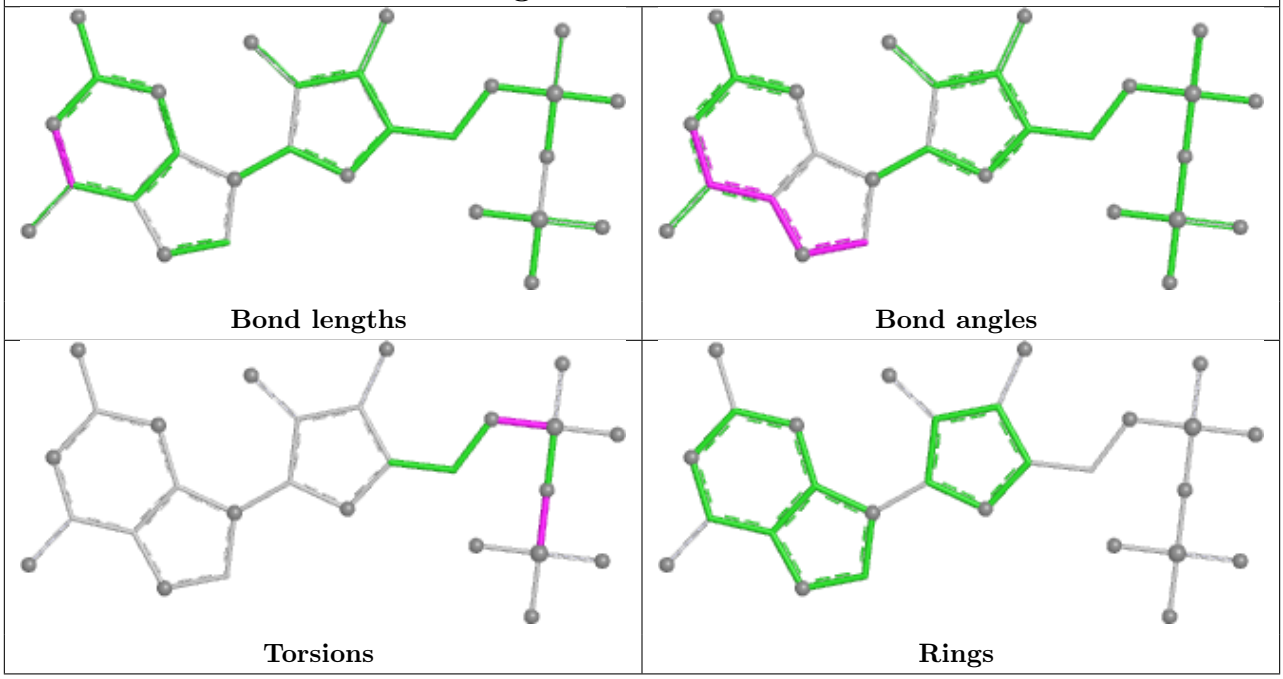

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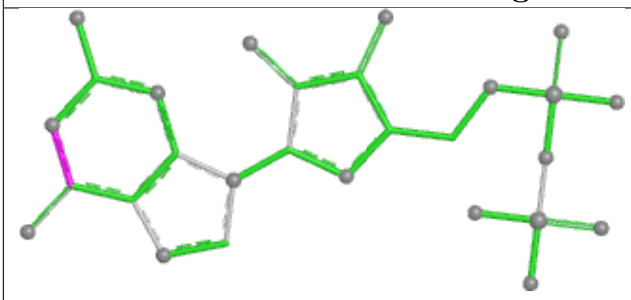
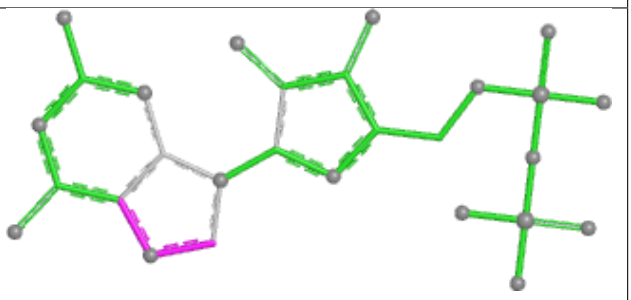
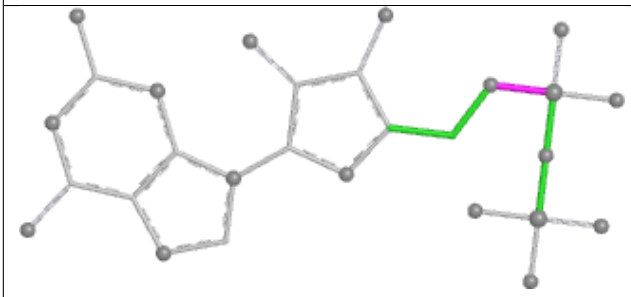
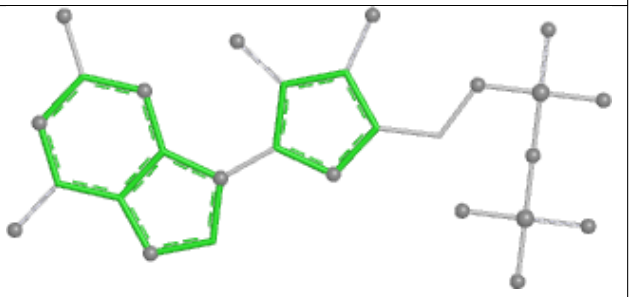
 Bond lengths	 Bond angles
 Torsions	 Rings

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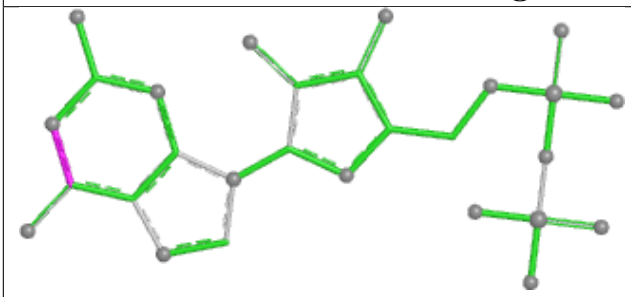
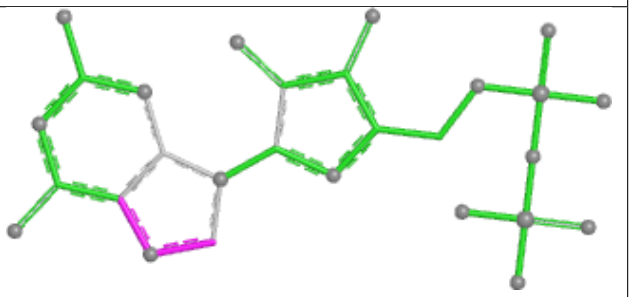
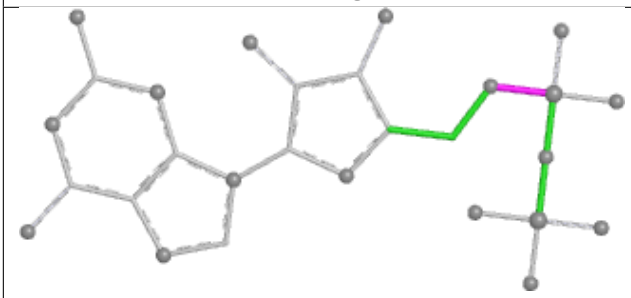
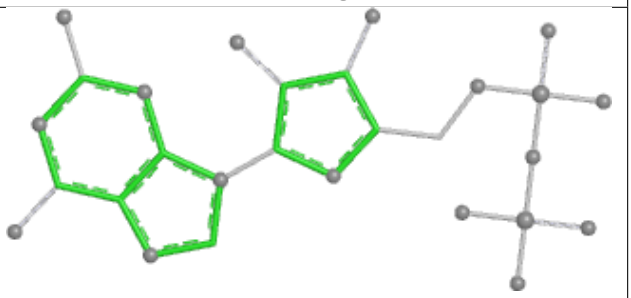
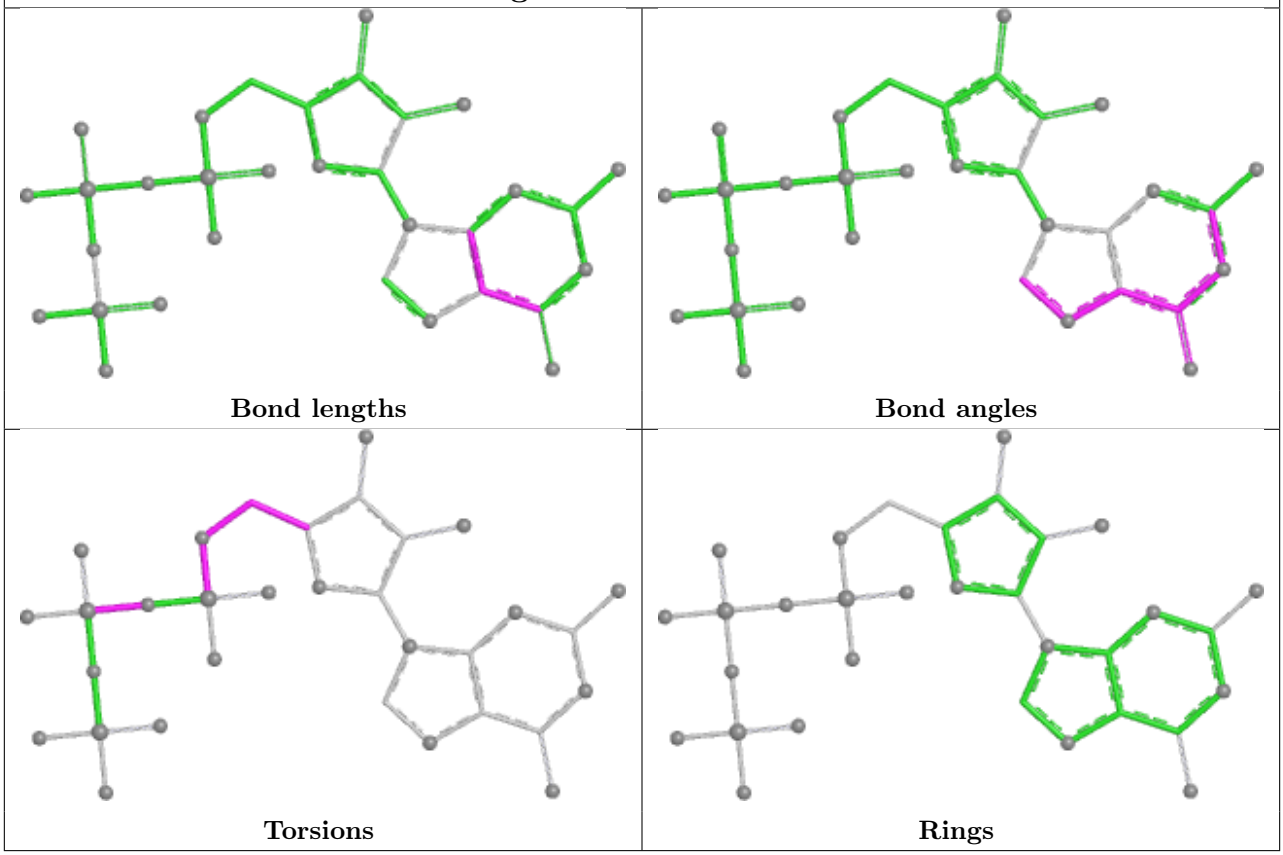
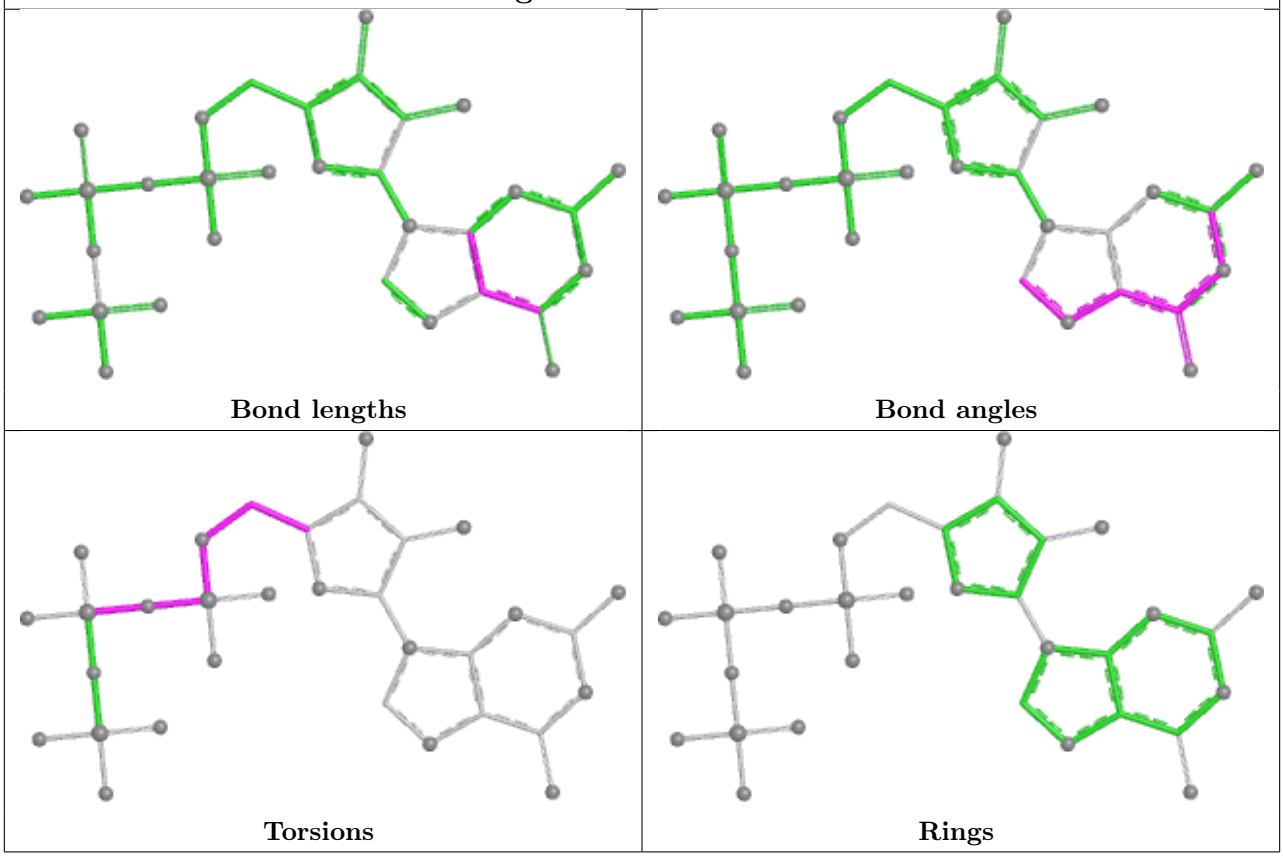
 Bond lengths	 Bond angles
 Torsions	 Rings

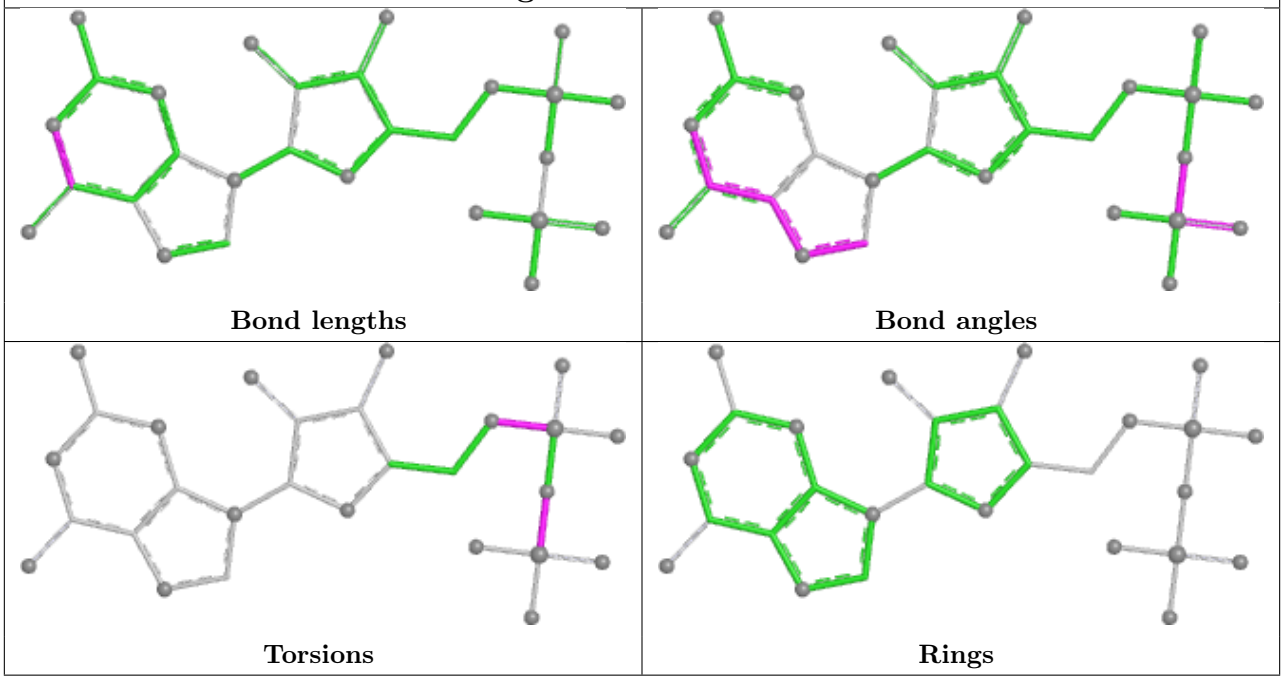
Ligand GTP M7 501



Ligand GTP P6 501



Ligand GDP J8 502



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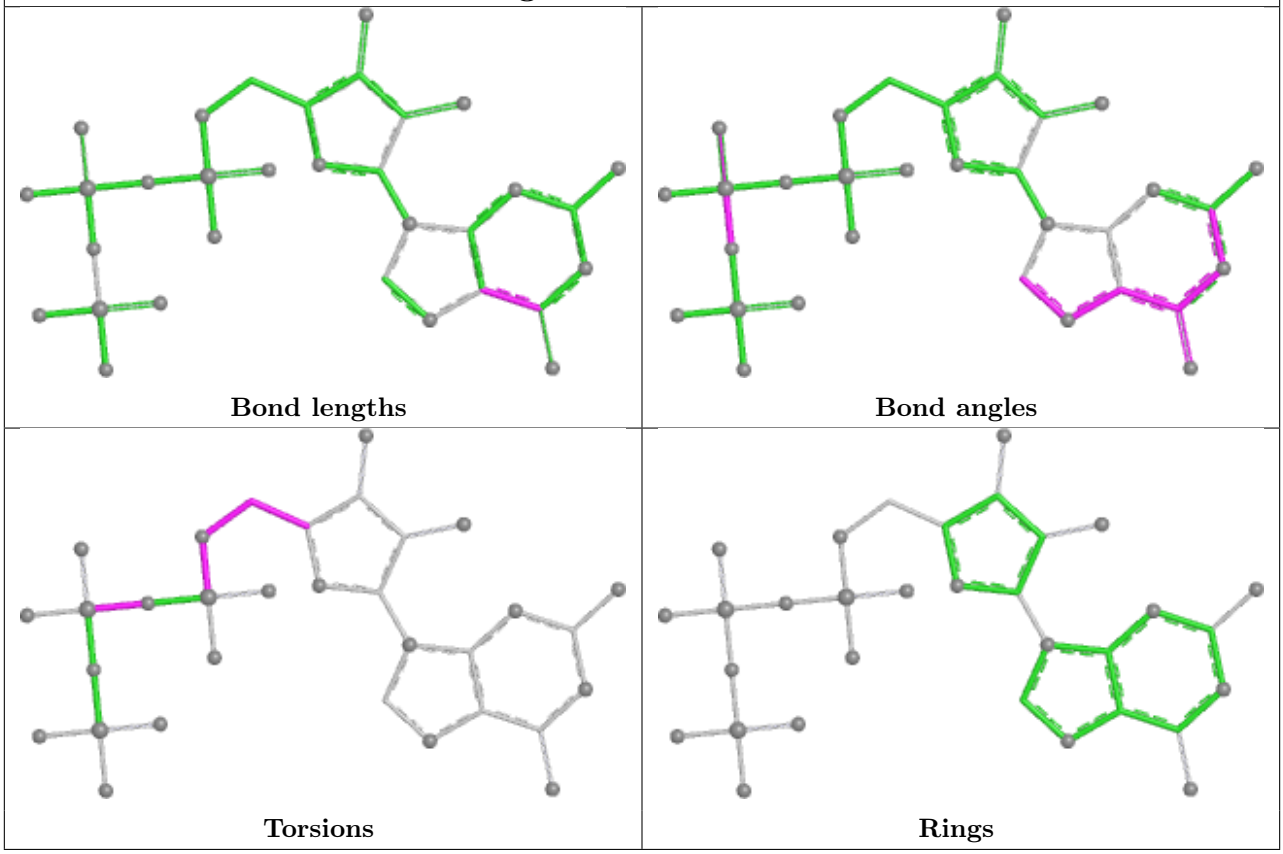
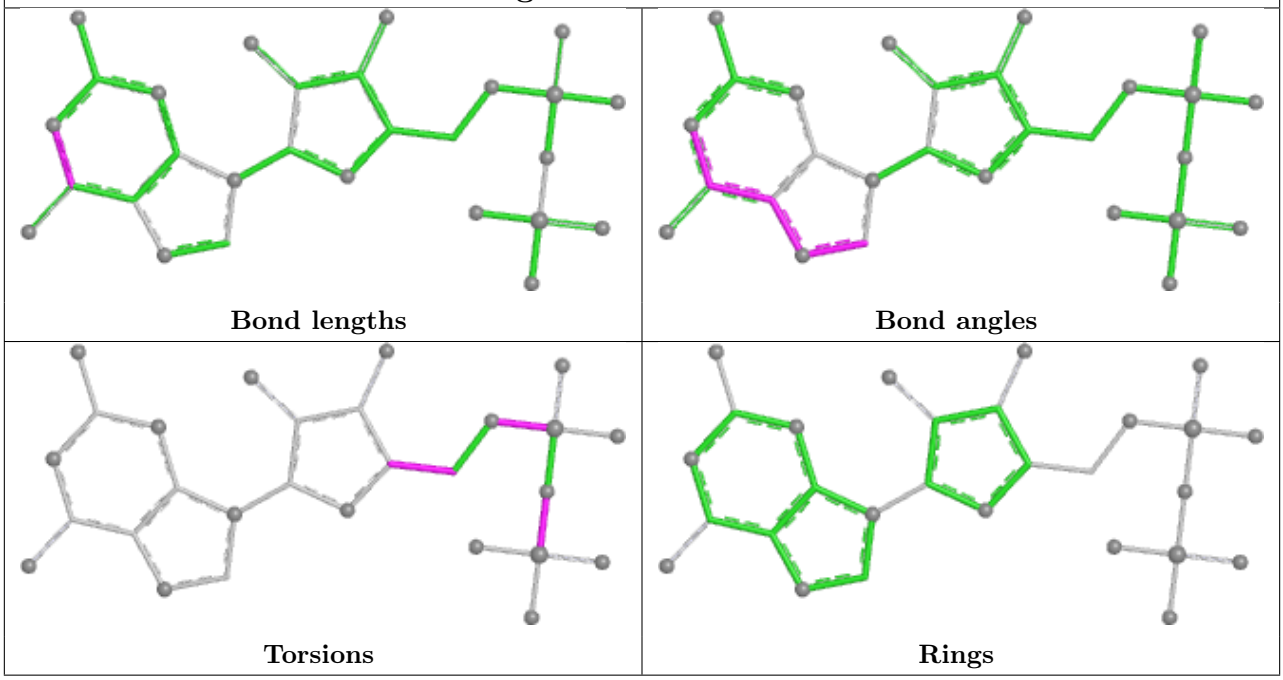


Ligand GDP S6 501



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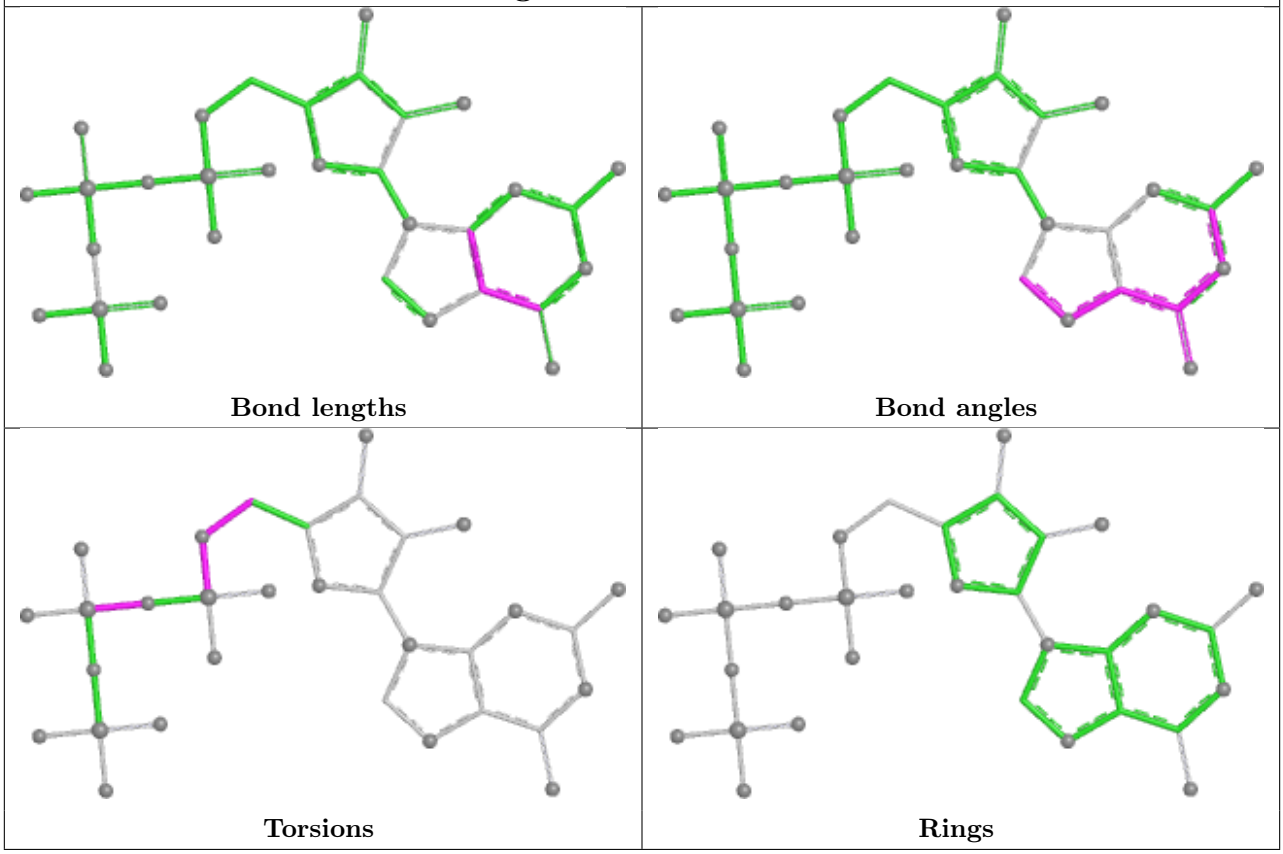

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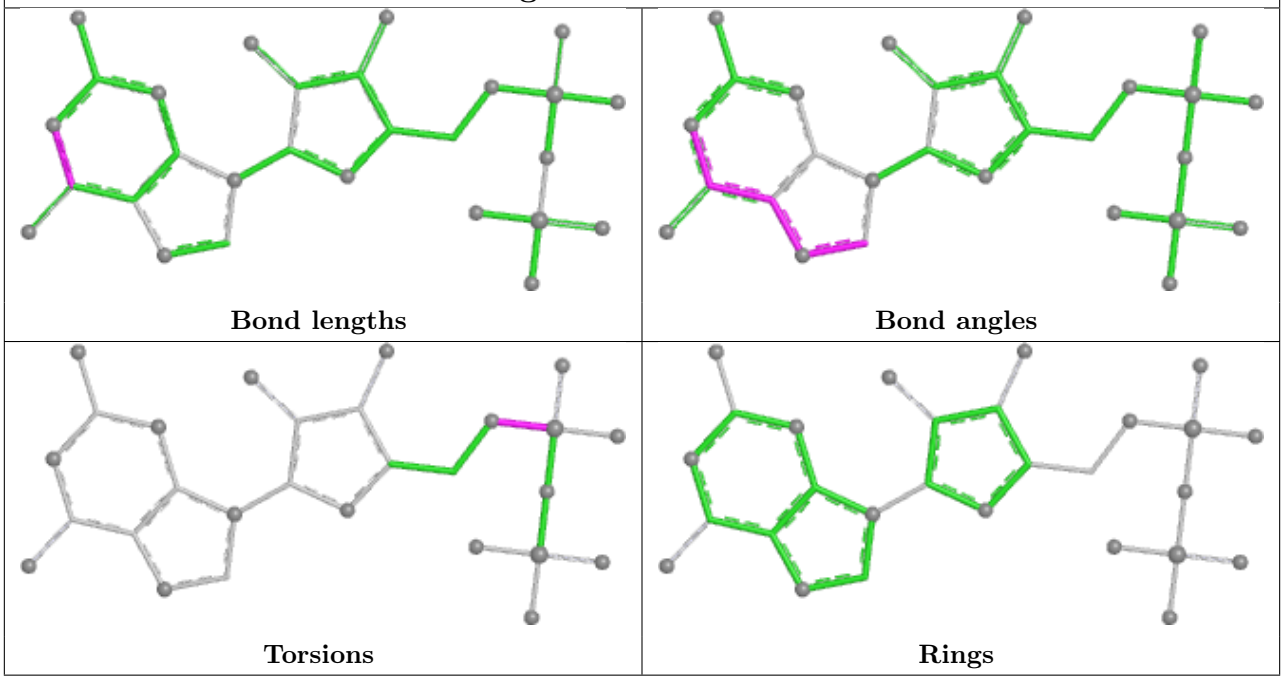
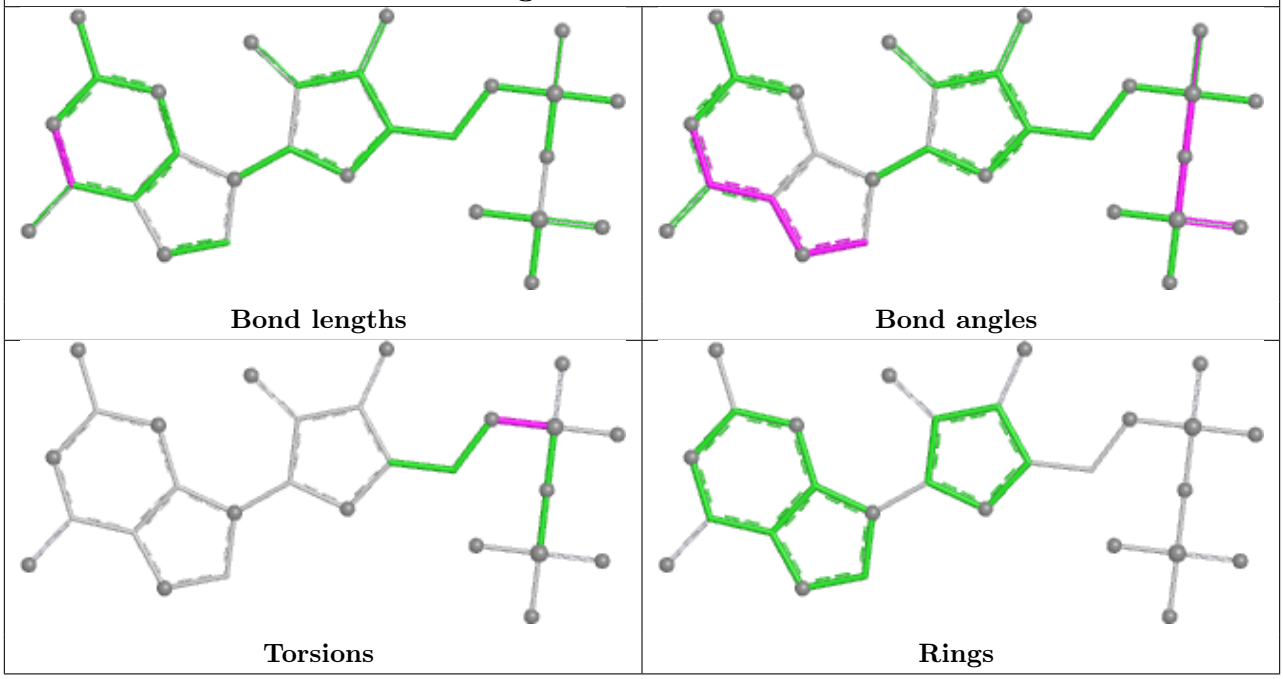


Ligand GDP J6 502



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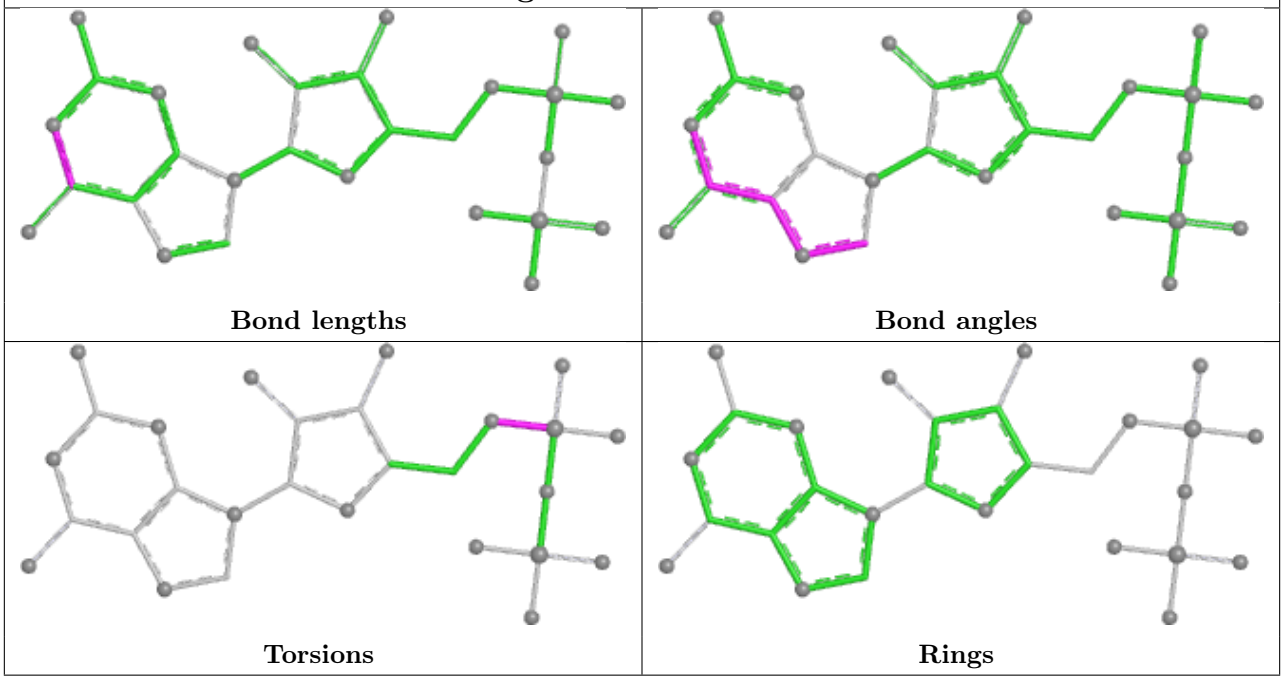
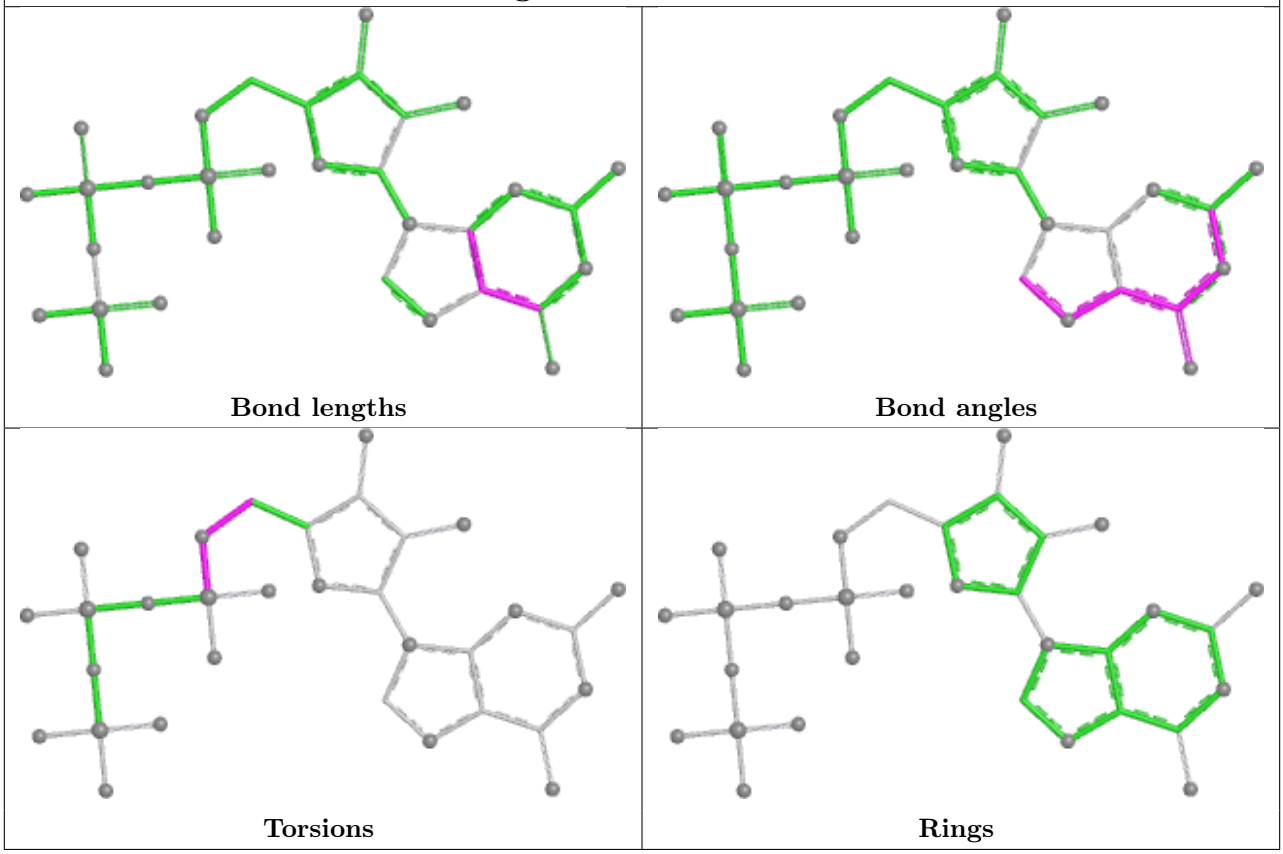


Ligand GTP D5 501



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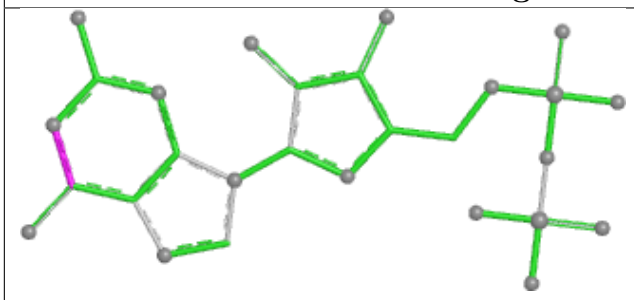
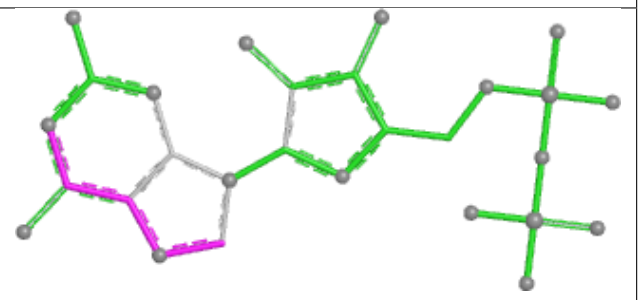
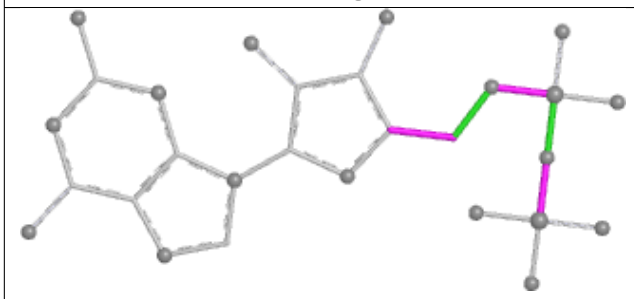


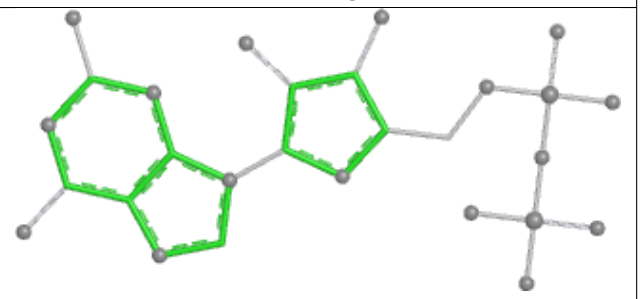
Bond lengths



Bond angles

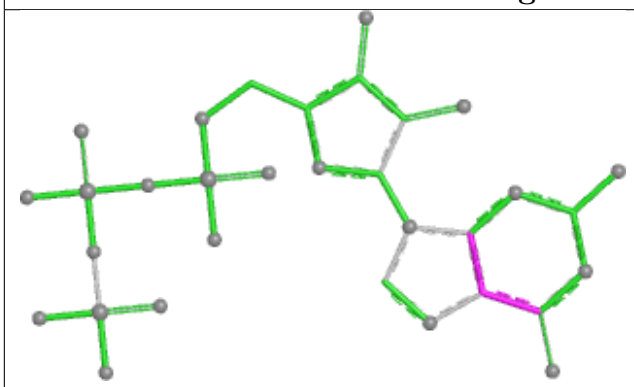


Torsions



Rings

Ligand GTP J4 501



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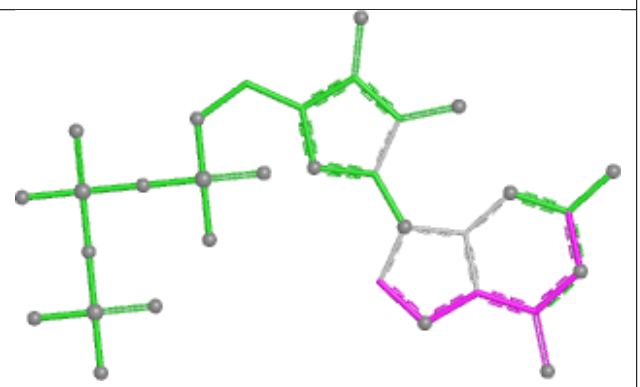
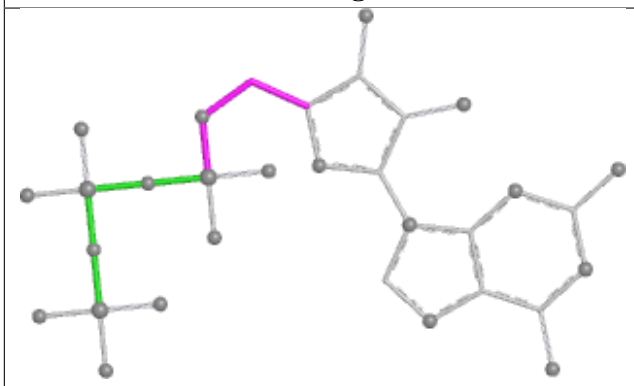


Bond angles



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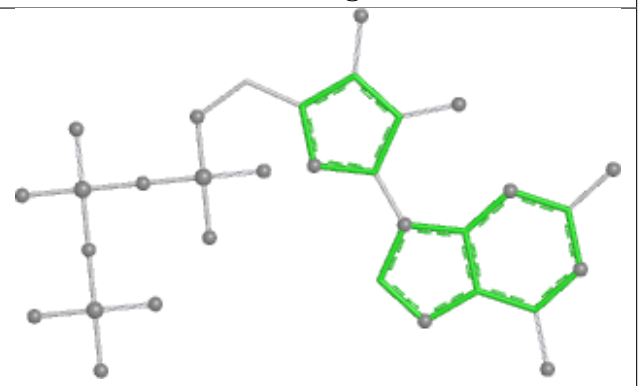
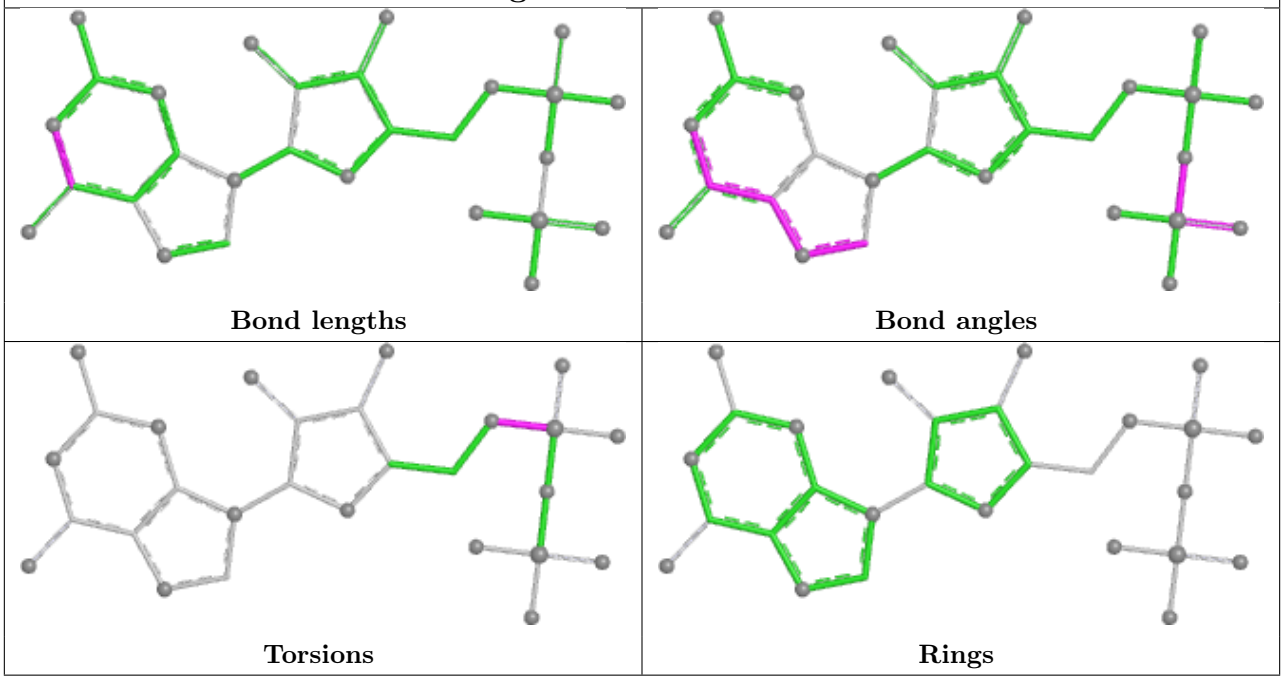
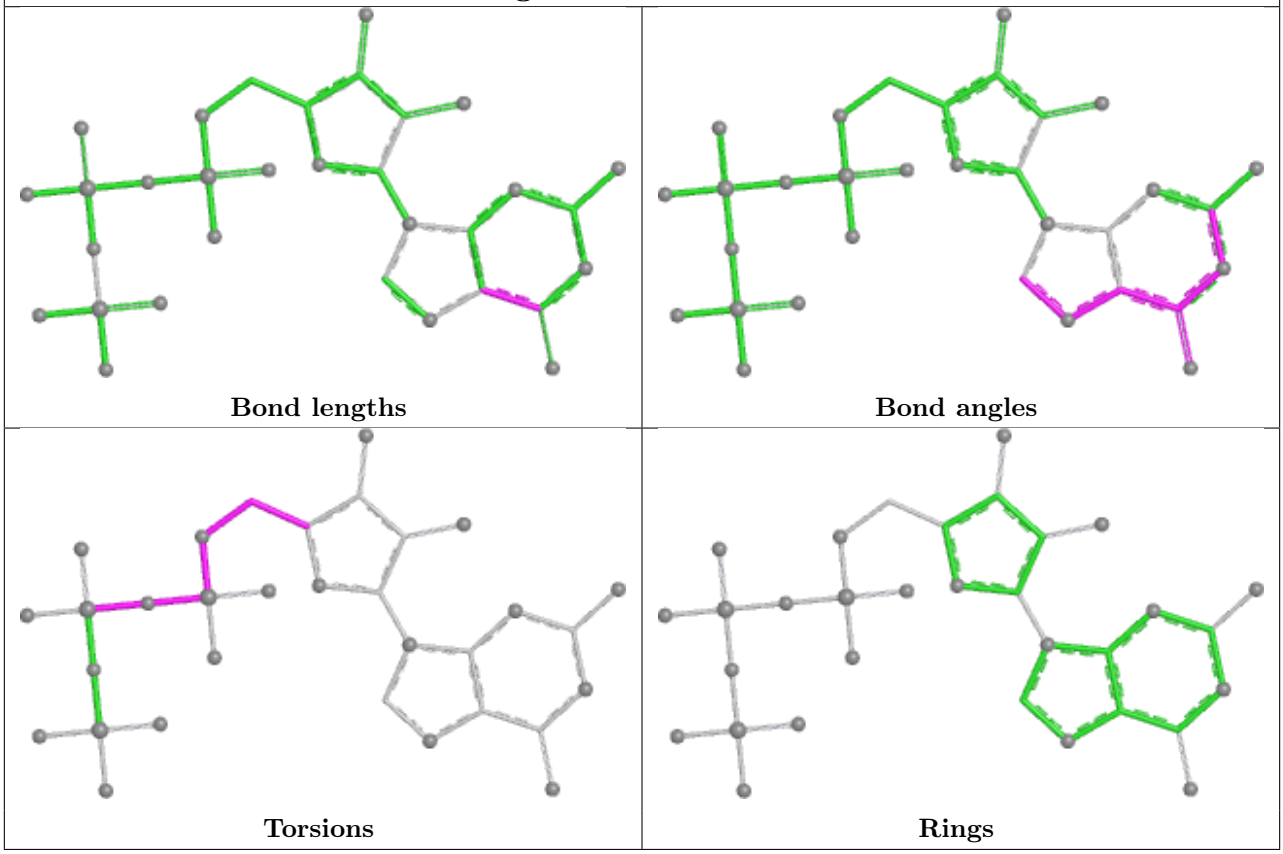


Rings

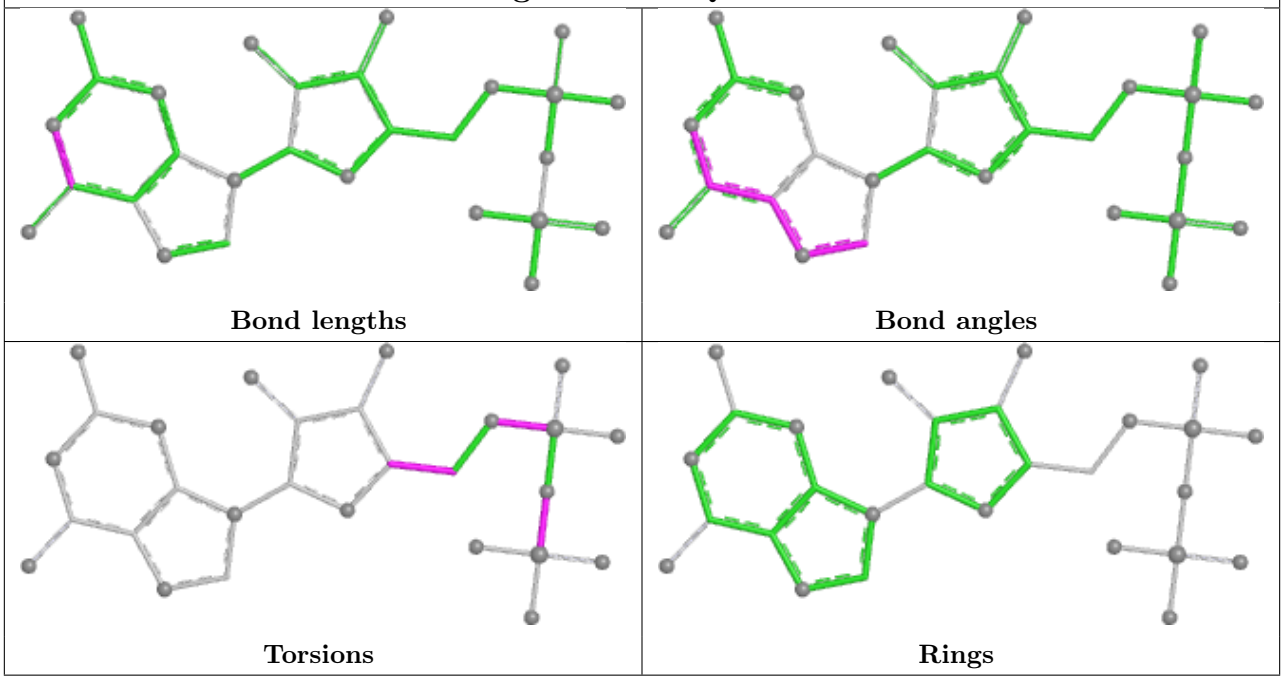
Ligand GDP 1M 501



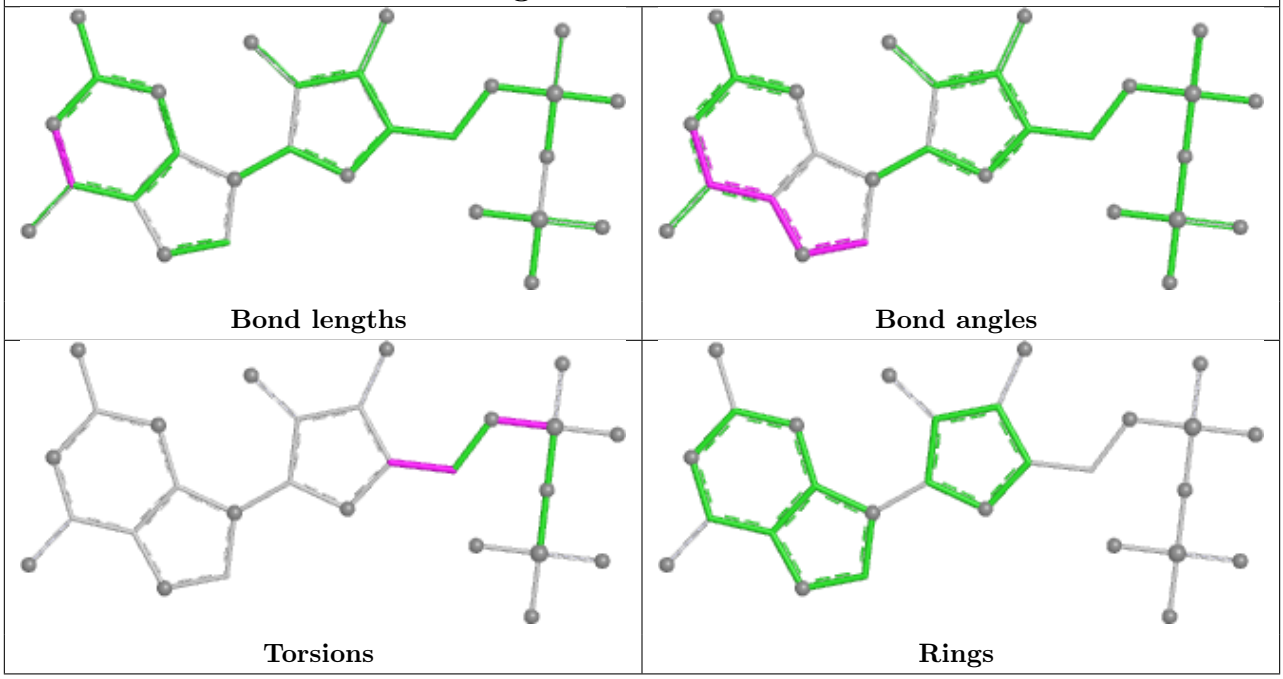
Ligand GTP 1C 501



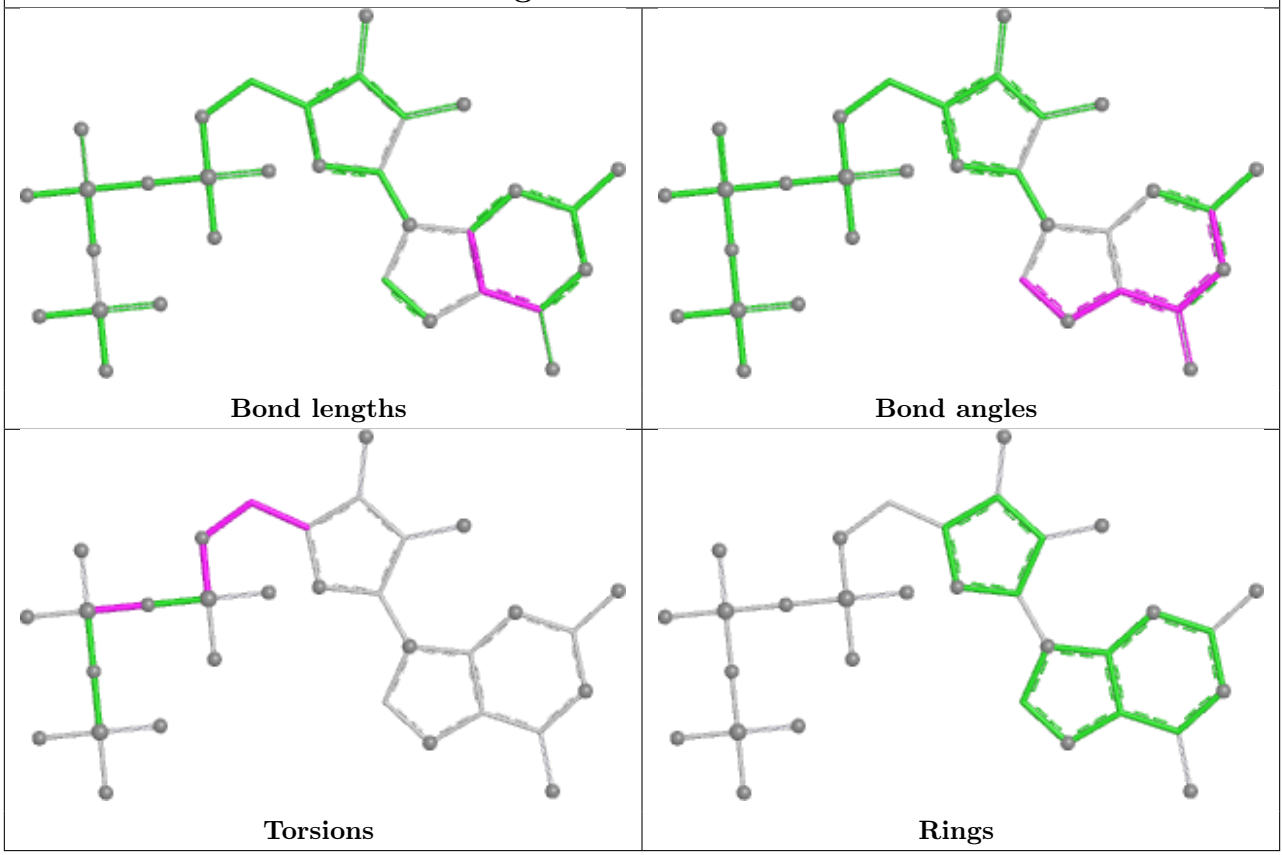
Ligand GDP Q6 502



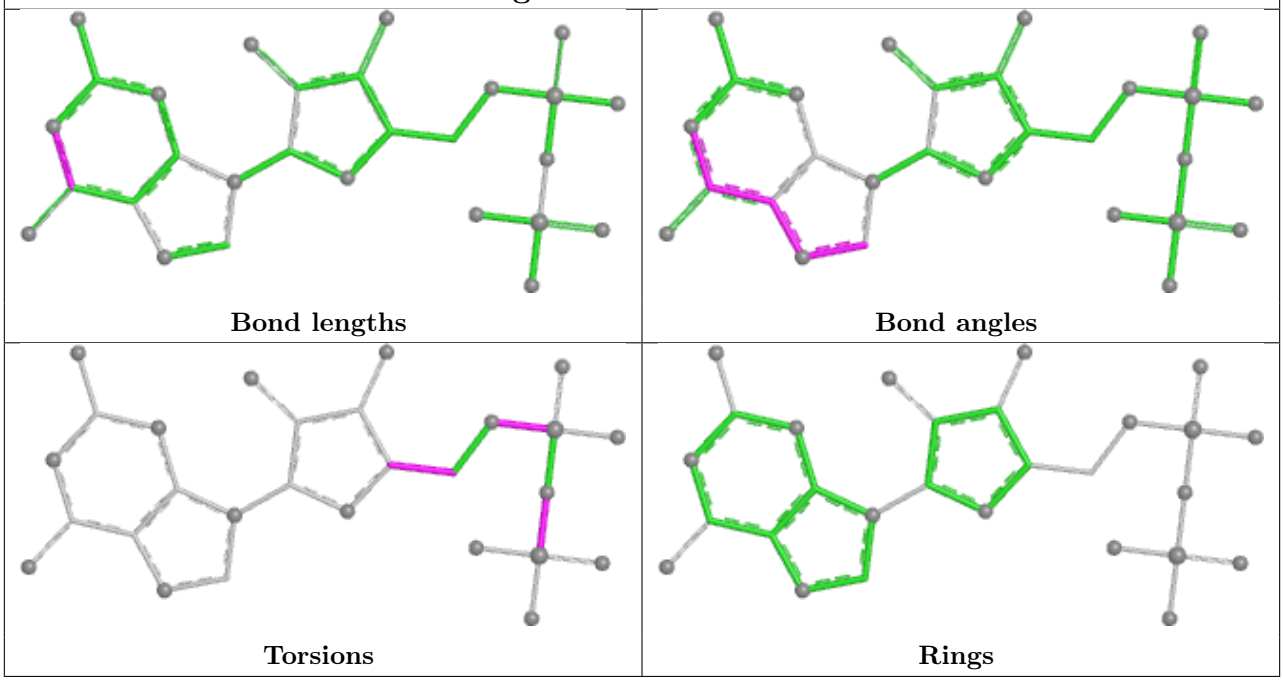
Ligand GDP U6 502



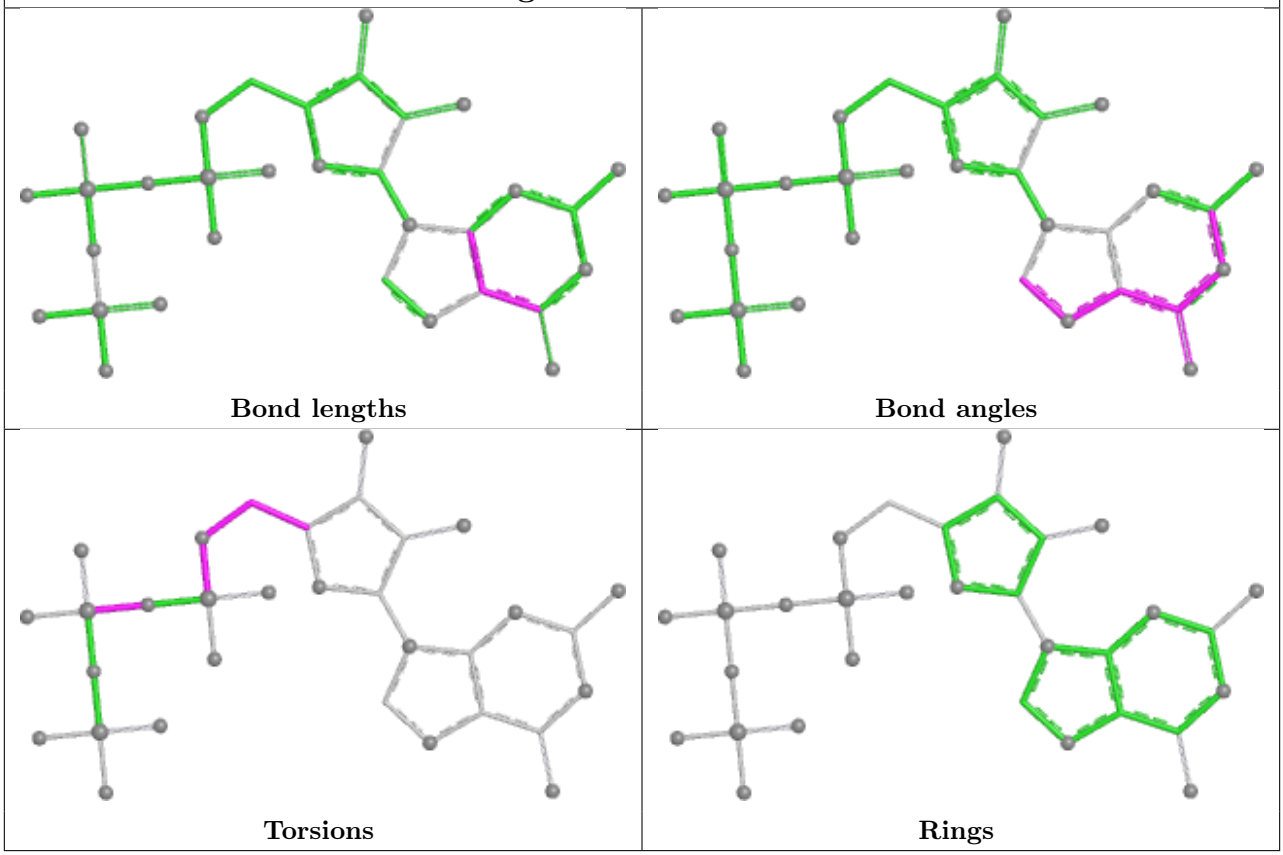
Ligand GTP O0 501



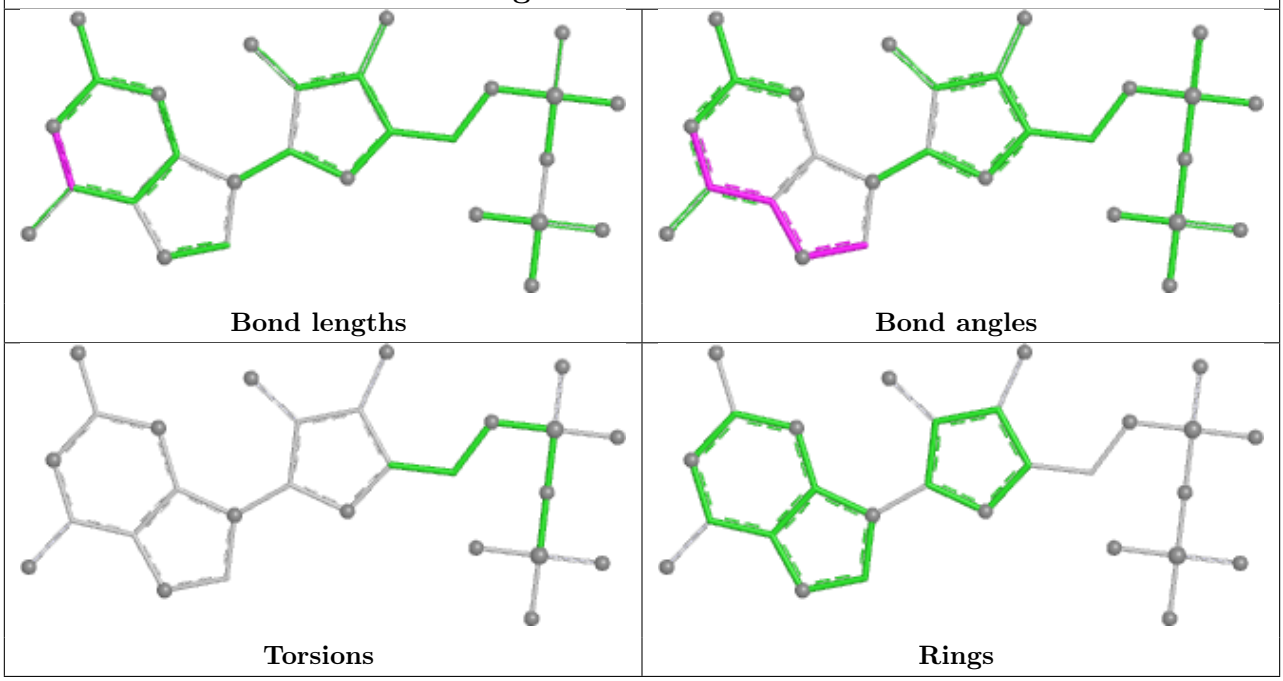
Ligand GDP A1 502



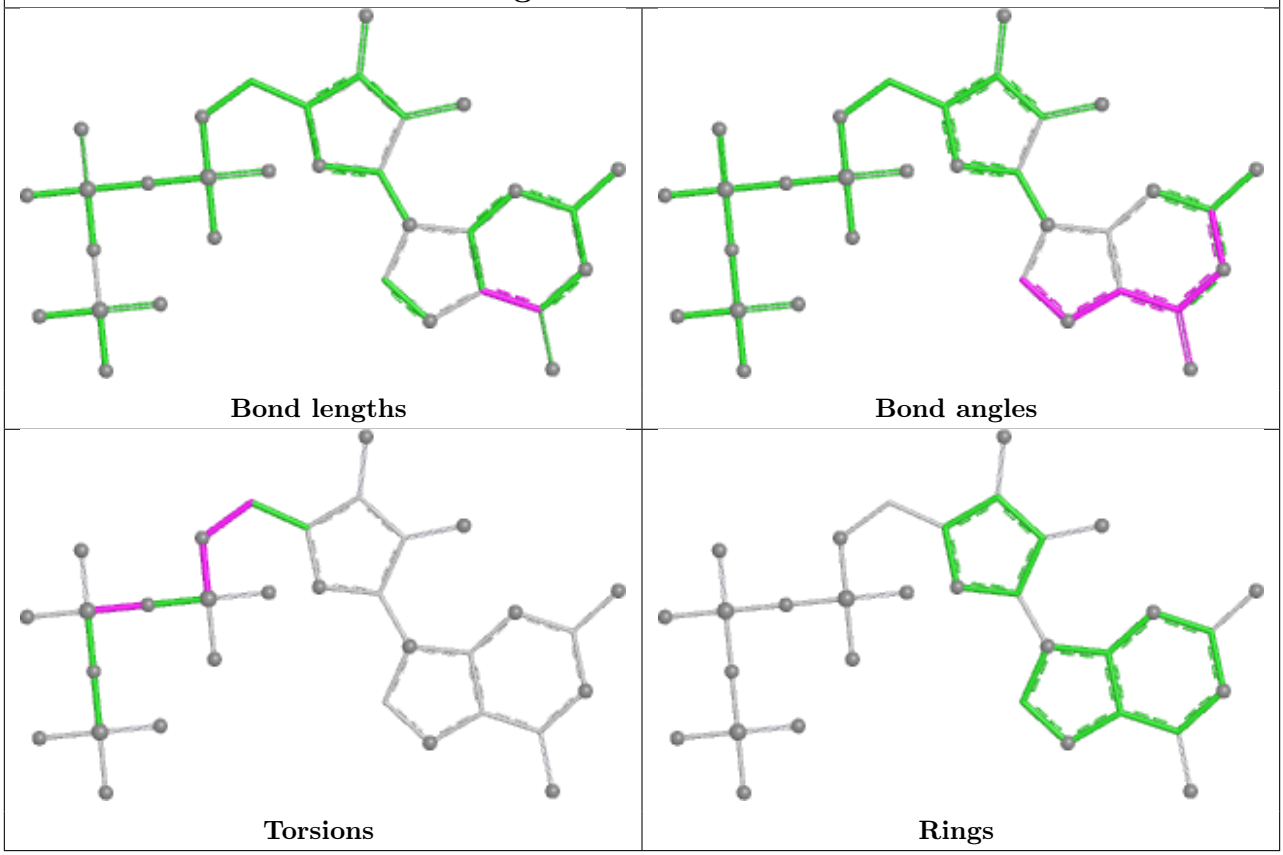
Ligand GTP S0 501



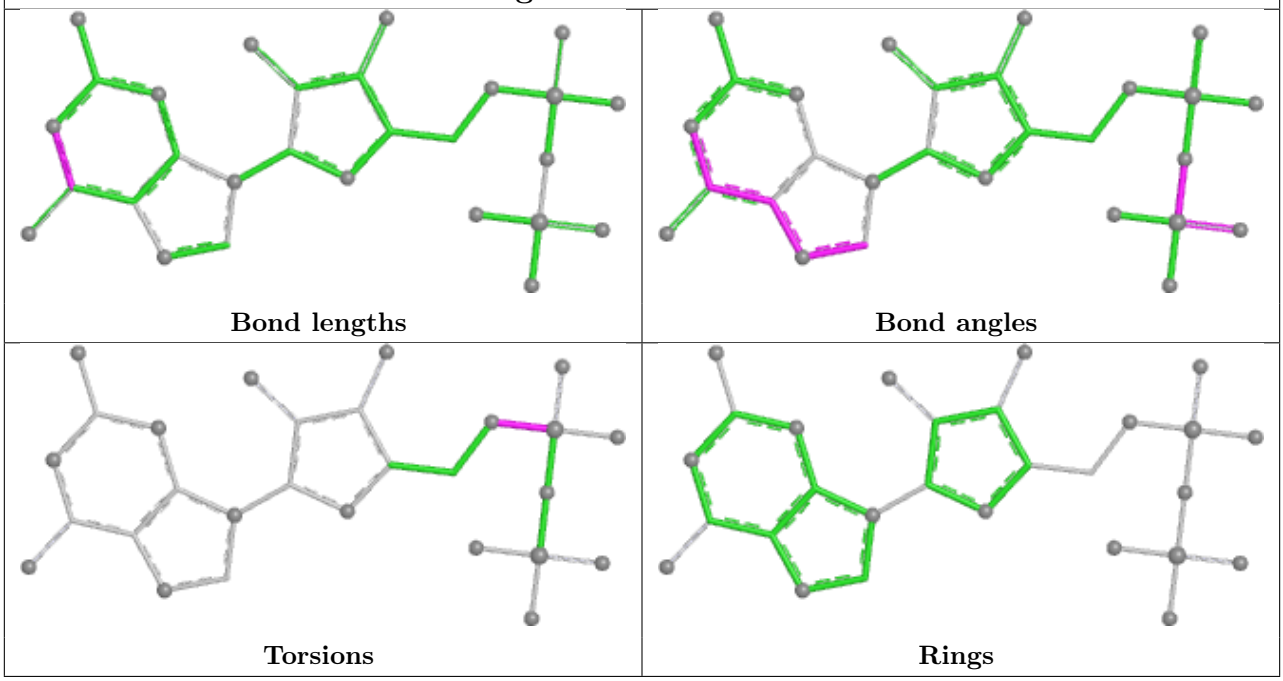
Ligand GDP 2A 502

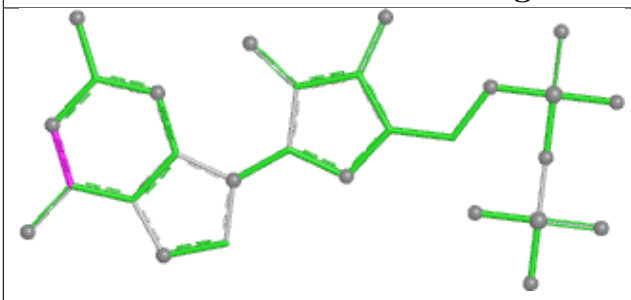
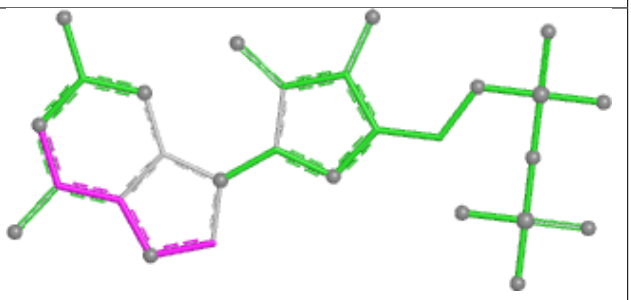
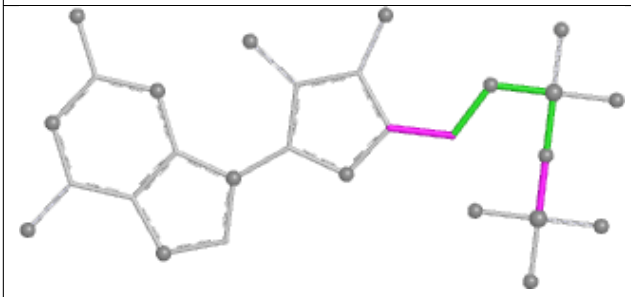
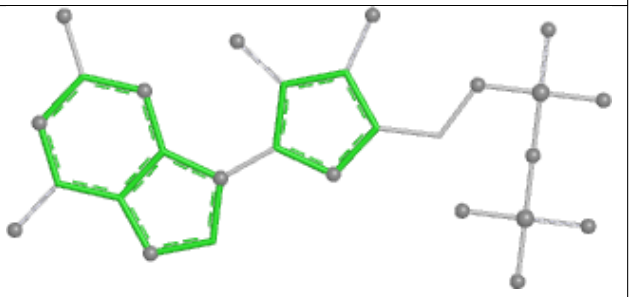


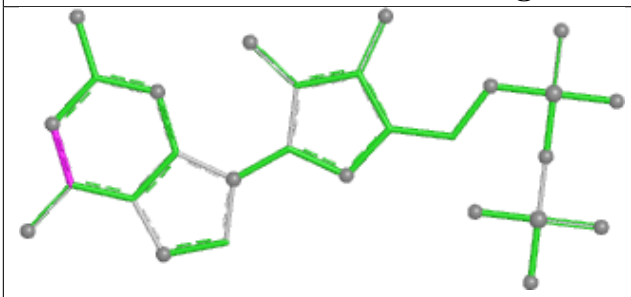
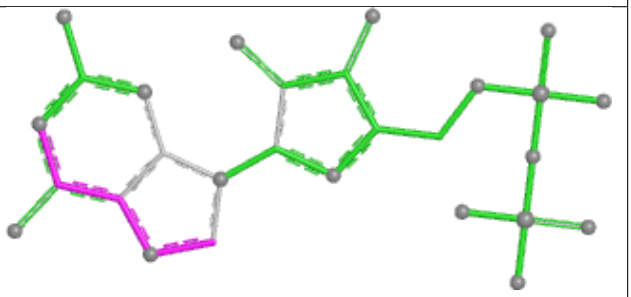
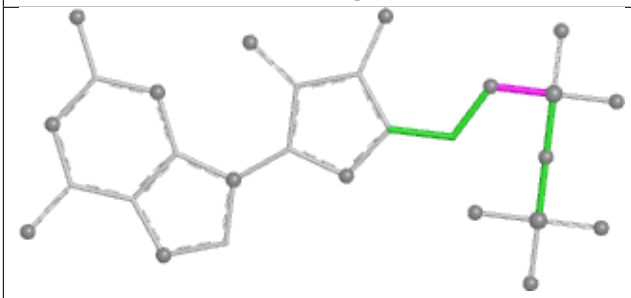
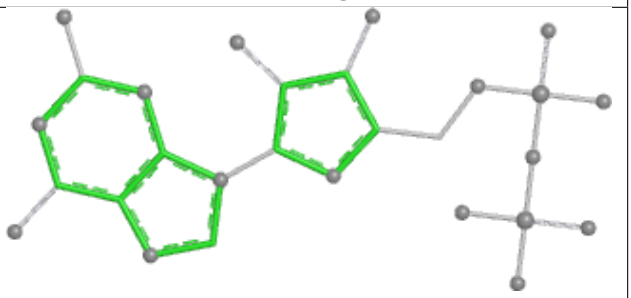
Ligand GTP V2 501



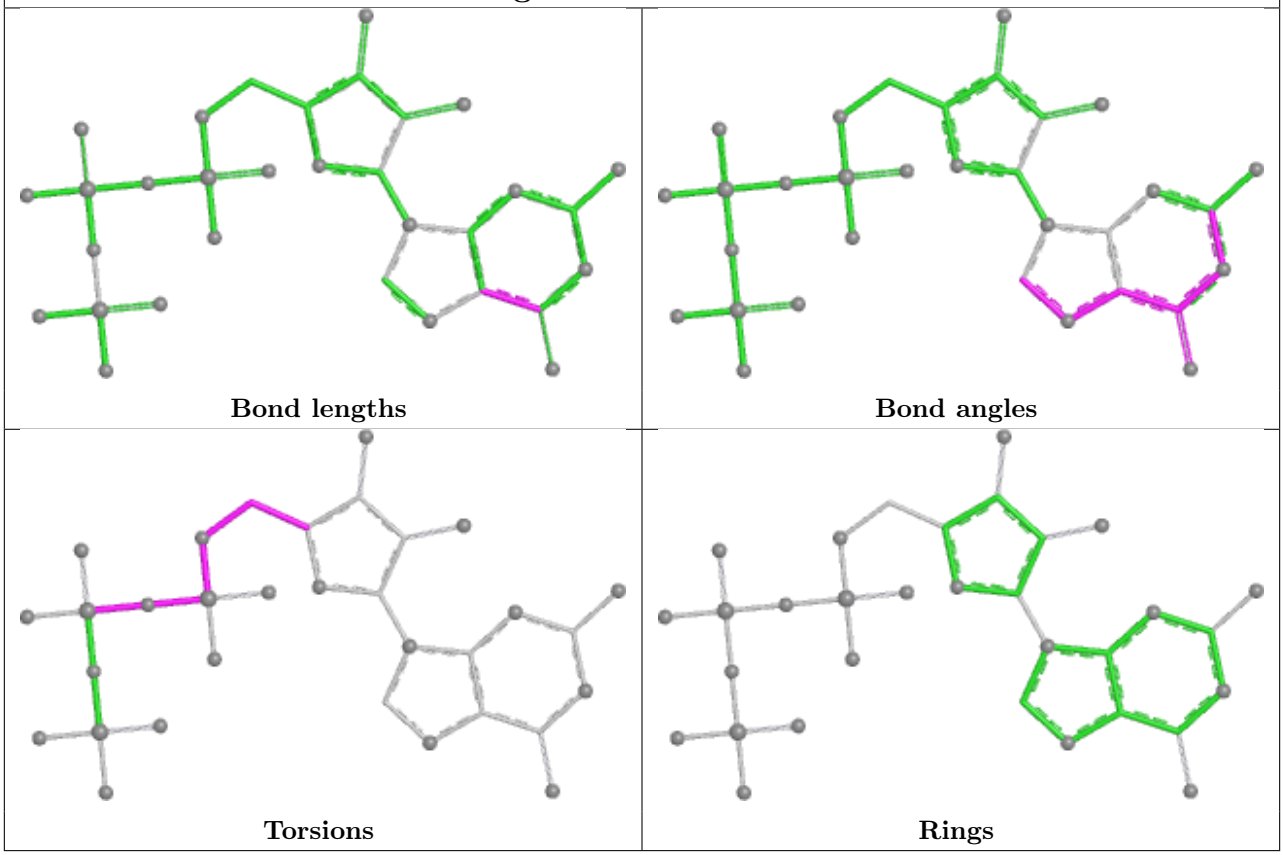
Ligand GDP L4 502



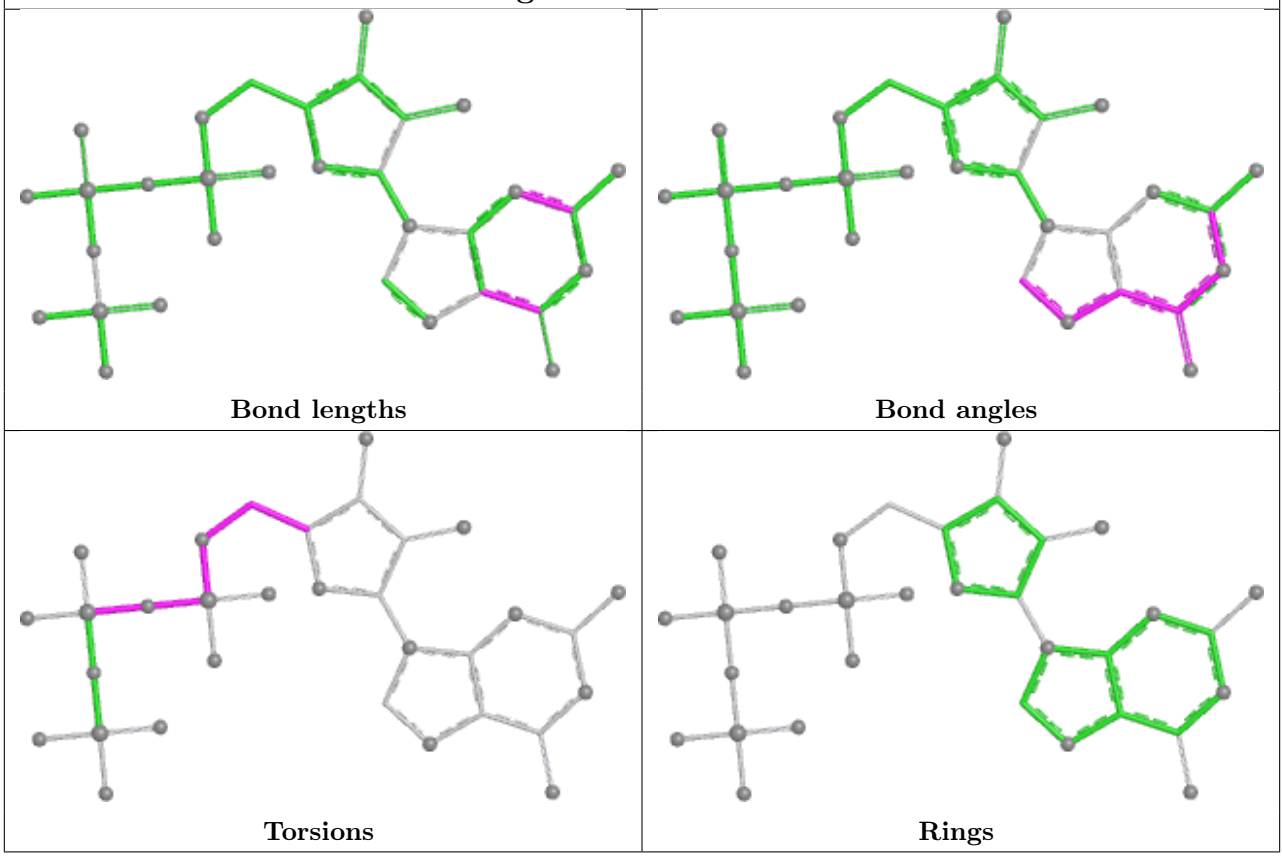
Ligand GDP E2 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP 1S 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

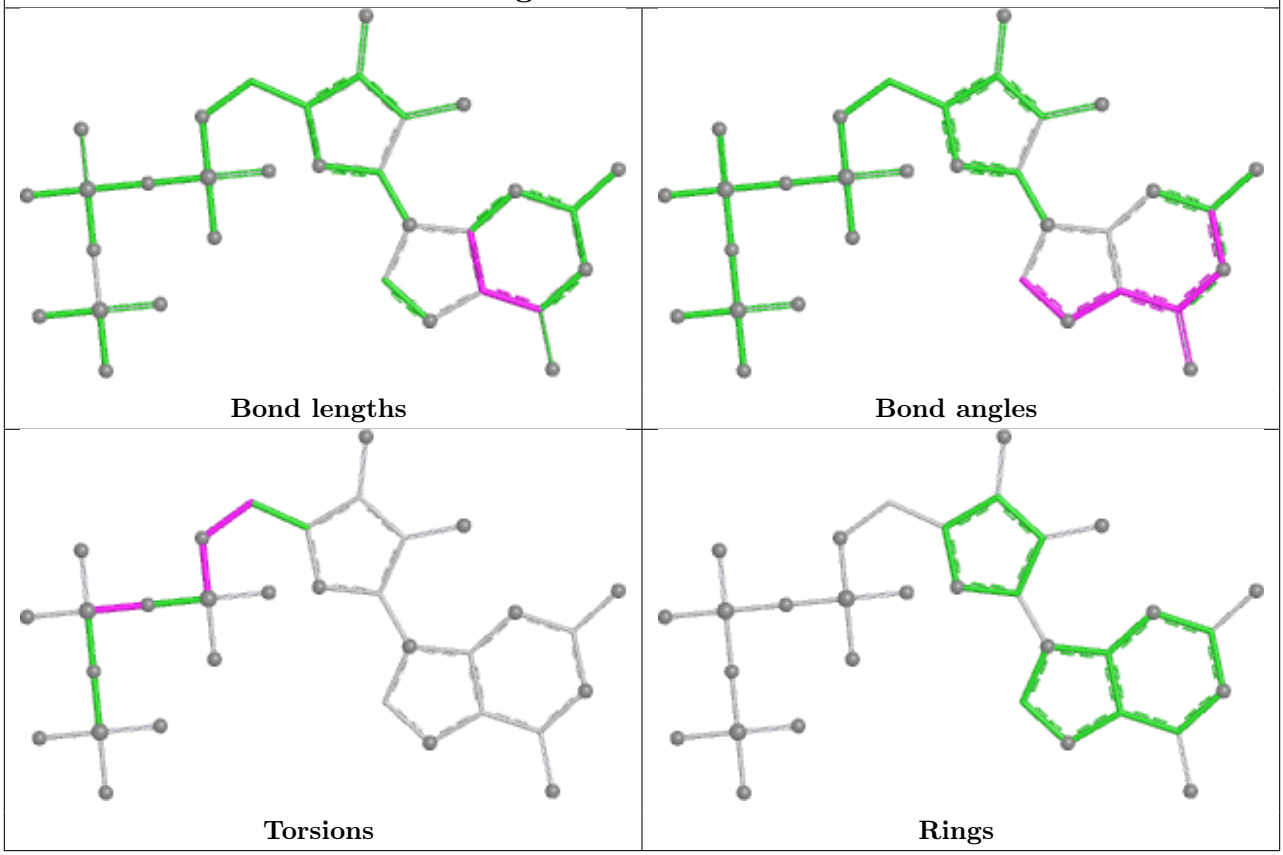
Ligand GTP H6 501



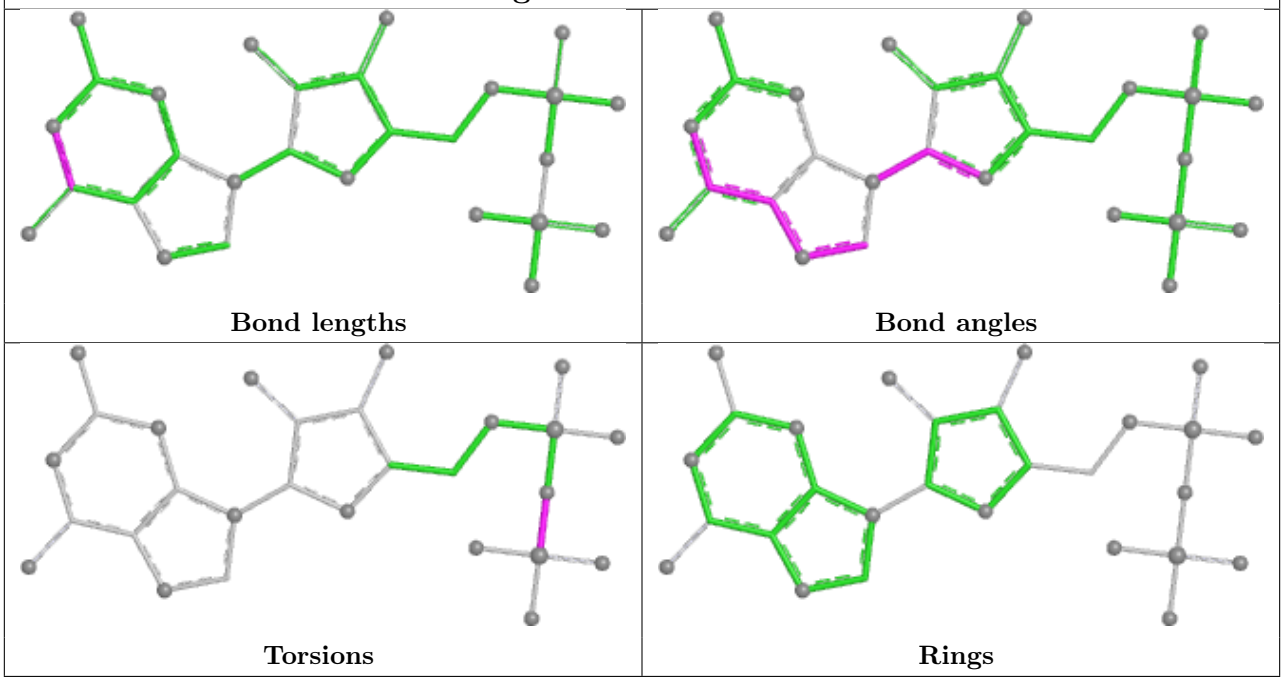
Ligand GTP Z0 501



Ligand GTP T4 501



Ligand GDP Y2 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.

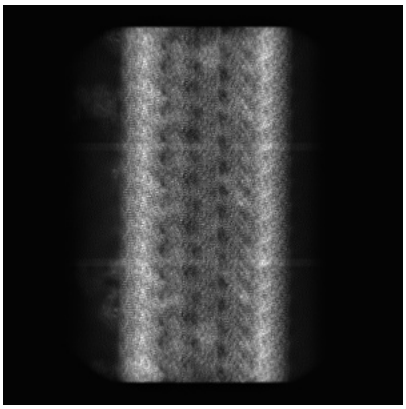
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20631. These allow visual inspection of the internal detail of the map and identification of artifacts.

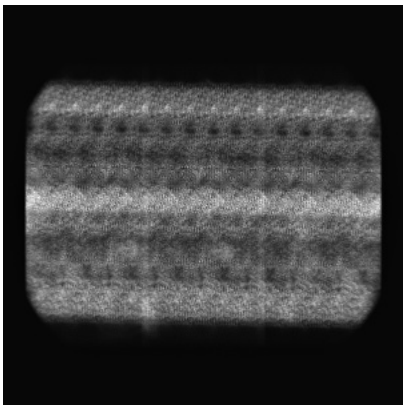
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

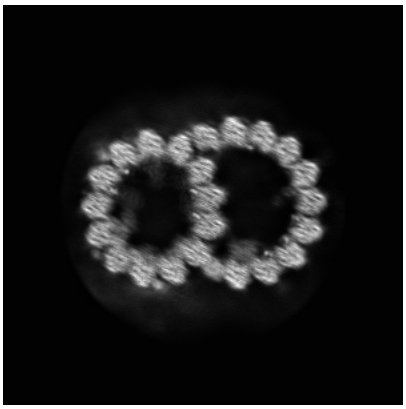
6.1.1 Primary map



X

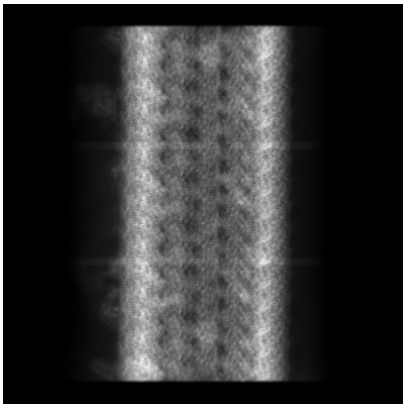


Y

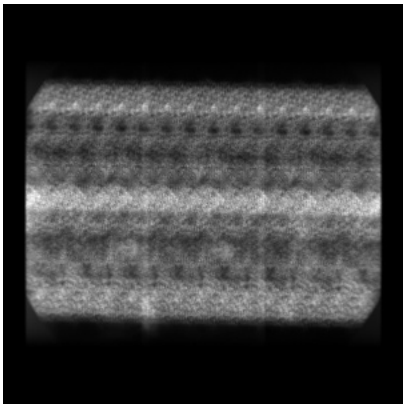


Z

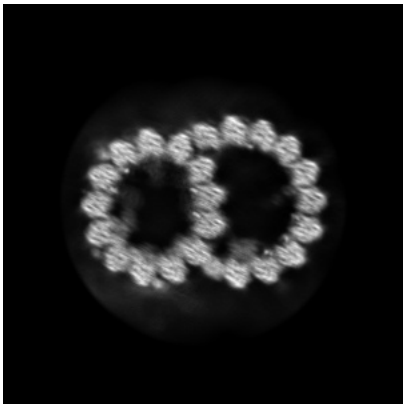
6.1.2 Raw map



X



Y

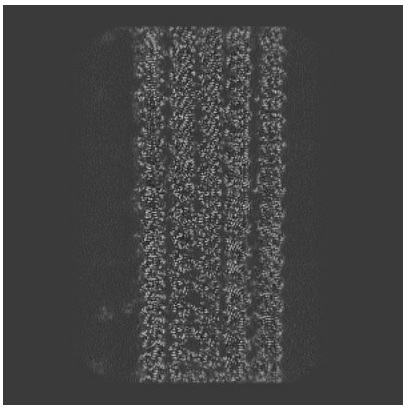


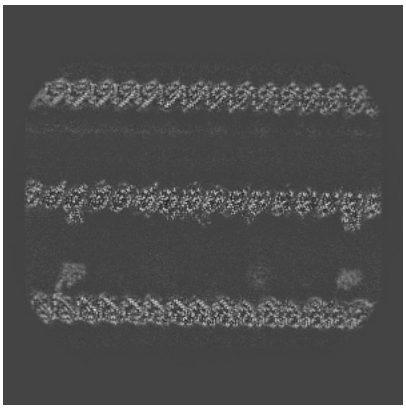
Z

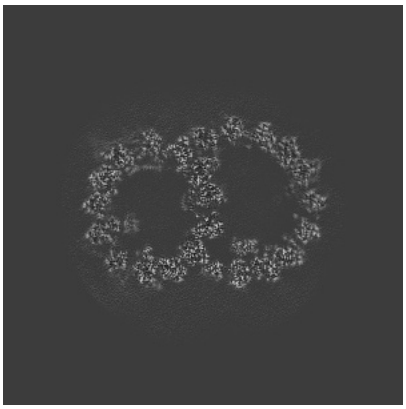
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

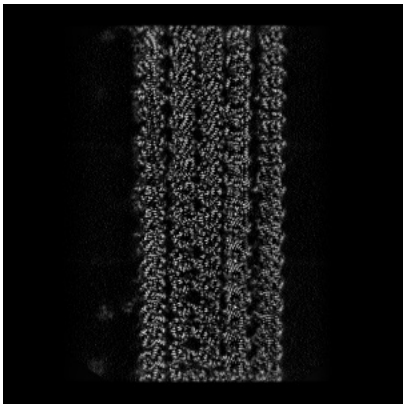
6.2.1 Primary map

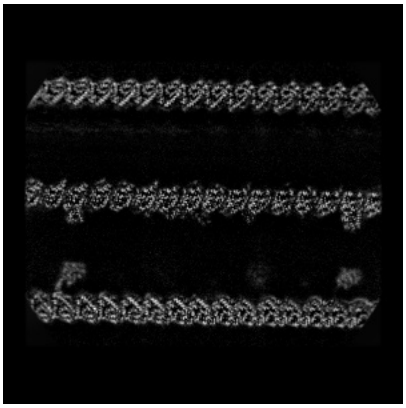

X Index: 256

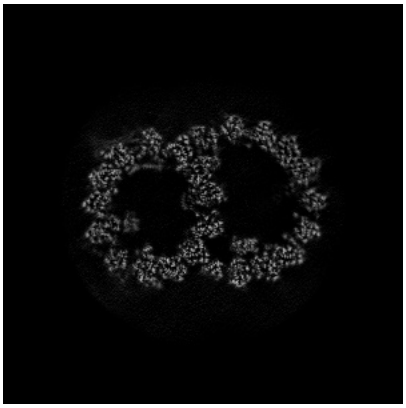

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

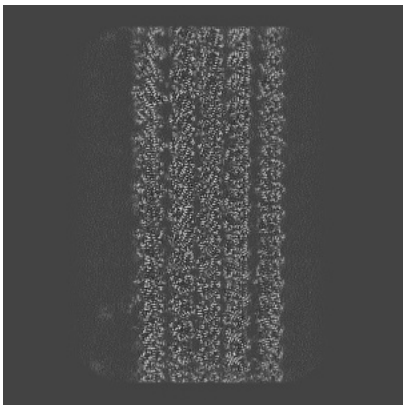

Y Index: 256

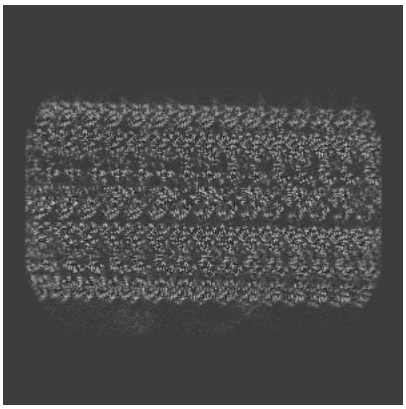

Z Index: 256

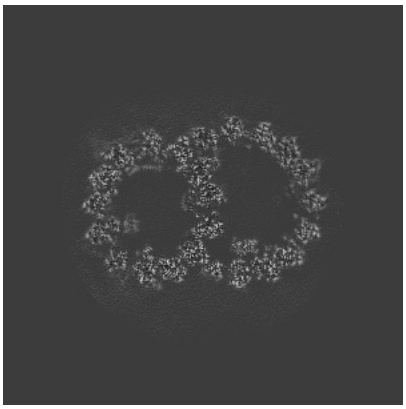
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

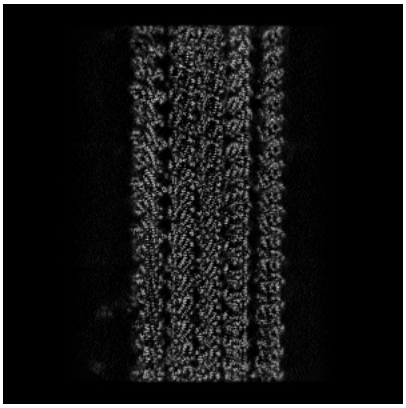
6.3.1 Primary map

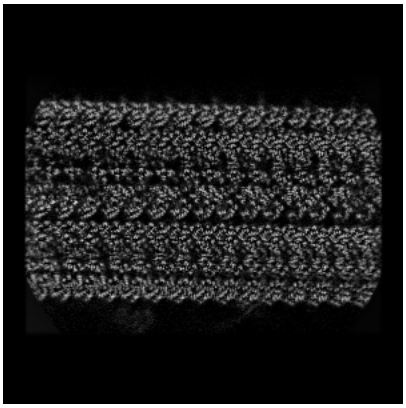

X Index: 258

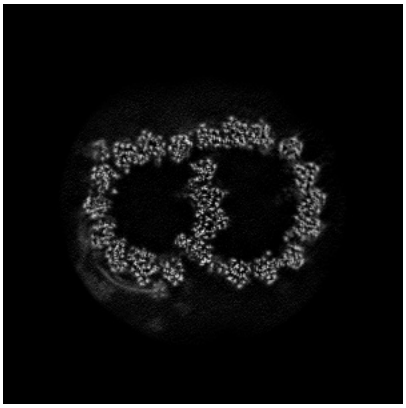

Y Index: 180


Z Index: 256

6.3.2 Raw map


X Index: 260

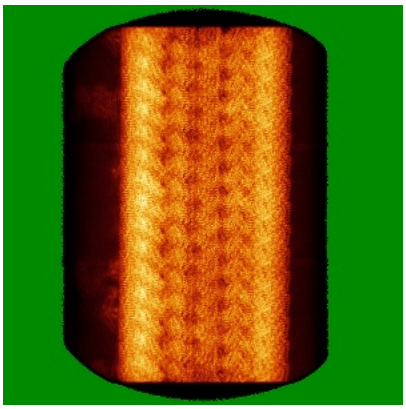

Y Index: 180

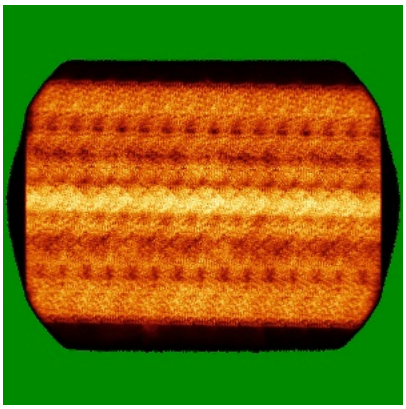

Z Index: 181

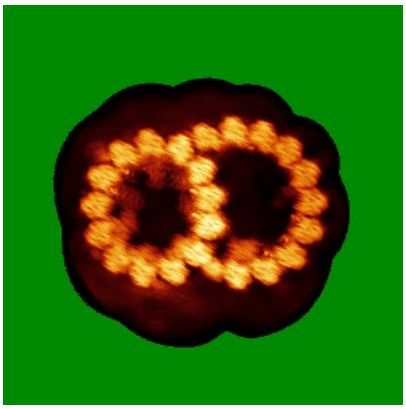
The images above show the largest variance slices of the map in three orthogonal directions.

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

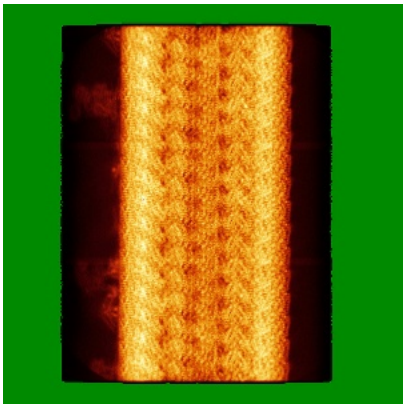
6.4.1 Primary map

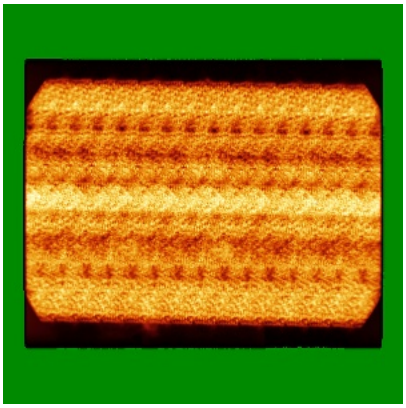

X


Y


Z

6.4.2 Raw map


X

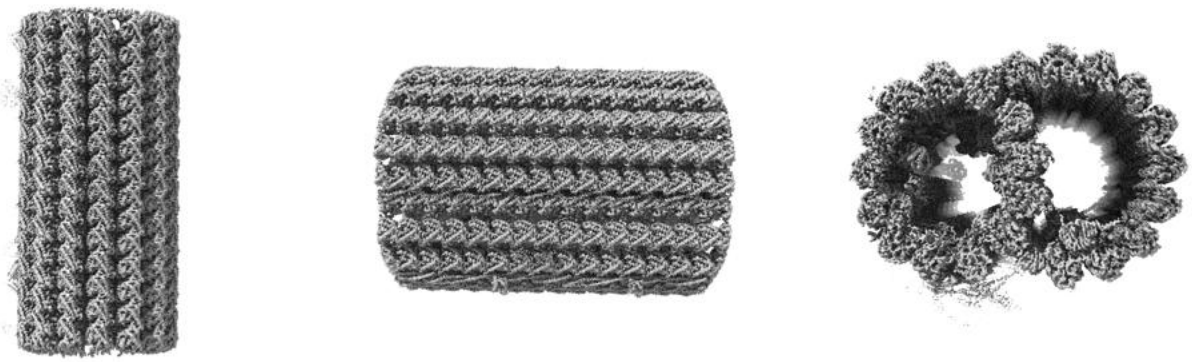

Y

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)

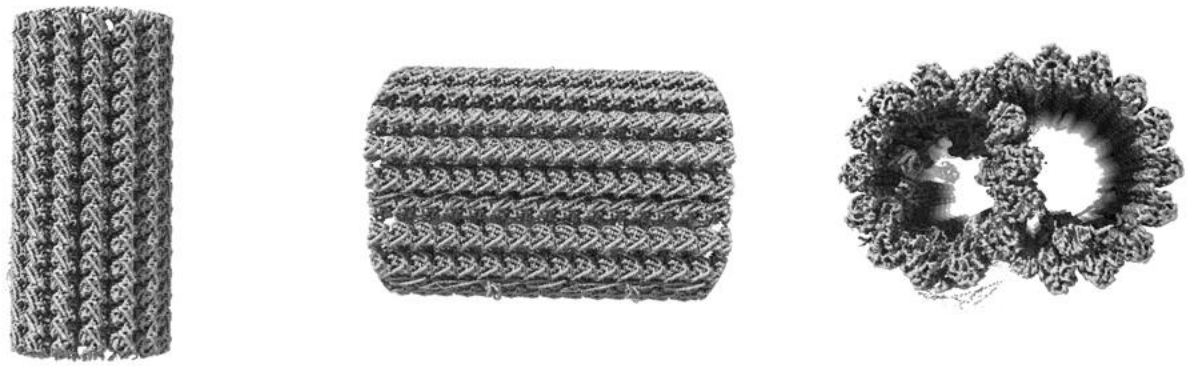
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

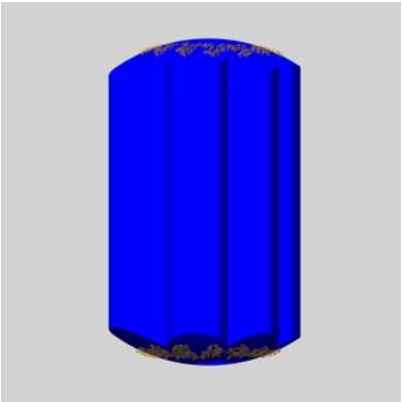
6.6 Mask visualisation (i)

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

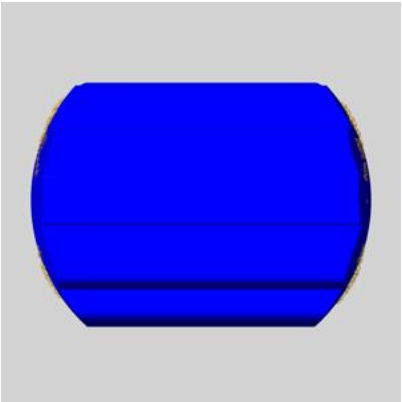
A mask typically either:

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

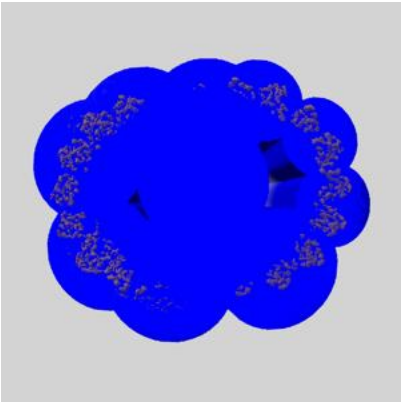
6.6.1 emd_20631_msk_1.map (i)



X



Y

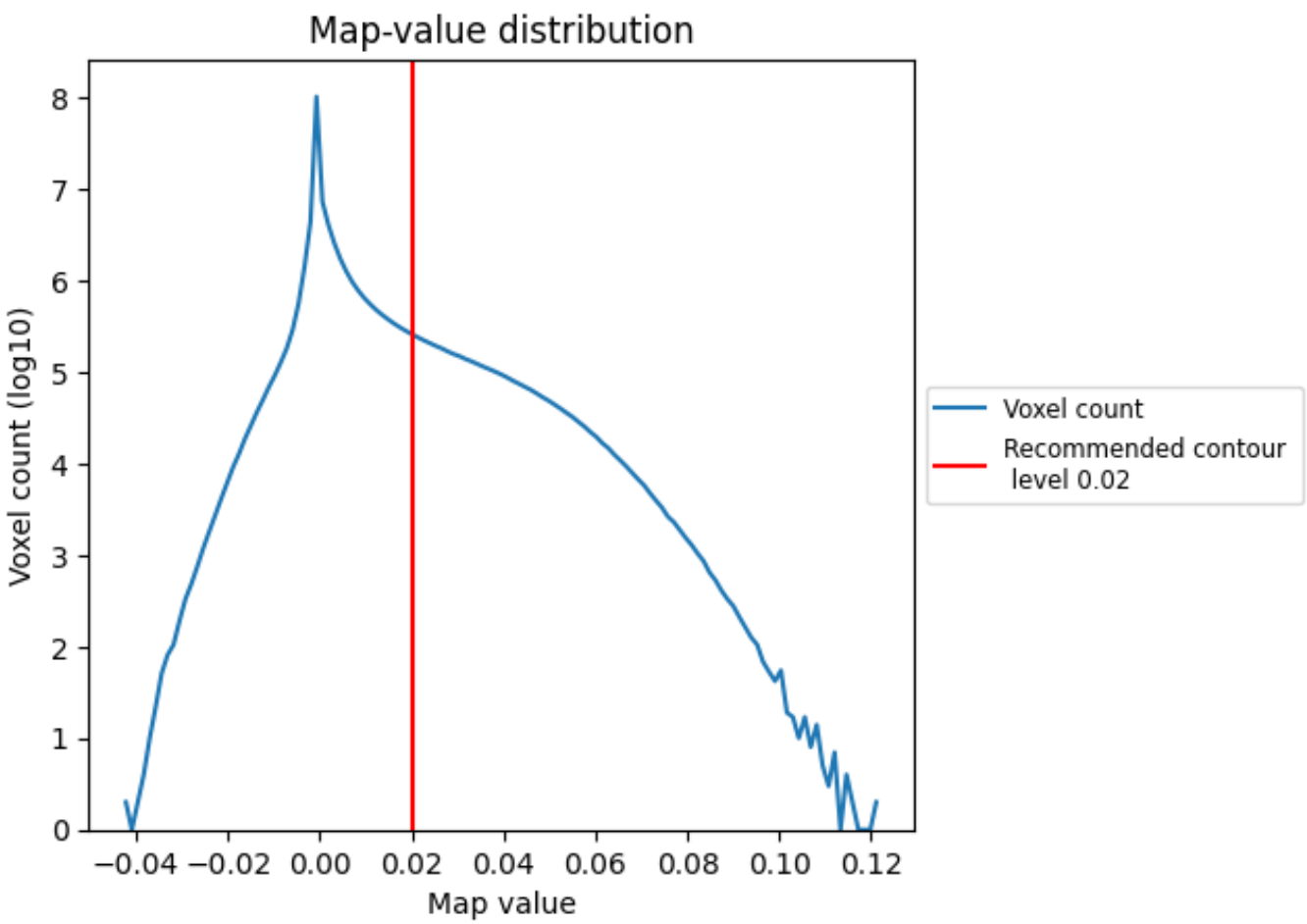


Z

7 Map analysis (i)

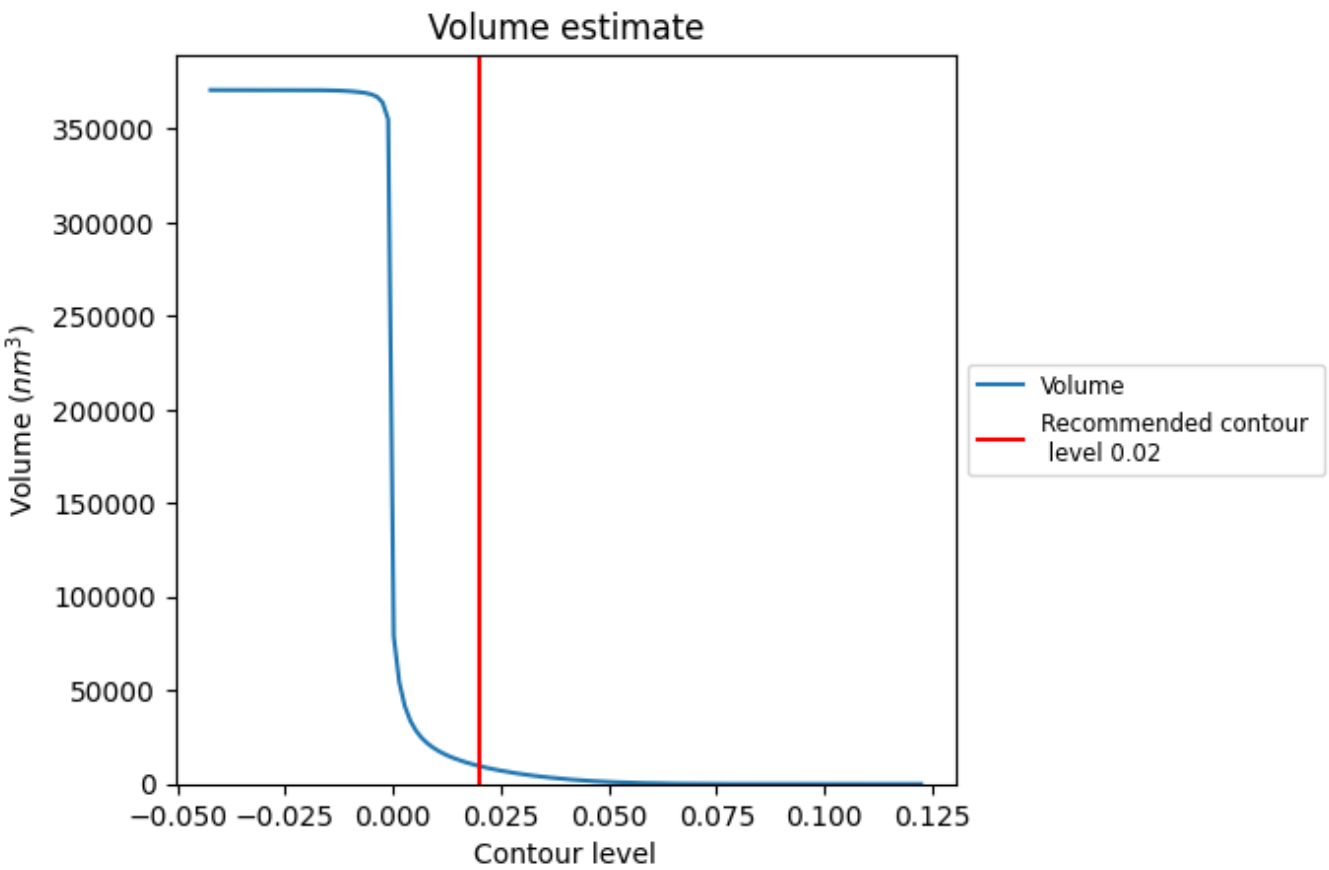
This section contains the results of statistical analysis of the map.

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.

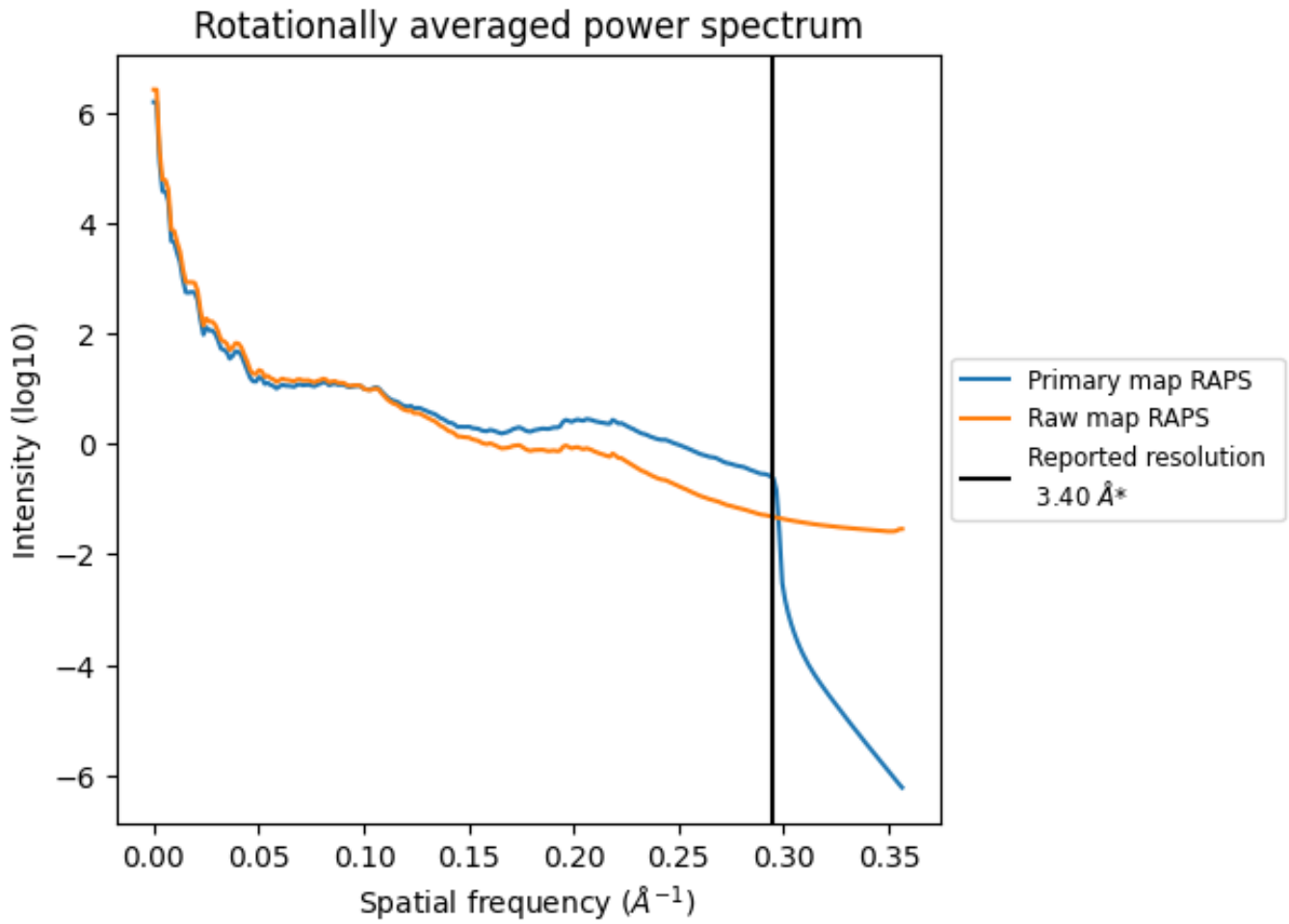
7.2 Volume estimate (i)



The volume at the recommended contour level is 9602 nm^3; this corresponds to an approximate mass of 8673 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

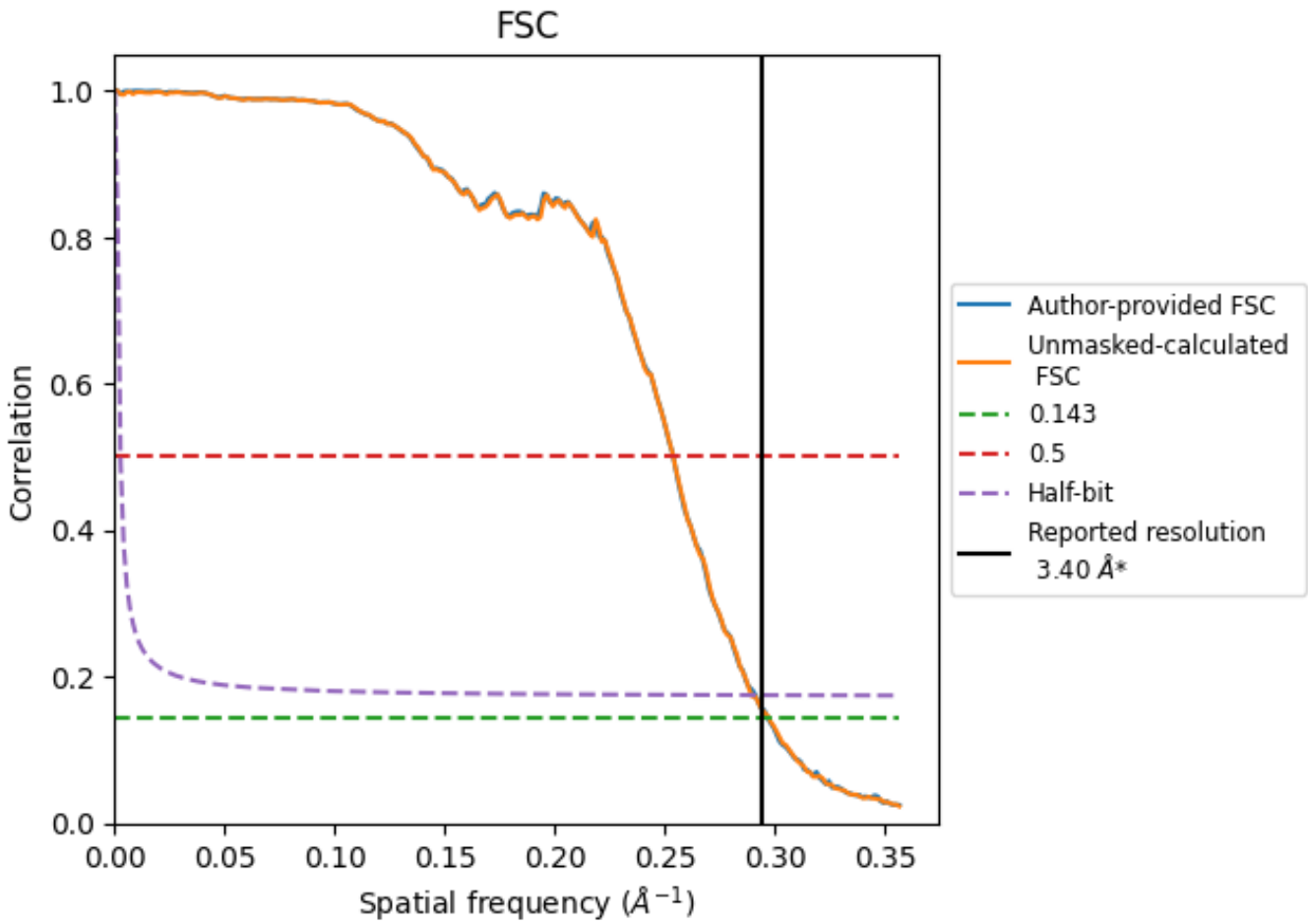


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

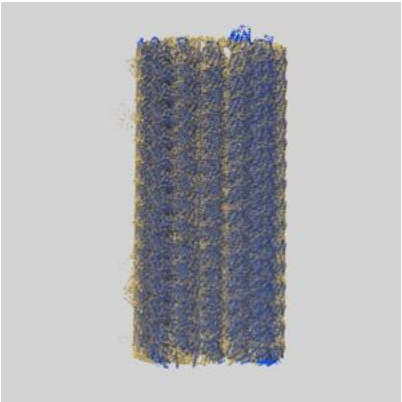
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	3.94	3.44
Unmasked-calculated*	3.36	3.94	3.46

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

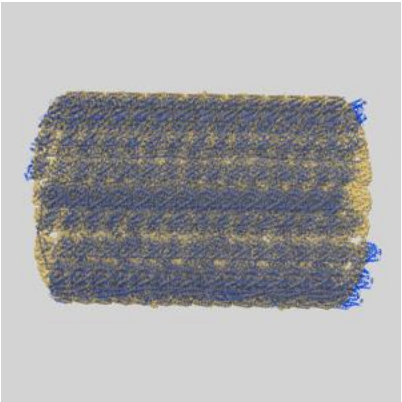
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20631 and PDB model 6U42. Per-residue inclusion information can be found in section 3 on page 72.

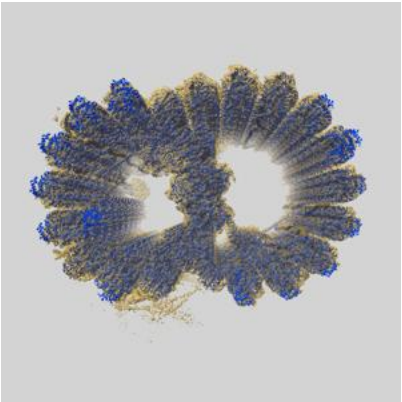
9.1 Map-model overlay (i)



X



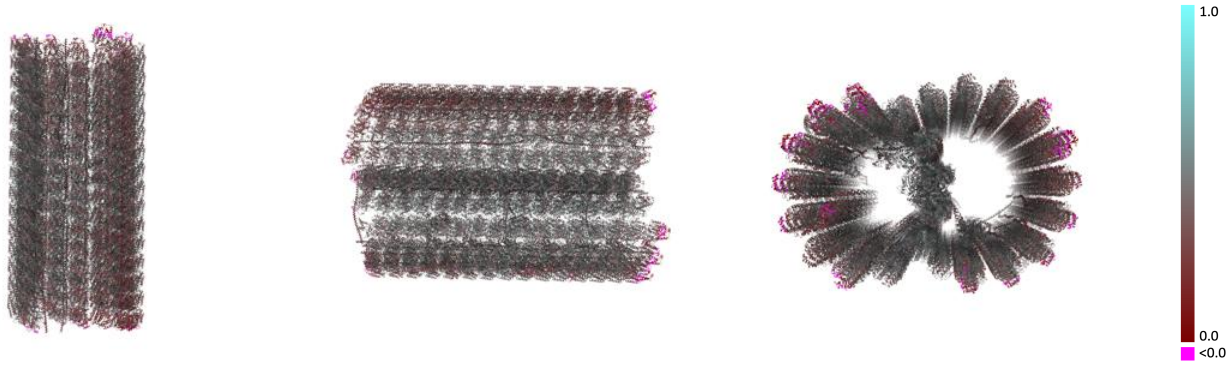
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

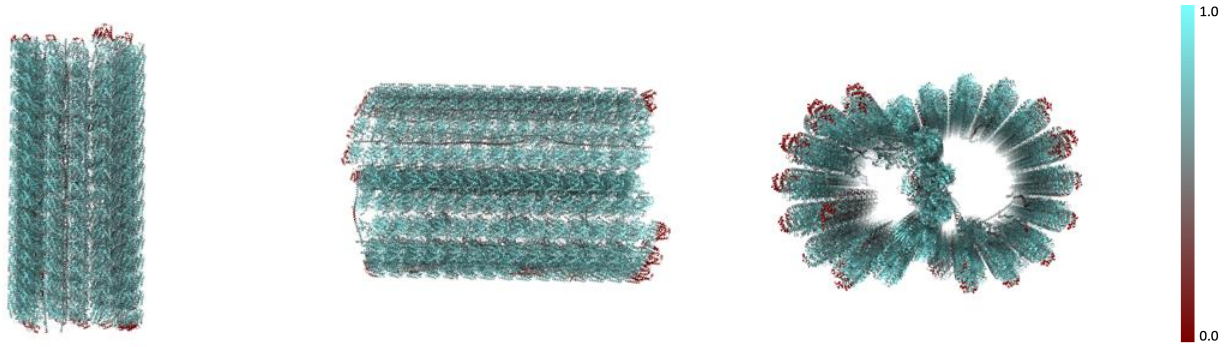
9.2 Q-score mapped to coordinate model (i)



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.

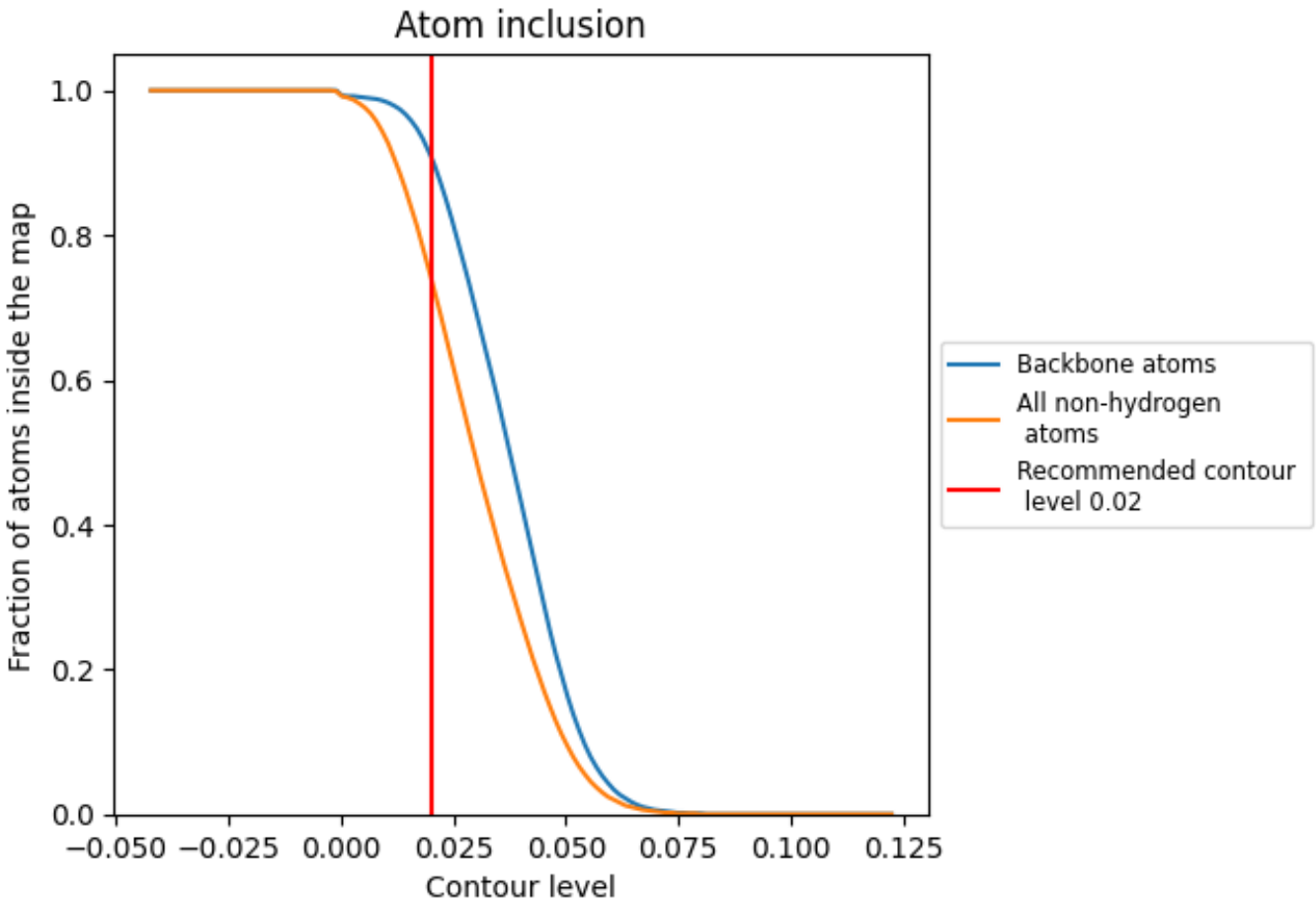
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 74% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7420	0.4300
0A	0.7370	0.3560
0B	0.7300	0.3380
0C	0.6090	0.2820
0E	0.6220	0.2650
0F	0.7110	0.3210
0G	0.7250	0.3350
0H	0.7080	0.3340
0I	0.7020	0.3280
0J	0.6960	0.3710
0K	0.7160	0.3810
0L	0.7100	0.3780
0M	0.7210	0.3860
0N	0.6800	0.3580
0O	0.7050	0.3580
0P	0.7180	0.3690
0Q	0.7280	0.3680
0R	0.6960	0.3390
0S	0.3710	0.1900
0U	0.6160	0.3050
0V	0.6750	0.3450
0W	0.6970	0.3680
0X	0.6900	0.3660
0Y	0.6880	0.3750
0Z	0.6990	0.4020
1	0.8460	0.4750
1A	0.7080	0.4140
1B	0.6970	0.4010
1C	0.7020	0.4050
1D	0.6760	0.3670
1E	0.6920	0.3710
1F	0.6760	0.3630
1G	0.6810	0.3540
1H	0.6020	0.3050
1K	0.7220	0.3540

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Chain	Atom inclusion	Q-score
1L	0.7570	0.4050
1M	0.7560	0.4150
1N	0.7490	0.4090
1O	0.7350	0.4050
1P	0.7560	0.4270
1Q	0.7620	0.4410
1R	0.7500	0.4280
1S	0.7590	0.4280
1T	0.7370	0.3960
1U	0.7350	0.4000
1V	0.7480	0.3950
1W	0.7480	0.3900
1X	0.6230	0.3180
1Z	0.5680	0.3280
2	0.8290	0.4910
2A	0.7580	0.3980
2B	0.7750	0.4290
2C	0.7720	0.4320
2D	0.7590	0.4220
2E	0.7580	0.4090
2F	0.7880	0.4410
2G	0.8020	0.4510
2H	0.7920	0.4450
2I	0.7920	0.4380
2J	0.7650	0.4280
2K	0.7690	0.4340
2L	0.7770	0.4340
2M	0.7770	0.4210
2N	0.6510	0.3500
2P	0.7520	0.4220
2Q	0.7670	0.4430
2R	0.7700	0.4550
2S	0.7630	0.4540
2T	0.7640	0.4410
2U	0.7840	0.4560
2V	0.7940	0.4650
2W	0.8040	0.4760
2X	0.7850	0.4630
2Y	0.8010	0.4600
2Z	0.7770	0.4590
3	0.8190	0.4990
3A	0.7870	0.4640

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Chain	Atom inclusion	Q-score
3B	0.7770	0.4490
3C	0.7820	0.4420
3D	0.6800	0.3770
3F	0.7980	0.4370
3G	0.8110	0.4600
3H	0.8170	0.4660
3I	0.8100	0.4710
3J	0.8080	0.4530
3K	0.8120	0.4600
3L	0.8240	0.4740
3M	0.8270	0.4790
3N	0.8130	0.4610
3O	0.8070	0.4530
3P	0.8080	0.4590
3Q	0.7960	0.4580
3R	0.8040	0.4500
3S	0.8000	0.4340
3T	0.6390	0.3450
3V	0.7570	0.4190
3W	0.8250	0.4700
3X	0.4290	0.4080
3Y	0.8420	0.4940
3Z	0.7490	0.4500
4	0.8180	0.5050
4A	0.8370	0.4820
4B	0.6770	0.4350
4C	0.8400	0.4870
4D	0.7600	0.4640
4E	0.8240	0.4770
4F	0.6740	0.4240
4G	0.8180	0.4720
4H	0.7500	0.4430
4I	0.8100	0.4610
4J	0.4450	0.4210
4L	0.6120	0.3360
4M	0.6680	0.3820
4N	0.6150	0.3210
4O	0.5690	0.3260
4P	0.7030	0.4020
4Q	0.7620	0.4420
4R	0.7290	0.4650
4S	0.7250	0.4290

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Chain	Atom inclusion	Q-score
4T	0.7480	0.4530
4U	0.7630	0.4690
4V	0.5860	0.3590
4W	0.4820	0.3340
4X	0.7070	0.3980
4Y	0.6020	0.3570
4Z	0.5290	0.3180
5	0.8130	0.5050
5A	0.5170	0.3020
5B	0.5230	0.3210
5C	0.5780	0.3700
5D	0.5790	0.3640
5E	0.4110	0.4750
5F	0.7330	0.4860
5G	0.7340	0.4760
5H	0.7840	0.4550
5I	0.7730	0.4790
5J	0.7460	0.4650
5K	0.7860	0.4650
5L	0.7520	0.4530
5M	0.7710	0.4660
5N	0.7270	0.4380
5O	0.6520	0.4170
5P	0.7600	0.4460
5Q	0.7260	0.4750
5R	0.7440	0.4490
5S	0.6280	0.4090
5T	0.6360	0.4180
5U	0.5900	0.4360
5V	0.6240	0.4190
5X	0.6870	0.4420
5Y	0.6880	0.4480
5Z	0.5550	0.4350
6	0.8280	0.5080
6A	0.6660	0.4470
6B	0.5020	0.4190
6C	0.5750	0.4210
6D	0.6180	0.4090
6E	0.7370	0.4770
6F	0.7860	0.4820
6G	0.5490	0.4760
6H	0.5180	0.4640

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Chain	Atom inclusion	Q-score
6I	0.6550	0.3670
6J	0.6510	0.4100
6K	0.6410	0.4100
6L	0.6480	0.4420
6M	0.6410	0.4300
6N	0.5920	0.4080
6O	0.6220	0.4010
6P	0.5000	0.3060
6Q	0.6940	0.4520
6R	0.7120	0.4470
6S	0.6340	0.4170
6T	0.7050	0.4190
6U	0.7010	0.4500
6V	0.7060	0.4470
6W	0.7330	0.4860
6X	0.7030	0.4560
6Y	0.6740	0.4450
6Z	0.6920	0.4280
7	0.8200	0.5030
7A	0.7340	0.4460
7B	0.7120	0.4780
7C	0.6090	0.4370
7D	0.7610	0.4860
7E	0.7810	0.4910
7F	0.5520	0.4700
7G	0.6800	0.4610
7H	0.6870	0.4210
7I	0.6410	0.4360
7J	0.7150	0.4510
7K	0.6800	0.4330
7L	0.7160	0.4460
7M	0.6090	0.4630
7N	0.5460	0.4640
7O	0.7120	0.4240
7P	0.6860	0.4690
7Q	0.5990	0.4710
7R	0.5080	0.3480
7S	0.5430	0.3390
7T	0.5130	0.3420
7U	0.5160	0.3280
7V	0.4630	0.2830
7W	0.3500	0.2580

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Chain	Atom inclusion	Q-score
7X	0.6080	0.3760
7Y	0.4930	0.4670
7Z	0.6180	0.4010
8	0.8340	0.5150
8A	0.5740	0.4280
8B	0.5720	0.4460
8C	0.6410	0.4510
8D	0.5470	0.4280
9	0.8260	0.5090
A0	0.8080	0.4950
A1	0.8130	0.4890
A2	0.8150	0.5000
A3	0.8150	0.5010
A4	0.8140	0.4850
A5	0.8230	0.4760
A7	0.8250	0.4540
A8	0.8240	0.4800
A9	0.8320	0.5000
B0	0.8210	0.4910
B1	0.8230	0.4910
B2	0.8260	0.4990
B3	0.8380	0.5040
B4	0.8210	0.5030
B5	0.8300	0.5050
B7	0.7970	0.4790
B8	0.8050	0.4810
B9	0.8140	0.4840
C0	0.8210	0.4840
C1	0.7940	0.4580
C2	0.8070	0.4400
C4	0.8190	0.4250
C5	0.8300	0.4740
C6	0.8300	0.4800
C7	0.8170	0.4700
C8	0.8200	0.4720
C9	0.8200	0.4870
D0	0.8320	0.4980
D1	0.8170	0.4950
D2	0.8100	0.4900
D3	0.7770	0.4570
D4	0.7820	0.4610
D5	0.8130	0.4710

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Chain	Atom inclusion	Q-score
D6	0.8170	0.4670
D7	0.7770	0.4310
D8	0.6030	0.3340
E0	0.7710	0.3970
E1	0.7770	0.4380
E2	0.7900	0.4500
E3	0.7640	0.4440
E4	0.7490	0.4130
E5	0.7540	0.4420
E6	0.7650	0.4450
E7	0.7510	0.4420
E8	0.7480	0.4360
E9	0.6990	0.4040
F0	0.7160	0.4180
F1	0.7310	0.4140
F2	0.7350	0.4050
F3	0.6670	0.3580
F5	0.3640	0.1850
F6	0.7310	0.3650
F7	0.7540	0.4080
F8	0.7610	0.4210
F9	0.7200	0.4040
G0	0.7440	0.4010
G1	0.7540	0.4320
G2	0.7700	0.4420
G3	0.7610	0.4330
G4	0.7690	0.4290
G5	0.7170	0.4070
G6	0.7400	0.4190
G7	0.7400	0.4040
G8	0.7300	0.3980
G9	0.5770	0.3110
H1	0.5200	0.2780
H2	0.7230	0.3820
H3	0.7720	0.4350
H4	0.7740	0.4360
H5	0.7520	0.4130
H6	0.7700	0.4190
H7	0.7930	0.4490
H8	0.7910	0.4550
H9	0.7840	0.4440
I0	0.7730	0.4390

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Chain	Atom inclusion	Q-score
I1	0.7530	0.4300
I2	0.7640	0.4360
I3	0.7500	0.4220
I4	0.7380	0.4080
I5	0.4760	0.2690
I7	0.7090	0.3880
I8	0.7800	0.4340
I9	0.7970	0.4590
J0	0.8060	0.4710
J1	0.7750	0.4340
J2	0.7990	0.4580
J3	0.8050	0.4680
J4	0.8200	0.4810
J5	0.8070	0.4580
J6	0.8090	0.4580
J7	0.7850	0.4490
J8	0.8010	0.4610
J9	0.7760	0.4350
K0	0.7730	0.4290
K1	0.4200	0.2380
K3	0.7840	0.4140
K4	0.8080	0.4440
K5	0.8090	0.4590
K6	0.8110	0.4600
K7	0.7850	0.4330
K8	0.7950	0.4530
K9	0.8070	0.4680
L0	0.8200	0.4720
L1	0.7950	0.4550
L2	0.8060	0.4490
L3	0.8020	0.4630
L4	0.8250	0.4720
L5	0.8050	0.4520
L6	0.8090	0.4340
L7	0.4370	0.2510
L9	0.7920	0.4340
M0	0.7990	0.4520
M1	0.7950	0.4550
M2	0.7690	0.4520
M3	0.7670	0.4420
M4	0.7760	0.4590
M5	0.8030	0.4690

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Chain	Atom inclusion	Q-score
M6	0.7900	0.4690
M7	0.7820	0.4560
M8	0.7790	0.4540
M9	0.7890	0.4680
N0	0.8020	0.4700
N1	0.7940	0.4490
N2	0.8040	0.4370
N3	0.4190	0.2430
N5	0.8060	0.4260
N6	0.8130	0.4580
N7	0.8060	0.4600
N8	0.8110	0.4730
N9	0.7720	0.4520
O0	0.8030	0.4610
O1	0.8000	0.4640
O2	0.8180	0.4810
O3	0.8000	0.4660
O4	0.8190	0.4720
O5	0.8020	0.4630
O6	0.8180	0.4820
O7	0.8060	0.4670
O8	0.8210	0.4640
O9	0.8120	0.4370
P3	0.8130	0.4570
P4	0.7910	0.4720
P5	0.7840	0.4730
P6	0.7710	0.4670
P7	0.7670	0.4630
P8	0.7710	0.4690
P9	0.7790	0.4740
Q0	0.7880	0.4790
Q1	0.7860	0.4740
Q2	0.7910	0.4770
Q3	0.7850	0.4770
Q4	0.8040	0.4860
Q5	0.7990	0.4820
Q6	0.8150	0.4740
Q8	0.4780	0.3100
Q9	0.7840	0.4690
R0	0.7770	0.4860
R1	0.7580	0.4820
R2	0.7630	0.4830

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Chain	Atom inclusion	Q-score
R3	0.7640	0.4780
R4	0.7690	0.4930
R5	0.7660	0.4890
R6	0.7710	0.4880
R7	0.7780	0.4950
R8	0.7820	0.4880
R9	0.7430	0.4760
S0	0.7650	0.4840
S1	0.7740	0.4820
S2	0.7930	0.4720
S4	0.6990	0.4180
S5	0.8070	0.4810
S6	0.7990	0.4910
S7	0.7800	0.4800
S8	0.7840	0.4990
S9	0.7900	0.4940
T0	0.8050	0.5010
T1	0.8010	0.4940
T2	0.8030	0.5020
T3	0.8010	0.4950
T4	0.7930	0.4910
T5	0.7720	0.4850
T6	0.7830	0.4830
T7	0.7880	0.4780
T8	0.8070	0.4720
U1	0.7370	0.4110
U2	0.7450	0.4330
U3	0.7530	0.4410
U4	0.7400	0.4470
U5	0.7130	0.4290
U6	0.7160	0.4420
U7	0.7480	0.4550
U8	0.7460	0.4600
U9	0.7500	0.4570
V0	0.7350	0.4470
V1	0.7460	0.4530
V2	0.7590	0.4580
V3	0.7510	0.4490
V4	0.7550	0.4490
V6	0.5190	0.2730
V7	0.7680	0.3980
V8	0.7720	0.4180

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Chain	Atom inclusion	Q-score
V9	0.7720	0.4290
W0	0.7810	0.4360
W1	0.7720	0.4290
W2	0.7920	0.4490
W3	0.7920	0.4570
W4	0.8090	0.4620
W5	0.7900	0.4530
W6	0.7900	0.4430
W7	0.7950	0.4490
W8	0.8080	0.4530
W9	0.7920	0.4390
X0	0.7890	0.4140
X2	0.5910	0.2770
X3	0.7280	0.3540
X4	0.7310	0.3750
X5	0.7300	0.3740
X6	0.7390	0.3940
X7	0.7310	0.3930
X8	0.7470	0.4150
X9	0.7610	0.4240
Y0	0.7570	0.4320
Y1	0.7270	0.4070
Y2	0.7390	0.4020
Y3	0.7550	0.4150
Y4	0.7600	0.4230
Y5	0.7510	0.4060
Y6	0.7510	0.3900
Y8	0.5500	0.2440
Y9	0.6850	0.2980
Z0	0.6910	0.3170
Z1	0.6750	0.3180
Z2	0.6700	0.3180
Z3	0.6850	0.3580
Z4	0.7150	0.3830
Z5	0.7070	0.3800
Z6	0.7170	0.3830
Z7	0.6850	0.3560
Z8	0.7020	0.3340
Z9	0.7220	0.3560