Full wwPDB EM Validation Report (i)

Nov 5, 2024 – 05:47 AM EST

PDB ID	:	8SNB
EMDB ID	:	EMD-40619
Title	:	atomic model of sea urchin sperm doublet microtubule (48-nm periodicity)
Authors	:	Zeng, J.; Zhang, R.
Deposited on	:	2023-04-26
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM Validation 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:

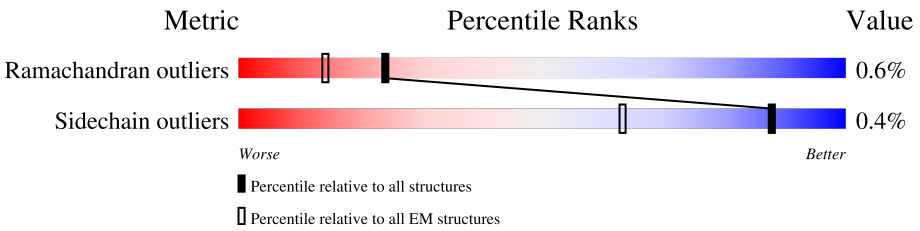
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.30 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	1A	309	11% 13% 86%
1	1B	309	72% 84% • 14%
2	1E	448	91% 93% • 6%
2	1F	448	38% 38% 62%
2	1G	448	64% 65% • 34%
2	1H	448	94% 92% • 6%
3	1K	696	25% 25% • 75%
3	1L	696	25% 25% • 75%
3	1M	696	25% 25% 75%

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Mol	Chain	Length	Quality of chain
3	1v	696	30% 29% 70%
3	1w	696	12% 12% 88%
3	1x	696	36% 35% 64%
3	1y	696	28% 28% 72%
3	1z	696	12% 12% 88%
3	2a	696	8% 7% 92%
4	1P	204	57% 100%
4	1Q	204	49% 67% 32%
5	1T	429	31% 52% 47%
5	1U	429	12% 26% 74%
5	1V	429	33% 52% 47%
5	1W	429	15% 24% 75%
6	1Y	139	74% 85% 14%
7	1a	251	50% 52% 47%
7	1b	251	48% 46% 51%
7	5E	251	44% 61% 39%
7	5F	251	25% 43% 55%
7	5G	251	35% 55% 43%
7	5H	251	27% 45% 53%
7	5I	251	10% 10% 89%
7	5J	251	63% 91% 7%
7	5K	251	27% 51% 47%
7	5L	251	22% 48% 50%
7	5M	251	5% 94%
7	5N	251	57% 96%

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Mol	Chain	Length	Quality of chain
7	5O	251	6% / 6% / 94%
8	1d	359	28% / 28% / 72%
9	1f	206	12% / 17% / 83%
9	1g	206	18% / 25% / 75%
10	1i	188	14% / 18% / 82%
10	1j	188	15% / 15% / 84%
10	9M	188	39% / 45% / 55%
10	9N	188	35% / 44% / 55%
10	9O	188	22% / 20% / 78%
11	1l	176	22% / 22% / 78%
11	1m	176	22% / 22% / 78%
12	1o	142	15% / 19% / 80%
12	1p	142	10% / 21% / 79%
12	1q	142	22% / 32% / 68%
12	1r	142	11% / 18% / 81%
13	2A	258	74% / 95%
13	2B	258	74% / 93%
13	2C	258	72% / 95%
13	2D	258	24% / 29% / 69%
14	2G	235	69% / 96%
15	2J	141	73% / 76% / 24%
15	2K	141	70% / 74% / 24%
15	2L	141	59% / 74% / 24%
16	2O	120	81% / 99%
17	2R	499	17% / 24% / 76%

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Mol	Chain	Length	Quality of chain
17	2S	499	62% 75% 25%
18	2V	292	60% 95%
18	2W	292	55% 96%
19	3A	195	28% 95%
19	3B	195	31% 94%
19	3C	195	54% 92% 8%
19	3D	195	47% 89% 10%
19	3E	195	31% 95% 5%
19	3F	195	52% 96%
19	3G	195	32% 95% 5%
20	3J	592	58% 80% 16%
20	3K	592	11% 11% 88%
21	3N	560	26% 45% 54%
21	3O	560	32% 48% 50%
22	3R	172	80% 92%
22	3S	172	61% 71% 26%
22	3T	172	79% 94%
23	3W	541	66% 69% 29%
23	3X	541	49% 58% 42%
23	3Y	541	17% 19% 81%
23	3Z	541	26% 31% 68%
24	4A	635	63% 97%
24	4B	635	52% 96%
24	4C	635	57% 97%
25	4F	516	40% 61% 39%

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Mol	Chain	Length	Quality of chain
25	4G	516	25% 39% 60%
26	4J	380	61% 97%
26	4K	380	73% 98%
27	4N	243	49% 60% 38%
27	4O	243	44% 44% 56%
27	4P	243	59% 61% 38%
27	4Q	243	37% 37% 62%
28	4T	231	62% 60% 38%
28	4U	231	62% 61% 38%
28	4V	231	6% 6% 94%
29	4Y	302	56% 98%
30	5A	277	12% 12% 87%
30	5B	277	58% 74% 23%
30	9Y	277	50% 47% 49%
30	9Z	277	36% 35% 64%
31	6A	236	38% 94% 5%
31	6B	236	92% 92% 7%
31	6C	236	64% 94% 6%
31	6D	236	40% 95% 5%
31	6E	236	39% 94% 5%
31	6F	236	41% 95% 5%
32	6I	123	37% 63% 37%
32	6J	123	28% 43% 57%
33	6M	469	49% 83% 17%
33	6N	469	12% 17% 83%

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Mol	Chain	Length	Quality of chain
34	6Q	310	32% 65% 35%
34	6R	310	16% 23% 77%
35	6U	379	26% 39% 61%
35	6V	379	36% 71% 28%
35	6W	379	31% 63% 36%
35	6X	379	19% 32% 68%
36	7A	744	64% 95%
36	7B	744	53% 60% 39%
36	7C	744	46% 71% 27%
36	7D	744	61% 95%
37	7G	645	44% 80% 18%
37	7H	645	47% 79% 18%
37	7I	645	62% 93%
38	7M	322	44% 80% 18%
38	7N	322	11% 21% 79%
39	7Q	185	50% 77% 22%
39	7R	185	72% 76% 23%
40	7U	200	43% 42% 54%
40	7V	200	23% 26% 74%
41	7Y	204	65% 95%
41	7Z	204	29% 30% 69%
42	8A	268	66% 88% 9%
43	8D	462	37% 85% 14%
43	8E	462	21% 38% 61%
43	8F	462	27% 57% 43%

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Mol	Chain	Length	Quality of chain
43	8G	462	44% 85% 14%
44	8J	430	36% 93% 6%
44	8K	430	39% 75% 25%
44	8L	430	43% 93% 6%
44	8M	430	13% 30% 70%
44	8N	430	96%
45	8Q	402	5% 95%
45	8R	402	45% 98%
45	8S	402	33% 74% 24%
45	8T	402	37% 99%
45	8U	402	10% 30% 70%
46	8X	119	87% 87% 13%
46	8Y	119	85% 86% 13%
46	8Z	119	87% 83% 13%
47	9A	220	65% 90% 6%
48	9D	171	47% 56% 44%
49	9G	150	57% 97%
50	9J	179	54% 56% 44%
51	9R	153	44% 93% 7%
52	9T	83	64% 90% 10%
53	9V	294	8% 6% 92%
53	9W	294	24% 24% 76%
54	AA	451	35% 96%
54	AB	451	36% 97%
54	AE	451	33% 96%

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Mol	Chain	Length	Quality of chain
54	AG	451	40% 96%
54	AI	451	26% 97%
54	AK	451	56% 96%
54	AM	451	61% 97%
54	BA	451	42% 96%
54	BB	451	49% 96%
54	BE	451	45% 96%
54	BG	451	57% 96%
54	BI	451	48% 96%
54	BK	451	68% 96%
54	BM	451	53% 96%
54	CA	451	34% 96%
54	CB	451	37% 96%
54	CE	451	33% 96%
54	CG	451	61% 96%
54	CI	451	39% 96%
54	CK	451	79% 96%
54	CM	451	54% 96%
54	DA	451	51% 97%
54	DB	451	59% 96%
54	DE	451	44% 96%
54	DG	451	63% 96%
54	DI	451	56% 96%
54	DK	451	93% 96%
54	DM	451	56% 96%

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Mol	Chain	Length	Quality of chain
54	EA	451	51% 87% 10%
54	EC	451	57% 96%
54	EE	451	56% 96%
54	EG	451	62% 96%
54	EI	451	63% 96%
54	EK	451	53% 96%
54	FA	451	38% 86% 10%
54	FB	451	42% 96%
54	FE	451	42% 85% 10%
54	FG	451	43% 96%
54	FI	451	49% 89% 8%
54	FK	451	43% 96%
54	GA	451	42% 96%
54	GB	451	34% 96%
54	GE	451	47% 96%
54	GG	451	39% 96%
54	GI	451	45% 96%
54	GK	451	41% 96%
54	HA	451	43% 96%
54	HB	451	30% 96%
54	HE	451	47% 95%
54	HG	451	34% 95%
54	HI	451	38% 97%
54	HK	451	25% 96%
54	IA	451	51% 96%

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Mol	Chain	Length	Quality of chain
54	IB	451	35% 96%
54	IE	451	70% 97%
54	IG	451	40% 96%
54	II	451	45% 96%
54	IK	451	37% 96%
54	IM	451	90% 96%
54	JA	451	39% 95%
54	JB	451	37% 96%
54	JE	451	42% 96%
54	JG	451	52% 96%
54	JI	451	45% 96%
54	JK	451	45% 97%
54	KA	451	34% 96%
54	KB	451	32% 95%
54	KE	451	40% 96%
54	KG	451	34% 96%
54	KI	451	47% 96%
54	KK	451	32% 97%
54	LA	451	33% 96%
54	LB	451	33% 96%
54	LE	451	41% 96%
54	LG	451	37% 96%
54	LI	451	32% 96%
54	LK	451	34% 97%
54	MA	451	33% 96%

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Mol	Chain	Length	Quality of chain
54	MB	451	37% 96%
54	ME	451	37% 96%
54	MG	451	37% 97%
54	MI	451	21% 96%
54	MK	451	79% 96%
54	ML	451	38% 97%
54	NA	451	46% 96%
54	NB	451	55% 96%
54	NE	451	50% 97%
54	NG	451	74% 96%
54	NI	451	57% 96%
54	NL	451	52% 96%
54	OA	451	20% 96%
54	OB	451	31% 95%
54	OE	451	19% 96%
54	OG	451	27% 96%
54	OI	451	20% 96%
54	OK	451	83% 96%
54	OL	451	22% 97%
54	PA	451	20% 96%
54	PB	451	37% 96%
54	PE	451	19% 96%
54	PG	451	33% 96%
54	PI	451	25% 96%
54	PK	451	67% 96%

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Mol	Chain	Length	Quality of chain
54	PL	451	35% 97%
54	QA	451	20% 96%
54	QB	451	36% 96%
54	QE	451	24% 96%
54	QG	451	29% 96%
54	QI	451	17% 96%
54	QK	451	36% 95%
54	QL	451	54% 96%
54	RA	451	22% 96%
54	RB	451	31% 95%
54	RE	451	23% 95%
54	RG	451	27% 96%
54	RI	451	22% 96%
54	RK	451	28% 96%
54	RL	451	74% 96%
54	SA	451	22% 96%
54	SB	451	28% 96%
54	SE	451	16% 96%
54	SG	451	22% 96%
54	SI	451	17% 96%
54	SK	451	19% 96%
54	TA	451	23% 96%
54	TB	451	23% 96%
54	TE	451	23% 96%
54	TG	451	26% 96%

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Mol	Chain	Length	Quality of chain
54	TI	451	20% 96%
54	TK	451	16% 96%
54	UA	451	50% 96%
54	UB	451	47% 95%
54	UE	451	57% 96%
54	UG	451	59% 96%
54	UI	451	54% 96%
54	UK	451	38% 96%
54	VA	451	51% 96%
54	VB	451	41% 97%
54	VE	451	51% 96%
54	VG	451	45% 96%
54	VI	451	54% 96%
54	VK	451	47% 96%
54	WA	451	44% 96%
54	WB	451	34% 96%
54	WE	451	52% 96%
54	WG	451	39% 96%
54	WI	451	39% 96%
54	WK	451	36% 95%
55	AC	447	40% 95%
55	AD	447	32% 96%
55	AF	447	35% 95%
55	AH	447	30% 95%
55	AJ	447	26% 95%

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Mol	Chain	Length	Quality of chain
55	AL	447	31% 95%
55	BC	447	41% 95%
55	BD	447	42% 95%
55	BF	447	55% 95%
55	BH	447	44% 96%
55	BJ	447	47% 96%
55	BL	447	46% 95%
55	CC	447	37% 95%
55	CD	447	37% 94%
55	CF	447	45% 96%
55	CH	447	36% 95%
55	CJ	447	46% 95%
55	CL	447	37% 95%
55	DC	447	46% 95%
55	DD	447	52% 95%
55	DF	447	53% 95%
55	DH	447	60% 95%
55	DJ	447	50% 95%
55	DL	447	54% 95%
55	EB	447	50% 95%
55	ED	447	62% 94%
55	EF	447	51% 95%
55	EH	447	67% 95%
55	EJ	447	45% 96%
55	EL	447	86% 95%

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Mol	Chain	Length	Quality of chain
55	EM	447	66% 94%
55	FC	447	36% 95%
55	FD	447	51% 95%
55	FF	447	37% 96%
55	FH	447	66% 96%
55	FJ	447	38% 94%
55	FL	447	73% 94%
55	FM	447	63% 95%
55	GC	447	34% 96%
55	GD	447	59% 96%
55	GF	447	33% 95%
55	GH	447	61% 95%
55	GJ	447	44% 96%
55	GL	447	65% 96%
55	GM	447	70% 96%
55	HC	447	37% 95%
55	HD	447	62% 95%
55	HF	447	35% 95%
55	HH	447	49% 95%
55	HJ	447	33% 95%
55	HL	447	62% 95%
55	HM	447	84% 95%
55	IC	447	43% 96%
55	ID	447	47% 95%
55	IF	447	36% 96%

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Mol	Chain	Length	Quality of chain
55	IH	447	59% 96%
55	IJ	447	40% 95%
55	IL	447	68% 95%
55	JC	447	30% 95%
55	JD	447	53% 95%
55	JF	447	37% 94%
55	JH	447	34% 94%
55	JJ	447	32% 95%
55	JL	447	72% 95%
55	JM	447	51% 95%
55	KC	447	34% 95%
55	KD	447	38% 95%
55	KF	447	34% 96%
55	KH	447	35% 95%
55	KJ	447	43% 95%
55	KL	447	54% 96%
55	KM	447	64% 96%
55	LC	447	38% 95%
55	LD	447	32% 96%
55	LF	447	35% 95%
55	LH	447	29% 96%
55	LJ	447	31% 95%
55	LL	447	33% 95%
55	LM	447	81% 95%
55	MC	447	40% 95%

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Mol	Chain	Length	Quality of chain
55	MD	447	30% 95%
55	MF	447	35% 96%
55	MH	447	29% 95%
55	MJ	447	32% 95%
55	MM	447	36% 95%
55	NC	447	58% 95%
55	ND	447	48% 95%
55	NF	447	48% 95%
55	NH	447	51% 95%
55	NJ	447	70% 94%
55	NK	447	84% 95%
55	NM	447	49% 95%
55	OC	447	30% 95%
55	OD	447	26% 96%
55	OF	447	17% 95%
55	OH	447	19% 95%
55	OJ	447	34% 95%
55	OM	447	26% 95%
55	PC	447	34% 94%
55	PD	447	22% 95%
55	PF	447	22% 95%
55	PH	447	26% 95%
55	PJ	447	42% 95%
55	PM	447	28% 95%
55	QC	447	27% 94%

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Mol	Chain	Length	Quality of chain
55	QD	447	24% 96%
55	QF	447	27% 95%
55	QH	447	27% 95%
55	QJ	447	24% 95%
55	QM	447	17% 95%
55	RC	447	23% 95%
55	RD	447	26% 95%
55	RF	447	21% 95%
55	RH	447	23% 96%
55	RJ	447	17% 95%
55	RM	447	24% 95%
55	SC	447	21% 95%
55	SD	447	18% 95%
55	SF	447	21% 95%
55	SH	447	24% 96%
55	SJ	447	17% 95%
55	SL	447	83% 95%
55	SM	447	28% 95%
55	TC	447	23% 95%
55	TD	447	24% 95%
55	TF	447	20% 96%
55	TH	447	30% 95%
55	TJ	447	16% 95%
55	TL	447	70% 96%
55	TM	447	36% 95%

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Mol	Chain	Length	Quality of chain
55	UC	447	54% 94%
55	UD	447	57% 95%
55	UF	447	54% 95%
55	UH	447	66% 94%
55	UJ	447	53% 95%
55	UL	447	75% 95%
55	UM	447	71% 95%
55	VC	447	41% 95%
55	VD	447	49% 95%
55	VF	447	45% 96%
55	VH	447	64% 94%
55	VJ	447	57% 95%
55	VL	447	57% 94%
55	VM	447	69% 95%
55	WC	447	34% 95%
55	WD	447	42% 95%
55	WF	447	35% 94%
55	WH	447	51% 96%
55	WJ	447	30% 96%
55	WL	447	36% 95%

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 1270897 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 CFAP96(C4orf47).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	42	324	205	55	61	3	0	0
1	1B	267	2033	1284	371	373	5	0	0

- Molecule 2 is a protein called Coiled-coil domain-containing protein 105.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1E	419	3281	2005	647	619	10	0	0
2	1F	170	1281	781	237	257	6	0	0
2	1G	294	2355	1440	478	432	5	0	0
2	1H	420	3294	2012	649	623	10	0	0

- Molecule 3 is a protein called Coiled-coil domain-containing protein 81.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1K	175	1406	897	246	257	6	0	0
3	1L	175	1406	897	246	257	6	0	0
3	1M	175	1393	889	244	254	6	0	0
3	1v	207	1719	1051	329	333	6	0	0
3	1w	87	727	441	145	138	3	0	0
3	1x	250	2088	1276	406	401	5	0	0
3	1y	198	1639	999	315	319	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1z	87	727	441	145	138	3	0	0
3	2a	54	452	276	83	90	3	0	0

- Molecule 4 is a protein called FAM166C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1P	203	1628	993	310	317	8	0	0
4	1Q	138	1130	686	223	217	4	0	0

- Molecule 5 is a protein called Protein FAM166B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1T	228	1845	1171	328	337	9	0	0
5	1U	111	898	575	158	161	4	0	0
5	1V	229	1857	1180	329	339	9	0	0
5	1W	107	871	549	156	162	4	0	0

- Molecule 6 is a protein called CFAP144(FAM183A).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	1Y	119	1009	638	176	191	4	0	0

- Molecule 7 is a protein called Outer dense fiber protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	1a	134	1030	647	184	193	6	0	0
7	1b	122	922	578	169	171	4	0	0
7	5E	154	1158	727	211	215	5	0	0
7	5F	112	861	542	153	160	6	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
7	5G	142	Total C N O S 1074 675 194 201 4	0	0
7	5H	117	Total C N O S 896 563 160 167 6	0	0
7	5I	27	Total C N O S 198 126 35 36 1	0	0
7	5J	233	Total C N O S 1776 1115 321 330 10	0	0
7	5K	134	Total C N O S 1011 635 184 188 4	0	0
7	5L	125	Total C N O S 958 603 170 179 6	0	0
7	5M	14	Total C N O 112 71 18 23	0	0
7	5N	244	Total C N O S 1856 1166 335 345 10	0	0
7	5O	15	Total C N O 117 78 20 19	0	0

- Molecule 8 is a protein called Tex33.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	1d	101	Total C N O S 808 521 136 148 3	0	0

- Molecule 9 is a protein called C20Orf85.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	1f	36	Total C N O 339 216 70 53	0	0
9	1g	51	Total C N O S 473 300 91 81 1	0	0

- Molecule 10 is a protein called ATP6V1FNB.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	1i	34	Total C N O 304 197 52 55	0	0
10	1j	31	Total C N O 275 177 48 50	0	0
10	9M	84	Total C N O S 705 453 125 124 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	9N	84	705	453	125	124	3	0	0
			Total	C	N	O			
10	9O	41	344	222	62	60		0	0

- Molecule 11 is a protein called Tex26(LOC100888047).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	1l	39	300	193	50	55	2	0	0
			Total	C	N	O	S		
11	1m	39	300	193	50	55	2	0	0

- Molecule 12 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	1o	29	252	155	51	44	2	0	0
			Total	C	N	O	S		
12	1p	30	261	160	52	47	2	0	0
			Total	C	N	O	S		
12	1q	46	382	240	69	72	1	0	0
			Total	C	N	O	S		
12	1r	27	235	146	49	38	2	0	0

- Molecule 13 is a protein called Enkurin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	2A	250	2045	1285	363	388	9	0	0
			Total	C	N	O	S		
13	2B	251	2051	1289	366	387	9	0	0
			Total	C	N	O	S		
13	2C	251	2054	1290	365	390	9	0	0
			Total	C	N	O	S		
13	2D	79	637	402	110	123	2	0	0

- Molecule 14 is a protein called CFAP107.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	2G	227	1874	1159	364	346	5	0	0

- Molecule 15 is a protein called Cilia- and flagella-associated protein 126.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	2J	107	862	534	161	164	3	0	0
15	2K	107	862	534	161	164	3	0	0
15	2L	107	862	534	161	164	3	0	0

- Molecule 16 is a protein called Flagellar FliJ protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	2O	119	978	611	184	182	1	0	0

- Molecule 17 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	2R	120	1035	628	200	202	5	0	0
17	2S	376	3254	1957	631	647	19	0	0

- Molecule 18 is a protein called Cilia- and flagella-associated protein 161.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	2V	284	2215	1382	392	427	14	0	0
18	2W	284	2215	1382	392	427	14	0	0

- Molecule 19 is a protein called CFA20 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	3A	187	1550	996	273	274	7	0	0
19	3B	187	1550	996	273	274	7	0	0
19	3C	180	1496	963	265	261	7	0	0
19	3D	176	1463	942	259	255	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	3E	186	1542	990	272	273	7	0	0
19	3F	187	1550	996	273	274	7	0	0
19	3G	186	1542	990	272	273	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	3J	495	3933	2460	699	763	11	0	0
20	3K	70	550	340	103	103	4	0	0

- Molecule 21 is a protein called Trichohyalin-plectin-homology domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	3N	258	2126	1306	406	405	9	0	0
21	3O	278	2329	1429	444	450	6	0	0

- Molecule 22 is a protein called CFAP276.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	3R	165	1317	820	242	252	3	0	0
22	3S	127	1006	625	191	188	2	0	0
22	3T	165	1317	820	242	252	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	3W	384	3224	1971	601	640	12	0	0
23	3X	315	2661	1623	506	523	9	0	0
23	3Y	104	862	523	168	168	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	3Z	172	1415	865	259	284	7	0	0

- Molecule 24 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	4A	617	4804	3030	841	902	31	0	0
			Total	C	N	O	S		
24	4B	615	4792	3022	839	901	30	0	0
			Total	C	N	O	S		
24	4C	617	4804	3030	841	902	31	0	0

- Molecule 25 is a protein called Trichohyalin-plectin-homology domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	4F	313	2613	1593	502	502	16	0	0
			Total	C	N	O	S		
25	4G	206	1753	1065	343	333	12	0	0

- Molecule 26 is a protein called Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	4J	378	2987	1875	520	569	23	0	0
			Total	C	N	O	S		
26	4K	376	2976	1869	518	566	23	0	0

- Molecule 27 is a protein called Cilia- and flagella-associated protein 77.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	4N	151	1237	772	235	224	6	0	0
			Total	C	N	O	S		
27	4O	108	878	553	162	159	4	0	0
			Total	C	N	O	S		
27	4P	150	1220	761	230	223	6	0	0
			Total	C	N	O	S		
27	4Q	93	744	462	146	133	3	0	0

- Molecule 28 is a protein called Cilia- and flagella-associated protein 97.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	4T	143	1221	767	234	211	9	0	0
28	4U	143	1221	767	234	211	9	0	0
28	4V	14	116	77	19	19	1	0	0

- Molecule 29 is a protein called HeLo_like_N(LOC577943).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	4Y	300	2422	1513	448	453	8	0	0

- Molecule 30 is a protein called Outer dense fiber protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	5A	35	265	168	50	46	1	0	0
30	5B	213	1650	1038	306	299	7	0	0
30	9Y	140	1083	677	208	193	5	0	0
30	9Z	101	783	495	145	140	3	0	0

- Molecule 31 is a protein called PACRG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	6A	225	1792	1151	310	323	8	0	0
31	6B	219	1737	1116	299	314	8	0	0
31	6C	223	1769	1139	304	318	8	0	0
31	6D	224	1784	1147	308	321	8	0	0
31	6E	224	1784	1147	308	321	8	0	0
31	6F	224	1784	1147	308	321	8	0	0

- Molecule 32 is a protein called Pierce1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	6I	78	632	397	112	119	4	0	0
32	6J	53	410	258	69	78	5	0	0

- Molecule 33 is a protein called Protein phosphatase 1 regulatory subunit 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	6M	391	3107	1936	567	593	11	0	0
33	6N	80	648	406	121	119	2	0	0

- Molecule 34 is a protein called RIB35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	6Q	201	1634	1028	292	306	8	0	0
34	6R	72	598	384	107	104	3	0	0

- Molecule 35 is a protein called RIB43A-like with coiled-coils protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	6U	149	1242	750	239	249	4	0	0
35	6V	274	2273	1370	435	458	10	0	0
35	6W	243	2035	1227	391	408	9	0	0
35	6X	121	1030	627	200	200	3	0	0

- Molecule 36 is a protein called EF-hand domain-containing family member C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	7A	725	5901	3763	1025	1093	20	0	0
36	7B	455	3734	2386	641	694	13	0	0
36	7C	543	4414	2816	773	810	15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	7D	724	5894	3758	1024	1092	20	0	0

- Molecule 37 is a protein called Flagellar protofilament ribbon protein rib74.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	7G	529	4301	2746	733	805	17	0	0
37	7H	529	4301	2746	733	805	17	0	0
37	7I	616	4996	3177	856	942	21	0	0

- Molecule 38 is a protein called SAXO3(LOC115918676).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	7M	263	2153	1350	401	391	11	0	0
38	7N	68	527	339	82	101	5	0	0

- Molecule 39 is a protein called TEPP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	7Q	145	1199	760	220	215	4	0	0
39	7R	142	1140	713	213	210	4	0	0

- Molecule 40 is a protein called SPATA48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	7U	93	755	476	136	134	9	0	0
40	7V	53	456	289	89	78		0	0

- Molecule 41 is a protein called Sperm-associated antigen 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	7Y	200	1593	991	270	327	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	7Z	64	491	297	89	103	2	0	0

- Molecule 42 is a protein called Testicular haploid expressed gene protein-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	8A	243	1931	1213	359	354	5	0	0

- Molecule 43 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	8D	397	3244	1990	594	640	20	0	0
			Total	C	N	O	S		
43	8E	178	1476	906	268	295	7	0	0
			Total	C	N	O	S		
43	8F	265	2142	1309	397	421	15	0	0
			Total	C	N	O	S		
43	8G	397	3244	1990	594	640	20	0	0

- Molecule 44 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	8J	403	3272	1986	606	668	12	0	0
			Total	C	N	O	S		
44	8K	322	2623	1594	485	534	10	0	0
			Total	C	N	O	S		
44	8L	403	3272	1986	606	668	12	0	0
			Total	C	N	O	S		
44	8M	128	1041	632	190	216	3	0	0
			Total	C	N	O	S		
44	8N	17	144	84	30	29	1	0	0

- Molecule 45 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O			
45	8Q	21	176	112	34	30		0	0
			Total	C	N	O	S		
45	8R	400	3241	1979	597	650	15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	8S	304	2476	1513	453	499	11	0	0
45	8T	400	3241	1979	597	650	15	0	0
45	8U	120	958	584	180	189	5	0	0

- Molecule 46 is a protein called Tex43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	8X	104	879	553	164	157	5	0	0
46	8Y	104	879	553	164	157	5	0	0
46	8Z	104	879	553	164	157	5	0	0

- Molecule 47 is a protein called Tex36(CFAP95, C9orf135).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	9A	207	1704	1053	314	334	3	0	0

- Molecule 48 is a protein called CFAP90(C5orf49).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	9D	96	808	504	157	145	2	0	0

- Molecule 49 is a protein called Tex49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	9G	150	1229	787	216	221	5	0	0

- Molecule 50 is a protein called Tex49_homologue(LOC580808).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	9J	101	822	513	157	147	5	0	0

- Molecule 51 is a protein called CFAP68(UPF0686, C11orf1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	9R	142	1166	736	208	220	2	0	0

- Molecule 52 is a protein called SPATA45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	9T	75	629	388	119	117	5	0	0

- Molecule 53 is a protein called C4orf45.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	9V	24	190	117	39	34	0	0
			Total	C	N	O		
53	9W	70	602	391	107	104	0	0

- Molecule 54 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	AA	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	AB	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	AE	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	AG	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	AI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	AK	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	AM	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	BA	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	BB	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	BE	437	3414	2164	581	647	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	BG	437	3414	2164	581	647	22	0	0
54	BI	437	3414	2164	581	647	22	0	0
54	BK	437	3414	2164	581	647	22	0	0
54	BM	437	3414	2164	581	647	22	0	0
54	CA	437	3414	2164	581	647	22	0	0
54	CB	437	3414	2164	581	647	22	0	0
54	CE	437	3414	2164	581	647	22	0	0
54	CG	437	3414	2164	581	647	22	0	0
54	CI	437	3414	2164	581	647	22	0	0
54	CK	437	3414	2164	581	647	22	0	0
54	CM	437	3414	2164	581	647	22	0	0
54	DA	437	3414	2164	581	647	22	0	0
54	DB	437	3414	2164	581	647	22	0	0
54	DE	437	3414	2164	581	647	22	0	0
54	DG	437	3414	2164	581	647	22	0	0
54	DI	437	3414	2164	581	647	22	0	0
54	DK	437	3414	2164	581	647	22	0	0
54	DM	437	3414	2164	581	647	22	0	0
54	EA	437	3414	2164	581	647	22	0	0
54	EC	437	3414	2164	581	647	22	0	0
54	EE	437	3414	2164	581	647	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	EG	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	EI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	EK	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	FA	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	FB	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	FE	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	FG	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	FI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	FK	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	GA	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	GB	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	GE	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	GG	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	GI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	GK	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	HA	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	HB	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	HE	432	3382	2144	575	641	22	0	0
			Total	C	N	O	S		
54	HG	435	3406	2160	579	645	22	0	0
			Total	C	N	O	S		
54	HI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	HK	435	3406	2160	579	645	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	IA	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	IB	434	3398	2154	578	644	22	0	0
			Total	C	N	O	S		
54	IE	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	IG	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	II	435	3402	2156	579	645	22	0	0
			Total	C	N	O	S		
54	IK	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	IM	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	JA	432	3387	2148	576	641	22	0	0
			Total	C	N	O	S		
54	JB	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	JE	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	JG	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	JI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	JK	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	KA	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	KB	434	3398	2154	578	644	22	0	0
			Total	C	N	O	S		
54	KE	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	KG	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	KI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	KK	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	LA	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	LB	437	3414	2164	581	647	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	LE	437	3414	2164	581	647	22	0	0
54	LG	437	3414	2164	581	647	22	0	0
54	LI	437	3414	2164	581	647	22	0	0
54	LK	437	3414	2164	581	647	22	0	0
54	MA	437	3414	2164	581	647	22	0	0
54	MB	437	3414	2164	581	647	22	0	0
54	ME	437	3414	2164	581	647	22	0	0
54	MG	437	3414	2164	581	647	22	0	0
54	MI	437	3414	2164	581	647	22	0	0
54	MK	437	3414	2164	581	647	22	0	0
54	ML	437	3414	2164	581	647	22	0	0
54	NA	435	3406	2160	579	645	22	0	0
54	NB	437	3414	2164	581	647	22	0	0
54	NE	437	3414	2164	581	647	22	0	0
54	NG	437	3414	2164	581	647	22	0	0
54	NI	434	3398	2154	578	644	22	0	0
54	NL	433	3391	2150	577	642	22	0	0
54	OA	437	3414	2164	581	647	22	0	0
54	OB	434	3398	2154	578	644	22	0	0
54	OE	437	3414	2164	581	647	22	0	0
54	OG	437	3414	2164	581	647	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	OI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	OK	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	OL	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	PA	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	PB	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	PE	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	PG	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	PI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	PK	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	PL	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	QA	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	QB	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	QE	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	QG	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	QI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	QK	433	3391	2150	577	642	22	0	0
			Total	C	N	O	S		
54	QL	436	3410	2162	580	646	22	0	0
			Total	C	N	O	S		
54	RA	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	RB	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	RE	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	RG	437	3414	2164	581	647	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	RI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	RK	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	RL	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	SA	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	SB	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	SE	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	SG	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	SI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	SK	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	TA	436	3410	2162	580	646	22	0	0
			Total	C	N	O	S		
54	TB	436	3410	2162	580	646	22	0	0
			Total	C	N	O	S		
54	TE	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	TG	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	TI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	TK	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	UA	436	3410	2162	580	646	22	0	0
			Total	C	N	O	S		
54	UB	434	3395	2152	578	643	22	0	0
			Total	C	N	O	S		
54	UE	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	UG	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	UI	437	3414	2164	581	647	22	0	0
			Total	C	N	O	S		
54	UK	437	3414	2164	581	647	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	VA	437	3414	2164	581	647	22	0	0
54	VB	437	3414	2164	581	647	22	0	0
54	VE	437	3414	2164	581	647	22	0	0
54	VG	435	3406	2160	579	645	22	0	0
54	VI	437	3414	2164	581	647	22	0	0
54	VK	437	3414	2164	581	647	22	0	0
54	WA	437	3414	2164	581	647	22	0	0
54	WB	436	3410	2162	580	646	22	0	0
54	WE	437	3414	2164	581	647	22	0	0
54	WG	437	3414	2164	581	647	22	0	0
54	WI	437	3414	2164	581	647	22	0	0
54	WK	437	3414	2164	581	647	22	0	0

- Molecule 55 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	AC	431	3383	2124	579	653	27	0	0
55	AD	431	3383	2124	579	653	27	0	0
55	AF	431	3383	2124	579	653	27	0	0
55	AH	431	3383	2124	579	653	27	0	0
55	AJ	431	3383	2124	579	653	27	0	0
55	AL	431	3383	2124	579	653	27	0	0
55	BC	431	3383	2124	579	653	27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	BD	431	3383	2124	579	653	27	0	0
55	BF	431	3383	2124	579	653	27	0	0
55	BH	431	3383	2124	579	653	27	0	0
55	BJ	431	3383	2124	579	653	27	0	0
55	BL	431	3383	2124	579	653	27	0	0
55	CC	431	3383	2124	579	653	27	0	0
55	CD	431	3383	2124	579	653	27	0	0
55	CF	431	3383	2124	579	653	27	0	0
55	CH	431	3383	2124	579	653	27	0	0
55	CJ	431	3383	2124	579	653	27	0	0
55	CL	431	3383	2124	579	653	27	0	0
55	DC	431	3383	2124	579	653	27	0	0
55	DD	431	3383	2124	579	653	27	0	0
55	DF	431	3383	2124	579	653	27	0	0
55	DH	431	3383	2124	579	653	27	0	0
55	DJ	431	3383	2124	579	653	27	0	0
55	DL	431	3383	2124	579	653	27	0	0
55	EB	431	3383	2124	579	653	27	0	0
55	ED	431	3383	2124	579	653	27	0	0
55	EF	431	3383	2124	579	653	27	0	0
55	EH	431	3383	2124	579	653	27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	EJ	431	3383	2124	579	653	27	0	0
55	EL	431	3383	2124	579	653	27	0	0
55	EM	431	3383	2124	579	653	27	0	0
55	FC	431	3383	2124	579	653	27	0	0
55	FD	431	3383	2124	579	653	27	0	0
55	FF	431	3383	2124	579	653	27	0	0
55	FH	431	3383	2124	579	653	27	0	0
55	FJ	431	3383	2124	579	653	27	0	0
55	FL	431	3383	2124	579	653	27	0	0
55	FM	431	3383	2124	579	653	27	0	0
55	GC	431	3383	2124	579	653	27	0	0
55	GD	431	3383	2124	579	653	27	0	0
55	GF	431	3383	2124	579	653	27	0	0
55	GH	431	3383	2124	579	653	27	0	0
55	GJ	431	3383	2124	579	653	27	0	0
55	GL	431	3383	2124	579	653	27	0	0
55	GM	431	3383	2124	579	653	27	0	0
55	HC	431	3383	2124	579	653	27	0	0
55	HD	431	3383	2124	579	653	27	0	0
55	HF	431	3383	2124	579	653	27	0	0
55	HH	431	3383	2124	579	653	27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	HJ	431	3383	2124	579	653	27	0	0
55	HL	431	3383	2124	579	653	27	0	0
55	HM	431	3383	2124	579	653	27	0	0
55	IC	431	3383	2124	579	653	27	0	0
55	ID	431	3383	2124	579	653	27	0	0
55	IF	431	3383	2124	579	653	27	0	0
55	IH	431	3383	2124	579	653	27	0	0
55	IJ	431	3383	2124	579	653	27	0	0
55	IL	431	3383	2124	579	653	27	0	0
55	JC	431	3383	2124	579	653	27	0	0
55	JD	431	3383	2124	579	653	27	0	0
55	JF	431	3383	2124	579	653	27	0	0
55	JH	431	3383	2124	579	653	27	0	0
55	JJ	431	3383	2124	579	653	27	0	0
55	JL	431	3383	2124	579	653	27	0	0
55	JM	431	3383	2124	579	653	27	0	0
55	KC	431	3383	2124	579	653	27	0	0
55	KD	431	3383	2124	579	653	27	0	0
55	KF	431	3383	2124	579	653	27	0	0
55	KH	431	3383	2124	579	653	27	0	0
55	KJ	431	3383	2124	579	653	27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	KL	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	KM	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	LC	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	LD	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	LF	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	LH	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	LJ	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	LL	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	LM	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	MC	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	MD	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	MF	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	MH	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	MJ	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	MM	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	NC	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	ND	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	NF	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	NH	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	NJ	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	NK	431	3383	2124	579	653	27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	NM	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	OC	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	OD	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	OF	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	OH	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	OJ	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	OM	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	PC	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	PD	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	PF	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	PH	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	PJ	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	PM	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	QC	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	QD	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	QF	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	QH	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	QJ	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	QM	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	RC	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	RD	431	3383	2124	579	653	27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	RF	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	RH	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	RJ	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	RM	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	SC	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	SD	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	SF	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	SH	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	SJ	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	SL	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	SM	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	TC	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	TD	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	TF	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	TH	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	TJ	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	TL	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	TM	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	UC	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	UD	431	3383	2124	579	653	27	0	0
			Total	C	N	O	S		
55	UF	431	3383	2124	579	653	27	0	0

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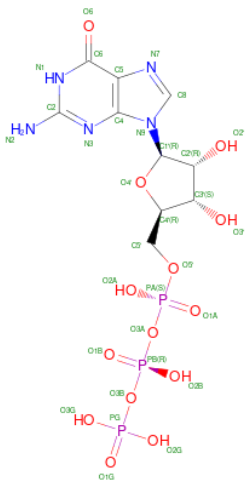
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	UH	431	3383	2124	579	653	27	0	0
55	UJ	431	3383	2124	579	653	27	0	0
55	UL	431	3383	2124	579	653	27	0	0
55	UM	431	3383	2124	579	653	27	0	0
55	VC	431	3383	2124	579	653	27	0	0
55	VD	431	3383	2124	579	653	27	0	0
55	VF	431	3383	2124	579	653	27	0	0
55	VH	431	3383	2124	579	653	27	0	0
55	VJ	431	3383	2124	579	653	27	0	0
55	VL	431	3383	2124	579	653	27	0	0
55	VM	431	3383	2124	579	653	27	0	0
55	WC	431	3383	2124	579	653	27	0	0
55	WD	431	3383	2124	579	653	27	0	0
55	WF	431	3383	2124	579	653	27	0	0
55	WH	431	3383	2124	579	653	27	0	0
55	WJ	431	3383	2124	579	653	27	0	0
55	WL	431	3383	2124	579	653	27	0	0

- Molecule 56 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

GTP



Mol	Chain	Residues	Atoms					AltConf
56	AA	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AB	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AG	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AI	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AK	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AM	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BA	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BB	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BG	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BI	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BK	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BM	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	
56	CA	1	32	10	5	14	3	0
56	CB	1	32	10	5	14	3	0
56	CE	1	32	10	5	14	3	0
56	CG	1	32	10	5	14	3	0
56	CI	1	32	10	5	14	3	0
56	CK	1	32	10	5	14	3	0
56	CM	1	32	10	5	14	3	0
56	DA	1	32	10	5	14	3	0
56	DB	1	32	10	5	14	3	0
56	DE	1	32	10	5	14	3	0
56	DG	1	32	10	5	14	3	0
56	DI	1	32	10	5	14	3	0
56	DK	1	32	10	5	14	3	0
56	DM	1	32	10	5	14	3	0
56	EA	1	32	10	5	14	3	0
56	EC	1	32	10	5	14	3	0
56	EE	1	32	10	5	14	3	0
56	EG	1	32	10	5	14	3	0
56	EI	1	32	10	5	14	3	0
56	EK	1	32	10	5	14	3	0
56	FA	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	FB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	FE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	FG	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	FI	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	FK	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	GA	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	GB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	GE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	GG	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	GI	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	GK	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	HA	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	HB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	HE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	HG	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	HI	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	HK	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	IA	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	IB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	IE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	IG	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	II	1	32	10	5	14	3	0
56	IK	1	32	10	5	14	3	0
56	IM	1	32	10	5	14	3	0
56	JA	1	32	10	5	14	3	0
56	JB	1	32	10	5	14	3	0
56	JE	1	32	10	5	14	3	0
56	JG	1	32	10	5	14	3	0
56	JI	1	32	10	5	14	3	0
56	JK	1	32	10	5	14	3	0
56	KA	1	32	10	5	14	3	0
56	KB	1	32	10	5	14	3	0
56	KE	1	32	10	5	14	3	0
56	KG	1	32	10	5	14	3	0
56	KI	1	32	10	5	14	3	0
56	KK	1	32	10	5	14	3	0
56	LA	1	32	10	5	14	3	0
56	LB	1	32	10	5	14	3	0
56	LE	1	32	10	5	14	3	0
56	LG	1	32	10	5	14	3	0
56	LI	1	32	10	5	14	3	0
56	LK	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	MA	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	MB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	ME	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	MG	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	MI	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	MK	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	ML	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	NA	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	NB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	NE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	NG	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	NI	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	NL	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	OA	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	OB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	OE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	OG	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	OI	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	OK	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	OL	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	PA	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	PB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	PE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	PG	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	PI	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	PK	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	PL	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	QA	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	QB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	QE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	QG	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	QI	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	QK	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	QL	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	RA	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	RB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	RE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	RG	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	RI	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	RK	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	RL	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	SA	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	SB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	SE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	SG	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	SI	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	SK	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	TA	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	TB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	TE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	TG	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	TI	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	TK	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	UA	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	UB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	UE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	UG	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	UI	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	UK	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	VA	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	VB	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	VE	1	32	10	5	14	3	0
			Total	C	N	O	P	
56	VG	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	VI	1	32	10	5	14	3	0
56	VK	1	32	10	5	14	3	0
56	WA	1	32	10	5	14	3	0
56	WB	1	32	10	5	14	3	0
56	WE	1	32	10	5	14	3	0
56	WG	1	32	10	5	14	3	0
56	WI	1	32	10	5	14	3	0
56	WK	1	32	10	5	14	3	0

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	AA	1	1	1	0
57	AB	1	1	1	0
57	AE	1	1	1	0
57	AG	1	1	1	0
57	AI	1	1	1	0
57	AK	1	1	1	0
57	AM	1	1	1	0
57	BA	1	1	1	0
57	BB	1	1	1	0
57	BE	1	1	1	0
57	BG	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	BI	1	1	1	0
57	BK	1	1	1	0
57	BM	1	1	1	0
57	CA	1	1	1	0
57	CB	1	1	1	0
57	CE	1	1	1	0
57	CG	1	1	1	0
57	CI	1	1	1	0
57	CK	1	1	1	0
57	CM	1	1	1	0
57	DA	1	1	1	0
57	DB	1	1	1	0
57	DE	1	1	1	0
57	DG	1	1	1	0
57	DI	1	1	1	0
57	DK	1	1	1	0
57	DM	1	1	1	0
57	EA	1	1	1	0
57	EC	1	1	1	0
57	EE	1	1	1	0
57	EG	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	EI	1	1	1	0
57	EK	1	1	1	0
57	FA	1	1	1	0
57	FB	1	1	1	0
57	FE	1	1	1	0
57	FG	1	1	1	0
57	FI	1	1	1	0
57	FK	1	1	1	0
57	GA	1	1	1	0
57	GB	1	1	1	0
57	GE	1	1	1	0
57	GG	1	1	1	0
57	GI	1	1	1	0
57	GK	1	1	1	0
57	HA	1	1	1	0
57	HB	1	1	1	0
57	HE	1	1	1	0
57	HG	1	1	1	0
57	HI	1	1	1	0
57	HK	1	1	1	0
57	IA	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	IB	1	1	1	0
57	IE	1	1	1	0
57	IG	1	1	1	0
57	II	1	1	1	0
57	IK	1	1	1	0
57	IM	1	1	1	0
57	JA	1	1	1	0
57	JB	1	1	1	0
57	JE	1	1	1	0
57	JG	1	1	1	0
57	JI	1	1	1	0
57	JK	1	1	1	0
57	KA	1	1	1	0
57	KB	1	1	1	0
57	KE	1	1	1	0
57	KG	1	1	1	0
57	KI	1	1	1	0
57	KK	1	1	1	0
57	LA	1	1	1	0
57	LB	1	1	1	0
57	LE	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	LG	1	1	1	0
57	LI	1	1	1	0
57	LK	1	1	1	0
57	MA	1	1	1	0
57	MB	1	1	1	0
57	ME	1	1	1	0
57	MG	1	1	1	0
57	MI	1	1	1	0
57	MK	1	1	1	0
57	ML	1	1	1	0
57	NA	1	1	1	0
57	NB	1	1	1	0
57	NE	1	1	1	0
57	NG	1	1	1	0
57	NI	1	1	1	0
57	NL	1	1	1	0
57	OA	1	1	1	0
57	OB	1	1	1	0
57	OE	1	1	1	0
57	OG	1	1	1	0
57	OI	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	OK	1	1	1	0
57	OL	1	1	1	0
57	PA	1	1	1	0
57	PB	1	1	1	0
57	PE	1	1	1	0
57	PG	1	1	1	0
57	PI	1	1	1	0
57	PK	1	1	1	0
57	PL	1	1	1	0
57	QA	1	1	1	0
57	QB	1	1	1	0
57	QE	1	1	1	0
57	QG	1	1	1	0
57	QI	1	1	1	0
57	QK	1	1	1	0
57	QL	1	1	1	0
57	RA	1	1	1	0
57	RB	1	1	1	0
57	RE	1	1	1	0
57	RG	1	1	1	0
57	RI	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	RK	1	1	1	0
57	RL	1	1	1	0
57	SA	1	1	1	0
57	SB	1	1	1	0
57	SE	1	1	1	0
57	SG	1	1	1	0
57	SI	1	1	1	0
57	SK	1	1	1	0
57	TA	1	1	1	0
57	TB	1	1	1	0
57	TE	1	1	1	0
57	TG	1	1	1	0
57	TI	1	1	1	0
57	TK	1	1	1	0
57	UA	1	1	1	0
57	UB	1	1	1	0
57	UE	1	1	1	0
57	UG	1	1	1	0
57	UI	1	1	1	0
57	UK	1	1	1	0
57	VA	1	1	1	0

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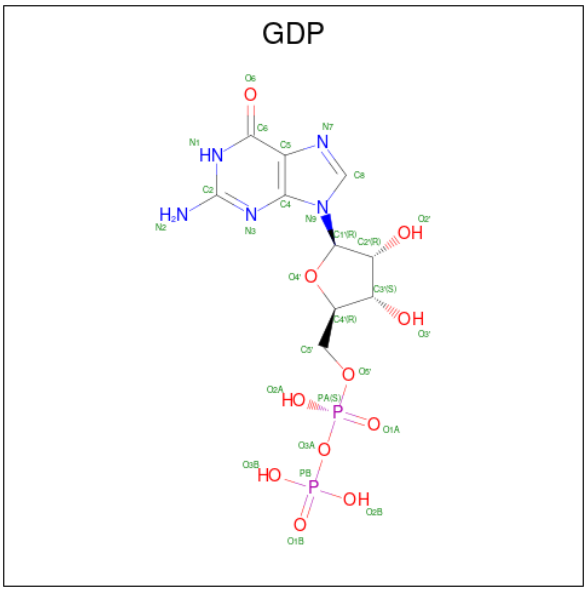
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	VB	1	1	1	0
57	VE	1	1	1	0
57	VG	1	1	1	0
57	VI	1	1	1	0
57	VK	1	1	1	0
57	WA	1	1	1	0
57	WB	1	1	1	0
57	WE	1	1	1	0
57	WG	1	1	1	0
57	WI	1	1	1	0
57	WK	1	1	1	0

- Molecule 58 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
58	AC	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	AD	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	AF	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	AH	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	AJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	AL	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	BC	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	BD	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	BF	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	BH	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	BJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	BL	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	CC	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	CF	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	CH	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	CJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	CL	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	DC	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	DD	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	DF	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	DH	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	
58	DJ	1	28	10	5	11	2	0
58	DL	1	28	10	5	11	2	0
58	EB	1	28	10	5	11	2	0
58	ED	1	28	10	5	11	2	0
58	EF	1	28	10	5	11	2	0
58	EH	1	28	10	5	11	2	0
58	EJ	1	28	10	5	11	2	0
58	EL	1	28	10	5	11	2	0
58	EM	1	28	10	5	11	2	0
58	FC	1	28	10	5	11	2	0
58	FD	1	28	10	5	11	2	0
58	FF	1	28	10	5	11	2	0
58	FH	1	28	10	5	11	2	0
58	FJ	1	28	10	5	11	2	0
58	FL	1	28	10	5	11	2	0
58	FM	1	28	10	5	11	2	0
58	GC	1	28	10	5	11	2	0
58	GD	1	28	10	5	11	2	0
58	GF	1	28	10	5	11	2	0
58	GH	1	28	10	5	11	2	0
58	GJ	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	GL	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	GM	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	HC	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	HD	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	HF	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	HH	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	HJ	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	HL	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	HM	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	IC	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	ID	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	IF	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	IH	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	IJ	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	IL	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	JC	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	JD	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	JF	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	JH	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	JJ	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	JL	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	JM	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	KC	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	KD	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	KF	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	KH	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	KJ	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	KL	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	KM	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	LC	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	LD	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	LF	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	LH	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	LJ	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	LL	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	LM	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	MC	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	MD	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	MF	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	MH	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	MJ	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	MM	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	NC	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	ND	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	NF	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	NH	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	NJ	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	NK	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	NM	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	OC	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	OD	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	OF	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	OH	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	OJ	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	OM	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	PC	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	PD	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	PF	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	PH	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	PJ	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	PM	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	QC	1	28	10	5	11	2	0
			Total	C	N	O	P	
58	QD	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	QF	1	28	10	5	11	2	0
58	QH	1	28	10	5	11	2	0
58	QJ	1	28	10	5	11	2	0
58	QM	1	28	10	5	11	2	0
58	RC	1	28	10	5	11	2	0
58	RD	1	28	10	5	11	2	0
58	RF	1	28	10	5	11	2	0
58	RH	1	28	10	5	11	2	0
58	RJ	1	28	10	5	11	2	0
58	RM	1	28	10	5	11	2	0
58	SC	1	28	10	5	11	2	0
58	SD	1	28	10	5	11	2	0
58	SF	1	28	10	5	11	2	0
58	SH	1	28	10	5	11	2	0
58	SJ	1	28	10	5	11	2	0
58	SL	1	28	10	5	11	2	0
58	SM	1	28	10	5	11	2	0
58	TC	1	28	10	5	11	2	0
58	TD	1	28	10	5	11	2	0
58	TF	1	28	10	5	11	2	0
58	TH	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	TJ	1	28	10	5	11	2	0
58	TL	1	28	10	5	11	2	0
58	TM	1	28	10	5	11	2	0
58	UC	1	28	10	5	11	2	0
58	UD	1	28	10	5	11	2	0
58	UF	1	28	10	5	11	2	0
58	UH	1	28	10	5	11	2	0
58	UJ	1	28	10	5	11	2	0
58	UL	1	28	10	5	11	2	0
58	UM	1	28	10	5	11	2	0
58	VC	1	28	10	5	11	2	0
58	VD	1	28	10	5	11	2	0
58	VF	1	28	10	5	11	2	0
58	VH	1	28	10	5	11	2	0
58	VJ	1	28	10	5	11	2	0
58	VL	1	28	10	5	11	2	0
58	VM	1	28	10	5	11	2	0
58	WC	1	28	10	5	11	2	0
58	WD	1	28	10	5	11	2	0
58	WF	1	28	10	5	11	2	0
58	WH	1	28	10	5	11	2	0

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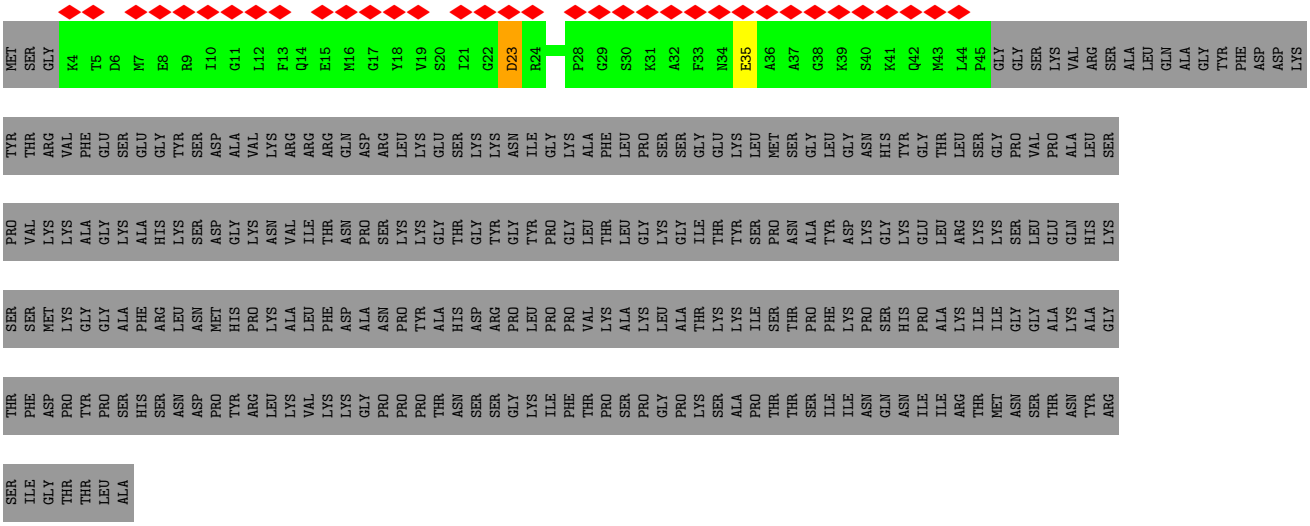
Mol	Chain	Residues	Atoms					AltConf
58	WJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	WL	1	Total	C	N	O	P	0
			28	10	5	11	2	

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.

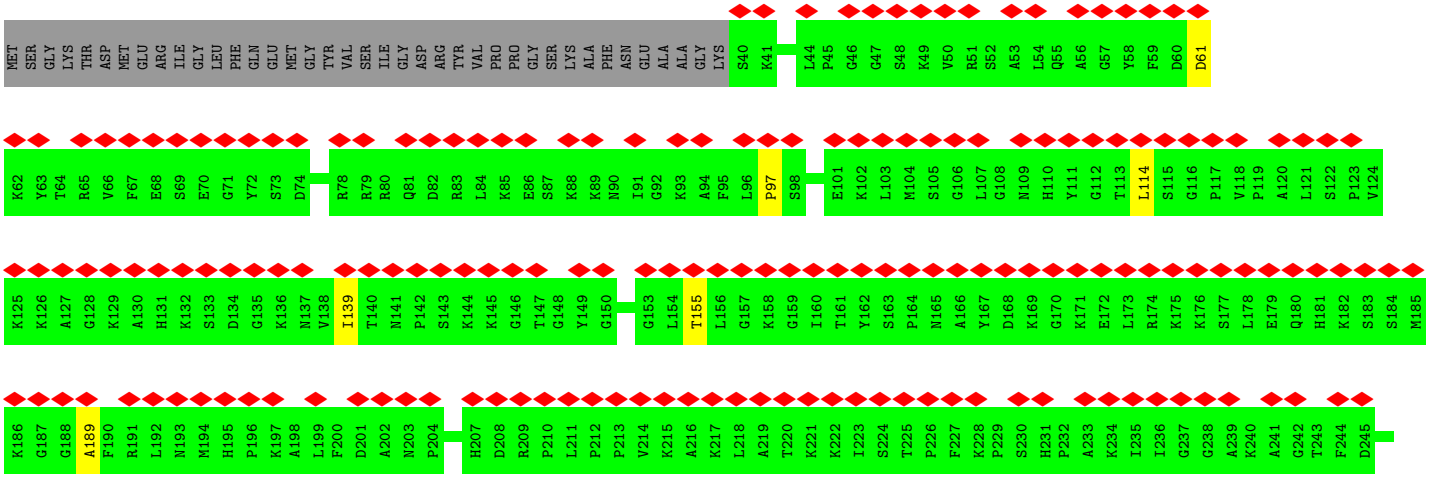
- Molecule 1: CFAP96(C4orf47)

Chain 1A:



- Molecule 1: CFAP96(C4orf47)

Chain 1B:



P248 S249 H250 S251 N252 D253 P254 Y255 R256 L257 K258 V259 K260 K261 G262 P263 P264 P265 T266 N267 S268 S269 G270 K271 I272 F273 T274 P275 S276 P277 G278 P279 K280 S281 T284 T285 S286 I287 I288 N289 Q290 N291 I292 I293 R294 T295 M296 N297 S298 T299 N300 Y301 R302 S303 I304 G305 T306 THR LEU

ALA

- Molecule 2: Coiled-coil domain-containing protein 105

Chain 1E: 91% 93% • 6%

MET MET SER THR ARG SER ARG THR GLN ILE PRO LEU ALA THR A15 T16 V17 G18 P19 Q20 S21 W22 S23 D24 A25 T26 V27 K28 E29 I30 K31 I32 S33 Q34 A35 A36 V37 E38 K39 T40 D41 T42 G43 Q44 E45 V46 G47 R48 S49 F50 D51 A52 L53 P54 S55 L56 R57 D58 N59 C60

A61 Q62 Q63 S64 N65 T66 V67 V68 H69 Q70 Y71 V72 R73 E74 C75 R76 I77 S78 L79 V80 K81 L82 R83 D84 S85 F86 L87 E88 T89 N90 E91 E92 V93 K94 S95 L96 I97 R98 G99 K100 E101 A102 L103 E104 K105 Q106 L107 E108 H109 I110 R111 K112 D113 I114 A115 L116 N117 K118 M119 S120

T121 E122 I123 R124 C125 T126 R127 P128 S129 R130 E131 R132 G133 R134 D135 G136 A137 D138 N139 V140 M141 E142 K143 E144 F145 R146 H147 L148 H149 Q150 L151 K152 K153 A154 L155 E156 L157 Q158 L159 R160 S161 V162 Q163 K164 Q165 L166 Q167 V168 L169 D170 Q171 C172 R173 K174 R175 L176 S177 A178 V179 I180

Q181 E182 R183 N184 R185 V186 L187 D188 L189 L190 C191 H192 A193 V194 S195 S196 V197 N198 GLY ARG ALA SER ARG GLY GLY GLY ARG VAL SER ARG GLN D212 K213 T214 M215 T216 F217 G218 G219 N220 G221 M222 G223 Y224 T225 R226 Q227 V228 N229 G230 N231 V232 A233 E234 L235 L236 G237 T238 G239 A240

S241 P242 P243 D244 A245 E246 N247 R248 S249 G250 T251 P252 P253 P254 D255 P256 L257 G258 P259 F260 T261 P262 E263 A264 A265 A266 A267 I268 A269 Q270 A271 R272 E273 A274 R275 Q276 R277 S278 Q279 F280 L281 R282 K283 D284 I285 R286 D287 A288 I289 E290 N291 T292 Q293 Q294 L295 Q296 Q297 A298 A299 H300

R301 A302 V303 N304 D305 G306 L307 N308 Q309 K310 V311 A312 E313 T314 I315 T316 L317 K318 Q319 H320 L321 T322 V323 A324 A325 G326 E327 N328 R329 H330 S331 I332 H333 R334 A335 Q336 R337 W338 Y339 D340 S341 T342 E343 K344 A345 L346 G347 Y348 T349 I350 G351 P352 E353 L354 Q355 S356 D357 L358 E359 T360

R361 E362 K363 L364 T365 R366 P367 I368 V369 R370 V371 F372 Q373 R374 H375 P376 G377 T378 N379 L380 P381 E382 A383 Q384 G385 I386 I387 R388 G389 A390 A391 G392 L393 D394 E395 S396 L397 L398 R399 T400 S401 R402 N403 I404 G405 L406 L407 Q408 L409 A410 Q411 G412 R413 L414 Q415 G416 D417 I418 R419 H420

K421 H422 A423 G424 A425 S426 V427 D428 S429 A430 I431 V432 R433 G434 R435 R436 R437 L438 A439 N440 H441 R442 W443 V444 M445 G446 SER VAL

- Molecule 2: Coiled-coil domain-containing protein 105

Chain 1F: 38% 38% 62%

MET MET SER THR ARG SER ARG THR GLN ILE PRO LEU ALA THR A15 T16 V17 G18 P19 Q20 S21 W22 S23 D24 A25 T26 V27 K28 E29 I30 K31 I32 S33 Q34 A35 A36 V37 E38 K39 T40 D41 T42 G43 Q44 E45 V46 G47 R48 S49 F50 D51 A52 L53 P54 S55 L56 R57 D58 N59 C60

A61 Q62 Q63 S64 N65 T66 V67 V68 H69 Q70 Y71 V72 R73 E74 C75 R76 I77 S78 L79 V80 K81 L82 R83 D84 S85 F86 L87 E88 T89 N90 GLU GLU VAL LYS SER LEU ILE ARG GLY LYS GLU ALA LEU GLU LYS GLN LEU GLU HIS ILE ARG LYS ASP ILE ALA LEU ASN LYS MET SER

THR GLU ILE ARG CYS THR ARG PRO SER ARG GLU ARG GLY ARG ASP GLY ALA ASP ASN VAL MET GLU LYS GLU PHE ARG HIS LEU HIS GLN LEU LYS LYS ALA LEU GLU LEU GLN LEU ARG SER VAL GLN LYS GLN LEU GLN VAL L169 D170 Q171 C172 R173 K174 R175 L176 S177 A178 V179 I180

Q181 E182 R183 N184 R185 V186 L187 D188 L189 L190 C191 H192 A193 V194 S195 S196 V197 N198 GLY ARG ALA SER ARG GLY GLY GLY ARG VAL SER ARG Q211 D212 K213 T214 M215 T216 F217 G218 G219 N220 G221 M222 G223 Y224 T225 R226 Q227 V228 N229 G230 N231 V232 A233 E234 L235 L236 G237 T238 G239 A240

S241 P242 P243 D244 A245 E246 N247 R248 S249 G250 T251 P252 P253 P254 D255 P256 L257 G258 P259 F260 T261 P262 E263 A264 A265 A266 A267 I268 A269 Q270 A271 R272 E273 A274 ARG GLN ARG SER GLN PHE LEU ARG LYS ASP ILE ARG ASP ALA ILE GLU ASN THR GLN GLN LEU GLN GLN ALA ALA HIS

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

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

LYS HIS ALA GLY ALA SER VAL ASP SER ALA ILE VAL ARG GLY ARG ARG ARG LEU ALA ASN HIS ARG TRP VAL MET GLY SER VAL

- Molecule 2: Coiled-coil domain-containing protein 105

Chain 1G:

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

ALA GLN GLN SER ASN THR VAL VAL HIS GLN TYR VAL ARG GLU CYS ARG I77 S78 L79 V80 K81 L82 R83 D84 S85 F86 L87 E88 T89 N90 E91 E92 V93 K94 S95 L96 I97 R98 G99 K100 E101 A102 L103 E104 K105 Q106 L107 E108 H109 I110 R111 K112 D113 I114 A115 L116 N117 K118 M119 S120

T121 E122 I123 R124 C125 T126 R127 P128 S129 R130 E131 R132 G133 R134 D135 G136 A137 D138 N139 V140 M141 E142 K143 E144 F145 R146 H147 L148 H149 Q150 L151 K152 K153 A154 L155 E156 L157 Q158 L159 R160 S161 V162 Q163 K164 Q165 L166 Q167 V168 L169 D170 Q171 C172 R173 K174 R175 L176 S177 A178 V179 I180

Q181 E182 R183 N184 ARG VAL LEU ASP LEU LEU CYS HIS ALA VAL SER SER VAL ASN GLY ARG ALA SER ARG GLY GLY GLY ARG VAL SER ARG GLN ASP LYS THR MET THR PHE GLY GLY ASN GLY MET GLY TYR THR ARG GLN VAL ASN GLY ASN VAL ALA GLU LEU LEU GLY THR GLY ALA

SER PRO PRO ASP ALA GLU ASN ARG SER GLY THR PRO PRO PRO ASP PRO LEU GLY PRO PHE T261 P262 E263 A264 A265 A266 A267 I268 A269 Q270 A271 R272 E273 A274 R275 Q276 R277 S278 Q279 F280 L281 R282 K283 D284 I285 R286 D287 A288 I289 E290 N291 T292 Q293 Q294 L295 Q296 Q297 A298 A299 H300

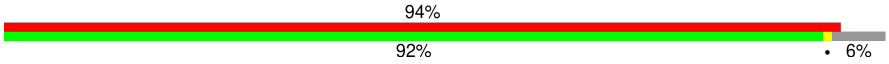
R301 A302 V303 N304 D305 G306 L307 N308 Q309 K310 V311 A312 E313 T314 I315 T316 L317 K318 Q319 H320 L321 T322 V323 A324 A325 G326 E327 N328 R329 H330 S331 I332 H333 R334 A335 Q336 R337 W338 Y339 D340 S341 T342 E343 K344 A345 L346 G347 Y348 T349 I350 G351 P352 E353 L354 Q355 S356 D357 L358 E359 T360

R361 E362 K363 L364 T365 R366 P367 I368 V369 R370 V371 F372 Q373 R374 H375 P376 G377 T378 N379 L380 P381 E382 A383 Q384 G385 I386 I387 R388 G389 A390 S391 G392 L393 D394 E395 S396 L397 L398 R399 T400 S401 R402 N403 I404 G405 L406 L407 Q408 L409 A410 Q411 G412 R413 L414 Q415 G416 D417 I418 R419 H420

K421 H422 A423 G424 A425 S426 V427 D428 S429 A430 I431 V432 R433 G434 R435 R436 R437 L438 A439 N440 H441 R442 W443 V444 M445 G446 SER VAL

• Molecule 2: Coiled-coil domain-containing protein 105

Chain 1H:



MET MET SER THR ARG SER ARG THR GLN ILE PRO LEU ALA THR A15 T16 V17 G18 P19 Q20 S21 W22 S23 D24 A25 T26 V27 K28 E29 I30 K31 I32 S33 Q34 A35 A36 V37 E38 K39 T40 D41 T42 G43 Q44 E45 V46 G47 R48 S49 F50 D51 A52 L53 P54 S55 L56 R57 D58 N59 C60

A61 Q62 Q63 S64 N65 T66 V67 V68 H69 Q70 Y71 V72 R73 E74 C75 R76 I77 S78 L79 V80 K81 L82 R83 D84 S85 F86 L87 E88 T89 N90 E91 E92 V93 K94 S95 L96 I97 R98 G99 K100 E101 A102 L103 E104 K105 Q106 L107 E108 H109 I110 R111 K112 D113 I114 A115 L116 N117 K118 M119 S120

T121 E122 I123 R124 C125 T126 R127 P128 S129 R130 E131 R132 G133 R134 D135 G136 A137 D138 N139 V140 M141 E142 K143 E144 F145 R146 H147 L148 H149 Q150 L151 K152 K153 A154 L155 E156 L157 Q158 L159 R160 S161 V162 Q163 K164 Q165 L166 Q167 V168 L169 D170 Q171 C172 R173 K174 R175 L176 S177 A178 V179 I180

Q181 E182 R183 N184 R185 V186 L187 D188 L189 L190 C191 H192 A193 V194 S195 S196 V197 N198 GLY ARG ALA SER ARG GLY GLY GLY ARG VAL SER ARG Q211 D212 K213 T214 M215 T216 F217 G218 G219 N220 G221 M222 G223 Y224 T225 R226 Q227 V228 N229 G230 N231 V232 A233 E234 L235 L236 G237 T238 G239 A240

S241 P242 P243 D244 A245 E246 N247 R248 S249 G250 T251 P252 P253 P254 D255 P256 L257 G258 P259 P260 T261 P262 E263 A264 A265 A266 A267 I268 A269 Q270 A271 R272 E273 A274 R275 Q276 R277 S278 Q279 F280 L281 R282 K283 D284 I285 R286 D287 A288 I289 E290 N291 T292 Q293 Q294 L295 Q296 Q297 A298 A299 H300

R301 A302 V303 N304 D305 G306 L307 N308 Q309 K310 V311 A312 E313 T314 I315 T316 L317 K318 Q319 H320 L321 T322 V323 A324 A325 G326 E327 N328 R329 H330 S331 I332 H333 R334 A335 Q336 R337 W338 Y339 D340 S341 T342 E343 K344 A345 L346 G347 Y348 T349 I350 G351 P352 E353 L354 Q355 S356 D357 L358 E359 T360

R361 E362 K363 L364 T365 R366 P367 I368 V369 R370 V371 F372 Q373 R374 H375 P376 G377 T378 N379 L380 P381 E382 A383 Q384 G385 I386 I387 R388 G389 A390 A391 G392 L393 D394 E395 S396 L397 L398 R399 T400 S401 R402 N403 I404 G405 L406 L407 Q408 L409 A410 Q411 G412 R413 L414 Q415 G416 D417 I418 R419 H420

K421 H422 A423 G424 A425 S426 V427 D428 S429 A430 I431 V432 R433 G434 R435 R436 R437 L438 A439 N440 H441 R442 W443 V444 M445 G446 SER VAL

• Molecule 3: Coiled-coil domain-containing protein 81

Chain 1K:

M1 T2 E3 V4 L5 S6 E7 L8 V9 S10 D11 A12 K13 R14 H15 K16 F17 S18 T19 I20 P21 K22 L23 S24 D25 D26 D27 I28 V29 S30 V31 W32 E33 N34 V35 A36 N37 F38 V39 E40 R41 H42 M43 A44 L45 Q46 K47 G48 V49 Q50 I51 H52 G53 L54 G55 T56 F57 T58 F59 T60

Q61 K62 K63 I64 D65 I66 G67 N68 N69 K70 F71 I72 L73 I74 Q75 R76 P77 V78 F79 V80 L81 S82 E83 K84 F85 A86 Q87 T88 H89 R90 L91 S92 Y93 T94 K95 H96 F97 T98 S99 G100 Q101 V102 P103 I104 V105 Q106 L107 N108 F109 A110 V111 L112 S113 N114 E115 S116 P117 F118 D119 R120

D121 S122 V123 E124 G125 C126 V127 R128 E129 V130 L131 Q132 A133 L134 S135 R136 A137 V138 Q139 S140 K141 R142 N143 V144 E145 F146 S147 F148 T149 G150 I151 G152 R153 L154 T155 I156 R157 D158 S159 K160 V161 K162 M163 K164 F165 Y166 K167 D168 F169 L170 T171 M172 S173 D174 G175 SER GLY HIS LEU VAL

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

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

PRO SER PRO ARG PRO GLN SER ARG GLY LEU LYS GLY THR PRO SER PRO PRO PRO GLY LYS PRO PRO SER PRO LYS GLU GLU LEU PRO PRO PRO ARG LEU ALA ALA GLU ILE ARG GLU SER LEU ALA ASN GLU ALA GLU ALA MET GLU ARG ALA GLU SER ALA SER CYS SER HIS ALA HIS

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

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

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

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

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

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

• Molecule 3: Coiled-coil domain-containing protein 81

Chain 1L: 25% 25% 75%

M1 T2 E3 V4 L5 S6 E7 L8 V9 S10 D11 A12 K13 R14 H15 K16 F17 S18 T19 I20 P21 K22 L23 S24 D25 D26 D27 I28 V29 S30 V31 W32 E33 N34 V35 A36 N37 F38 V39 E40 R41 H42 M43 A44 L45 Q46 K47 G48 V49 Q50 I51 H52 G53 L54 G55 T56 F57 T58 F59 T60

Q61 K62 K63 I64 D65 I66 G67 N68 N69 K70 F71 I72 L73 I74 Q75 R76 P77 V78 F79 V80 L81 S82 E83 K84 F85 A86 Q87 T88 H89 R90 L91 S92 Y93 T94 K95 H96 F97 T98 S99 G100 Q101 V102 P103 I104 V105 Q106 L107 N108 F109 A110 V111 L112 S113 N114 E115 S116 P117 F118 D119 R120

D121 S122 V123 E124 G125 C126 V127 R128 E129 V130 L131 Q132 A133 L134 S135 R136 A137 V138 Q139 S140 K141 R142 N143 V144 E145 F146 S147 F148 T149 G150 T151 G152 R153 L154 T155 I156 R157 D158 S159 K160 V161 K162 M163 K164 F165 Y166 K167 D168 F169 L170 T171 M172 M173 D174 G175 SER GLY HIS LEU VAL

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

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

PRO SER PRO ARG PRO GLN SER ARG GLY LEU LYS GLY THR PRO SER PRO PRO PRO GLY LYS PRO PRO SER PRO LYS GLU GLU LEU PRO PRO PRO ARG LEU ALA ALA GLU ILE ARG GLU SER LEU ALA ASN GLU ALA GLU ALA MET GLU ARG ALA GLU SER ALA SER CYS SER HIS ALA HIS

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

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

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

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

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

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

- Molecule 3: Coiled-coil domain-containing protein 81

Chain 1M: 25% 25% 75%

M1 T2 E3 V4 L5 S6 E7 L8 V9 S10 D11 A12 K13 R14 H15 K16 F17 S18 T19 I20 P21 K22 L23 S24 D25 D26 D27 I28 V29 S30 V31 W32 E33 N34 V35 A36 N37 F38 V39 E40 R41 H42 M43 A44 L45 Q46 K47 G48 V49 Q50 I51 H52 G53 L54 G55 T56 F57 T58 F59 T60

Q61 K62 K63 I64 D65 I66 G67 N68 M69 K70 F71 I72 L73 I74 Q75 R76 P77 V78 F79 V80 L81 S82 E83 K84 F85 A86 Q87 T88 H89 R90 L91 S92 Y93 T94 K95 H96 F97 T98 S99 G100 Q101 V102 P103 I104 V105 Q106 L107 N108 F109 A110 V111 L112 S113 N114 E115 S116 P117 F118 D119 R120

D121 S122 V123 E124 G125 C126 V127 R128 E129 V130 L131 Q132 A133 L134 S135 R136 A137 V138 Q139 S140 K141 R142 N143 V144 E145 F146 S147 F148 T149 G150 I151 G152 R153 L154 T155 I156 R157 D158 S159 K160 V161 K162 M163 K164 F165 Y166 K167 D168 F169 L170 T171 M172 M173 D174 G175 SER GLY HIS LEU VAL

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

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

PRO SER PRO ARG PRO GLN SER ARG GLY LEU LYS GLY THR PRO SER PRO PRO PRO GLY LYS PRO PRO SER PRO LYS GLY GLU LEU PRO PRO PRO ARG LEU ALA ALA GLU ILE ARG GLU SER LEU ALA ASN GLU ALA GLU ALA MET GLU ARG ALA GLU SER ALA SER CYS SER HIS ALA HIS

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

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

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

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

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

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

- Molecule 3: Coiled-coil domain-containing protein 81

Chain 1v: 30% 29% 70%

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

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

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

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

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

PRO SER PRO ARG PRO GLN SER ARG GLY LEU LYS GLY THR PRO SER PRO PRO PRO GLY LYS PRO PRO SER PRO LYS GLY GLU LEU PRO PRO ARG LEU ALA ALA GLU ILE ARG GLU SER LEU ALA ASN GLU ALA GLU ALA MET GLU ARG ALA GLU SER ALA SER CYS SER HIS ALA HIS

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

LYS HIS HIS SER GLN LYS ILE ALA ALA PHE ASN LEU GLY VAL SER GLU ALA ILE LYS ASN LYS GLN LYS GLU ARG SER THR GLU PHE ASN ARG SER TYR VAL PHE GLN ASN ARG ALA ARG THR PRO P463 R464 F465 L466 K467 Q468 E469 E470 Y471 A472 T473 D474 L475 G476 S477 Q478 V479 E480

A481 K482 A483 V484 D485 K486 I487 K488 R489 R490 Q491 D492 T493 D494 F495 L496 E497 R498 L499 E500 Q501 V502 Q503 L504 A505 E506 E507 L508 S509 A510 Q511 R512 E513 R514 Y515 L516 R517 D518 K519 H520 Q521 Q522 T523 D524 M525 Y526 R527 K528 A529 L530 S531 A532 Q533 V534 R535 F536 K537 P538 L539 P540

L541 P542 G543 A544 V545 ALA ASP SER LYS GLU PRO ILE PHE GLY LYS PHE ASP ALA T559 N560 E561 Q562 L563 A564 E565 R566 R567 R568 R569 A570 I571 E572 V573 F574 Q575 D576 Q577 I578 S579 T580 V581 E582 N583 R584 R585 K586 N587 N588 L589 T590 N591 H592 V593 K594 T595 Q596 N597 D598 E599 T600

D601 M602 L603 E604 K605 T606 R607 R608 E609 L610 I611 A612 D613 R614 A615 A616 R617 F618 E619 Q620 A621 F622 Q623 T624 R625 K626 S627 L628 E629 E630 T631 W632 K633 E634 A635 D636 A637 L638 K639 K640 S641 R642 E643 E644 E645 Q646 V647 L648 K649 L650 Q651 S652 S653 G654 I655 L656 L657 H658 E659 Q660

C661 D662 Q663 Y664 H665 R666 C667 E668 Q669 C670 L671 R672 V673 L674 K675 M676 C677 G678 E679 S680 N681 I682 TRP SER GLU SER ARG TYR ILE PRO GLY SER ARG LEU ILE MET

- Molecule 3: Coiled-coil domain-containing protein 81

Chain 1w: 12% 12% 88%

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

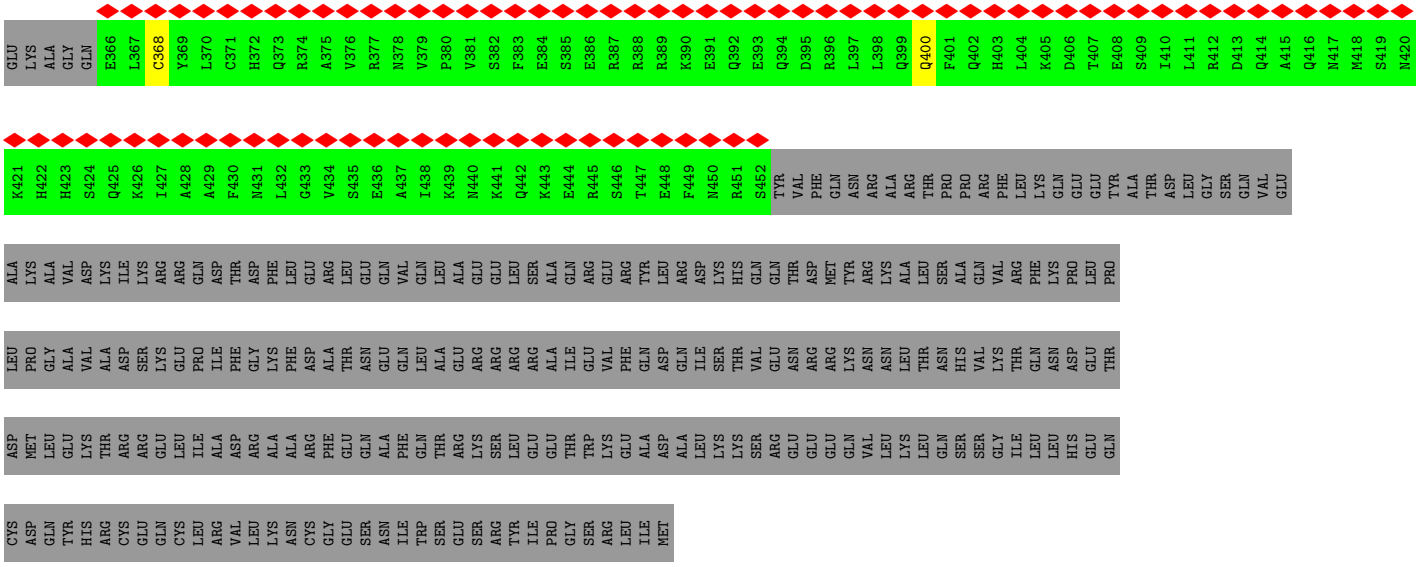
GLN LYS LYS ILE ASP ILE GLY ASN ASN LYS PHE ILE LEU ILE GLN ARG PRO VAL PHE VAL LEU SER GLU LYS PHE ALA GLN THR HIS ARG LEU SER TYR THR LYS HIS PHE THR SER GLY GLN VAL PRO ILE VAL GLN LEU ASN PHE ALA VAL LEU SER ASN GLU SER PRO PHE ASP ARG

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

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

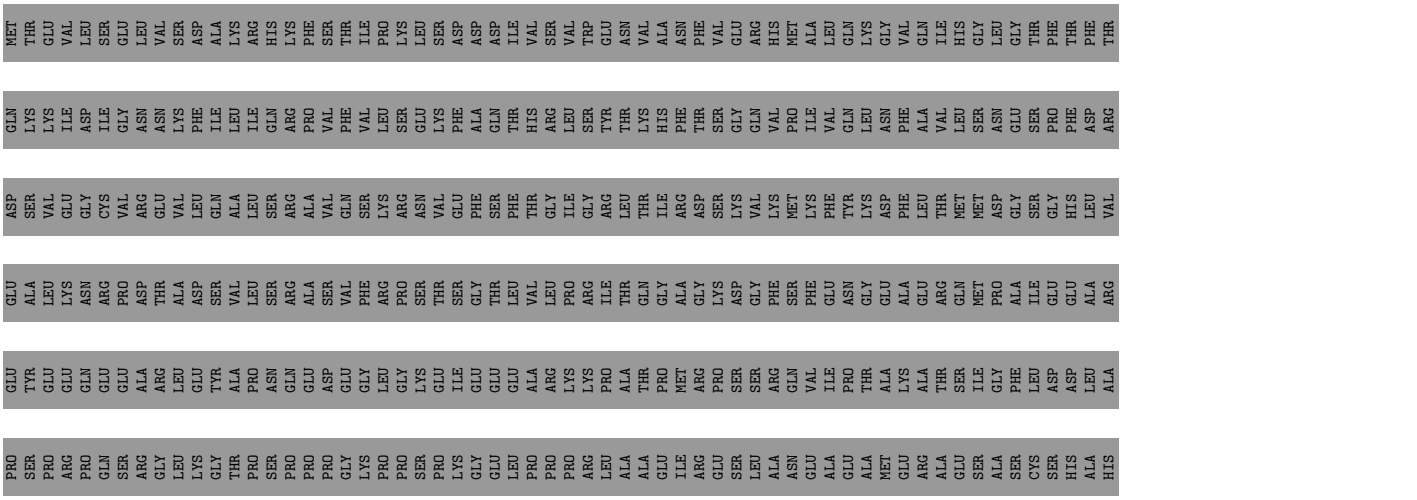
GLU TYR GLU GLU GLN GLU GLU ALA ARG LEU GLU TYR ALA PRO ASN GLN GLU ASP GLU GLY LEU GLY LYS GLU ILE GLY GLU GLU GLU ARG LYS LYS PRO ALA THR PRO MET ARG PRO SER SER ARG GLN VAL ILE PRO THR ALA LYS ALA THR SER ILE GLY PHE LEU ASP ASP LEU ALA

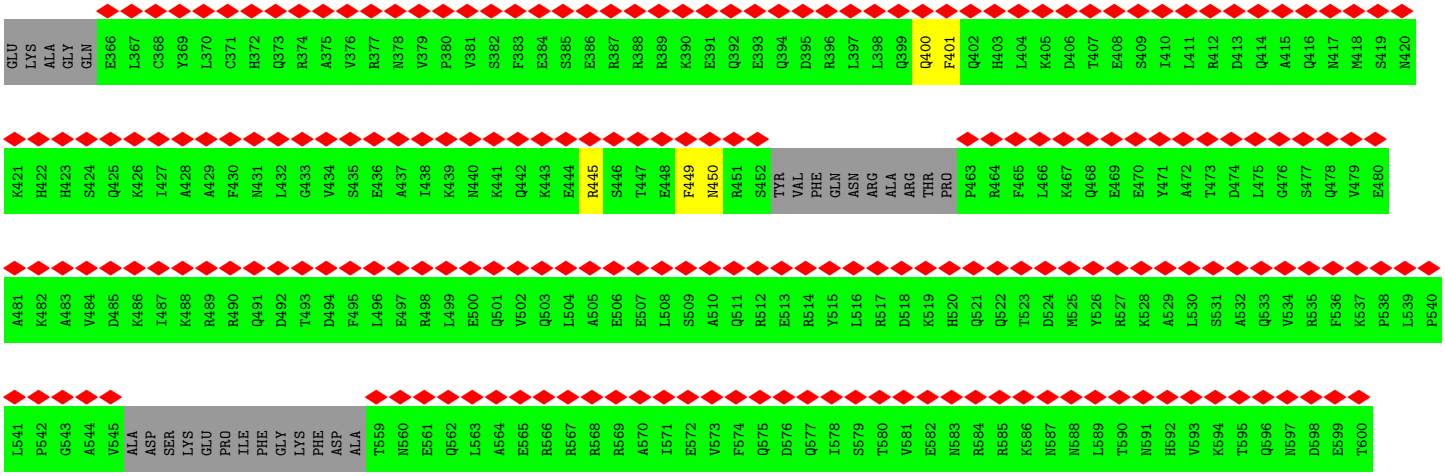
PRO SER PRO ARG PRO GLN SER ARG GLY LEU LYS GLY THR PRO SER PRO PRO PRO GLY LYS PRO PRO SER PRO LYS GLY GLU LEU PRO PRO ARG LEU ALA ALA GLU ILE ARG GLU SER LEU ALA ASN GLU ALA GLU ALA MET GLU ARG ALA GLU SER ALA SER CYS SER HIS ALA HIS



- Molecule 3: Coiled-coil domain-containing protein 81

Chain 1x:





D601 M602 L603 E604 K605 T606 R607 R608 E609 L610 I611 A612 D613 R614 A615 A616 R617 F618 E619 Q620 A621 F622 Q623 T624 R625 K626 S627 L628 E629 E630 T631 W632 K633 E634 A635 D636 A637 L638 LYS LYS SER ARG GLU GLU GLU GLN VAL LEU LYS LEU GLN SER SER GLY ILE LEU LEU HIS GLU GLN

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

• Molecule 3: Coiled-coil domain-containing protein 81

Chain 1y: 28% 28% 72%

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

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

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

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

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

PRO SER PRO ARG PRO GLN SER ARG GLY LEU LYS GLY THR PRO SER PRO PRO PRO GLY LYS PRO PRO SER PRO LYS GLY GLU LEU PRO PRO PRO ARG LEU ALA ALA GLU ILE ARG GLU SER LEU ALA ASN GLU ALA GLU ALA MET GLU ARG ALA GLU SER ALA SER CYS SER HIS ALA HIS

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

LYS HIS HIS SER GLN LYS ILE ALA ALA PHE ASN LEU GLY VAL SER GLU ALA ILE LYS ASN LYS GLN LYS GLU ARG SER THR GLU PHE ASN ARG SER TYR VAL PHE GLN ASN ARG ALA ARG THR PRO PRO ARG PHE LEU LYS GLN GLU GLU Y471 A472 T473 D474 L475 G476 S477 Q478 V479 E480

A481 K482 A483 V484 D485 K486 I487 K488 R489 R490 Q491 D492 T493 D494 F495 L496 E497 R498 L499 E500 Q501 V502 Q503 L504 A505 E506 E507 L508 S509 A510 Q511 R512 E513 R514 Y515 L516 R517 D518 K519 H520 Q521 Q522 T523 D524 M525 Y526 R527 K528 A529 L530 S531 A532 Q533 V534 R535 F536 K537 P538 L539 P540

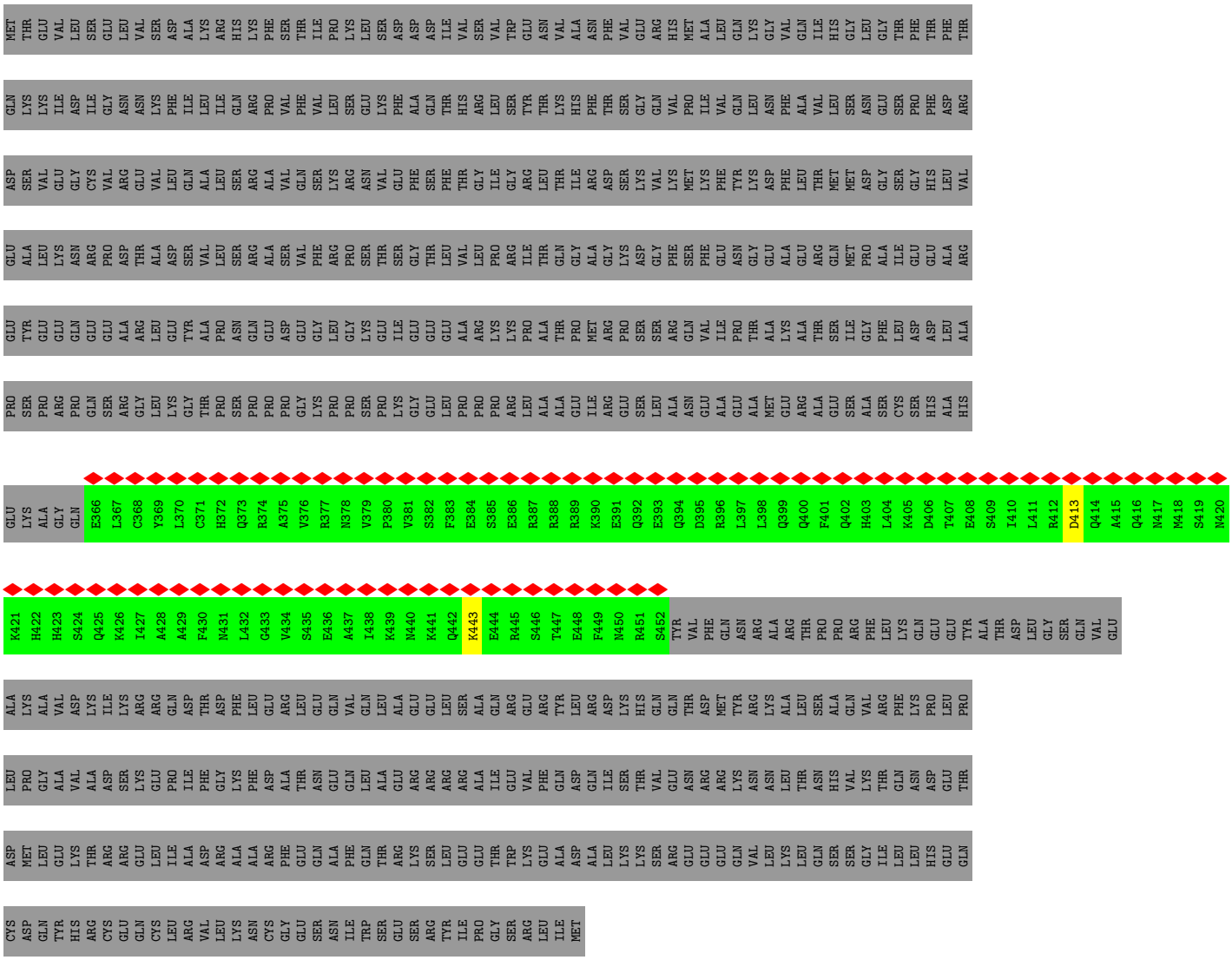
L541 P542 G543 A544 VAL ALA ASP SER LYS GLU PRO ILE PHE GLY LYS PHE ASP ALA T559 N560 E561 Q562 L563 A564 E565 R566 R567 R568 R569 A570 I571 E572 V573 F574 Q575 D576 Q577 I578 S579 T580 V581 E582 N583 R584 R585 K586 N587 N588 L589 T590 N591 H592 V593 K594 T595 Q596 N597 D598 E599 T600

D601 M602 L603 E604 K605 T606 R607 R608 E609 L610 I611 A612 D613 R614 A615 A616 R617 F618 E619 Q620 A621 F622 Q623 T624 R625 K626 S627 L628 E629 E630 T631 W632 K633 E634 A635 D636 A637 L638 L639 K640 S641 R642 E643 E644 E645 Q646 V647 L648 K649 L650 Q651 S652 S653 G654 I655 L656 L657 H658 E659 Q660

C661 D662 Q663 Y664 H665 R666 C667 E668 Q669 C670 L671 R672 V673 L674 K675 N676 C677 G678 E679 S680 N681 I682 TRP SER GLU SER ARG TYR ILE PRO GLY SER ARG LEU ILE MET

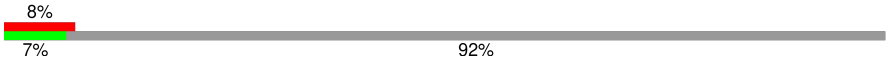
• Molecule 3: Coiled-coil domain-containing protein 81

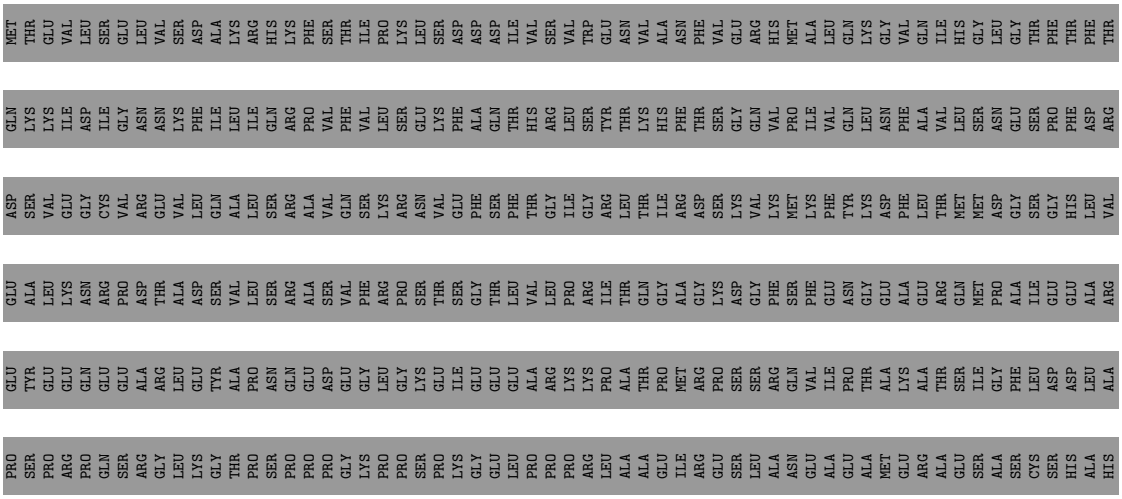
Chain 1z: 12% 12% 88%



• Molecule 3: Coiled-coil domain-containing protein 81

Chain 2a:





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

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

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

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

ASP MET LEU GLU LYS THR ARG ARG GLU LEU ILE ALA ASP ARG ALA ALA ARG PHE E619 Q620 A621 F622 Q623 T624 R625 K626 S627 S628 L629 E630 T631 W632 K633 E634 A635 D636 A637 L638 K639 K640 S641 R642 E643 E644 E645 Q646 V647 L648 K649 L650 Q651 S652 S653 G654 I655 L656 L657 H658 E659 Q660

C661 D662 Q663 Y664 H665 R666 C667 E668 Q669 C670 L671 R672 VAL LEU LYS ASN CYS GLY GLU SER ASN ILE TRP SER GLU SER ARG TYR ILE PRO GLY SER ARG LEU ILE MET

- Molecule 4: FAM166C

Chain 1P: 57% 100%

MET S2 R3 S4 A5 L8 T11 H12 Q13 R20 L21 M22 H28 C29 M32 K33 F34 D35 Y36 G37 E38 G41 N42 A43 D50 Y51 R52 N68 S59 K60 T61 N65 Q68 F69 D78 D85 R90 P95 Q96 Y97 S98 L99 S100 N101 H104

D105 E108 D109 I110 N111 D114 K115 E119 E122 K125 D126 T130 V131 G132 R133 V134 N135 E136 F137 L138 R141 Q144 E145 M146 Y147 H148 Q149 D150 S151 A152 L153 I154 D155 E156 H157 V158 D159 M160 R161 E162 E163 A164 S165 T166 N167 M168 A169 R170 N171 I172 P173 V174

E175 R176 M177 S178 I179 P180 P181 I182 R183 T184 F185 S186 K187 S188 S189 T190 V191 R192 D193 R194 A195 M196 R197 D198 V199 H200 Y201 E202 H203 R204

- Molecule 4: FAM166C

Chain 1Q: 49% 67% 32%

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

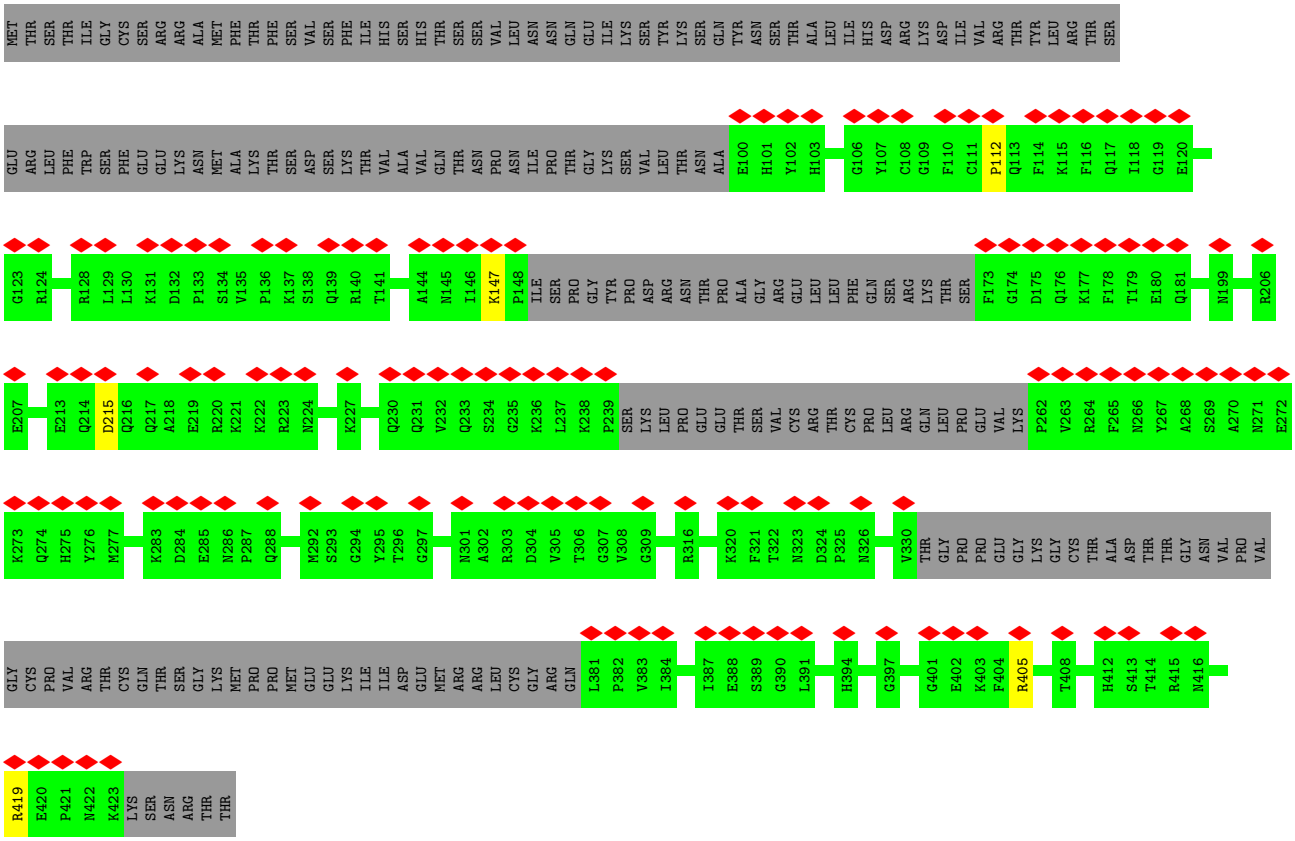
THR ASN TYR SER ASN GLY G67 Q68 Y73 N76 P77 D78 G82 A83 R84 D85 R86 T87 R88 E89 R90 F91 R92 T93 T94 P95 Q96 Y97 S98 L99 S100 M101 H104 D105 E108 D109 D114 K115 E122 K125 D126 G132 R133 V134 N135 E136 F137 L138 I139 P140 R141

Q144 E145 M146 Y147 H148 Q149 D150 S151 A152 L153 I154 D155 E156 H157 V158 D159 M160 R161 E162 E163 A164 S165 T166 N167 M168 A169 R170 N171 I172 P173 V174 E175 R176 M177 S178 I179 P180 P181 I182 R183 T184 F185 S186 K187 S188 S189 T190 V191 R192 D193 R194 A195 M196 R197 D198 V199 H200 Y201 E202

H203 R204

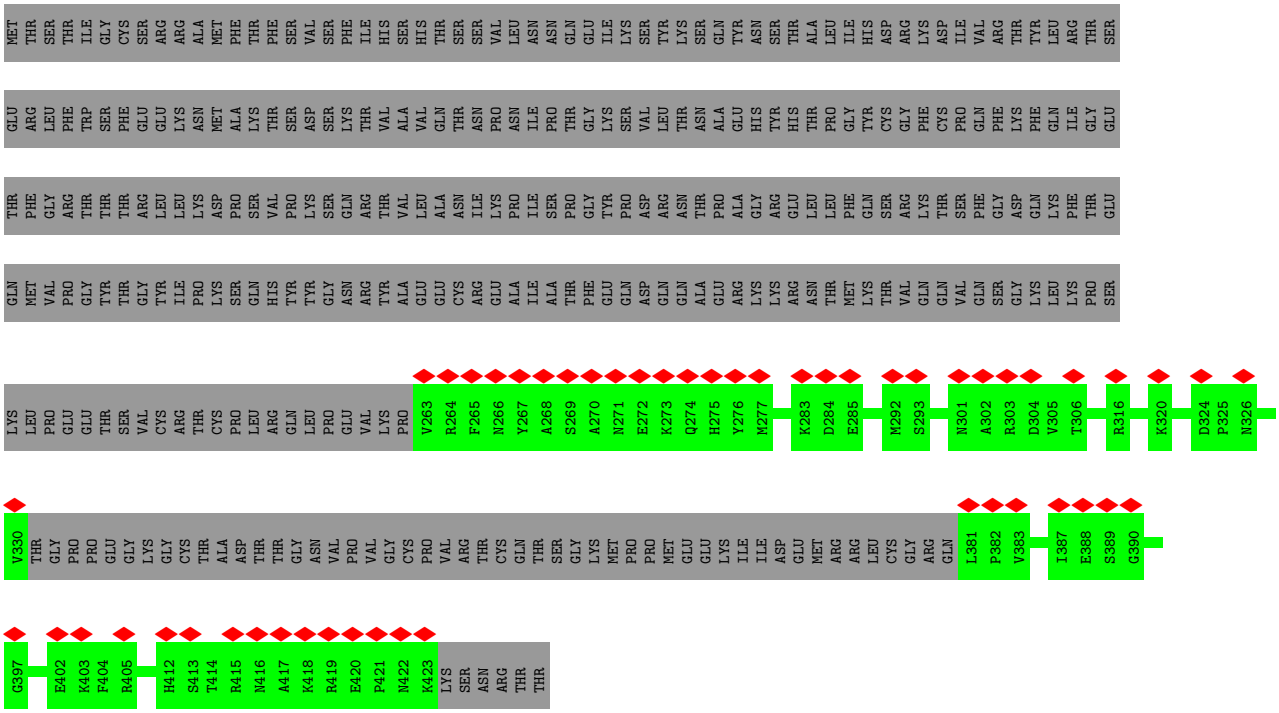
- Molecule 5: Protein FAM166B

Chain 1T:



- Molecule 5: Protein FAM166B

Chain 1U:



• Molecule 5: Protein FAM166B

Chain 1V: 33% 52% • 47%

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

GLU ARG LEU PHE TRP SER PHE GLU GLU LYS ASN MET ALA LYS THR SER ASP SER LYS THR VAL ALA VAL GLN THR ASN PRO ASN ILE PRO THR GLY LYS SER VAL LEU THR ASN ALA E100 H101 Y102 H103 T104 P105 C108 G109 F110 F114 K115 F116 Q117 I118 G119 E120 R124

R128 L129 L130 K131 D132 P133 S134 V135 P136 K137 S138 Q139 R140 T141 V142 L143 A144 N145 I146 K147 P148 ILE SER PRO GLY TYR PRO ASP ARG ASN THR PRO ALA GLY ARG GLU LEU LEU PHE GLN SER ARG LYS THR S172 F173 G174 D175 Q176 K177 F178 T179 E180 Q181 G188 K192 S193 Q194

H195 Y196 Y197 G198 E204 C205 R206 E207 E213 Q214 D215 Q216 Q217 A218 E219 R220 K221 K222 R223 N224 T225 M226 K227 T228 V229 Q230 Q231 V232 Q233 S234 G235 K236 L237 K238 P239 SER LYS LEU PRO GLU GLU THR SER VAL CYS ARG THR CYS PRO LEU ARG GLN LEU PRO GLU VAL LYS P262

V263 R264 F265 N266 Y267 A268 S269 A270 N271 E272 K273 Q274 H275 Y276 K283 D284 E285 Q288 M292 S293 G294 Y298 N301 A302 R303 D304 V305 T306 G307 N315 R316 K320 N323 D324 P325 N326 H327 P328 M329 V330 THR GLY PRO PRO GLU GLY LYS GLY CYS THR ALA ASP

THR THR GLY ASN VAL PRO VAL GLY CYS PRO VAL ARG THR CYS GLN THR SER GLY LYS MET PRO PRO MET GLU GLU LYS ILE ILE ASP GLU MET ARG ARG LEU CYS GLY ARG GLN L381 P382 V383 I384 Y385 P386 I387 E388 S389 G390 L391 V392 P393 H394 G397 G401 E402 K403 F404 R405

Y406 G407 T408 T409 H412 R415 N416 A417 K418 R419 E420 P421 N422 K423 LYS SER ASN ARG THR THR

• Molecule 5: Protein FAM166B

Chain 1W: 15% 24% 75%

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

GLU ARG LEU PHE TRP SER PHE GLU GLU LYS ASN MET ALA LYS THR SER ASP SER LYS THR VAL ALA VAL GLN THR ASN PRO ASN ILE PRO THR GLY LYS SER VAL LEU THR ASN ALA GLU HIS TYR HIS THR PRO GLY TYR CYS GLY F110 K115 F116 Q117 E120 R124 T125

R128 K131 D132 P133 S134 V135 P136 K137 S138 Q139 R140 T141 V142 L143 A144 N145 I146 K147 P148 ILE SER PRO GLY TYR PRO ASP ARG ASN THR PRO ALA GLY ARG GLU LEU LEU PHE GLN SER ARG LYS THR S172 F173 G174 D175 Q176 K177 F178 T179 E180 Q181 G188 Y189 Q194 H195

G198 R206 E207 E213 Q214 D215 Q216 Q217 A218 E219 R220 K221 K222 R223 N224 T225 M226 K227 T228 V229 Q230 Q231 V232 Q233 S234 G235 K236 L237 K238 P239 SER LYS LEU PRO GLU GLU THR SER VAL CYS ARG THR CYS PRO LEU ARG GLN LEU PRO GLU VAL LYS PRO VAL ARG PHE ASN TYR

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

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

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

- Molecule 6: CFAP144(FAM183A)

Chain 1Y:

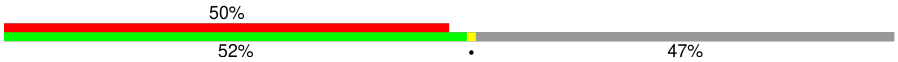
MET ALA ALA ALA GLN ALA LYS LYS PRO GLU LYS ASP P13 V14 N15 I16 V17 H18 Q19 N20 A21 I22 L23 C24 E25 T26 I27 K28 E29 E30 N31 E32 C33 Q34 R35 L36 Y37 T38 N39 Y40 S41 I42 N43 P44 F45 K46 K47 M48 Y49 T50 L51 T52 G53 K54 P55 N56 S57 L58 H59 D60

SER ALA ASP GLY GLU E66 D67 D68 N69 F70 L71 R72 I73 I74 K75 R76 S77 T78 Q79 E80 P81 G82 K83 K84 F85 E86 F87 P88 Q89 T90 E91 A92 Q93 E94 V95 G96 W97 Y98 Y99 K100 P101 L102 L103 P104 Q105 D106 R107 G108 D109 K110 R111 R116 Q117 E120 I121 T122 K123 Y124

M125 D126 E127 A128 W129 K130 Q131 K132 E133 Q134 Q135 E136 ASN LEU GLN

- Molecule 7: Outer dense fiber protein 3

Chain 1a:



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

PRO GLY PRO CYS HIS ASN PHE PRO ALA GLY VAL THR ARG LYS GLY ASN ASP GLY THR PRO LYS TYR SER LEU TYR ALA ARG SER LYS GLU LEU THR ALA PHE LYS THR PRO GLY PRO GLY SER TYR SER PRO GLU LYS ALA GLY ARG SER ALA HIS LEU HIS ALA P116 E117 H118 T119 F120

G121 S122 R123 T124 K125 G126 I127 T128 F129 D130 K131 S132 P133 A134 P135 N136 N137 Y138 S139 L140 P141 S142 I143 L144 G145 G146 R147 S148 C149 V150 K151 P152 S153 K154 P155 V156 Y157 S158 M159 R160 G161 R162 N163 K164 M165 G166 G167 F168 D169 E170 D171 L172 Q173 K174 T175 P176 G177 P178 G179 S180

Y181 D182 V183 V184 D185 P186 A187 I188 Y189 K190 N191 K192 S193 P194 M195 Y196 S197 I198 T199 G200 R201 N202 Q203 L204 P205 C206 D207 S208 T209 R210 K211 P214 G215 Q216 H217 S218 P219 E220 K221 V222 T223 V224 N225 K226 R227 M228 A229 P230 K231 F232 S233 F234 G235 H238 S239 Q240 Y241 T242

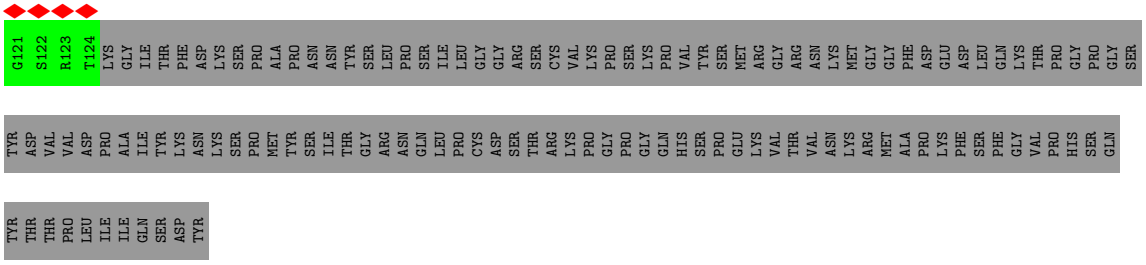
T243 P244 L245 I246 I247 Q248 S249 ASP TYR

- Molecule 7: Outer dense fiber protein 3

Chain 1b:

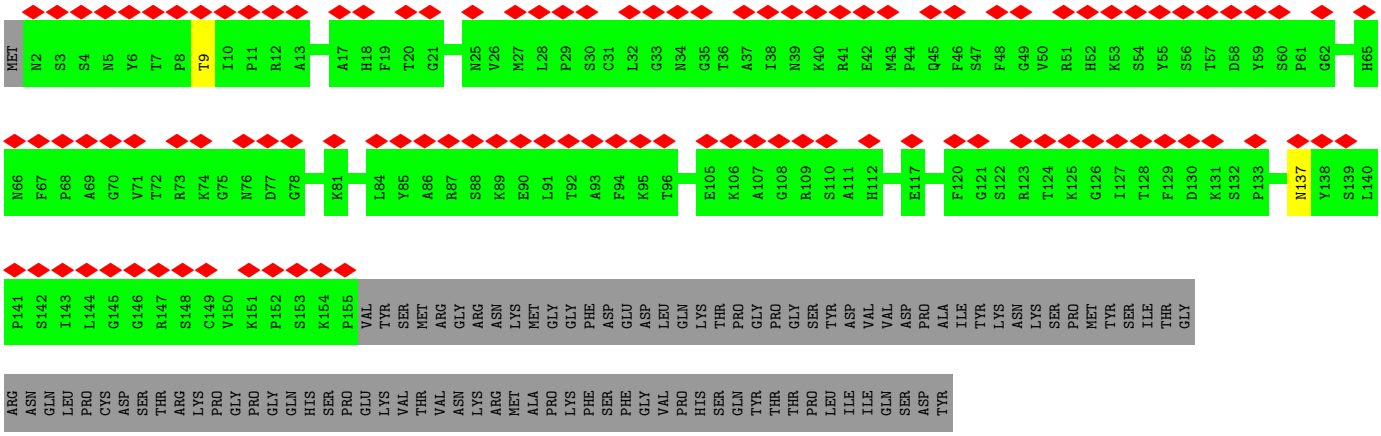
MET ASN S3 S4 N5 Y6 T7 P8 T9 I10 P11 R12 A13 P14 I15 A16 A17 H18 F19 T20 G21 P22 G23 P24 N25 V26 M27 L28 P29 S30 C31 L32 G33 N34 G35 T36 A37 I38 N39 K40 R41 E42 M43 P44 Q45 F46 S47 F48 G49 V50 R51 H52 K53 S54 Y55 S56 T57 D58 Y59 S60

P61 G62 P63 C64 H65 N66 F67 P68 A69 G70 V71 T72 R73 K74 G75 N76 D77 G78 T79 P80 K81 Y82 S83 L84 Y85 A86 R87 S88 K89 E90 L91 T92 A93 P94 K95 T96 P97 G98 P99 G100 S101 Y102 S103 P104 E105 K106 A107 G108 R109 S110 A111 H112 L113 H114 A115 P116 E117 H118 T119 F120



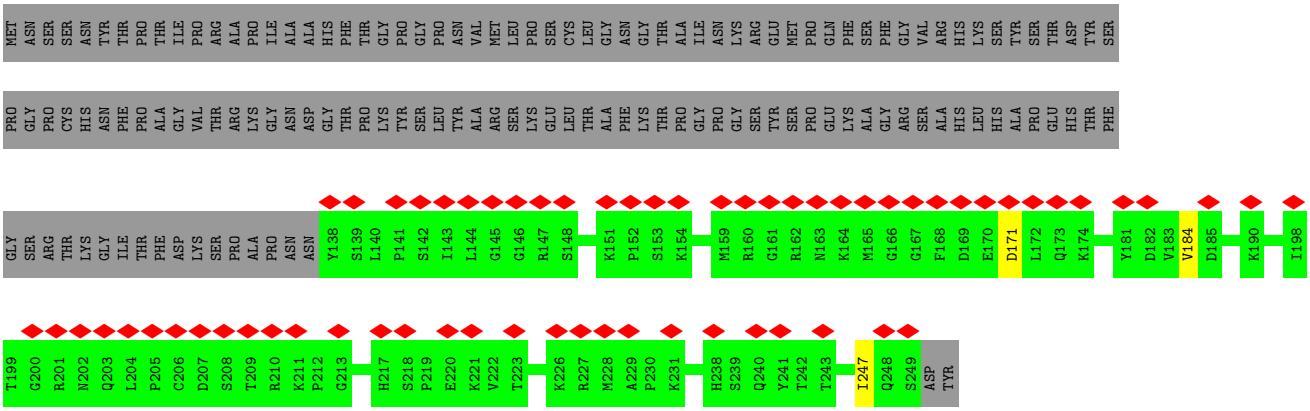
• Molecule 7: Outer dense fiber protein 3

Chain 5E:



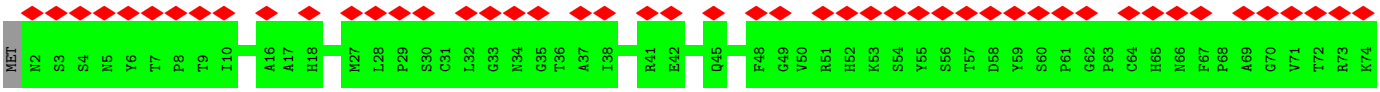
• Molecule 7: Outer dense fiber protein 3

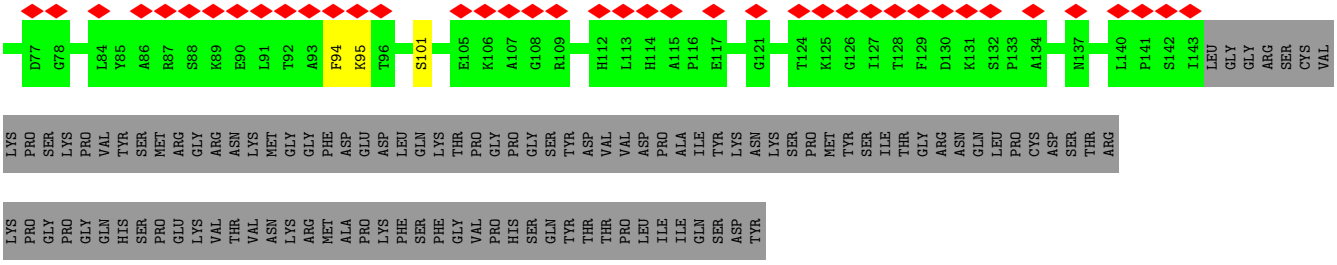
Chain 5F:



• Molecule 7: Outer dense fiber protein 3

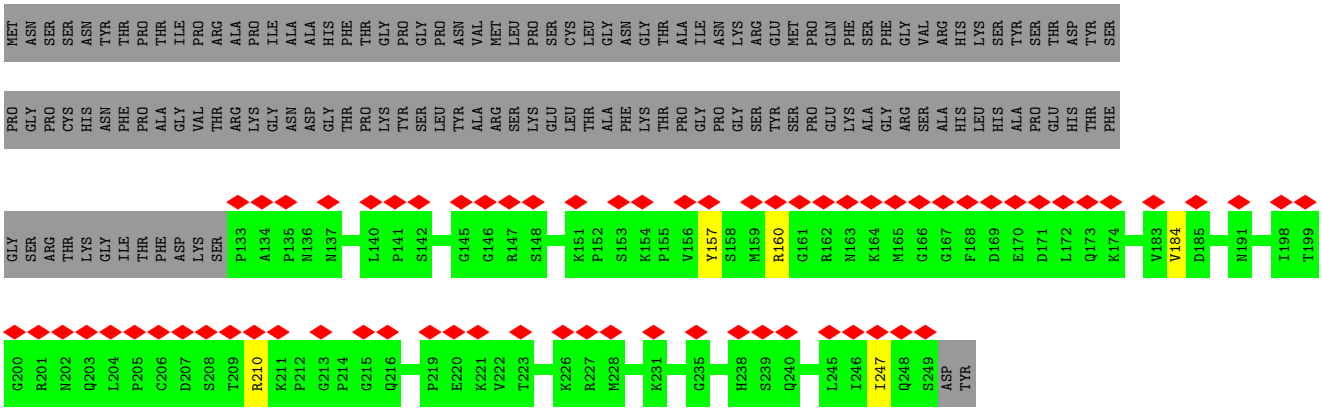
Chain 5G:





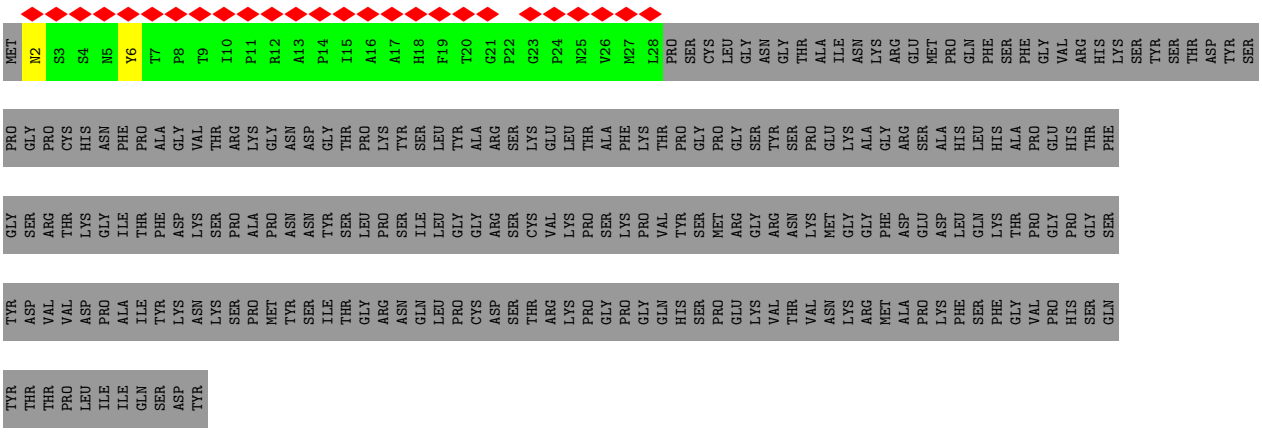
• Molecule 7: Outer dense fiber protein 3

Chain 5H:



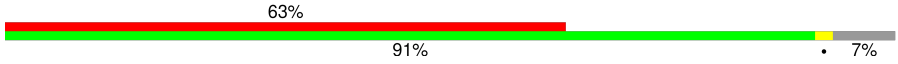
• Molecule 7: Outer dense fiber protein 3

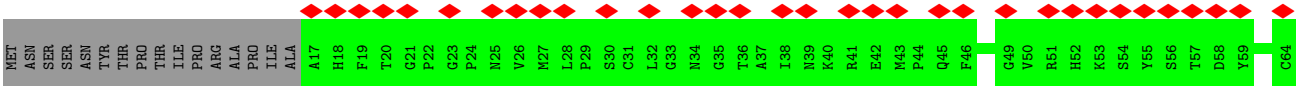
Chain 5I:

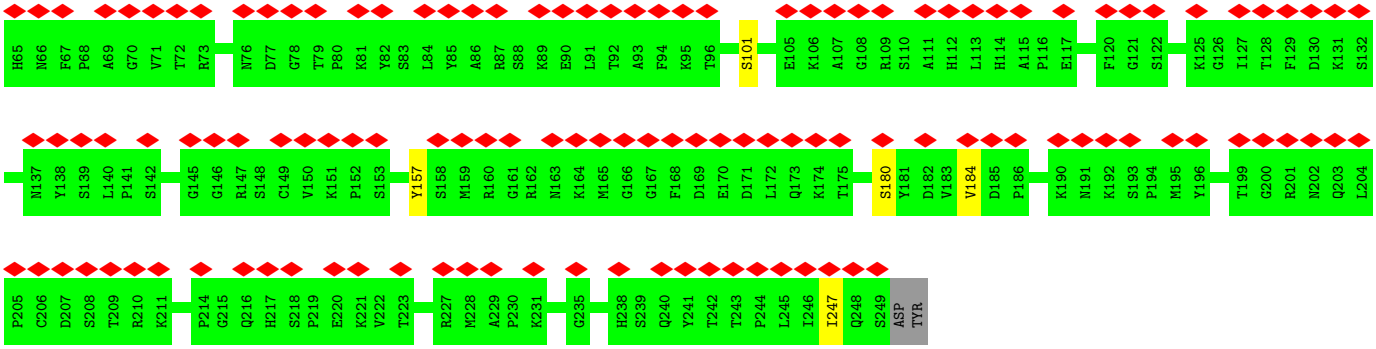


• Molecule 7: Outer dense fiber protein 3

Chain 5J:

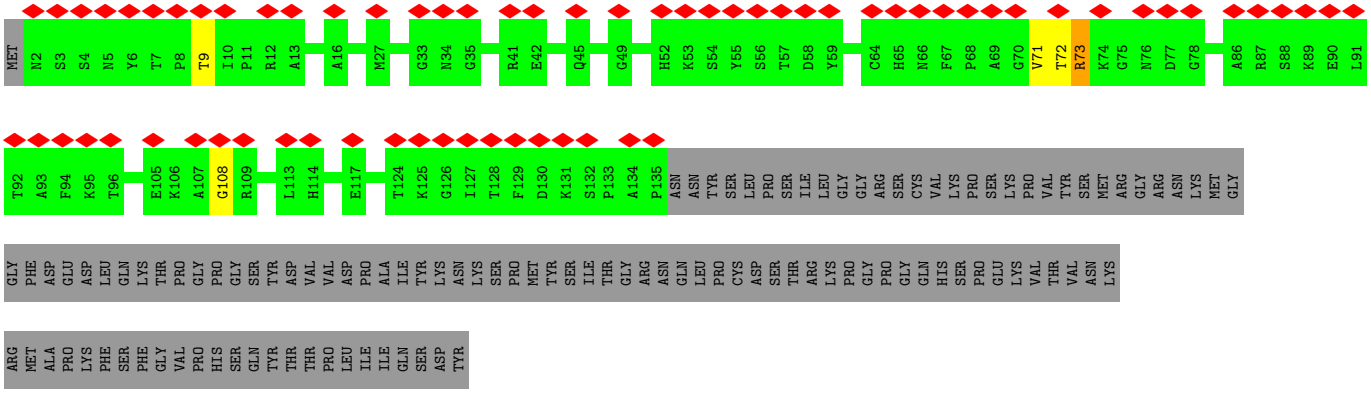






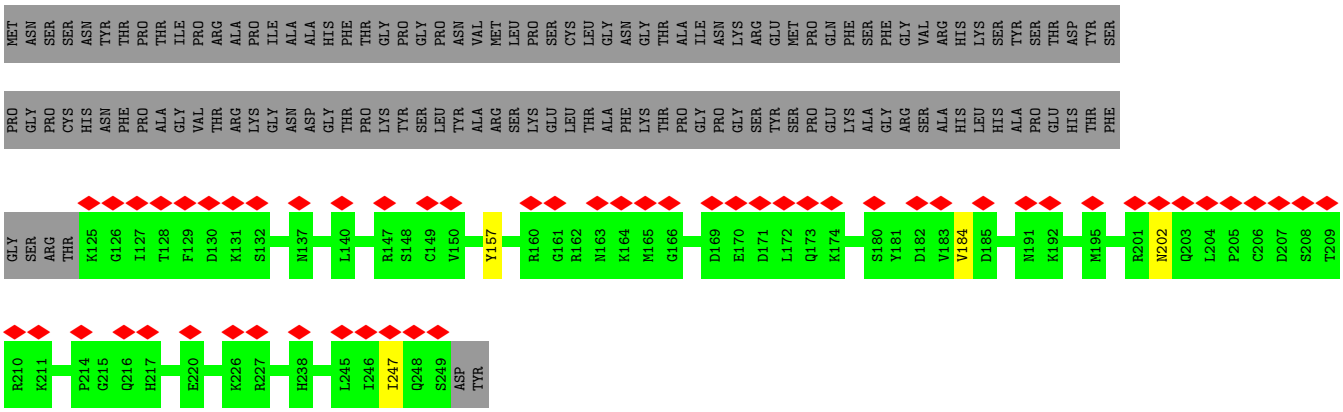
- Molecule 7: Outer dense fiber protein 3

Chain 5K:



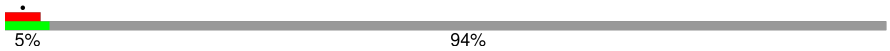
- Molecule 7: Outer dense fiber protein 3

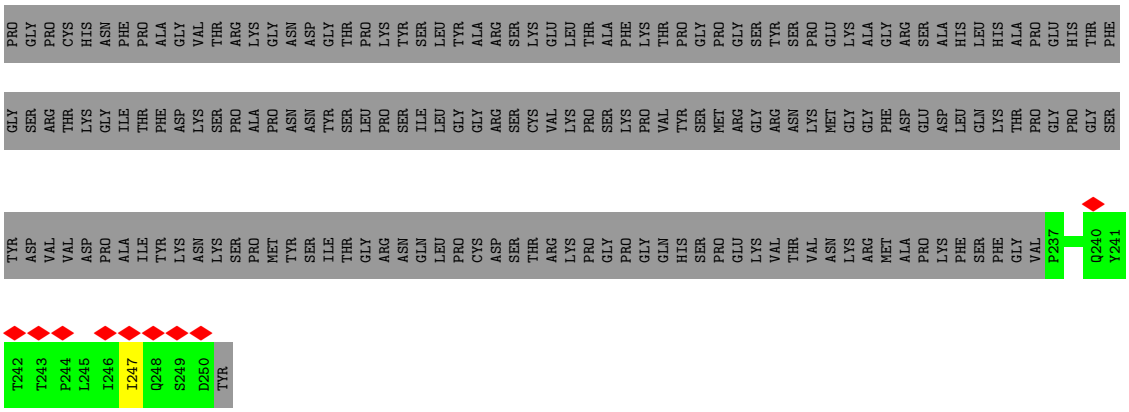
Chain 5L:



- Molecule 7: Outer dense fiber protein 3

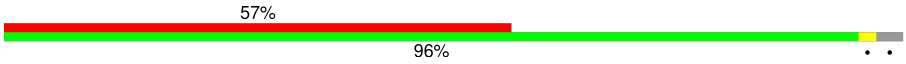
Chain 5M:

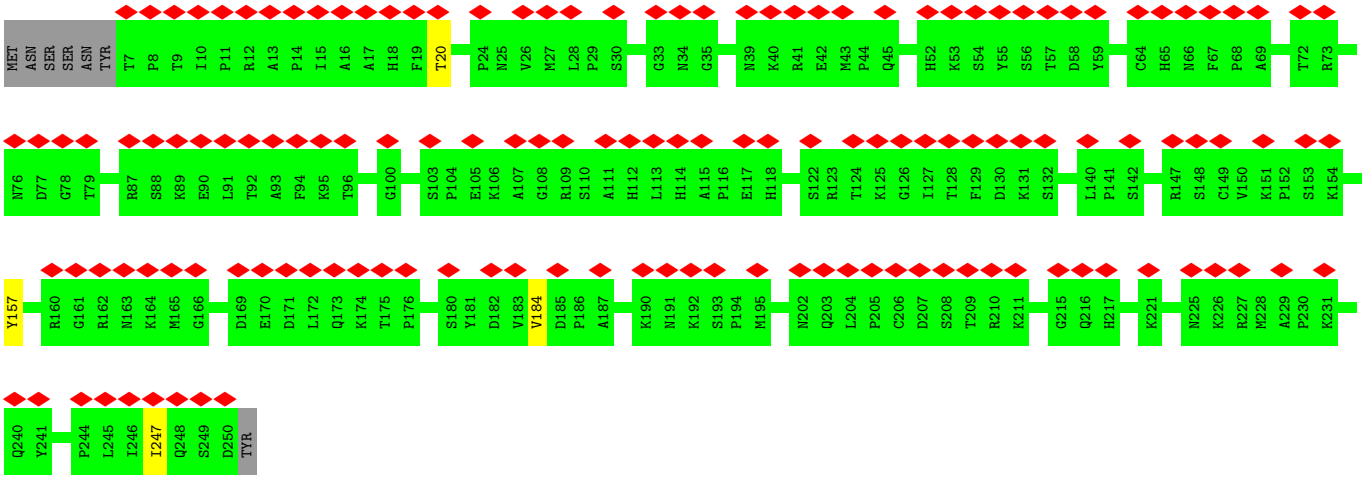




- Molecule 7: Outer dense fiber protein 3

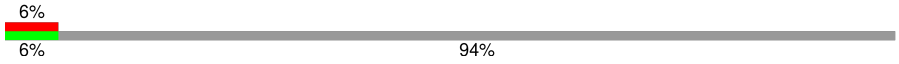
Chain 5N:

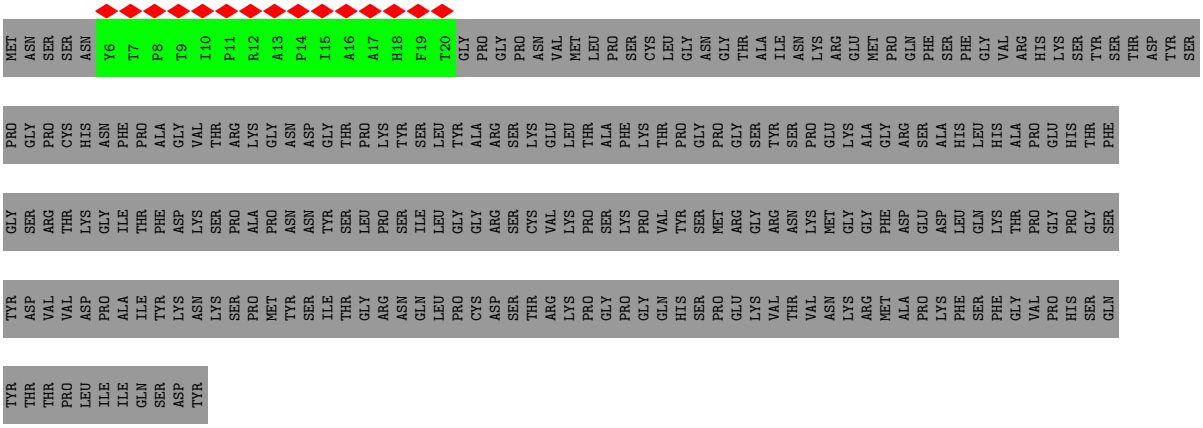




- Molecule 7: Outer dense fiber protein 3

Chain 5O:





- Molecule 8: Tex33

Chain 1d:

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

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

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

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

PHE LEU ARG LYS ALA THR PRO PRO PRO LYS ARG I252 P253 G254 P255 L256 I257 T258 A259 K260 F261 P262 P263 V264 K265 T266 S267 I268 S269 L270 D271 T272 D273 P274 M275 Y276 S277 A278 L279 G280 T281 S282 L283 K284 Q285 D286 I287 F288 N289 G290 V291 P292 H293 S294 H295 V296 K297 S298 L299 Y300

K301 S302 S303 F304 T305 Q306 D307 I308 H309 N310 K311 S312 V313 E314 V315 F316 P317 P318 K319 F320 A321 I322 Q323 R324 N325 Q326 D327 S328 K329 W330 N331 E332 D333 G334 V335 I336 R337 M338 K339 L340 Y341 K342 A343 W344 D345 A346 M347 T348 L349 E350 R351 L352 GLN ALA LYS GLY GLY GLY THR

- Molecule 9: C20Orf85

Chain 1f:

MET GLN ALA VAL ASN LEU LYS LYS ASN PRO N11 E17 R18 W19 K20 D21 H22 V23 R24 H25 E26 H27 R28 A29 W30 R31 N32 W33 P34 E35 R36 W37 G38 F39 I40 T41 N42 E43 Y44 T45 R46 MET TYR LYS ARG LEU ARG GLY GLU GLN VAL SER PRO ASP PRO GLU ASP LYS TYR

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

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

GLY ARG ASN ALA LYS GLY TYR LYS GLY ILE LEU LYS GLN PHE ASN TRP PRO MET GLN GLY ILE MET

- Molecule 9: C20Orf85

Chain 1g:

MET GLN ALA VAL ASN LEU LYS LYS ASN PRO ASN TYR VAL HIS ILE ALA GLU R18 W19 K20 D21 H22 V23 R24 H25 E26 H27 R28 A29 W30 R31 N32 E35 R36 F39 Y44 T45 R46 M47 Y48 K49 R50 L51 R52 G53 E54 Q55 V56 S57 P58 D59 P60 E61 D62 K63 Y64 F65

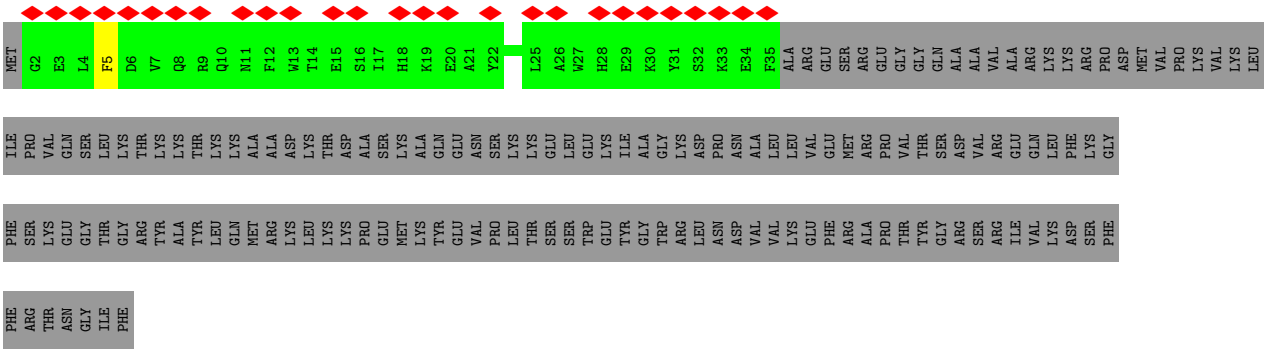
Y66 D67 D68 CYS GLU ARG ASP GLY GLU ARG GLU SER SER VAL GLY PRO ASP GLU SER ILE SER ARG ARG PHE HIS PRO SER ASP GLN SER VAL SER PRO SER HIS SER GLY ALA LYS LEU LYS HIS ALA SER ALA TYR SER ASP LEU PRO ASN ILE ILE ASN GLY SER SER TRP LYS GLU

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

ARG ASN ALA LYS GLY TYR LYS GLY ILE LEU LYS GLN PHE ASN TRP PRO MET GLN GLY ILE MET

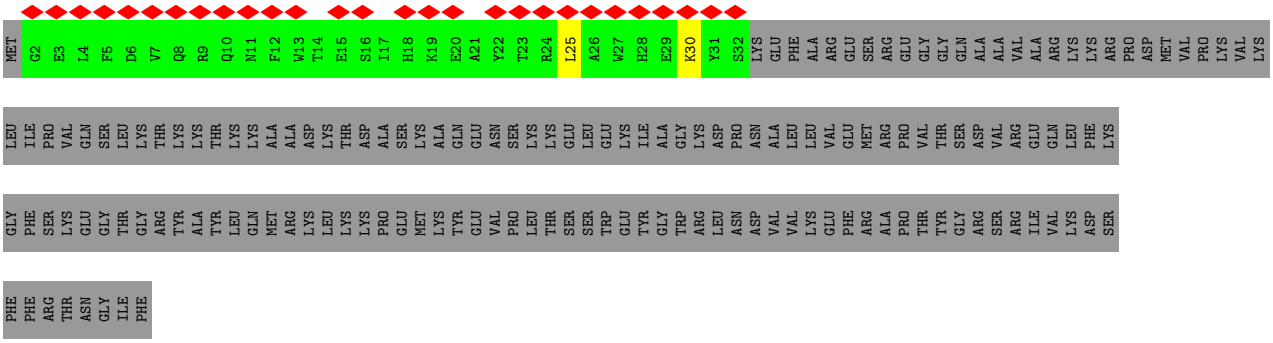
- Molecule 10: ATP6V1FNB

Chain 1i:



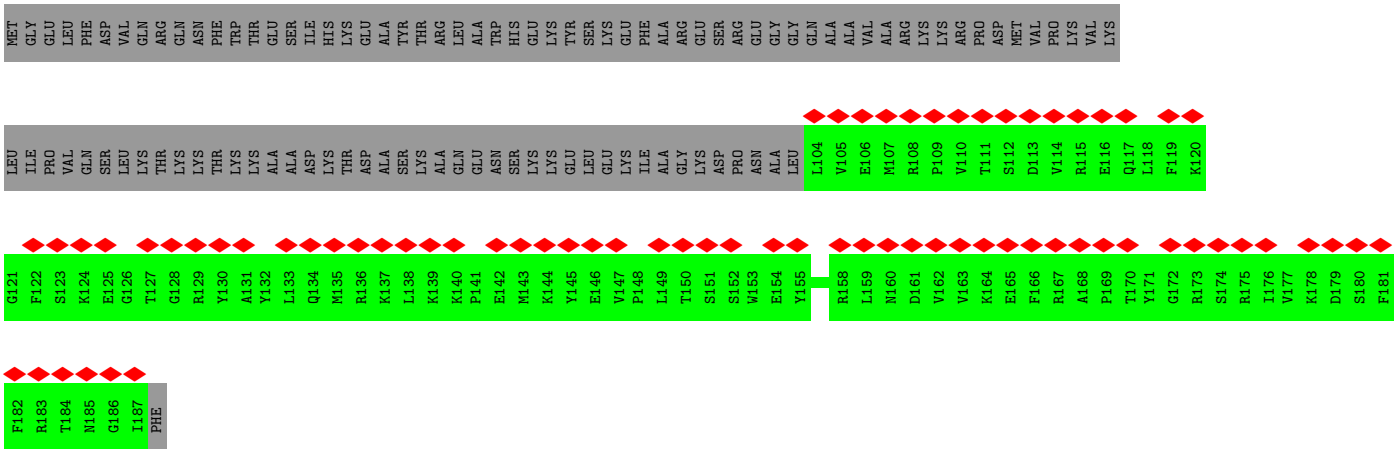
- Molecule 10: ATP6V1FNB

Chain 1j:



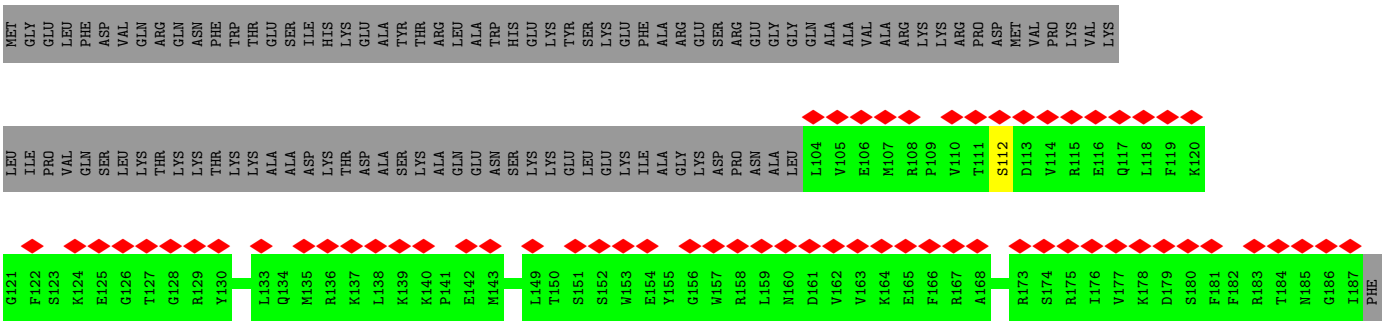
- Molecule 10: ATP6V1FNB

Chain 9M:



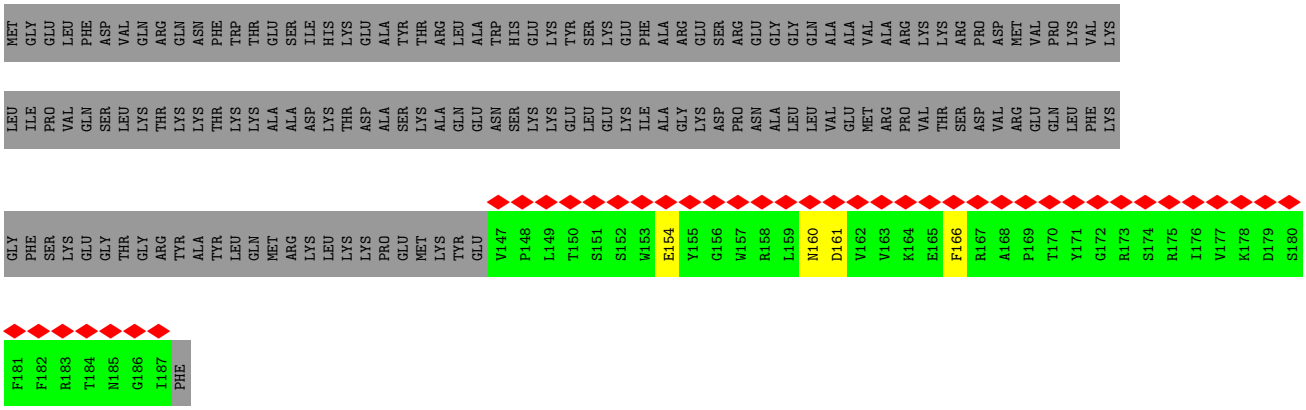
- Molecule 10: ATP6V1FNB

Chain 9N:



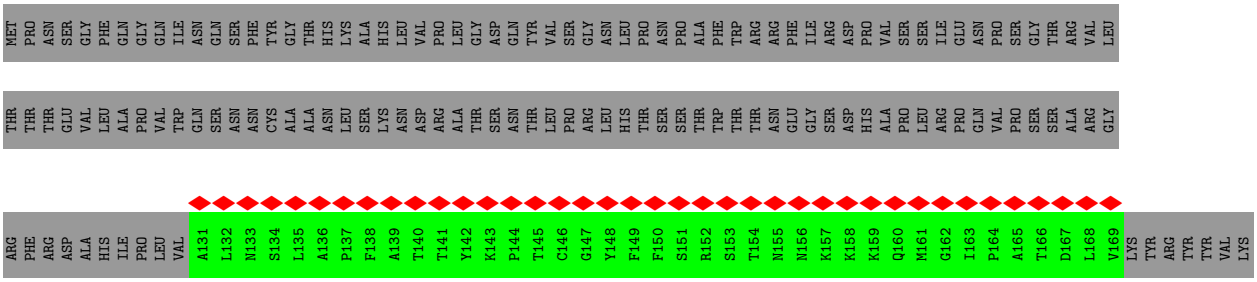
- Molecule 10: ATP6V1FNB

Chain 9O:



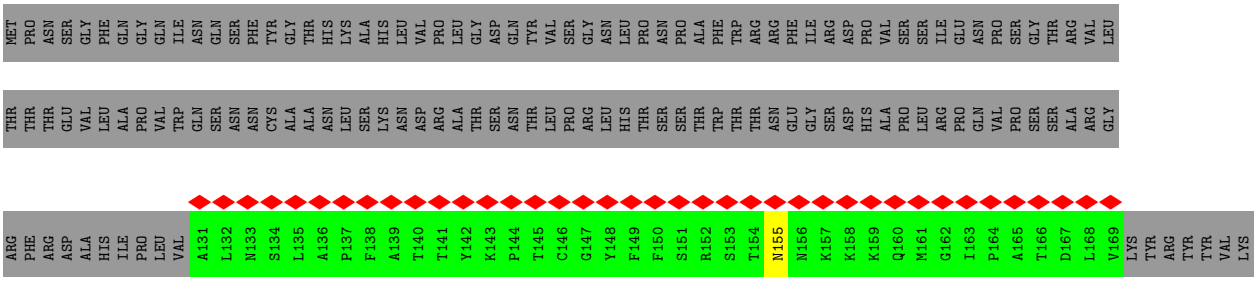
- Molecule 11: Tex26(LOC100888047)

Chain 1l:



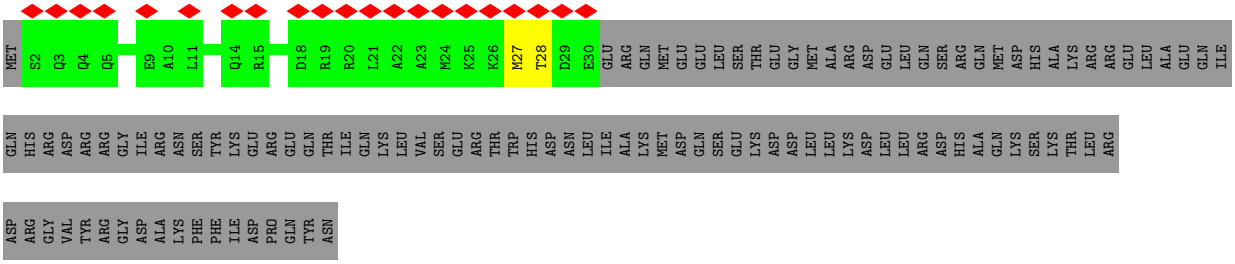
- Molecule 11: Tex26(LOC100888047)

Chain 1m:



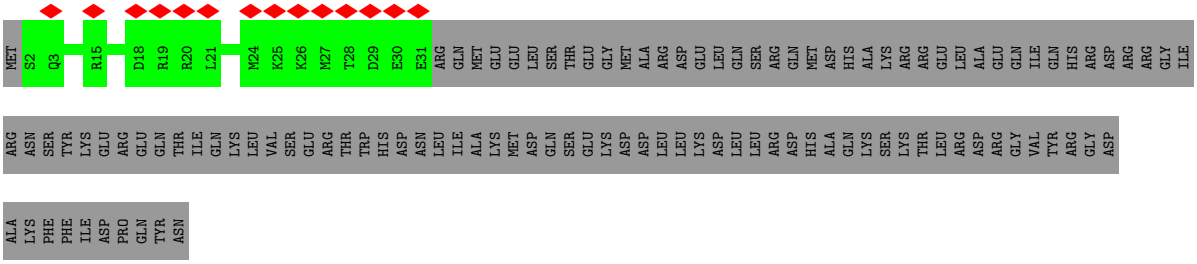
- Molecule 12: Meiosis-specific nuclear structural protein 1

Chain 1o:



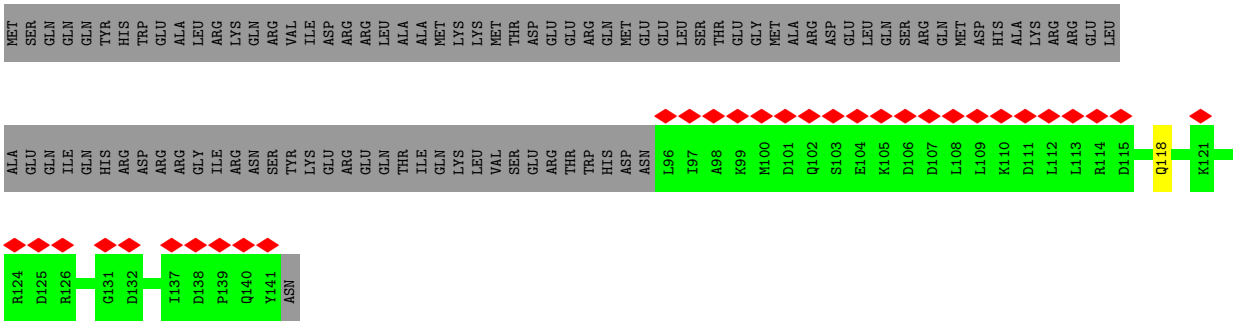
- Molecule 12: Meiosis-specific nuclear structural protein 1

Chain 1p:



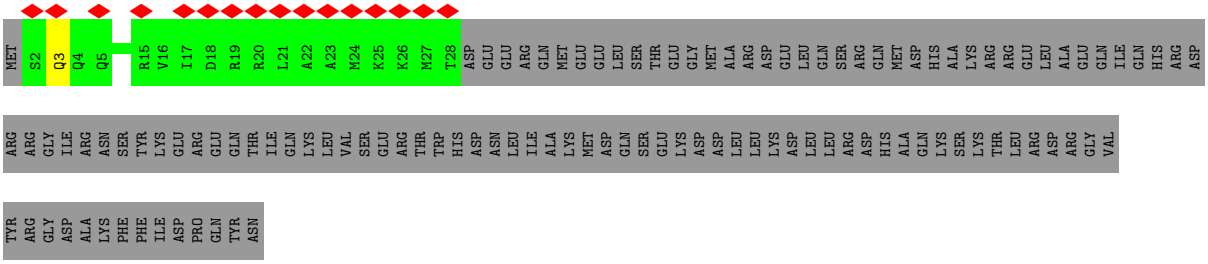
- Molecule 12: Meiosis-specific nuclear structural protein 1

Chain 1q:



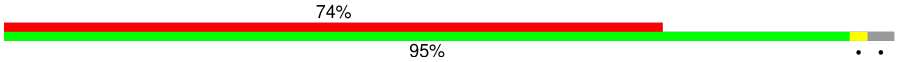
- Molecule 12: Meiosis-specific nuclear structural protein 1

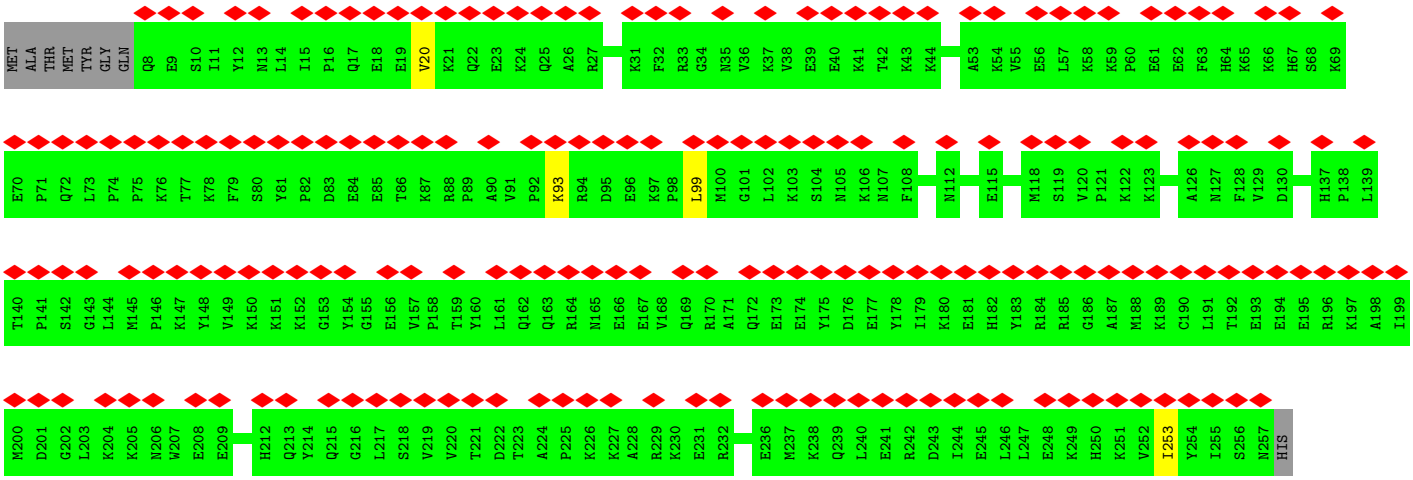
Chain 1r:



• Molecule 13: Enkurin domain-containing protein

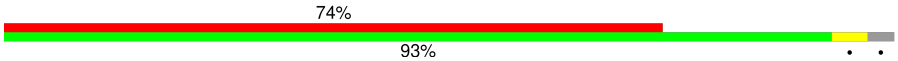
Chain 2A:

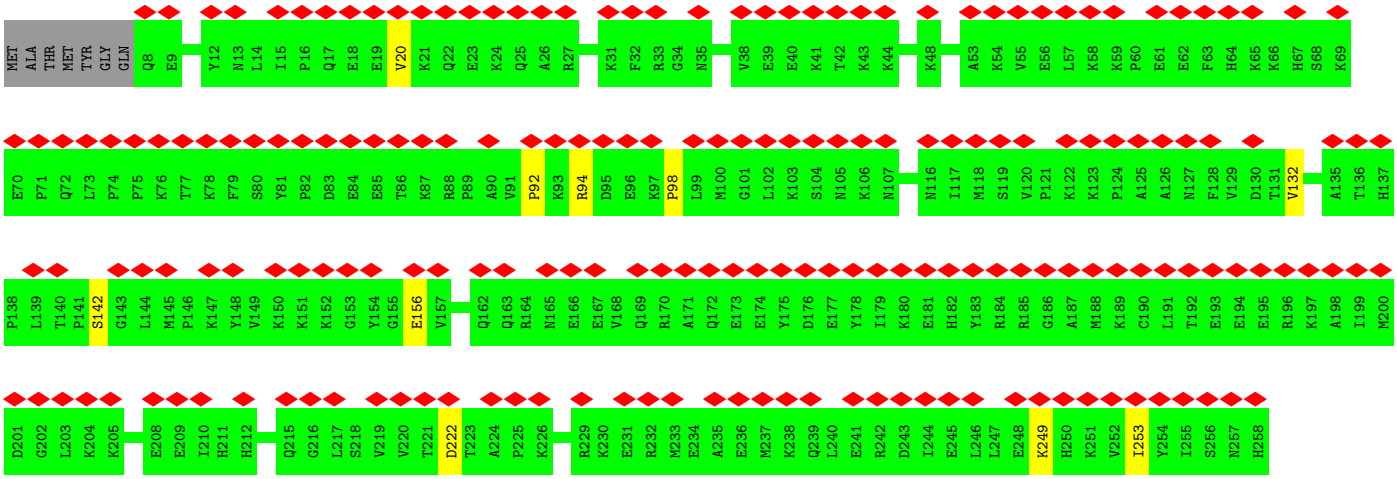




• Molecule 13: Enkurin domain-containing protein

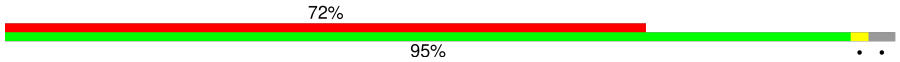
Chain 2B:

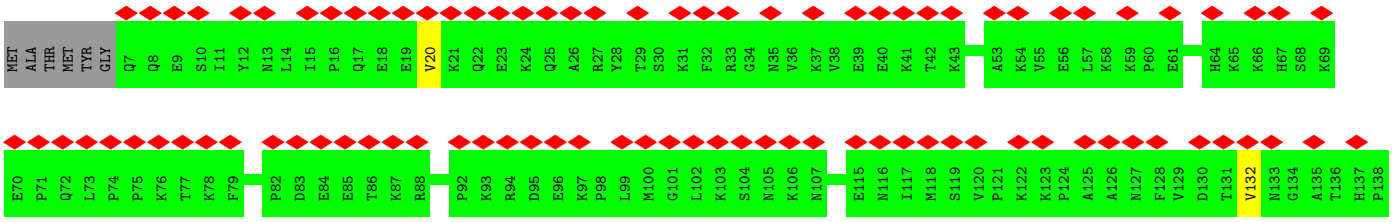




• Molecule 13: Enkurin domain-containing protein

Chain 2C:





L139 T140 P141 S142 G143 L144 M145 P146 K147 Y148 V149 K150 K151 K152 G153 Y154 G155 E156 V157 L161 Q162 Q163 R164 N165 E166 E167 V168 Q169 R170 A171 Q172 E173 E174 Y175 D176 E177 Y178 I179 K180 E181 H182 Y183 R184 R185 G186 A187 M188 K189 C190 L191 T192 E193 E194 E195 R196 K197 A198 I199 M200

D201 G202 L203 K204 K205 E208 E209 I210 H211 H212 Q213 G216 L217 V220 T221 D222 T223 A224 P225 K226 R229 K230 E231 R232 M233 K238 Q239 L240 E241 R242 D243 I244 E245 L246 L247 E248 K249 H250 K251 V252 I253 Y254 I255 S256 N257 HIS

- Molecule 13: Enkurin domain-containing protein

Chain 2D: 24% 29% 69%

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

GLU GLU PHE HIS LYS LYS HIS SER LYS GLU PRO GLN LEU PRO PRO LYS THR LYS PHE SER TYR PRO ASP GLU GLU THR LYS ARG PRO ALA VAL PRO LYS ARG ASP GLU LYS PRO LEU MET GLY LEU LYS SER ASN LYS N107 F108 V109 N110 E115 N116 I117 M118 S119 K122 K123 P124

A125 A126 N127 F128 V129 D130 T131 V132 N133 G134 A135 T136 H137 P138 L139 T140 P141 S142 G143 L144 M145 P146 K147 Y148 V149 K150 K151 K152 G153 E156 V157 P158 T159 Y160 L161 Q162 Q163 R164 N165 E166 E167 V168 Q169 R170 A171 Q172 E173 E174 Y175 D176 E177 Y178 I179 K180 E181 H182 Y183 R184 R185

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

LEU LEU GLU LYS HIS LYS VAL ILE TYR ILE SER ASN HIS

- Molecule 14: CFAP107

Chain 2G: 69% 96%

MET A2 H3 G4 D5 P6 Q7 K8 W9 N10 L11 P12 G13 W14 R15 I16 E17 Q18 R19 G22 N23 I26 G27 N28 E31 E32 R33 Q34 K35 F36 G37 R38 G39 G40 E41 K42 H43 T44 S45 T46 H47 R48 M49 D50 Y51 L52 N53 N54 R55 N56 F57 A58 P59 D60 V61 M62 T63

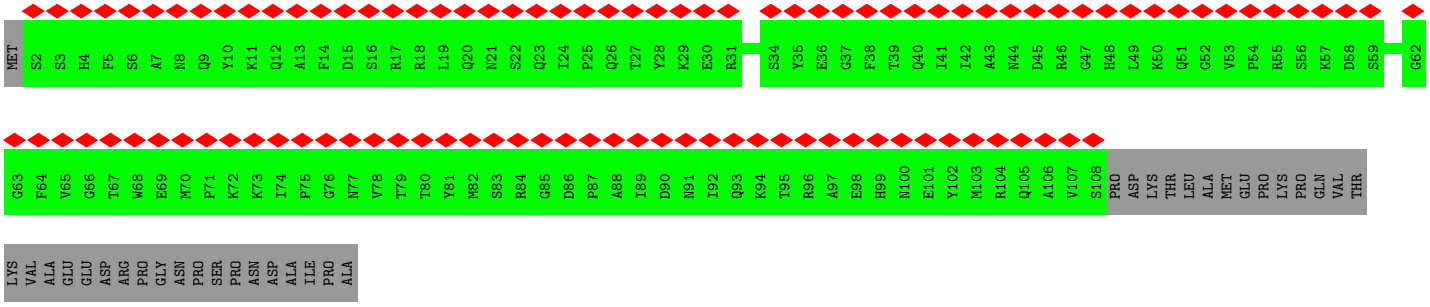
R64 K68 M69 R70 N71 E72 G73 L74 D75 Q76 T77 L78 L79 F80 N84 K85 N86 L87 K88 N89 N90 E97 N100 K101 R102 E103 R104 S105 G106 G107 D108 Q109 L110 P111 E112 L113 R114 H115 W116 D117 G118 Q119 K120 L121 E124 P125 E126 K127 T128 D129 H130 K133 G134

N138 F139 G140 L141 K142 D143 R144 E147 K148 W149 K150 T151 E152 E153 A154 D155 K156 K157 L158 S159 D160 Y161 S162 D168 Y169 K170 N171 K172 P173 R174 A175 A176 T179 E180 Q185 R186 A187 Q188 S189 S190 R191 M192 K197 I198 N199 K200 D201 T202 N203 L204 R205 S206 T207 S208 I209

L210 Q211 T212 P213 Q214 Q215 I216 H217 M218 R219 T220 R221 N222 E223 A224 V225 S226 R227 S228 GLY PRO ALA PRO VAL SER VAL

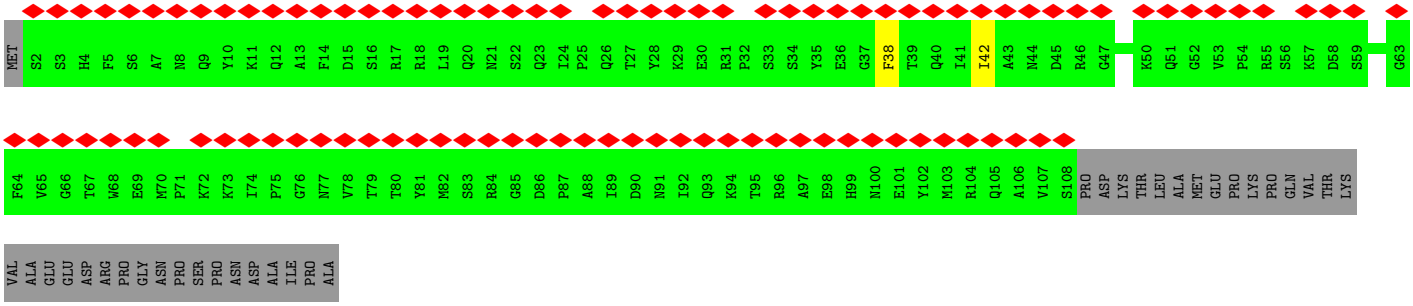
- Molecule 15: Cilia- and flagella-associated protein 126

Chain 2J: 73% 76% 24%



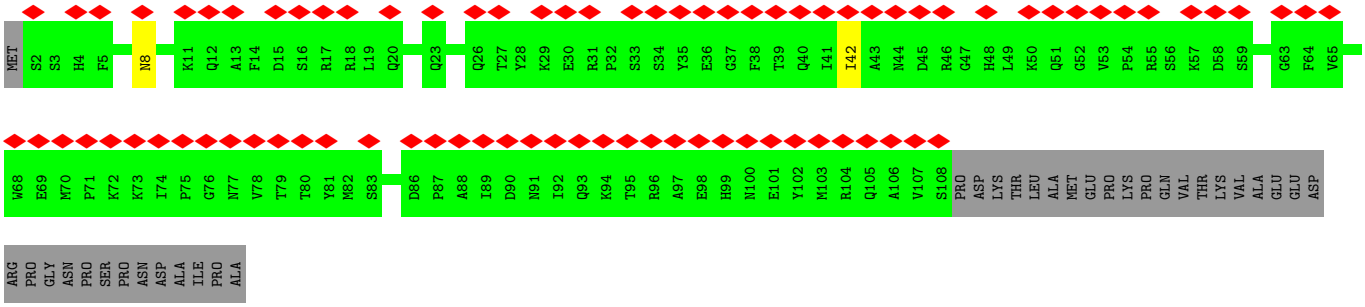
- Molecule 15: Cilia- and flagella-associated protein 126

Chain 2K:



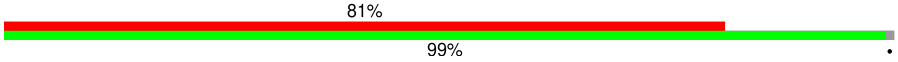
- Molecule 15: Cilia- and flagella-associated protein 126

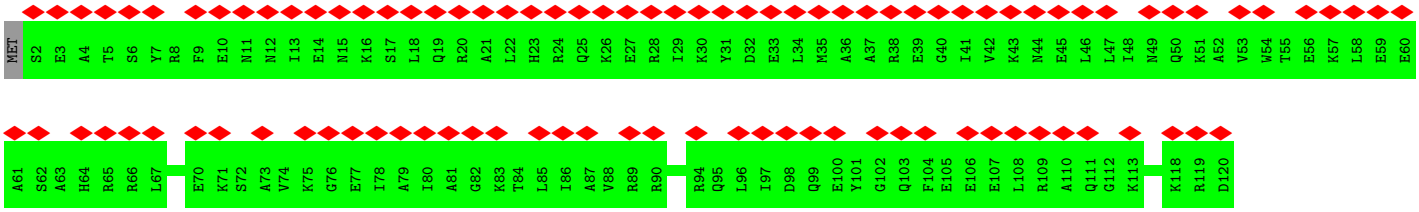
Chain 2L:



- Molecule 16: Flagellar FliJ protein

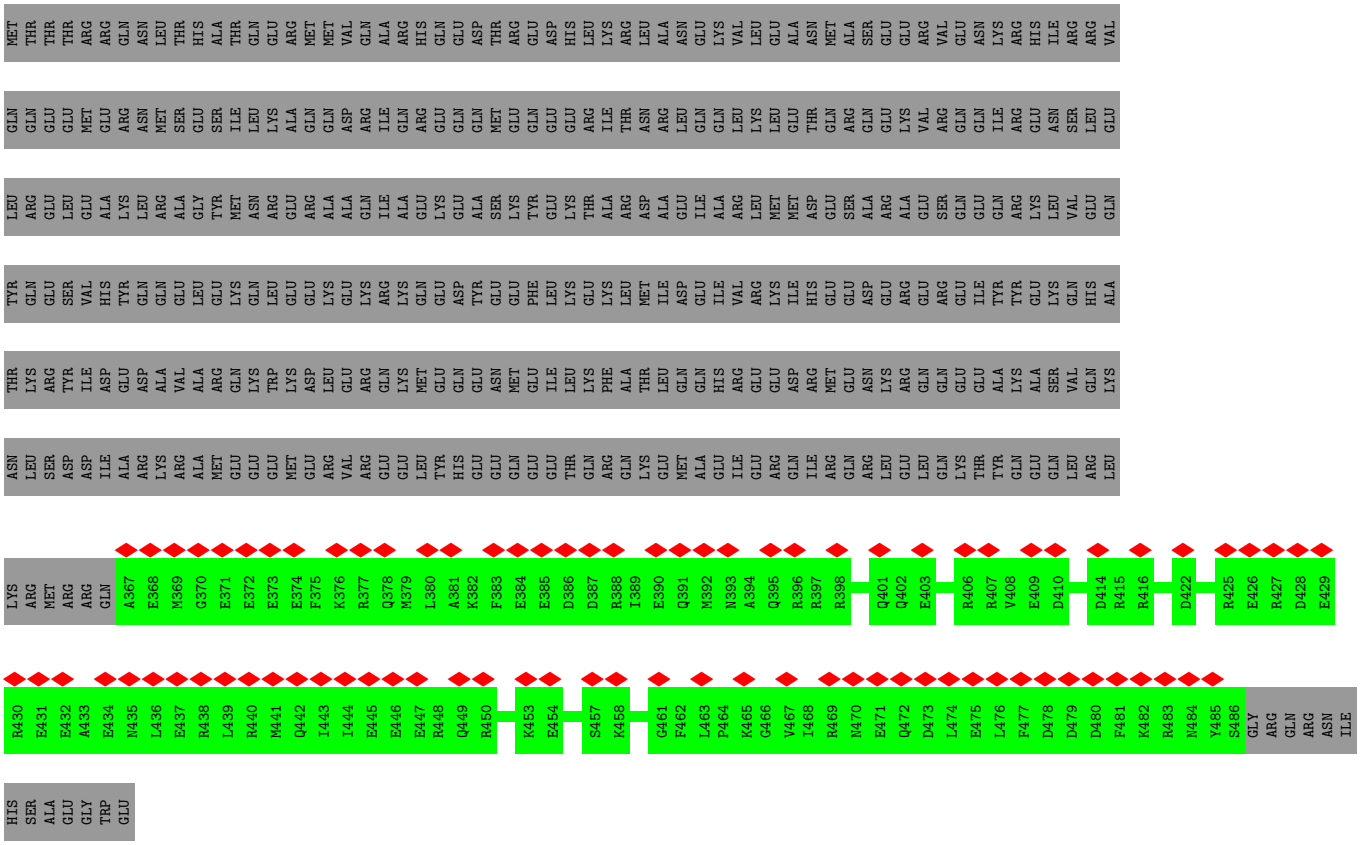
Chain 2O:





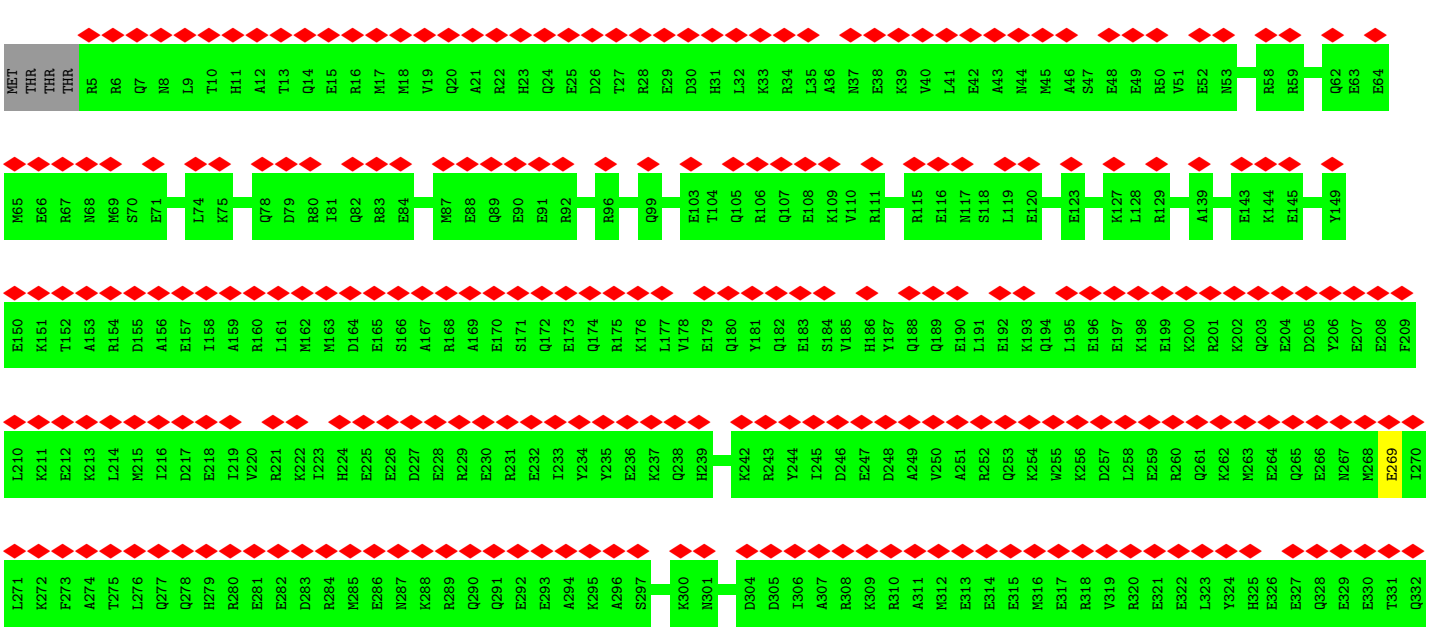
- Molecule 17: Meiosis-specific nuclear structural protein 1

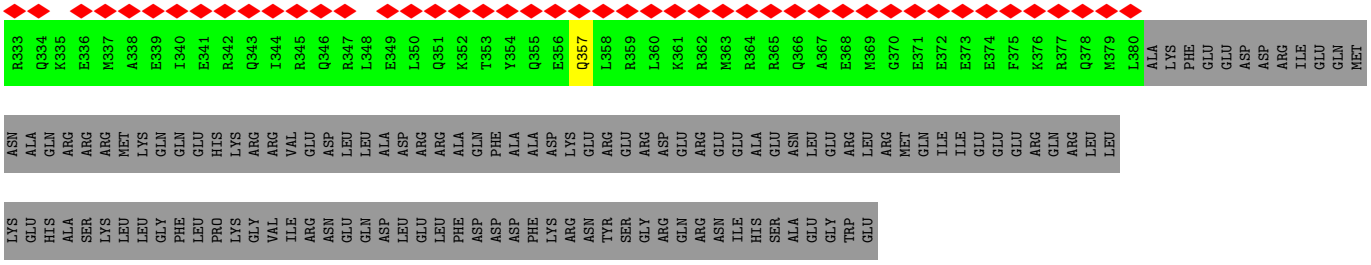
Chain 2R:



- Molecule 17: Meiosis-specific nuclear structural protein 1

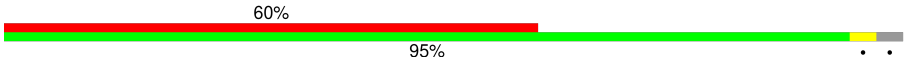
Chain 2S:

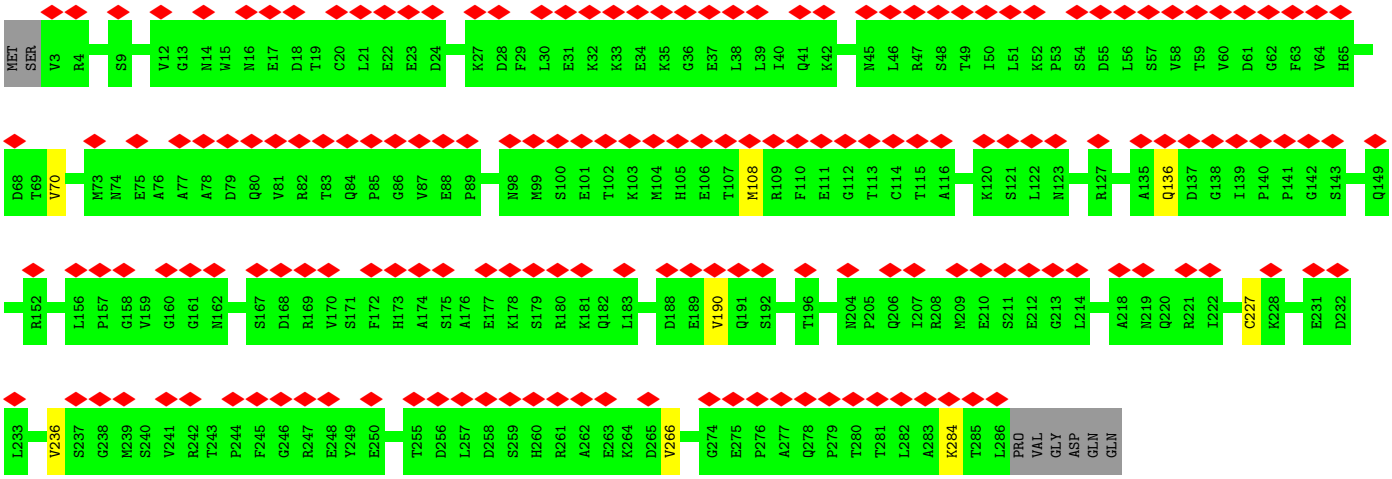




• Molecule 18: Cilia- and flagella-associated protein 161

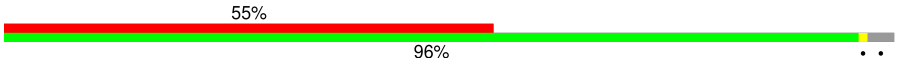
Chain 2V:

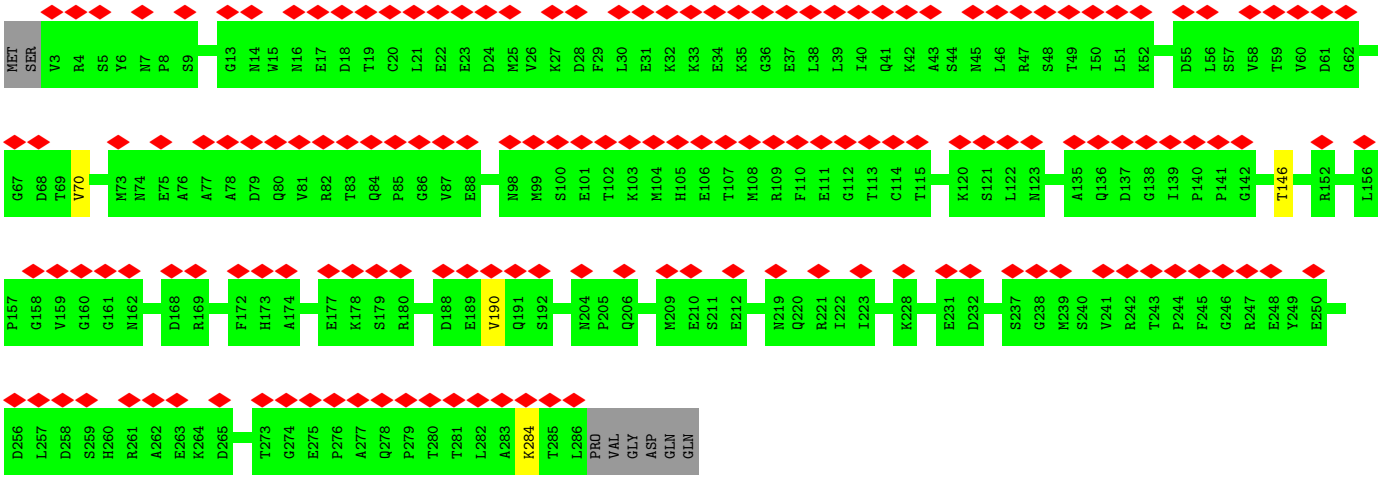




• Molecule 18: Cilia- and flagella-associated protein 161

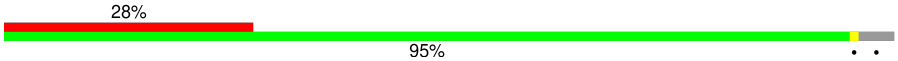
Chain 2W:

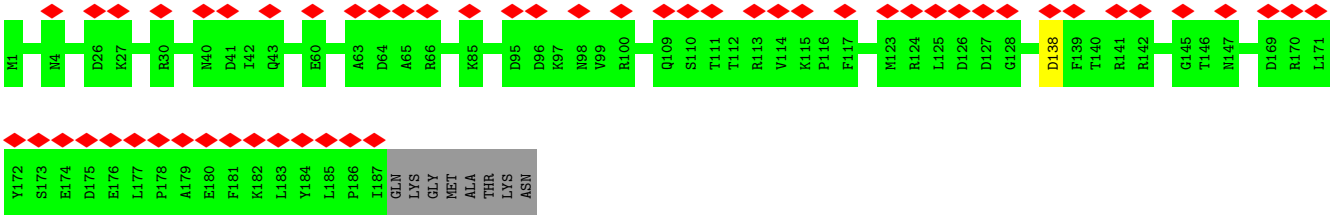




• Molecule 19: CFA20 domain-containing protein

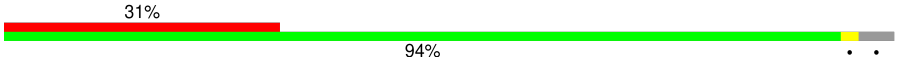
Chain 3A:

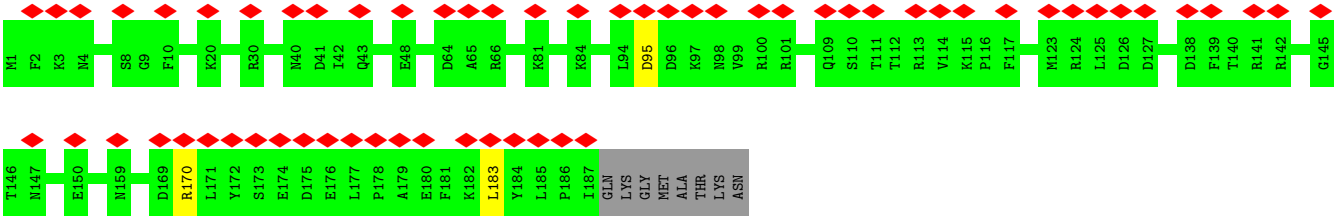




- Molecule 19: CFA20 domain-containing protein

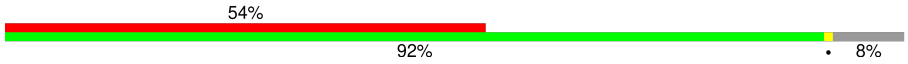
Chain 3B:

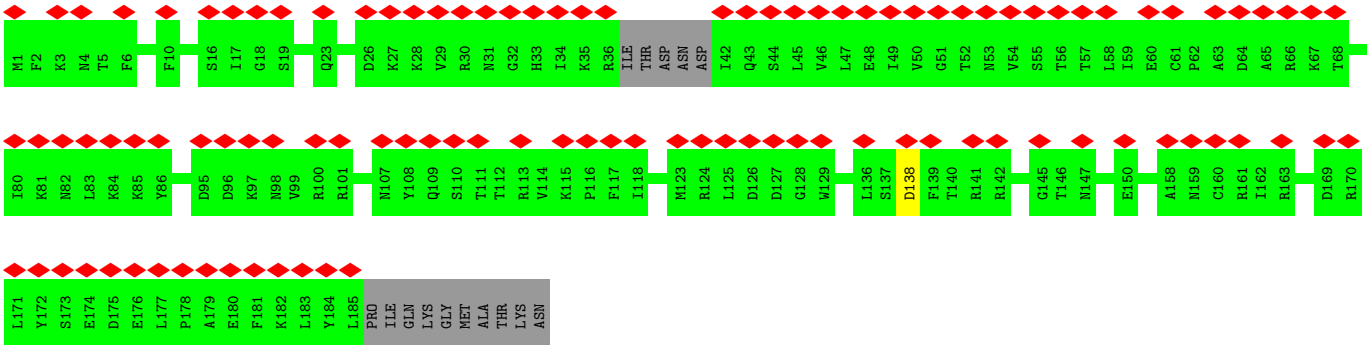




- Molecule 19: CFA20 domain-containing protein

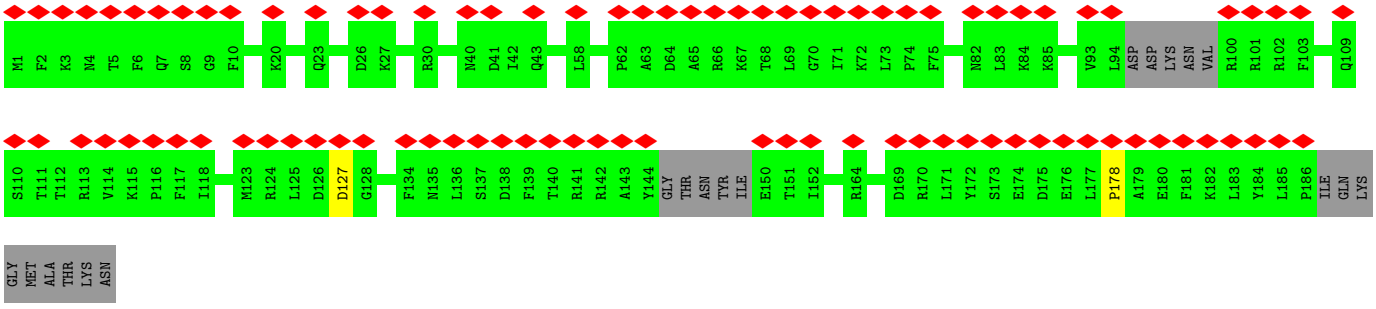
Chain 3C:





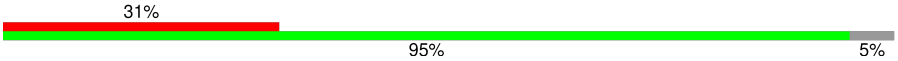
- Molecule 19: CFA20 domain-containing protein

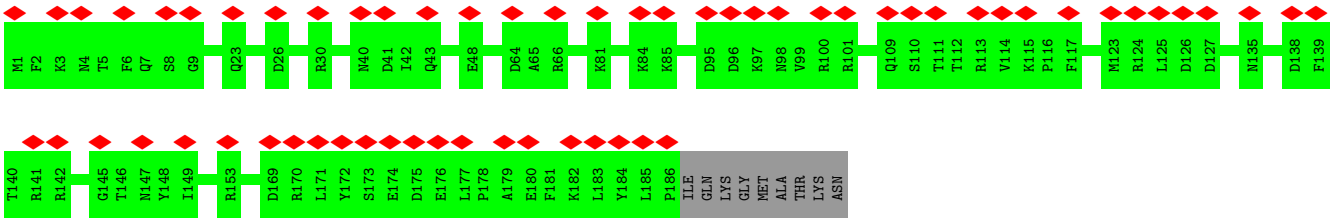
Chain 3D:



- Molecule 19: CFA20 domain-containing protein

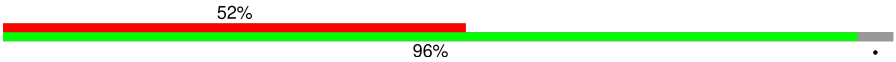
Chain 3E:

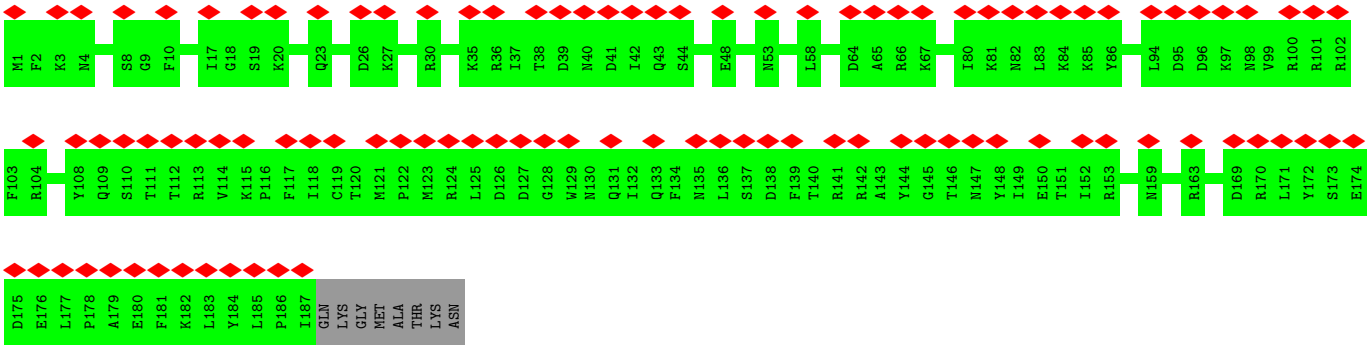




- Molecule 19: CFA20 domain-containing protein

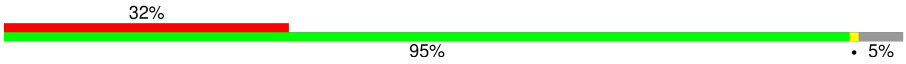
Chain 3F:

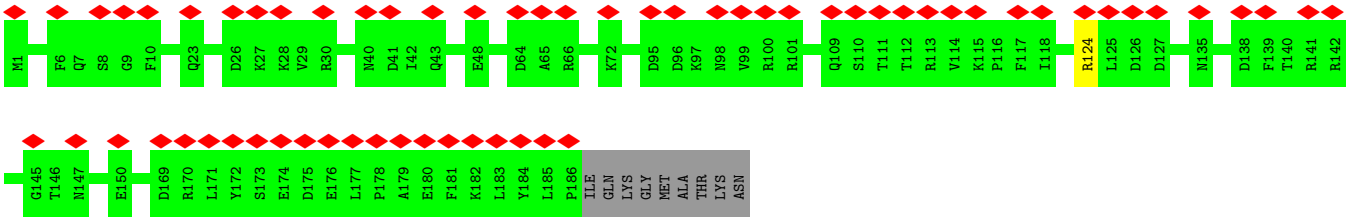




- Molecule 19: CFA20 domain-containing protein

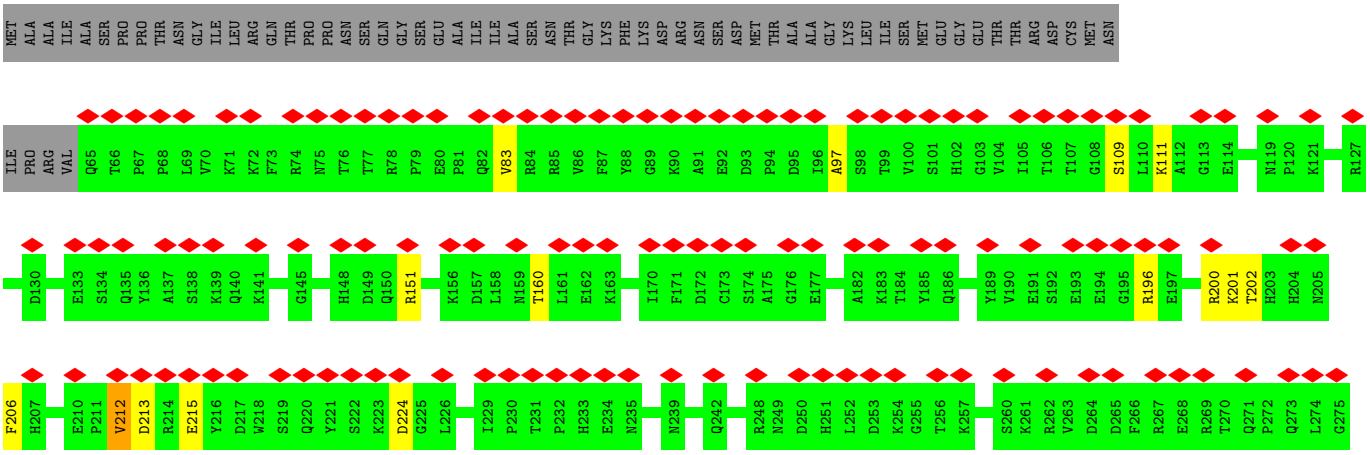
Chain 3G:





- Molecule 20: EF-hand domain-containing protein

Chain 3J:



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H340 N341 F342 N343 N344 L345 Q346 A347 A348 F349 N350 H351 Y352 D353 K354 N355 G356 D357 G358 K359 I360 D361 I362 N363 E364 L365 R366 L367 C368 G369 D370 Q371 F372 S373 L374 P375 I376 E377 P378 E379 L380 L381 E382 Q383 L384 I385 L386 Y387 C388 D389 A390 N391 T392 N393 G394 C395 I396 D397 Y398 F399

E400 F401 A402 N403 F404 L405 N406 W407 K408 D409 K410 M411 N412 E413 G414 E415 T416 LEU THR ASN PRO ALA SER ALA ALA VAL LYS GLY GLU SER GLN GLU SER LYS GLU GLY THR PRO GLU ARG LEU LYS LYS GLN ILE ASP GLN A447 I448 G449 G450 H451 R452 T453 M457 I458 N459 A460

G463 G464 V465 S466 T467 K468 G469 Y470 D481 I482 A483 R486 R489 I490 S491 D492 T493 K494 D498 E499 S500 D501 A502 F503 M510 K514 G515 I516 Y517 E518 K519 D520 F521 F522 E526 P527 E528 Q529 I530 K531 G532 I533 F534 S535 D536 I537 G538 V539 E540 M541 D542 P543 E544

T545 F546 H547 K548 L549 W550 S551 V552 A553 T554 S555 R556 S557 D558 Q559 G560 Q561 V562 R568 N569 D572 E573 V574 Q575 A576 L577 Q578 L579 A580 D581 E582 A583 Q584 N585 L586 G587 R588 P589 GLU LEU VAL

- Molecule 20: EF-hand domain-containing protein

Chain 3K: 11% 11% 88%

MET ALA ALA ILE ALA SER PRO PRO THR ASN GLY ILE LEU ARG GLN THR PRO PRO ASN SER GLN GLY SER GLU A25 I26 I27 A28 S29 N30 T31 G32 K33 F34 K35 D36 R37 N38 S39 D40 M41 T42 K46 L47 I48 S49 M50 E51 G52 E53 T54 T55 R56 D57 C58 M59 N60 I61 P62

R63 V64 Q65 T66 P67 P68 L69 V70 K71 K72 F73 R74 N75 T76 T77 R78 P79 E80 P81 Q82 V83 R84 R85 V86 F87 Y88 G89 K90 A91 E92 D93 P94 ASP ILE ALA SER THR VAL SER HIS GLY VAL ILE THR THR GLY SER LEU LYS ALA GLY GLU VAL VAL ASN PRO ASN PRO LYS THR

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

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

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

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

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

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

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

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

- Molecule 21: Trichohyalin-plectin-homology domain-containing protein

Chain 3N:

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

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

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

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

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

ILE PHE A303 A304 A305 K306 K307 K308 M309 T310 K311 L312 R313 R314 K315 R316 E317 K318 E319 L320 W321 Q322 E323 K324 Q325 D326 M327 V328 T329 R330 M331 V332 N333 D334 L335 D336 S337 Q338 M339 K340 A341 K342 A343 D344 D345 E346 D347 D348 R349 I350 A351 K352 A353 V354 A355 D356 R357 E358 A359 A360

R361 E362 K363 E364 M365 Q366 E367 K368 E369 S370 R371 L372 E373 D374 D375 L376 K377 Q378 M379 A380 L381 H382 R383 T384 Q385 Q386 M387 K388 Q389 K390 E391 K392 E393 E394 R395 Q396 E397 R398 R399 R400 E401 L402 E403 A404 L405 H406 L407 K408 I409 E410 A411 D412 R413 L414 F415 A416 T417 K418 Q419 E420

E421 K422 M423 K424 R427 Q442 E443 R444 H445 E446 L447 K448 R452 Q455 L456 E457 M458 D459 N462 I463 D464 E475 E486 G487 V491 R499 D511 N523 D524 R525 V528 Q534 E540 H545 I546 G547 K548 P549 R553 K554 R555 W560

- Molecule 21: Trichohyalin-plectin-homology domain-containing protein

Chain 3O:

MET ALA GLN GLU GLN VAL ARG HIS GLY ARG ARG ARG GLY GLN LYS LYS ASN SER PRO ILE GLY ASN ARG SER GLY GLY ALA PRO PRO ALA GLY PRO GLY MET MET LEU PRO ASP GLY SER ASP LEU ARG Q44 V45 T46 V47 L48 S49 K50 A51 D52 W53 S54 R55 I56 R57 A58 Q59 L60

E61 R62 K63 Q64 R65 E66 E67 E68 A69 F70 R71 A72 K73 R74 E75 A76 K77 E78 A79 L80 H81 Q82 Q83 S84 K85 D86 M87 V88 K89 N90 W91 S92 N93 T94 I95 A96 G97 Q98 R99 L100 Q101 K102 L103 E104 A105 R106 K107 I108 R109 E110 E111 K112 E113 E114 A115 E116 R117 V118 Q119 I120

D121 I122 E123 K126 Y127 Q128 A129 E130 K131 E134 D137 D148 E165 R166 D167 D171 L172 K173 R174 A175 R176 E177 M180 E181 G182 N183 D184 M185 E186 L187 Y188 L189 R190 R193 E194 L195 E196 E197 G198 I199 L200 A201 D202 Q203 E204 R209 M210 Q211 D212 R213

E218 Q222 Q229 E232 I233 D234 D238 V239 R240 E241 G242 R243 E244 L245 K246 E247 D250 Y251 Y252 N253 A254 E255 R256 A257 K258 I259 E260 R261 I262 R263 E266 K267 Q268 D269 L270 M271 H272 S273 H274 L275 A279 D280 R281 D282 L283 I284 R285 A286 A287 Q288 E289 Q290 K291

E292 E293 E294 E295 E296 E297 R300 A304 A305 K306 K307 K311 L312 R313 R314 K315 R316 E317 K318 E319 L320 W321 GLN GLU LYS GLN ASP ASN VAL THR ARG MET VAL ASN ASP LEU ASP SER GLN MET LYS ALA LYS ALA ASP ASP GLU ASP ASP ARG ILE ALA LYS ALA VAL ALA ASP

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

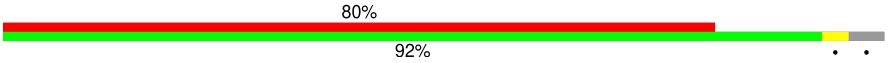
THR LYS GLN GLU GLU LYS MET LYS GLN ILE ARG GLN GLU ASN GLU ASN LEU LYS GLY PHE HIS SER ASN GLN ILE GLN GLU ARG HIS GLU LEU LYS LEU LEU GLY ARG ALA GLU GLU GLN LEU GLU MET ASP LYS LYS ASN ILE ASP LEU LEU ALA LEU GLU GLU GLN GLN PHE GLN GLU TYR

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

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

- Molecule 22: CFAP276

Chain 3R:



MET SER ASN ILE GLU MET S7 N8 R9 D10 F14 E15 K16 L17 E18 N19 D20 T21 S22 F23 F24 G25 T26 N27 E28 T29 Q30 K31 M32 P33 Y34 G35 E36 P37 T38 H39 I40 A41 Q42 T43 K44 D45 R49 L50 N51 S52 T53 C54 A57 S58 R61 E62 V63 Y64 H65 H66

D67 P68 K69 A70 P71 R72 D73 S74 L75 D76 F77 N82 Y83 D84 H85 H86 G87 E88 L89 L90 R93 S94 E95 M98 Q99 P100 E101 T102 L103 G104 A105 N106 H107 G108 R109 I110 L111 K112 N113 R114 V115 P116 E117 K118 V119 A120 E121 P122 V123 S124 P125 T126 G127 K128 L129 T130 I131

V132 S133 I134 H135 T136 P137 K138 K139 E140 S141 I142 H143 S144 V145 K146 G147 A148 I149 E150 S151 H152 H153 T154 P155 A156 T157 N158 Q159 G160 F161 S162 R163 K164 H165 D166 G167 G168 F169 Y170 T171 THR

- Molecule 22: CFAP276

Chain 3S:

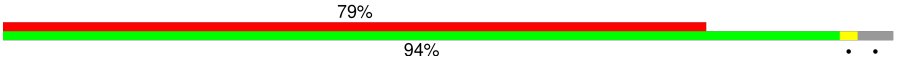
MET SER ASN ILE GLU MET SER ASN ARG ASP PRO TYR PRO PHE GLU LYS LEU GLU ASN ASP THR SER PHE PHE GLY THR ASN GLU THR GLN LYS MET PRO TYR GLY GLU PRO THR HIS ILE ALA GLN THR LYS D45 P46 W47 Q48 R49 L50 N51 S52 T53 C54 T55 S58 S59 R60 R61

E62 V63 Y64 H65 H66 D67 P68 K69 A70 P71 R72 D73 D76 K80 A81 N82 Y83 D84 H85 H86 G87 E88 L89 L90 K91 N92 R93 S94 E95 T96 L97 M98 Q99 P100 E101 T102 L103 G104 A105 N106 H107 G108 R109 I110 L111 K112 N113 R114 V115 P116 E117 K118 V119 A120 E121 P122 V123 S124

P125 T126 G127 K128 L129 T130 I131 V132 S133 I134 H135 T136 P137 K138 K139 E140 S141 I142 H143 S144 V145 K146 G147 A148 I149 E150 S151 H152 H153 T154 P155 A156 T157 N158 Q159 G160 F161 S162 R163 K164 H165 D166 F169 Y170 T171 THR

- Molecule 22: CFAP276

Chain 3T:



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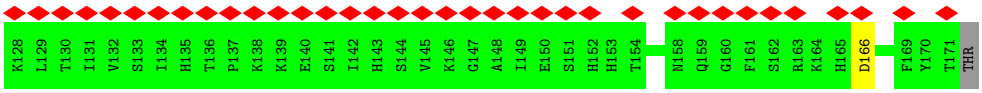
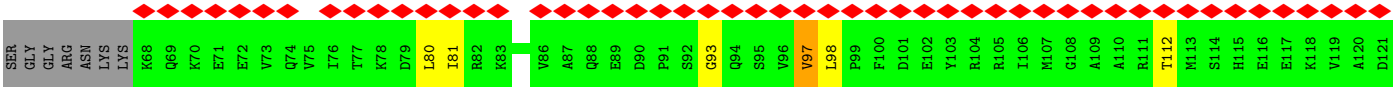
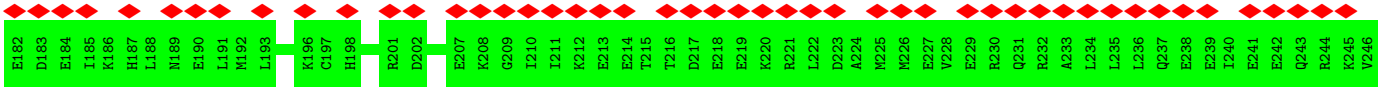
H66 D67 P68 K69 A70 P71 R72 D73 S74 L75 D76 K80 A81 N82 Y83 D84 H85 H86 G87 E88 L89 L90 K91 N92 R93 S94 E95 T96 L97 M98 Q99 P100 E101 T102 L103 G104 A105 N106 H107 G108 R109 I110 L111 K112 N113 R114 V115 P116 E117 K118 V119 A120 E121 P122 V123 S124 P125 T126 G127

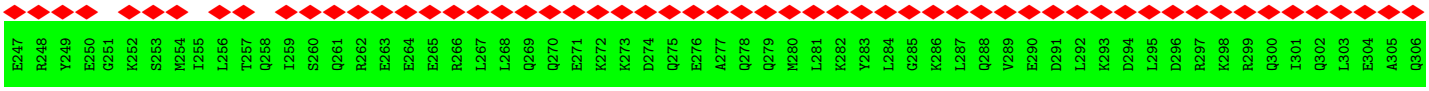


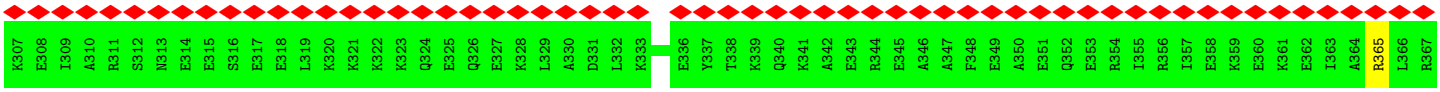
• Molecule 23: Cilia- and flagella-associated protein 45

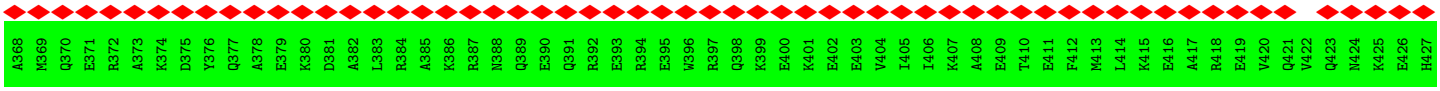
Chain 3W:

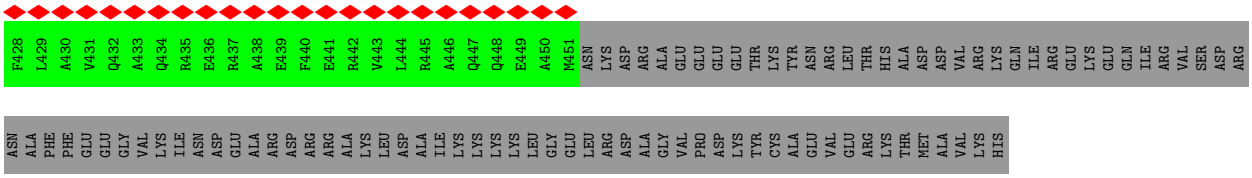






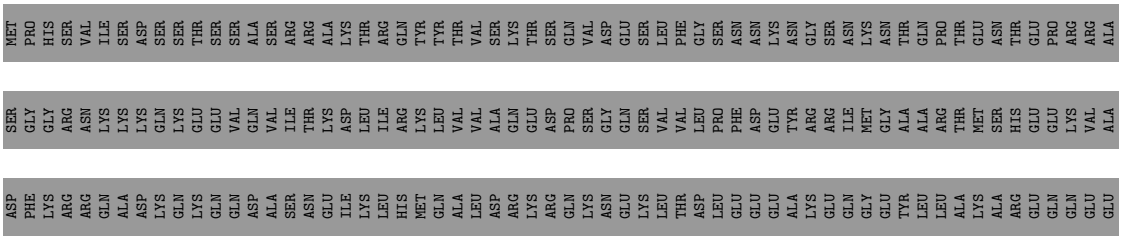






• Molecule 23: Cilia- and flagella-associated protein 45

Chain 3X:



GLN GLU ASP GLU ILE LYS HIS LEU ASN GLU LEU MET LEU ASN ALA LYS CYS HIS ALA ILE ARG ASP ALA GLN ILE LEU GLU LYS GLY ILE ILE LYS GLU GLU THR THR ASP GLU GLU LYS ARG LEU ASP A224 M225 M226 E227 V228 E229 R230 Q231 R232 A233 L234 L235 L236 Q237 E238 E239 I240

E241 E242 Q243 R244 E247 R248 Y249 E250 Q251 K252 L256 I259 S260 Q261 R262 E263 E264 E265 R266 L267 L268 Q269 Q270 E271 K272 K273 D274 Q275 E276 A277 Q278 Q279 M280 L281 K282 Y283 L284 G285 K286 L287 Q288 V289 E290 D291 L292 K293 D294 L295 D296 R297 K298 R299 Q300 I301 Q302 L303 E304

A305 Q306 K307 E308 I309 A310 R311 S312 N313 E314 E315 S316 E317 E318 L319 K320 K321 K322 K323 Q324 E325 Q326 E327 K328 L329 A330 D331 L332 K333 V334 N335 E336 Y337 T338 K339 Q340 K341 A342 E343 R344 E345 A346 A347 F348 E349 A350 E351 Q352 E353 R354 I355 R356 I357 E358 K359 E360 K361 E362 I363 A364

R365 L366 R367 A368 M369 Q370 E371 R372 A373 K374 D375 Y376 Q377 A378 E379 K380 D381 A382 L383 R384 A385 K386 R387 N388 Q389 E390 Q391 R392 E393 R394 E395 W396 R397 Q398 K399 E400 K401 E402 E403 V404 I405 I406 K407 A408 E409 T410 E411 F412 M413 L414 K415 E416 A417 R418 E419 V420 Q421 V422 Q423 N424

K425 E426 H427 F428 L429 A430 V431 Q432 A433 Q434 R435 E436 R437 A438 E439 F440 E441 R442 V443 L444 R445 A446 Q447 Q448 E449 A450 M451 N452 K453 D454 R455 A456 E457 E458 E459 E460 T461 K462 R465 D470 D471 V472 R473 K474 R477 E478 K479 E480 Q481 I482 R483 D486 R487 N488 A489 F490

F491 E492 E493 K496 I497 N498 D499 E500 A501 R502 D503 R504 R505 L508 D509 K512 K513 K514 K515 L516 G517 E518 L519 R520 D521 A522 G523 D526 K527 Y528 C529 A530 E531 V532 E533 R534 K535 T536 M537 A538 VAL LYS HIS

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

Chain 3Y:

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

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

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

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

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

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

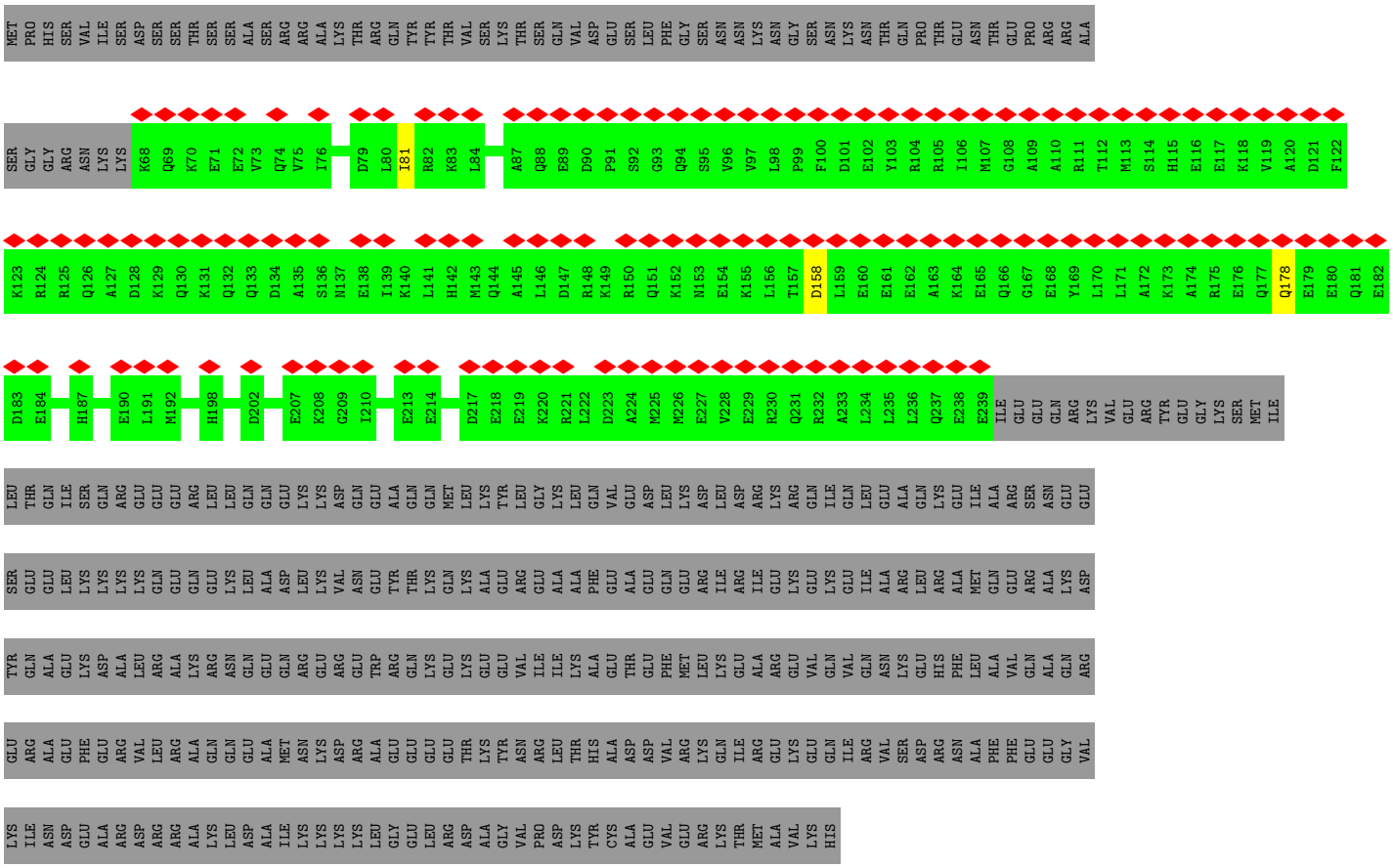
LYS GLU ILE ALA ARG LEU ARG ALA MET GLN GLU ARG ALA LYS ASP TYR GLN ALA GLU LYS ASP ALA LEU ARG ALA LYS ARG ASN GLN GLU GLN ARG GLU GLU TRP ARG GLN LYS GLU LYS GLU VAL ILE ILE LYS ALA GLU THR GLU PHE MET LEU LYS GLU ALA ARG GLU VAL

GLN VAL GLN ASN LYS GLU HIS PHE LEU ALA VAL GLN ALA GLN ARG E436 R437 A438 E439 F440 E441 R442 V443 L444 R445 A446 Q447 Q448 E449 A450 M451 N452 K453 D454 R455 A456 E457 E458 E459 E460 T461 K462 Y463 N464 R465 L466 D470 D471 V472 R473 K474 R477 E478 K479 E480 Q481 I482 R483

D486 R487 N488 A489 F490 F491 E492 E493 G494 V495 K496 I497 N498 D499 E500 A501 R502 D503 R504 R505 A506 K507 L508 D509 A510 I511 K512 K513 K514 K515 L516 G517 E518 L519 R520 D521 A522 G523 V524 P525 D526 K527 Y528 C529 A530 E531 V532 E533 R534 K535 T536 M537 A538 V539 LYS HIS

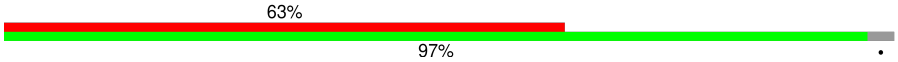
• Molecule 23: Cilia- and flagella-associated protein 45

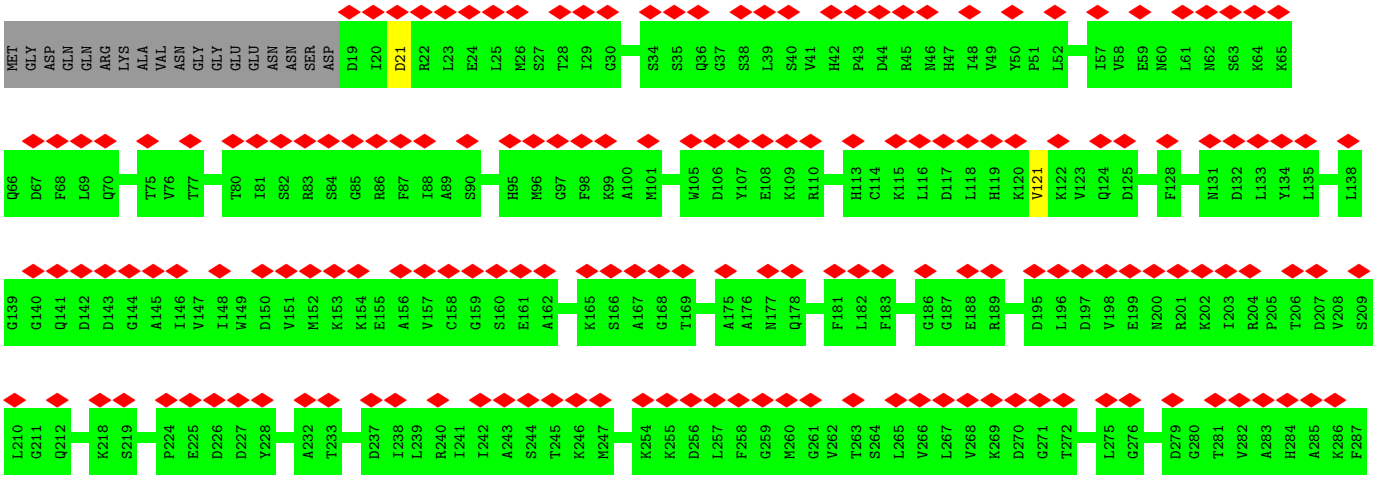
Chain 3Z:

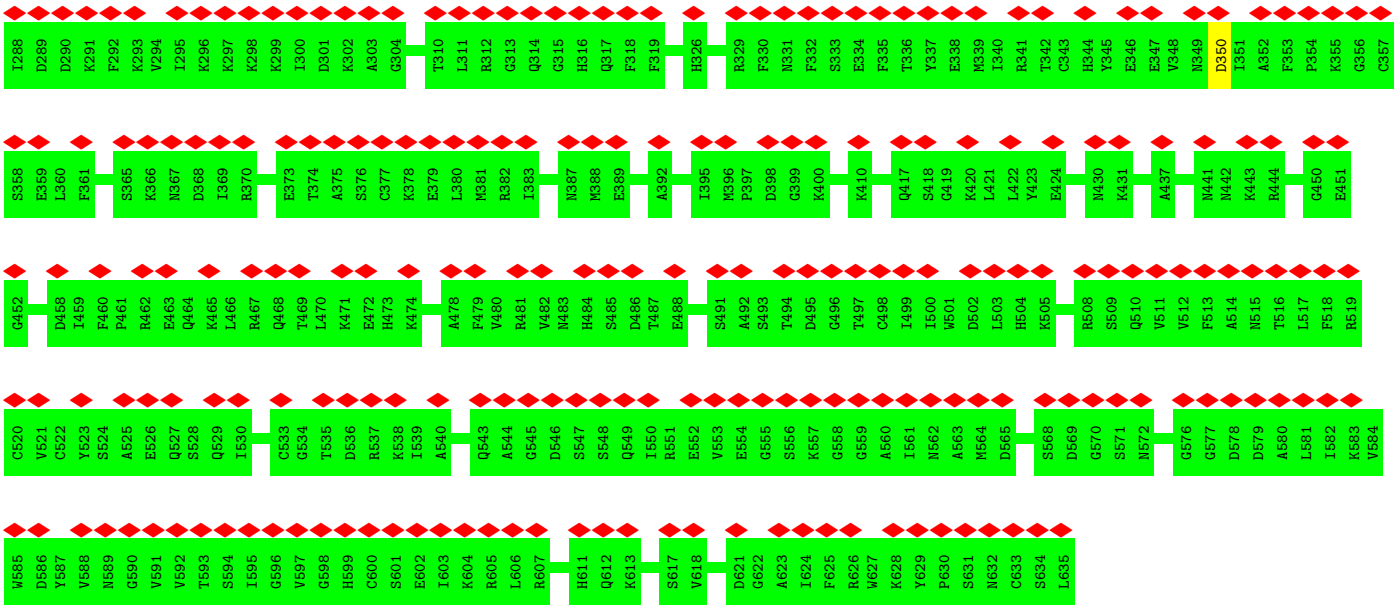


• Molecule 24: Cilia- and flagella-associated protein 52

Chain 4A:

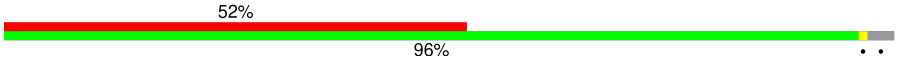


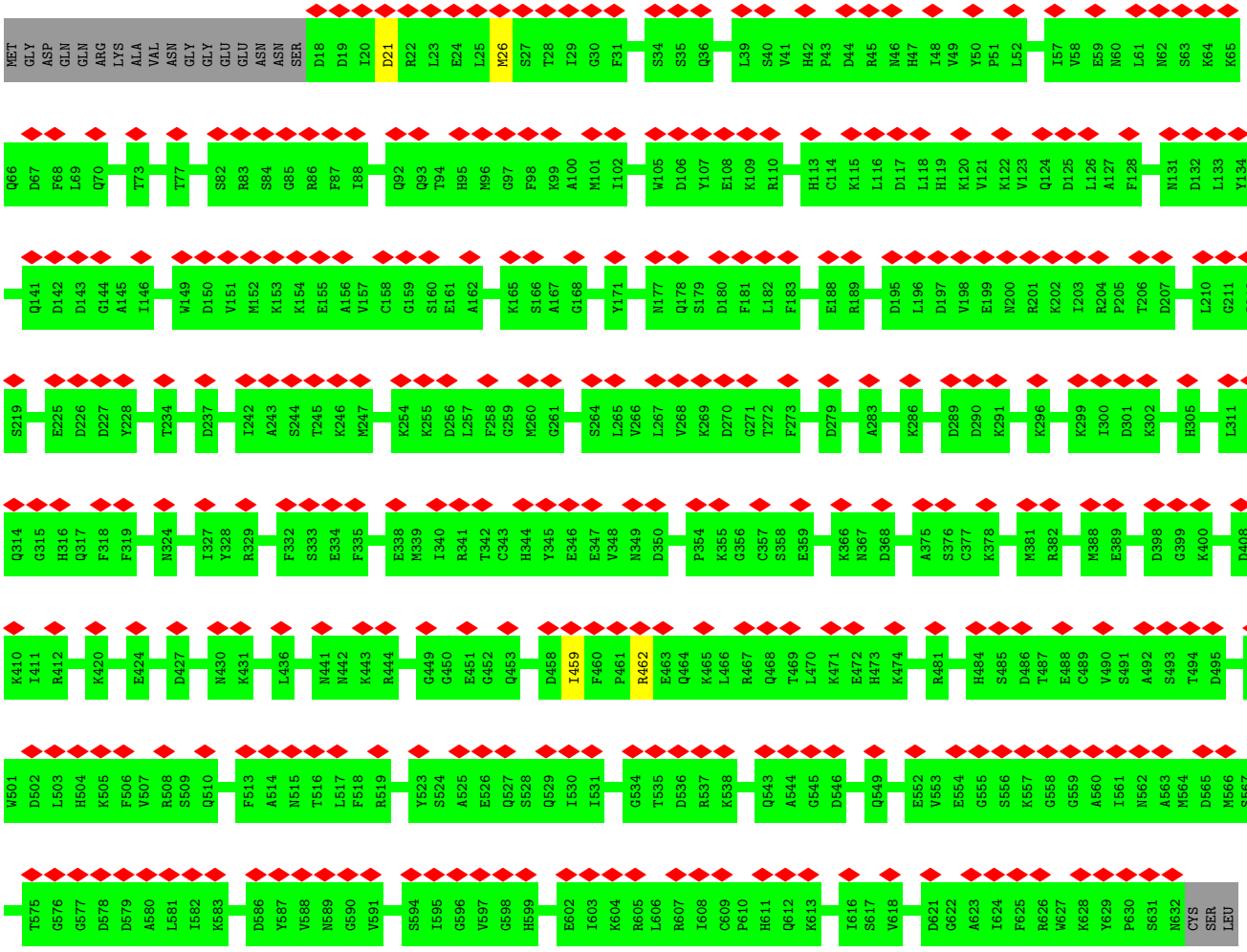




- Molecule 24: Cilia- and flagella-associated protein 52

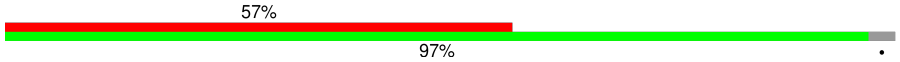
Chain 4B:

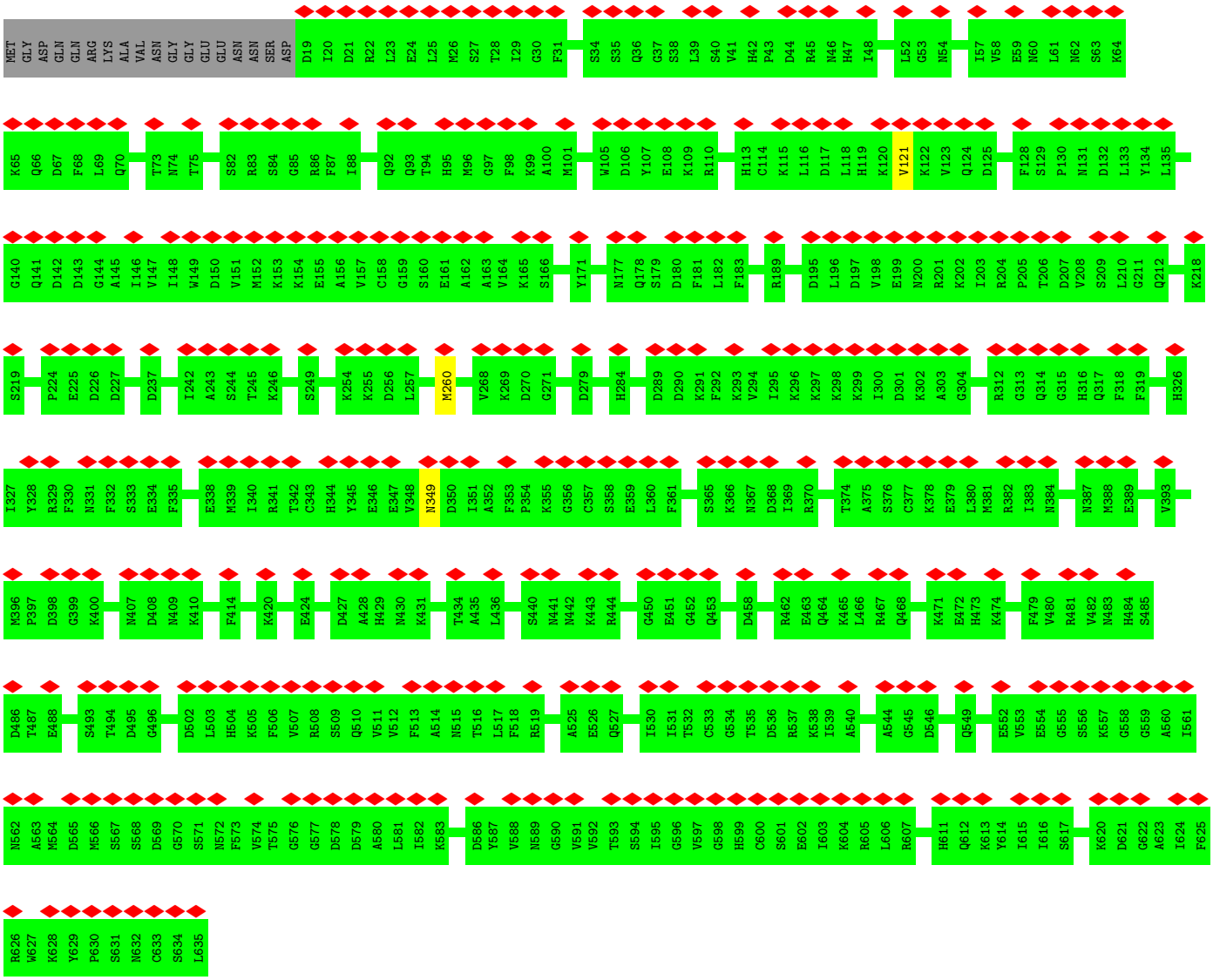




• Molecule 24: Cilia- and flagella-associated protein 52

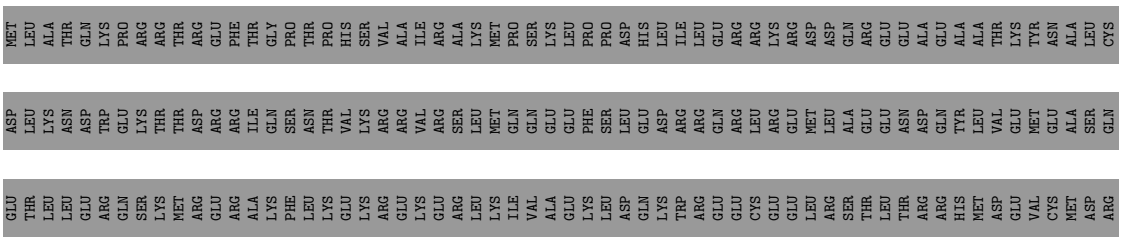
Chain 4C:





• Molecule 25: Trichohyalin-plectin-homology domain-containing protein

Chain 4F:



SER HIS GLN LEU GLU THR LYS ALA ARG MET GLN ALA HIS ASP GLN GLU V197 E198 R199 M200 D203 K207 D208 K212 E213 A214 K215 E216 E217 K218 Q221 R226 N227 M228 Q235 M238 E242 A243 K244 R245 Q246 E247 E248 K249 Q250 L251 R252 I253 D254 G255 G256 K257

L258 R259 K260 E261 E262 A263 A264 L265 R266 K267 L268 E269 E270 Q271 R272 A273 M274 A275 E276 K277 R278 A279 L280 Q281 Q282 E283 M284 R285 D286 D289 Q290 N291 I292 K293 L294 K295 A296 K297 R298 M299 A300 K301 E302 V303 Q304 E305 E306 L307 A308 L309 D310 M311 K312 I313 L314 E315 K316 L317 L318

E319 E320 S321 R322 N323 E324 A325 M326 E327 I328 T329 Q330 R331 K332 K333 E334 L335 R336 Q337 E338 D339 Q340 R341 Y342 R343 K344 Y345 L346 Q347 E348 Q349 M350 R351 L352 E353 Q354 Q355 R356 E357 A358 E359 I360 D361 R362 M363 E367 V368 E369 R370 Q371 W372 Q373 K374 R375 L376 S377 Q378 W379 A380

K381 E382 R383 N384 A385 R386 K387 R388 L389 M390 E391 E392 V393 L394 R397 R398 Q399 Q400 V401 E402 E403 R404 L405 A406 A407 N408 A409 N410 A411 Q412 A413 E414 L415 A416 K417 E418 R419 E420 A421 M422 Q423 A424 A425 M426 E427 E428 H429 K430 R431 L432 D433 D434 E435 K436 Q437 A438 L441

Q461 D467 E468 E469 Y470 R471 E472 H475 E478 T479 E480 R493 I496 D497 K498 A499 R504 Q505 H506 M507 S508 A509 ARG LYS SER PRO GLN ILE ALA

- Molecule 25: Trichohyalin-plectin-homology domain-containing protein

Chain 4G:

MET LEU ALA THR GLN LYS P7 R8 R9 E12 H19 R24 A25 K26 M27 P28 S29 K30 L31 P32 P33 D34 H35 L36 I37 L38 E39 R40 R41 K42 R43 D44 D45 Q46 R47 E48 E49 A50 E51 A52 K55 Y56 N57 A58 L59 C60 D61 L62 K63 N64 D65 W66 E67 K68 D71

R72 R73 K80 R81 R82 V83 R84 M87 Q88 E91 D96 Q99 R100 E103 M104 E107 E108 N109 D110 Q111 Y112 L113 V114 E115 M116 E117 A118 S119 Q120 E121 T122 L123 L124 E125 R126 Q127 S128 K129 M130 R131 E132 R133 A134 K135 F136 L137 K138 E139 K140 R141 E142 K143 E144

K147 E151 D154 Q155 E159 E160 C161 E162 E163 L164 R170 M173 D174 E175 D179 H182 Q183 L184 E185 T186 K187 A188 R189 M190 D194 Q195 E196 V197 E198 R199 D203 L204 W205 E206 K207 D208 R209 L210 A211 K212 GLU ALA LYS GLU GLU LYS ILE ALA GLN GLU

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

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

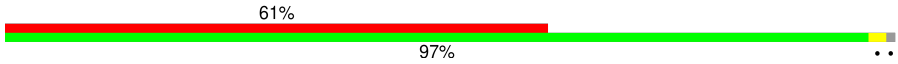
ARG LYS TYR LEU GLN GLU GLN MET ARG LEU GLU GLN GLN ARG GLU ALA GLU ILE ASP ARG MET ILE SER ALA GLU VAL GLU ARG GLN TRP GLN LYS ARG LEU SER GLN TRP ALA ALA LYS GLU ARG ASN ALA ARG LYS ARG LEU MET GLU GLU VAL LEU ALA ILE ARG ARG GLN GLN VAL GLU

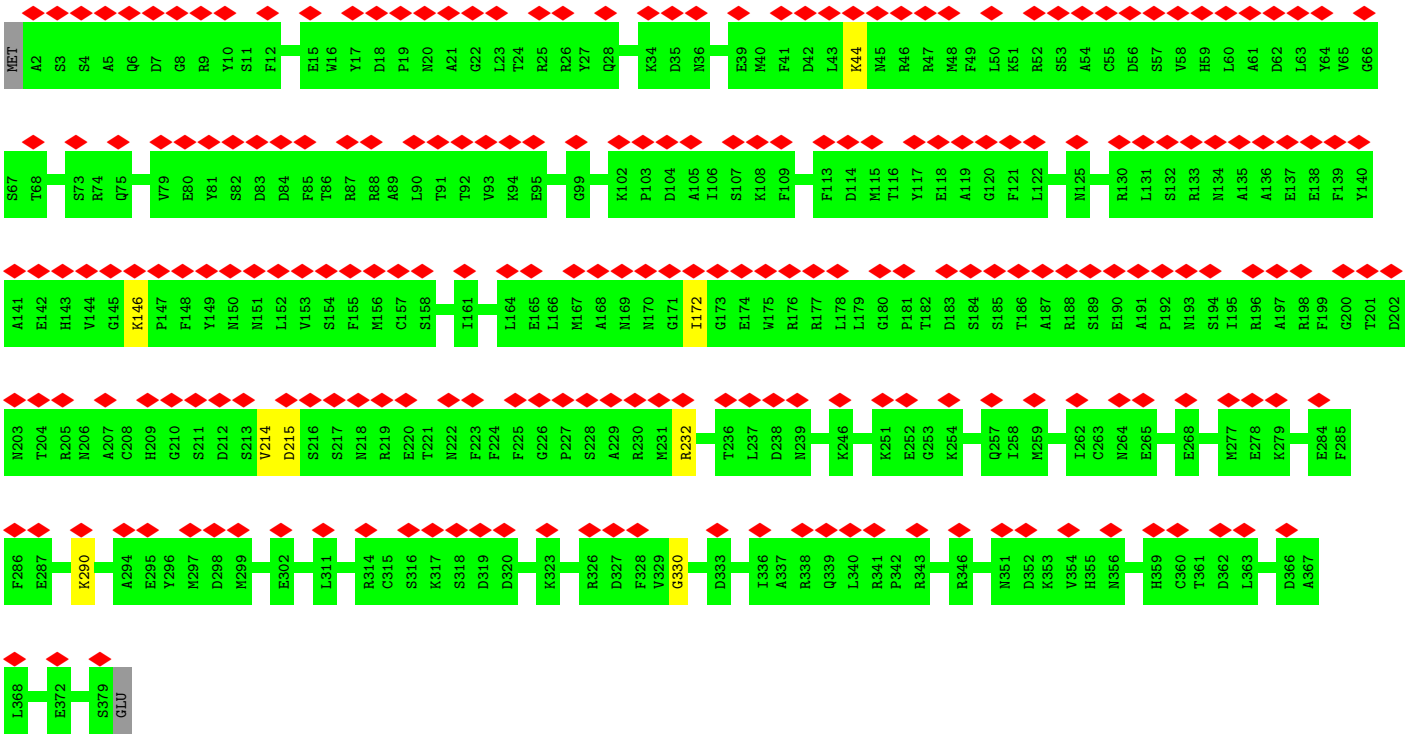
GLU ARG LEU ALA ASN ALA ALA ASN ALA GLN ALA GLU LEU ALA LYS GLU ARG GLU ALA MET GLN ALA ALA MET GLU GLU LYS GLU ALA ARG LEU ASP ASP GLU LYS GLN ALA ALA ILE LEU ALA ARG ASN LYS ASN TYR GLU GLN ASN LEU LEU GLN GLN

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

- Molecule 26: Nucleoside diphosphate kinase

Chain 4J:





- Molecule 26: Nucleoside diphosphate kinase

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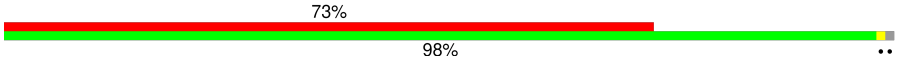
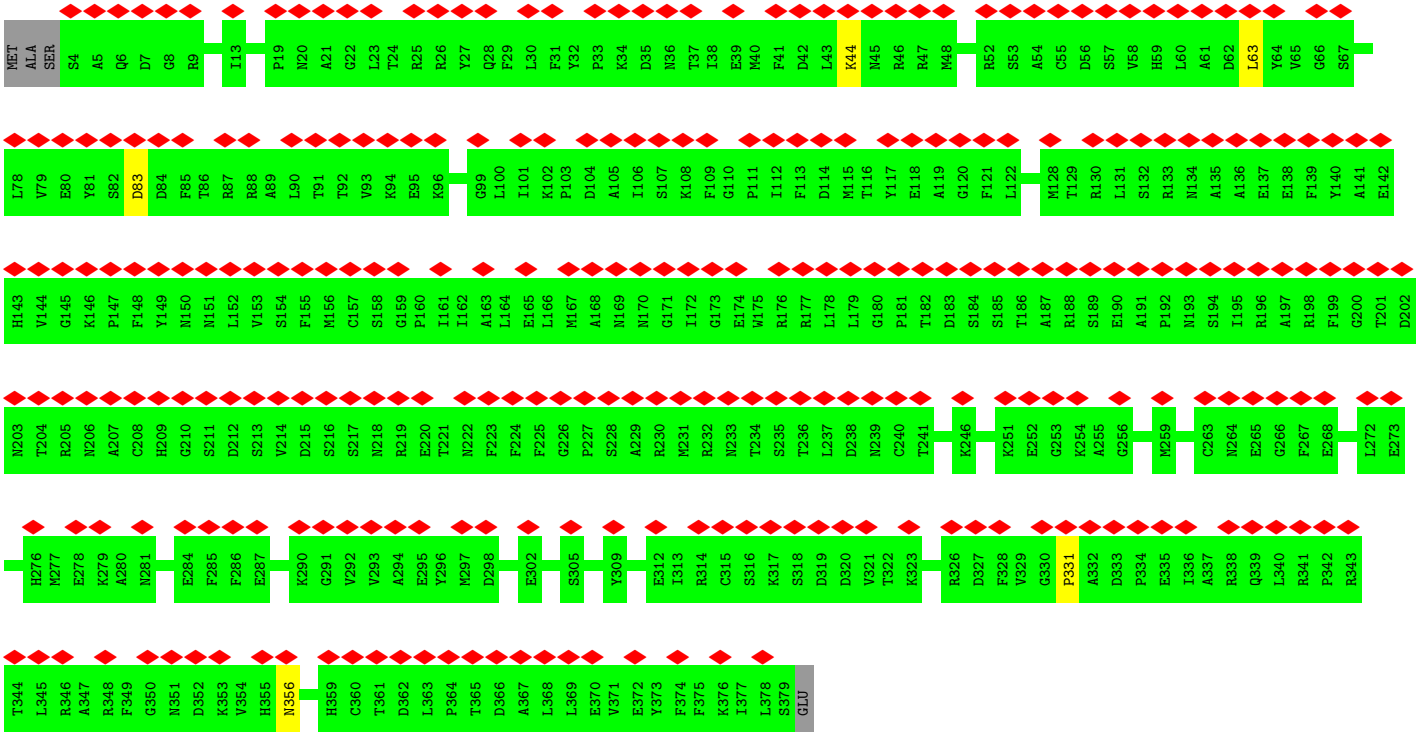
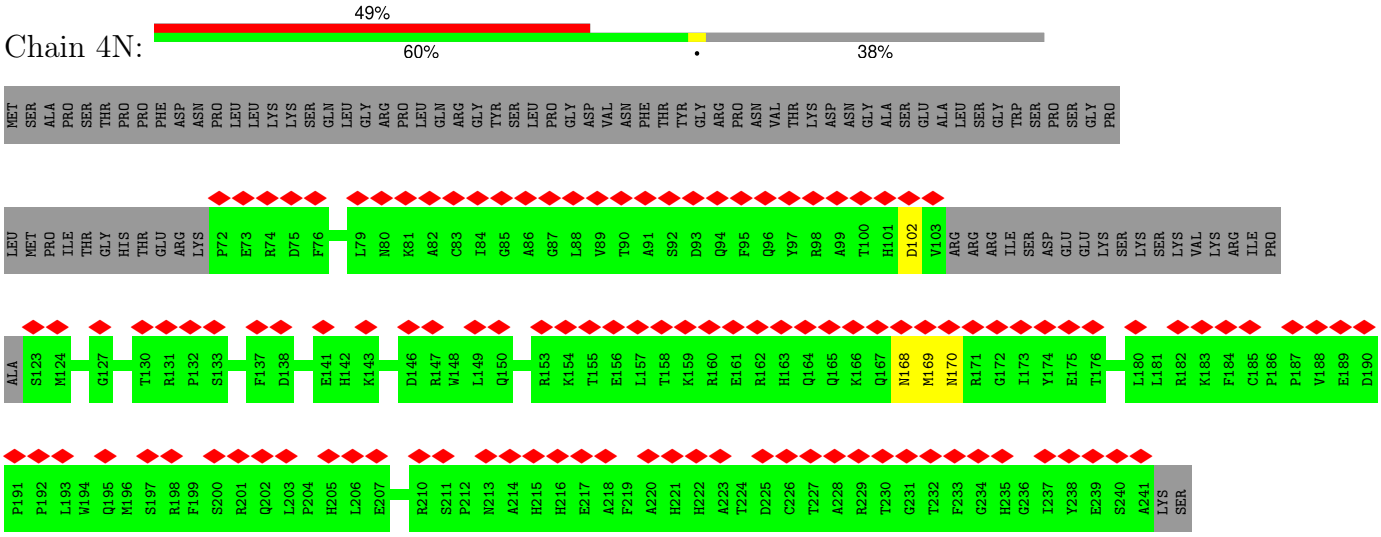




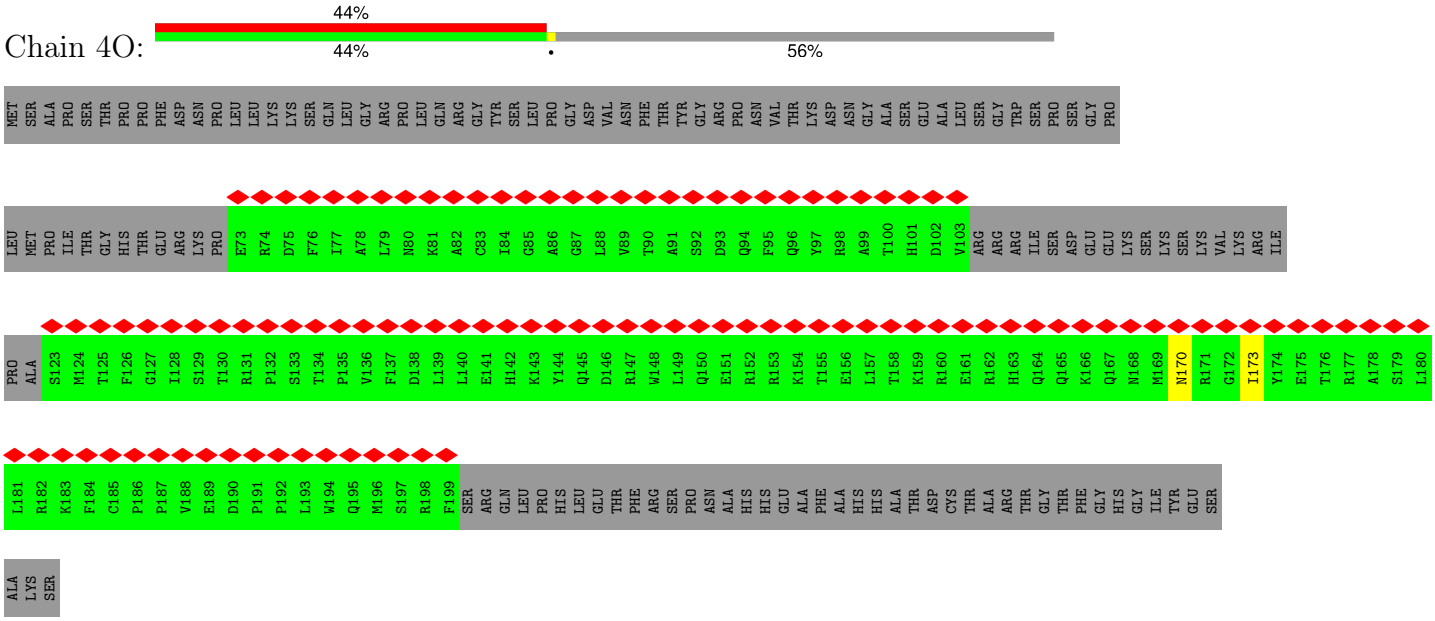
- Molecule 27: Cilia- and flagella-associated protein 77

Chain 4N:



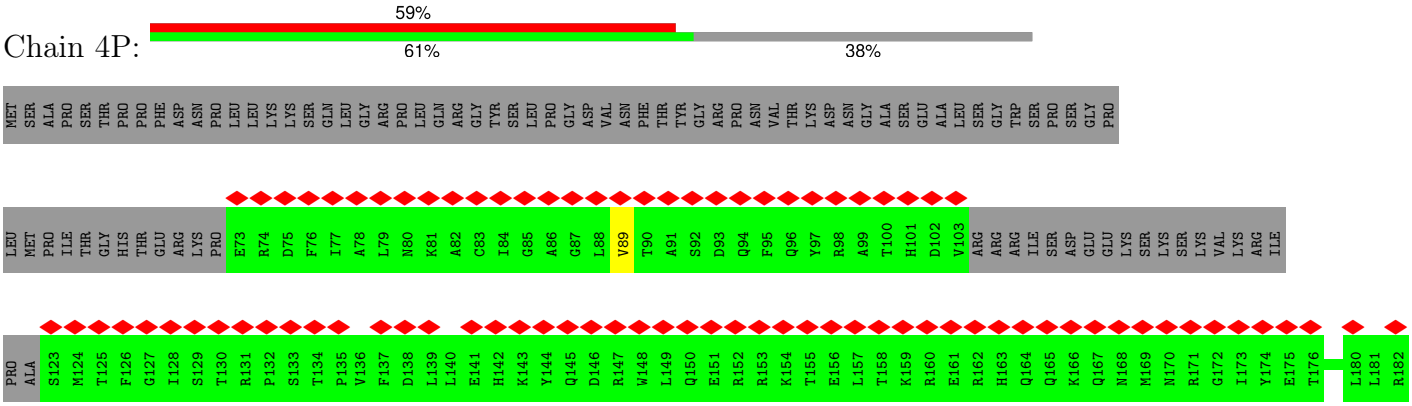
• Molecule 27: Cilia- and flagella-associated protein 77

Chain 4O:



• Molecule 27: Cilia- and flagella-associated protein 77

Chain 4P:



K183 F184 C185 P186 P187 V188 E189 D190 P191 P192 L193 W194 Q195 M196 S197 R198 F199 S200 R201 Q202 L203 P204 H205 L206 E207 T208 F209 R210 S211 P212 N213 A214 H215 H216 E217 A218 F219 A220 H221 H222 A223 T224 D225 C226 T227 A228 R229 T230 G231 T232 F233 G234 H235 G236 I237 Y238 E239 S240 A241 LYS

SER

• Molecule 27: Cilia- and flagella-associated protein 77

Chain 4Q: 37% 37% 62%

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

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

PRO ALA SER MET THR PHE GLY ILE SER THR ARG PRO SER THR PRO VAL PHE ASP LEU LEU GLU HIS LYS TYR GLN ASP ARG TRP L149 Q150 E151 R152 R153 K154 T155 E156 L157 T158 K159 R160 E161 R162 H163 Q164 Q165 K166 Q167 N168 M169 N170 R171 G172 I173 Y174 E175 T176 R177 A178 S179 L180

L181 R182 K183 F184 C185 P186 P187 V188 E189 D190 P191 P192 L193 W194 Q195 M196 S197 R198 F199 S200 R201 Q202 L203 P204 H205 L206 E207 T208 F209 R210 S211 P212 N213 A214 H215 H216 E217 A218 F219 A220 H221 H222 A223 T224 D225 C226 T227 A228 R229 T230 G231 T232 F233 G234 H235 G236 I237 Y238 E239 S240

A241 LYS SER

• Molecule 28: Cilia- and flagella-associated protein 97

Chain 4T: 62% 60% 38%

MET HIS ARG ALA TYR GLN PRO ILE THR PRO ALA N12 N13 K14 L15 L16 K17 K18 R19 W20 D21 E22 K23 R24 F25 D26 N27 H28 L29 Q30 K31 V32 Q33 S34 A35 R36 P37 V38 I39 D40 D41 K42 P43 P44 K45 T46 Y47 V48 H49 L50 H51 L52 K53 L54 K55 K56 M57 Q58 M59 E60

E61 E62 R63 L64 T65 I66 I67 E68 R69 D70 N71 R72 I73 L74 L75 E76 K77 M78 C79 H80 I81 M82 L83 T84 R85 G86 M87 V88 D89 N90 K91 N92 F93 Y94 D95 G96 K97 S98 L99 N100 R101 M102 A103 R104 Q105 R106 E107 L108 L109 R110 V111 T112 H113 E114 N115 Q116 A117 I118 M119 R120

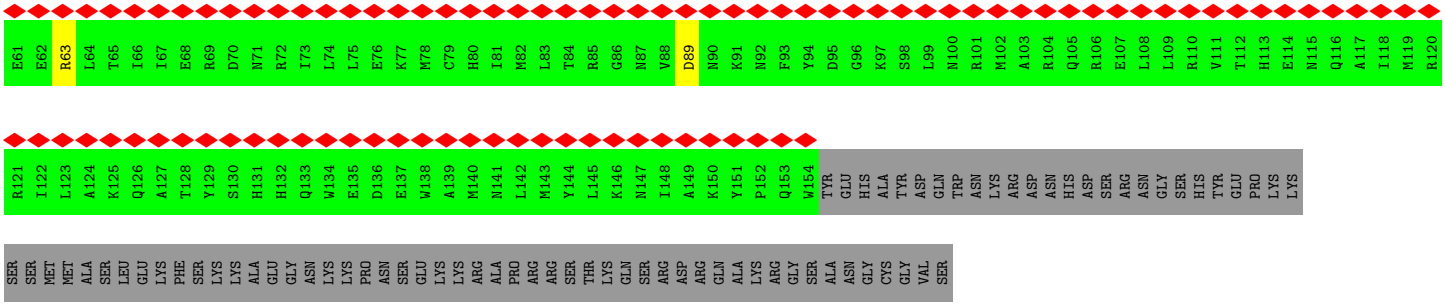
R121 I122 L123 A124 K125 Q126 A127 T128 Y129 S130 H131 H132 Q133 W134 E135 D136 E137 W138 A139 M140 N141 L142 M143 Y144 L145 K146 N147 I148 A149 K150 Y151 P152 Q153 W154 TYR GLU HIS ALA TYR ASP GLN TRP ASN LYS ARG ASP ASN HIS ASP SER ARG ASN GLY SER HIS TYR GLU PRO LYS LYS

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

• Molecule 28: Cilia- and flagella-associated protein 97

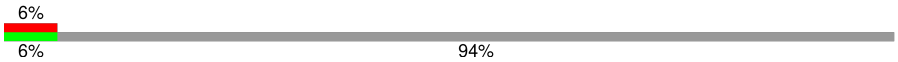
Chain 4U: 62% 61% 38%

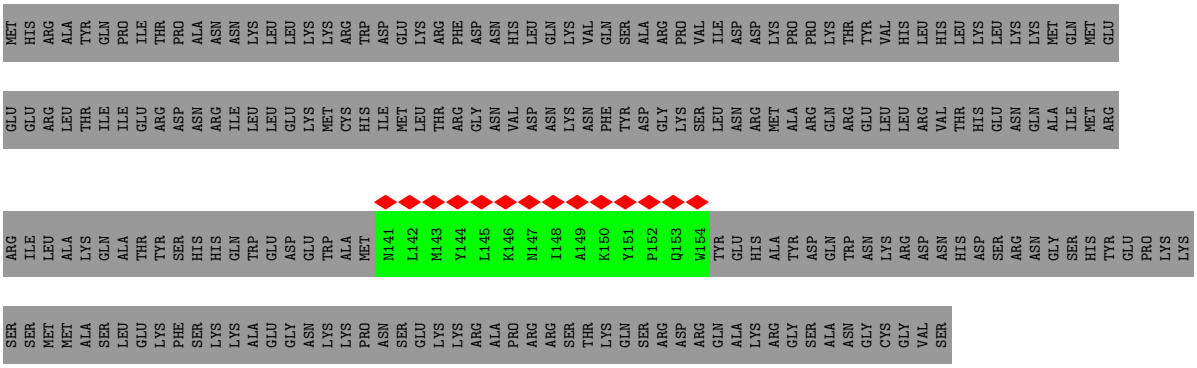
MET HIS ARG ALA TYR GLN PRO ILE THR PRO ALA N12 N13 K14 L15 L16 K17 K18 R19 W20 D21 E22 K23 R24 F25 D26 N27 H28 L29 Q30 K31 V32 Q33 S34 A35 R36 P37 V38 I39 D40 D41 K42 P43 P44 K45 T46 Y47 V48 H49 L50 H51 L52 K53 L54 K55 K56 M57 Q58 M59 E60



• Molecule 28: Cilia- and flagella-associated protein 97

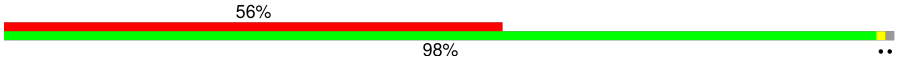
Chain 4V:

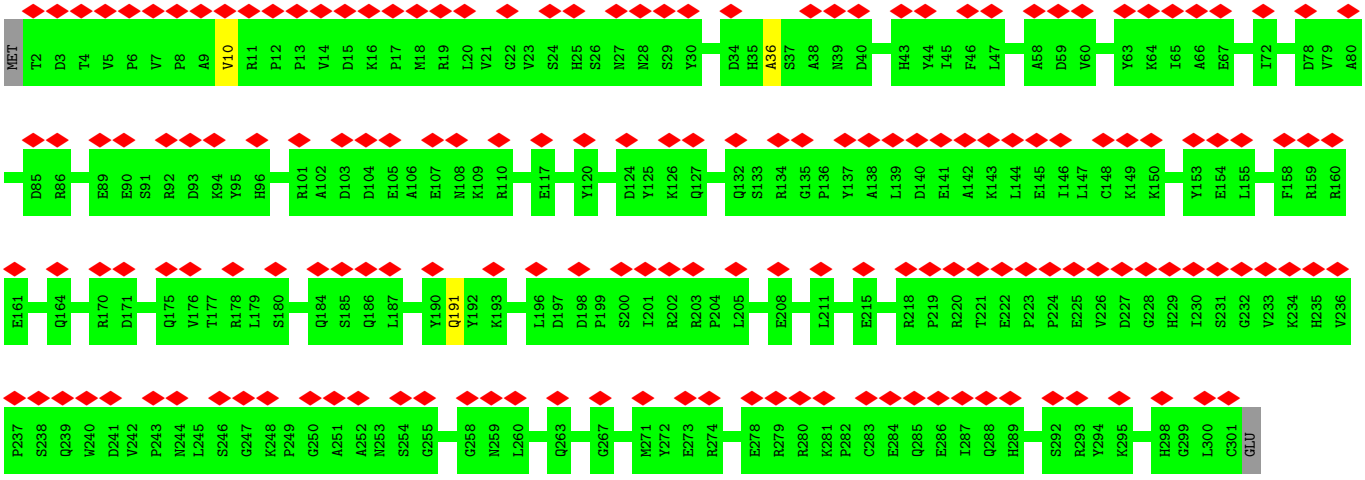




• Molecule 29: HeLo_like_N(LOC577943)

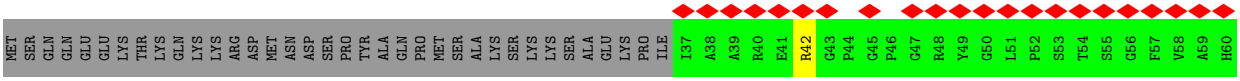
Chain 4Y:





• Molecule 30: Outer dense fiber protein 3

Chain 5A:



D61 F62 T63 K64 H65 M66 K67 P68 A69 Y70 S71 PHE GLY HIS ARG LEU GLU ASN SER MET PHE GLN LYS ASP CYS SER PRO GLY PRO GLY TYR LYS ILE HIS SER GLU ILE THR ARG VAL GLY LYS ASP GLY THR PRO ALA TYR SER MET LEU ALA ARG GLN LYS ASP PRO ASN THR PHE

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

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

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

- Molecule 30: Outer dense fiber protein 3

Chain 5B: 58% 74% • 23%

MET SER GLN GLN GLU GLU LYS THR LYS GLN LYS LYS ARG ASP MET ASN ASP SER PRO TYR ALA GLN PRO MET SER ALA LYS SER LYS LYS SER ALA GLU LYS PRO ILE ILE ALA ALA ARG GLU ARG GLY PRO GLY PRO GLY ARG TYR GLY LEU PRO SER THR S55 G56 F57 V58 A59 H60

D61 F62 T63 K64 H65 M66 K67 P68 A69 Y70 S71 F72 G73 H74 R75 L76 E77 ASN SER MET PHE GLN LYS ASP CYS S86 P87 G88 P89 G90 Y91 K92 I93 H94 S95 E96 I97 T98 R99 V100 G101 K102 D103 G104 T105 P106 A107 Y108 S109 M110 L111 A112 R113 Q114 K115 D116 P117 N118 T119 F120

I121 T122 P123 S124 P125 Y126 A127 Y128 S129 P130 E131 K132 V133 H134 P135 Q136 G137 E138 R139 H140 A141 P142 V143 H144 S145 M146 T150 R153 K154 R155 D156 Q157 A158 Y164 D165 V168 L169 L170 G171 S172 K173 N176 K177 Y178 S182 H183 S184 M185 T186 G187 R188 P189 H190 V191

G192 S193 Y194 L195 E196 D197 H198 A199 K200 C201 P202 G203 P204 G205 S206 H207 D208 A209 I210 H211 P212 D213 V214 T215 K216 F217 K218 K219 S223 M224 L225 G226 R227 H228 D229 L230 A231 N232 D233 S234 A235 T236 K237 H243 E246 K247 N251 K252 R253 K254 Y255 S259 L260 G261 I262

R263 H264 S265 E266 I272 V273 V274 V275 LYS ASP

- Molecule 30: Outer dense fiber protein 3

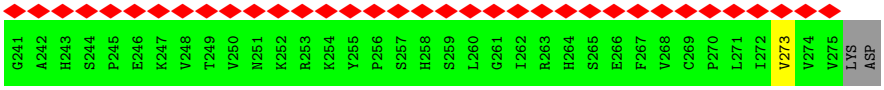
Chain 9Y: 50% 47% • 49%

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

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

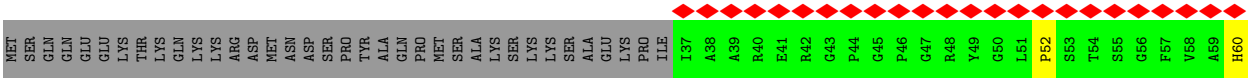
ILE THR PRO SER PRO TYR ALA TYR S129 P130 E131 K132 V133 H134 P135 Q136 G137 E138 R139 H140 A141 P142 V143 H144 S145 M146 G147 S148 R149 T150 R151 F152 R153 K154 R155 D156 Q157 A158 P159 A160 P161 N162 S163 Y164 D165 L166 P167 V168 L169 L170 G171 S172 K173 V174 P175 N176 K177 Y178 S179 S180

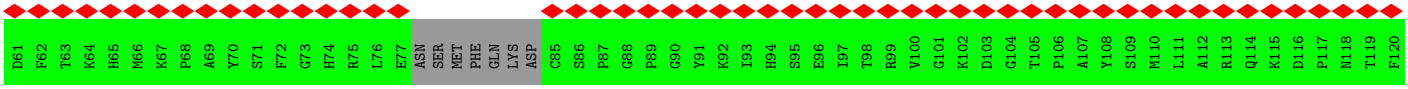
A181 S182 H183 S184 M185 T186 G187 R188 P189 H190 V191 G192 S193 Y194 L195 E196 D197 H198 A199 K200 C201 P202 G203 P204 G205 S206 H207 D208 A209 I210 H211 P212 D213 V214 T215 K216 F217 K218 K219 P220 S221 Y222 S223 M224 L225 G226 R227 H228 D229 LEU ALA ASN ASP SER ALA THR K237 P238 G239 P240

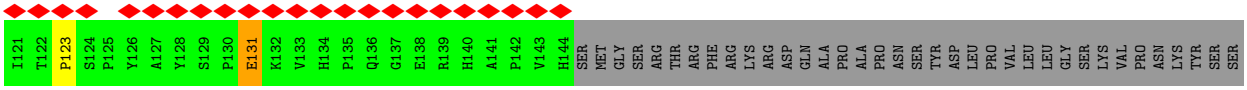


- Molecule 30: Outer dense fiber protein 3

Chain 9Z:

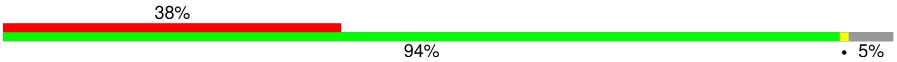


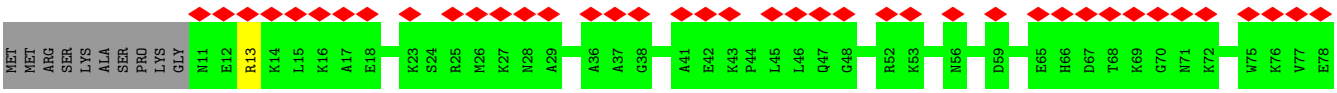


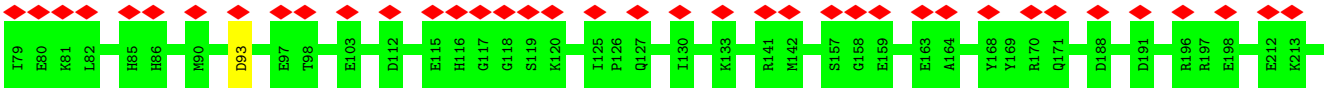


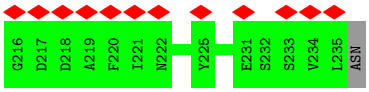
- Molecule 31: PACRG

Chain 6A:



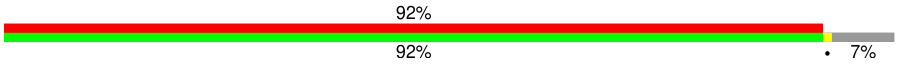


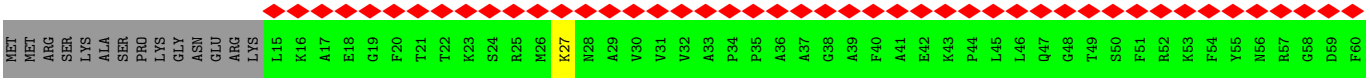


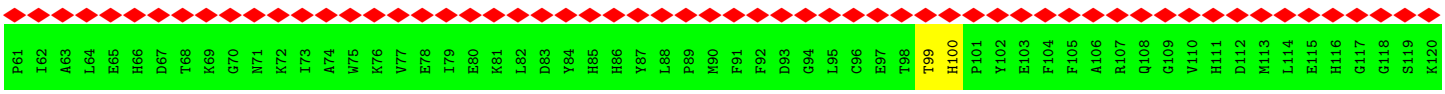


- Molecule 31: PACRG

Chain 6B:







- Molecule 31: PACRG

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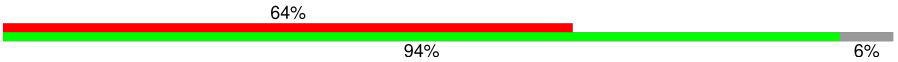
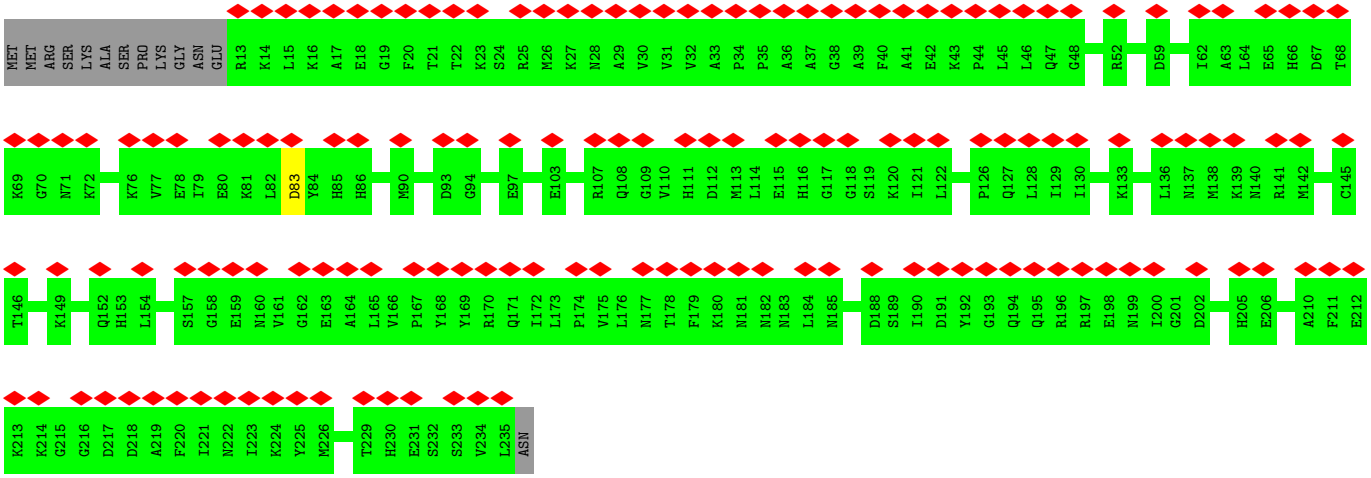
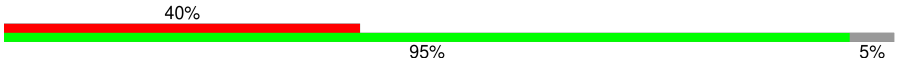
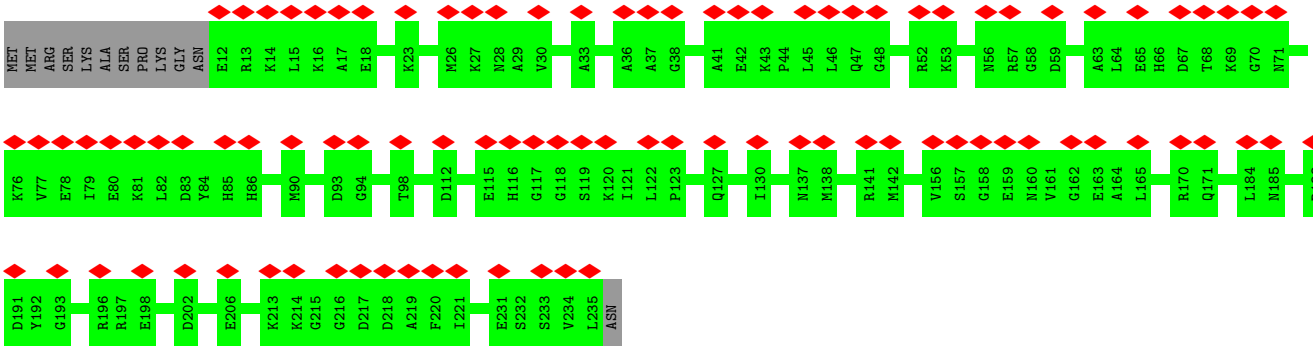




- Molecule 31: PACRG

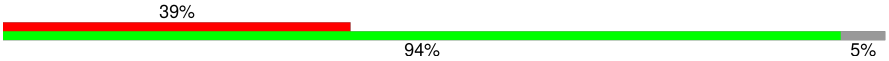
Chain 6D:

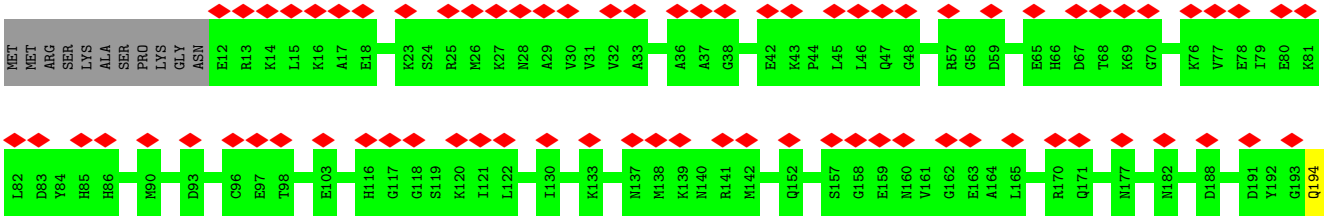


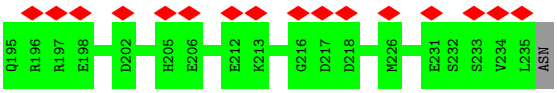


- Molecule 31: PACRG

Chain 6E:

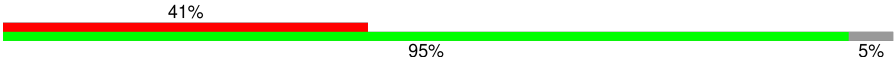


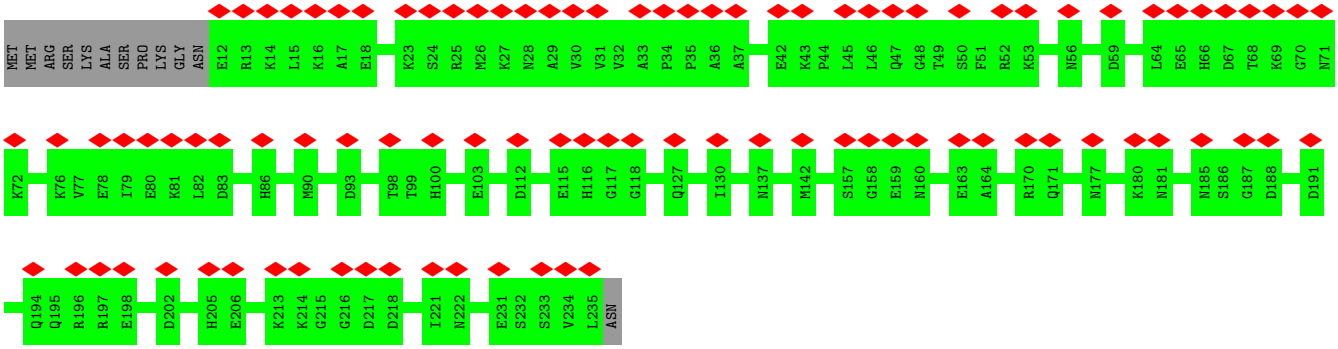




• Molecule 31: PACRG

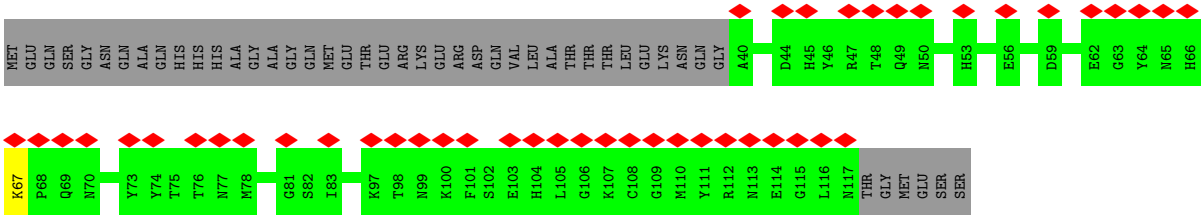
Chain 6F:





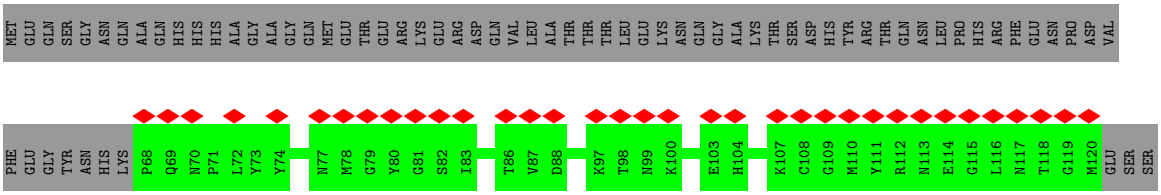
• Molecule 32: Pierce1

Chain 6I:



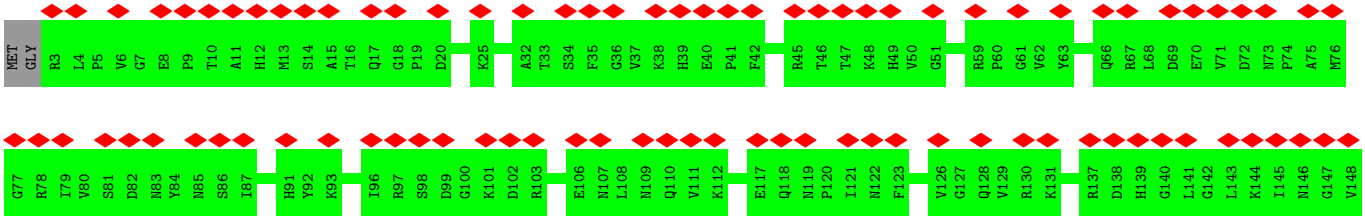
• Molecule 32: Pierce1

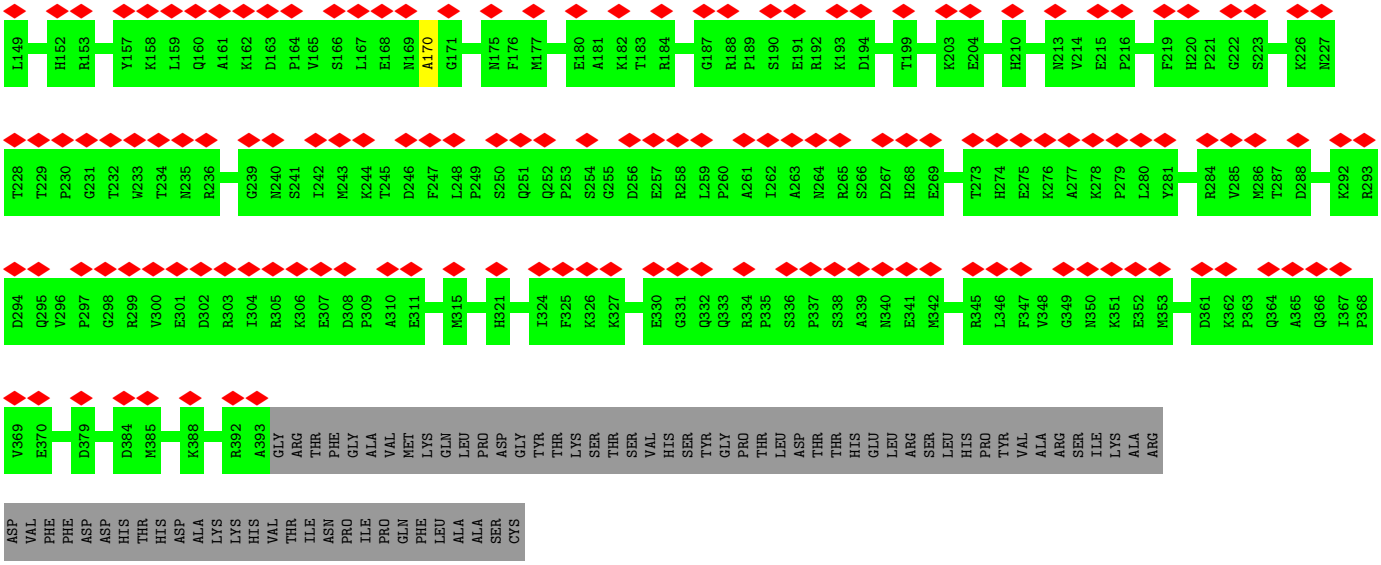
Chain 6J:



• Molecule 33: Protein phosphatase 1 regulatory subunit 32

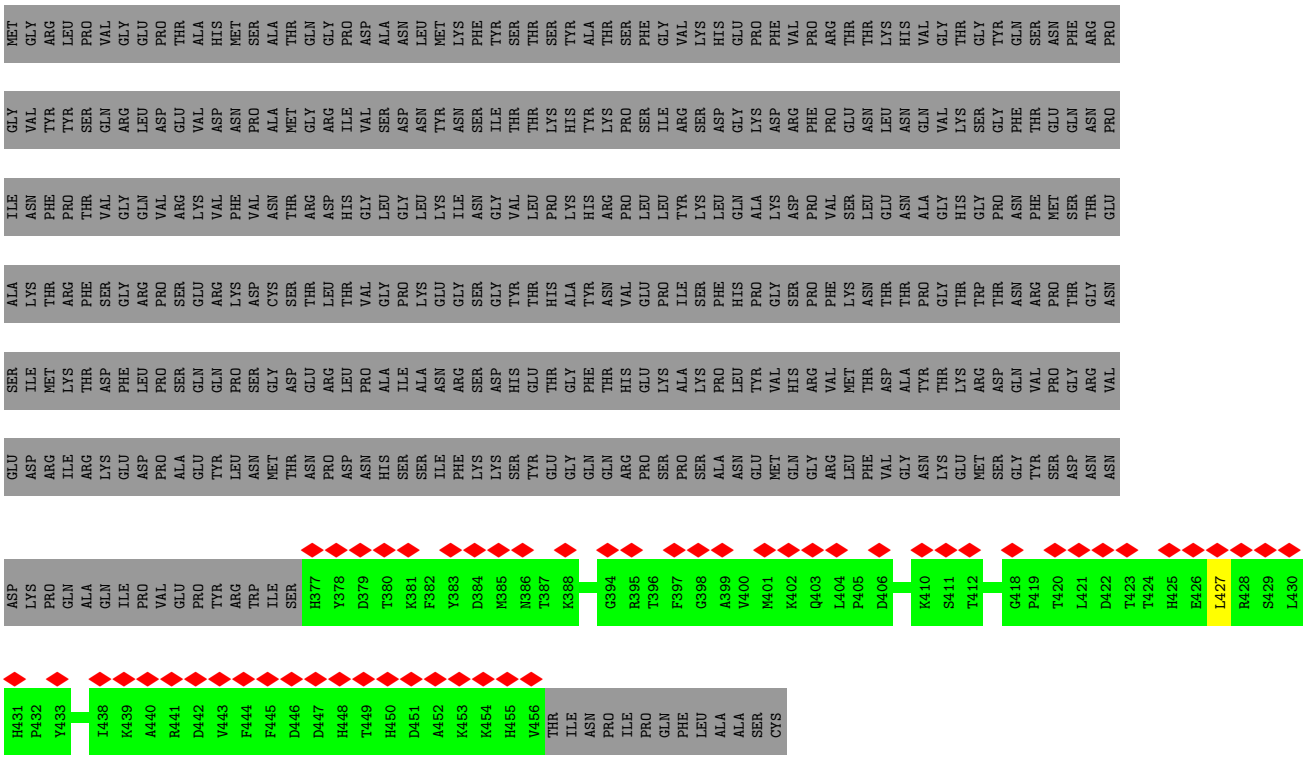
Chain 6M:





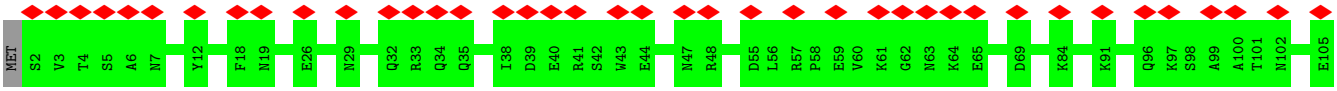
- Molecule 33: Protein phosphatase 1 regulatory subunit 32

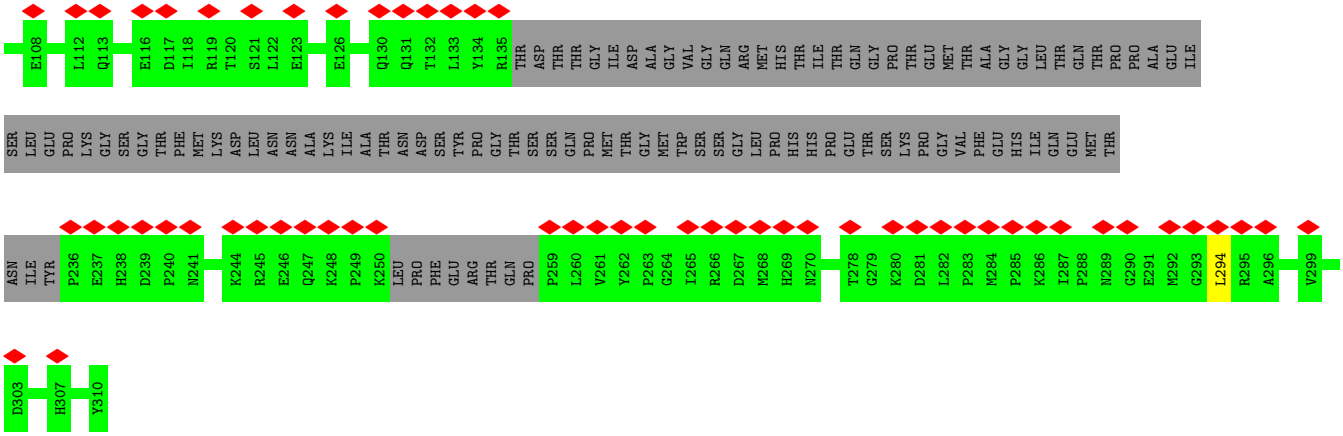
Chain 6N:



- Molecule 34: RIB35

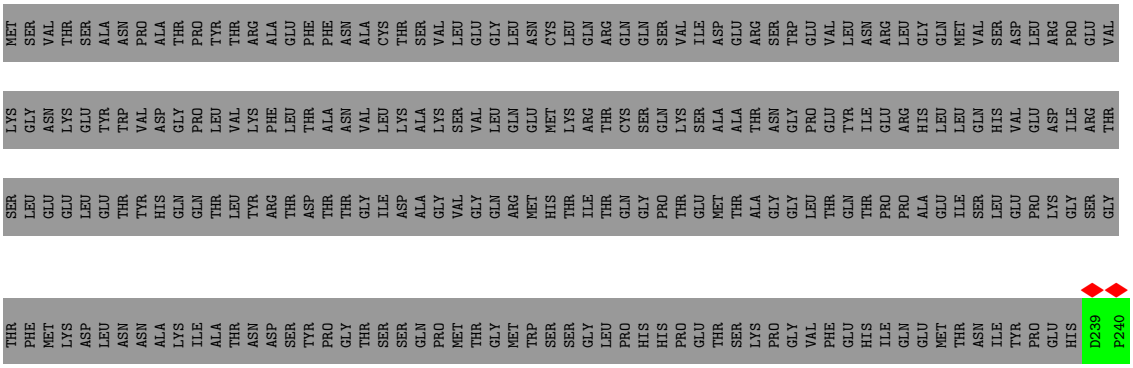
Chain 6Q:





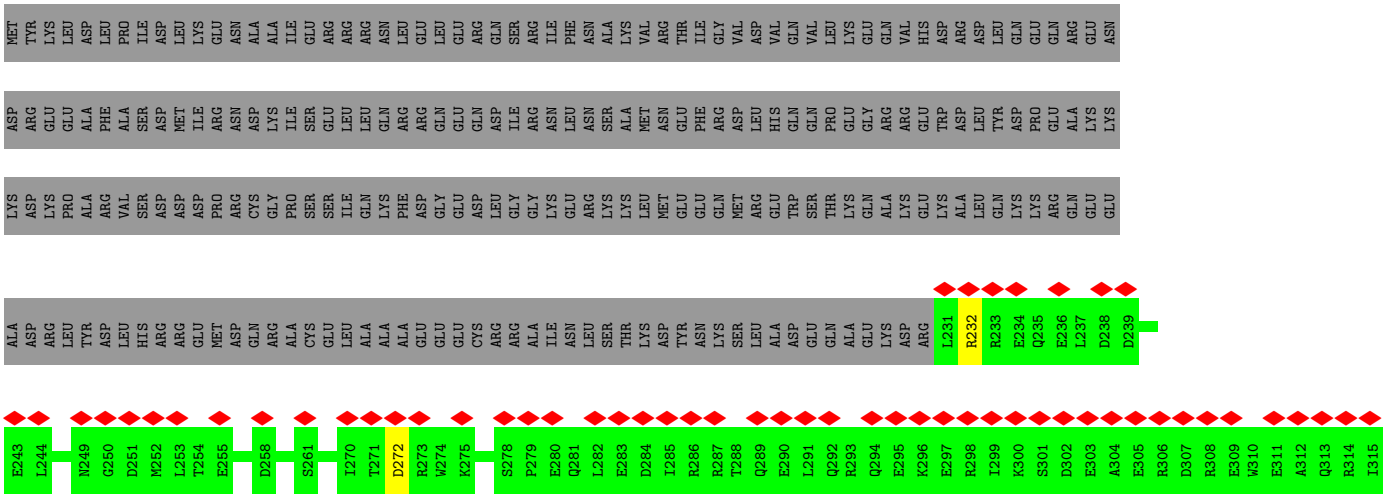
• Molecule 34: RIB35

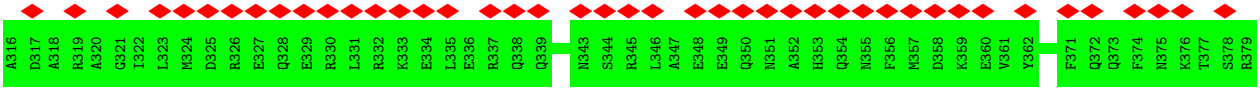
Chain 6R:



• Molecule 35: RIB43A-like with coiled-coils protein 2

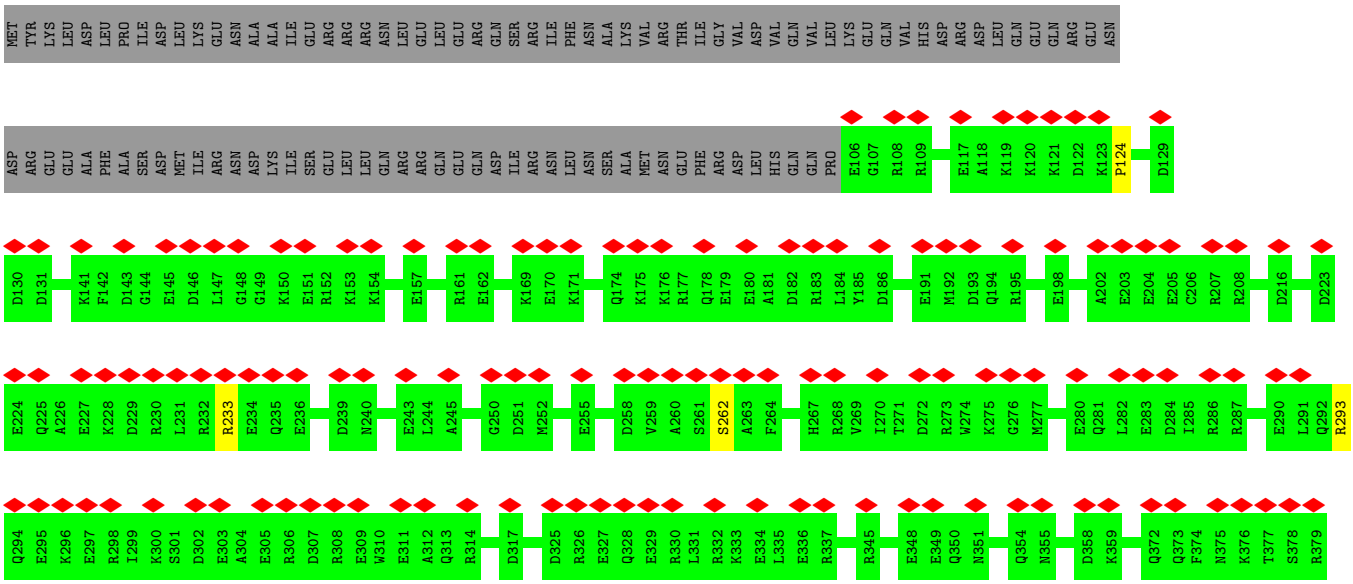
Chain 6U:





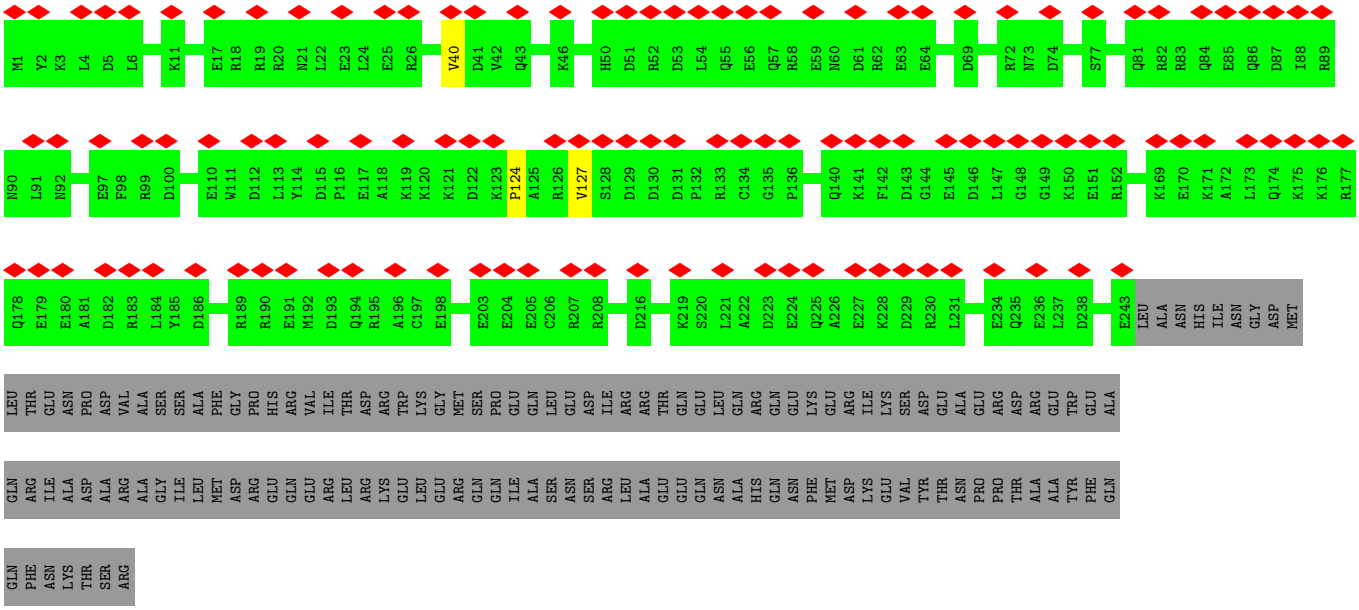
- Molecule 35: RIB43A-like with coiled-coils protein 2

Chain 6V:



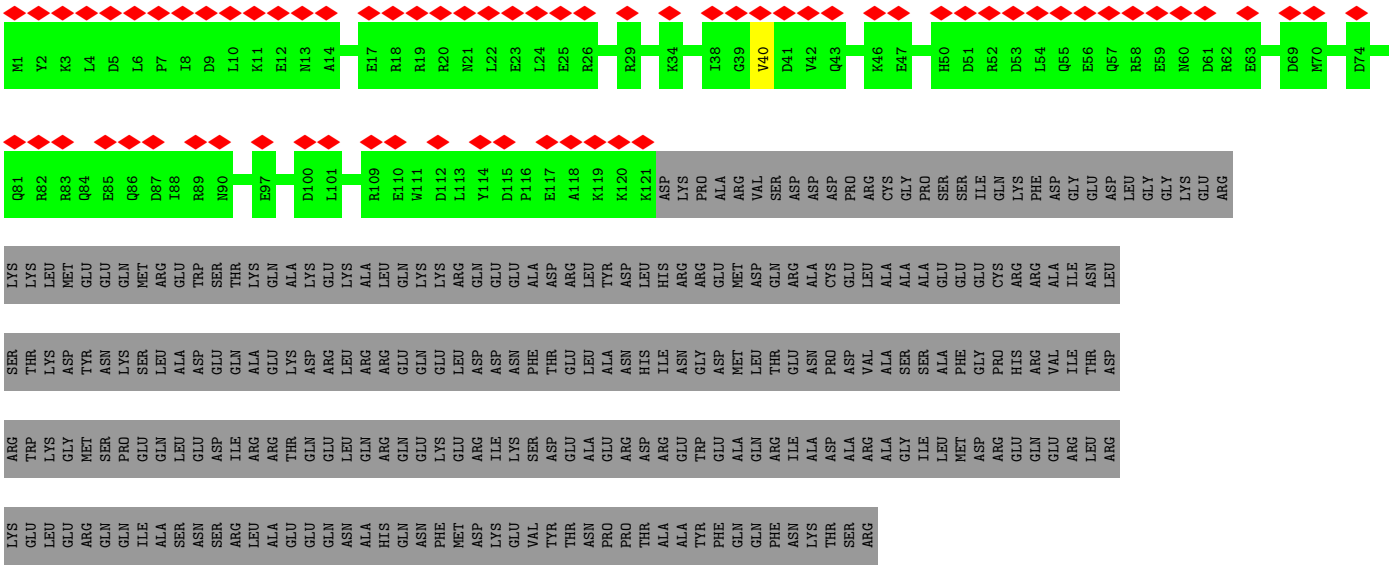
- Molecule 35: RIB43A-like with coiled-coils protein 2

Chain 6W:



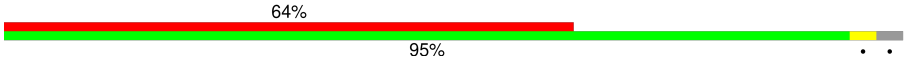
- Molecule 35: RIB43A-like with coiled-coils protein 2

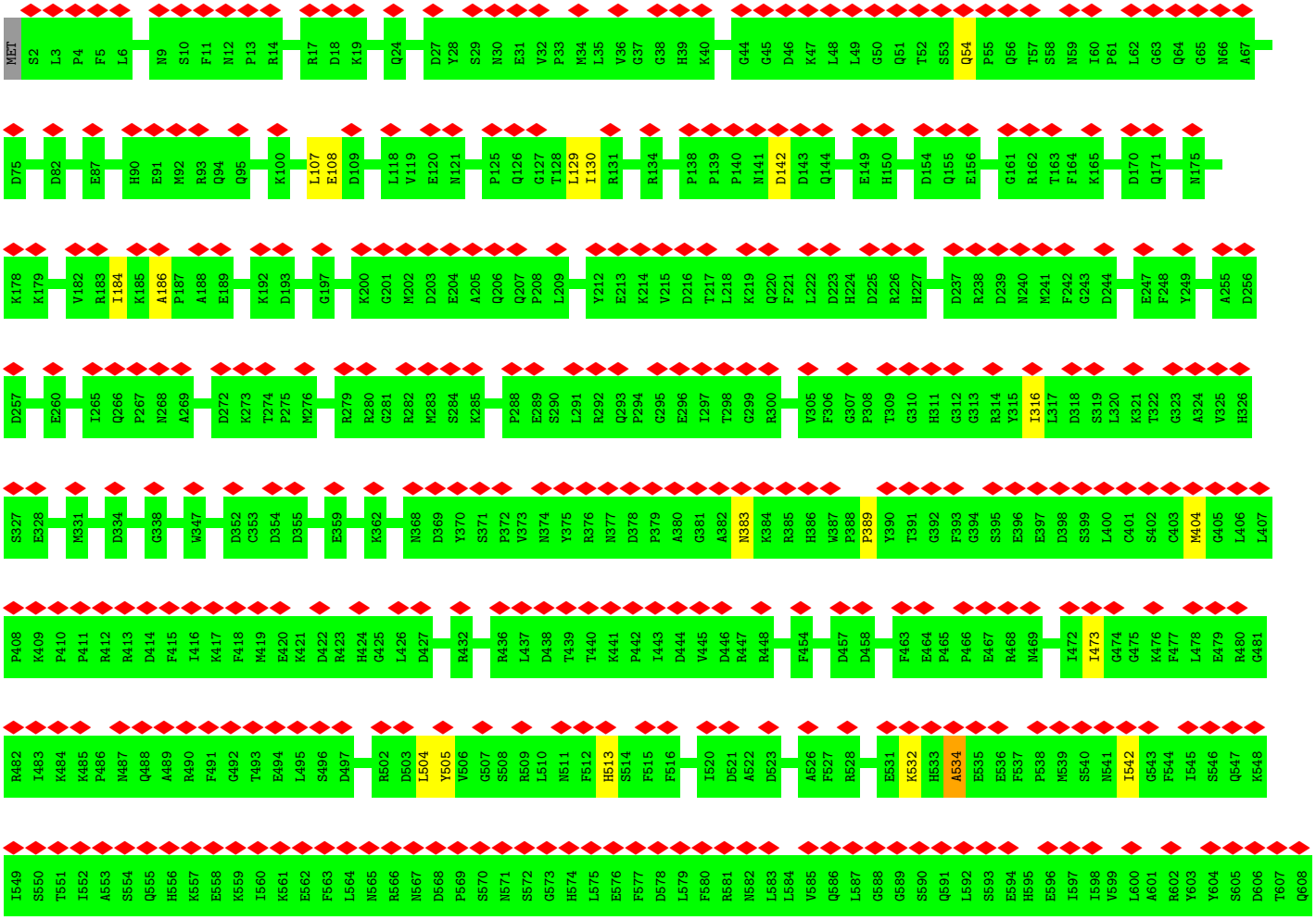
Chain 6X:



- Molecule 36: EF-hand domain-containing family member C2

Chain 7A:





D609 V610 K611 L612 S613 V614 E615 T616 L617 V618 S619 I620 V621 Q622 E623 Q624 L625 K626 K627 N628 S629 F630 E631 N632 F633 T634 K635 L636 L637 E638 G639 F640 L641 Q642 H643 D644 T645 D646 K647 S648 G649 Y650 L651 D652 G653 A654 L655 V656 R657 S658 N661 A662 F663 H664 L665 P666 L667 P668 D669

D670 L671 L672 R673 A674 L675 I676 S677 R678 L679 E680 A681 N682 E683 D684 G685 L686 V687 N688 Y689 N690 A691 L692 V693 T694 Y695 L696 N697 W698 R699 D700 H701 P702 M703 T704 T705 A706 Q707 Y708 V709 A710 P711 PRO ALA ASN PHE ASP GLU SER TRP THR GLY LYS ASP ASN GLY ASP ARG VAL LYS

R730 V731 N732 Y733 I734 A735 L736 L737 Q738 S739 I740 F741 P742 D743 M744

- Molecule 36: EF-hand domain-containing family member C2

Chain 7B: 53% 60% 39%

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

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

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

GLY VAL ARG ILE LYS ALA PRO ALA GLU THR PRO LYS ASP PRO TYR THR GLY PHE ARG LYS GLY MET ASP GLU ALA GLN GLN P208 L209 R210 P211 Y212 E213 K214 V215 D216 T217 L218 K219 Q220 F221 L222 D223 H224 D225 R226 H227 V228 L229 R230 F231 L232 C233 F234 TRP ASP ASP ARG ASP ASN

MET PHE GLY ASP L245 R246 E247 F248 Y249 L250 H251 Y252 F253 D256 D257 T258 I259 E260 I261 K262 E263 I264 I265 Q266 P267 N268 A269 G270 R271 D272 K273 T274 P275 M276 F277 L278 R279 R280 G281 R282 MET SER LYS ILE SER PRO GLU SER LEU ARG GLN PRO GLY GLU ILE THR GLY ARG THR

VAL LEU ASN VAL PHE GLY PRO THR GLY HIS GLY GLY ARG TYR ILE LEU ASP SER LEU LYS THR GLY ALA VAL HIS SER GLU PHE Y330 M331 E332 N333 D334 L335 T336 I337 G338 S339 T340 ILE ASN ALA ASN GLY ARG TRP LEU T349 L350 A351 D352 C353 D354 D355 F356 E359 K362 Q363

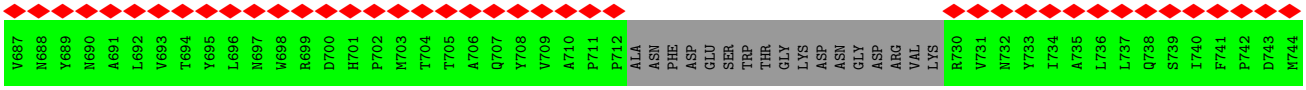
N368 D369 Y370 S371 P372 V373 N374 Y375 R376 N377 D378 P379 A380 G381 A382 N383 K384 R385 H386 W387 P388 P389 Y390 T391 G392 F393 G394 S395 E396 E397 D398 S399 L400 C401 S402 C403 M404 G405 L406 L407 P408 K409 P410 P411 R412 R413 D414 F415 I416 F418 M419 E420 K421 D422 R423 H424 G425 L426

D427 R432 R436 L437 D438 T439 T440 K441 P442 I443 D444 V445 D446 R447 R448 L455 S456 D457 D458 F463 P466 E467 R468 N469 S470 G471 I472 I473 G474 G475 K476 F477 L478 E479 R480 G481 R482 I483 K484 K485 P486 N487 Q488 A489 R490 F491 G492 T493 E494 L495 S496 D497 Y498 A501

R502 D503 L504 Y505 V506 G507 S508 R509 L510 N511 F512 H513 S514 F515 F516 F517 D521 A522 D523 E524 R528 Y529 M530 E531 K532 H533 A534 E535 E536 F537 P538 M539 S540 N541 I542 G543 F544 I545 S546 Q547 K548 I549 S550 T551 I552 A553 S554 Q555 H556 K557 E558 K559 I560 K561 E562 F563 L564 N565

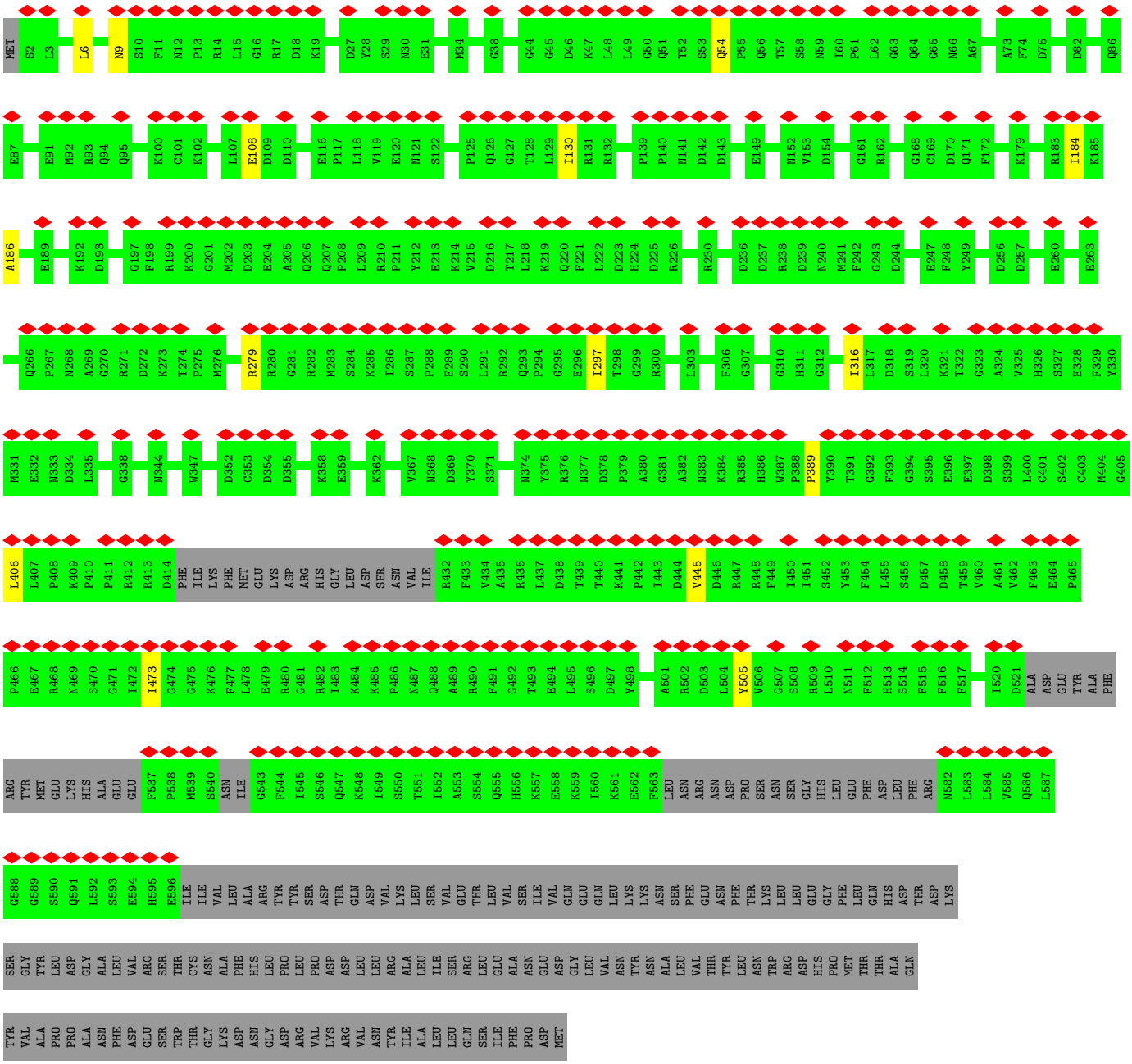
R566 N567 D568 P569 S570 N571 S572 G573 H574 L575 E576 F577 D578 L579 F580 R581 N582 L583 L584 V585 Q586 L587 G588 G589 S590 Q591 L592 S593 E594 H595 E596 I597 I598 V599 L600 A601 R602 Y603 Y604 S605 D606 T607 Q608 D609 V610 K611 L612 S613 V614 E615 T616 L617 V618 S619 I620 V621 Q622 E623 Q624 L625

K626 K627 N628 S629 F630 E631 N632 F633 T634 K635 L636 L637 E638 G639 F640 L641 Q642 H643 D644 T645 D646 K647 S648 G649 Y650 L651 D652 G653 A654 L655 V656 R657 S658 N661 A662 F663 H664 L665 P666 L667 P668 D669 D670 L671 L672 R673 A674 L675 I676 S677 R678 L679 E680 A681 N682 E683 D684 G685 L686



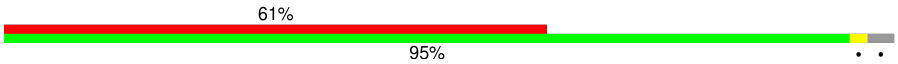
• Molecule 36: EF-hand domain-containing family member C2

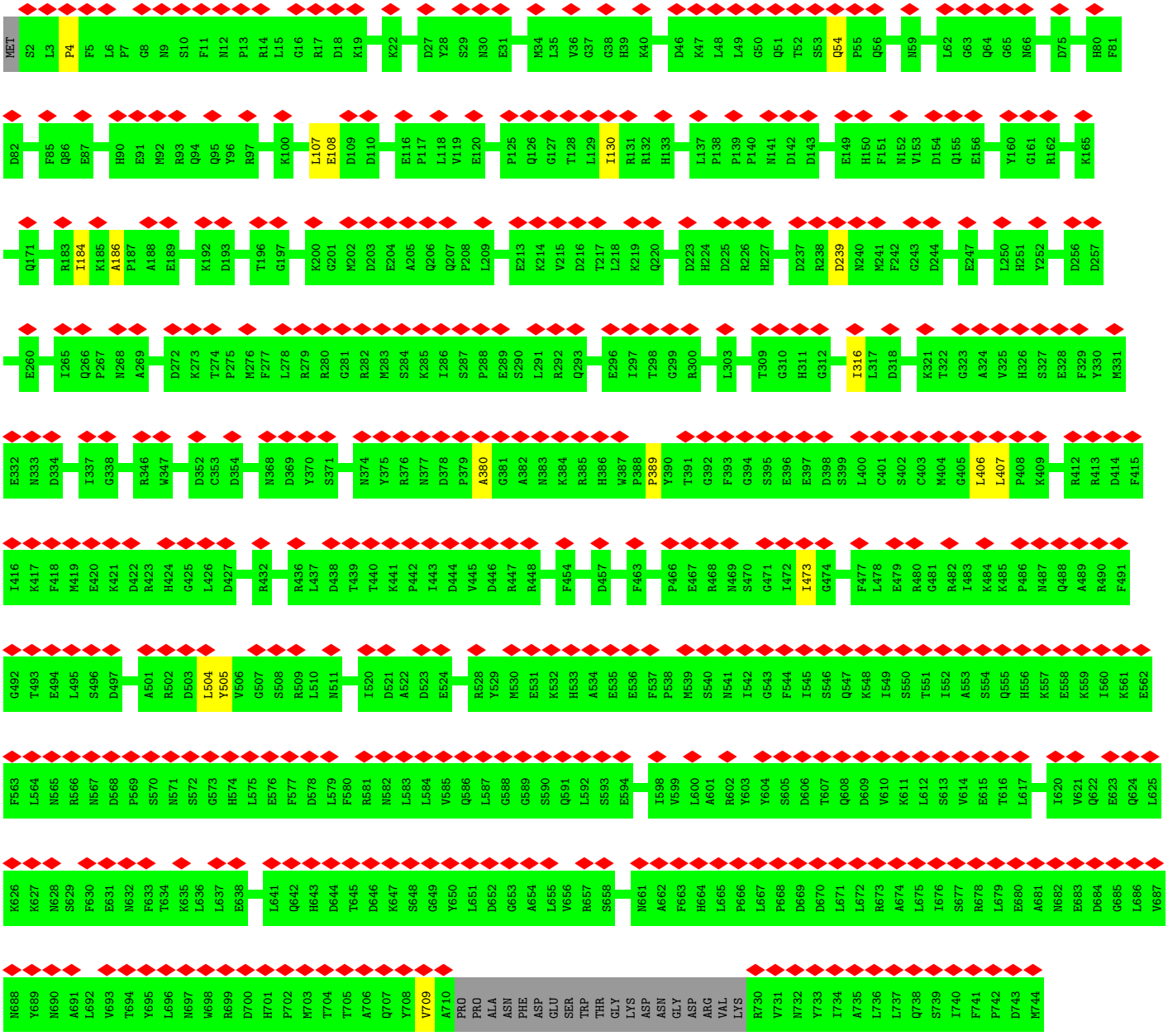
Chain 7C:



• Molecule 36: EF-hand domain-containing family member C2

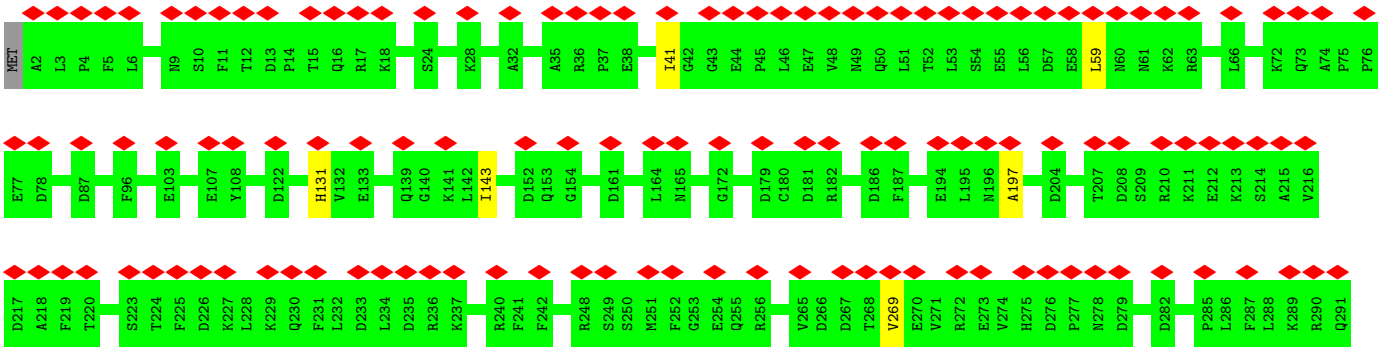
Chain 7D:

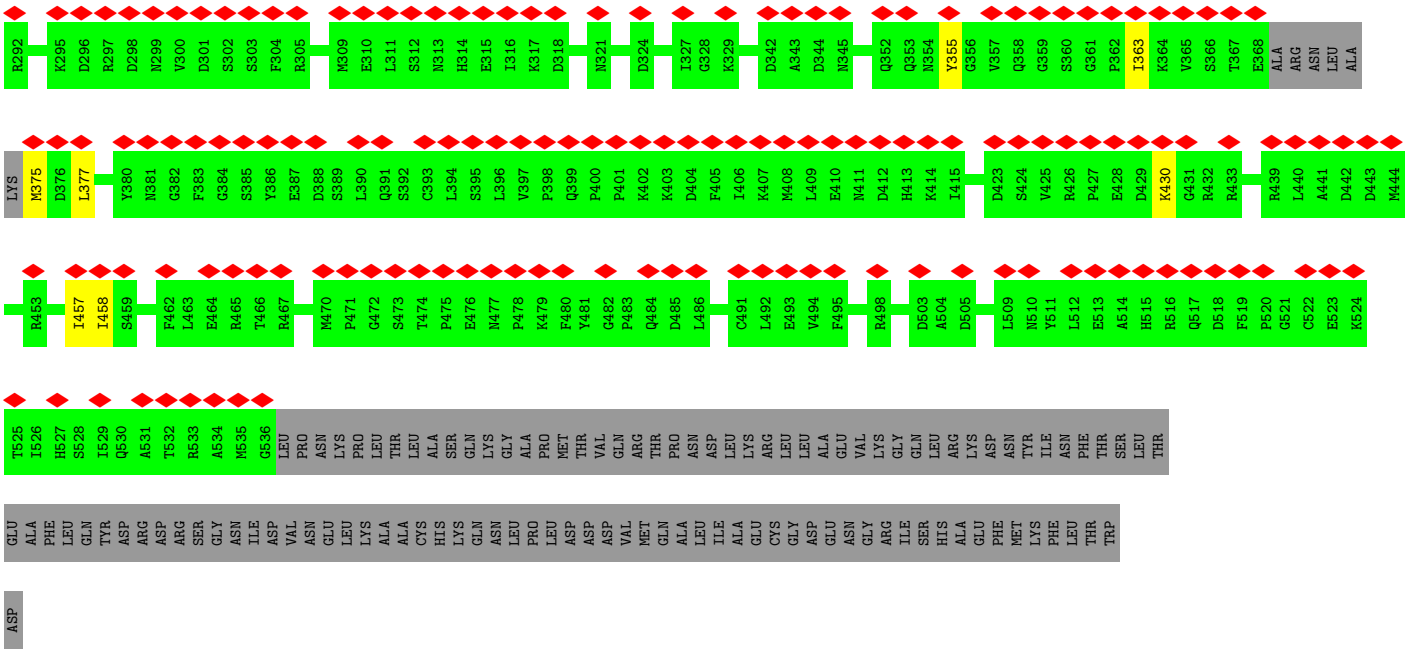




- Molecule 37: Flagellar protofilament ribbon protein rib74

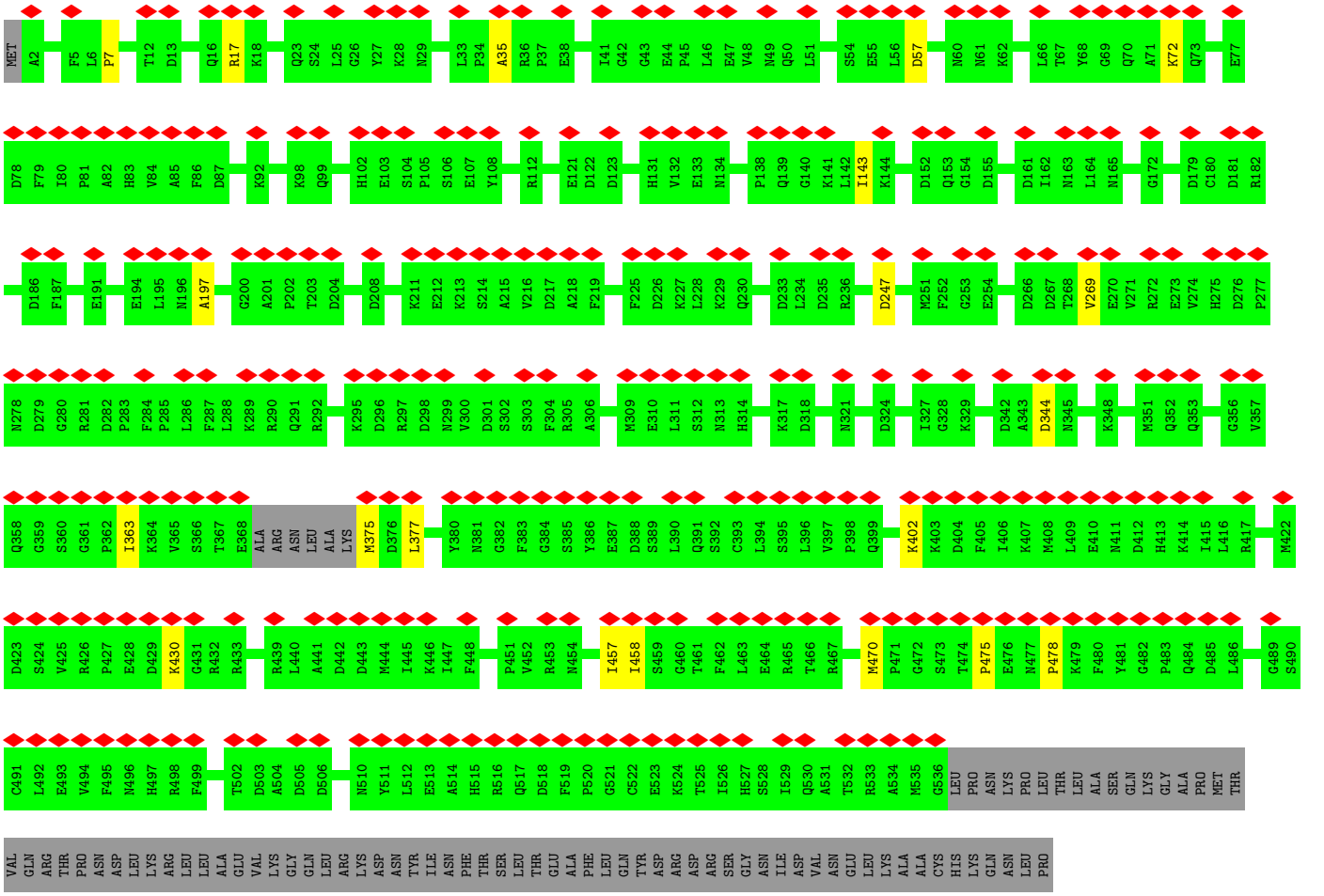
Chain 7G:





- Molecule 37: Flagellar protofilament ribbon protein rib74

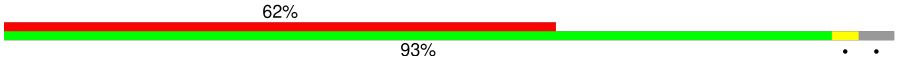
Chain 7H:



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

- Molecule 37: Flagellar protofilament ribbon protein rib74

Chain 7I:



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R63 P64 T65 L66 G69 Q70 A71 K72 Q73 A74 P75 P76 E77 D78 H83 D87 F96 H102 E103 S104 P105 S106 E107 Y108 R112 P113 L116 E121 D122 P130 H131 V132 E133 G136 M137 P138 Q139 G140 K141 L142 T143 K144 R147 K150 N151 D152 Q153 G154

D155 H156 K160 D161 I162 N163 L164 N165 I166 Y171 G172 D179 R182 D186 F187 E194 L195 N196 A197 A201 P202 T203 D204 D208 K211 E212 K213 S214 A215 V216 D217 A218 F219 S223 T224 F225 D226 K227 L228 K229 D233 L234 D235 R236 K237 V238 L239 R240 F241

F242 R248 S249 S250 M251 F252 G253 E254 Q261 Y262 V265 D266 D267 T268 V269 E270 V271 R272 E273 V274 H275 D276 P277 N278 D279 G280 R281 D282 P283 F284 P285 L286 K289 R290 Q291 R292 K295 D296 R297 D298 N299 V300 D301 S302 S303 F304 R305 A306 M309 E310 L311 S312 N313 H314

E315 I316 K317 D318 N321 D324 F325 G326 I327 G328 K329 N335 D342 A343 D344 N345 Q352 Q353 G356 V357 Q358 G359 S360 G361 P362 I363 K364 V365 S366 T367 E368 ALA ARG ASN LEU ALA LYS M375 D376 L377 P378 P379 Y380 N381 G382 F383 G384 S385 Y386 E387 D388 S389 L390 Q391

S392 C393 L394 S395 L396 V397 P398 Q399 P400 P401 K402 K403 D404 F405 I406 K407 M408 L409 E410 N411 D412 H413 K414 I415 L416 R417 M422 D423 S424 V425 R426 P427 E428 D429 K430 G431 R432 R433 R439 L440 A441 D442 D443 M444 I445 K446 I447 F448 R453 I457 I458 S459 E464 R465 T466

R467 M470 P471 G472 S473 T474 P475 E476 N477 P478 K479 Q484 D485 L486 E493 V494 F495 N496 H497 R498 D503 A504 D505 D506 L512 E513 A514 H515 R516 Q517 D518 F519 P520 G521 C522 E523 K524 T525 I526 H527 S528 I529 Q530 A531 T532 R533 A534 M535 G536 LEU PRO ASN LYS PRO LEU

THR LEU ALA SER GLN LYS GLY ALA PRO MET THR VAL GLN ARG T557 P558 N559 D560 L561 K562 R563 L564 L565 A566 E567 V568 K569 G570 Q571 L572 R573 K574 D575 N576 Y577 I578 N579 F580 T581 S582 L583 T584 E585 A586 F587 L588 Q589 Y590 D591 R592 D593 R594 S595 G596 N597 I598 D599 V600 N601 E602

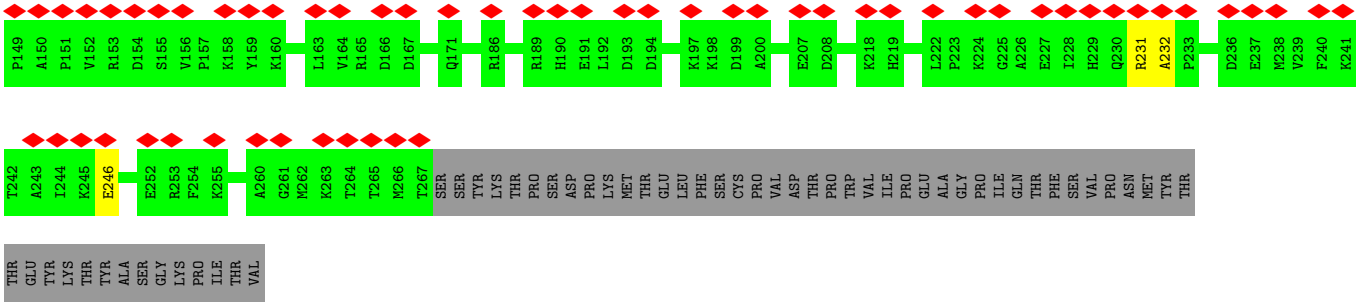
L603 K604 A605 A606 C607 H608 K609 Q610 N611 L612 P613 L614 D615 D616 D617 V618 M619 Q620 A621 L622 I623 A624 E625 C626 G627 D628 E629 N630 G631 R632 I633 S634 H635 A636 E637 F638 M639 K640 F641 L642 T643 TRP ASP

- Molecule 38: SAXO3(LOC115918676)

Chain 7M:

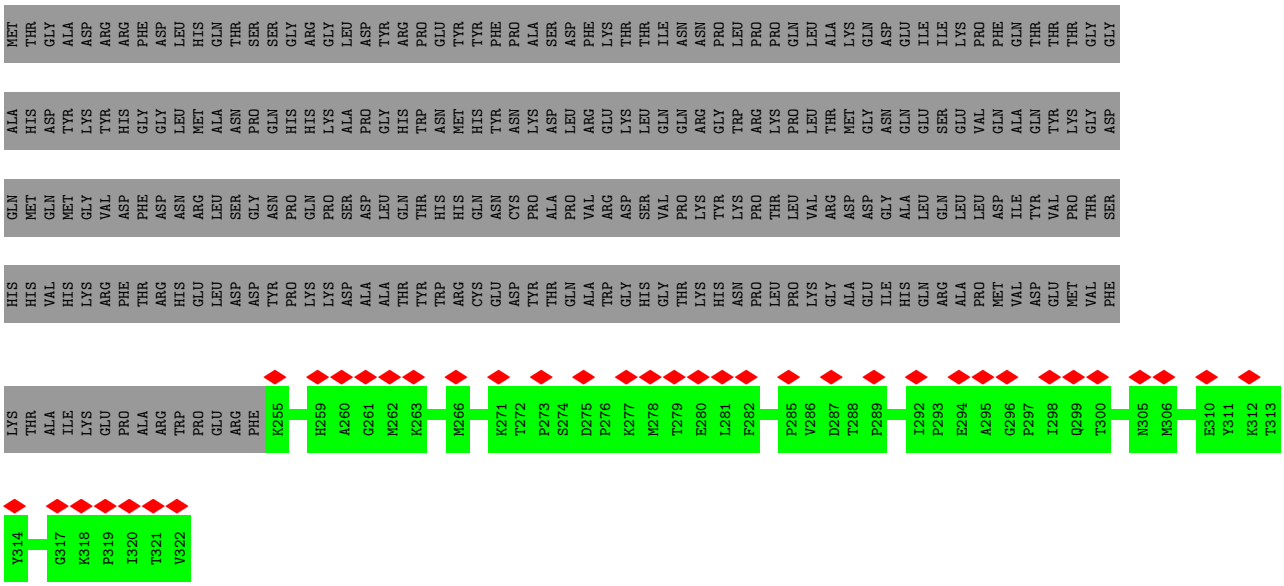
MET THR GLY ALA D5 R6 R7 F8 D9 L10 H11 Q12 S15 G16 R17 G18 L19 D20 Y25 Y26 F27 S30 D31 F32 K33 T34 T35 I36 N37 N38 P39 L40 Q43 K46 Q47 D48 E49 K52 Q55 T56 T57 G60 A61 H62 D63 Y64 K65 Y66 H67 G68 G69 L70

M71 A72 N73 P74 Q75 H76 H77 K78 M85 D90 K94 L95 Q96 K102 M106 G107 N108 Q109 E110 S111 E112 V113 Q114 A115 Q116 Y117 K118 G119 D120 Q121 M122 Q123 M124 G125 V126 D127 F128 D129 N130 R131 L132 S133 G134 N135 P136 S139 D140 L141 Q142 H145 Q146 N147 C148



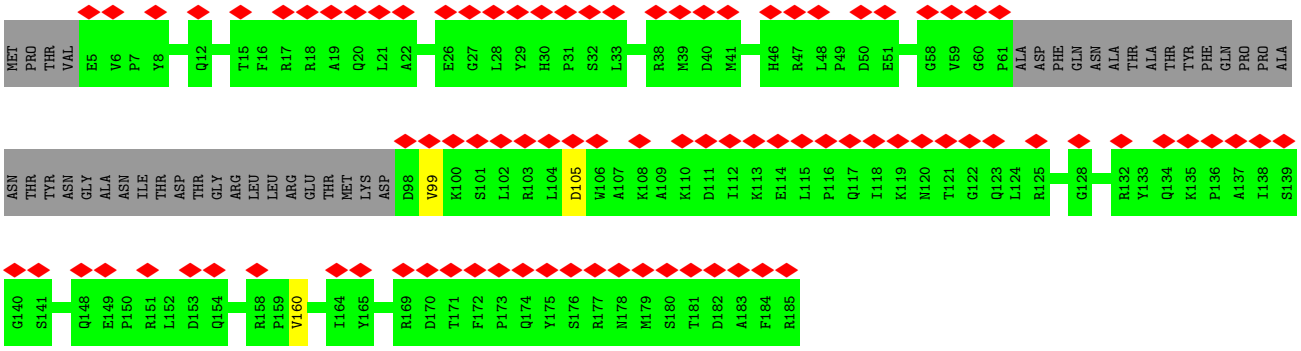
- Molecule 38: SAXO3(LOC115918676)

Chain 7N:



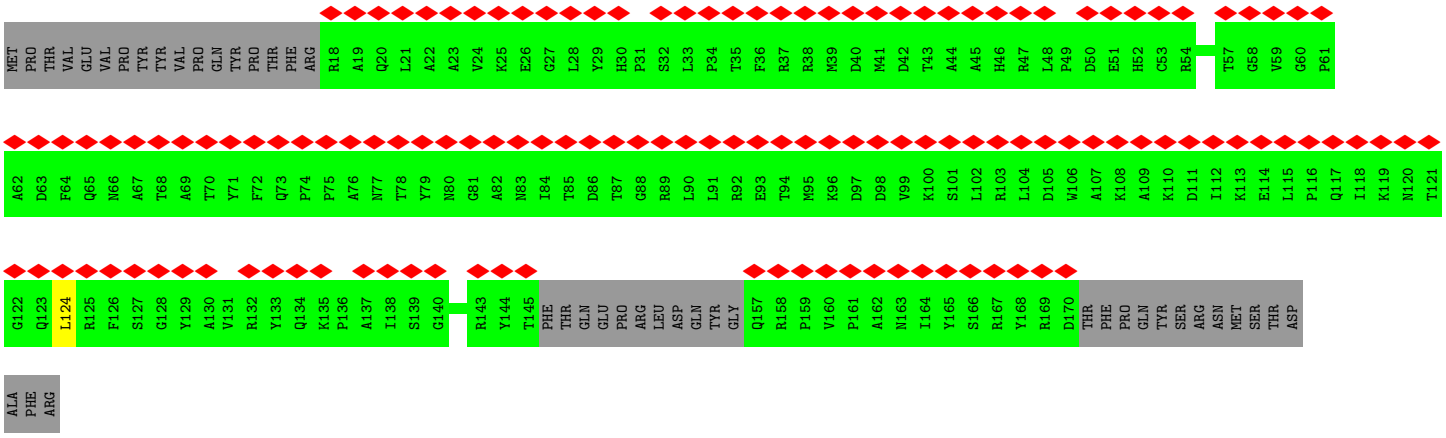
- Molecule 39: TEPP protein

Chain 7Q:



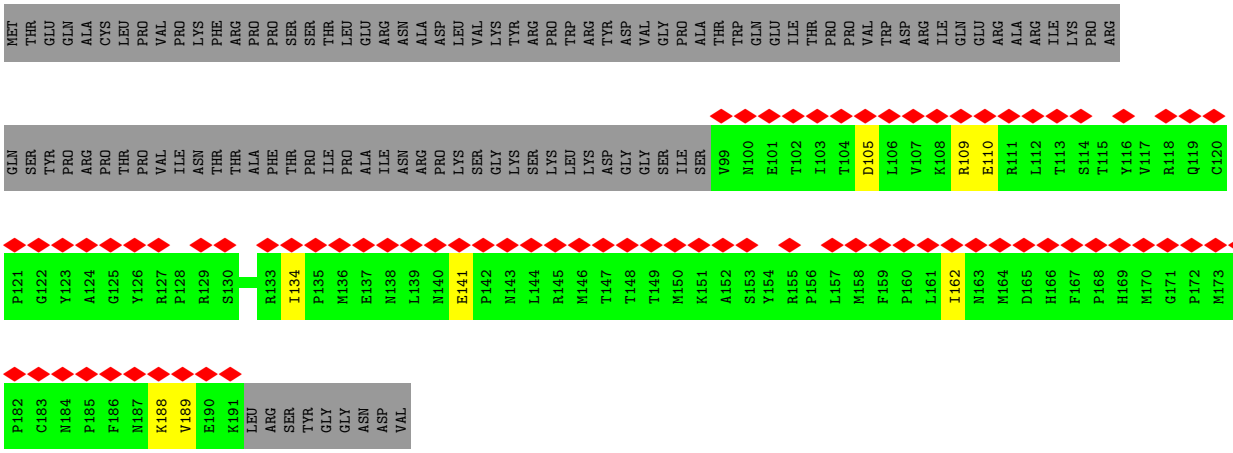
- Molecule 39: TEPP protein

Chain 7R:



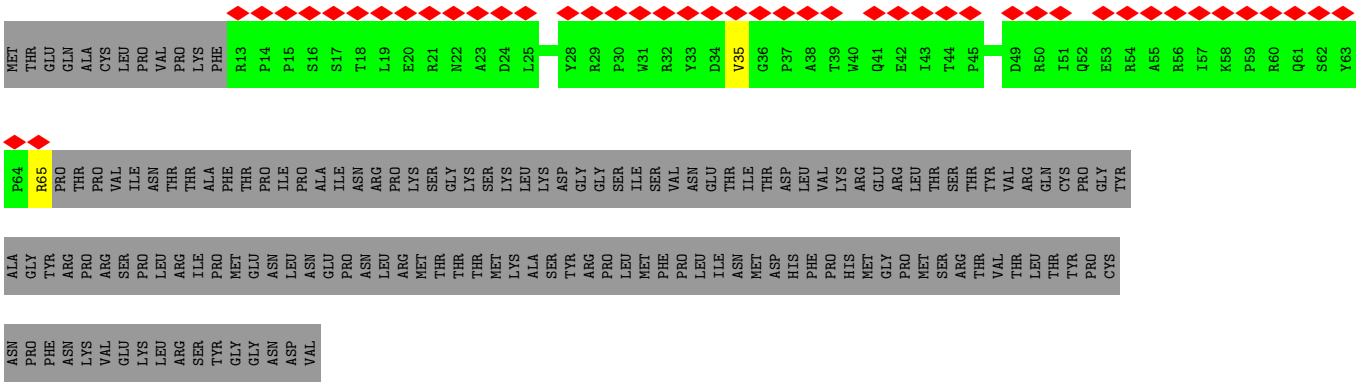
• Molecule 40: SPATA48

Chain 7U:



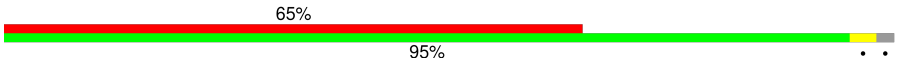
• Molecule 40: SPATA48

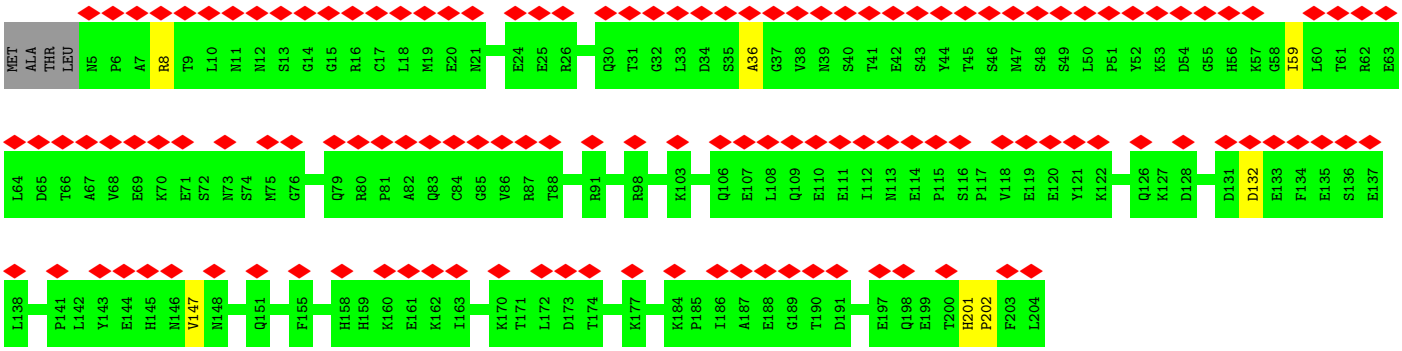
Chain 7V:



• Molecule 41: Sperm-associated antigen 8

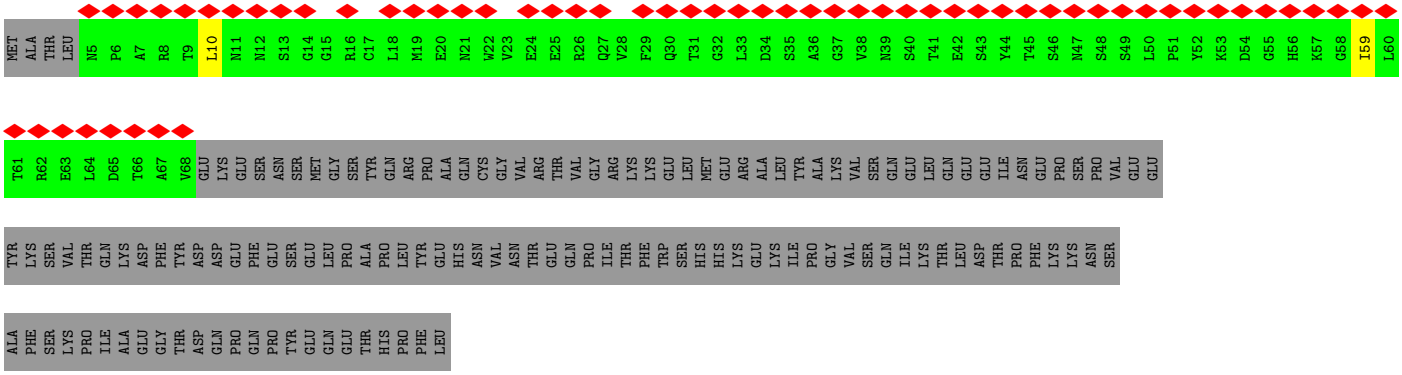
Chain 7Y:





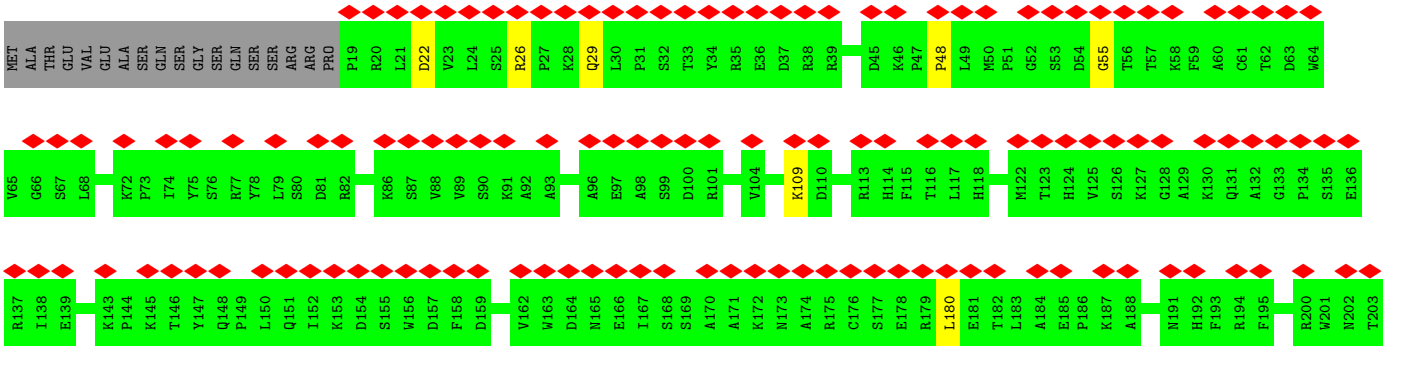
• Molecule 41: Sperm-associated antigen 8

Chain 7Z:



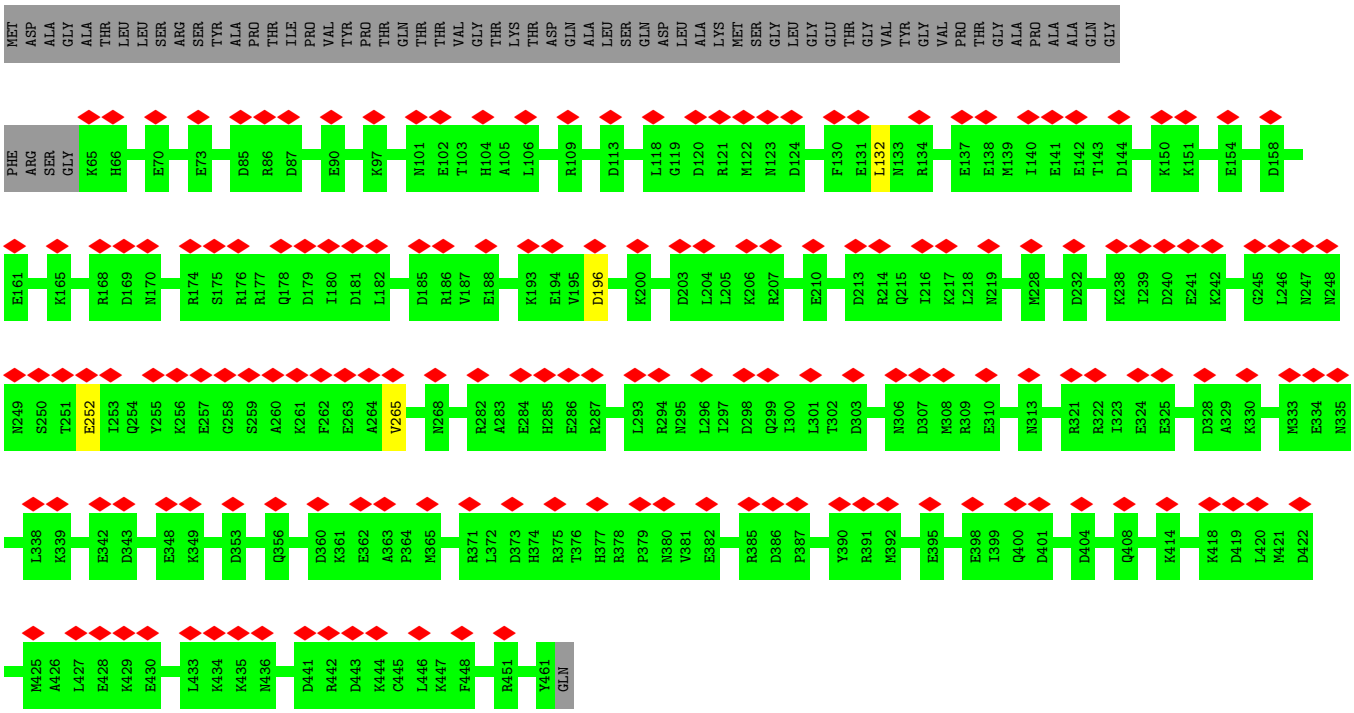
• Molecule 42: Testicular haploid expressed gene protein-like

Chain 8A:



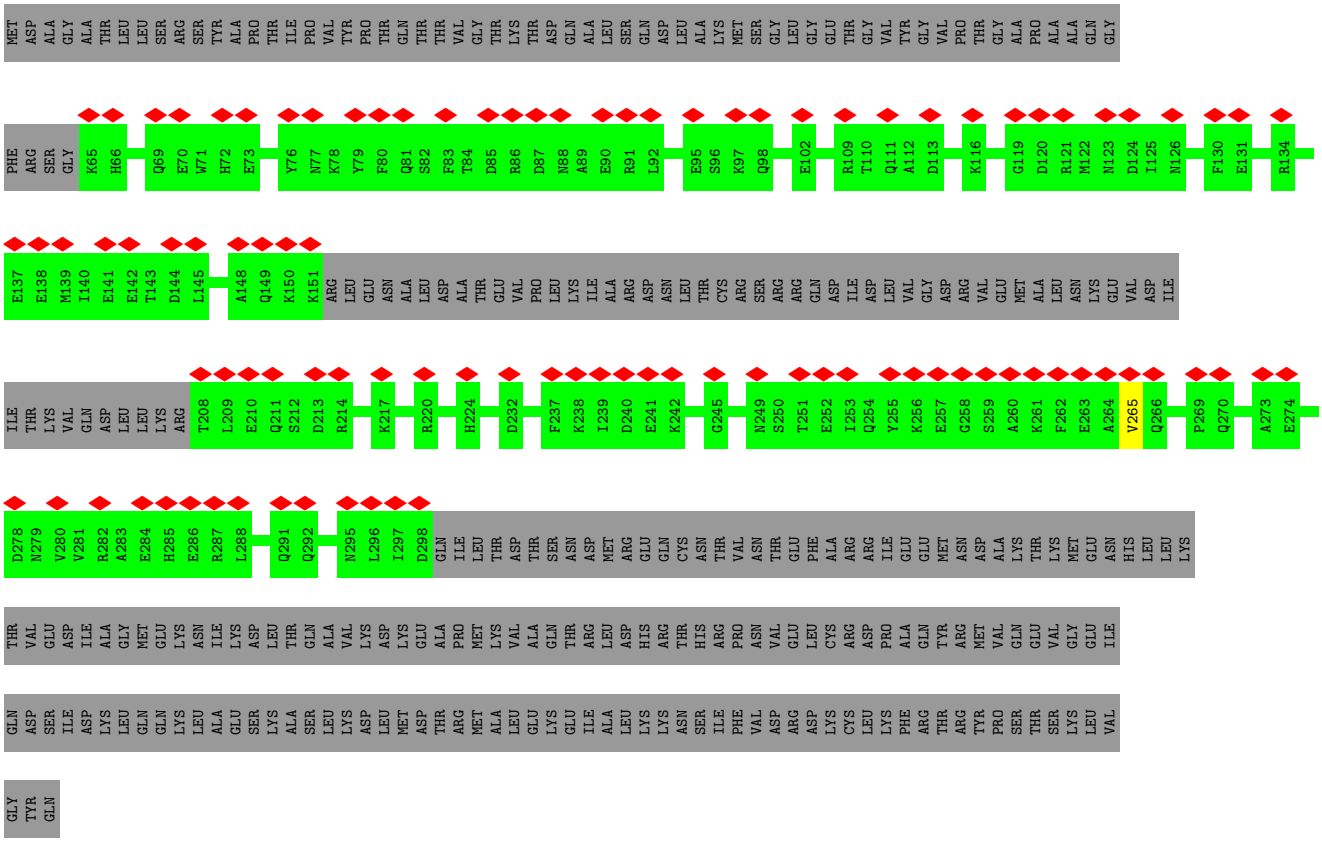
• Molecule 43: Tektin

Chain 8D:



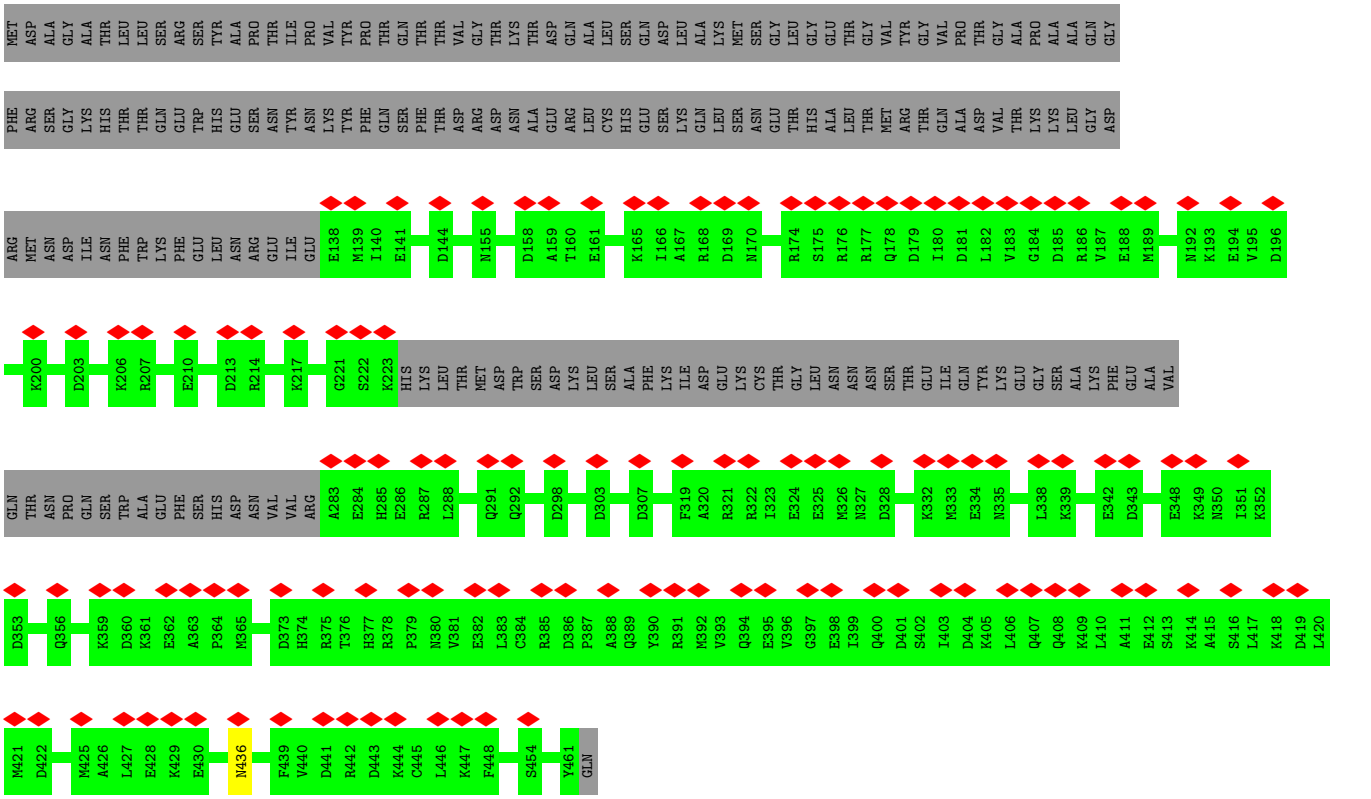
- Molecule 43: Tektin

Chain 8E:



- Molecule 43: Tektin

Chain 8F:

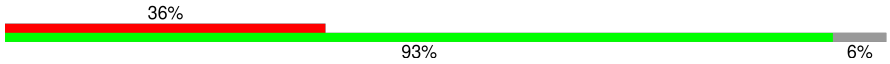


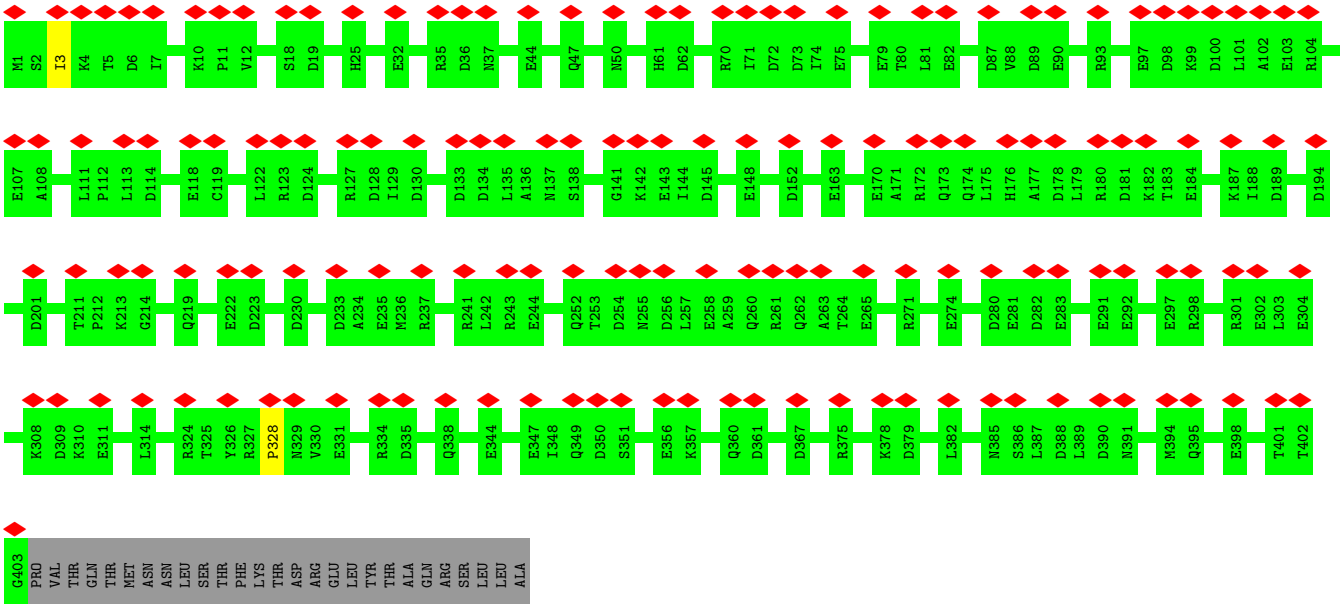
- Molecule 43: Tektin

Chain 8G:

- Molecule 44: Tektin

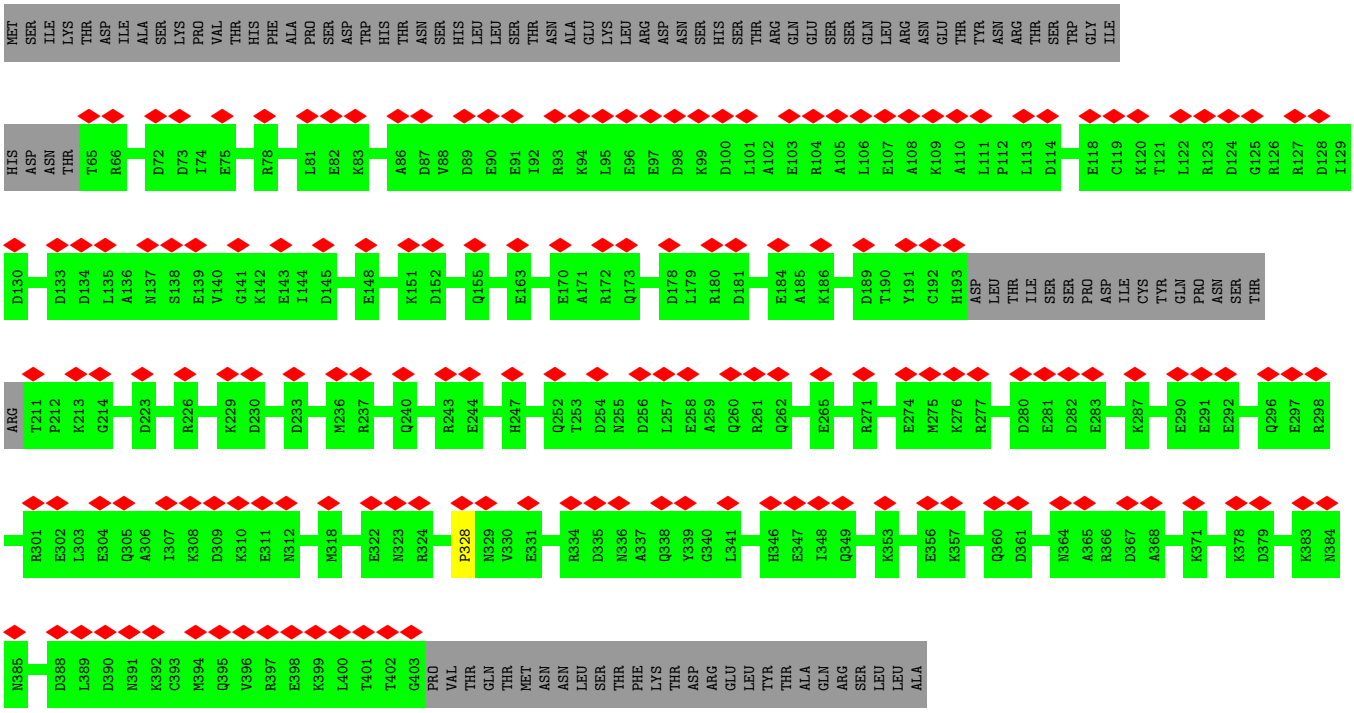
Chain 8J:





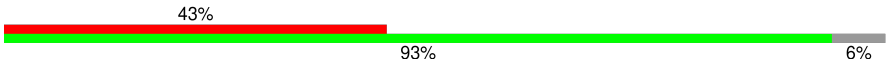
- Molecule 44: Tektin

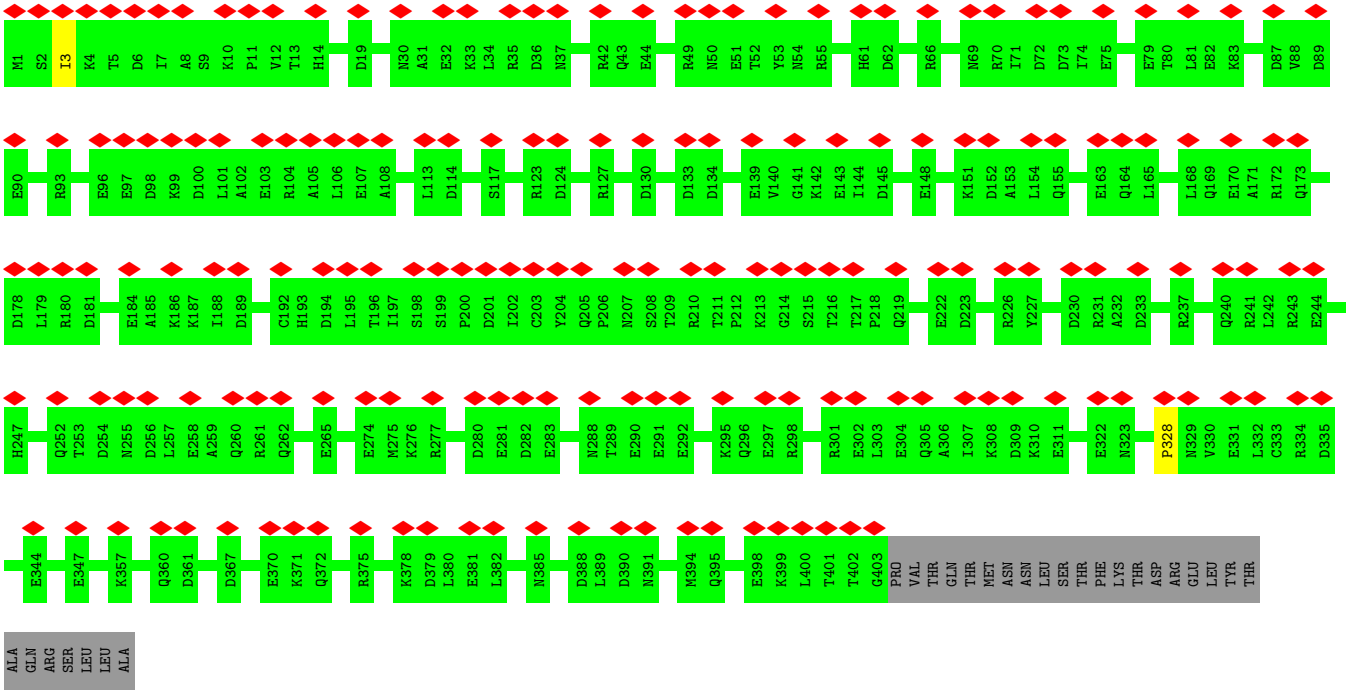
Chain 8K:



- Molecule 44: Tektin

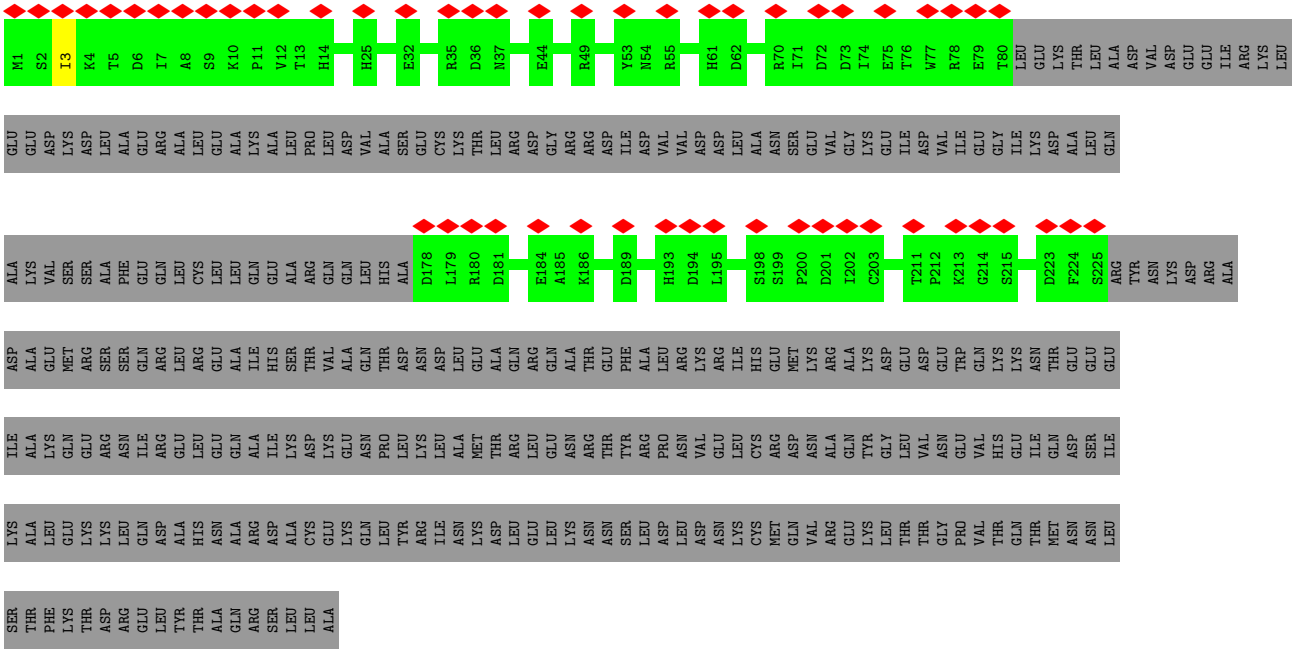
Chain 8L:





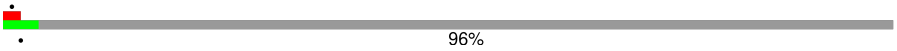
- Molecule 44: Tektin

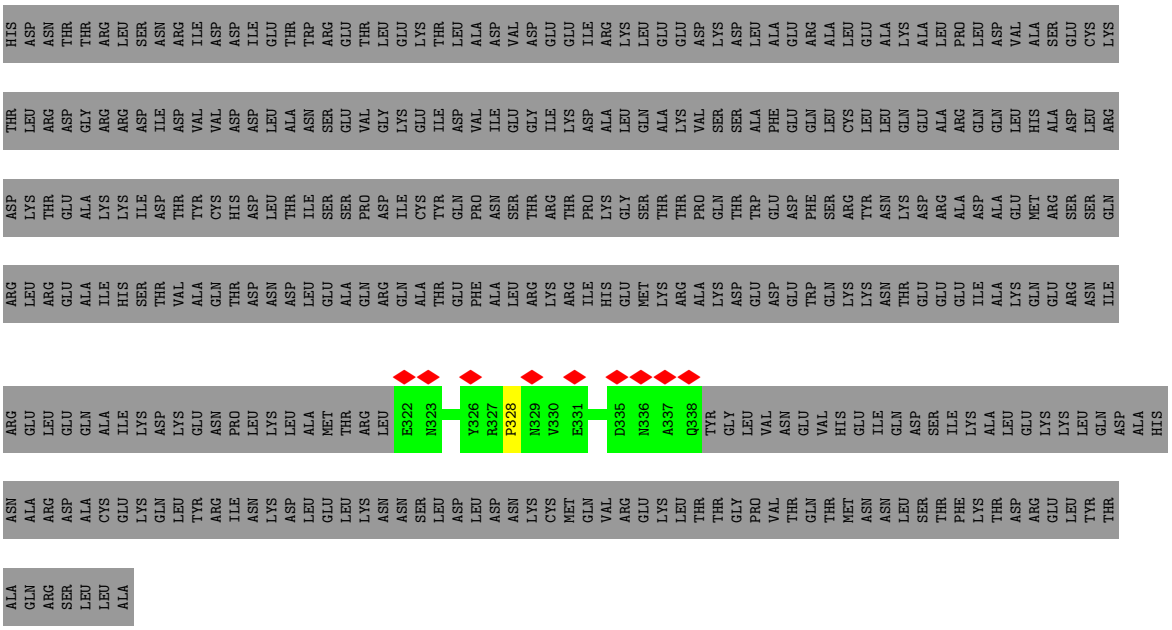
Chain 8M:



- Molecule 44: Tektin

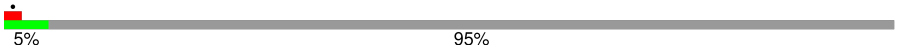
Chain 8N:





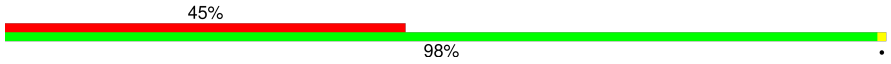
- Molecule 45: Tektin

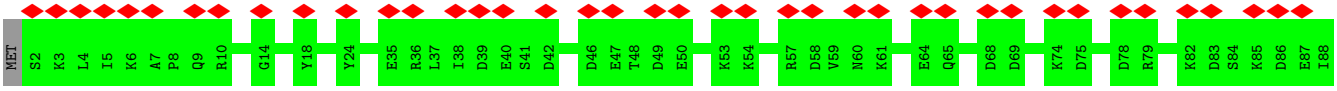
Chain 8Q:

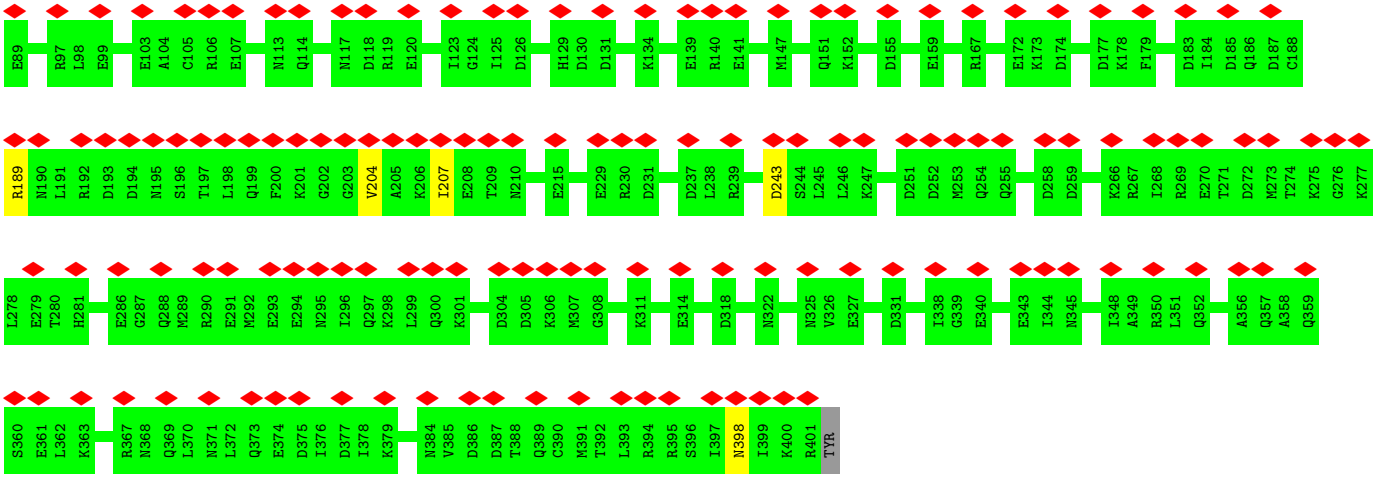


- Molecule 45: Tektin

Chain 8R:

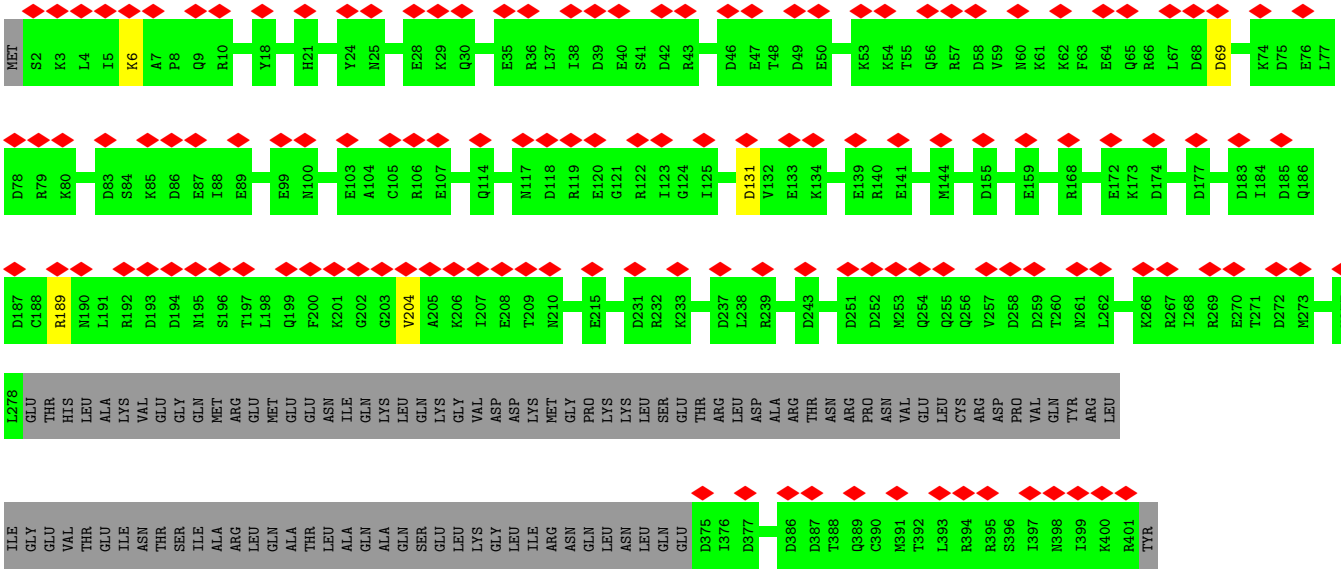






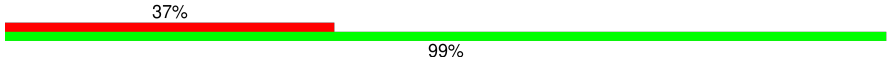
- Molecule 45: Tektin

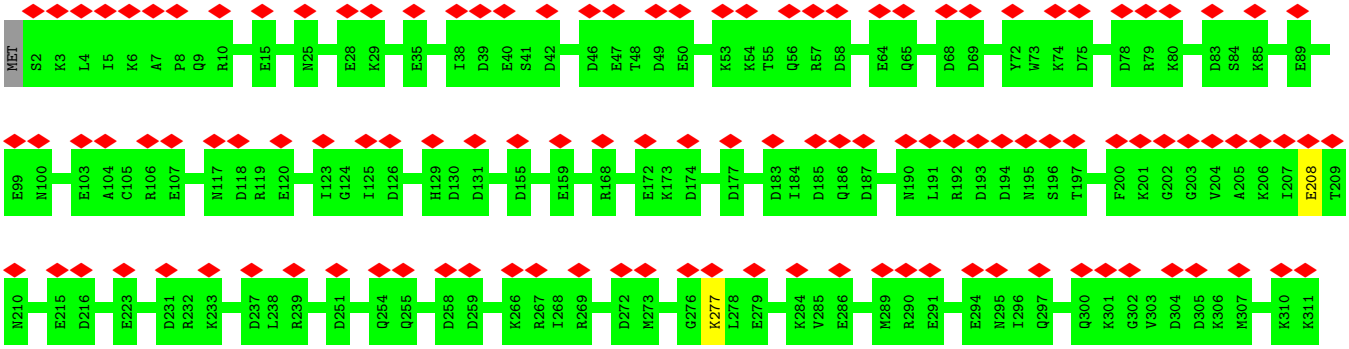
Chain 8S:

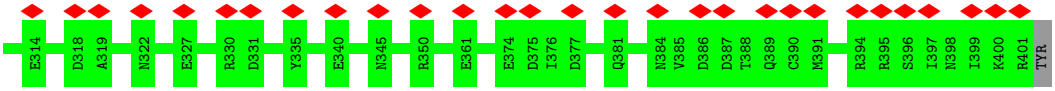


- Molecule 45: Tektin

Chain 8T:

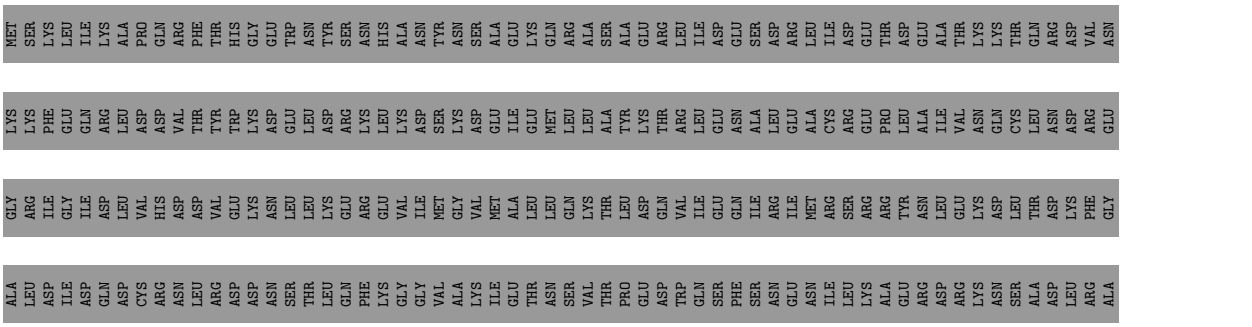


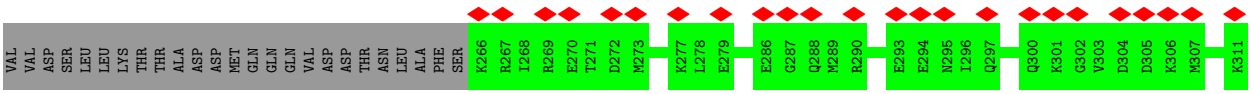


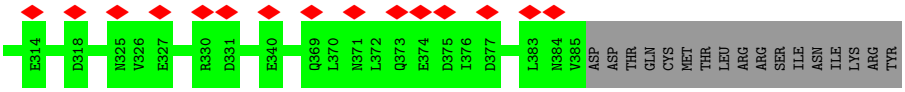


- Molecule 45: Tektin

Chain 8U:

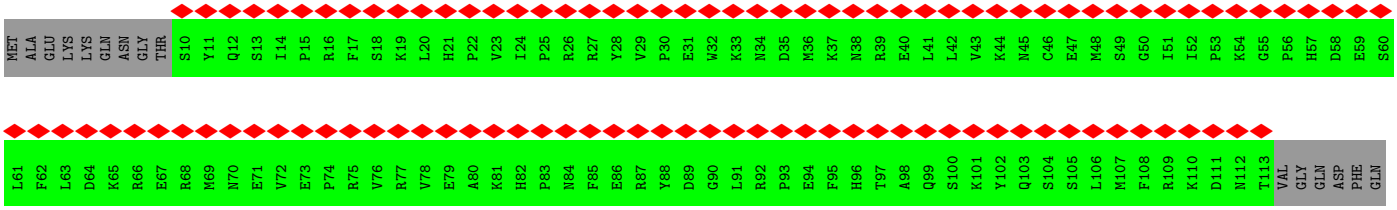






- Molecule 46: Tex43

Chain 8X:



- Molecule 46: Tex43

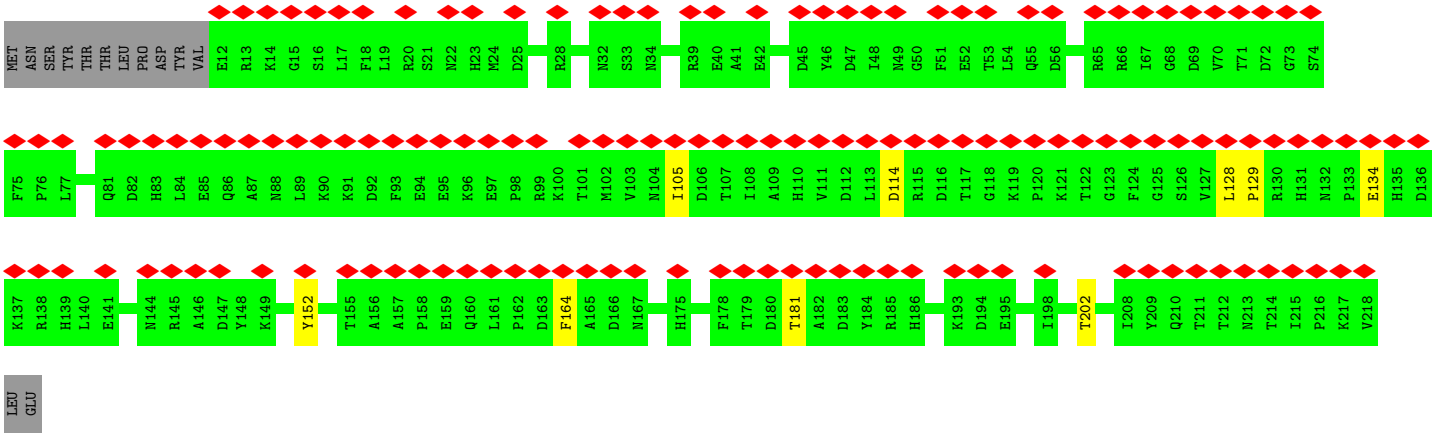
Chain 8Y:

- Molecule 46: Tex43

Chain 8Z:

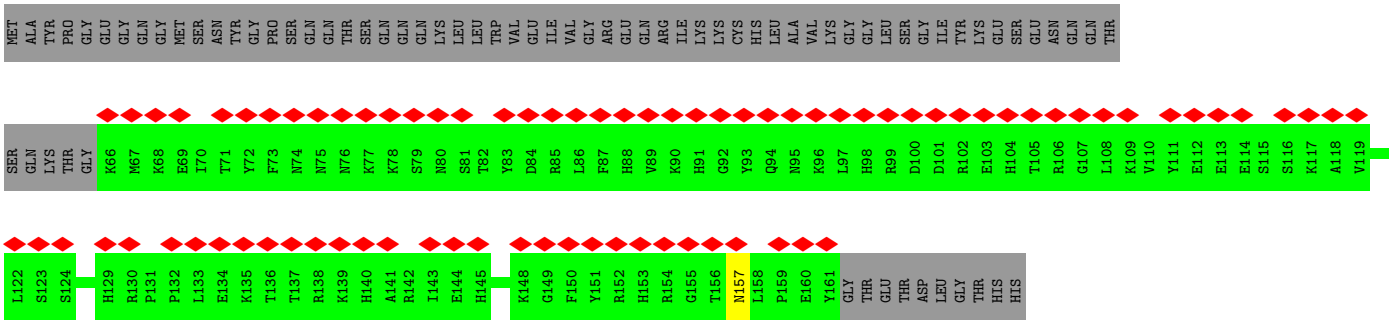
- Molecule 47: Tex36(CFAP95, C9orf135)

Chain 9A:



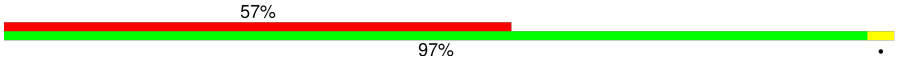
- Molecule 48: CFAP90(C5orf49)

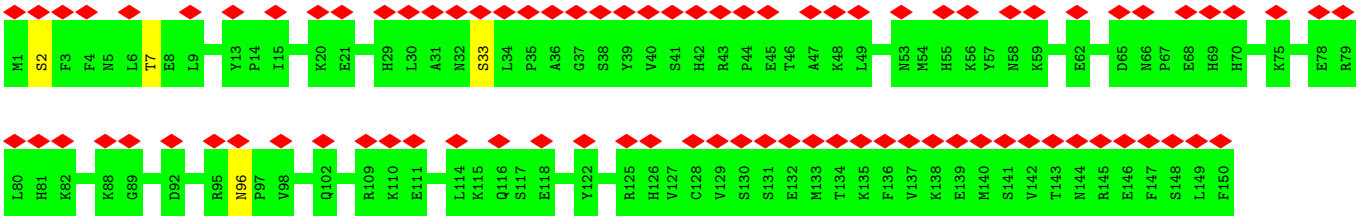
Chain 9D:



- Molecule 49: Tex49

Chain 9G:





- Molecule 50: Tex49_homologue(LOC580808)

Chain 9J:

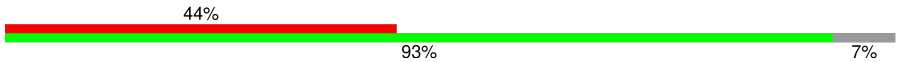
MET THR ALA GLN CYS MET GLY ASN PHE GLY ALA HIS LYS TRP ARG TYR PRO GLU PHE MET ALA ASP ARG TYR GLY ARG SER ASN GLY SER VAL ASP PRO GLU SER ARG HIS LYS GLN TYR ASP ALA GLY VAL SER ASP GLN THR VAL TRP VAL ASN LYS ARG TYR ILE PRO THR ASP LEU

ARG SER THR ALA PRO VAL PRO ARG ARG LYS LEU LEU ALA SER ALA ARG LEU P78 H79 V80 E81 R82 D83 W84 V85 P86 L87 G88 E89 A90 S91 C92 R93 Q94 I95 S96 R97 A98 M99 E100 E101 R102 Q103 L104 Y105 V106 S107 Q108 P109 S110 T111 R112 S113 E114 D115 W116 S117 T118 L119 R120

Q121 I122 L123 P124 S125 K126 G127 L128 P129 L130 R131 D132 S133 P134 P135 N136 W137 G138 T139 G140 N141 A142 Y143 A144 P145 P146 M147 L148 G149 A150 R151 Q152 R153 R154 H157 I158 N159 S160 P161 M162 T163 R164 Y165 T166 D167 N168 M169 H170 T171 T172 H173 K174 L175 F176 K177 L178 HIS

- Molecule 51: CFAP68(UPF0686, C11orf1)

Chain 9R:

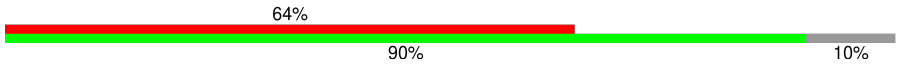


MET ALA SER GLY ASP E6 V7 A8 F9 R10 S11 M12 G15 S16 G17 L18 G19 E20 H24 D27 L28 E29 K30 F31 Q32 G35 W36 R37 T38 T39 T40 K41 E42 D43 C44 D48 N53 E56 E57 K62 R63 V66 P67 K68 S72 D75 D79

K83 S88 G89 P90 K91 P92 V93 P94 K95 H96 I97 R103 E104 S105 A110 E114 L115 D116 K121 E122 R123 E128 R132 D137 L140 R141 K142 N143 P144 V145 H146 Q147 THR GLU THR SER GLN ARG

- Molecule 52: SPATA45

Chain 9T:

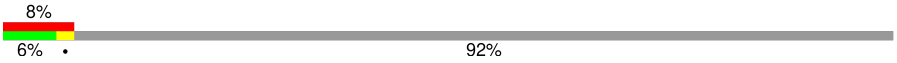


M1 D2 P3 Q4 K5 N6 Y7 E8 M9 N10 N11 Q12 R13 E20 L21 S22 P23 L24 Q25 D26 W27 C28 K29 S30 E31 R32 K33 H34 H35 G36 E37 N38 F39 K40 S41 S42 V43 F44 N45 A46 LYS GLN GLY GLN PRO GLU SER GLU A55 R56 C57 T58 F59 E60 V61 N62 D63 K64 T65

H66 R67 R70 N74 K75 T76 S77 Y78 S79 H80 L81 A82 I83

- Molecule 53: C4orf45

Chain 9V:



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

ARG MET VAL GLY ILE GLY THR MET SER Q70 E71 G72 T73 S74 D75 L76 Q77 Y78 I79 W80 R81 G82 A83 P84 G85 A86 P87 P88 P89 R90 R91 R92 S93 GLN TRP VAL GLY GLU VAL GLY TRP PHE ILE PRO PRO TYR HIS ASP THR LYS ASN THR LEU SER GLY ASN GLN ILE GLN LEU

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

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

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

- Molecule 53: C4orf45

Chain 9W: 24% 24% 76%

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

ARG MET VAL GLY ILE GLY THR MET SER GLN GLU GLY THR SER ASP LEU GLN TYR ILE TRP ARG GLY ALA PRO GLY A86 P87 P88 P89 R90 R91 R92 S93 Q94 W95 V96 G97 E98 V99 G100 W101 F102 I103 P104 P105 Y106 H107 D108 T109 K110 N111 T112 L113 S114 G115 N116 Q117 I118 Q119 L120

K121 V122 F123 R124 K125 A126 Q127 E128 E129 K130 Y131 T132 H133 R134 F135 Q136 E137 P138 W139 Y140 L141 A142 P143 N144 D145 P146 D147 Y148 K149 Q150 N151 F152 P153 F154 T155 GLN GLY SER LYS ARG ASN TRP ARG ALA PRO GLY GLN GLN ARG SER ALA GLU GLN LEU PRO PRO ARG PRO HIS THR

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

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

- Molecule 54: Tubulin alpha chain

Chain AA: 35% 96%

M1 R2 E3 C4 I5 E22 L23 L26 E27 H28 G29 D33 G34 Q35 S38 D39 K40 G43 G44 G45 D46 D47 N50 T51 F52 E55 T56 G57 A58 G59 K60 H61 D69 L70 E71 F72 T73 D76 E77 V78 R79 T80 G81 R84 Q85 L86 F87 E90

I93 T94 G95 K96 E97 D98 H107 Y108 T109 I110 G111 K112 E113 D116 L117 D120 R121 I122 R123 K124 L125 A126 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136 F141 G142 A150 M154 E155 R156 V159 D160 Y161 G162 K163 K164 S165 F169 A170 I171 Y172 P173 A174 P175

Q176 I177 S178 T179 I188 H192 T193 H197 S198 D199 C200 M203 V204 D205 Y210 D211 R214 D218 I219 E220 R221 L230 S237 D245 N249 V250 D251 L252 T253 E254 F255 Q256 R264 L269 E279 K280 A281 E284 Q285 E297 K304 C305 D306

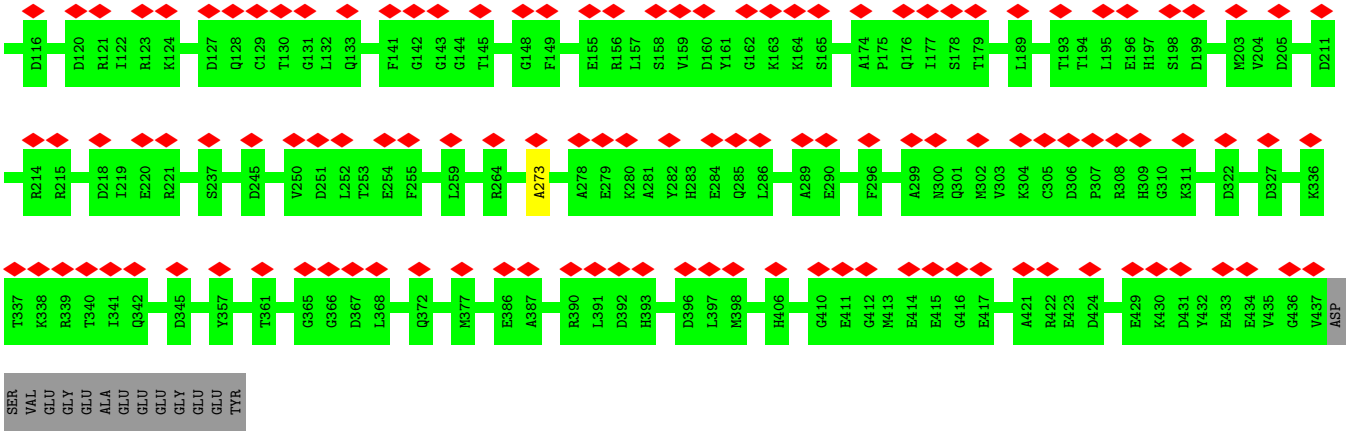
H309 A314 D322 K336 T337 K338 R339 Q342 D345 T361 V362 V363 P364 G365 G366 D367 K370 L378 E386 R390 L391 D392 H393 D396 L397 M398 Y399 A400 K401 G410 E411 G412 M413 E414 E415 G416 E417 R422 E423 D424 L425 E429 K430 D431 Y432

E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

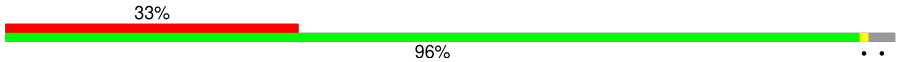
Chain AB: 36% 97%

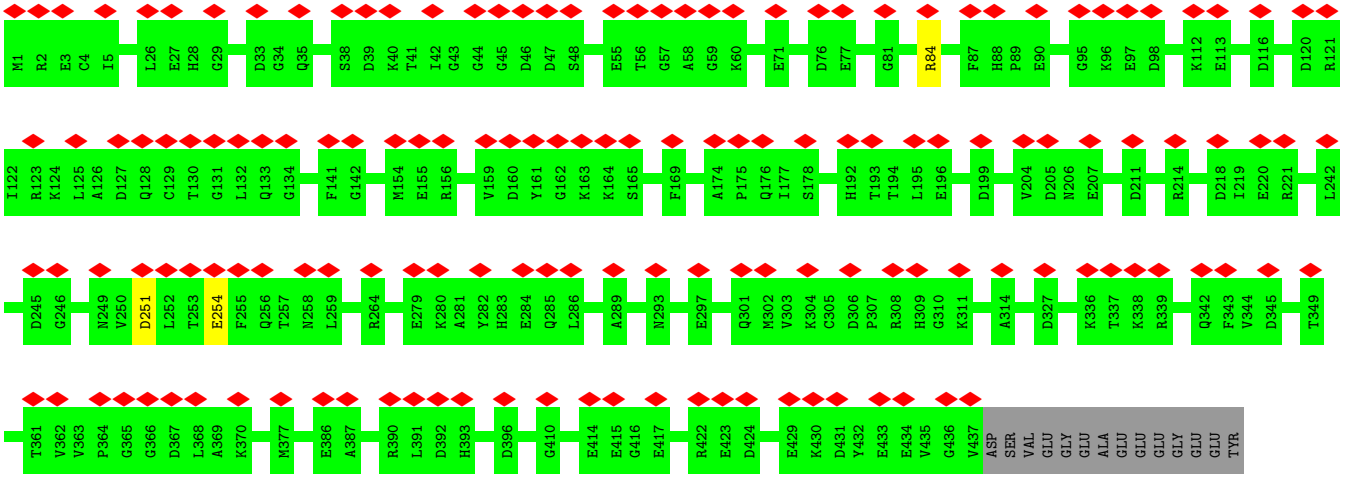
M1 R2 E3 G29 D33 G34 Q35 M36 P37 S38 D39 K40 G43 G44 G45 D46 D47 S48 F49 E55 T56 G57 A58 G59 E71 D76 E77 V78 R79 R84 Q85 L86 F87 E90 T94 G95 K96 E97 D98 A99 A100 N101 R105 G106 H107 Y108 T109 I110 E113



- Molecule 54: Tubulin alpha chain

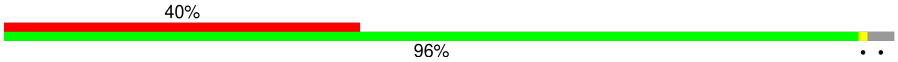
Chain AE:

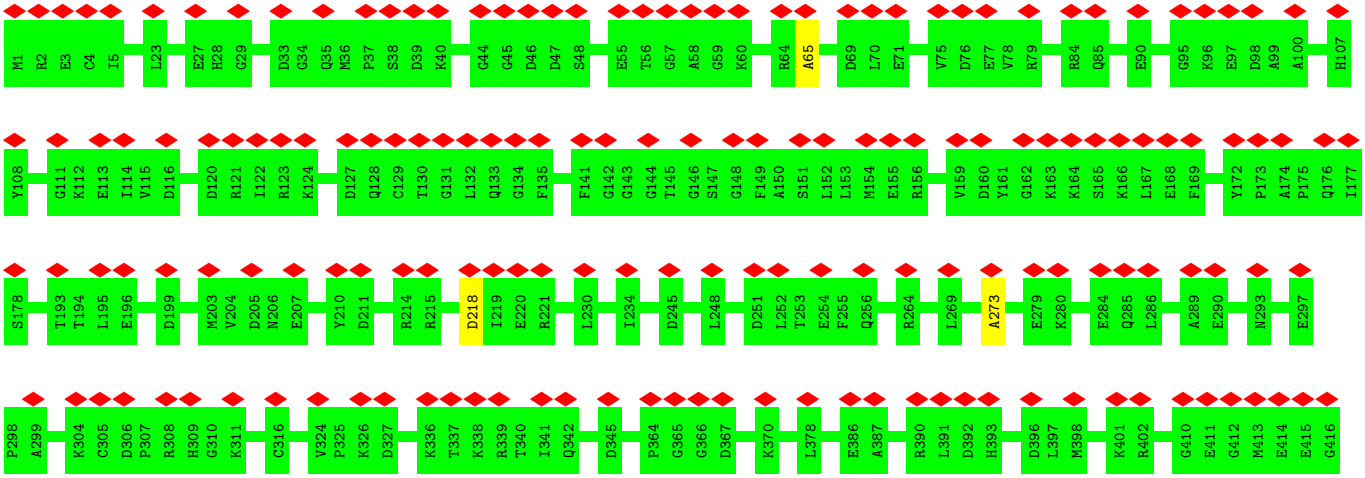


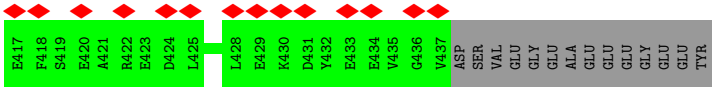


- Molecule 54: Tubulin alpha chain

Chain AG:

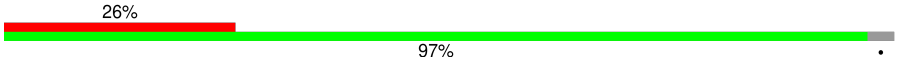


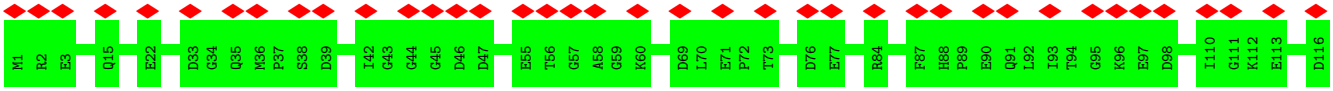


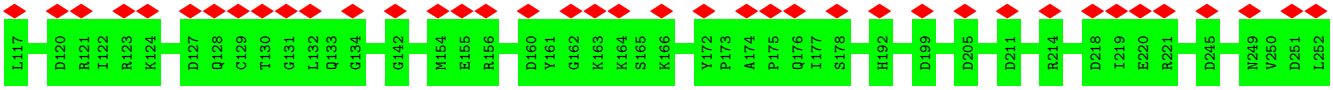


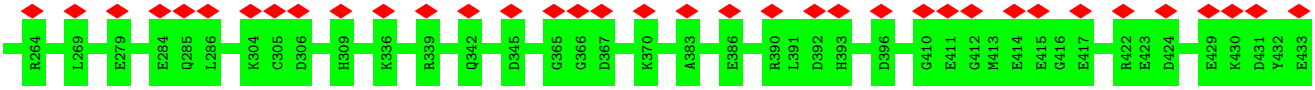
• Molecule 54: Tubulin alpha chain

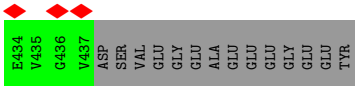
Chain AI:





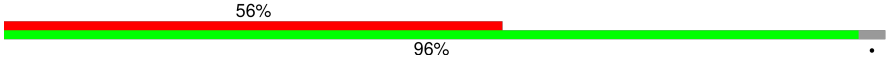


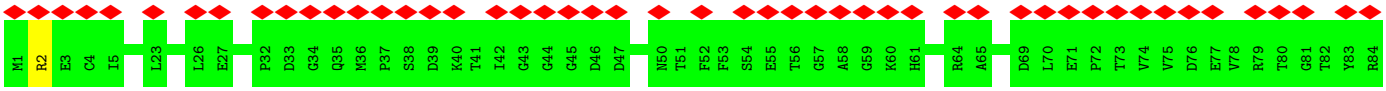


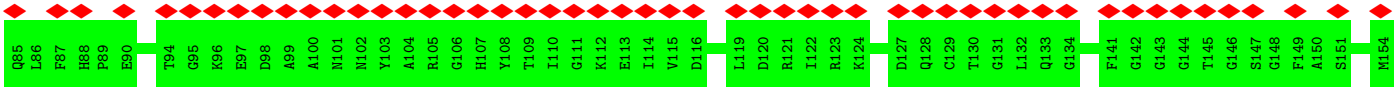


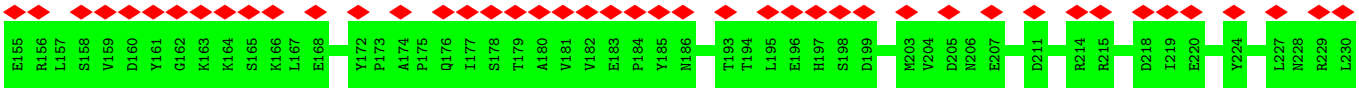
• Molecule 54: Tubulin alpha chain

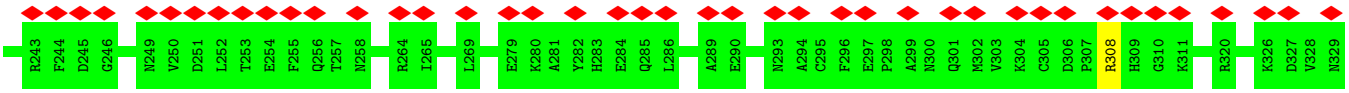
Chain AK:

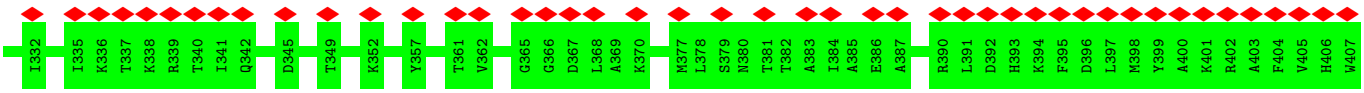


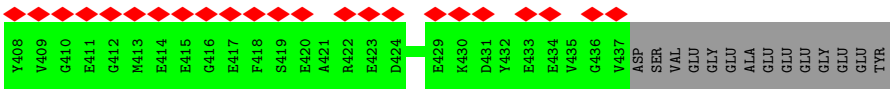












• Molecule 54: Tubulin alpha chain

Chain AM: 61% 97%

M1 R2 E3 C4 I5 I16 E22 L23 L26 E27 H28 G29 D33 G34 Q35 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 S48 F49 N50 T51 F52 F53 S54 E55 T56 G57 A58 G59 K60 H61 R64 D69 L70 E71 D76 E77 V78 R79 R84 Q85 L86

E90 K96 E97 D98 H107 Y108 T109 K112 E113 D116 D120 R121 I122 R123 K124 A126 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 F141 G142 T145 M154 E155 R156 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 A174 P175 Q176 I177 S178 H192

L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 D211 R214 R215 D218 I219 E220 Q233 I234 V235 S236 S237 I238 T239 A240 S241 L242 R243 F244 D245 G246 A247 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 L259 V260 P261 Y262 P263 R264 I265 H266 L269 A270 T271

Y272 A273 P274 V275 I276 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 A294 C295 F296 E297 P298 A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 Y312 M313 A314 C315 C316 M317 L318 Y319 R320 G321 D322 V323 V324 P325 K326 D327 V328 N329 A330 A331 I332

A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 K352 V353 G354 I355 N356 Y357 Q358 P359 P360 T361 V362 G365 G366 D367 L368 A369 K370 V371 Q372 R373 A374 V375 C376 M377 L378 S379 N380 T381 T382 A383 I384 A385 E386 A387 W388 A389 R390 L391 D392 H393

D396 G410 E411 G412 M413 E414 E415 G416 E417 E420 A421 R422 E423 D424 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain BA: 42% 96%

M1 R2 E3 C4 G17 E22 L26 D33 D39 K40 T41 I42 G43 G44 G45 D46 D47 S48 F49 N50 E55 A65 D69 L70 E71 E77 T80 G81 E90 Q91 K96 E97 D98 I110 G111 K112 E113 D116 D120 R121 I122 R123 K124 D127

Q128 C129 T130 G131 L132 Q133 G134 F135 L136 F141 G142 L153 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 Q176 H192 T193 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 N206 E207 A208 I209 Y210 D211 I212 C213 R214 R215 D218 I219 E220

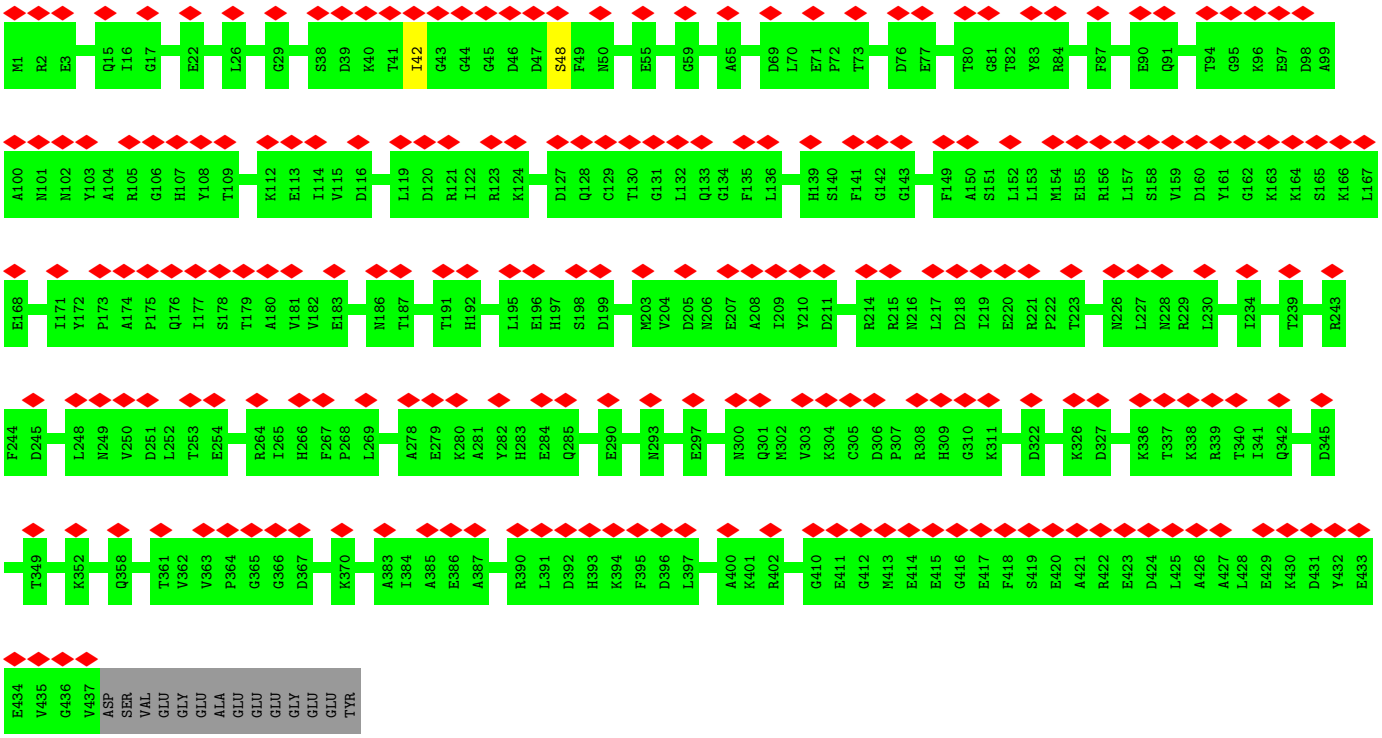
R221 P222 T223 L227 L230 I231 S237 I238 T239 A240 S241 L242 D245 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 R264 L269 P274 V275 A278 E279 K280 A281 Y282 H283 E284 Q285 L286 E290 W293 A294 C295 F296 E297 N300 Q301 M302 V303 K304

C305 D306 P307 R308 H309 G310 K311 M317 L318 D322 K326 D327 V328 N329 I335 K336 T337 K338 R339 T340 I341 Q342 D345 T349 G350 F351 K352 Y357 Q358 T361 V362 V363 P364 G365 G366 D367 L368 A369 K370 V371 Q372 R373 M377 A383 E386 A387 R390 L391

D392 H393 D396 L397 R402 E411 G412 M413 E414 E415 G416 E417 R422 E423 A426 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

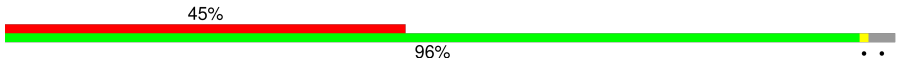
- Molecule 54: Tubulin alpha chain

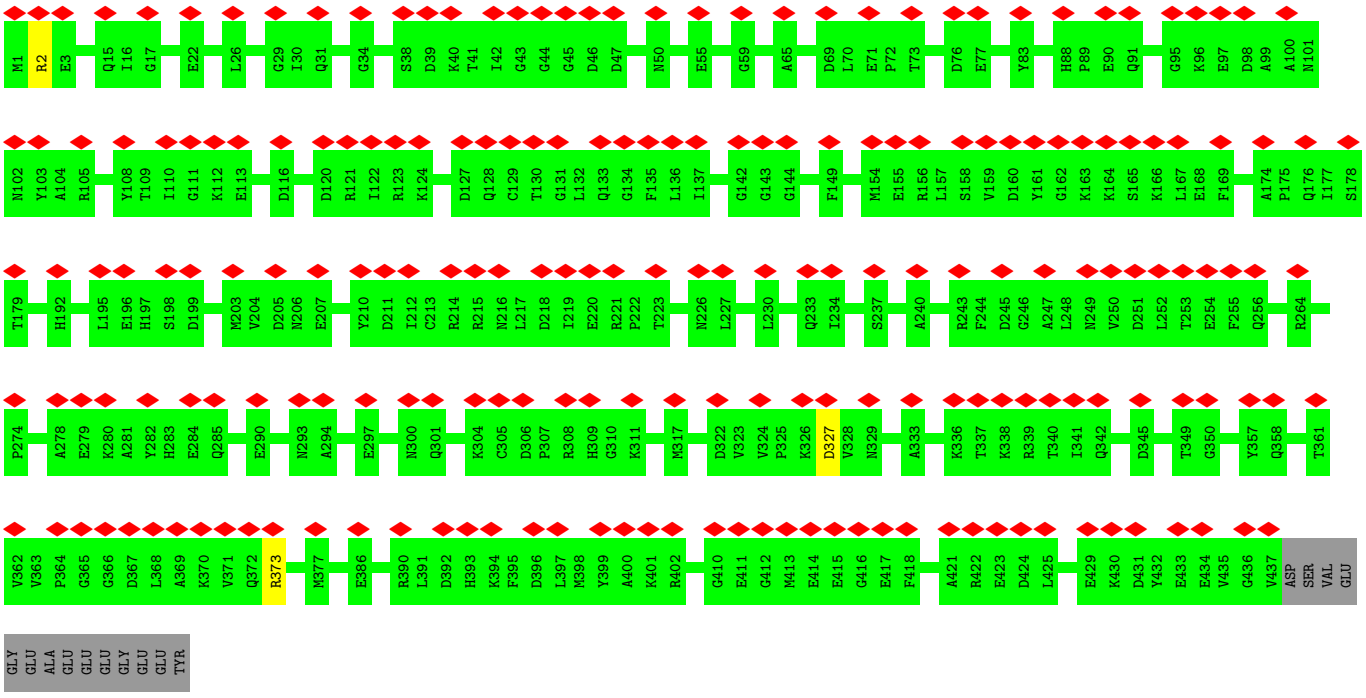
Chain BB: 49% 96%



• Molecule 54: Tubulin alpha chain

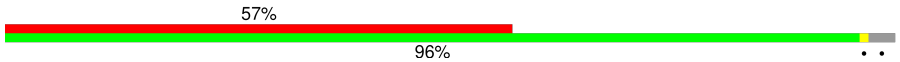
Chain BE:

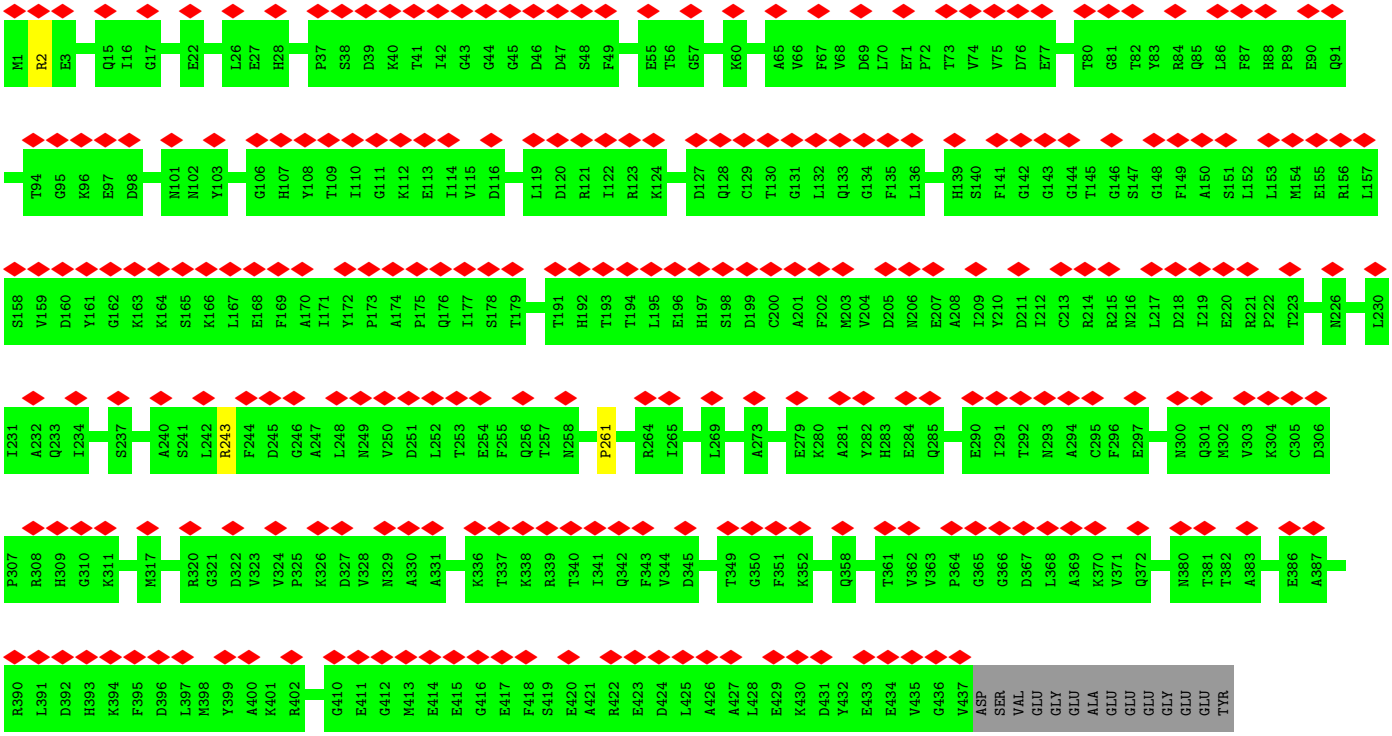




• Molecule 54: Tubulin alpha chain

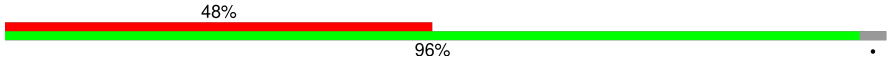
Chain BG:

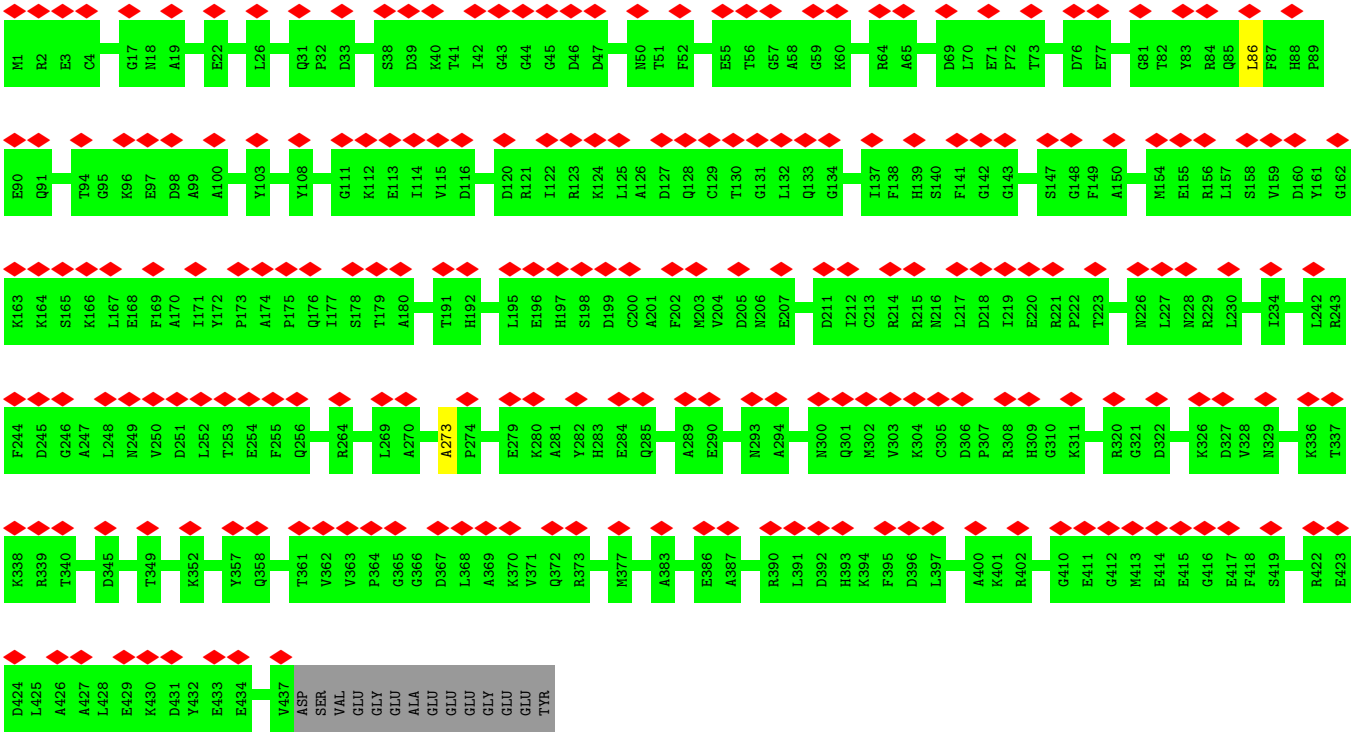




- Molecule 54: Tubulin alpha chain

Chain BI:





- Molecule 54: Tubulin alpha chain

Chain BK: 68% 96%

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E90 Q91 L92 I93 T94 G95 K96 E97 D98 A99 A100 N101 N102 Y103 A104 R105 G106 H107 Y108 T109 I110 G111 K112 E113 I114 V115 D116 L117 V118 L119 D120 R121 I122 R123 K124 L125 A126 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 H139 S140 F141 G142 G143 G144 T145 G146 S147 G148 F149 A150 S151

L152 L153 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 A170 I171 Y172 P173 A174 P175 Q176 I177 S178 T179 A180 V181 V182 E183 P184 Y185 N186 T187 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 M203 V204 D205 N206 E207 A208 I209 Y210 D211 I212 C213

R214 R215 N216 L217 D218 I219 E220 R221 P222 T223 Y224 T225 N226 L227 N228 R229 L230 I231 I234 R243 F244 D245 G246 A247 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 R264 L269 A270 T271 Y272 A273 A278 E279 Y282 H283 E284 Q285 L286 S287 V288 A289 E290 N293

A294 C295 F296 E297 P298 A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 M317 L318 Y319 R320 G321 D322 V323 V324 P325 K326 D327 V328 N329 A330 A331 I332 I335 K336 T337 K338 R339 T340 I341 Q342 D345 T349 G350 F351 K352 Q358 T361 P364 G365 G366 D367

L368 A369 K370 R373 A383 E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 A403 F404 V405 H406 W407 Y408 V409 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437

ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain BM: 53% 96%

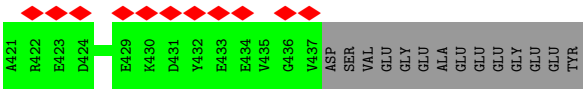
M1 R2 E3 G17 E22 L26 E27 H28 G29 I30 Q31 P32 D33 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 S48 F49 N50 S54 E55 T56 G57 A58 G59 K60 D69 D76 E77 G81 R84 F87 E90 Q91 K96 E97 D98 A99 A100 N101

Y108 T109 I110 G111 K112 E113 D116 L119 D120 R123 K124 D127 Q128 C129 T130 G131 L132 Q133 F141 G142 G143 S147 S151 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 Y172 P173 A174 P175 Q176 I177 S178 T179 T191 H192 L195

E196 H197 S198 D199 C200 M203 V204 D205 N206 E207 D211 R214 R215 D218 I219 E220 R221 P222 T223 L230 S237 A240 S241 L242 R243 F244 D245 G246 A247 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 L259 V260 P261 Y262 P263 R264 F267 P268 L269 A270 A278

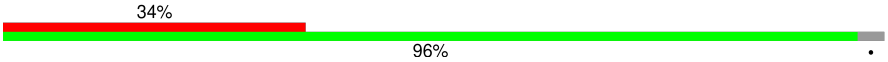
E279 K280 A281 Y282 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 A294 C295 F296 E297 Q301 K304 C305 D306 P307 R308 H309 G310 K311 Y312 M313 A314 C315 C316 M317 L318 Y319 R320 G321 D322 V323 V324 P325 K326 D327 V328 N329 A330 A331 I332 A333 T334 I335 K336 T337 K338 R339 T340 I341

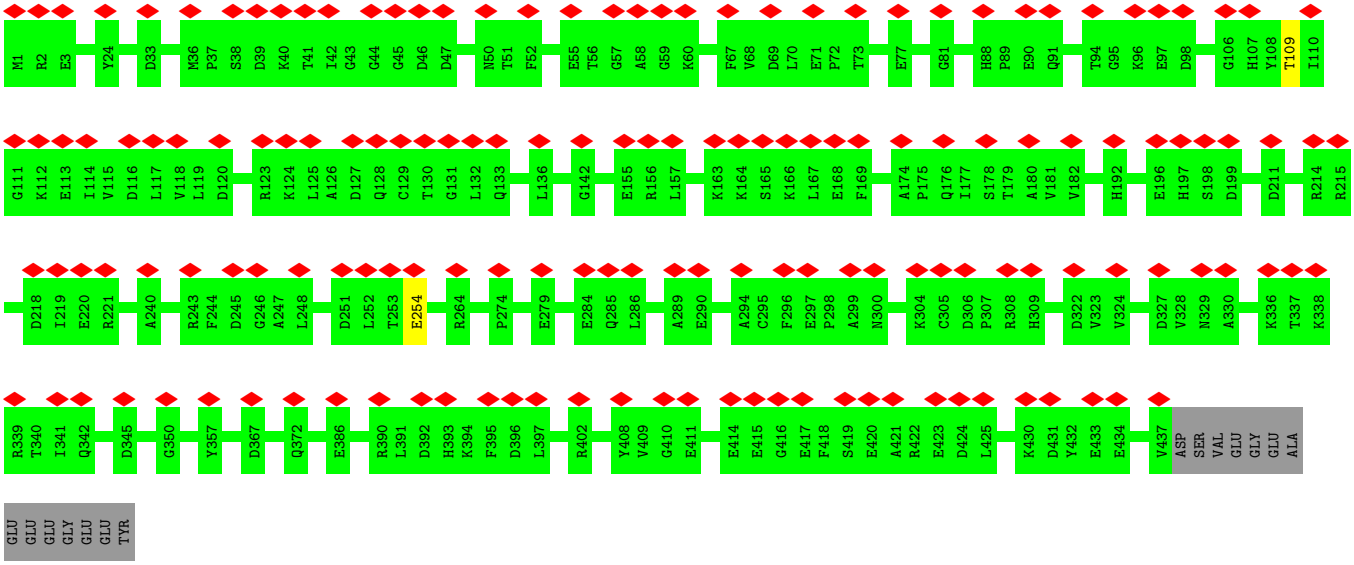
Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 K352 V353 G354 I355 N356 Y357 Q358 P359 P360 T361 P364 G365 G366 D367 K370 V371 Q372 R373 A383 E386 A387 R390 L391 D392 H393 K394 F395 D396 K401 R402 H406 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420



• Molecule 54: Tubulin alpha chain

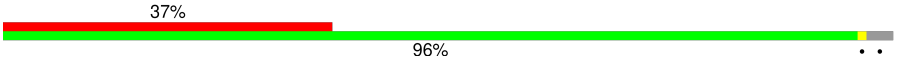
Chain CA:





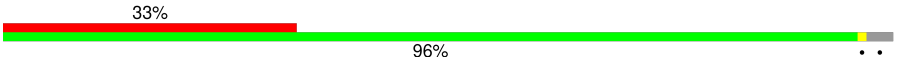
• Molecule 54: Tubulin alpha chain

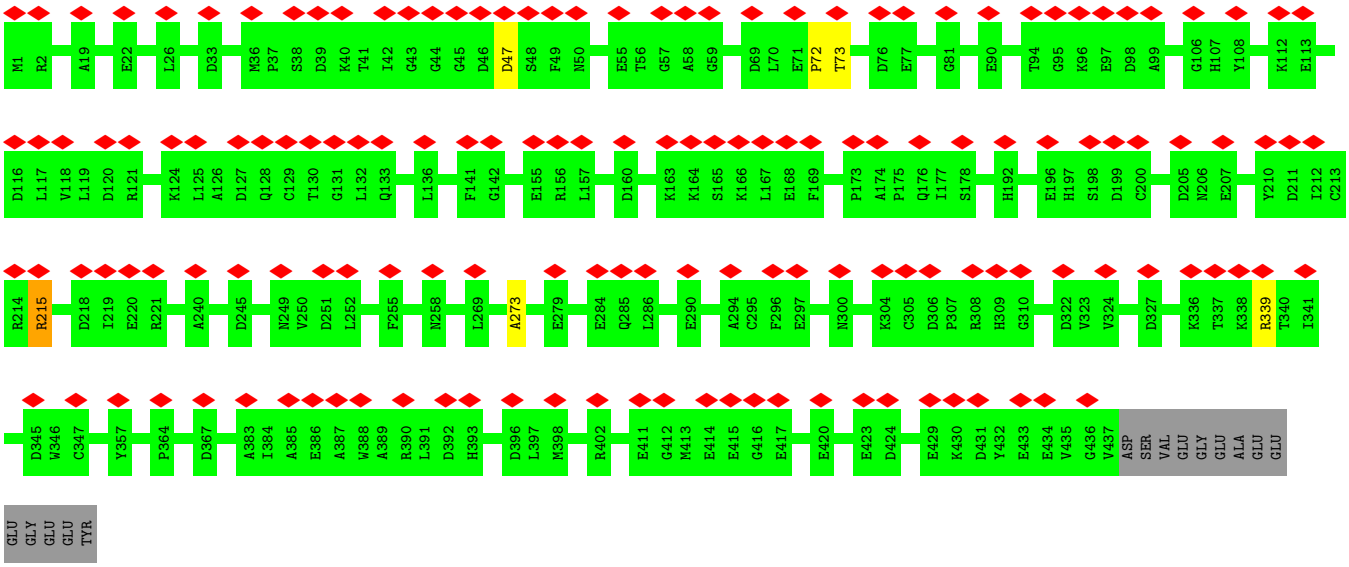
Chain CB:



• Molecule 54: Tubulin alpha chain

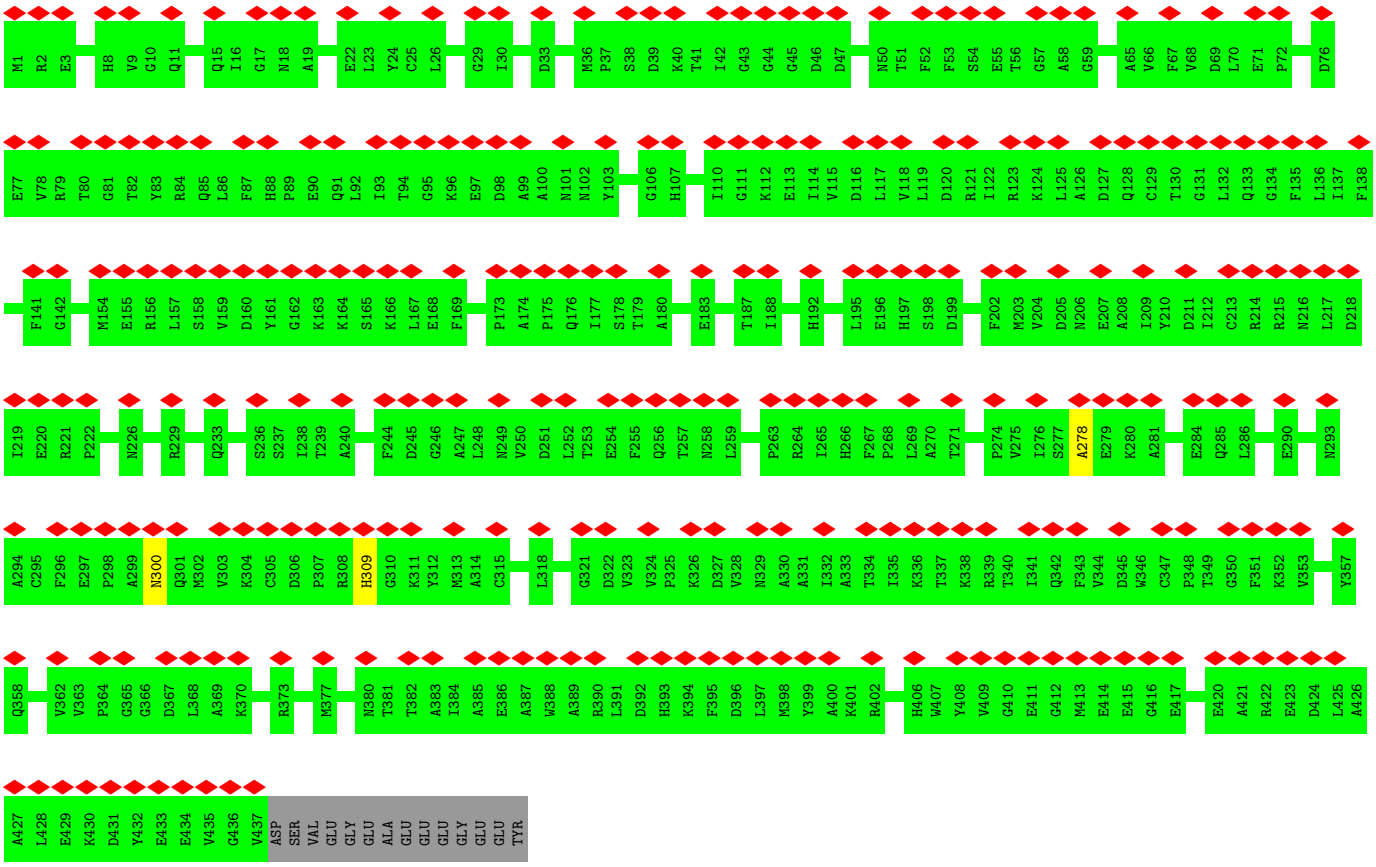
Chain CE:





• Molecule 54: Tubulin alpha chain

Chain CG: 61% 96%



• Molecule 54: Tubulin alpha chain

Chain CI: 39% 96%

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E113 I114 V115 D116 L117 V118 L119 D120 D127 Q128 C129 T130 G131 L132 Q133 L136 I137 F138 R156 V159 K163 K164 S165 K166 L167 E168 F169 A174 P175 Q176 I177 S178 T179 A180 E196 H197 S198 D199 F202 M203 V204 D205 N206 E207 A208 I209 Y210 D211 R214 R215 N216

L217 D218 I219 E220 R221 I231 A232 Q233 I238 F244 D245 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 H266 F267 P268 L269 P274 A278 E279 K280 A281 E284 Q285 L286 E290 A294 C295 F296 E297 Q301 K304 C305 D306 P307 R308 H309 M313

M317 D322 V323 V324 P325 K326 D327 V328 N329 A330 K336 T337 K338 R339 T340 I341 Q342 D345 P348 T349 G350 F351 K352 Y357 T361 V362 V363 P364 G365 G366 D367 L368 A369 K370 V371 Q372 R373 M377 A383 I384 A385 E386 A387 R390 L391 D392 H393 K394 F395 D396

L397 M398 Y399 R402 E411 E414 E415 A421 R422 E423 D424 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain CK: 79% 96%

M1 R2 E3 C4 I5 S6 I7 H8 V9 G10 Q11 A12 G13 V14 Q15 I16 G17 N18 A19 C20 W21 E22 L23 Y24 C25 L26 G29 I30 Q31 P32 D33 G34 Q35 M36 P37 S38 D39 T42 G43 G44 G45 D46 D47 S48 F49 N50 T51 F52 F53 S54 E55 T56 G57 A58 G59 K60 H61 V62

P63 R64 A65 V66 F67 V68 D69 L70 E71 P72 T73 V74 V75 D76 E77 V78 R79 T80 G81 T82 Y83 R84 Q85 L86 F87 H88 P89 E90 Q91 L92 I93 T94 G95 K96 E97 D98 A99 A100 N101 N102 Y103 A104 R105 G106 H107 Y108 T109 I110 G111 K112 E113 I114 V115 D116 L117 V118 L119 D120 R121 I122

R123 K124 L125 A126 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136 I137 F138 H139 S140 F141 G142 G143 G144 T145 G146 S147 G148 F149 A150 S151 L152 L153 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 A170 I171 Y172 P173 A174 P175 Q176 I177 S178 T179 A180 V181 V182

E183 P184 Y185 N186 T187 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 N206 E207 A208 I209 Y210 D211 I212 C213 R214 R215 N216 L217 D218 I219 E220 R221 P222 T223 Y224 T225 N226 L227 N228 R229 L230 I231 A232 Q233 I234 V235 S236 S237 I238 T239 A240 S241 L242

D245 N249 V250 D251 L252 T253 E254 F255 Q256 P263 R264 I265 H266 F267 P268 L269 A270 T271 Y272 A273 P274 V275 I276 S277 A278 E279 K280 A281 Q285 L286 E290 N293 A294 C295 F296 E297 P298 A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 L318 D322

V323 V324 P325 K326 D327 V328 N329 A330 K336 T337 K338 R339 T340 I341 D345 P348 Y357 T361 V362 V363 P364 G365 G366 D367 L368 A369 L378 A383 I384 A385 E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 A403 F404 V405 H406 W407 Y408

V409 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain CM: 54% 96%

M1 R2 E3 S6 A19 E22 L26 I30 D33 G34 Q35 S38 D39 G43 G44 G45 D46 D47 M50 E55 T56 G57 A58 G59 K60 F67 V68 D69 L70 E71 P72 T73 D76 E77 T80 G81 H88 I93 T94 G95 K96 E97 D98 A99 A100

N101 N102 I110 G111 K112 E113 I114 V115 D116 L117 V118 L119 D120 K124 L125 A126 D127 Q128 C129 T130 G131 L132 Q133 L136 I137 F138 G142 G143 M154 E155 R156 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 P173 A174 P175 Q176 I177 S178 T179 A180 E183

T187 I188 L189 H192 E196 H197 S198 D199 F202 M203 N206 E207 Y210 D211 R214 R215 N216 L217 D218 I219 E220 R221 P222 T223 N226 I231 A232 Q233 I234 S237 A240 S241 L242 R243 F244 D245 G246 A247 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 L259

Y262 P263 R264 I265 H266 F267 P268 L269 A270 T271 Y272 A273 P274 A278 E279 K280 A281 E284 Q285 L286 E290 N293 A294 C295 F296 E297 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 Y312 M313 A314 C315 C316 M317 L318 G321 D322 V323 V324 P325 K326 D327 V328

N329 A330 A331 I332 A333 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 K352 Y357 Q358 V362 V363 P364 G365 G366 D367 L368 A369 Q372 M377 L378 S379 N380 A383 I384 A385 E386 A387 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400

K401 R402 A403 F404 V405 H406 W407 Y408 V409 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain DA: 51% 97%

M1 R2 E3 C4 I5 W21 E22 C25 L26 G29 I30 Q31 P32 D33 G34 Q35 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 N50 E55 T56 G57 A58 G59 R64 F67 V68 D69 L70 E71 D76 T82 Y83 R84 Q85 H88 P89 E90 Q91 L92

G95 K96 E97 D98 N101 N102 Y103 A104 R105 G106 H107 Y108 T109 I110 G111 K112 E113 I114 V115 D116 L117 D120 R121 I122 R123 K124 L125 A126 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136 I137 F138 F141 G142 G146 S147 L153 M154 E155 R156 L157 S158 V159 D160 Y161 G162

K163 K164 S165 K166 L167 E168 F169 Y172 Q176 I177 S178 T179 A180 E183 T187 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 F202 M203 V204 D205 D211 R214 R215 D218 I219 E220 R221 R229 Q233 I238 T239 A240 R243 F244 D245 G246 A247

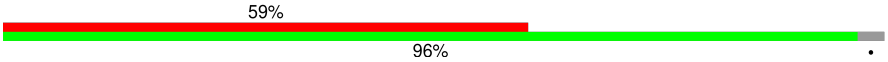
L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 L259 P263 R264 I265 H266 F267 P274 A278 E279 K280 E284 Q285 L286 S287 E290 N293 A294 E297 P298 A299 K304 C305 D306 P307 R308 H309 M313 L318 D322 K326 D327 A330 A331 T334 I335

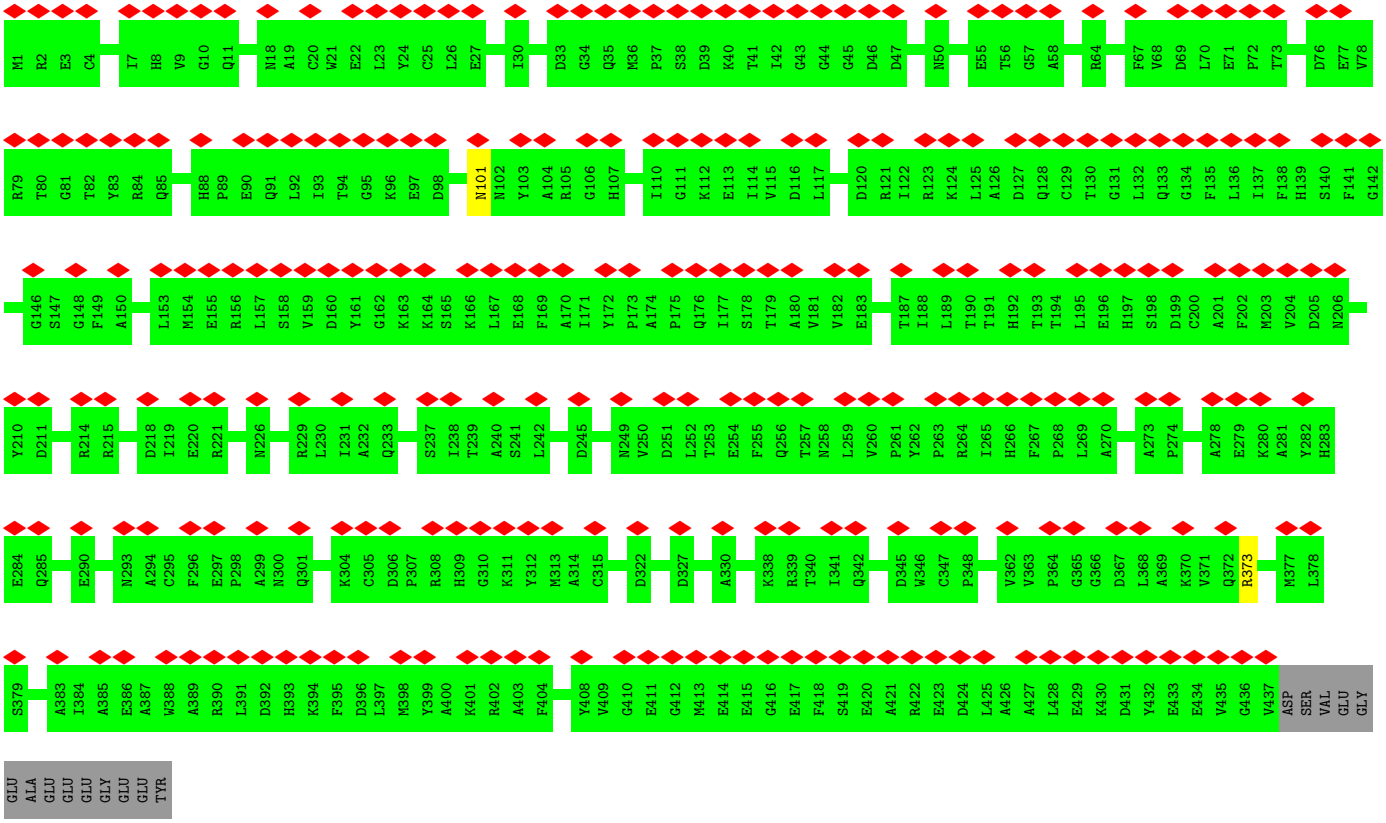
K338 R339 T340 I341 D345 W346 C347 P348 Y357 Q358 T361 V362 V363 P364 G365 G366 D367 L368 A369 K370 V371 Q372 N380 A383 I384 A385 E386 A387 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 R402 A403 F404 V409 G410 E411 G412 M413 E414 E415 G416 E417 F418

S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLU GLU GLY GLU GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain DB:





- Molecule 54: Tubulin alpha chain

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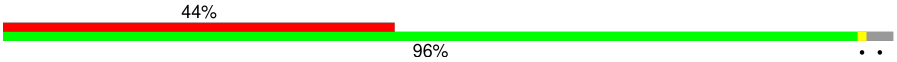
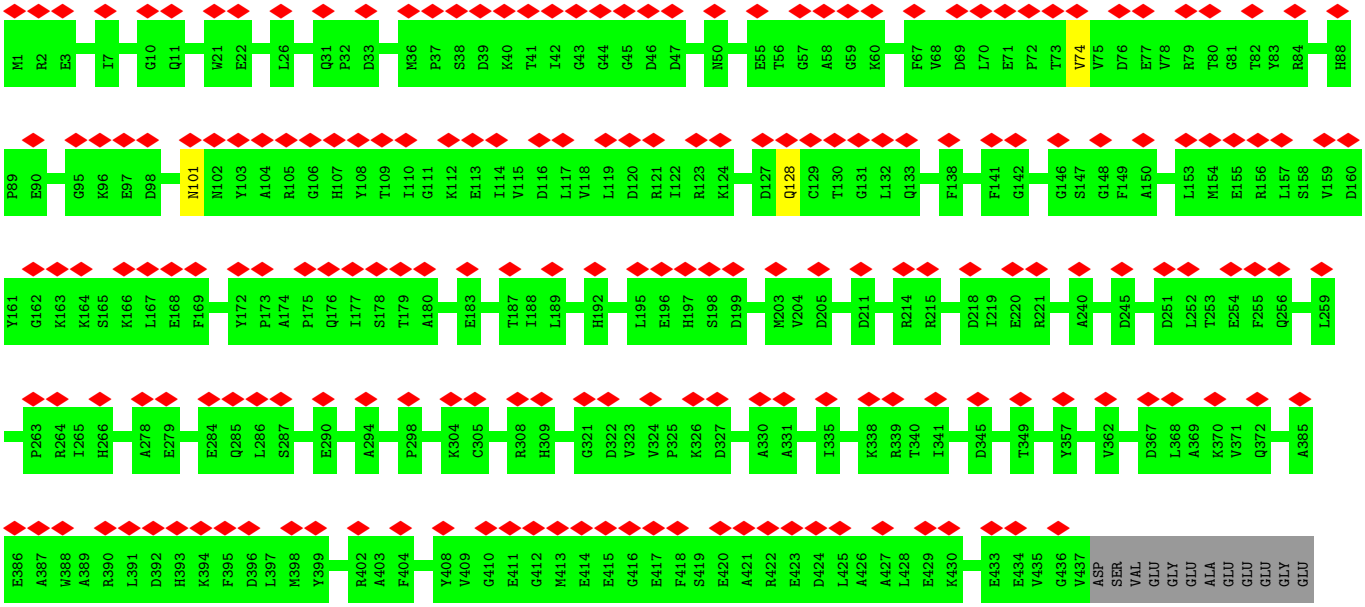




GLU
TYR

• Molecule 54: Tubulin alpha chain

Chain DG: 63% 96%

M1 R2 E3 I7 H8 V9 G10 N18 A19 C20 W21 E22 L23 Y24 C25 L26 E27 H28 G29 I30 Q31 P32 D33 G34 Q35 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 S48 F49 N50 F53 S54 E55 T56 G57 A58 G59 K60 H61 A65 V66 D69 L70 E71 P72

T73 V74 V75 D76 E77 V78 R79 T80 G81 R84 Q85 L86 F87 H88 P89 E90 Q91 G95 K96 E97 D98 N102 Y103 A104 R105 G106 H107 I110 G111 K112 E113 I114 V115 D116 L117 V118 L119 D120 R121 I122 R123 K124 L125 A126 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136 I137 F138

F141 G142 G148 L153 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 A170 I171 Y172 P175 S178 T179 A180 E183 T187 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 D211 R214 R215 N216

L217 D218 I219 E220 R221 R229 Q233 I238 T239 A240 S241 L242 R243 F244 D245 G246 A247 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 L259 V260 P261 Y262 P263 R264 I265 H266 F267 P268 L269 A270 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 V288 A289 E290 N293 A294 C295

F296 A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 Y312 M313 A314 C315 C316 M317 L318 Y319 R320 G321 D322 K326 D327 A330 A331 I332 A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 K352 Y357 Q358 T361 V362 V363

P364 G365 G366 D367 L368 A369 K370 V371 Q372 R373 A374 V375 C376 M377 L378 S379 T382 A383 I384 A385 E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 A403 Y408 V409 G410 E411 G412 M413 E414 E415 G416 E417 E420 A421 R422 E423 D424 L425 A426 A427 L428

E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

• Molecule 54: Tubulin alpha chain

Chain DI: 56% 96%

M1 R2 E3 I7 H8 V9 G10 Q11 N18 A19 C20 W21 E22 L23 Y24 C25 L26 E27 D33 G34 Q35 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 S48 F49 N50 F53 S54 E55 T56 G57 A58 G59 K60 H61 F67 V68 D69 L70 E71 P72 T73 D76 E77

V78 R79 R84 Q85 H88 P89 E90 Q91 L92 G95 K96 E97 D98 N101 N102 Y103 A104 R105 G106 H107 Y108 T109 I110 G111 K112 E113 I114 V115 D116 L117 D120 R121 I122 R123 K124 L125 A126 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136 I137 F138 H139 S140 F141 G142 G146

A150 L153 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 A170 I171 Y172 P173 A174 P175 Q176 I177 S178 T179 A180 E183 T187 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 N206 E207 A208 I209 Y210 D211

R214 R215 N216 L217 D218 I219 E220 R221 R229 Q233 A240 S241 L242 R243 F244 D245 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 L259 V260 P263 R264 I265 H266 F267 P268 L269 A270 S277 A278 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 E290 N293 A294 E297

P298 A299 N300 Q301 K304 C305 D306 P307 R308 H309 Y312 M313 L318 D322 V323 V324 P325 K326 D327 A330 A331 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 Y357 V362 V363 P364 G365 G366 D367 L368 A369 K370 V371 Q372 N380

A383 I384 A385 E386 A387 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 R402 A403 F404 Y408 V409 G410 E411 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU

GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain DK: 93% 96%

M1 R2 E3 C4 I5 S6 I7 H8 V9 G10 Q11 A12 G13 V14 Q15 I16 G17 N18 A19 C20 W21 E22 L23 Y24 C25 L26 E27 H28 G29 I30 Q31 P32 D33 G34 Q35 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 S48 F49 N50 T51 F52 F53 S54 E55 T56 G57 A58 G59 K60

H61 V62 P63 R64 A65 V66 F67 V68 D69 L70 E71 P72 T73 V74 V75 D76 E77 V78 R79 T80 G81 T82 Y83 R84 Q85 L86 F87 H88 P89 E90 Q91 L92 I93 T94 G95 K96 E97 D98 A99 A100 N101 N102 Y103 A104 R105 G106 H107 Y108 T109 I110 G111 K112 E113 I114 V115 D116 L117 V118 L119 D120

R121 I122 R123 K124 L125 A126 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136 I137 F138 H139 S140 F141 G142 G143 G144 T145 G146 S147 G148 F149 A150 S151 L152 L153 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 A170 I171 Y172 P173 A174 P175 Q176 I177 S178 T179 A180

V181 V182 E183 P184 Y185 N186 T187 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 N206 E207 A208 I209 Y210 D211 I212 C213 R214 R215 N216 L217 D218 I219 E220 R221 P222 T223 Y224 T225 N226 L227 N228 R229 L230 I231 A232 Q233 I234 V235 S236 S237 I238 T239 A240

S241 L242 R243 F244 D245 G246 A247 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 L259 V260 P261 Y262 P263 R264 I265 H266 F267 P268 L269 A270 T271 Y272 A273 P274 V275 I276 S277 A278 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 A294 C295 F296 E297 P298 A299 N300

Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 Y312 M313 A314 C315 C316 M317 L318 Y319 R320 G321 D322 V323 V324 P325 K326 D327 V328 N329 A330 A331 I332 A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 I355 N356 Y357 P360 T361 V362 V363

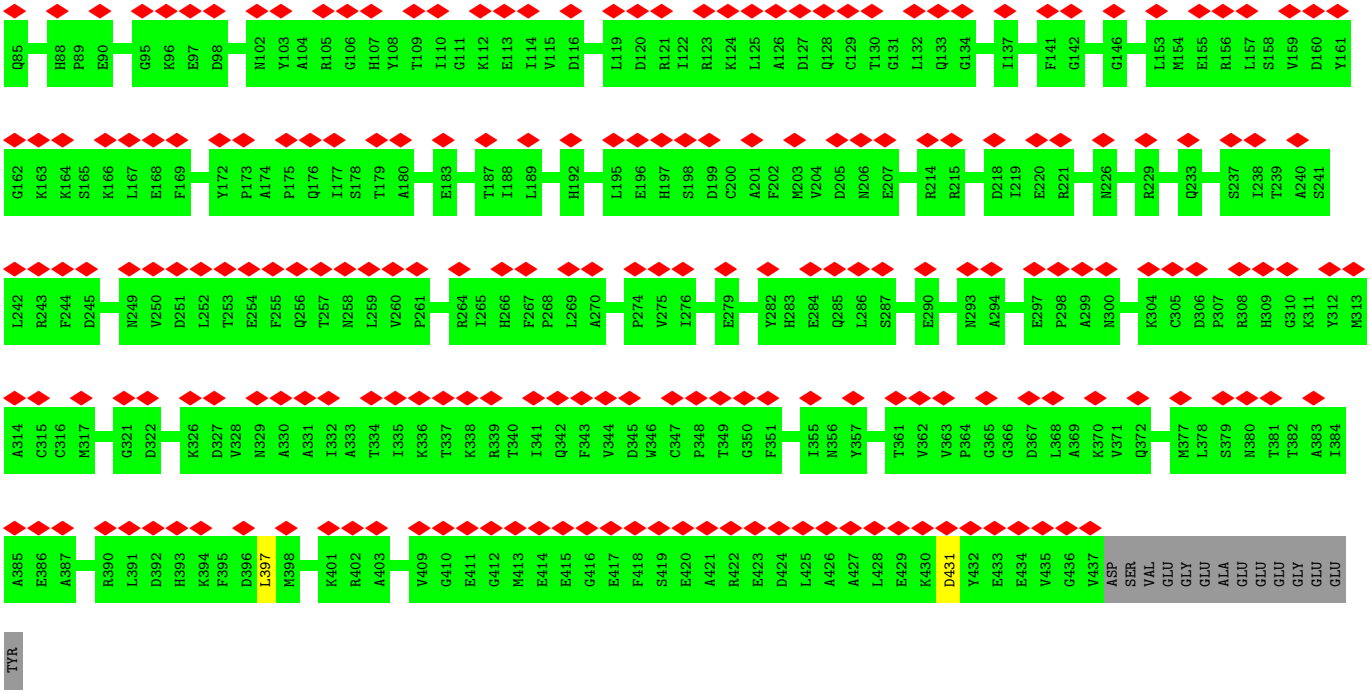
P364 G365 G366 D367 L368 A369 K370 V371 Q372 R373 A374 V375 C376 M377 L378 S379 N380 T381 T382 A383 I384 A385 E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 A403 F404 V405 H406 W407 Y408 V409 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423

D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

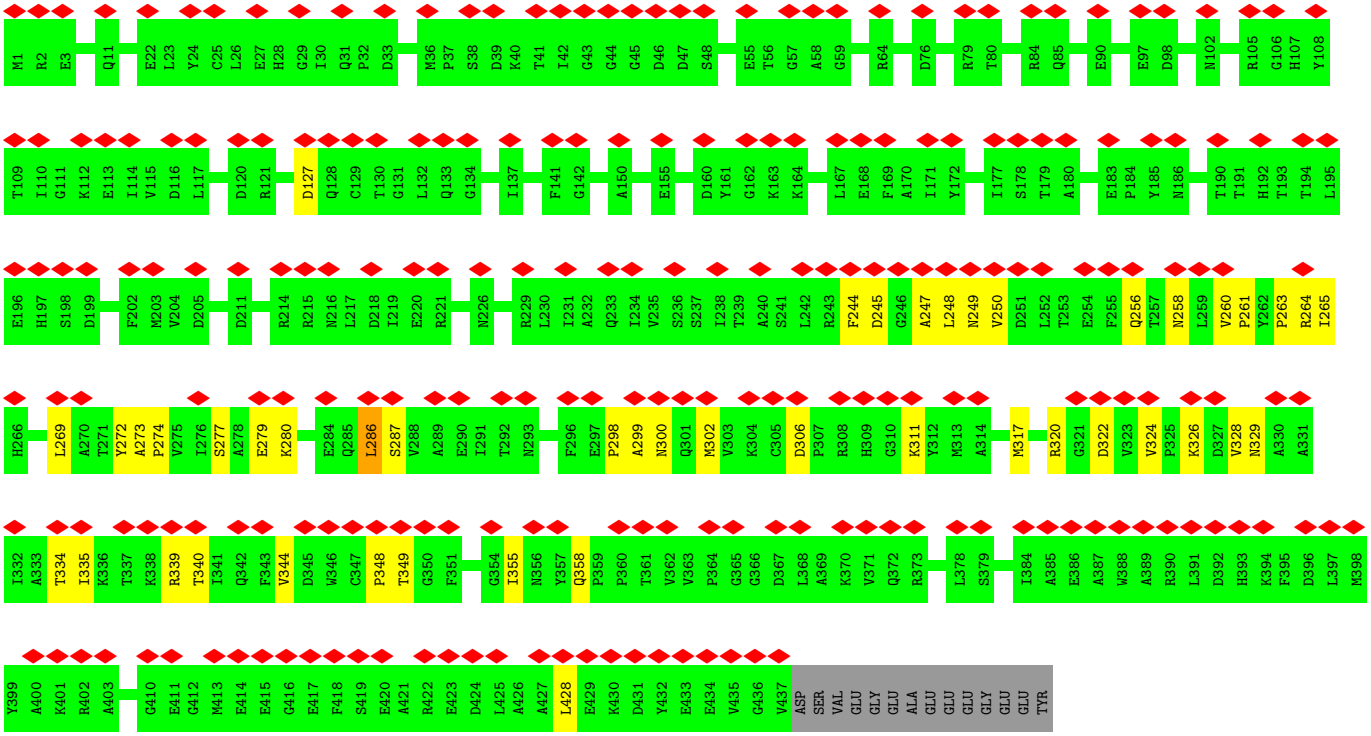
Chain DM: 56% 96%

M1 R2 E3 H8 V9 N18 W21 E22 C25 L26 Q31 P32 D33 G34 Q35 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 S48 F49 N50 F53 S54 E55 T56 G57 A58 G59 K60 F67 V68 D69 L70 E71 P72 T73 D76 R79 T80 G81 R84



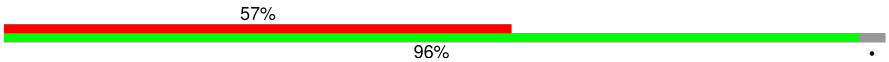
- Molecule 54: Tubulin alpha chain

Chain EA:



- Molecule 54: Tubulin alpha chain

Chain EC:



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G95 K96 E97 D98 R105 Y108 T109 I110 E113 I114 V115 D116 D120 D127 Q128 C129 T130 G134 F135 L136 H139 S140 F141 G142 G146 S147 A150 L153 M154 E155 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 A170 I171 Y172 P175 Q176 I177 S178 T179

E183 P184 Y185 N186 T187 I188 L189 H192 T193 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 N206 E207 Y210 D211 R214 R215 N216 L217 D218 I219 E220 L227 N228 R229 L230 I231 A232 Q233 I234 I238 T239 A240 S241 D245 G246 A247 L248 N249 V250 D251 L252 T253

E254 F255 Q256 T257 N258 L259 V260 P261 Y262 P263 R264 I265 H266 F267 P268 L269 A270 T271 Y272 A273 P274 V275 I276 S277 A278 E279 K280 E284 Q285 L286 A289 E290 I291 T292 N293 A294 C295 F296 E297 P298 A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 Y312 M313 A314 C315 C316

M317 L318 G321 D322 K326 D327 A330 A331 I332 A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 K352 V353 G354 Y357 V362 V363 P364 G365 G366 D367 L368 A369 K370 V371 Q372 R373 A374 V375 C376 M377 L378 S379 N380 T381 T382 A383 I384

A385 E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 A403 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU

GLU TYR

- Molecule 54: Tubulin alpha chain

Chain EE: 56% 96%

M1 R2 E3 G17 E22 L23 Y24 C25 L26 E27 H28 G29 I30 Q31 P32 D33 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 N50 T51 F52 E55 T56 G57 A58 G59 K60 H61 R64 A65 V66 F67 E71 V74 V75 D76 R79 T80 R84 Q85

E90 Q91 L92 I93 E97 D98 N102 R105 G106 I110 E113 I114 V115 D116 L117 D120 R121 I122 R123 K124 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136 I137 F138 H139 S140 F141 G142 T145 G146 S147 A150 L153 M154 E155 V159 D160 Y161 G162 K163

K164 S165 K166 L167 E168 F169 A170 I171 Y172 P175 Q176 I177 S178 T179 A180 E183 P184 Y185 N186 T187 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 F202 M203 V204 D205 N206 E207 D211 R214 R215 D218 I219 E220 T225 R229 L230 I231 A232 Q233 I234

I238 T239 A240 F244 D245 G246 A247 L248 D251 L252 T253 E254 F255 Q256 T257 N258 L259 V260 P263 R264 I265 H266 F267 P268 L269 A270 V275 E279 K280 A281 Y282 H283 E284 Q285 A289 E290 I291 T292 N293 A294 C295 F296 E297 P298 A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308

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T382 A383 I384 A385 E386 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 A403 V409 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU

GLU GLY GLU GLU TYR

• Molecule 54: Tubulin alpha chain

Chain EG: 62% 96%

M1 R2 E3 V9 G17 C20 Y24 E27 H28 D33 M36 P37 S38 I42 G43 G44 G45 D46 D47 N50 E55 T56 G57 A58 G59 R64 F67 V68 D69 L70 V74 V75 D76 E77 V78 R79 T80 G81 R84 Q85 L86 F87 E90 Q91 L92

I93 K96 E97 D98 N102 Y103 A104 R105 G106 H107 Y108 T109 I110 G111 K112 E113 I114 V115 D116 L117 D120 R121 I122 R123 K124 L125 A126 D127 Q128 C129 T130 Q133 G134 I137 F138 H139 S140 F141 G142 G143 G144 T145 G146 S147 G148 F149 A150 E155 R156 D160 Y161 G162 K163

K164 S165 K166 L167 E168 F169 Y172 P173 A174 P175 Q176 I177 S178 T179 A180 V181 V182 E183 N186 T187 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 N206 E207 A208 I209 Y210 D211 R214 R215 D218 I219 E220 T225 N226 L227 N228 R229 L230

I231 I234 I238 L242 R243 F244 D245 G246 A247 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 L259 V260 P261 Y262 P263 R264 I265 H266 F267 P268 L269 A270 T271 Y272 A273 P274 S277 A278 E279 K280 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 A294 C295 F296 E297 P298

A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 Y312 M313 A314 C315 C316 M317 L318 G321 D322 V323 K326 D327 V328 N329 A330 A331 I332 A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 G354 I355 N356 Y357 T361 G365

G366 D367 L368 A369 K370 V371 Q372 R373 M377 L378 S379 N380 T381 T382 A383 I384 A385 E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 A403 Y408 V409 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430

D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

• Molecule 54: Tubulin alpha chain

Chain EI: 63% 96%

M1 R2 E3 G10 Q11 G17 E22 L23 Y24 C25 L26 E27 H28 G29 I30 Q31 P32 D33 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 E55 T56 G57 A58 G59 K60 H61 A65 V66 F67 V68 D69 L70 E71 V74 V75 D76 R79 R84 Q85

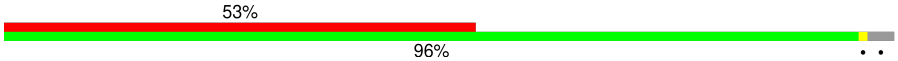
E90 Q91 L92 G95 K96 E97 D98 A99 N102 R105 G106 H107 Y108 K112 E113 D116 L117 D120 R121 I122 R123 K124 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136 I137 F138 H139 S140 F141 G142 G146 A150 L153 M154 E155 R156 D160 Y161 G162 K163 K164

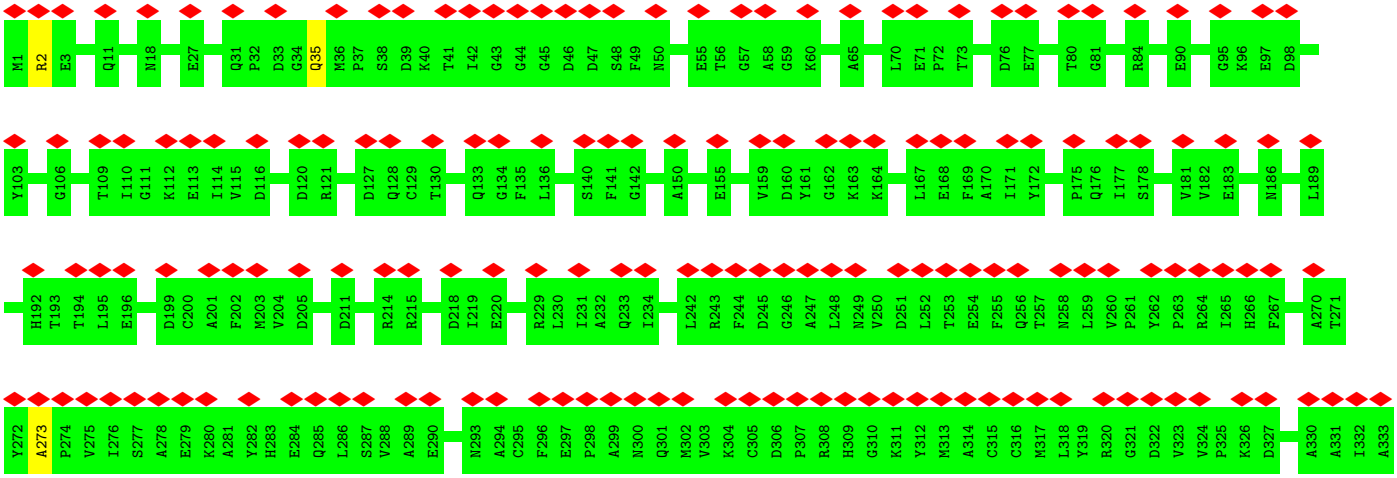
S165 K166 L167 E168 F169 A170 I171 Y172 P173 A174 P175 Q176 I177 S178 T179 A180 E183 P184 Y185 N186 T187 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 N206 E207 A208 I209 Y210 D211 I212 C213 R214 R215 N216 L217 D218 I219 E220 R221 L227 N228 R229

L230 I231 A232 Q233 I234 S237 A240 R243 F244 D245 G246 A247 L248 N249 V250 D251 L252 T253 E254 F255 Q256 L259 R264 I265 H266 F267 P268 L269 A270 T271 Y272 A273 P274 V275 I276 S277 A278 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 E290 I291 T292 N293 A294 C295 F296 E297

- Molecule 54: Tubulin alpha chain

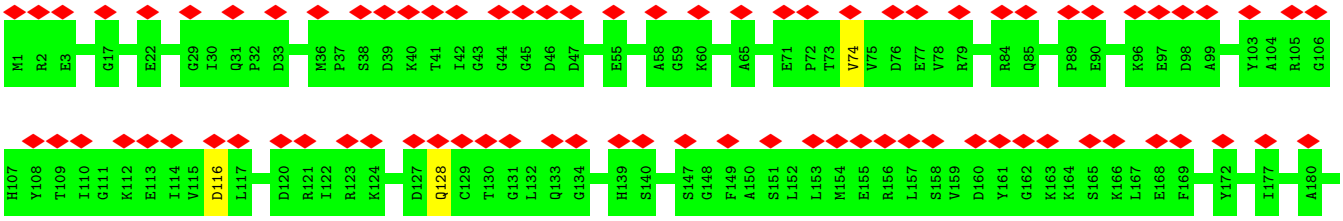
Chain EK:

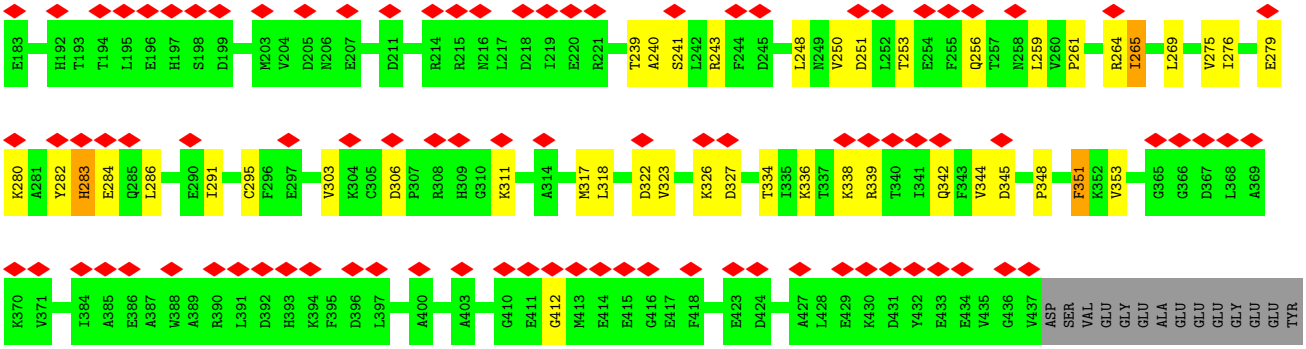




- Molecule 54: Tubulin alpha chain

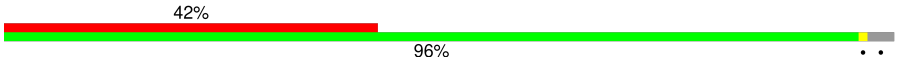
Chain FA:

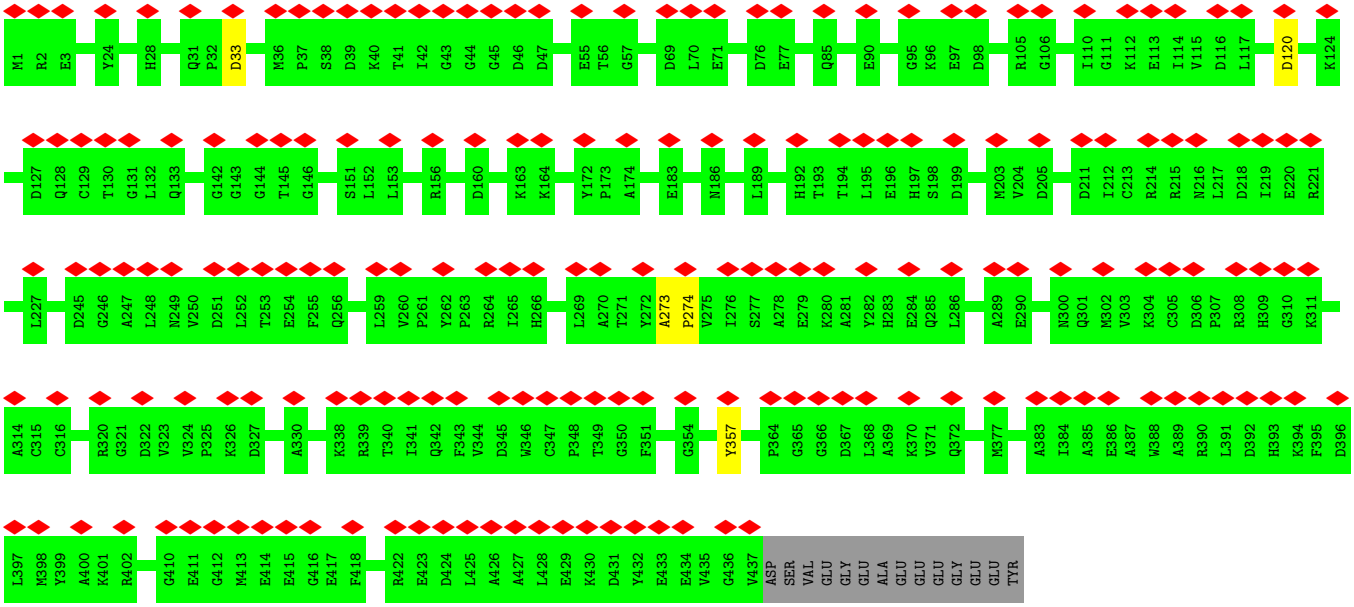




- Molecule 54: Tubulin alpha chain

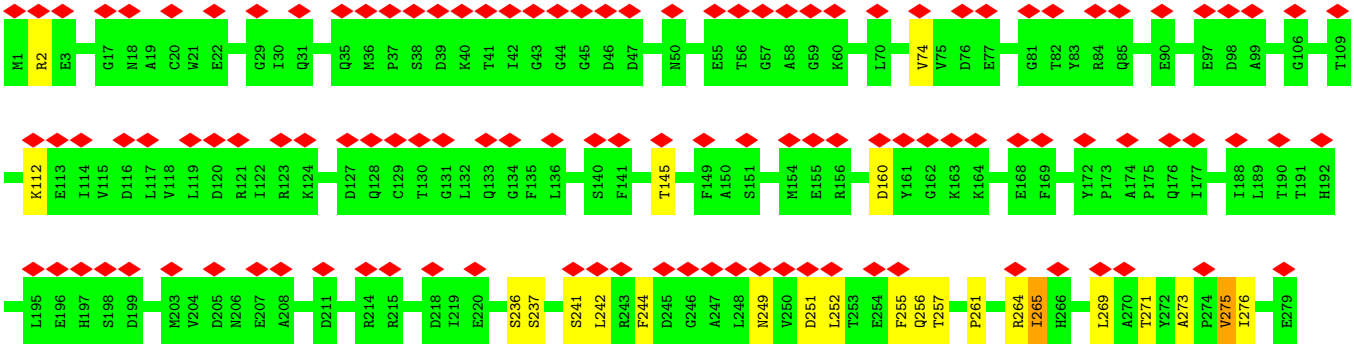
Chain FB:

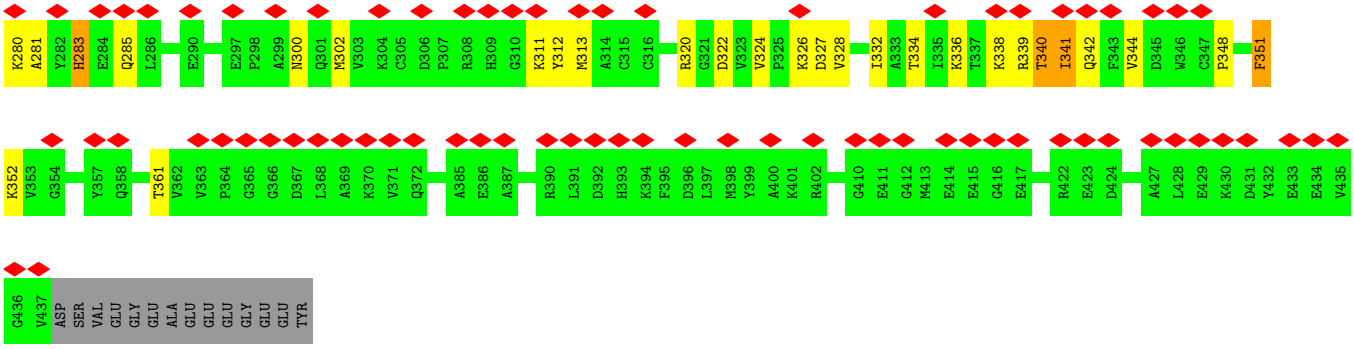




- Molecule 54: Tubulin alpha chain

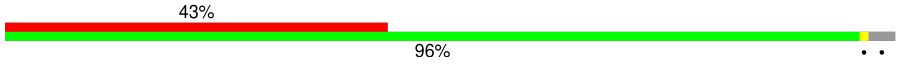
Chain FE:

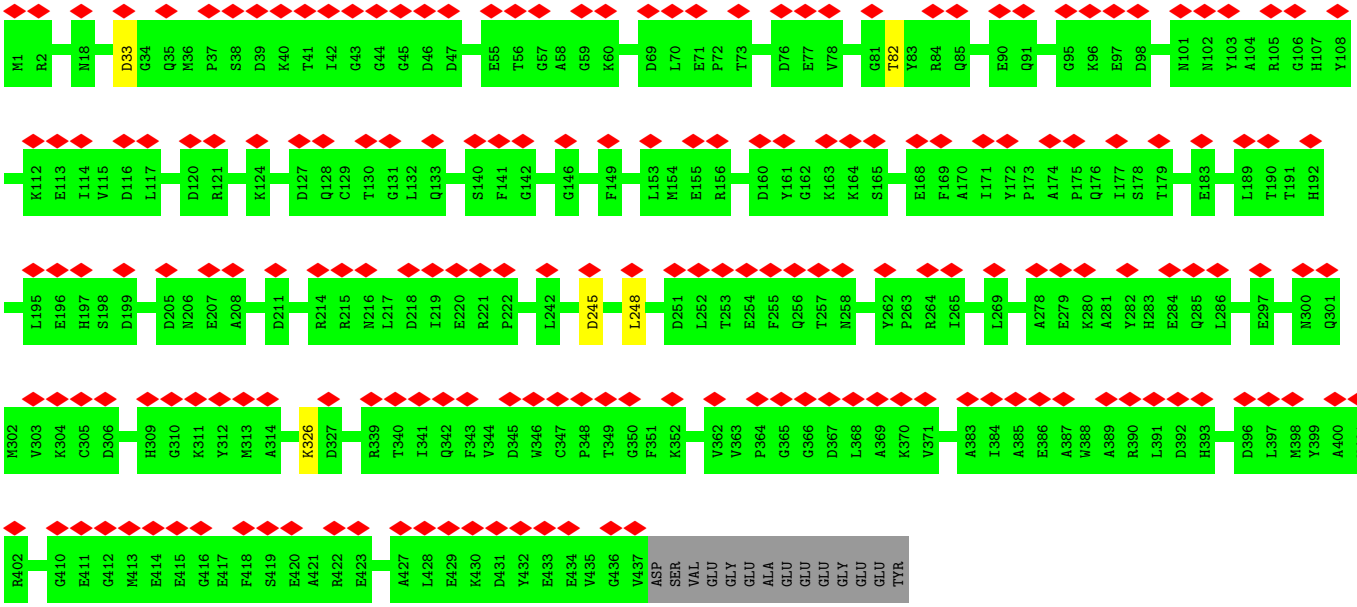




- Molecule 54: Tubulin alpha chain

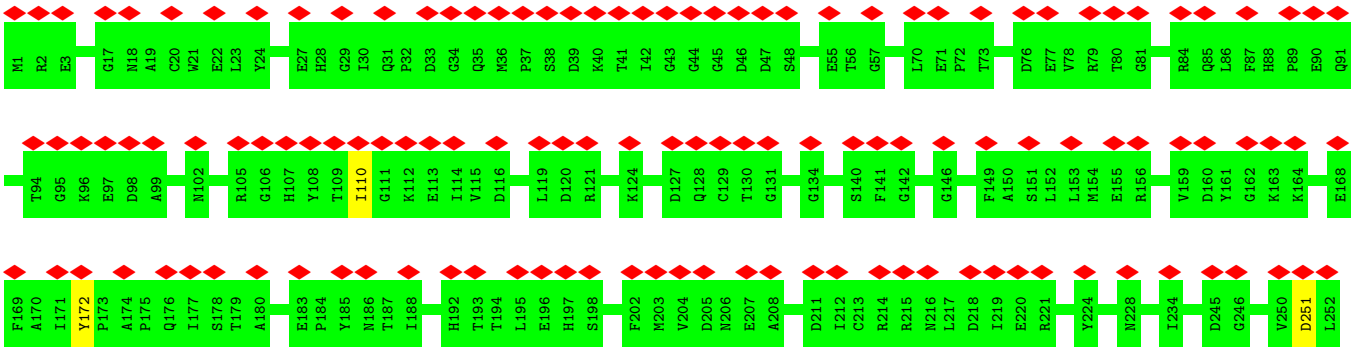
Chain FG:

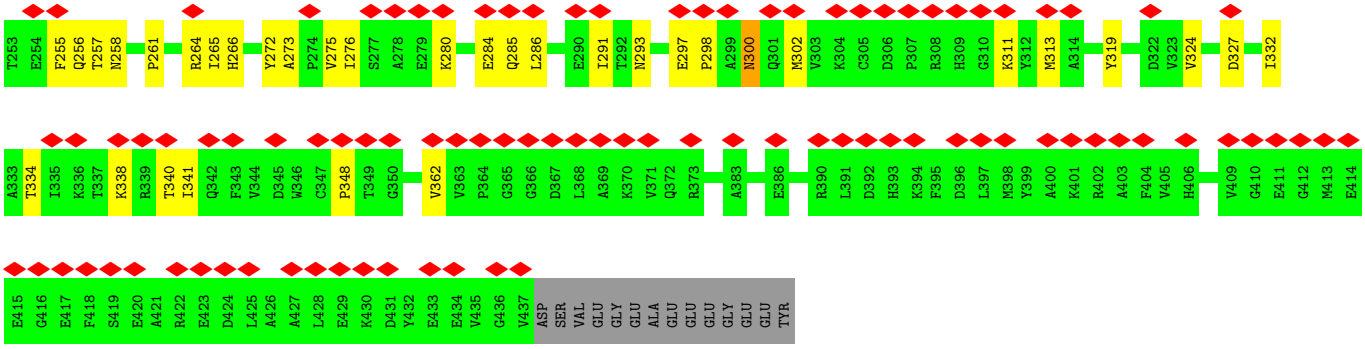




- Molecule 54: Tubulin alpha chain

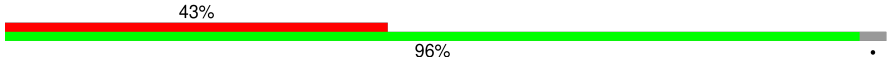
Chain FI:

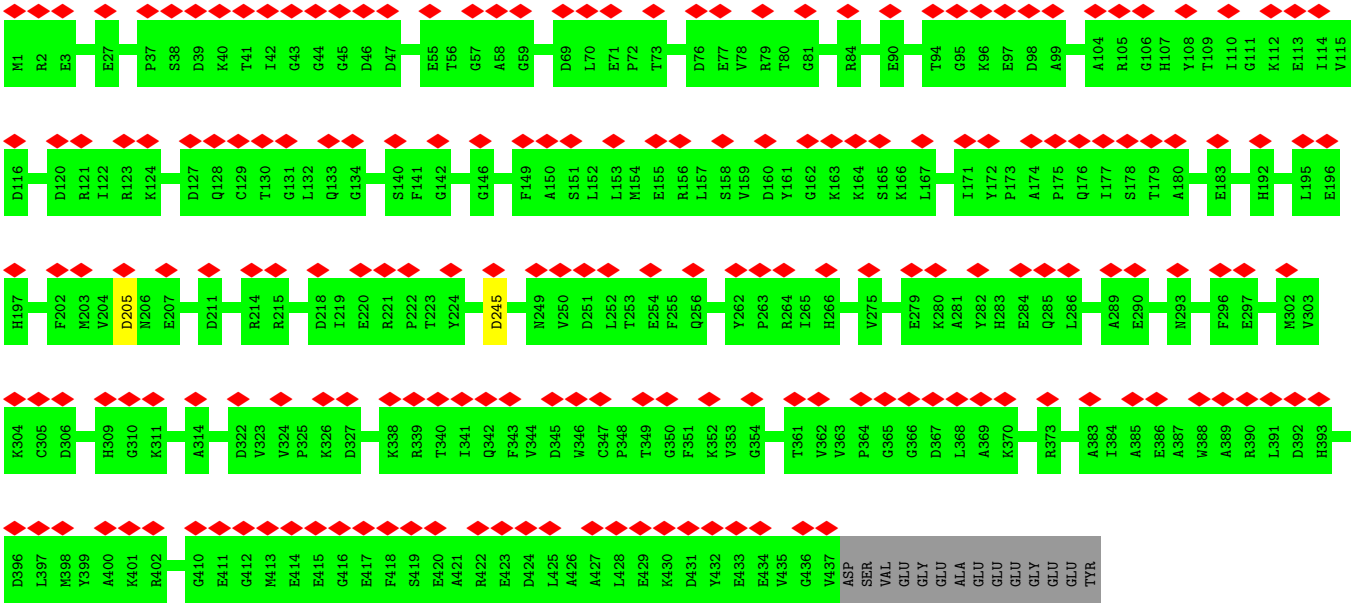




- Molecule 54: Tubulin alpha chain

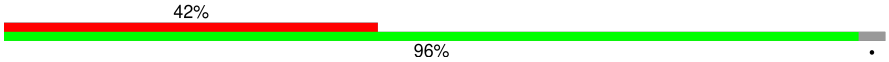
Chain FK:

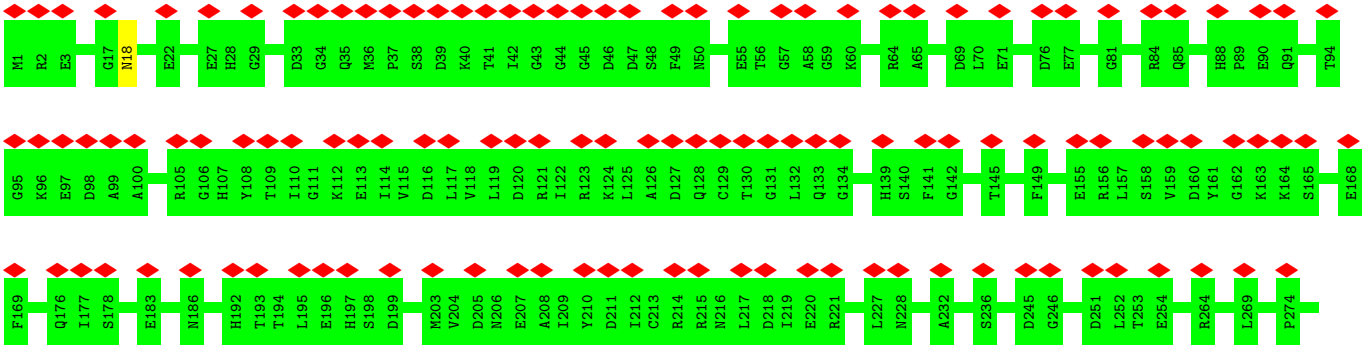


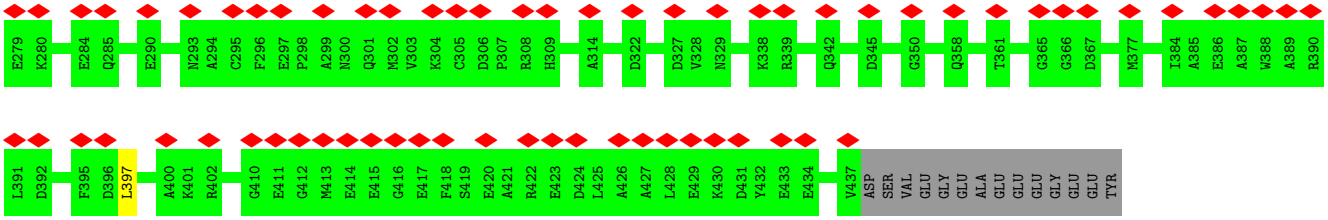


- Molecule 54: Tubulin alpha chain

Chain GA:

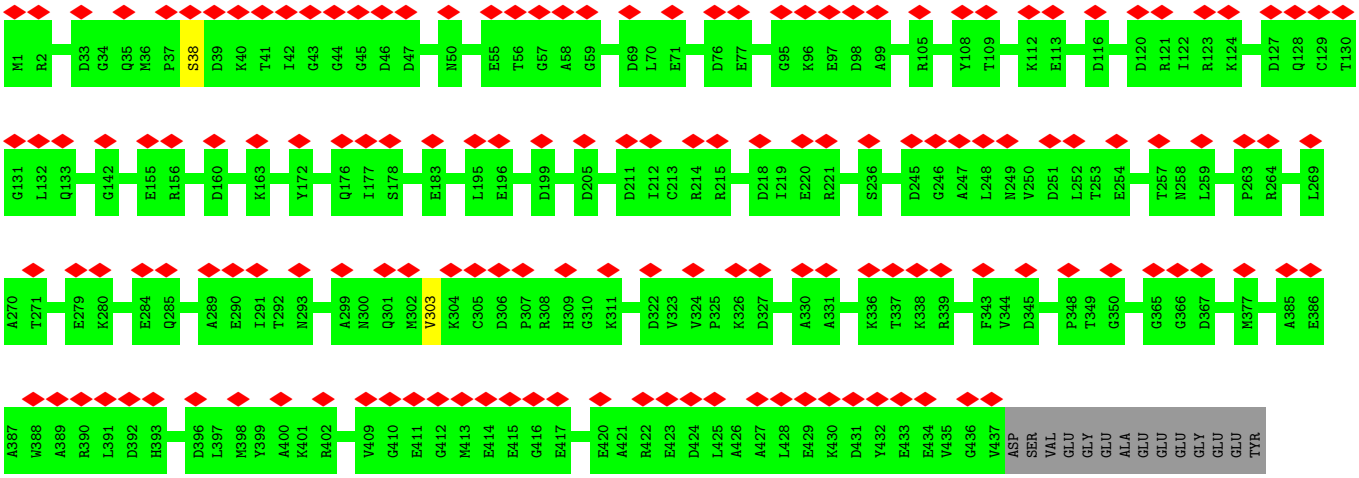






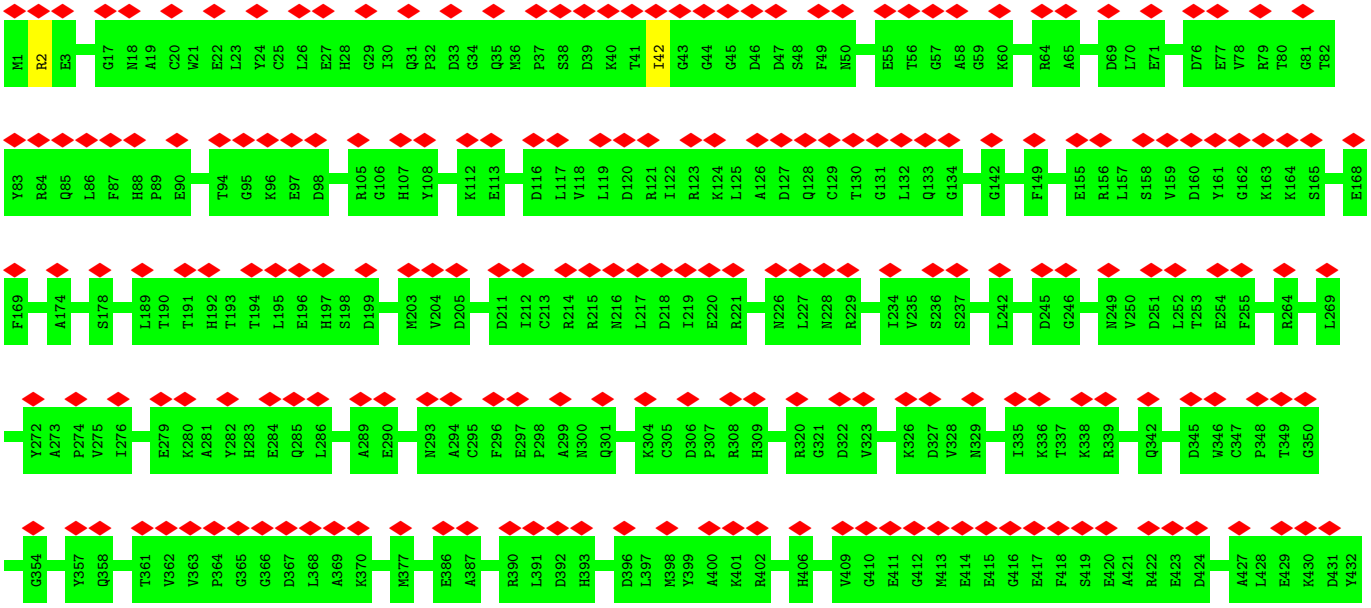
• Molecule 54: Tubulin alpha chain

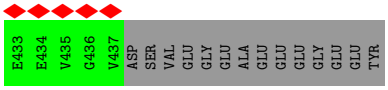
Chain GB: 34% 96%



• Molecule 54: Tubulin alpha chain

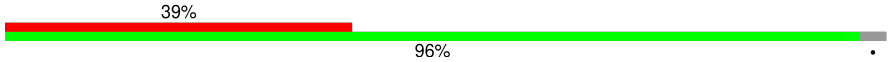
Chain GE: 47% 96%

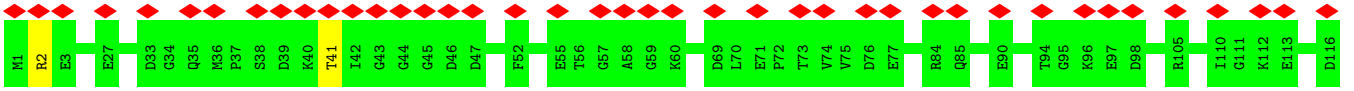


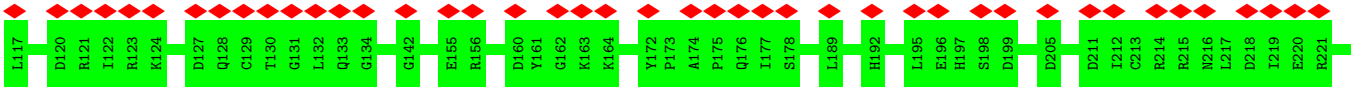


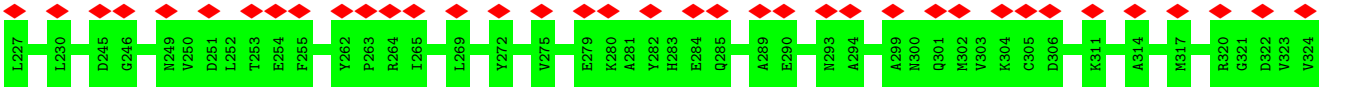
• Molecule 54: Tubulin alpha chain

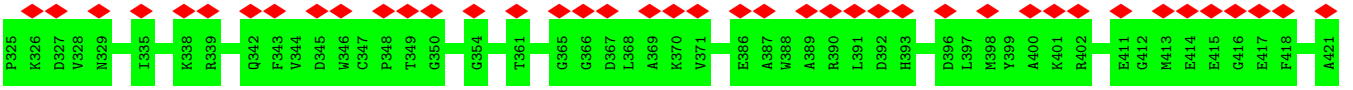
Chain GG:

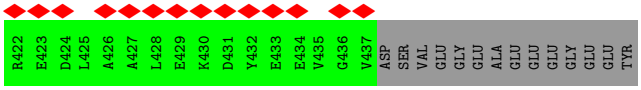






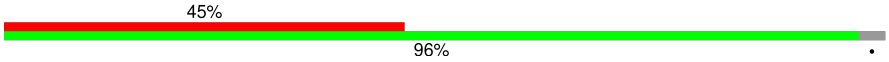


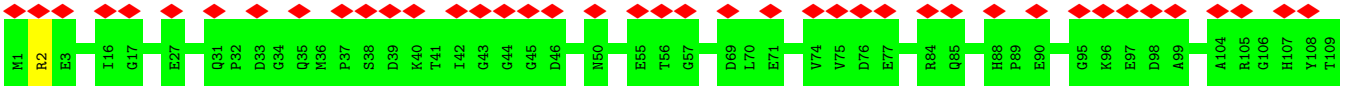


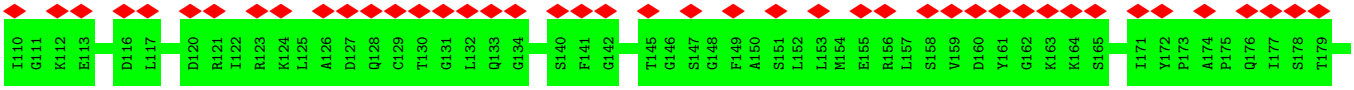


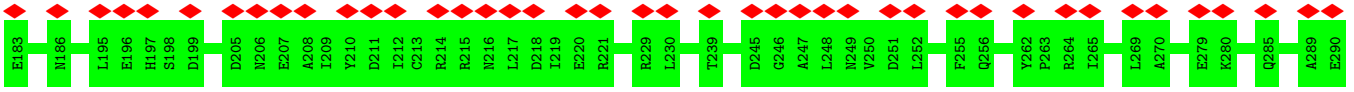
• Molecule 54: Tubulin alpha chain

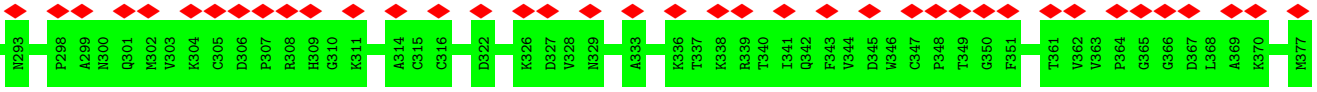
Chain GI:

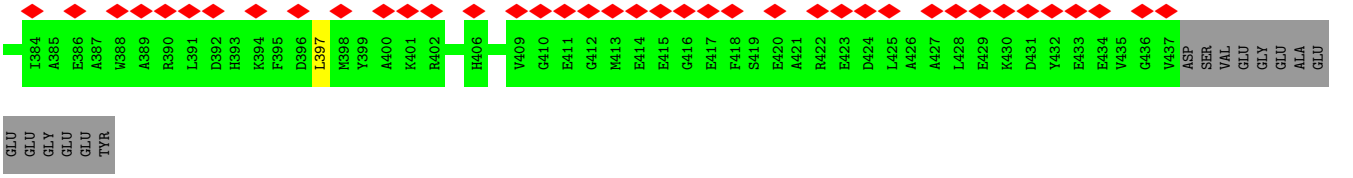






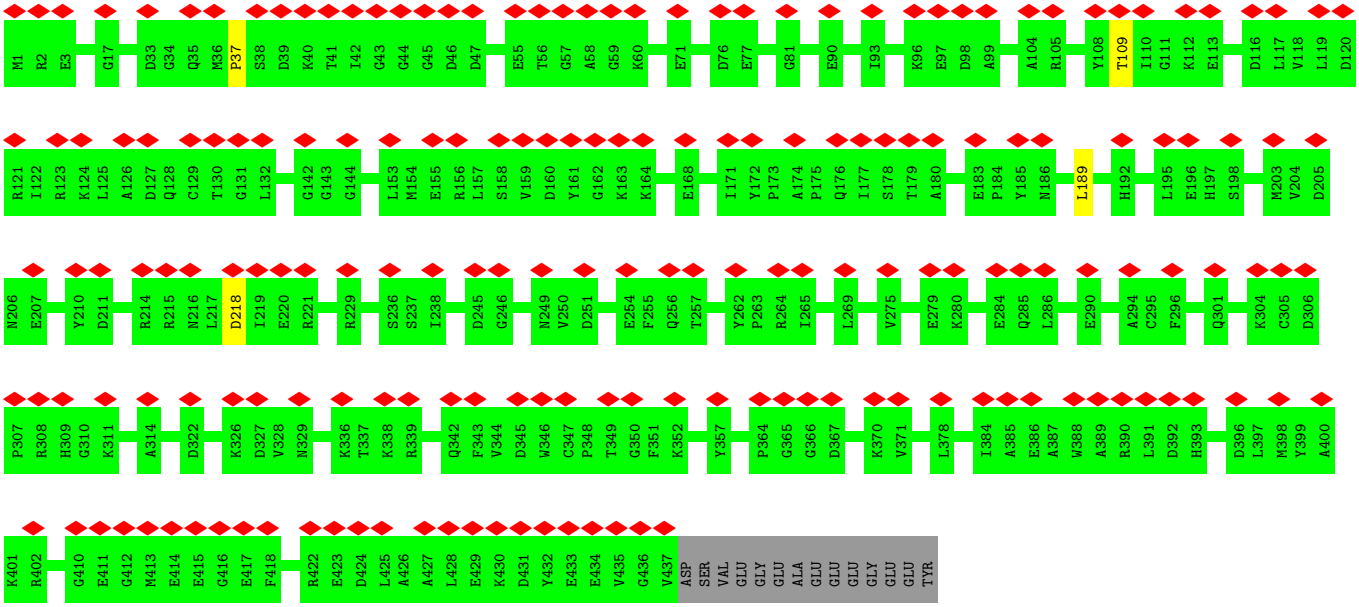






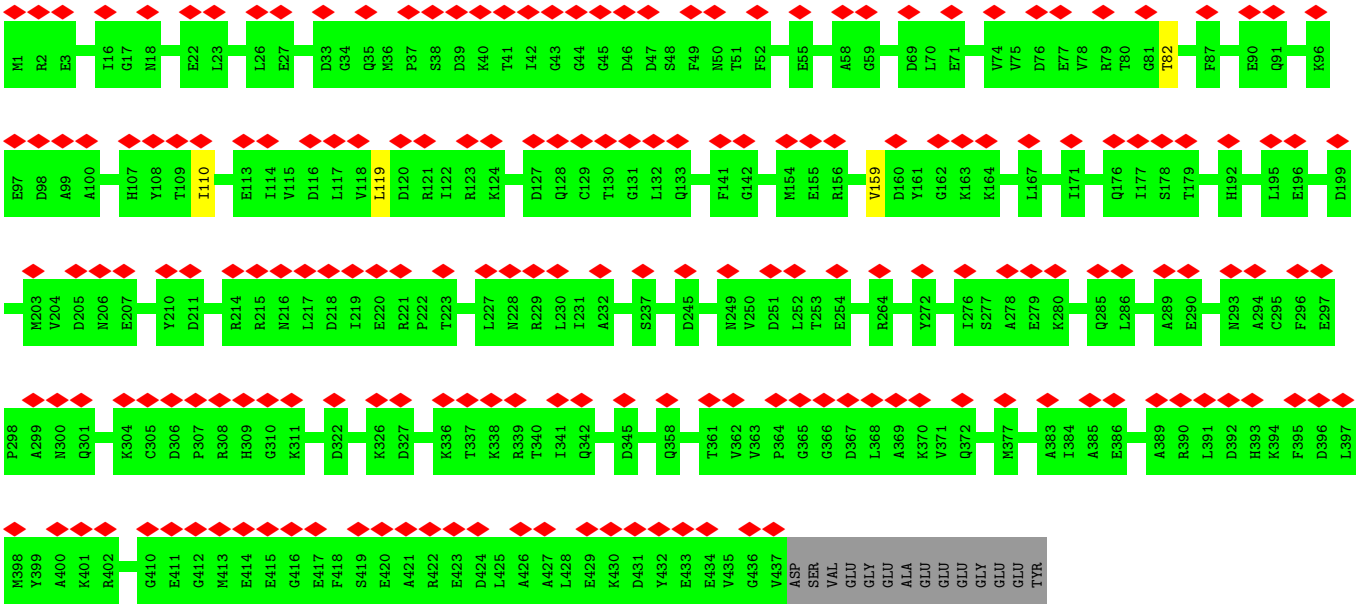
- Molecule 54: Tubulin alpha chain

Chain GK: 41% 96%



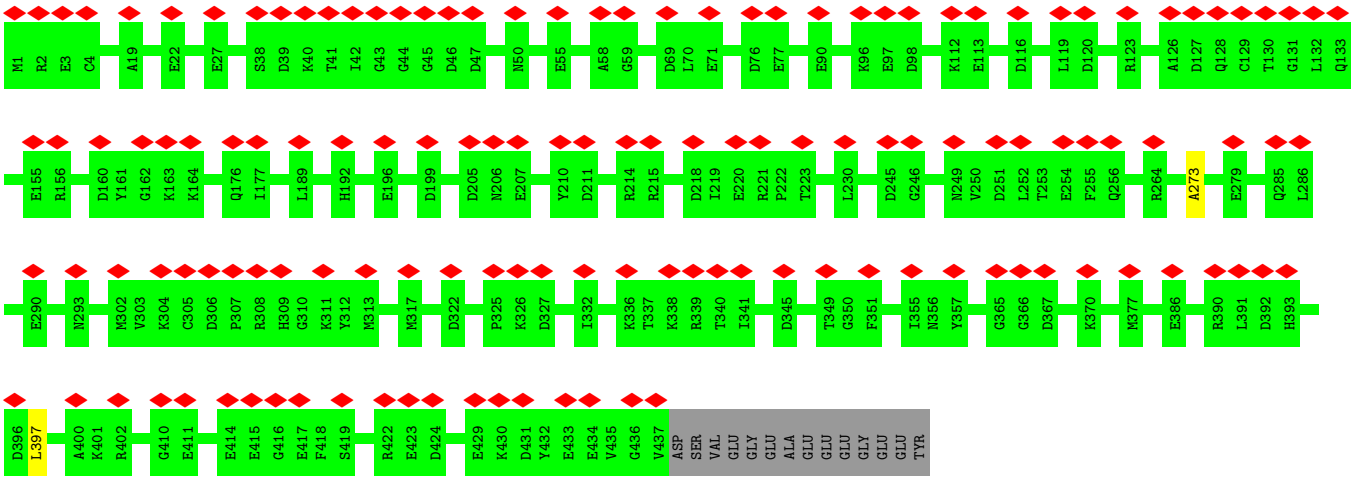
- Molecule 54: Tubulin alpha chain

Chain HA: 43% 96%



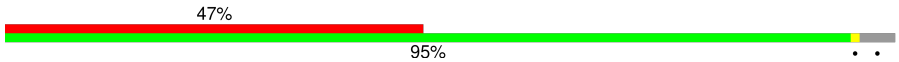
- Molecule 54: Tubulin alpha chain

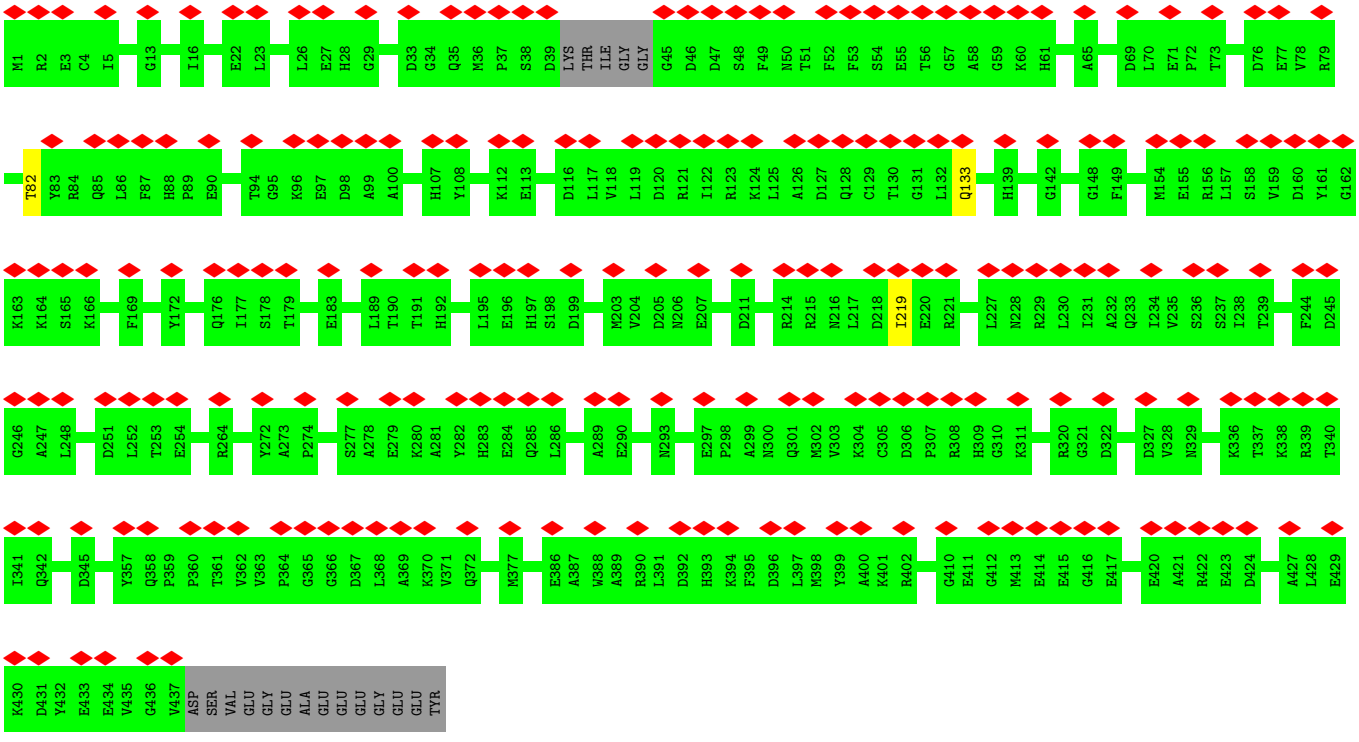
Chain HB: 30% 96%



- Molecule 54: Tubulin alpha chain

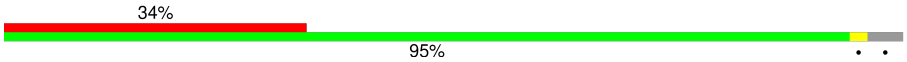
Chain HE:

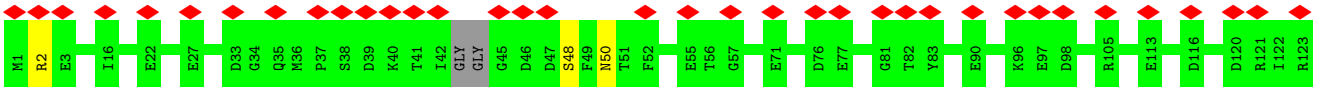


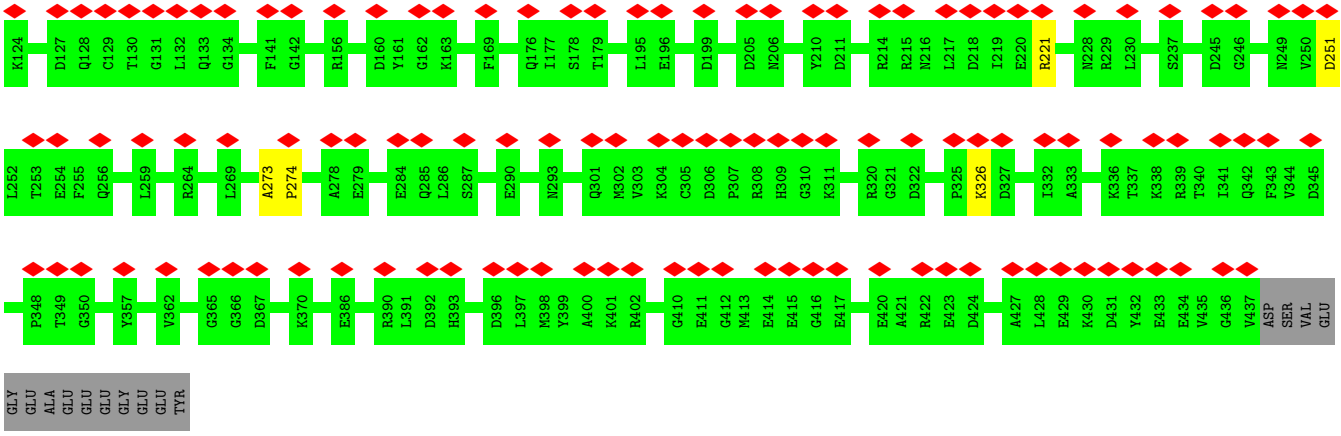


- Molecule 54: Tubulin alpha chain

Chain HG:

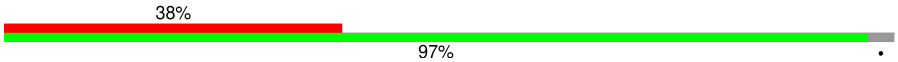


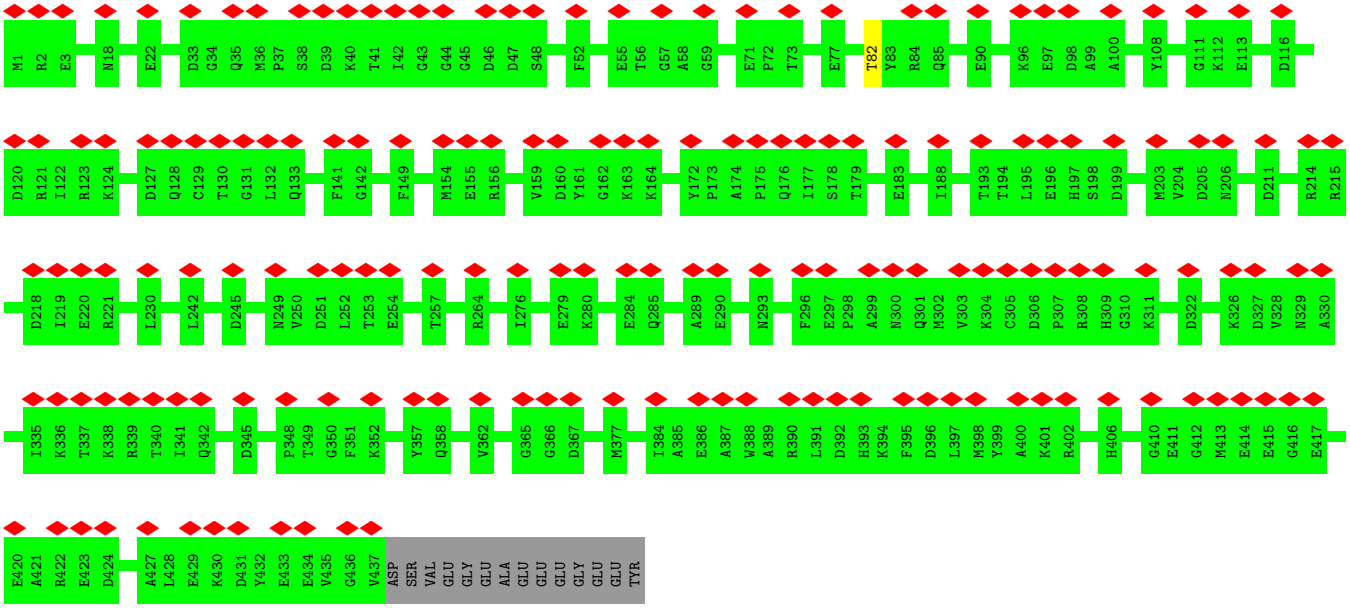




- Molecule 54: Tubulin alpha chain

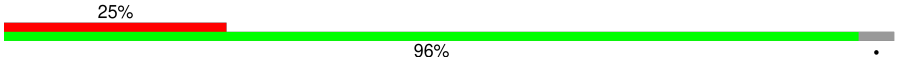
Chain HI:

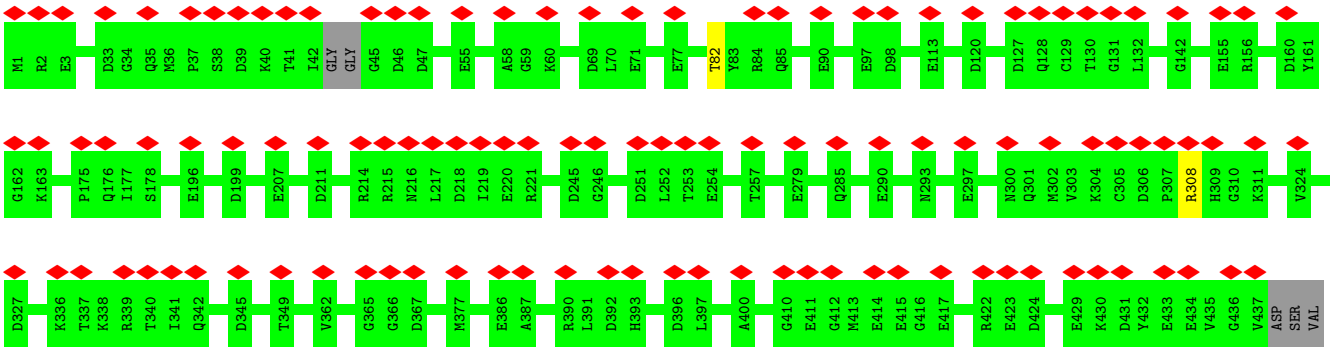




- Molecule 54: Tubulin alpha chain

Chain HK:

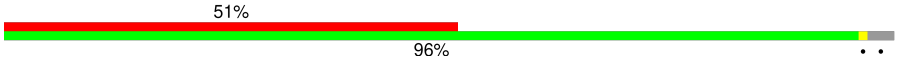




GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain IA:



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N102 Y103 A104 R105 G106 H107 Y108 T109 I110 G111 K112 E113 D116 L117 V118 L119 D120 R121 I122 R123 K124 L125 A126 D127 Q128 C129 T130 G131 L132 Q133 G134 F141 G142 G143 G144 T145 G146 S147 G148 L152 L153 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169

A170 I171 Y172 P173 A174 P175 Q176 I177 S178 T179 V182 E183 P184 Y185 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 N206 E207 Y210 D211 I212 C213 R214 R215 N216 L217 D218 I219 E220 R221 P222 A240 R243 F244 D245 V250 D251 L252

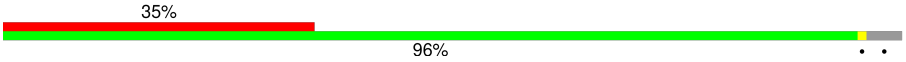
T253 E254 F255 R264 L269 E279 K280 Q285 L286 E290 F296 A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 M317 D322 V323 V324 D327 V328 N329 I332 A333 K336 T337 K338 R339 T340 I341 Q342 D345 W346 C347 P348 K352

Y357 Q358 V362 V363 P364 G365 G366 D367 M377 A385 E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 A403 F404 V405 H406 W407 Y408 V409 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432

E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain IB:



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G143 G144 G148 M154 E155 R156 V159 D160 Y161 G162 K163 K164 S165 A174 P175 Q176 I177 S178 T179 E183 I188 L195 E196 H197 S198 D199 D205 N206 D211 R214 R215 D218 I219 E220 D245 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258

R264 I265 H266 L269 A273 Q285 L286 E290 N293 M302 D306 P307 R308 H309 G310 K311 Y312 M313 M317 V324 D327 V328 N329 K336 T337 K338 R339 T340 I341 Q342 D345 W346 C347 P348 F351 K352 Y357 P364 G365 G366 D367 L378 A385

E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 H406 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU

GLU TYR

- Molecule 54: Tubulin alpha chain

Chain IE: 70% 97%

M1 R2 E3 C4 I5 S6 A12 G13 G17 N18 A19 E22 L23 Y24 C25 L26 E27 H28 G29 I30 Q31 P32 D33 G34 Q35 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 S48 F49 N50 T51 F52 F53 S54 E55 T56 G57 A58 G59 K60 H61 R64 A65 V66 F67 V68

D69 L70 E71 D76 E77 G81 T82 Y83 R84 Q85 L86 F87 H88 P89 E90 Q91 L92 K96 E97 D98 A99 A100 H107 Y108 G111 K112 E113 I114 V115 D116 L117 V118 L119 D120 R121 I122 R123 K124 L125 A126 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 F138 H139 S140 F141 G142

G143 G144 T145 G146 S147 G148 F149 A150 S151 L152 L153 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 A170 I171 Y172 P173 A174 P175 Q176 I177 S178 T179 E183 P184 Y185 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205

N206 E207 A208 I209 Y210 D211 I212 C213 R214 R215 N216 L217 D218 I219 E220 R221 P222 T223 L227 N228 R229 L230 I231 A232 Q233 I234 V235 S236 S237 I238 T239 A240 S241 L242 R243 F244 D245 G246 A247 L248 N249 V250 D251 L252 T253 E254 F255 Q256 L259 Y262 P263 R264 I265 H266 L269

Y272 I276 S277 A278 E279 K280 A281 Y282 H283 E284 Q285 L286 A289 E290 N293 A294 E297 P298 A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 Y312 M313 C316 M317 L318 Y319 R320 G321 D322 P325 K326 D327 V328 N329 A330 A331 I332 A333 T334 I335 K336 T337 K338

R339 T340 I341 Q342 D345 W346 F351 K352 V353 G354 Y357 Q358 T361 V362 V363 P364 G365 G366 D367 L368 A369 K370 M377 I384 A385 E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 A403 F404 V405 H406 V409 G410 E411 G412 M413 E414 E415

G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain IG: 40% 96%

M1 R2 E3 N18 E22 L26 D33 G34 Q35 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 E55 T56 G57 A58 G59 K60 D69 L70 E71 P72 T73 D76 E77 T80 G81 T82 Y83 R84 H88 P89 E90 Q91 G95 K96 E97 D98 A99 A100 N101

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E207 A208 I209 Y210 D211 R214 R215 D218 I219 E220 R221 L230 D245 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 Y262 P263 R264 I265 L269 A273 E279 Q285 A289 E290 N293 M302 V303 K304 C305 D306 P307 R308 H309 D322 K326 D327

A333 K336 T337 K338 R339 T340 I341 D345 W346 C347 P348 Y357 V362 V363 P364 G365 G366 D367 K370 M377 N380 A383 I384 A385 E386 A387 R390 L391 D392 H393 K394 F395 D396 L397 A400 K401 R402 A403 F404 V405 H406 G410 E411 G412 M413 E414 E415 G416

E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

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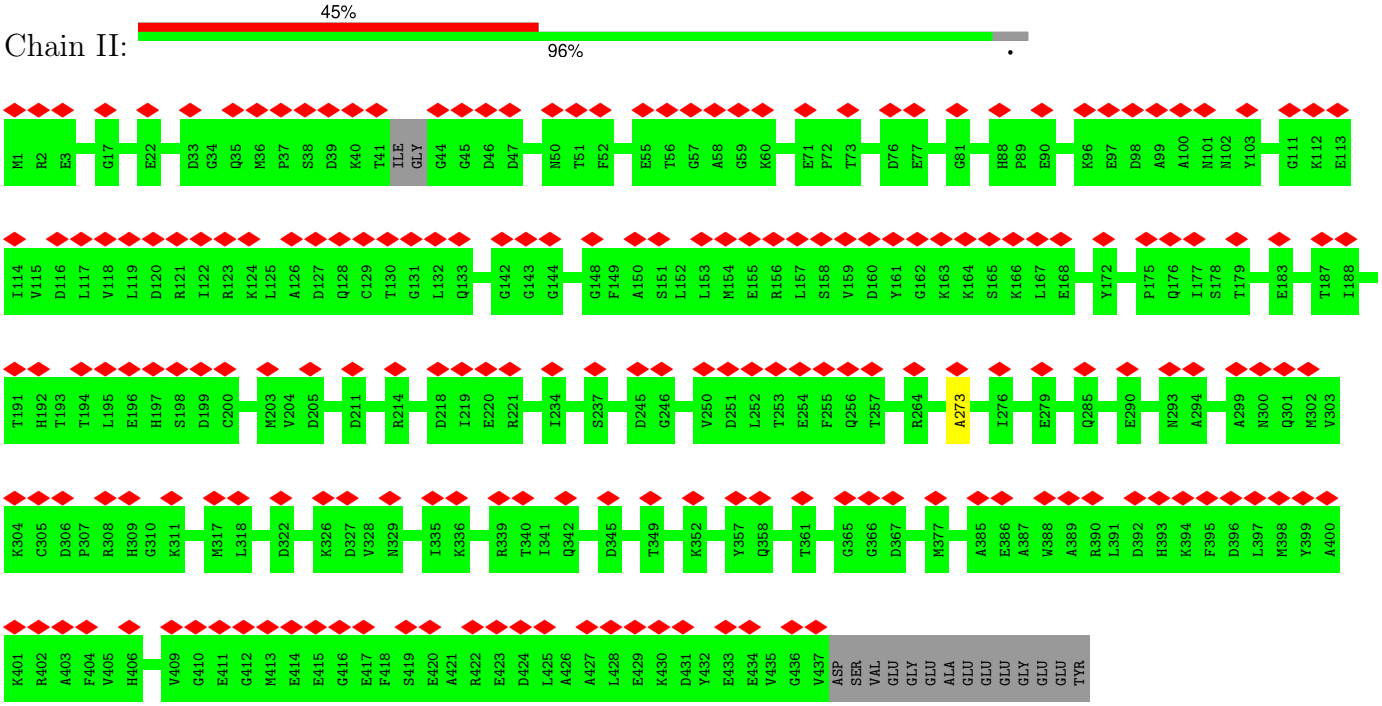

- Molecule 54: Tubulin alpha chain

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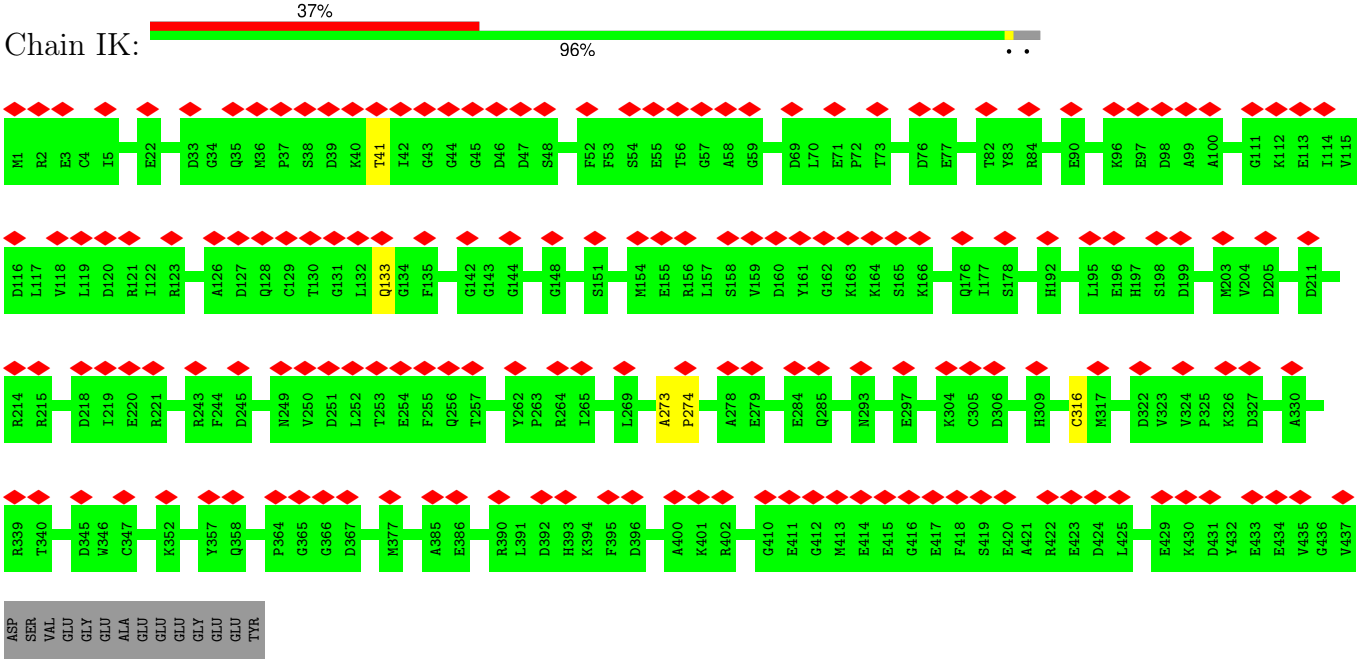

- Molecule 54: Tubulin alpha chain

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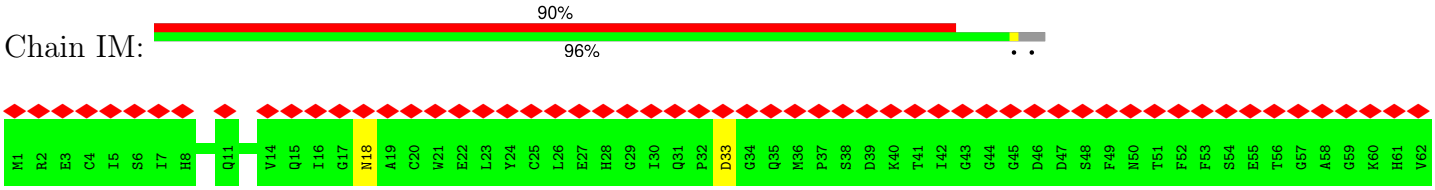

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R123 K124 L125 A126 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136 I137 F138 H139 S140 F141 G142 G143 G144 T145 G146 S147 G148 F149 L152 L153 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 A170 T171 Y172 P173 A174 P175 Q176 I177 S178 T179 A180 V181 V182 E183

P184 T187 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 N206 E207 A208 I209 Y210 D211 I212 C213 R214 R215 N216 L217 D218 I219 E220 R221 P222 N226 L227 N228 R229 L230 I231 A232 Q233 I234 V235 S236 S237 I238 T239 A240 S241 L242 R243 F244 D245 G246

A247 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 L259 V260 P261 Y262 P263 R264 I265 H266 F267 P268 L269 A270 T271 Y272 A273 P274 V275 I276 S277 A278 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 A294 C295 F296 E297 P298 A299 N300 Q301 M302 V303 K304 C305 D306

P307 R308 H309 G310 K311 Y312 M313 A314 C315 C316 M317 L318 Y319 R320 G321 D322 V323 V324 P325 K326 D327 V328 N329 A330 A331 I332 A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 K352 V353 G354 I355 N356 Y357 Q358 P359 P360 T361 V362 V363 P364 G365 G366

D367 L368 A369 K370 V371 Q372 R373 A374 V375 C376 M377 L378 S379 N380 T381 T382 A383 I384 A385 E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 A403 F404 V405 H406 W407 Y408 V409 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426

A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain JA: 39% 95%

M1 R2 E22 D33 P37 S38 D39 K40 THR ILE GLY GLY GLY D46 D47 E55 T56 G57 A58 D69 L70 E71 P72 T73 D76 T80 G81 R84 H88 P89 E90 Q91 L92 G95 K96 E97 D98 R105 G106 I110 G111 K112 E113 I114 V115 D116 L117

D120 R121 I122 R123 D127 Q128 C129 T130 G131 L132 Q133 G134 F141 G142 E155 R156 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 Q176 I177 S178 T179 A180 E183 H192 E196 D199 M203 V204 D205 N206 E207 D211 I212 C213 R214 R215 N216 L217 D218

I219 E220 R221 P222 T223 N226 L227 N228 Q233 A240 D245 N249 V250 D251 L252 T253 E254 F255 N258 L259 R264 A270 A273 P274 V275 I276 E279 K280 A281 E284 Q285 L286 E290 N293 A294 C295 F296 E297 P298 A299 N300 Q301 M302 V303 K304 C305 D306

P307 R308 H309 G310 K311 Y312 M313 A314 C315 C316 M317 D322 D327 V328 N329 K336 T337 K338 R339 T340 I341 Q342 D345 P348 T349 G350 Y357 V362 V363 P364 G365 G366 D367 L368 Q372 A385 E386 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402

V409 G410 E411 G412 M413 E414 E415 G416 E420 E423 D424 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

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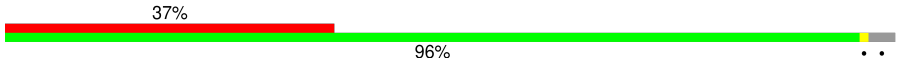
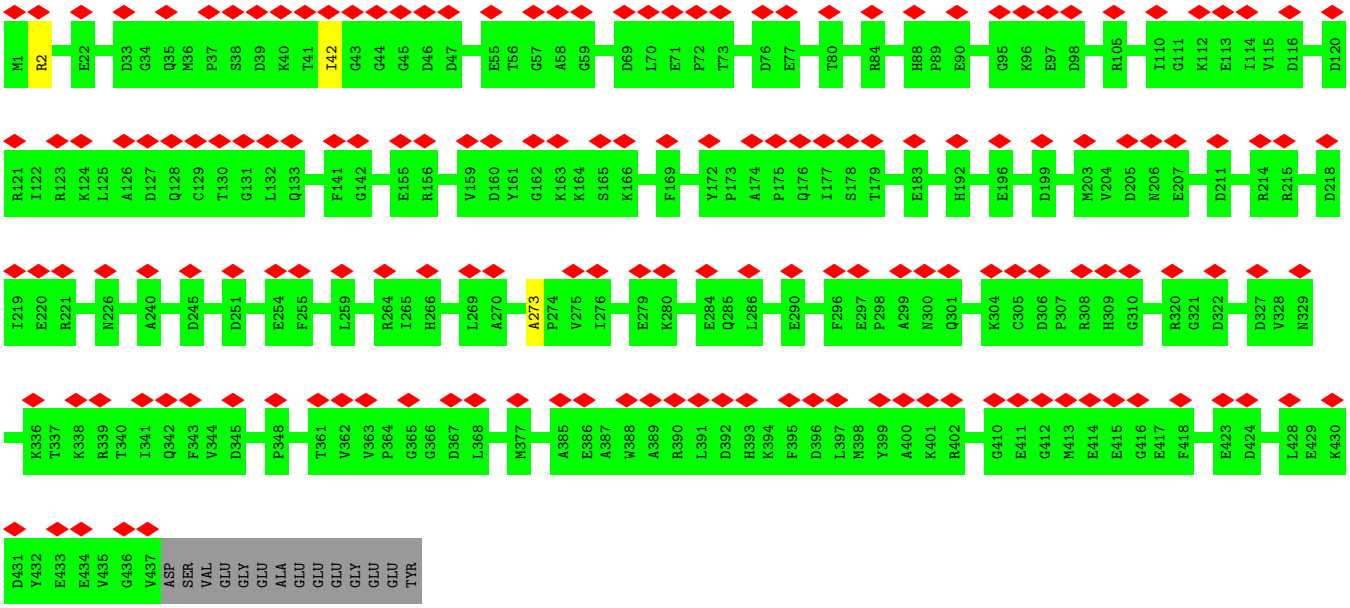
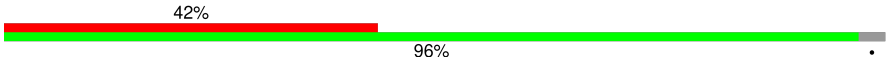
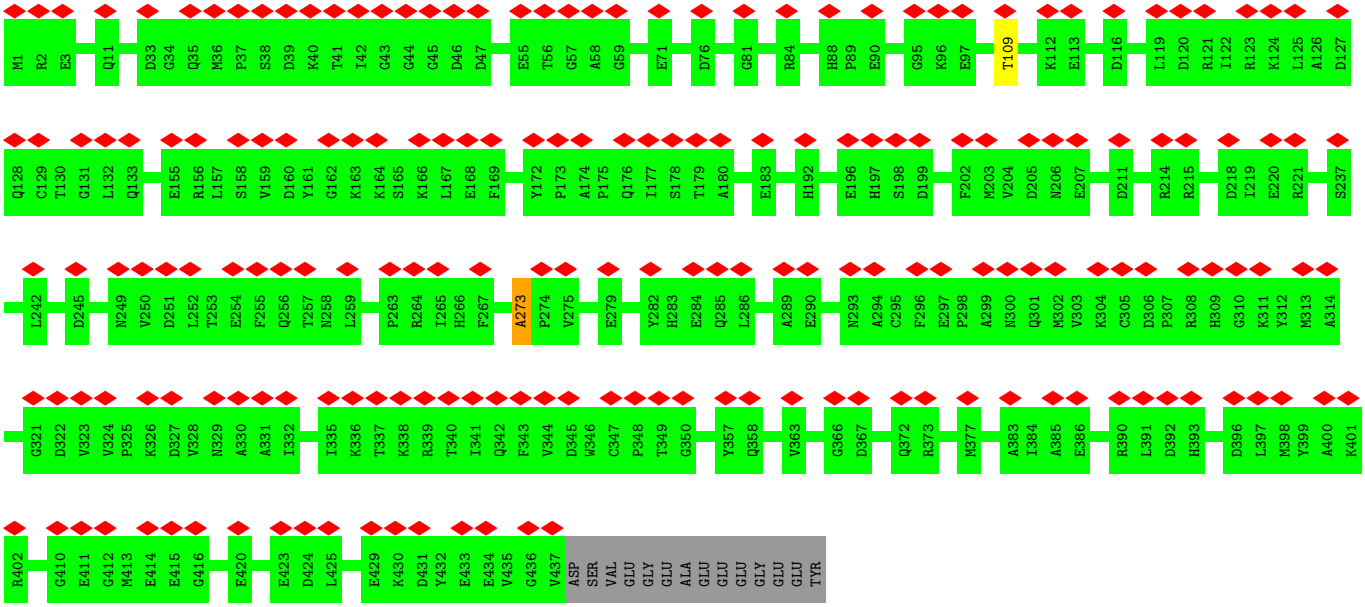




- Molecule 54: Tubulin alpha chain

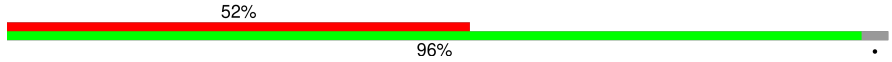
Chain JE:

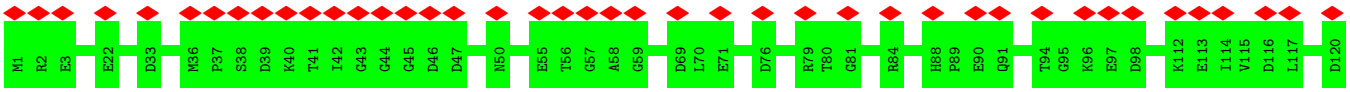


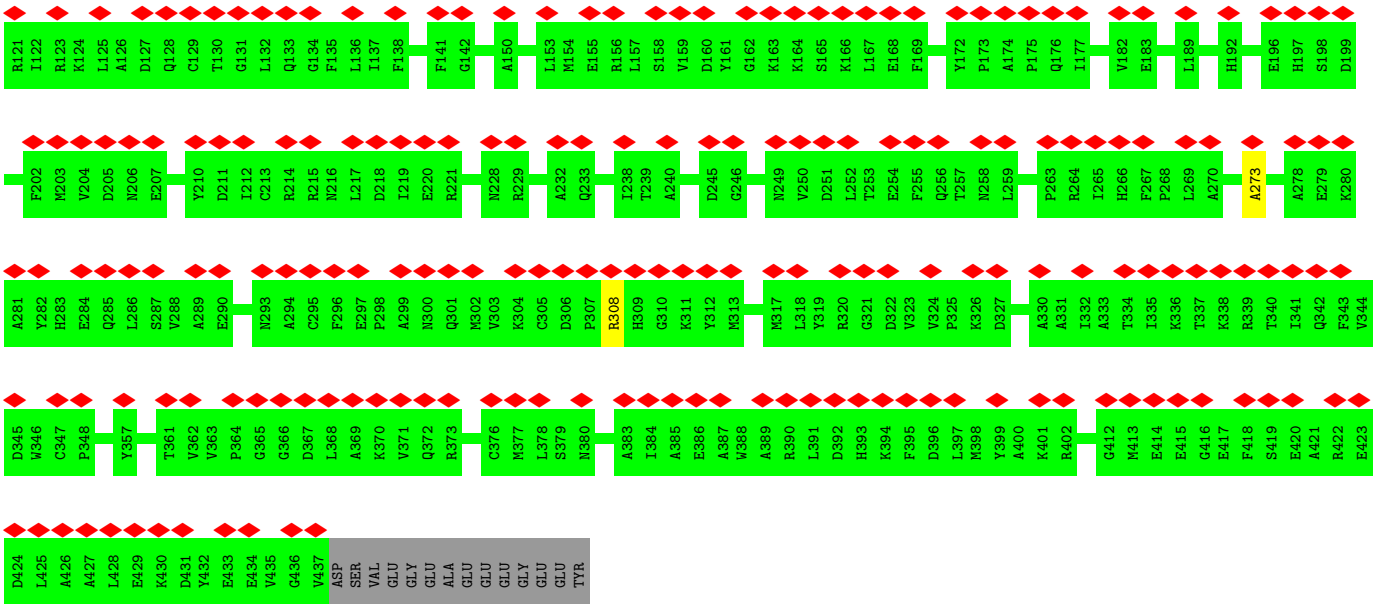


- Molecule 54: Tubulin alpha chain

Chain JG:

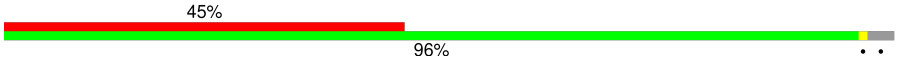


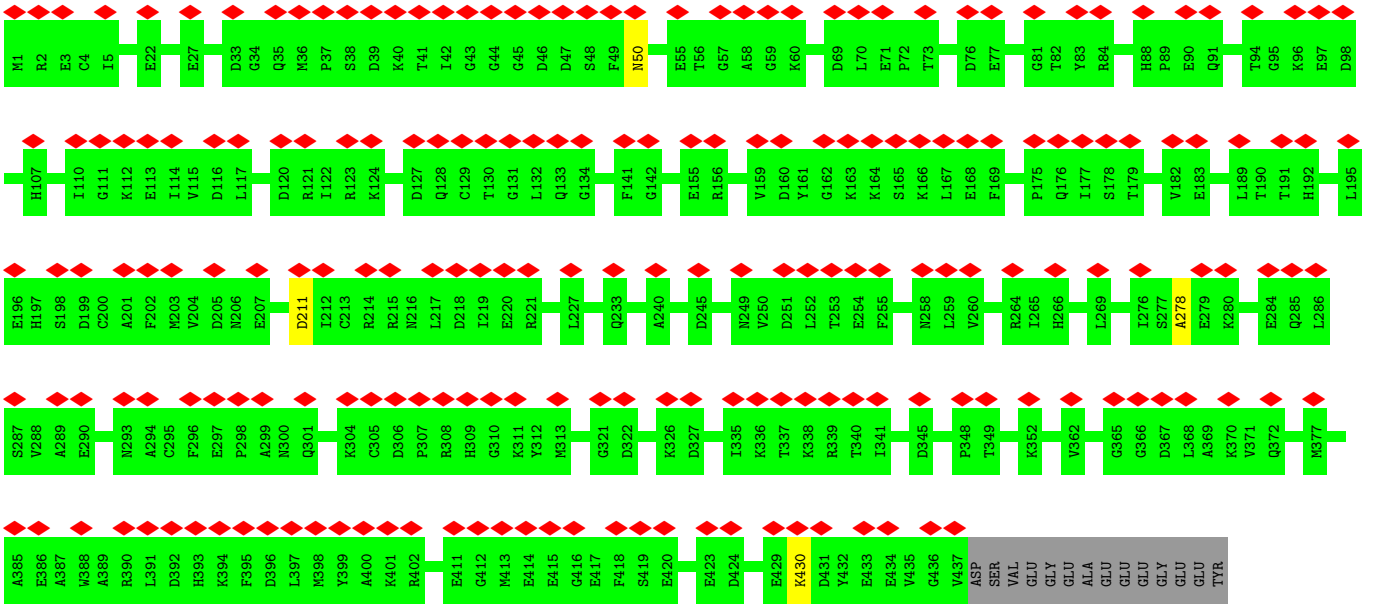




- Molecule 54: Tubulin alpha chain

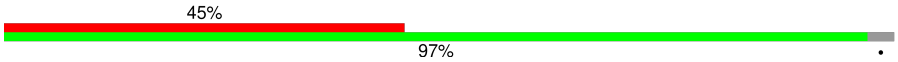
Chain JI:

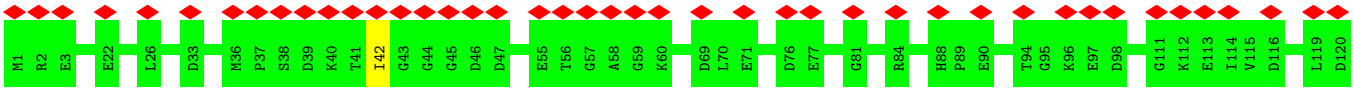


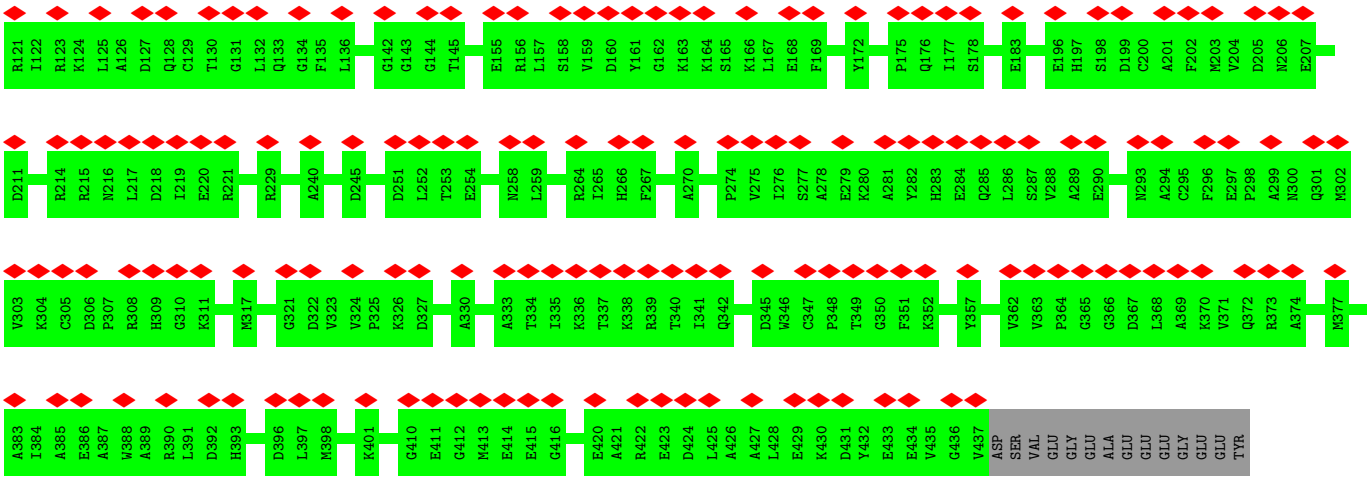


- Molecule 54: Tubulin alpha chain

Chain JK:







- Molecule 54: Tubulin alpha chain

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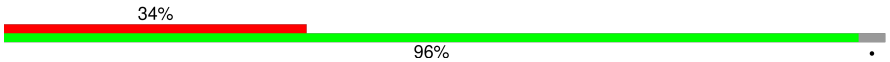
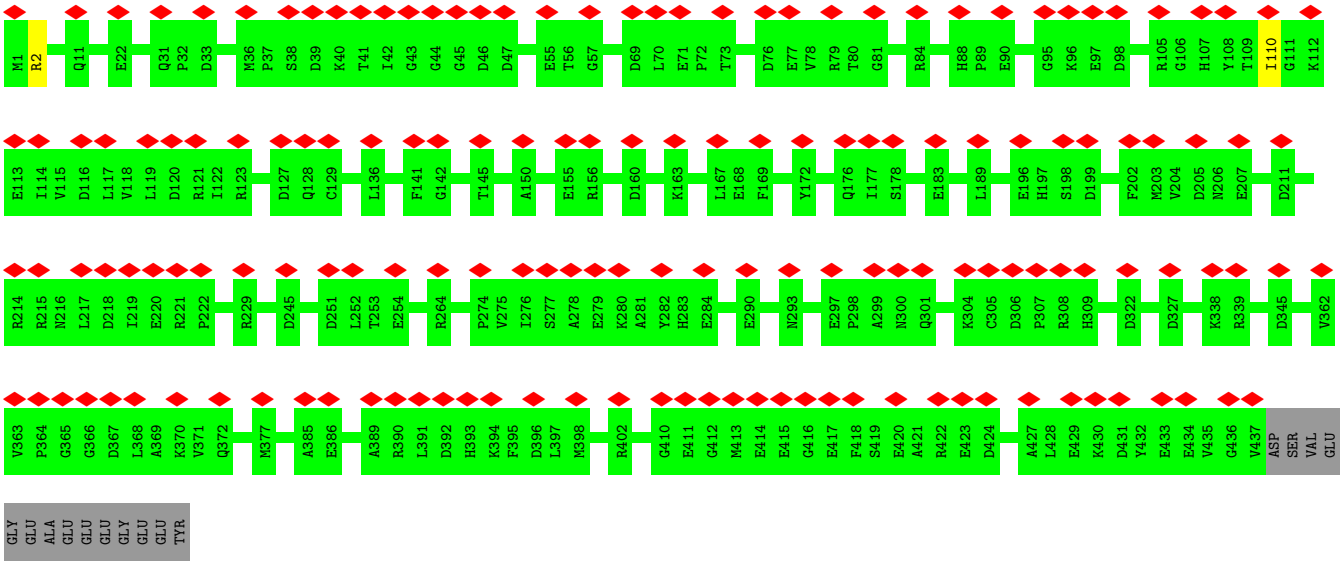
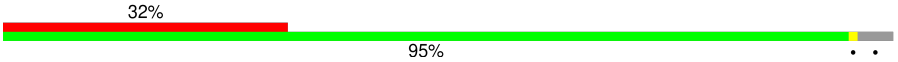
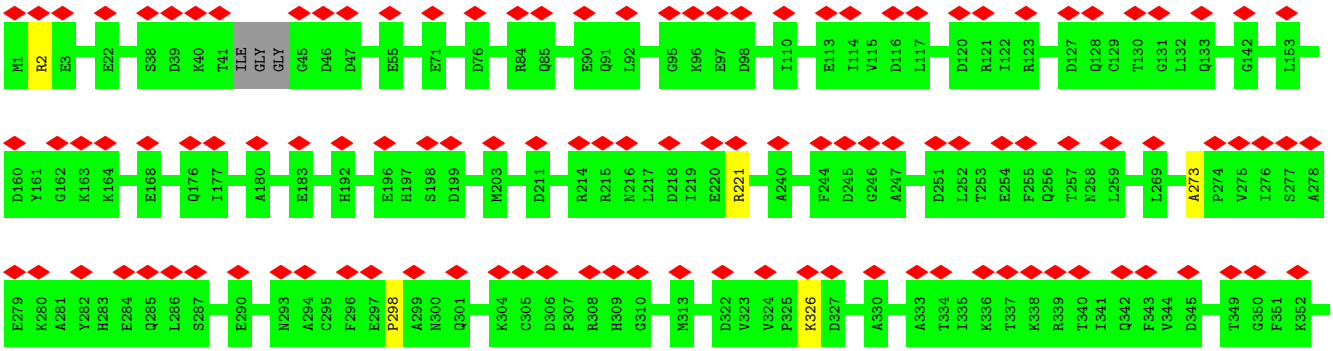


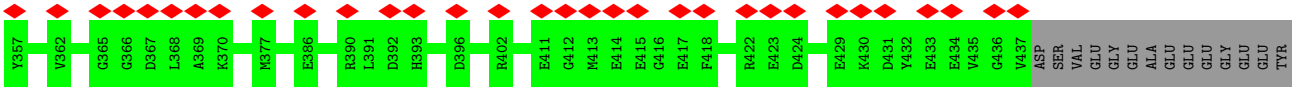


- Molecule 54: Tubulin alpha chain

Chain KB:

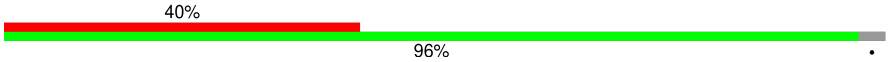


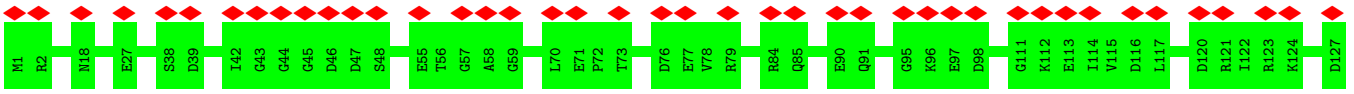


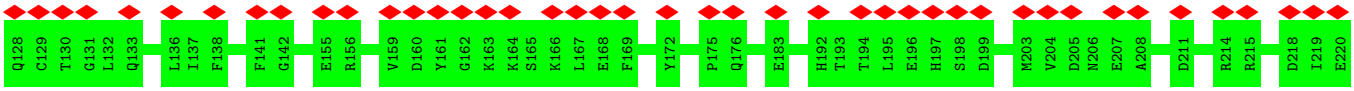


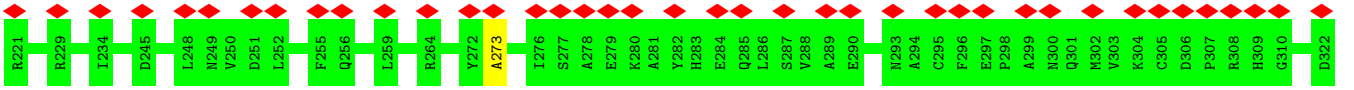
- Molecule 54: Tubulin alpha chain

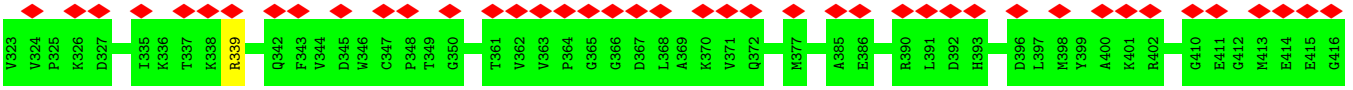
Chain KE:

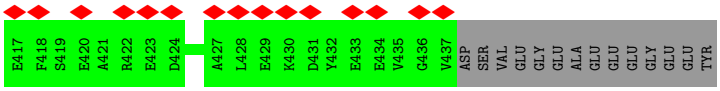






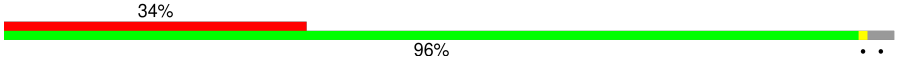


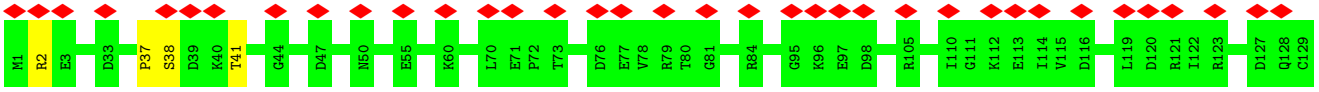


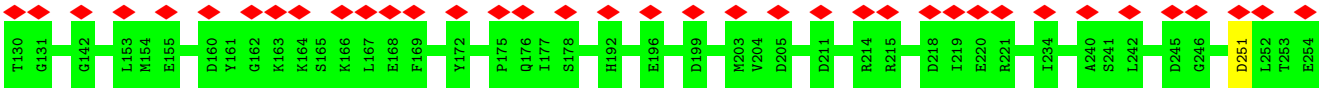


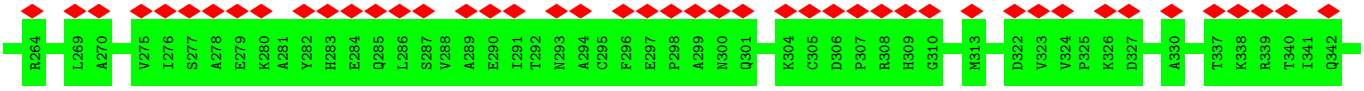
- Molecule 54: Tubulin alpha chain

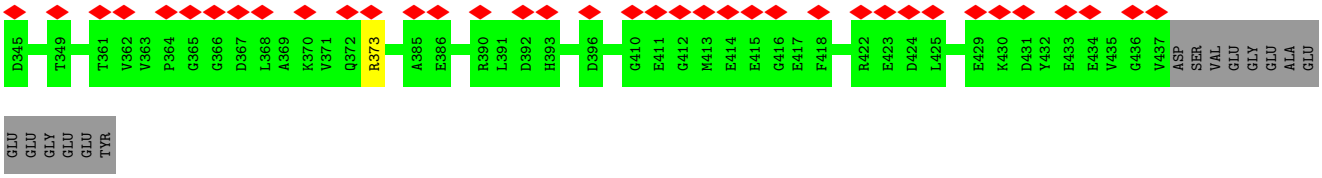
Chain KG:





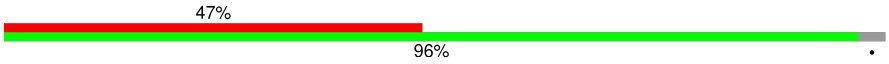


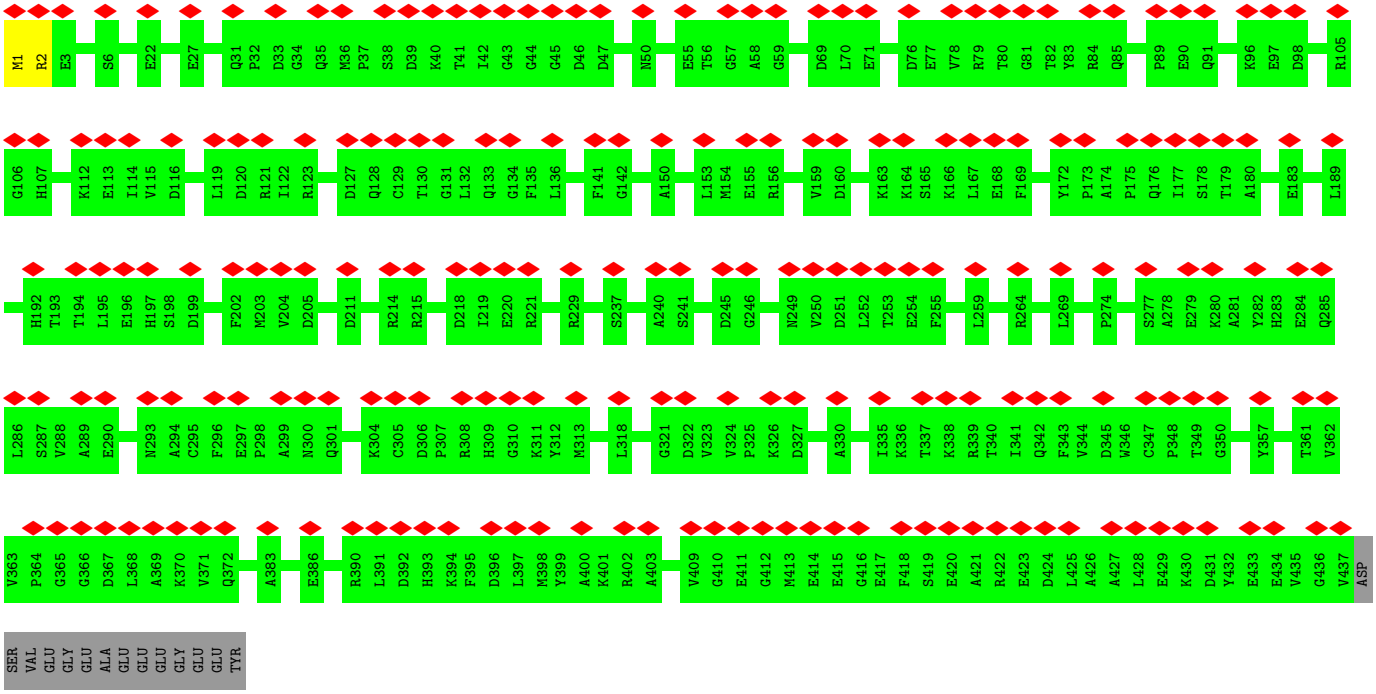




- Molecule 54: Tubulin alpha chain

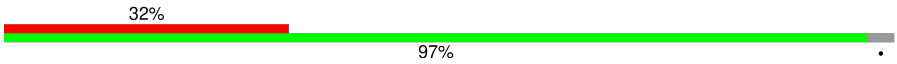
Chain KI:

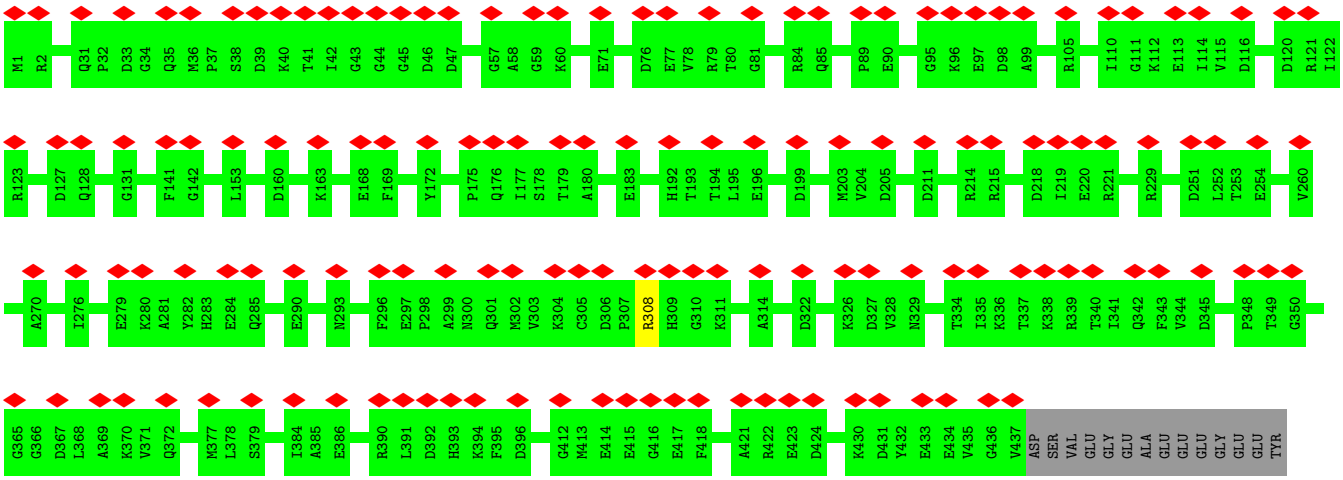




- Molecule 54: Tubulin alpha chain

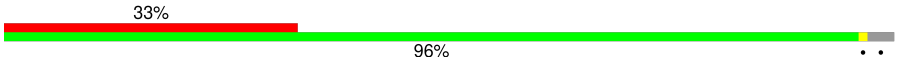
Chain KK:

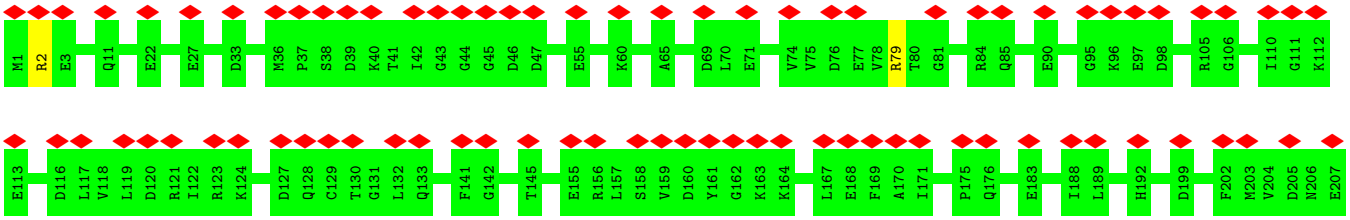


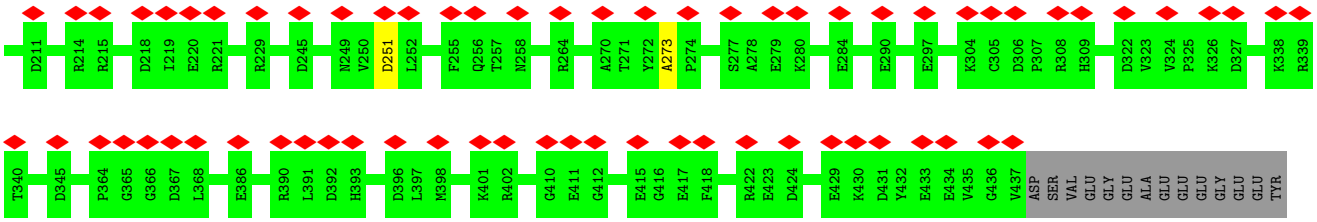


- Molecule 54: Tubulin alpha chain

Chain LA:

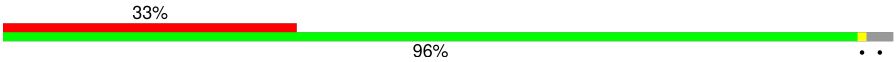


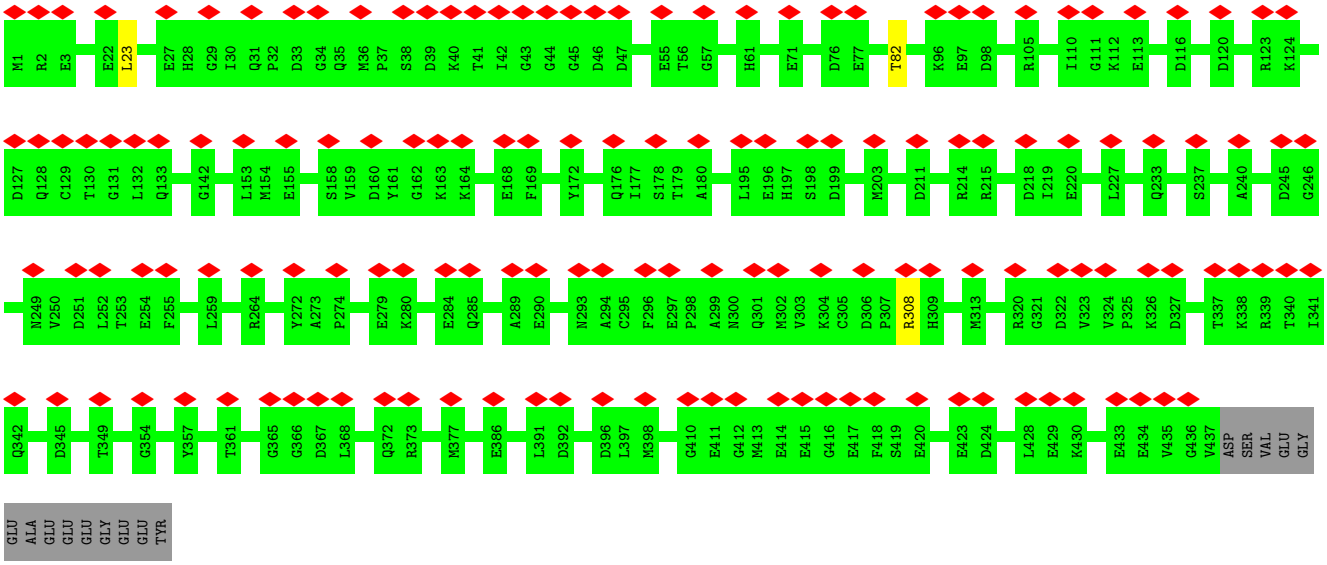




- Molecule 54: Tubulin alpha chain

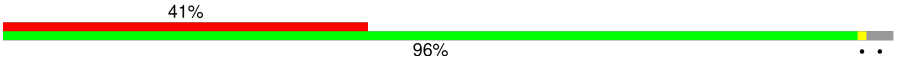
Chain LB:

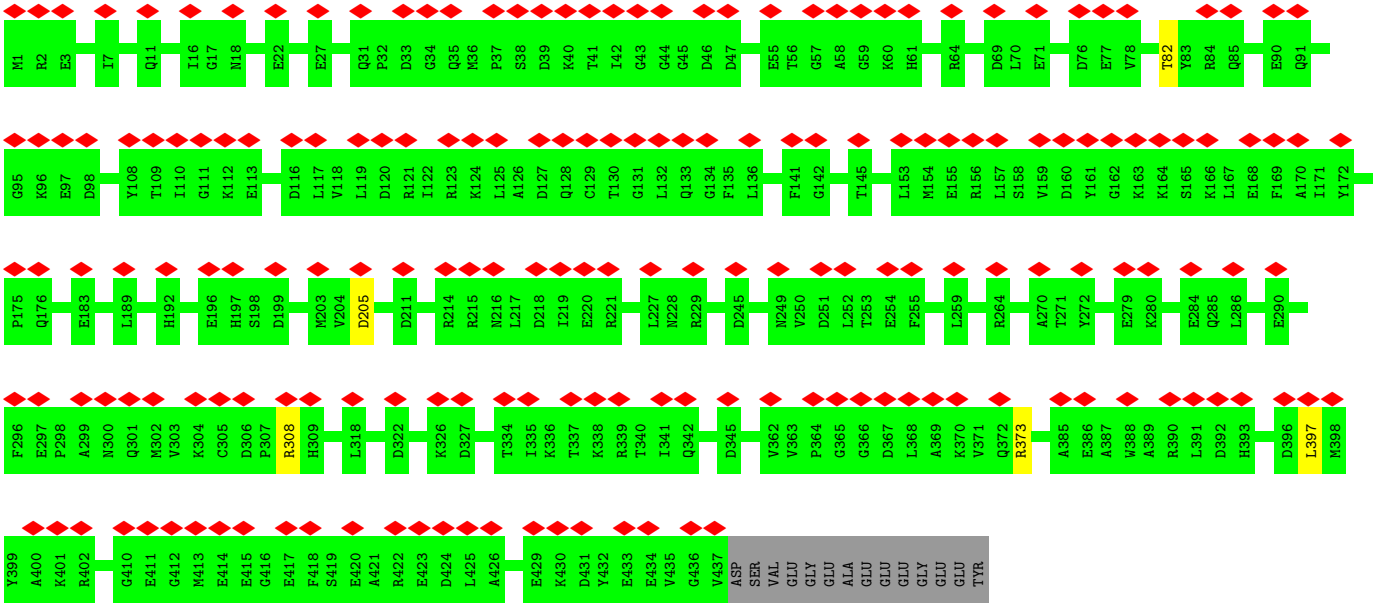




- Molecule 54: Tubulin alpha chain

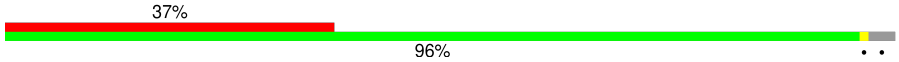
Chain LE:

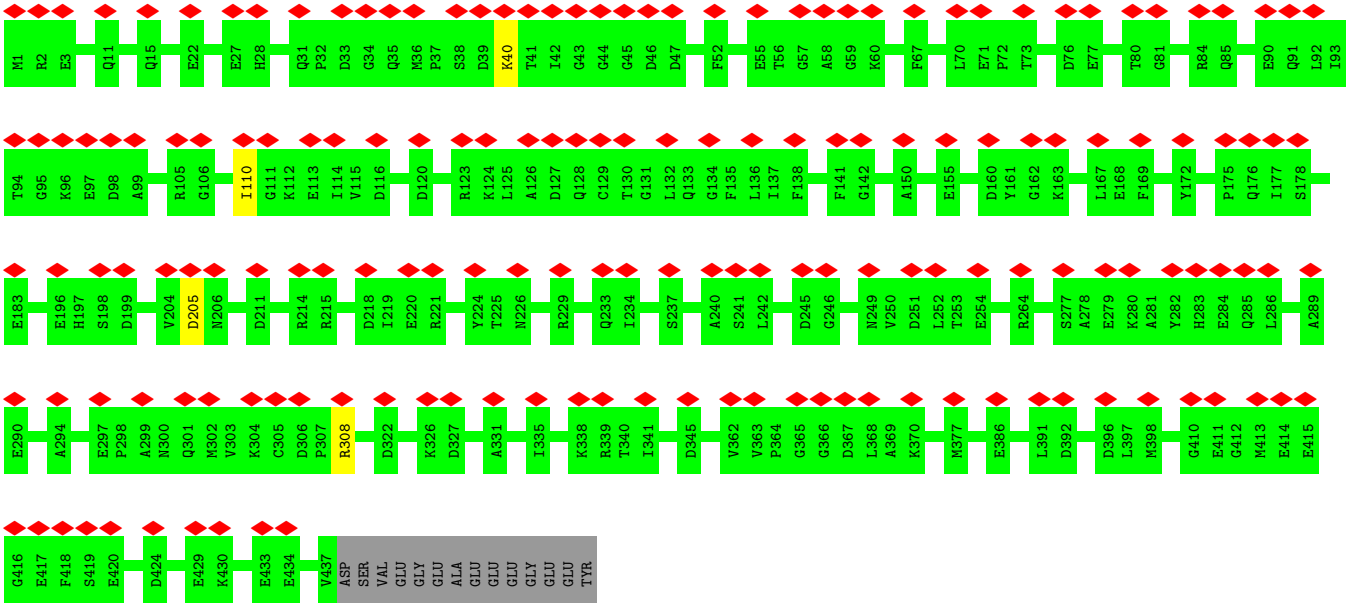




• Molecule 54: Tubulin alpha chain

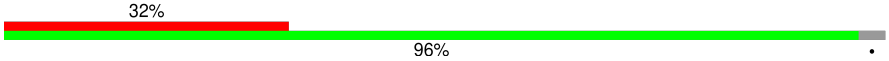
Chain LG:

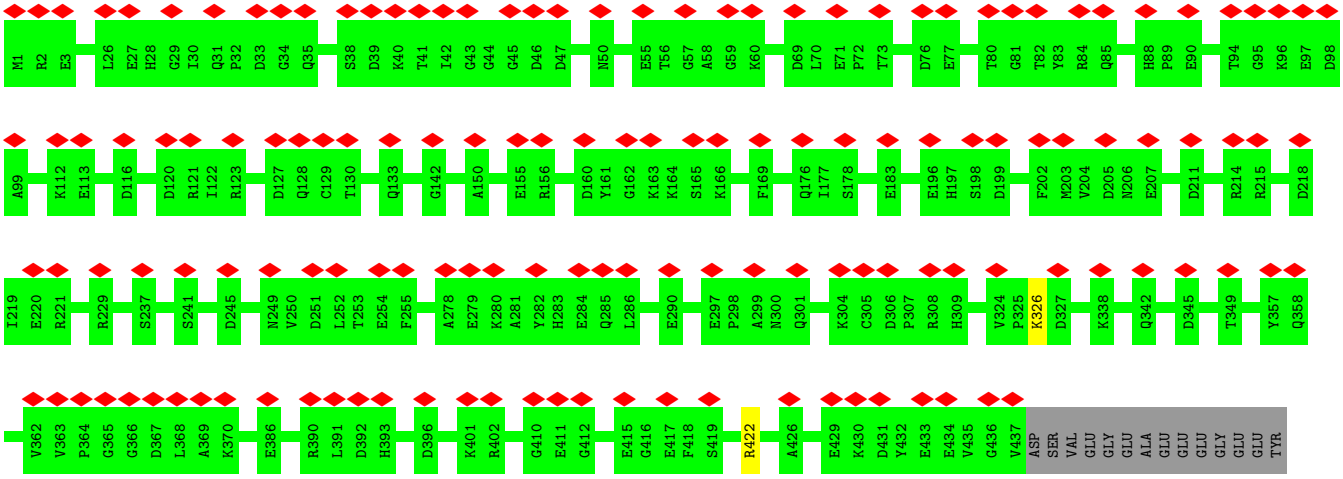




• Molecule 54: Tubulin alpha chain

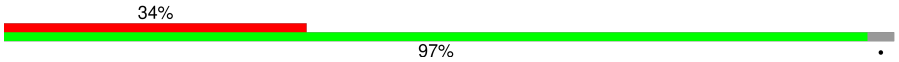
Chain LI:

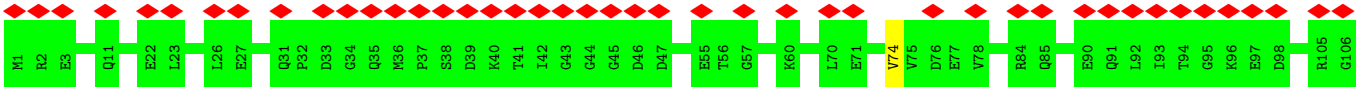


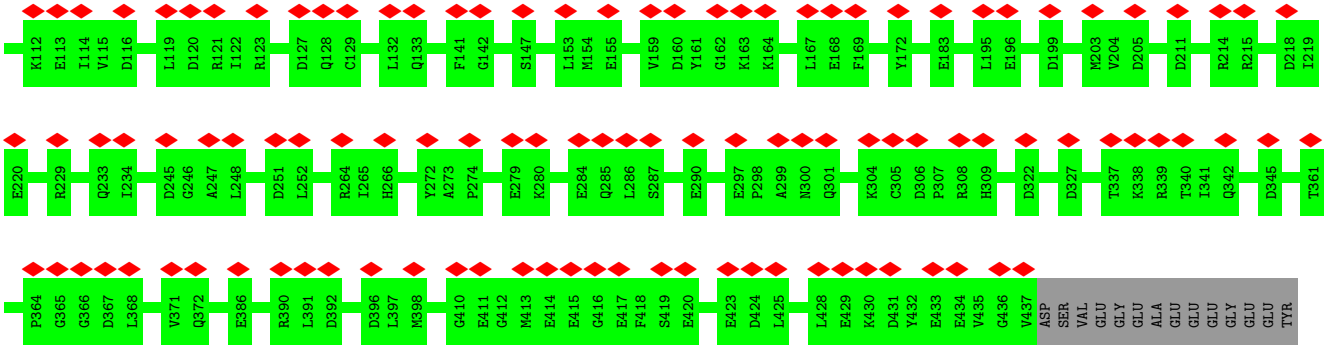


• Molecule 54: Tubulin alpha chain

Chain LK:

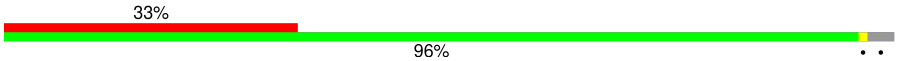


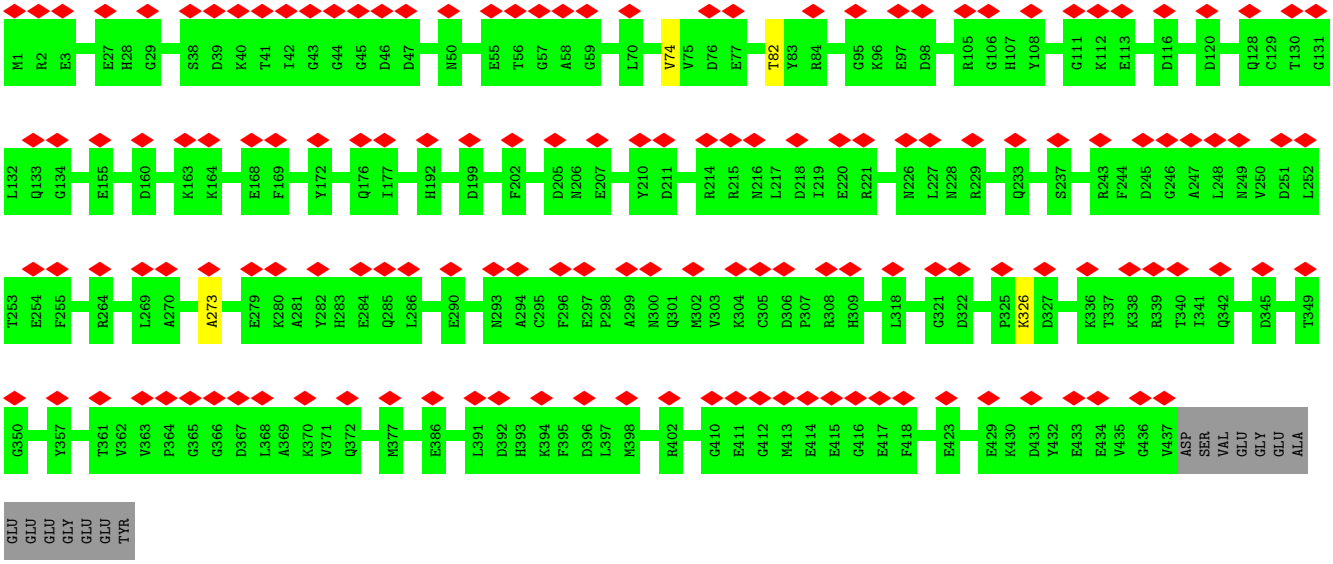




- Molecule 54: Tubulin alpha chain

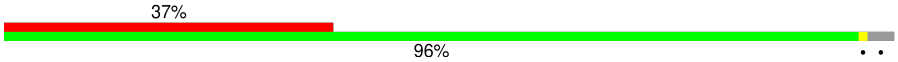
Chain MA:

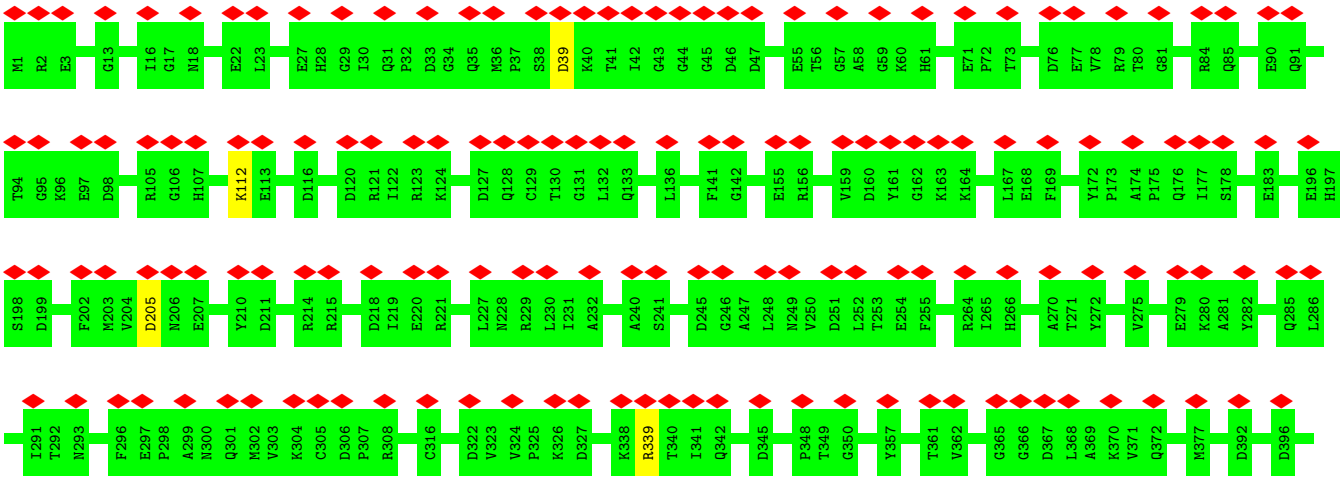


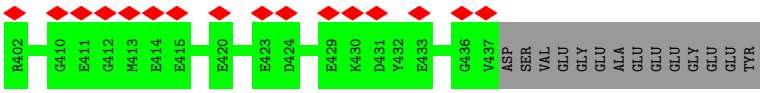


- Molecule 54: Tubulin alpha chain

Chain MB:

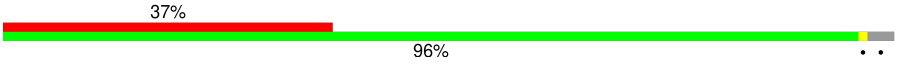


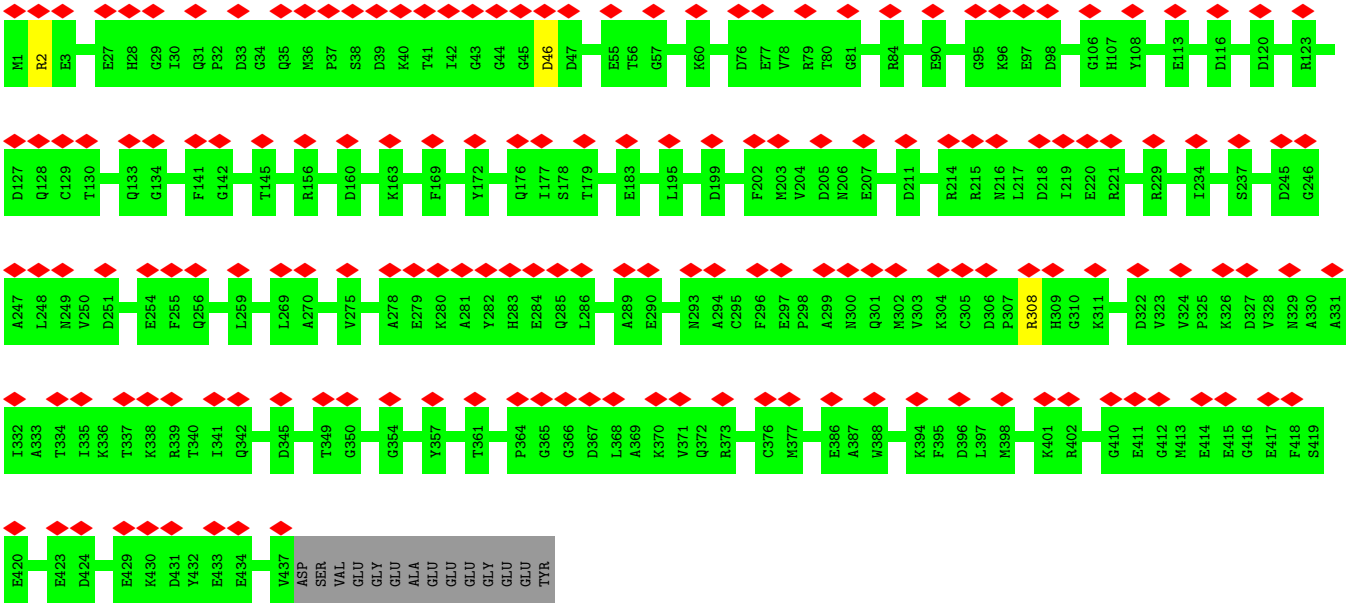




• Molecule 54: Tubulin alpha chain

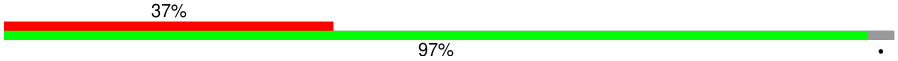
Chain ME:

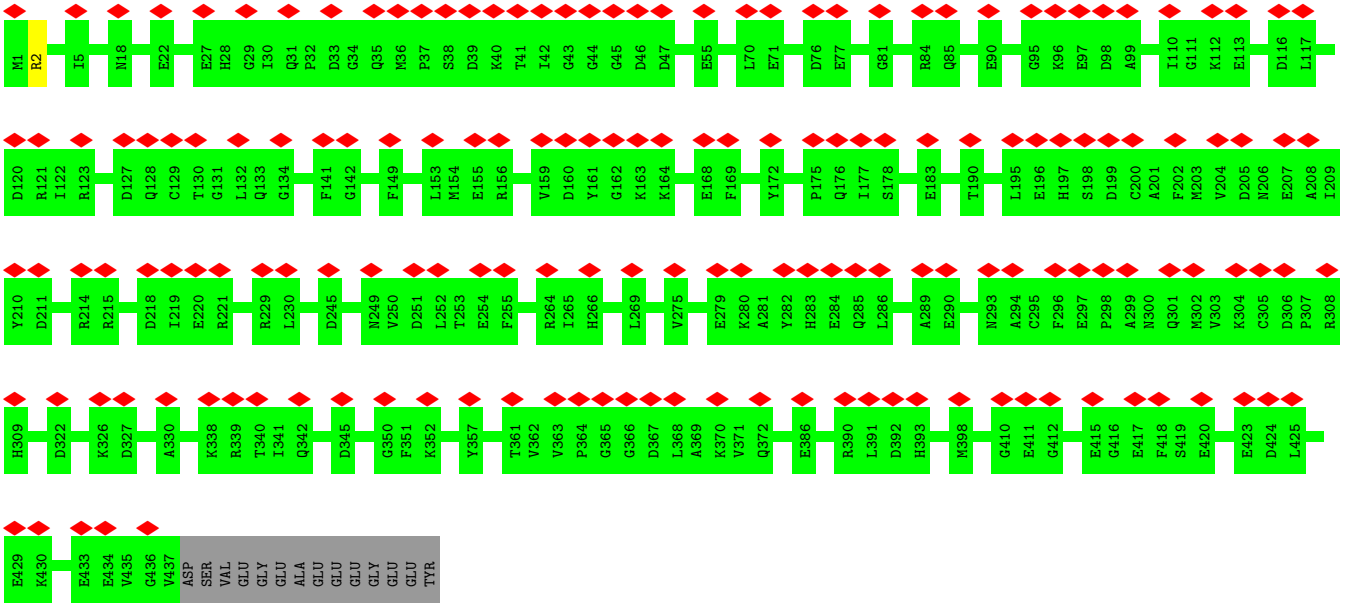




• Molecule 54: Tubulin alpha chain

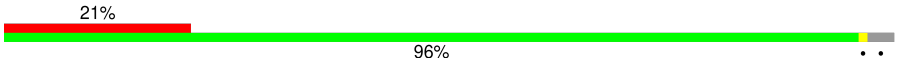
Chain MG:

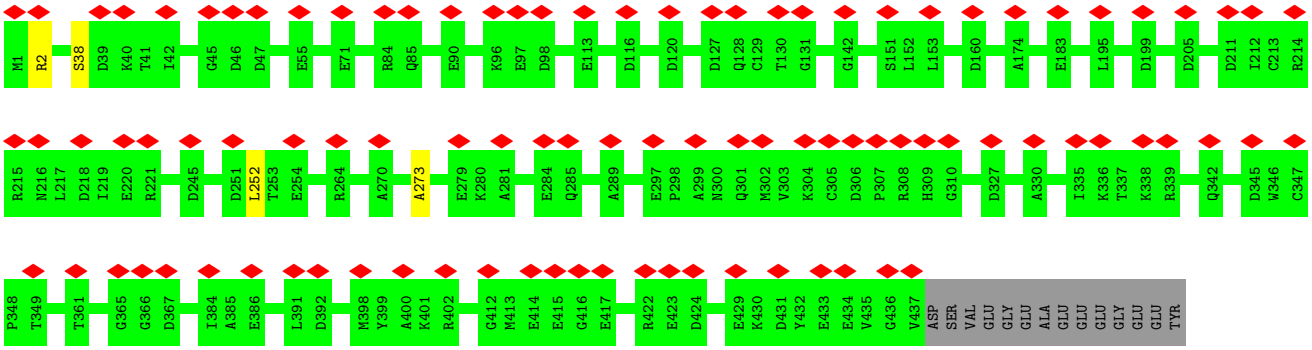




• Molecule 54: Tubulin alpha chain

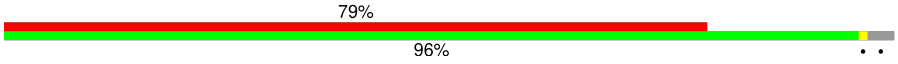
Chain MI:

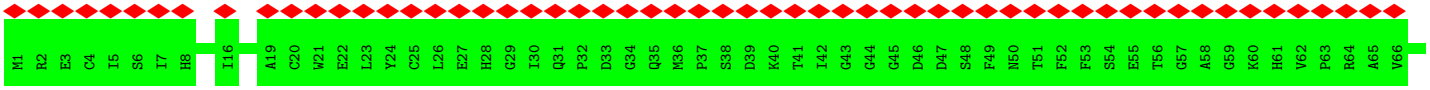


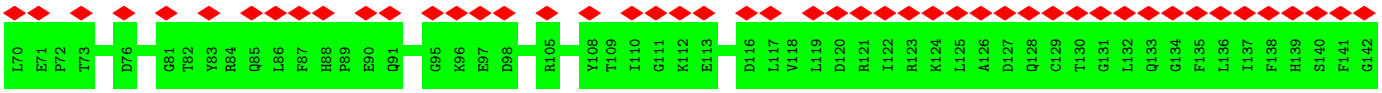


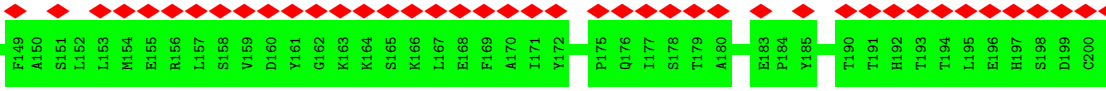
- Molecule 54: Tubulin alpha chain

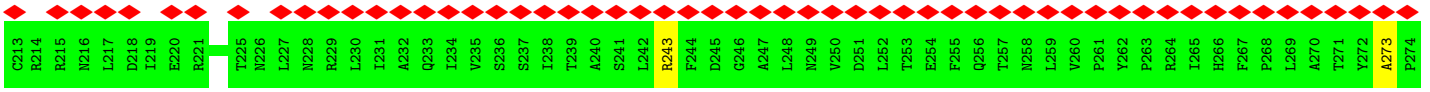
Chain MK:

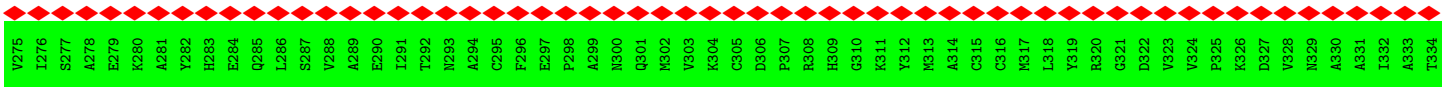


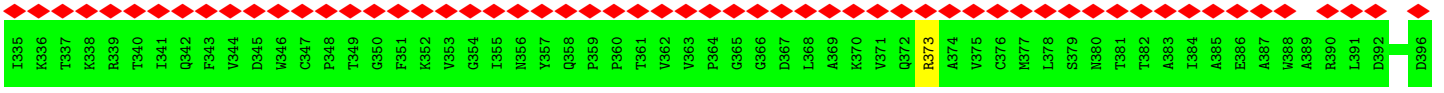


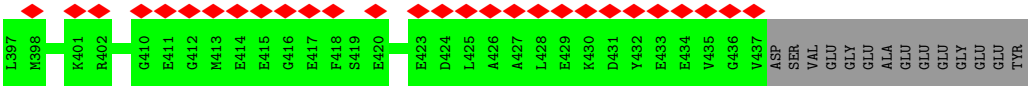






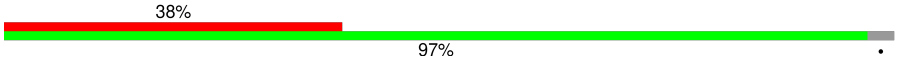


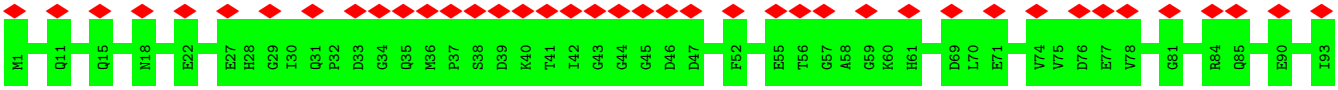


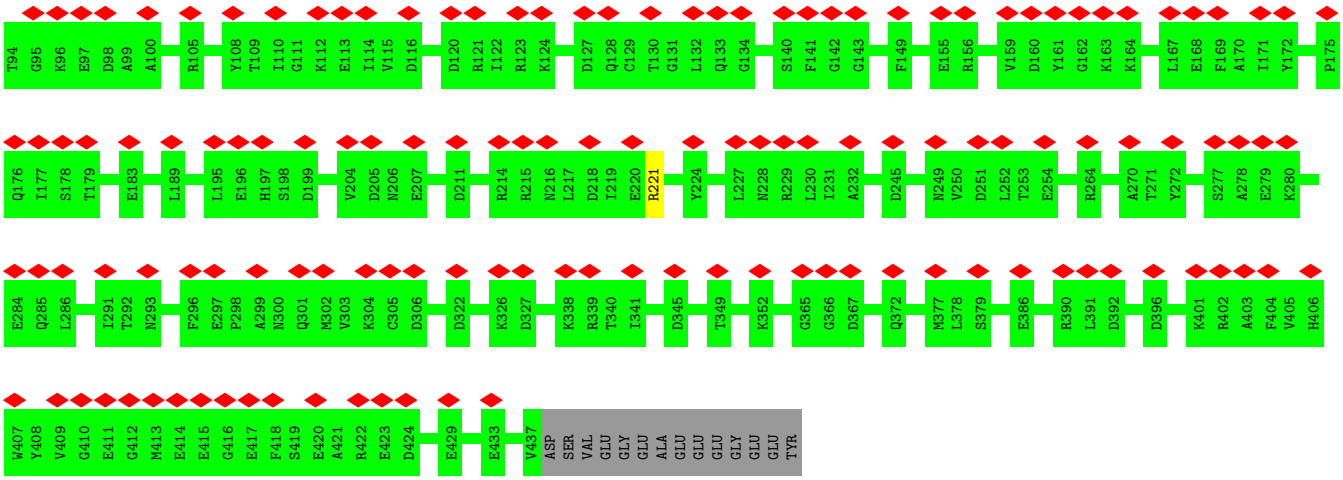


- Molecule 54: Tubulin alpha chain

Chain ML:

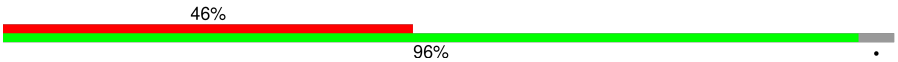


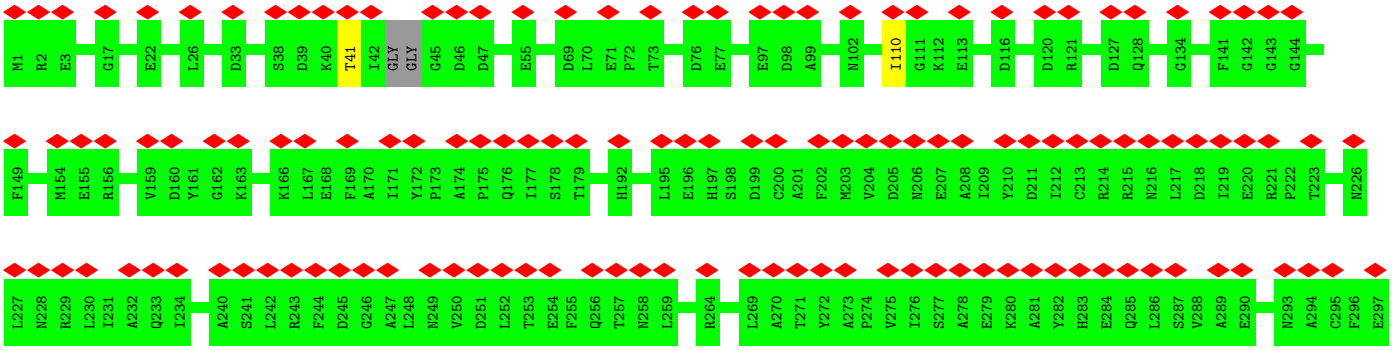




- Molecule 54: Tubulin alpha chain

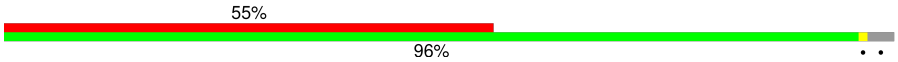
Chain NA:

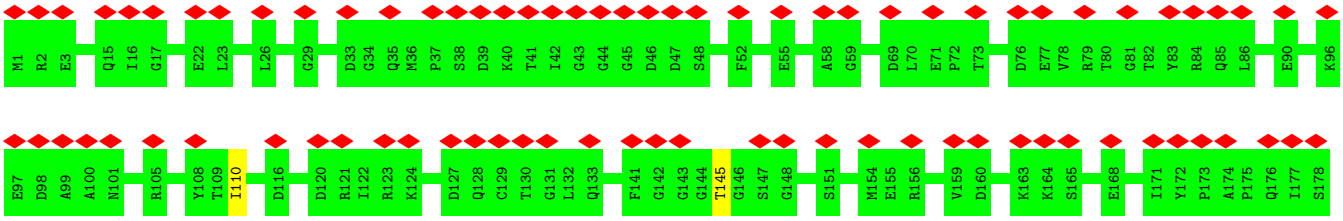




- Molecule 54: Tubulin alpha chain

Chain NB:





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F255 Q256 L259 R264 L269 Y272 A273 P274 V275 I276 S277 A278 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 A294 C295 F296 E297 F298 A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 C316 M317 L318 Y319 R320 G321 D322 P325 K326 D327

V328 N329 A330 A331 I332 A333 K336 T337 K338 R339 T340 I341 Q342 D345 W346 C347 P348 T349 G350 F351 N356 Y357 Q358 P359 P360 T361 V362 V363 P364 G365 G366 D367 L368 A369 K370 V371 Q372 R373 M377 L378 A385 E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399

A400 K401 R402 H406 W407 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLY GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain NE: 50% 97%

M1 R2 E3 G17 E22 L26 D33 G34 Q35 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 E55 T56 G57 A58 A65 E71 D76 E77 K96 E97 D98 I110 E113 D116 R123 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136

F141 G142 G143 M154 E155 R156 D160 K163 K164 S165 E168 F169 A170 I171 Y172 P173 A174 P175 Q176 I177 S178 T179 L189 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 N206 E207 A208 I209 Y210 D211 I212 C213 R214 R215 N216 L217 D218 I219 E220 R221 P222 T223

N226 L227 N228 R229 L230 I231 A232 Q233 S237 I238 F244 D245 G246 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 L259 V260 P263 R264 F267 P268 L269 A270 T271 Y272 A273 P274 V275 I276 S277 A278 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293

A294 C295 F296 E297 P298 A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 C316 M317 L318 Y319 R320 G321 D322 V323 V324 P325 K326 D327 V328 N329 A330 A331 I332 A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 D345 W346 C347 P348 T349 G350 F351 K352 Y357 Q358 T361

V362 V363 P364 G365 G366 D367 L368 A369 K370 V371 Q372 R373 M377 L378 T381 T382 A383 I384 A385 E386 A387 W388 A389 R390 L391 D392 H393 D396 R402 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437

ASP SER VAL GLU GLY GLU ALA GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain NG: 74% 96%

M1 R2 E3 C4 I5 Q11 A12 G13 V14 Q15 I16 G17 N18 A19 E22 L23 L26 E27 H28 G29 I30 Q31 P32 D33 G34 Q35 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 F52 E55 A58 G59 A65 D69 L70 E71 P72 T73 V74 V75 D76 E77

G81 T82 Y83 R84 E90 Q91 T94 G95 K96 E97 D98 A99 A100 N101 N102 Y103 A104 R105 G106 H107 Y108 T109 I110 G111 K112 E113 D116 L119 D120 R121 I122 R123 K124 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136 H139 S140 F141 G142 G143 G144 T145 G146 S147 G148

F149 A150 S151 L152 L153 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 A170 I171 Y172 P173 A174 P175 Q176 I177 S178 T179 A180 V181 V182 E183 P184 Y185 N186 T187 I188 L189 T190 T191 H192 T193 T194 L195 E196 H197 S198 D199 C200 A201 F202 M203 V204 D205 N206 E207 A208

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V275 I276 S277 A278 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 A294 C295 F296 E297 P298 A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 Y312 M313 A314 C315 C316 M317 L318 Y319 R320 G321 D322 V323 V324 P325 K326 D327 V328 N329 A330 A331 I332 A333

T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 K352 I355 N356 Y357 Q358 T361 V362 V363 P364 G365 G366 D367 L368 A369 K370 V371 Q372 R373 M377 L378 S379 N380 T381 A385 E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399

A400 K401 R402 A403 F404 V405 H406 W407 Y408 V409 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain NI: 57% 96%

M1 R2 E3 Q15 I16 G17 N18 A19 E22 L23 L26 D33 G34 Q35 M36 P37 S38 D39 K40 T41 ILE GLY GLY G45 D46 D47 N50 E55 T56 G57 A58 A65 D69 L70 E71 P72 T73 D76 E77 R84 H88 P89 E90 K96 E97 D98 N101

N102 R105 G106 H107 Y108 T109 I110 G111 K112 E113 D116 D120 R123 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136 F141 G142 G143 S147 S151 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 A170 I171 Y172 P173 A174 P175 Q176

I177 S178 T179 E183 H192 T193 T194 L195 E196 H197 S198 D199 M203 V204 D205 N206 E207 Y210 D211 I212 C213 R214 R215 N216 L217 D218 I219 E220 R221 P222 L227 N228 R229 L230 I231 A232 Q233 I234 S237 A240 S241 L242 R243 F244 D245 G246 A247 L248 N249 V250 D251 L252 T253

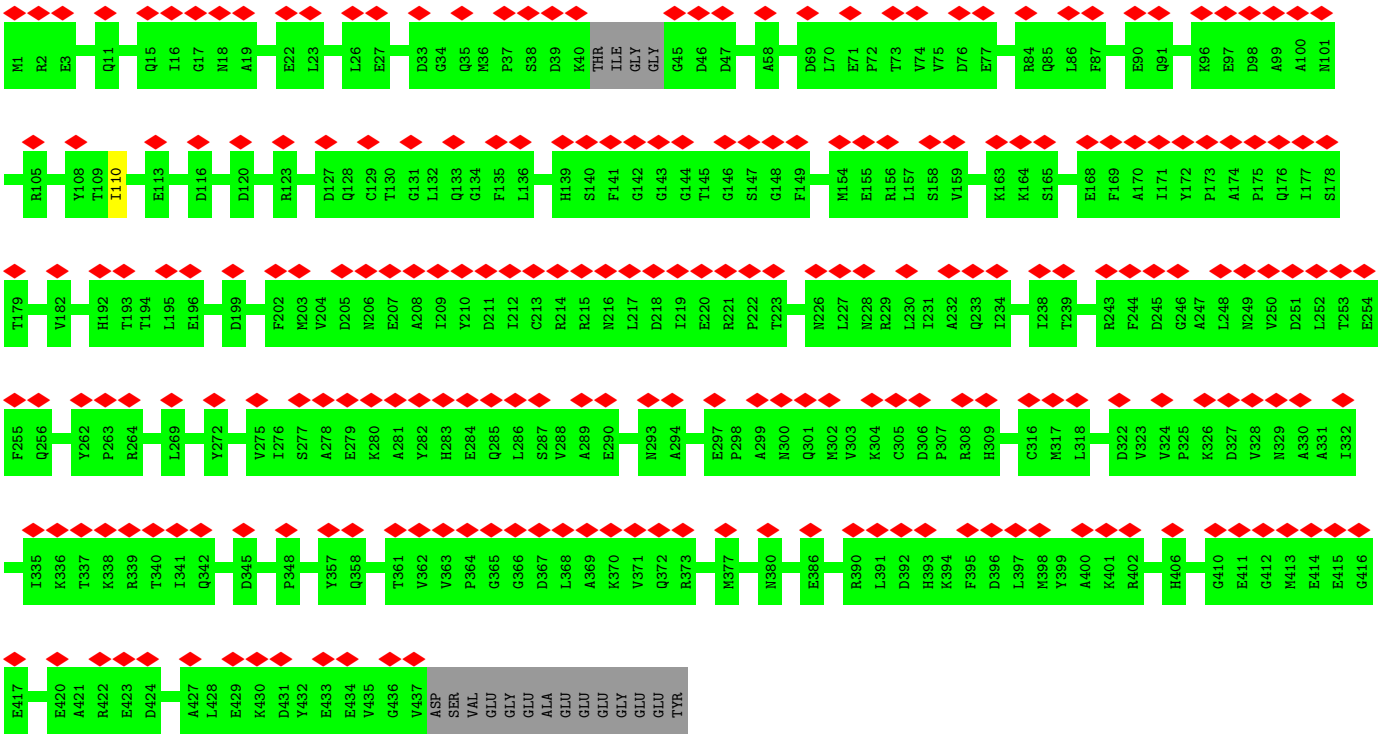
E254 F255 Q256 T257 Y262 P263 R264 I265 H266 F267 P268 L269 A270 T271 Y272 A273 P274 V275 I276 S277 A278 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 A294 C295 F296 E297 P298 A299 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 M313 M317 L318

G321 D322 V323 V324 P325 K326 D327 V328 N329 A330 T334 I335 K336 T337 K338 R339 T340 I341 Q342 D345 W346 C347 P348 T349 G350 F351 K352 Y357 Q358 T361 V362 V363 P364 G365 G366 D367 L368 A369 K370 V371 Q372 R373 M377 N380 T381 T382 A383 I384 A385 E386 A387 W388 A389 R390

L391 D392 H393 K394 F395 D396 L397 R402 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

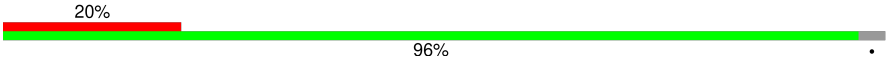
- Molecule 54: Tubulin alpha chain

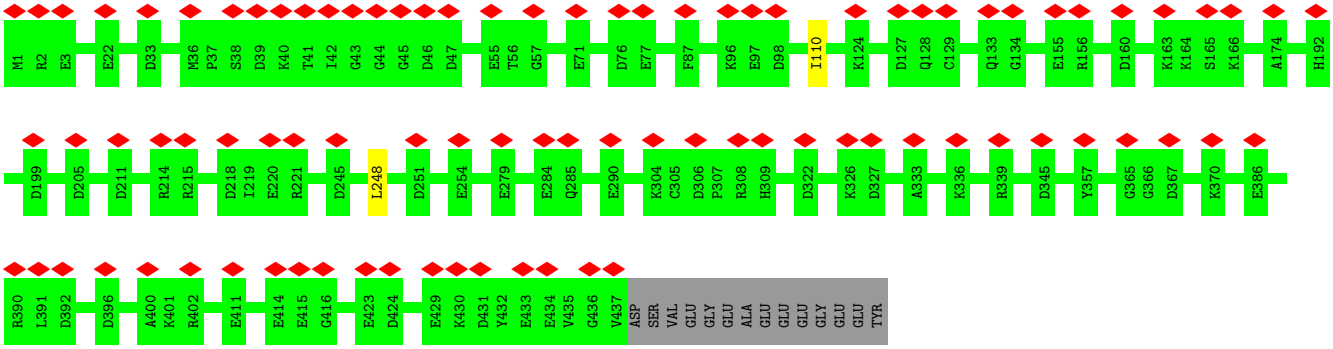
Chain NL: 52% 96%



- Molecule 54: Tubulin alpha chain

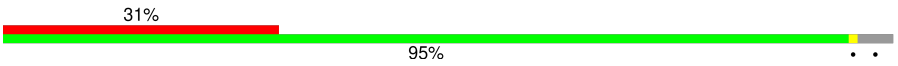
Chain OA:

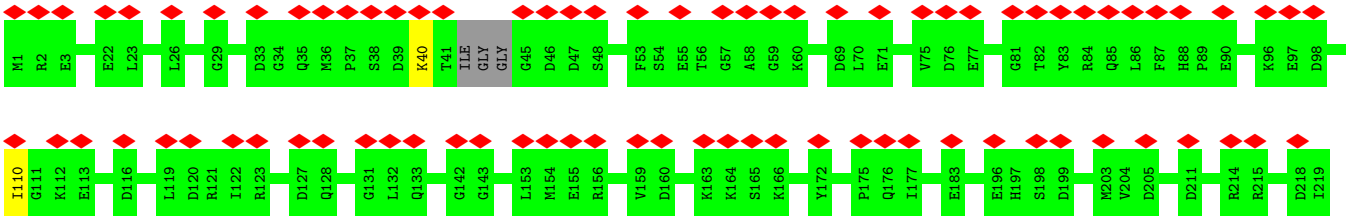


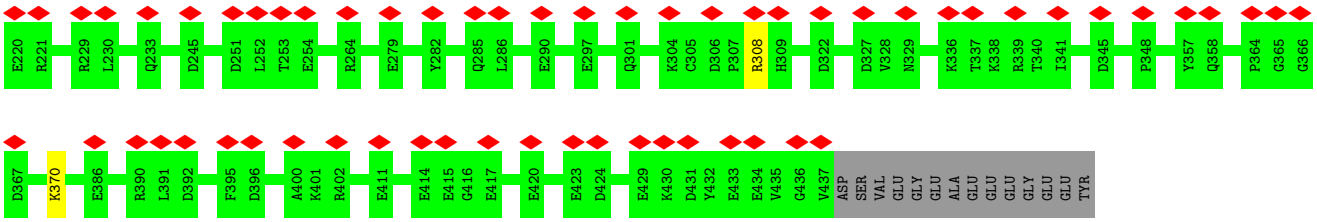


- Molecule 54: Tubulin alpha chain

Chain OB:

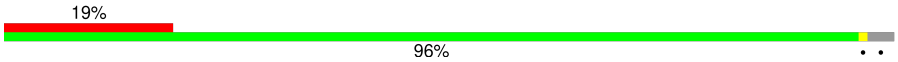


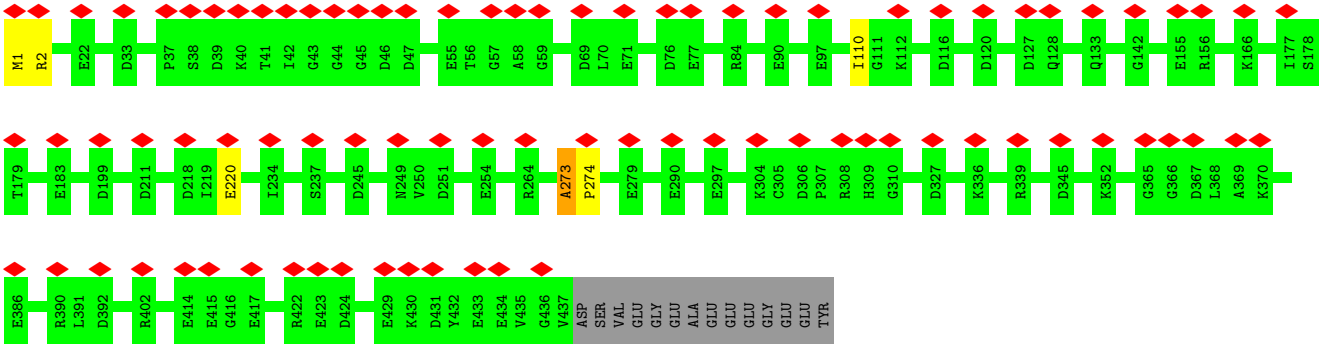




• Molecule 54: Tubulin alpha chain

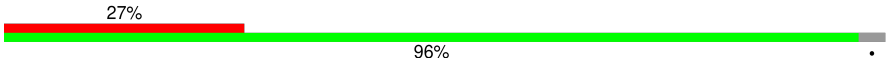
Chain OE:

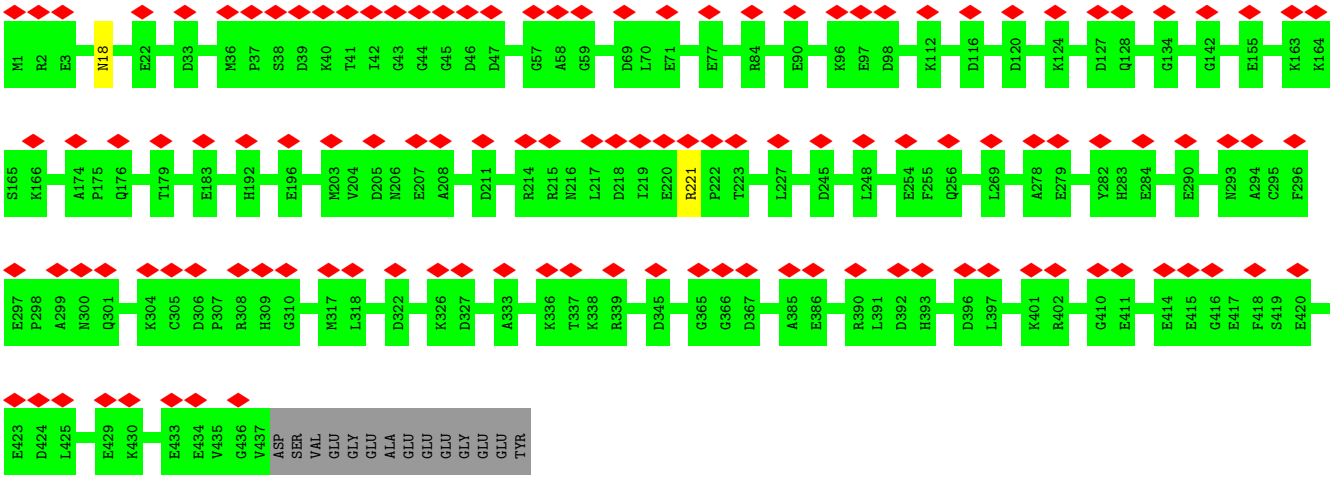




• Molecule 54: Tubulin alpha chain

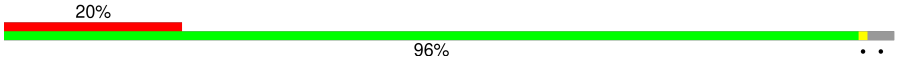
Chain OG:

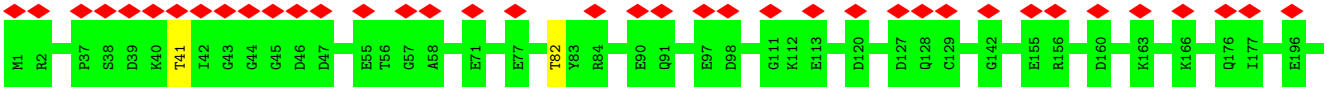


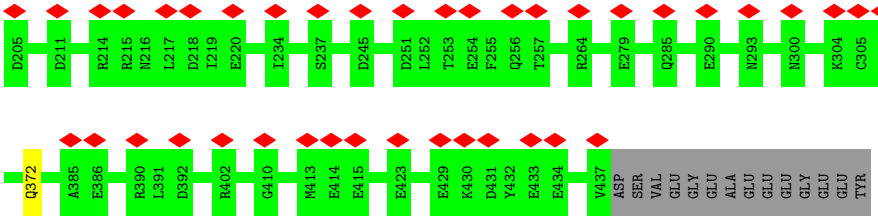


• Molecule 54: Tubulin alpha chain

Chain OI:

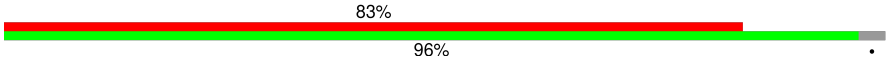


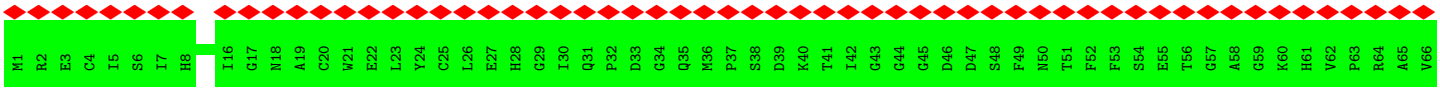


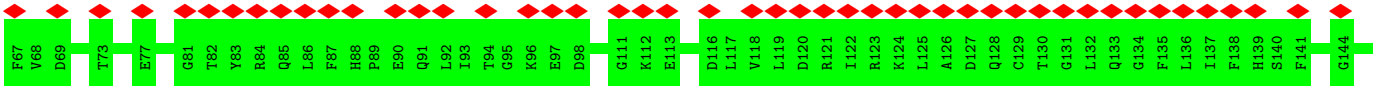


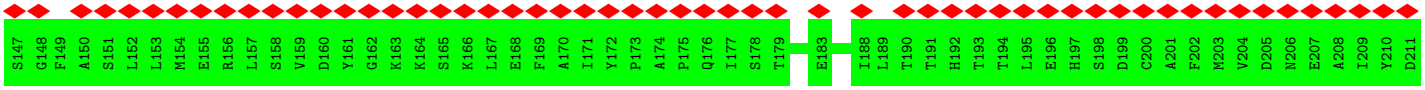
- Molecule 54: Tubulin alpha chain

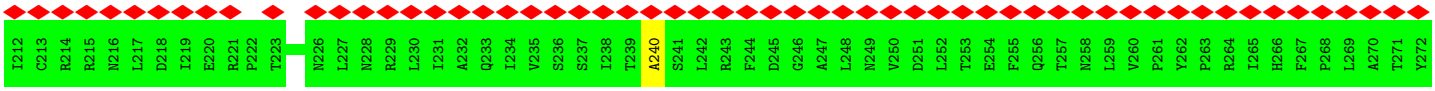
Chain OK:

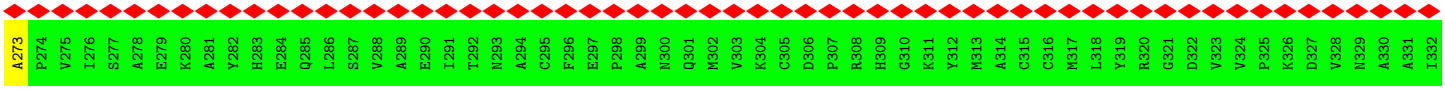


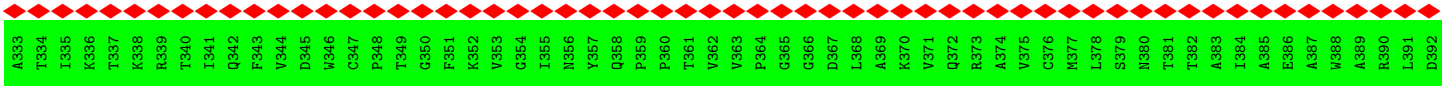


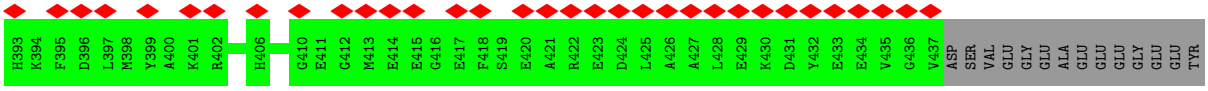






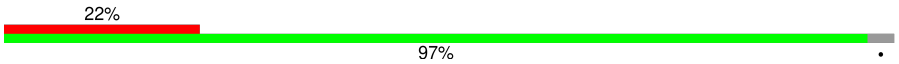


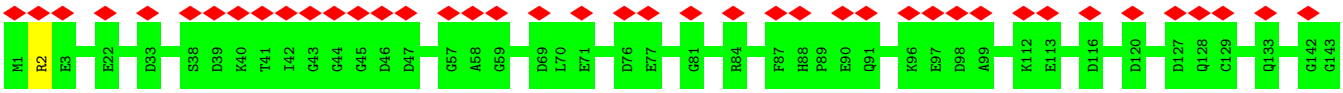


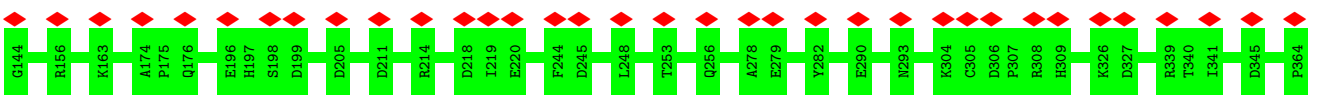


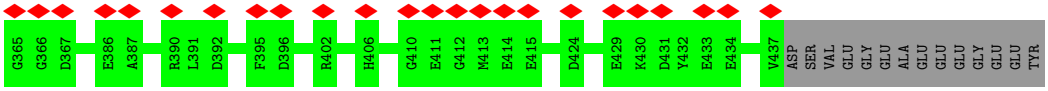
- Molecule 54: Tubulin alpha chain

Chain OL:



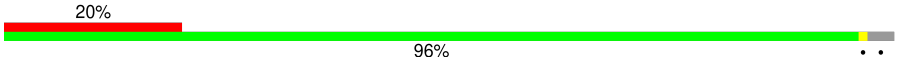


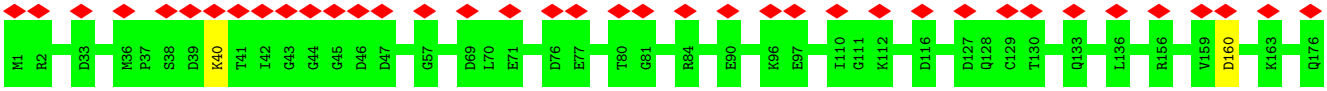


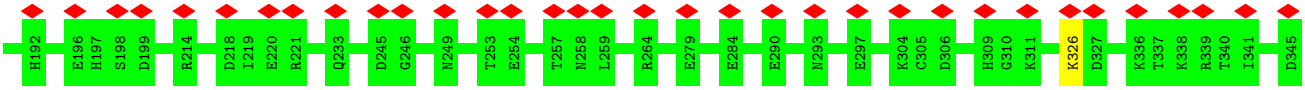


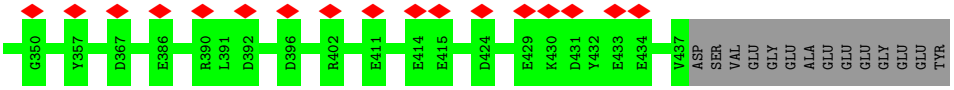
- Molecule 54: Tubulin alpha chain

Chain PA:



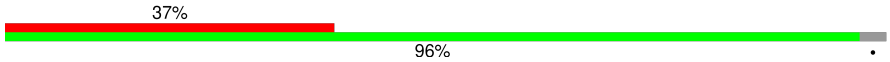


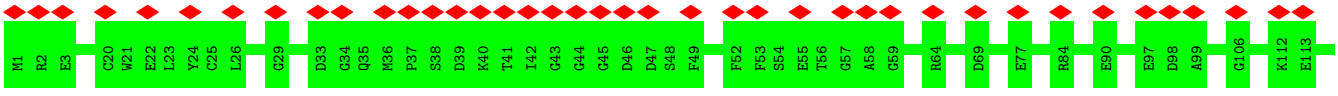


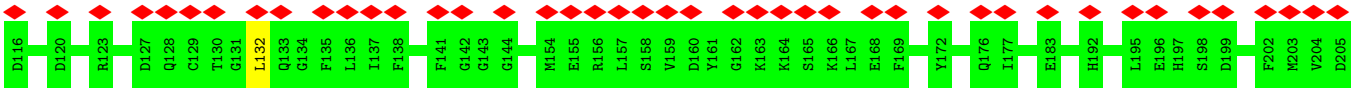


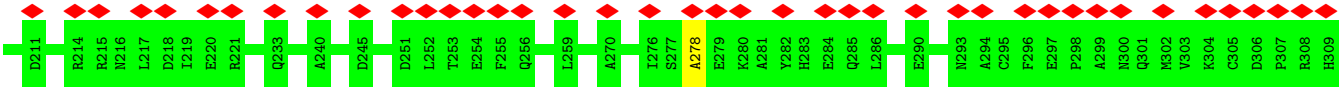
- Molecule 54: Tubulin alpha chain

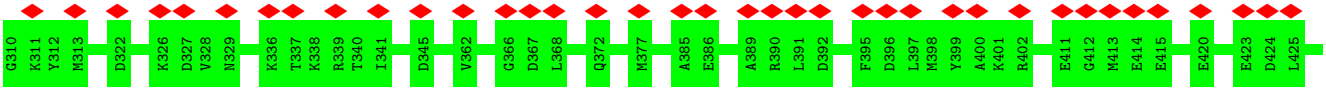
Chain PB:

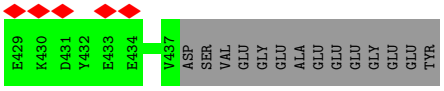






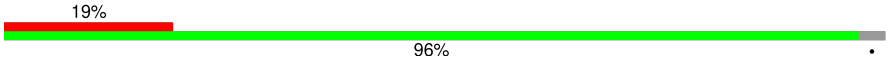


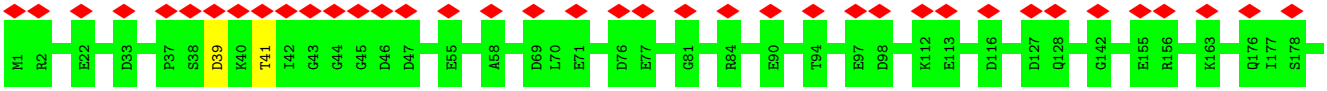


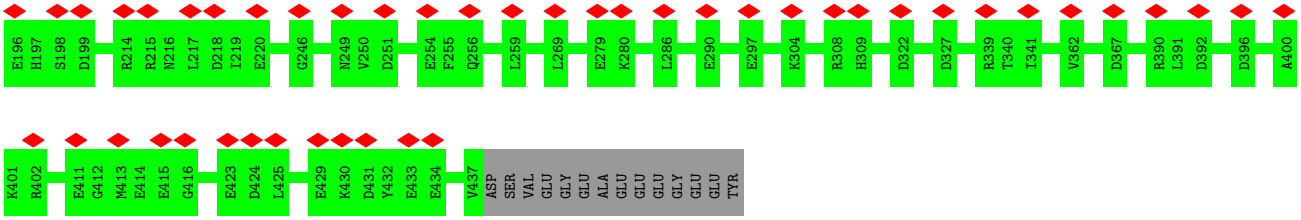


- Molecule 54: Tubulin alpha chain

Chain PE:

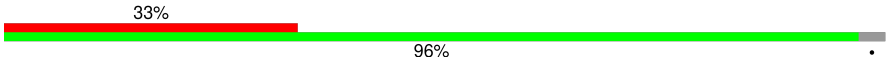


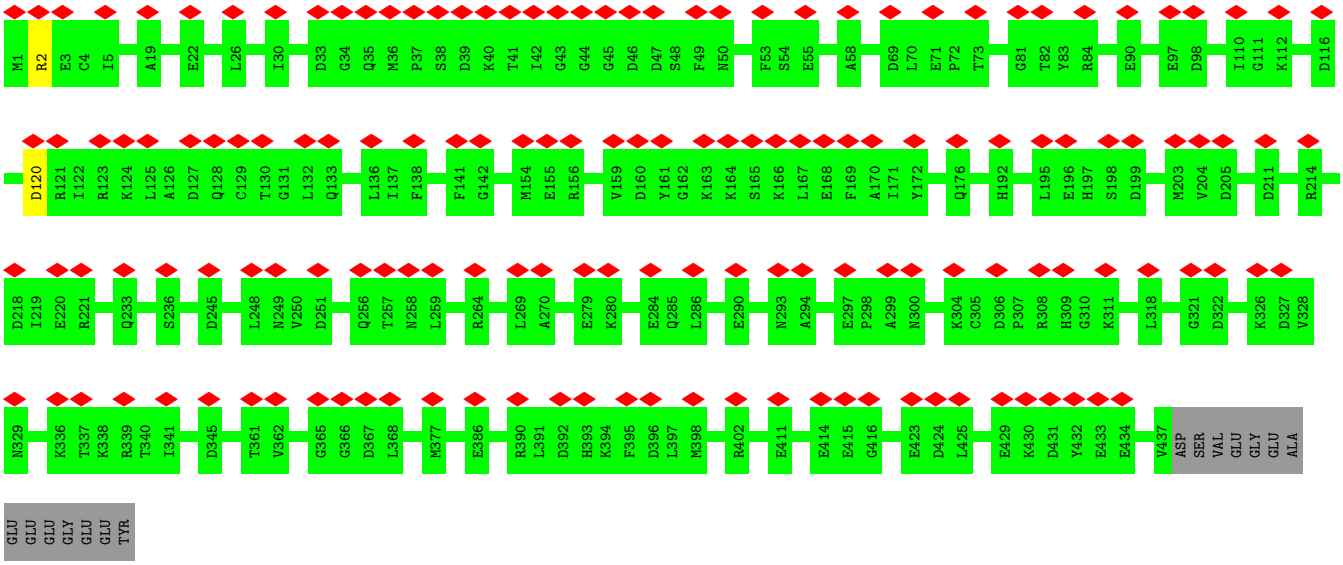




• Molecule 54: Tubulin alpha chain

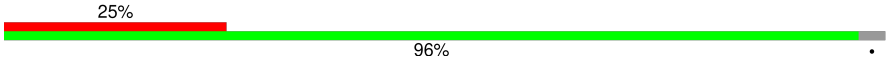
Chain PG:

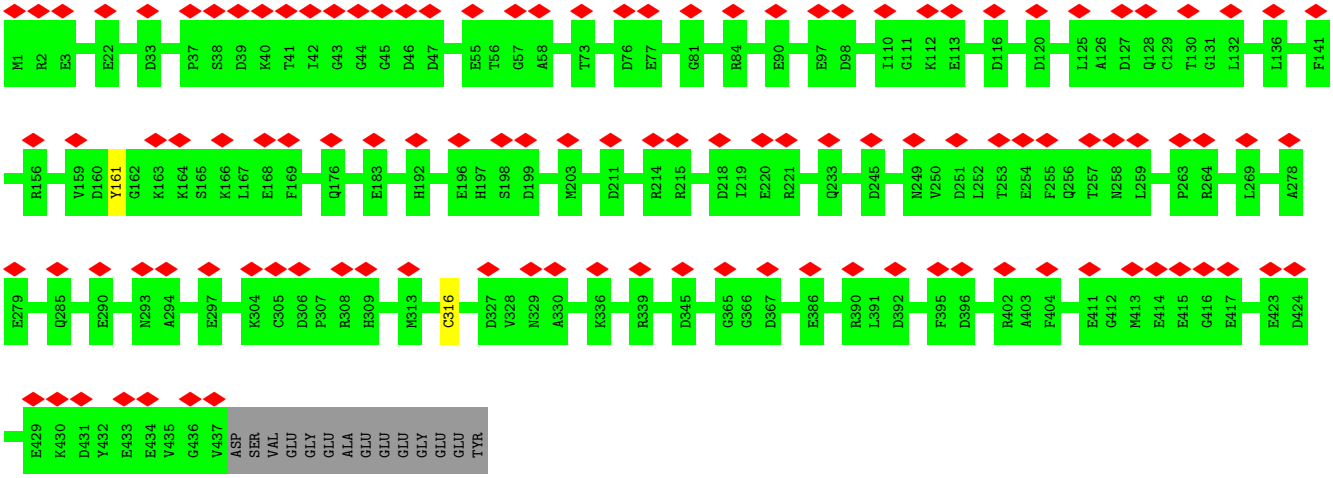




• Molecule 54: Tubulin alpha chain

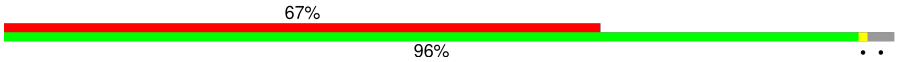
Chain PI:





• Molecule 54: Tubulin alpha chain

Chain PK:



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T80 G81 T82 Y83 R84 E90 Q91 L92 E97 D98 N101 I110 G111 K112 E113 D116 D120 R123 K124 L125 A126 D127 Q128 C129 T130 G131 L132 Q133 G134 F135 L136 G144 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 L167 E168 F169 A174 P175

Q176 I177 S178 T179 A180 H192 L195 E196 H197 S198 D199 C200 A201 F202 M203 N206 E207 D211 R214 R215 N216 L217 D218 I219 E220 R221 P222 T223 N226 L227 N228 I231 A232 Q233 I234 V235 S236 S237 I238 T239 A240 S241 L242 R243 F244 D245 G246 A247 L248 N249 V250 D251 L252

T253 E254 F255 Q256 T257 N258 L259 V260 P261 Y262 P263 R264 I265 H266 F267 P268 L269 A270 T271 Y272 A273 P274 V275 I276 S277 A278 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 A294 C295 F296 E297 P298 A299 N300 Q301 K304 C305 D306 P307 R308 H309 G310 K311 Y312 M313

A314 C315 C316 M317 L318 Y319 R320 G321 D322 V323 V324 P325 K326 D327 V328 N329 A330 A331 I332 A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 K352 V353 G354 I355 N356 Y357 Q358 P359 P360 T361 V362 V363 P364 G365 G366 D367 L368 A369 K370 V371 Q372 R373

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VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain PL: 35% 97%

M1 R2 A19 E22 D33 G34 Q35 M36 P37 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 F53 S54 E55 T56 G57 A58 D69 L70 E71 P72 T73 D76 E77 V78 R79 T80 G81 T82 Y83 R84 F87 E90 Q91 L92 I93 T94 G95 K96 E97 D98 A99 A100 N101

N102 Y103 A104 R105 Y108 T109 I110 G111 K112 E113 I114 V115 D116 L117 D127 Q128 L132 F138 F141 G142 G143 G144 L153 M154 E155 D160 Y161 G162 K163 K164 S165 F169 Y172 P173 A174 P175 Q176 I177 S178 T179 A180 V181 V182 E183 P184 Y185 E196 H197 S198

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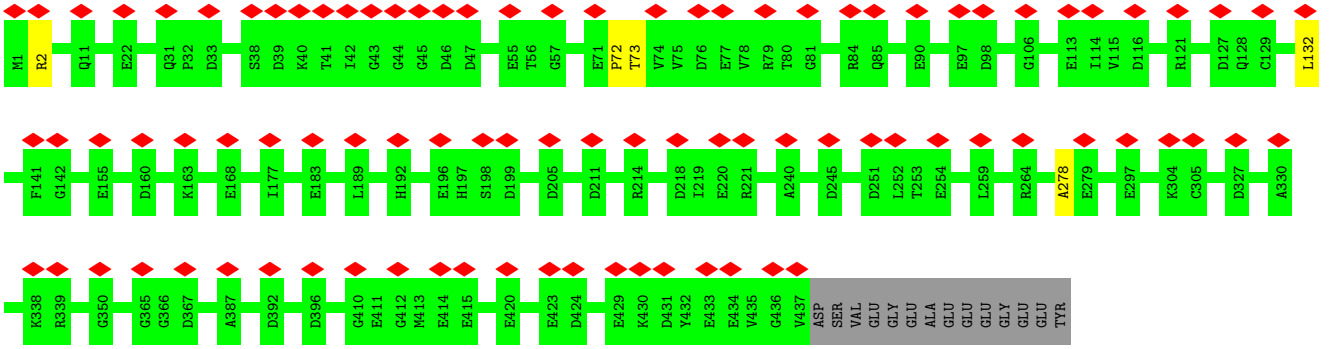
V362 G365 G366 D367 K370 E386 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 A403 F404 V405 H406 W407 Y408 V409 G410 E411 G412 M413 E414 E415 G416 E423 D424 K430 D431 Y432 E433 E434 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY

GLU GLU TYR

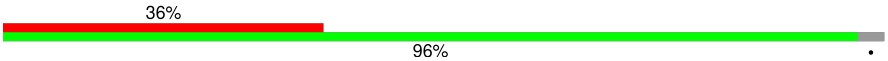
- Molecule 54: Tubulin alpha chain

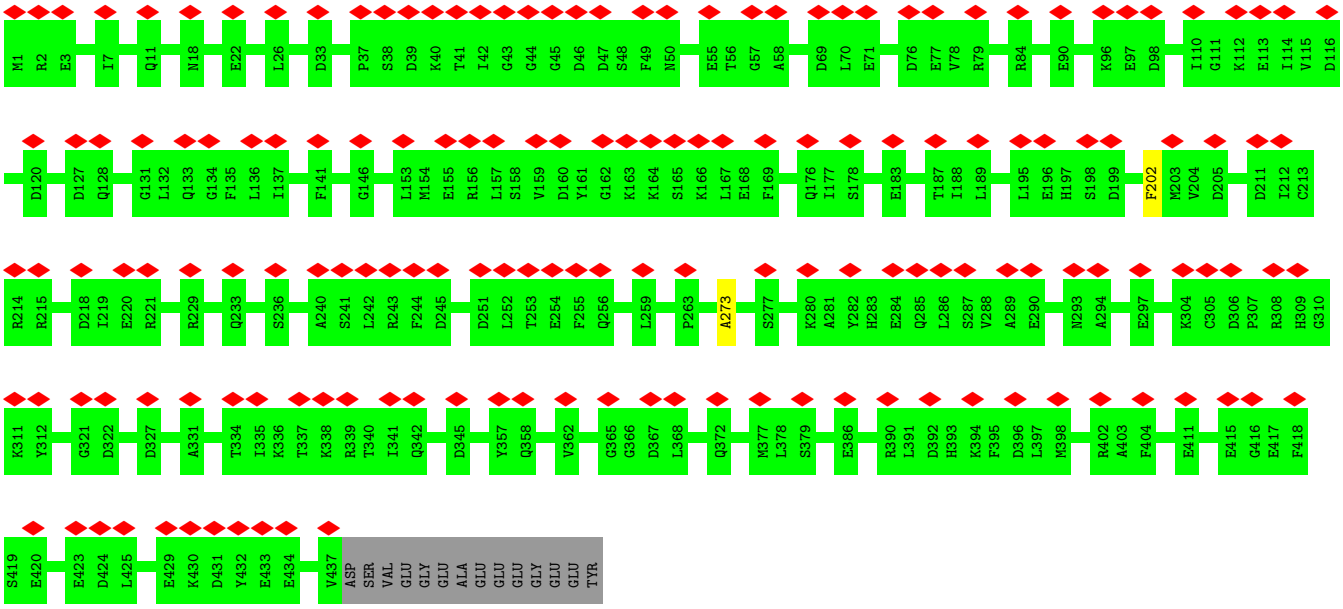
Chain QA: 20% 96%



- Molecule 54: Tubulin alpha chain

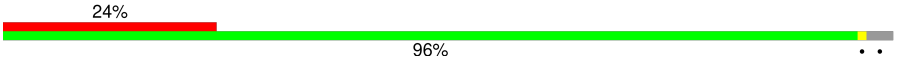
Chain QB:

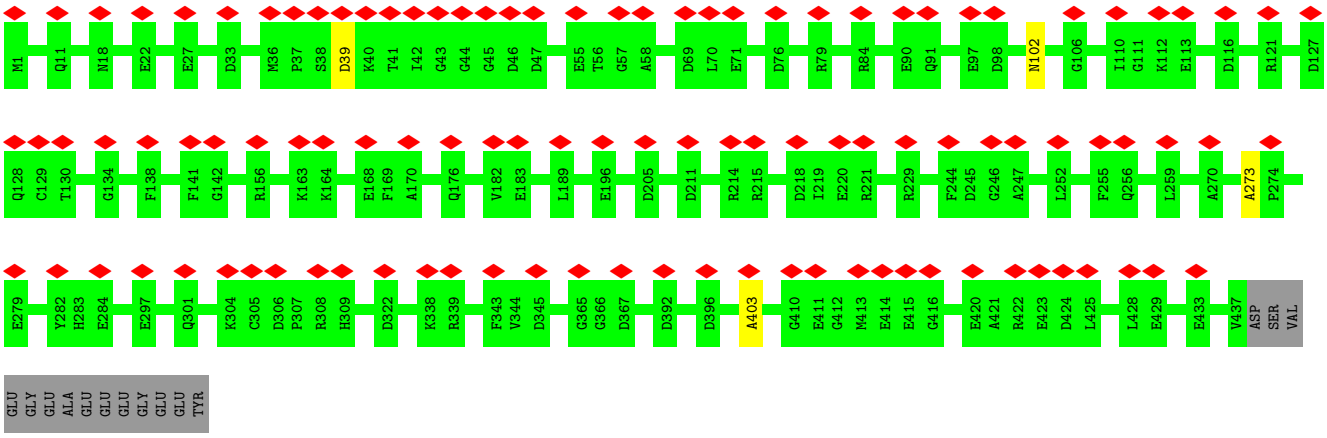




- Molecule 54: Tubulin alpha chain

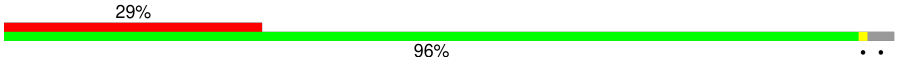
Chain QE:

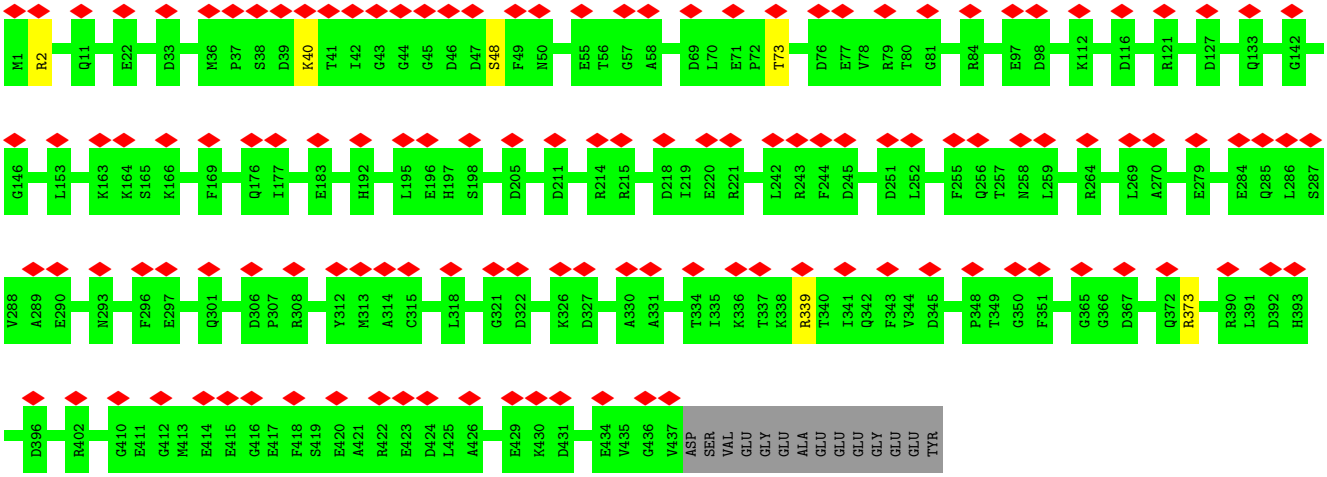




- Molecule 54: Tubulin alpha chain

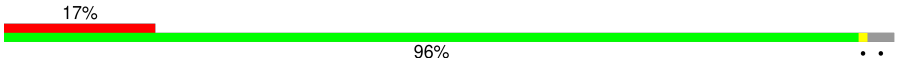
Chain QG:

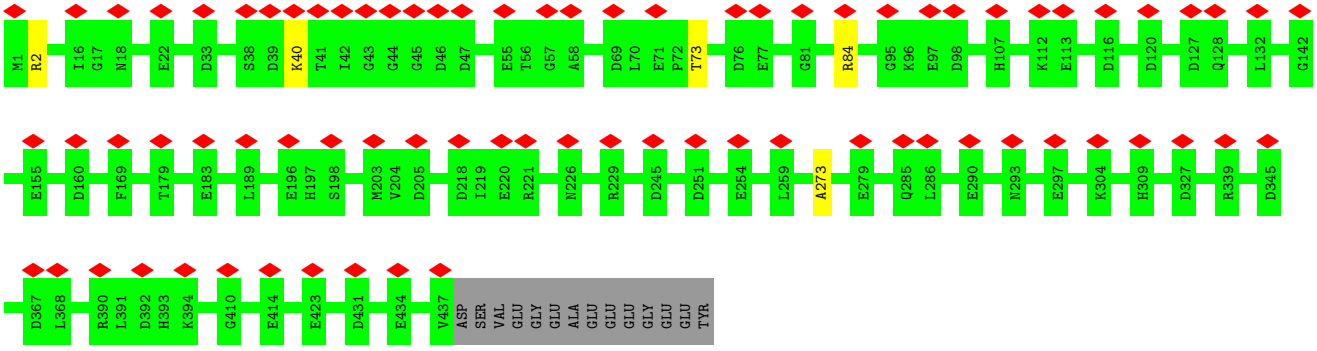




- Molecule 54: Tubulin alpha chain

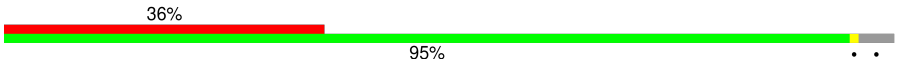
Chain QI:

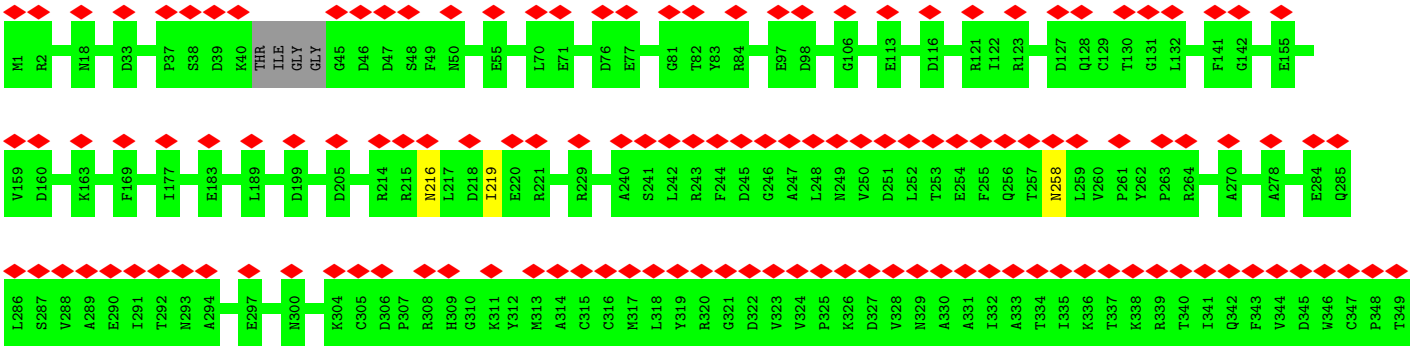


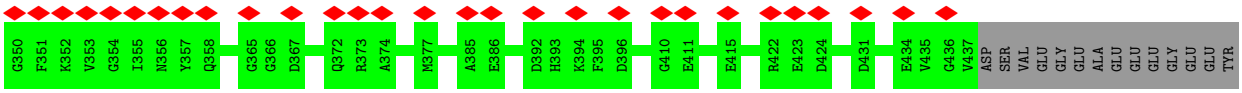


- Molecule 54: Tubulin alpha chain

Chain QK:

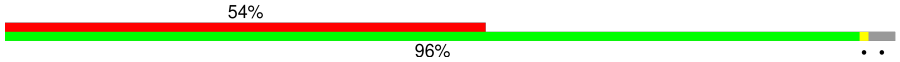


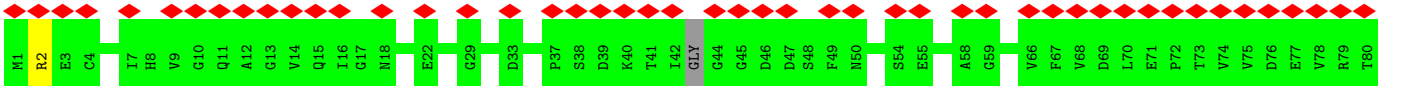


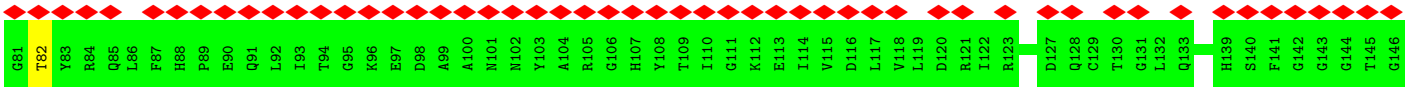


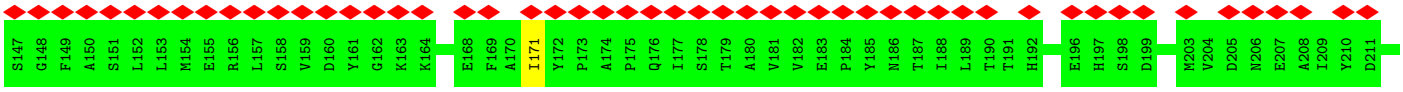
• Molecule 54: Tubulin alpha chain

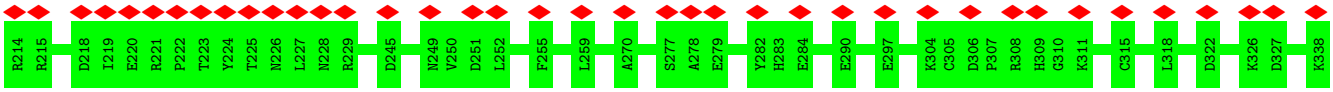
Chain QL:

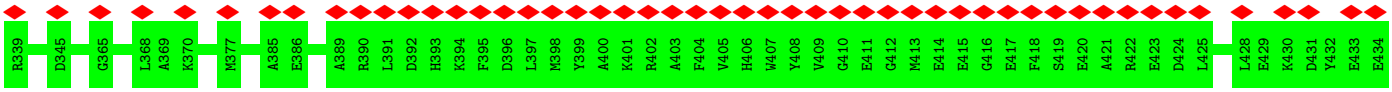






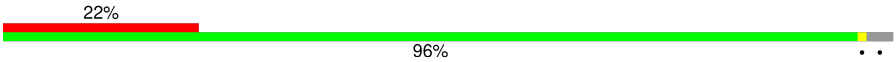


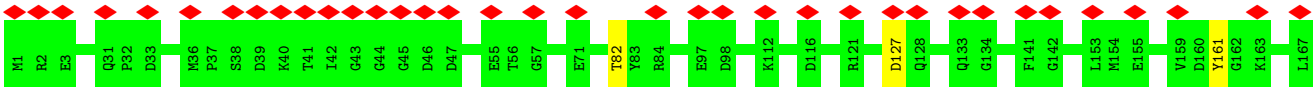


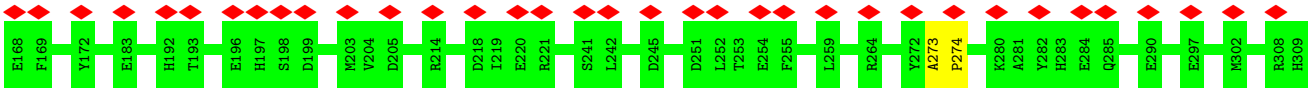


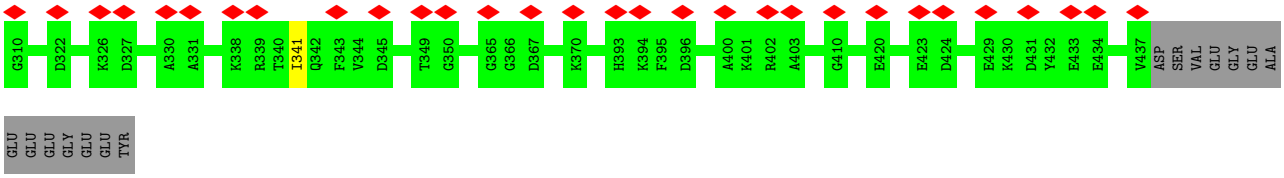
• Molecule 54: Tubulin alpha chain

Chain RA:



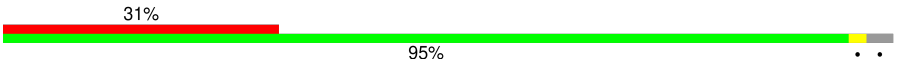


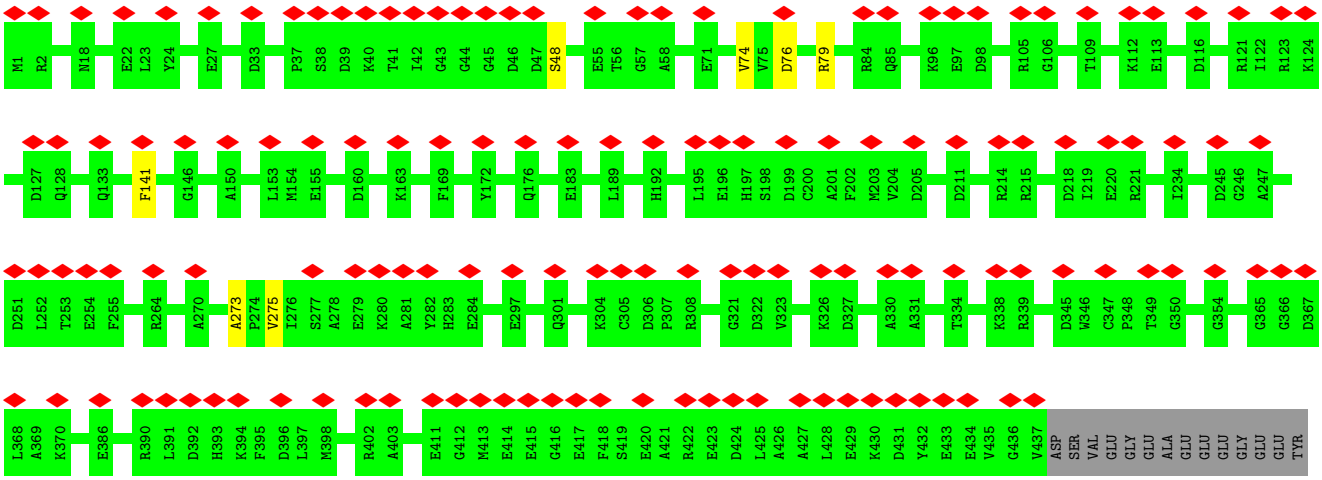




• Molecule 54: Tubulin alpha chain

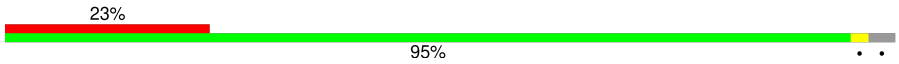
Chain RB:

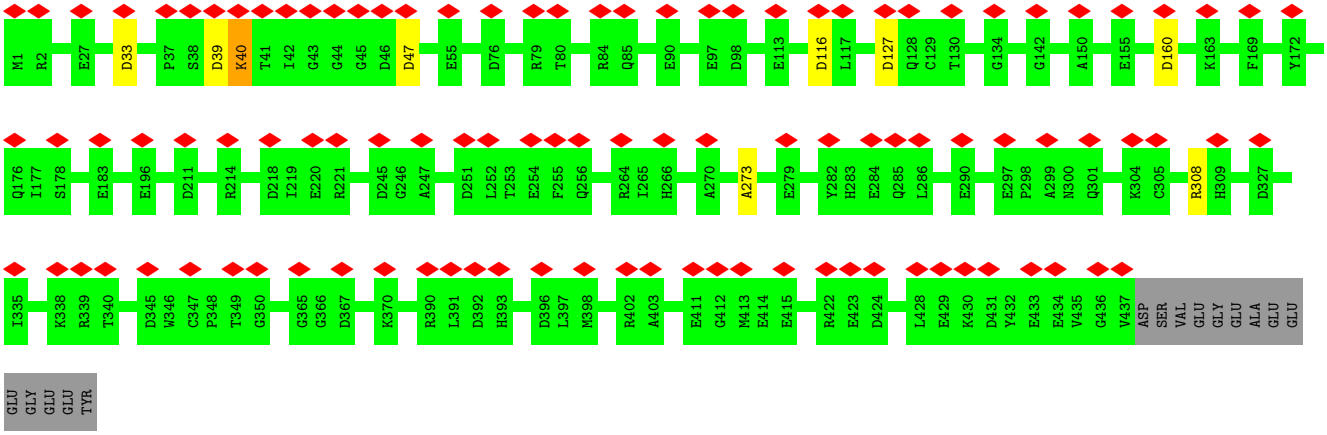




- Molecule 54: Tubulin alpha chain

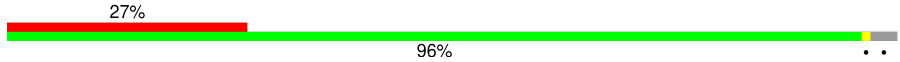
Chain RE:

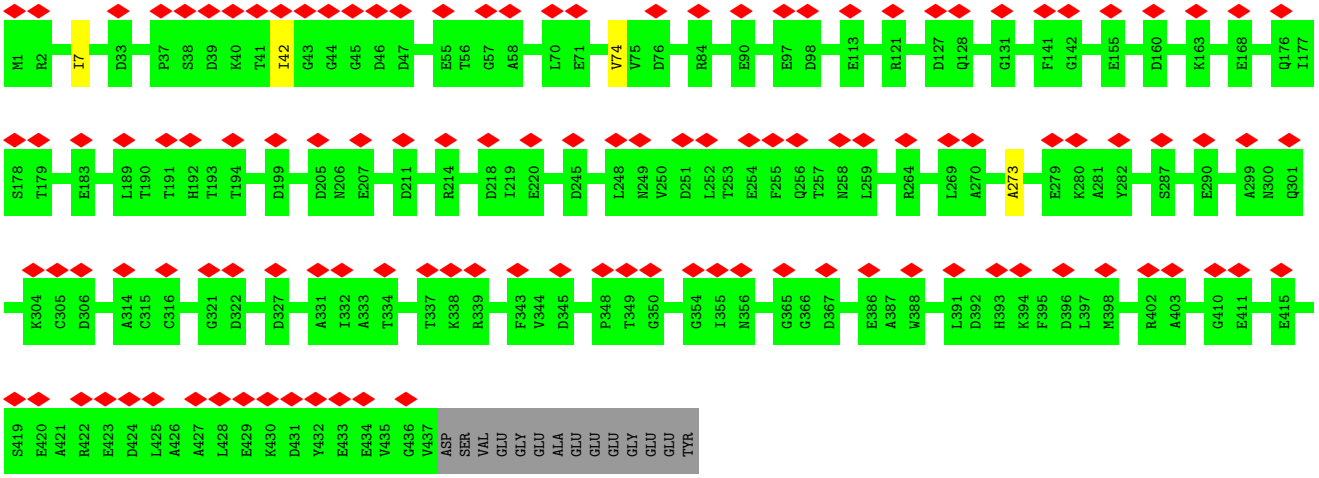




- Molecule 54: Tubulin alpha chain

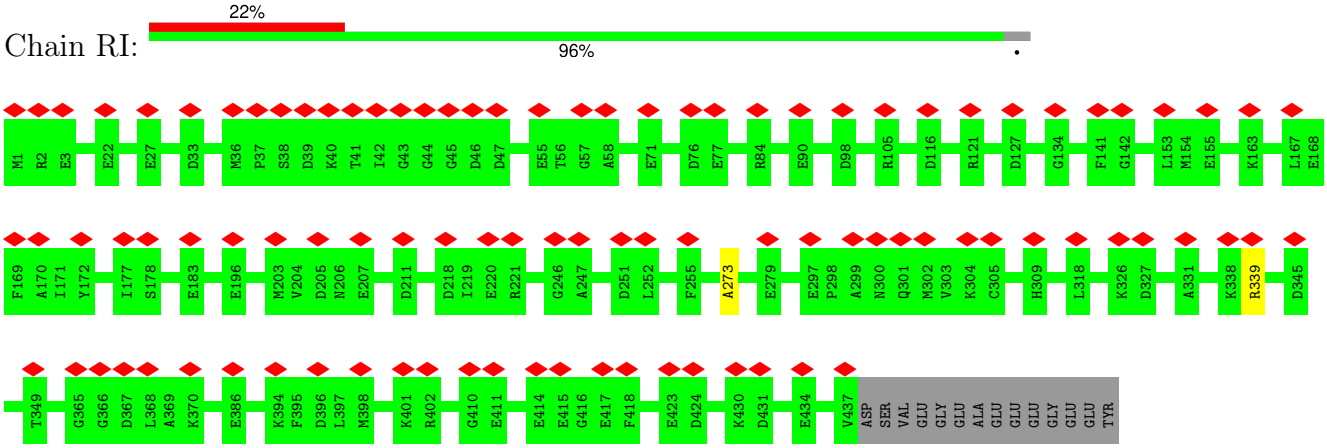
Chain RG:





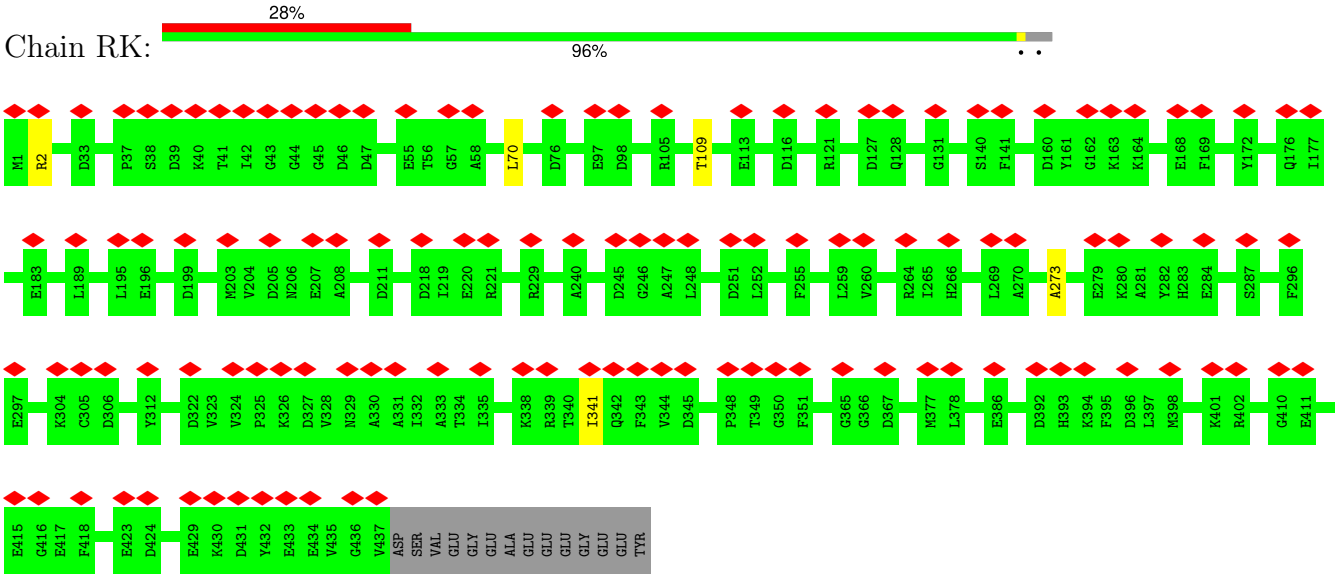
- Molecule 54: Tubulin alpha chain

Chain RI:



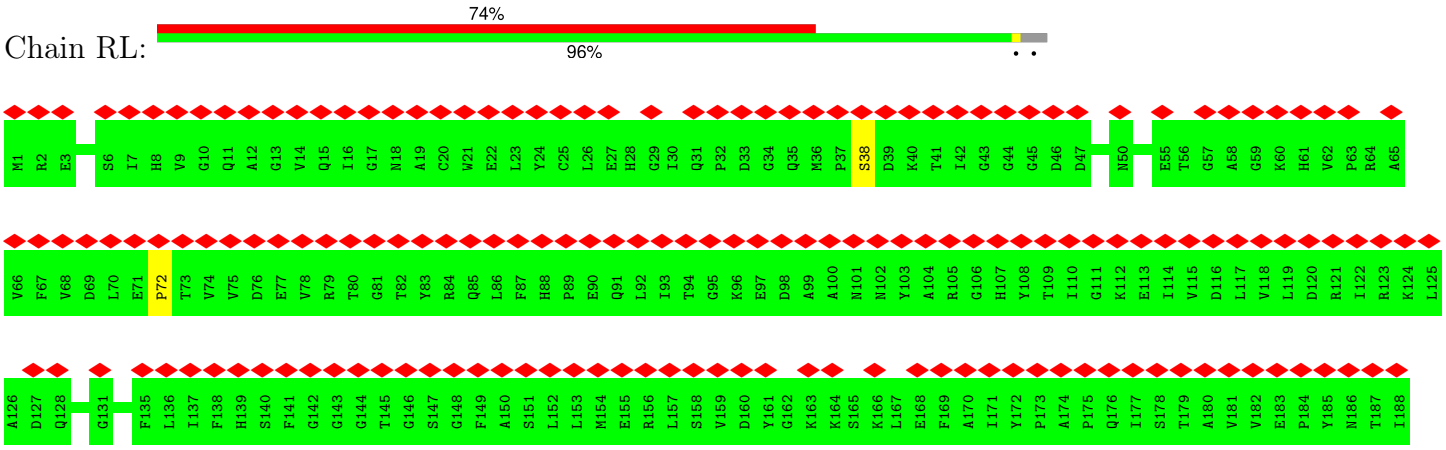
- Molecule 54: Tubulin alpha chain

Chain RK:



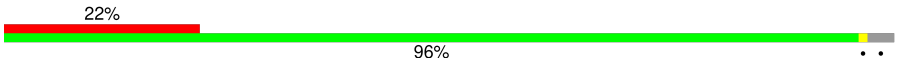
- Molecule 54: Tubulin alpha chain

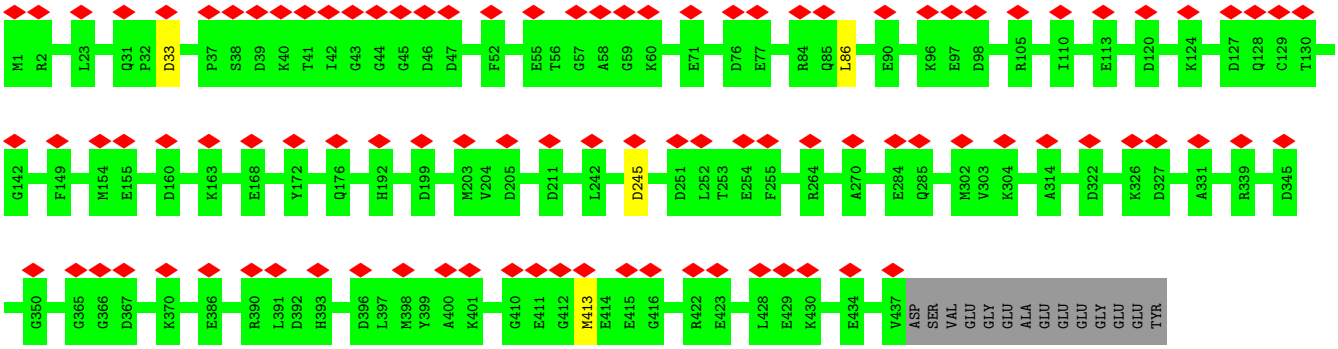
Chain RL:



- Molecule 54: Tubulin alpha chain

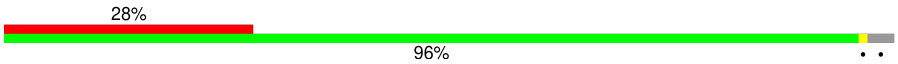
Chain SA:

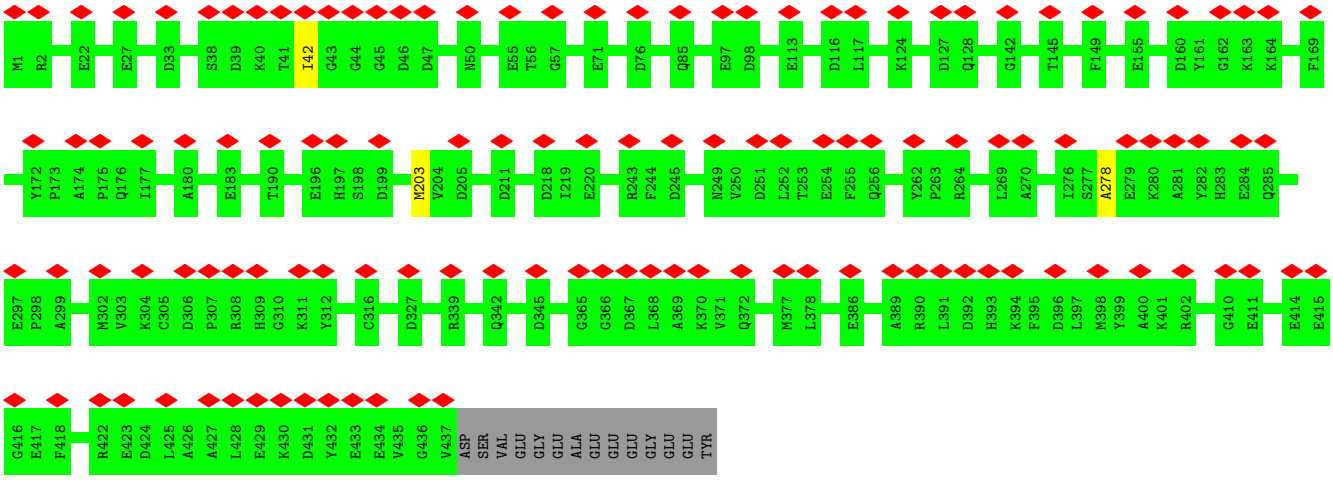




- Molecule 54: Tubulin alpha chain

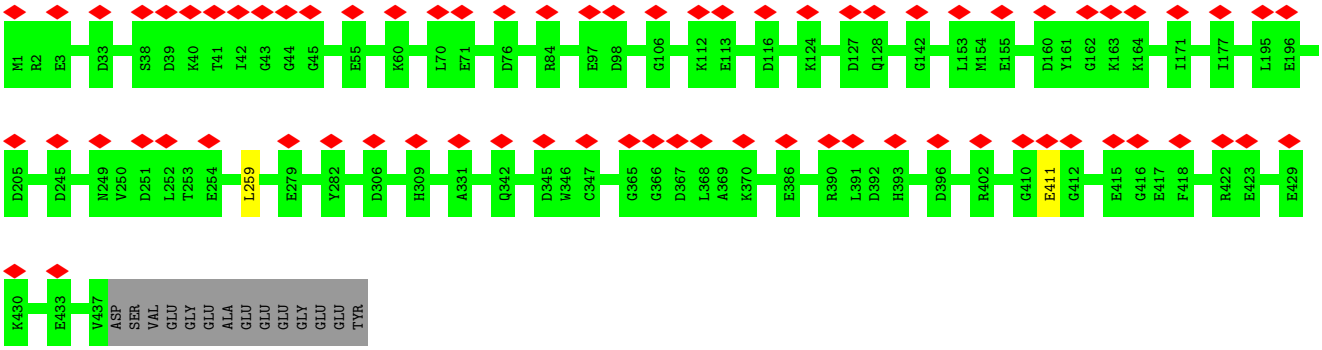
Chain SB:





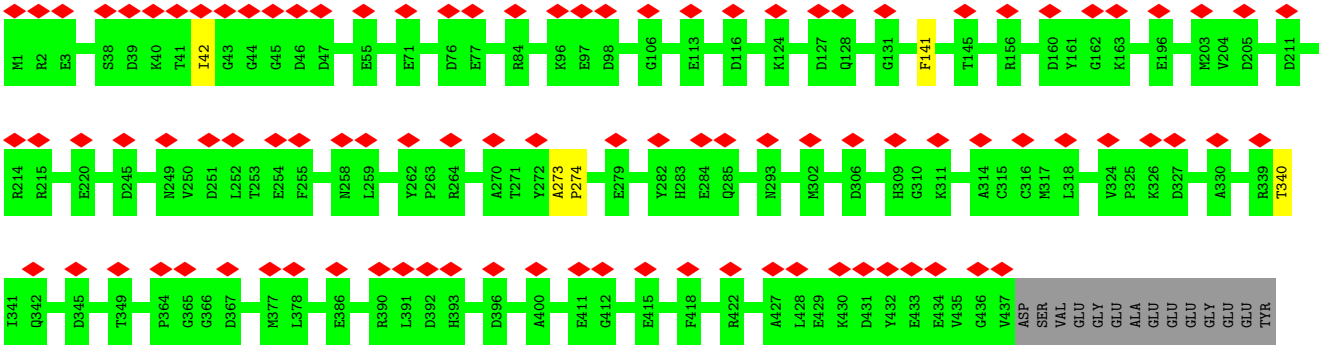
- Molecule 54: Tubulin alpha chain

Chain SE: 16% 96%



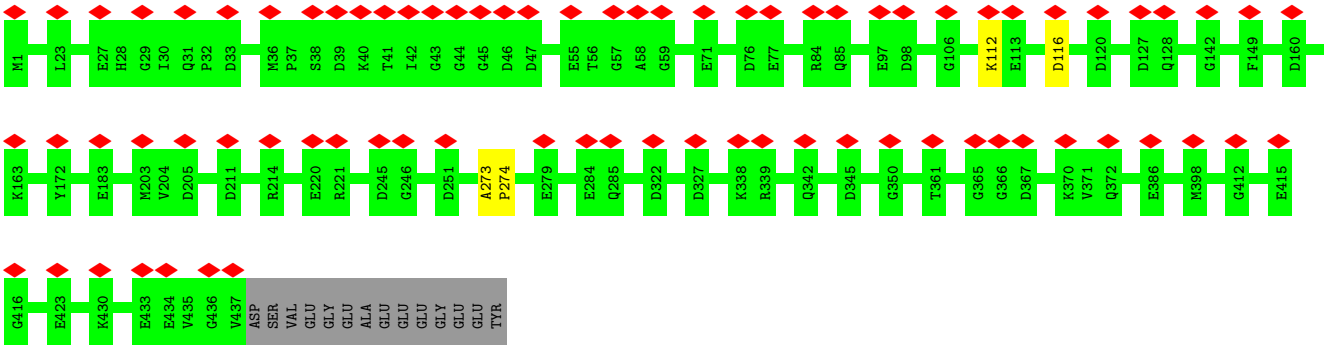
- Molecule 54: Tubulin alpha chain

Chain SG: 22% 96%



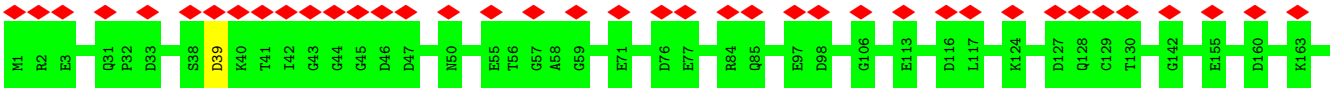
- Molecule 54: Tubulin alpha chain

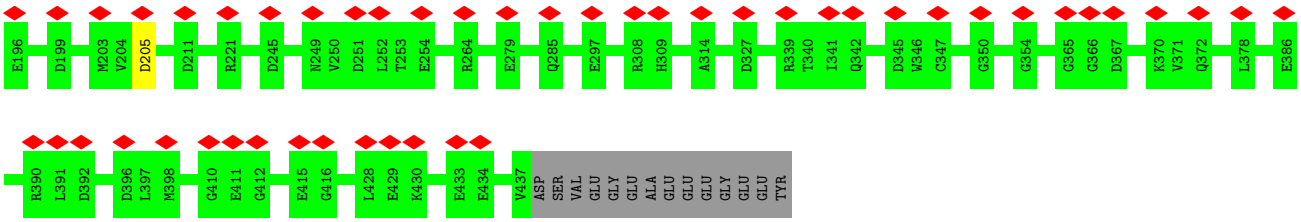
Chain SI: 17% 96%



- Molecule 54: Tubulin alpha chain

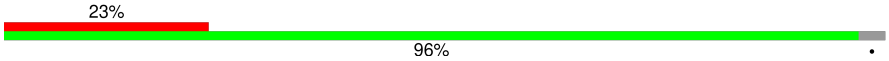
Chain SK: 19% 96%

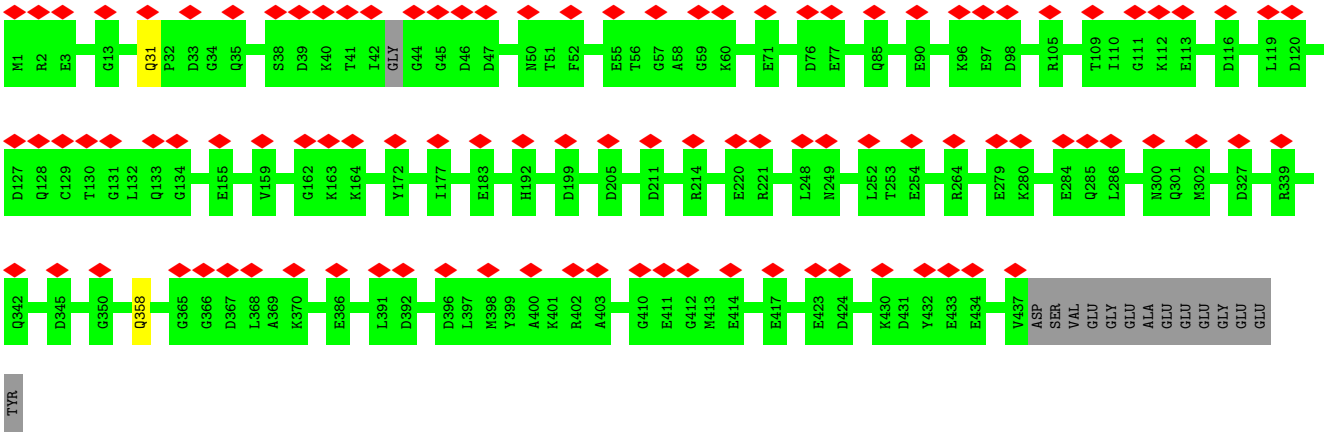




• Molecule 54: Tubulin alpha chain

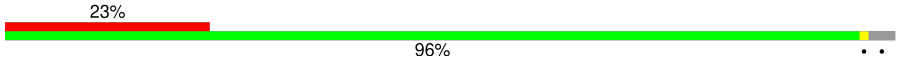
Chain TA:

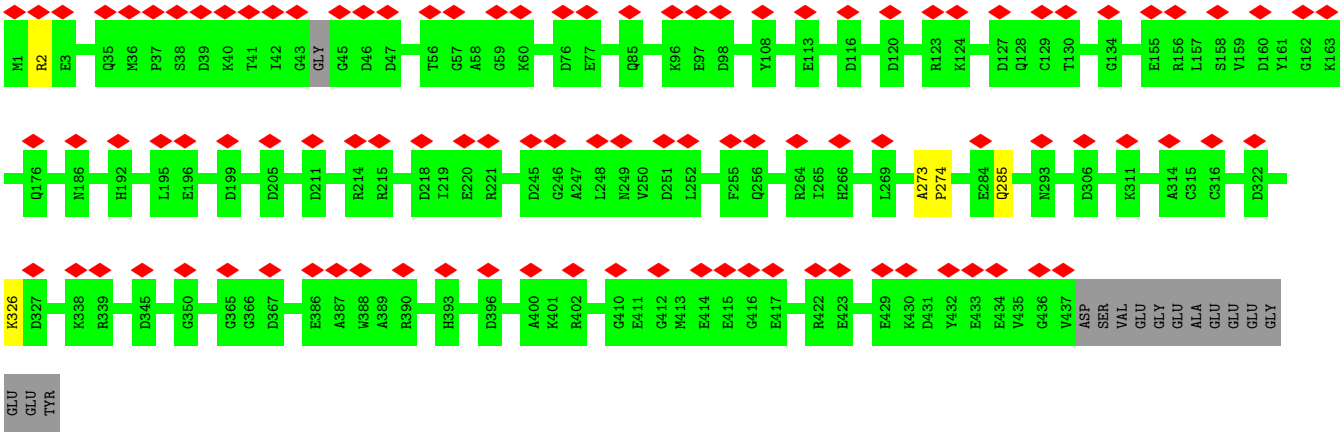




• Molecule 54: Tubulin alpha chain

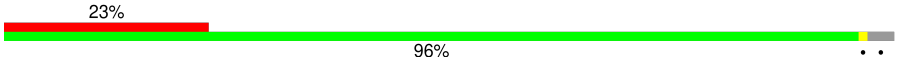
Chain TB:

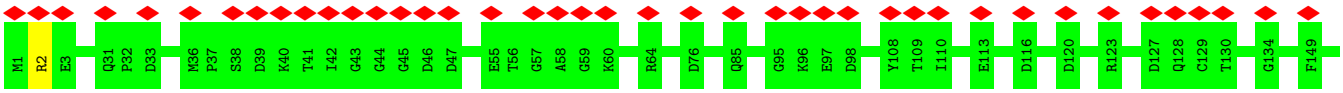


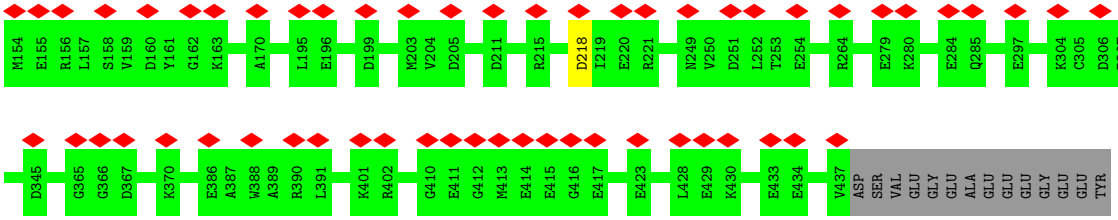


• Molecule 54: Tubulin alpha chain

Chain TE:

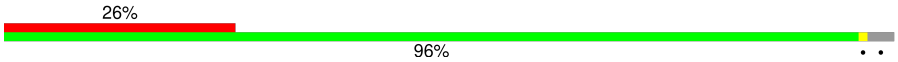


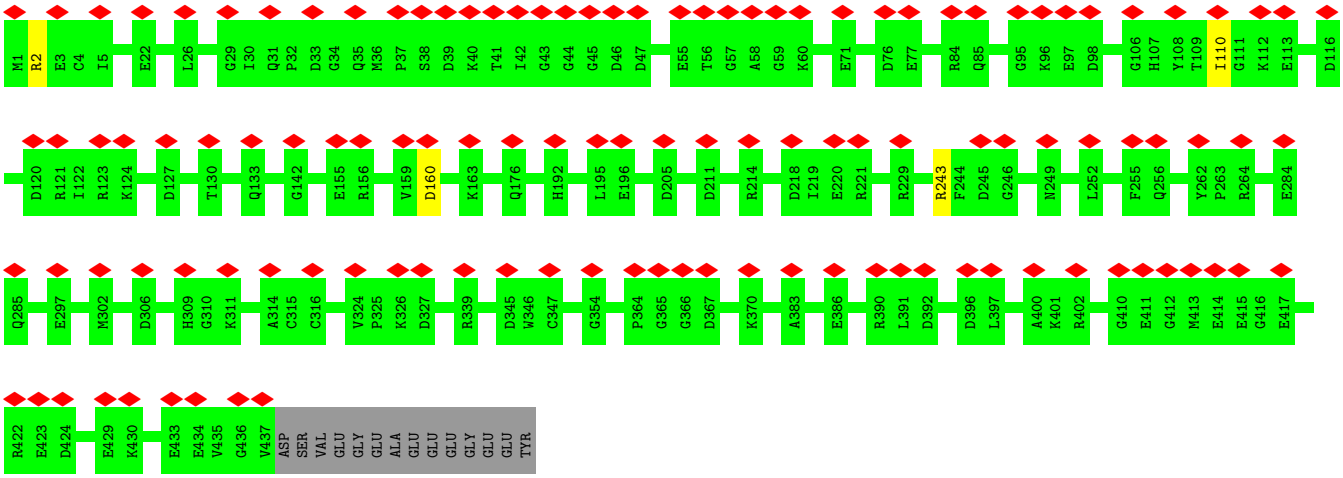




- Molecule 54: Tubulin alpha chain

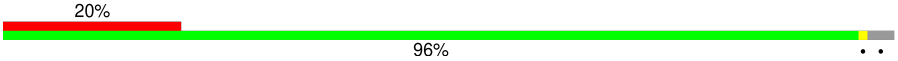
Chain TG:

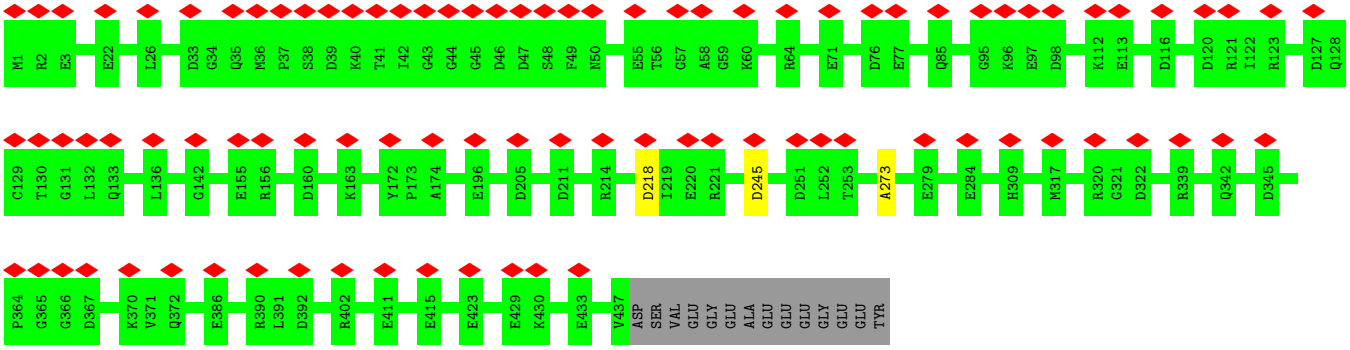




- Molecule 54: Tubulin alpha chain

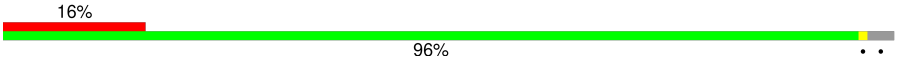
Chain TI:

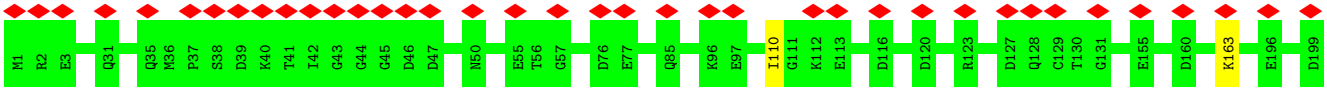


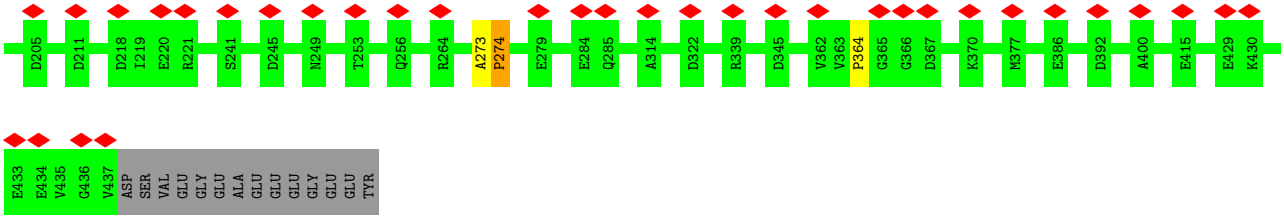


- Molecule 54: Tubulin alpha chain

Chain TK:

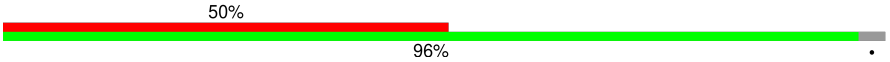


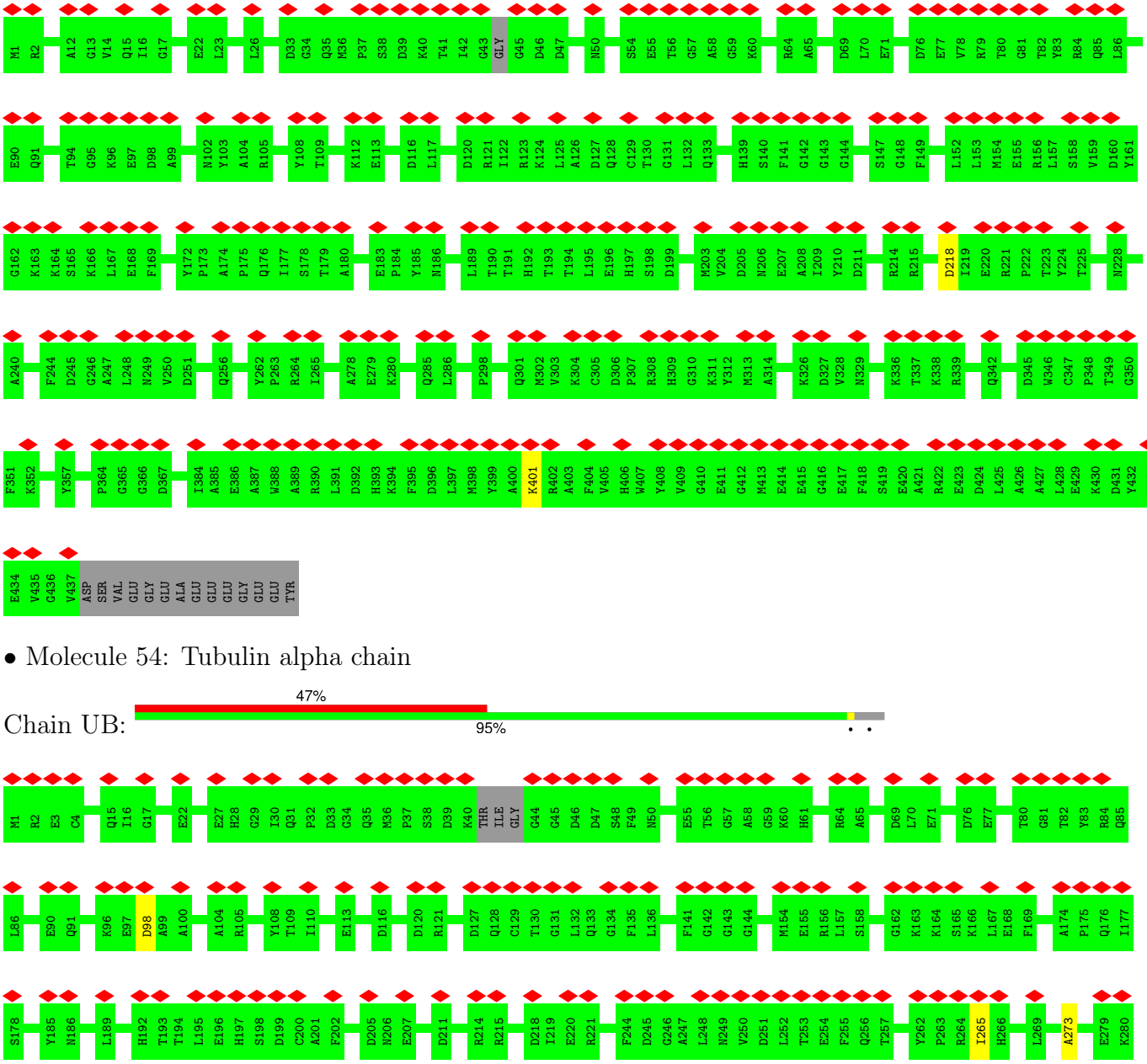




• Molecule 54: Tubulin alpha chain

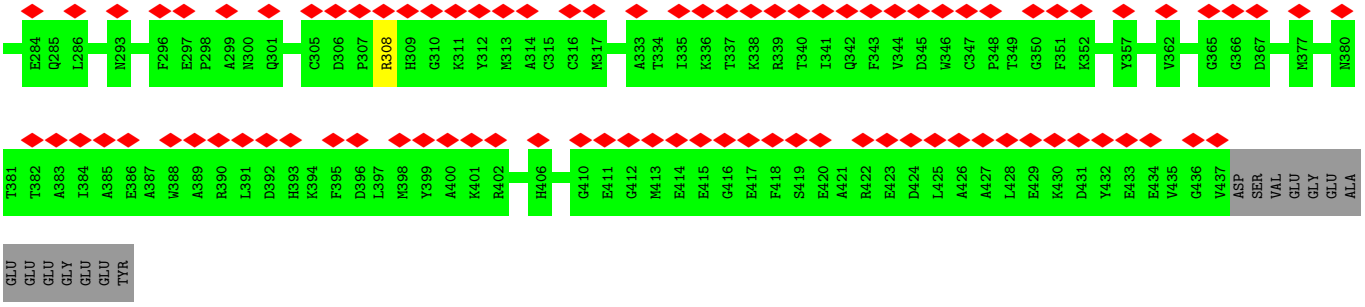
Chain UA:





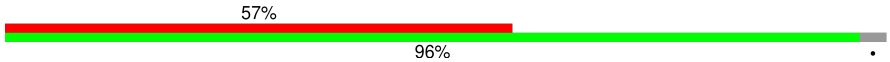
• Molecule 54: Tubulin alpha chain

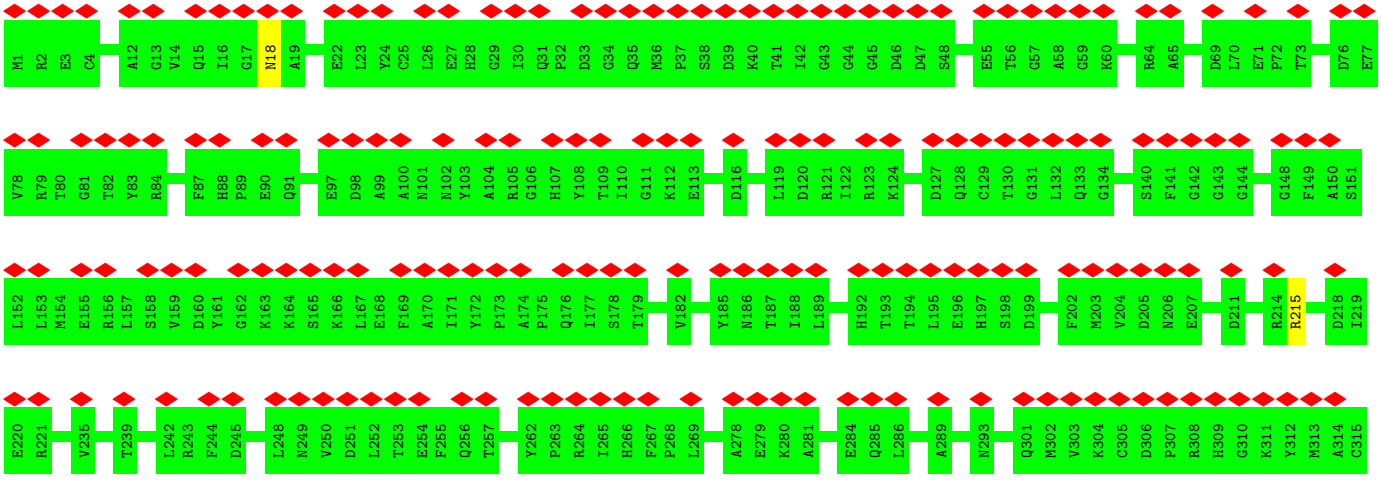
Chain UB:



- Molecule 54: Tubulin alpha chain

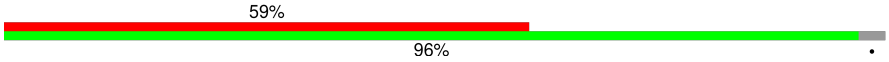
Chain UE:

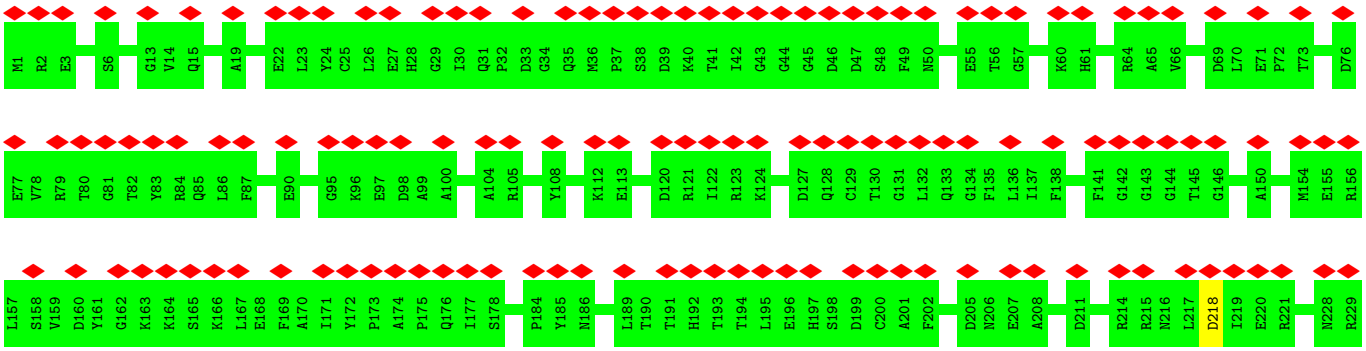


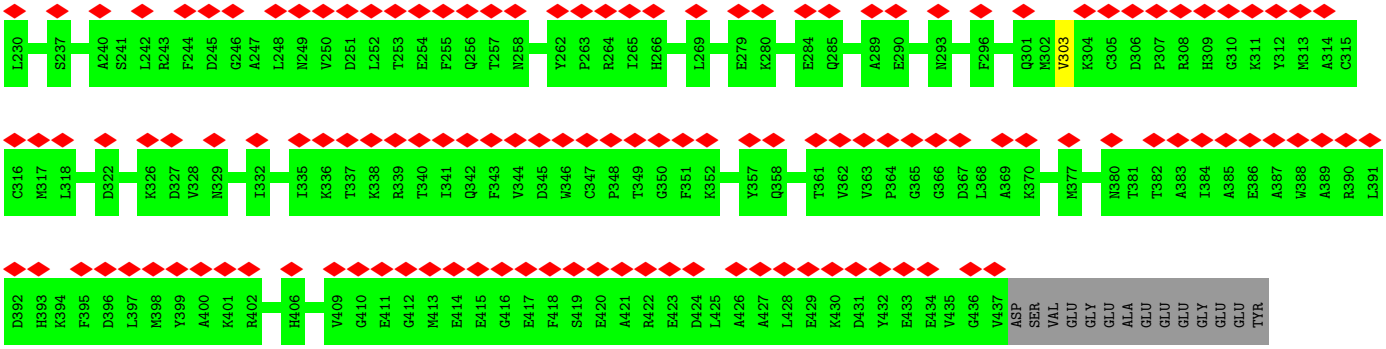


- Molecule 54: Tubulin alpha chain

Chain UG:

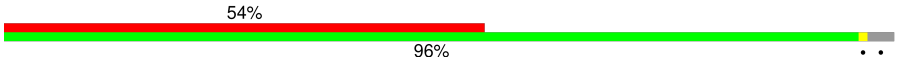


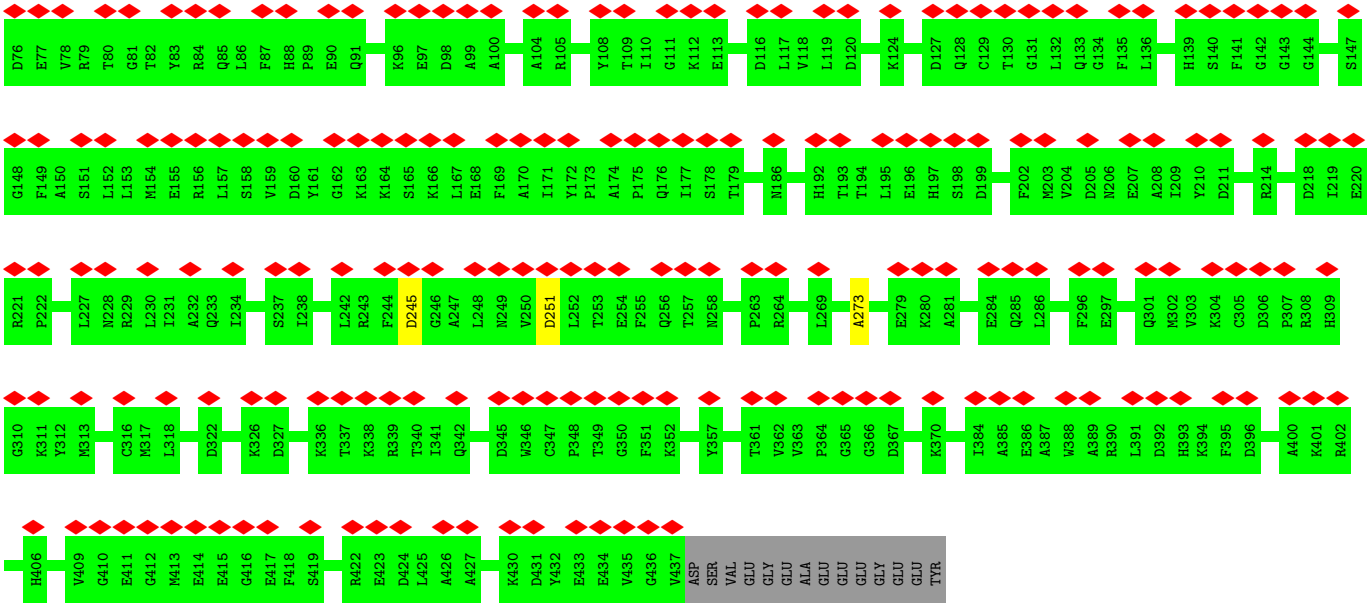




- Molecule 54: Tubulin alpha chain

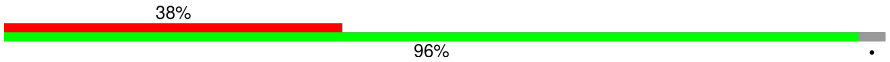
Chain UI:

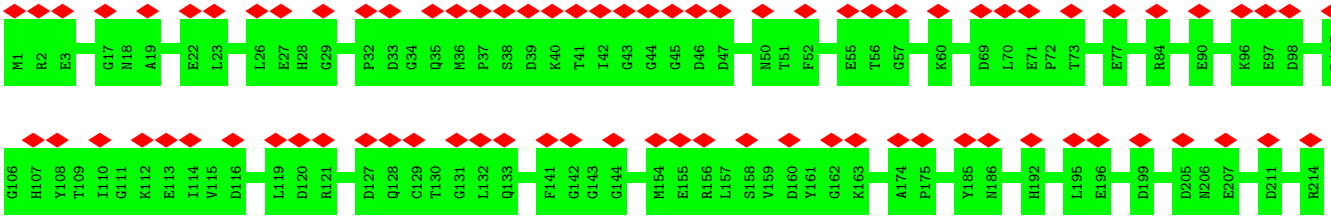


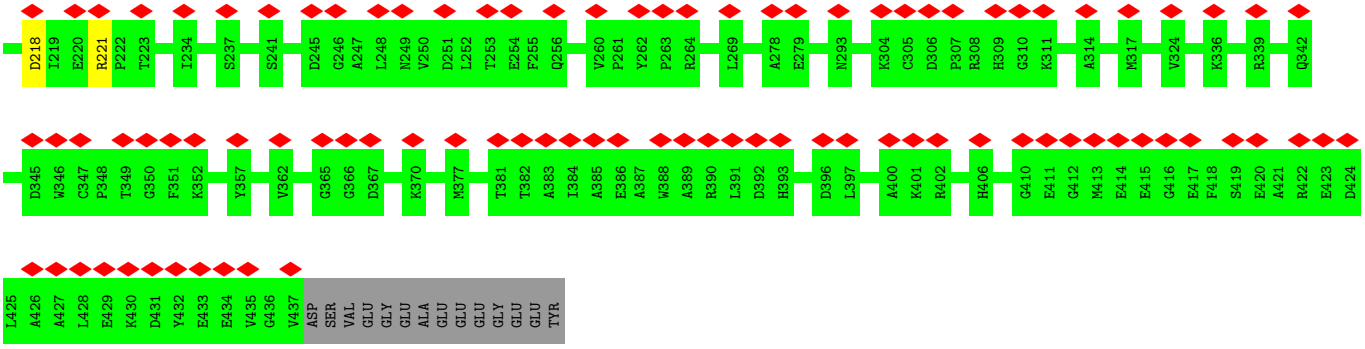


- Molecule 54: Tubulin alpha chain

Chain UK:

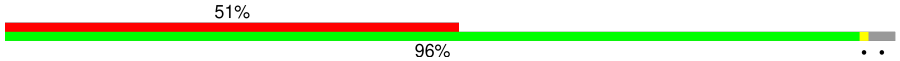


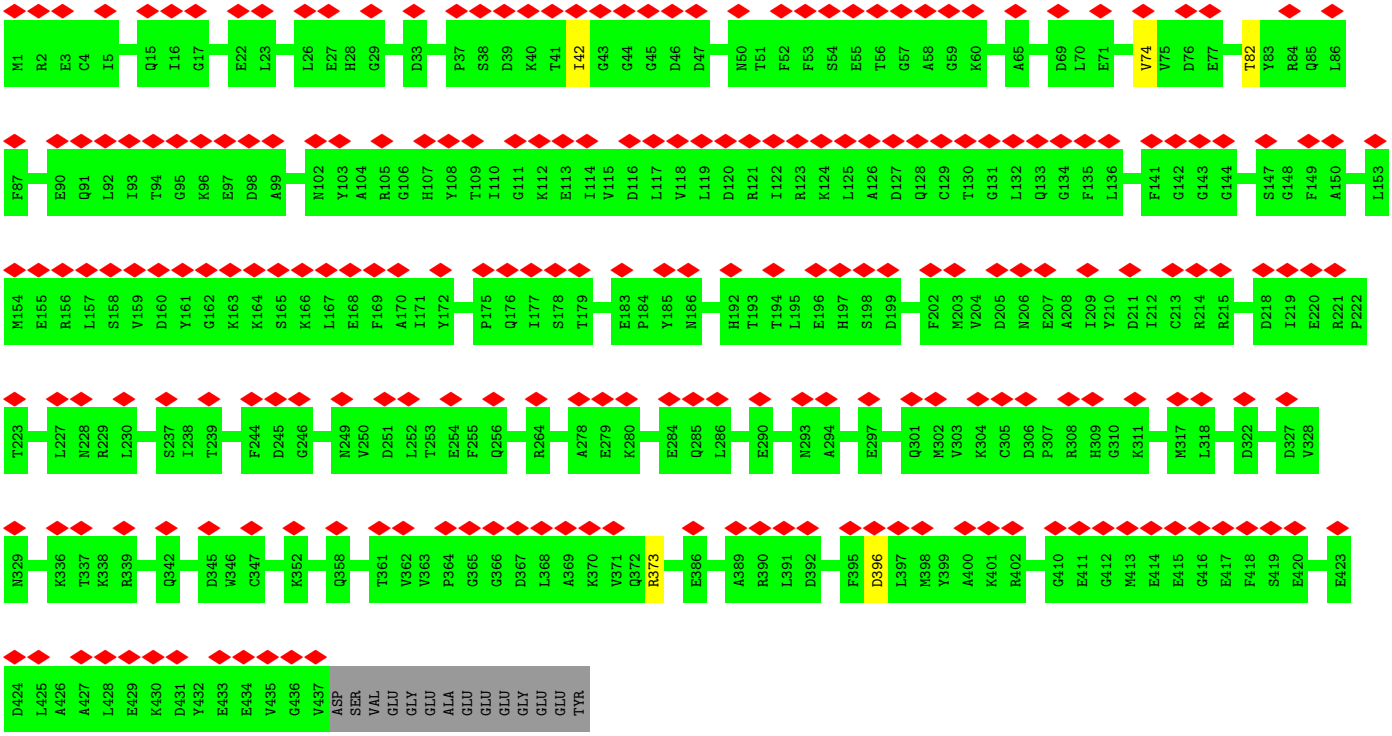




- Molecule 54: Tubulin alpha chain

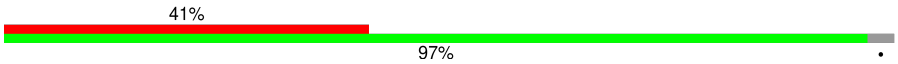
Chain VA:

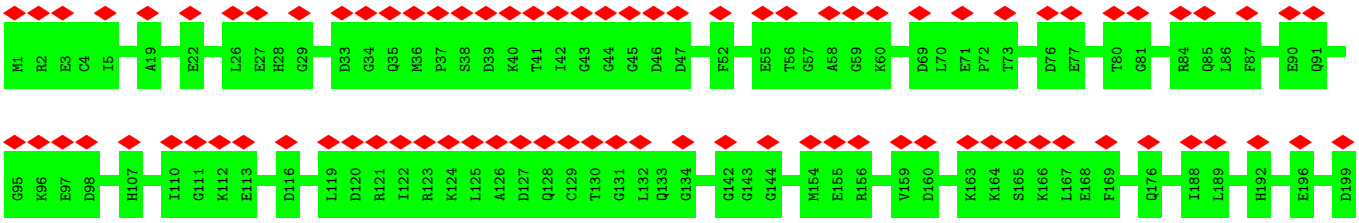


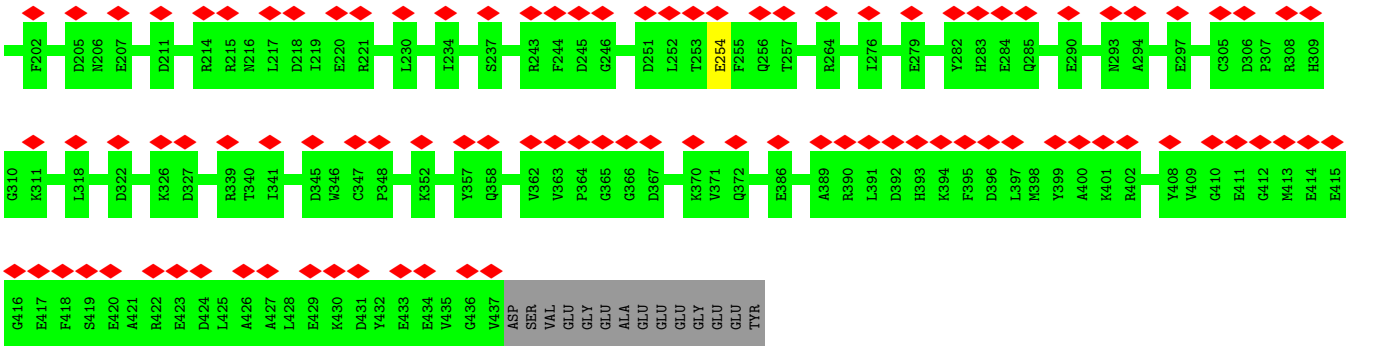


- Molecule 54: Tubulin alpha chain

Chain VB:

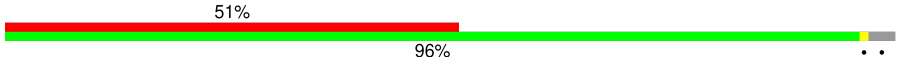


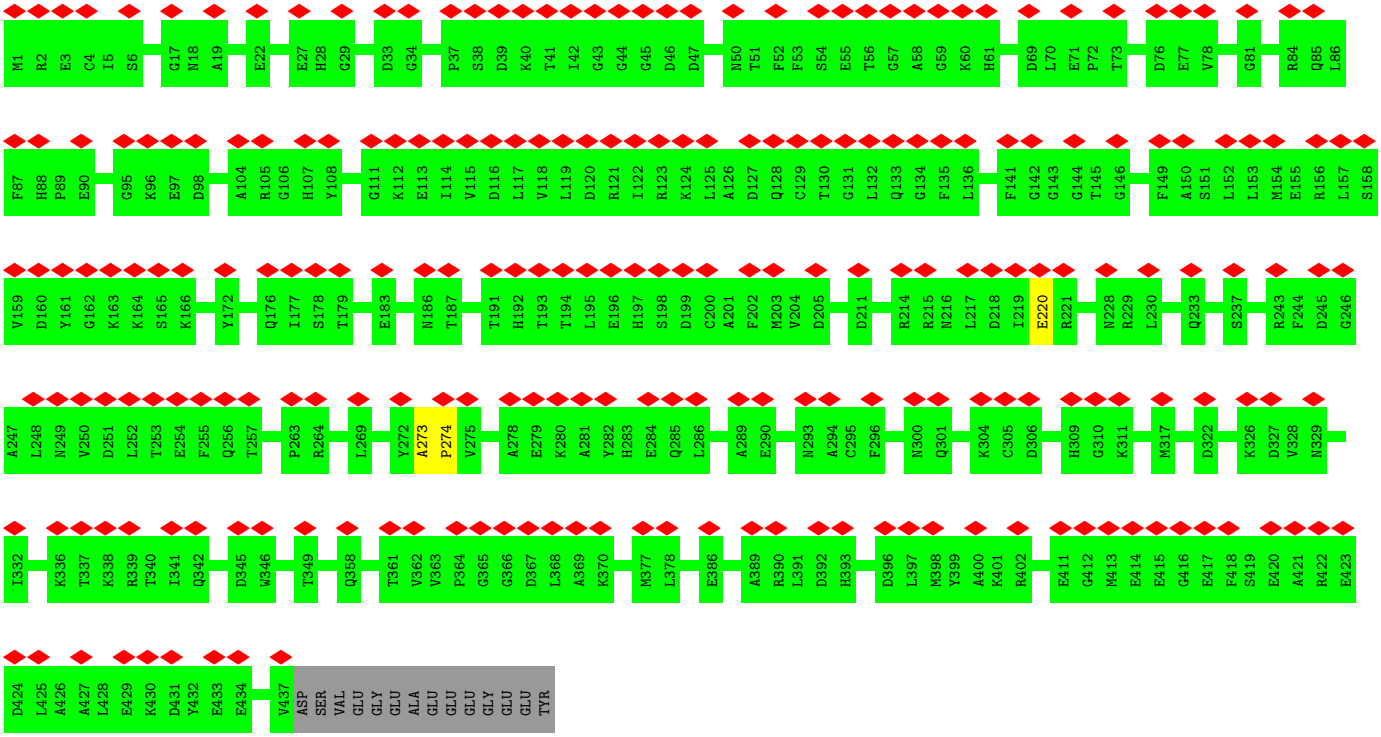




- Molecule 54: Tubulin alpha chain

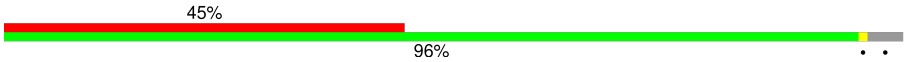
Chain VE:

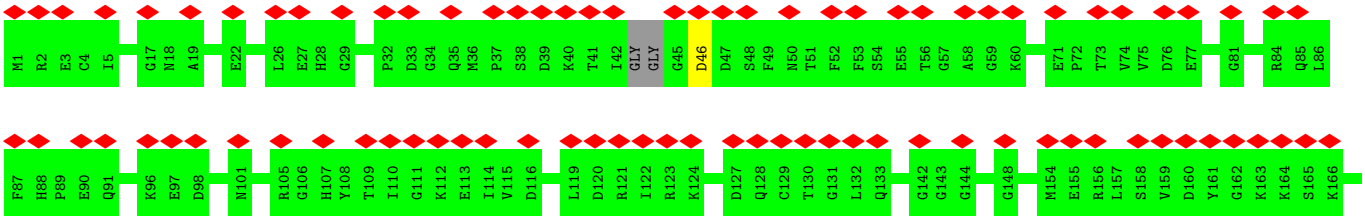


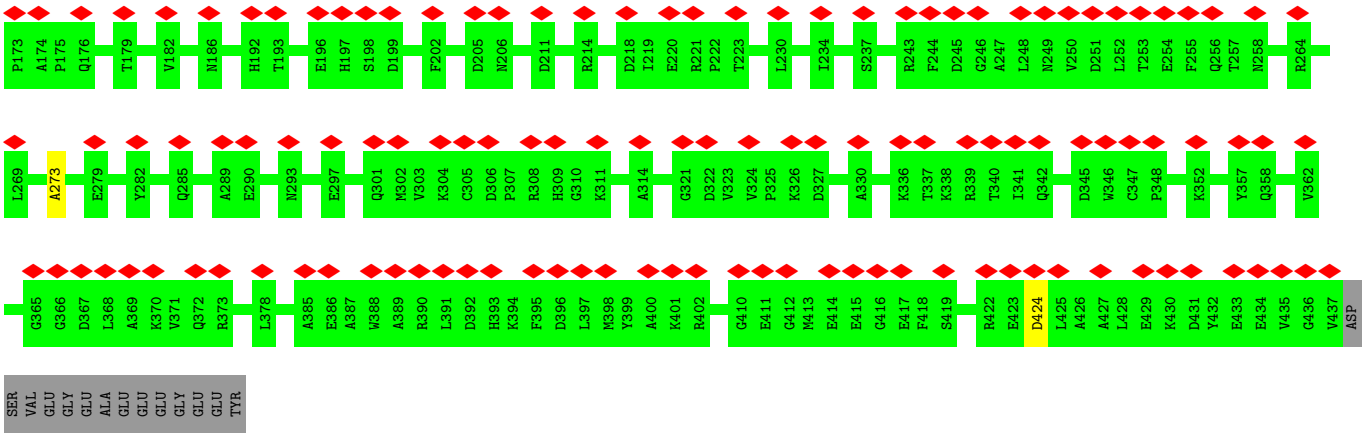


- Molecule 54: Tubulin alpha chain

Chain VG:

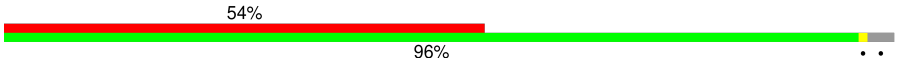


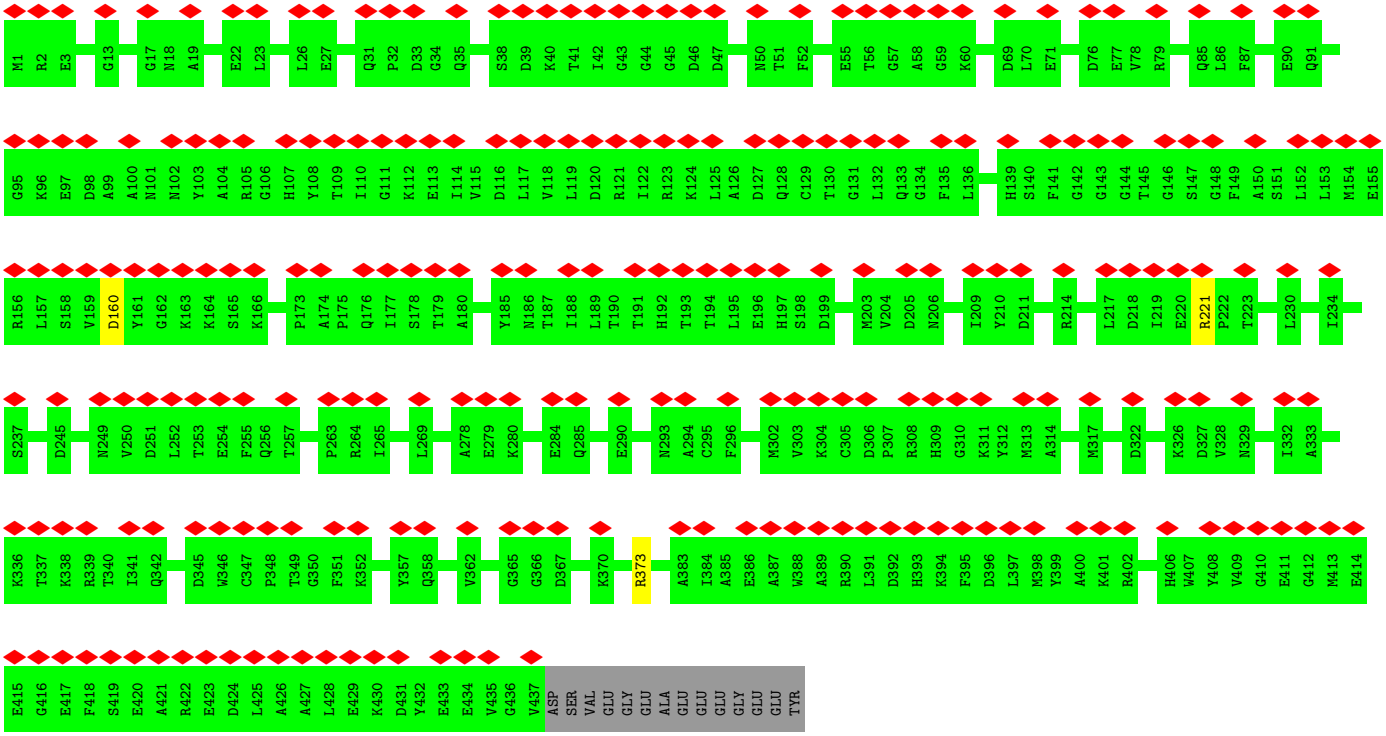




- Molecule 54: Tubulin alpha chain

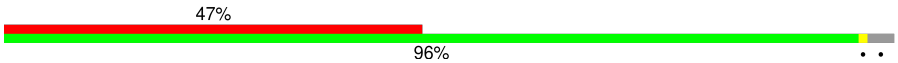
Chain VI:

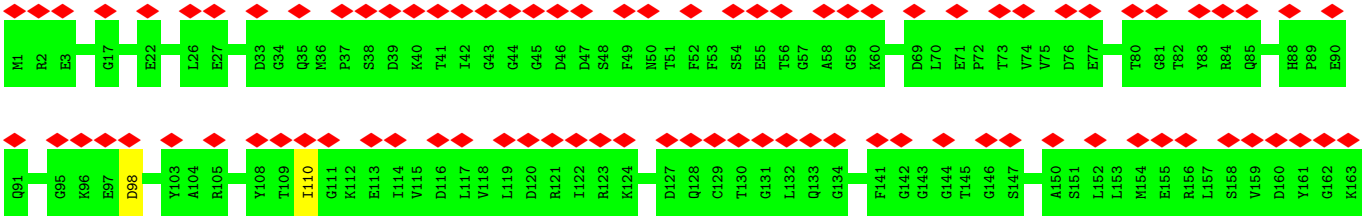




- Molecule 54: Tubulin alpha chain

Chain VK:





K164 S165 K166 L167 E168 F169 Y172 Q176 I177 S178 T179 E183 I188 H192 T193 T194 L195 E196 H197 S198 D199 M203 V204 D205 N206 D211 I212 C213 R214 R215 D218 I219 E220 R221 P222 T223 L230 D245 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258

R264 L269 A278 E279 K280 Q285 L286 E290 F296 E297 N300 Q301 M302 V303 K304 C305 D306 P307 R308 H309 G310 K311 Y312 M313 M317 D322 K326 D327 K336 T337 K338 R339 T340 I341 Q342 D345 W346 C347 P348 T349 G350 F351 K352 Y357 Q358 P364

G365 G366 D367 K370 V371 Q372 A385 E386 A387 W388 A389 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 A400 K401 R402 H406 W407 Y408 V409 G410 E411 G412 M413 E414 E415 G416 E417 F418 S419 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP

SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU TYR

- Molecule 54: Tubulin alpha chain

Chain WA: 44% 96%

M1 R2 E3 G17 N18 A19 E22 L26 D33 S38 D39 K40 T41 I42 G43 G44 G45 D46 D47 N50 E55 T56 G57 A58 G59 K60 F67 V68 D69 L70 E71 D76 E77 G81 T82 H88 P89 E90 K96 E97 D98 A99 I110 G111 K112 E113 I114

V115 D116 D120 R121 I122 R123 K124 L125 A126 D127 Q128 C129 Q133 G134 F135 F141 G142 L153 M154 E155 R156 L157 S158 V159 D160 Y161 G162 K163 K164 S165 K166 F169 A170 I171 Y172 P173 A174 P175 Q176 I177 S178 E183 H192 L195 E196 D199 F202 M203 V204 D205

N206 E207 R214 R215 N216 L217 D218 I219 E220 N226 I234 S237 A240 F244 D245 G246 N249 V250 D251 L252 T253 E254 F255 Q256 T257 R264 A273 I276 S277 A278 E279 Y282 H283 E284 Q285 L286 E290 N293 A294 C295 F296 E297 P298 A299 N300 Q301

K304 C305 D306 P307 R308 H309 G310 K311 Y312 M313 M317 D322 K326 D327 V328 N329 A330 A331 I332 A333 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 F351 K352 Y357 Q358 T361 V362 V363 P364 G365 G366 D367 L368 A369 K370 R373 M377 A385 E386 A387 W388

A389 R390 L391 D392 H393 K394 F395 D396 L397 K401 R402 A403 H406 E411 G412 M413 E414 E415 G416 E417 E420 A421 R422 E423 D424 L425 A426 A427 L428 E429 K430 D431 Y432 E433 E434 V435 G436 V437 ASP SER VAL GLU GLY GLU ALA GLU GLU GLU GLY GLU GLU GLU TYR

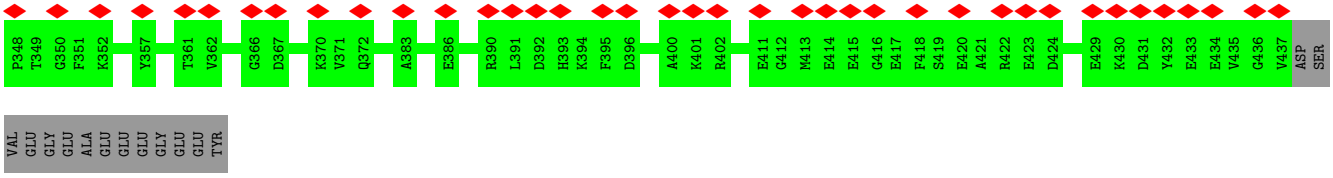
- Molecule 54: Tubulin alpha chain

Chain WB: 34% 96%

M1 R2 I5 G17 E22 L26 D33 M36 P37 S38 D39 K40 T41 I42 G43 GLY G45 D46 D47 S48 E55 T56 G57 A58 G59 K60 D69 L70 E71 P72 T73 D76 E77 R84 F87 H88 P89 E90 K96 E97 D98 K112 E113 D116 D120

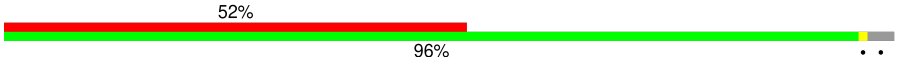
R121 I122 R123 D127 Q128 C129 Q133 F141 G142 M154 E155 R156 V159 K163 K164 S165 K166 F169 P175 Q176 I177 S178 I188 E196 H197 S198 D199 D205 N206 E207 R214 L217 D218 I219 E220 R221 D245 G246 N249 V250 D251 L252 T253 E254

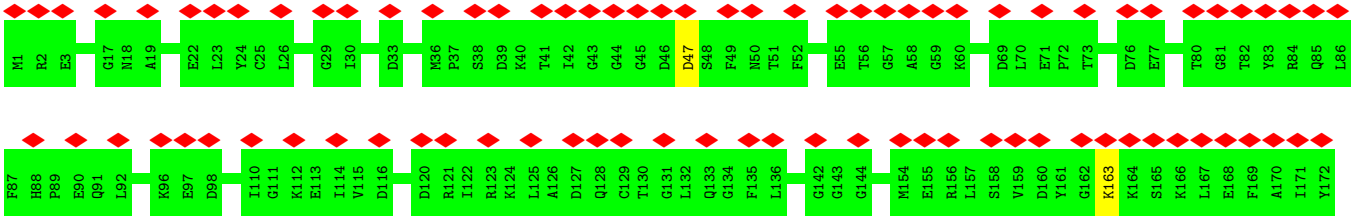
P261 Y262 P263 R264 A273 P274 A278 E279 K280 A281 Y282 H283 E284 Q285 L286 A289 E290 N293 F296 E297 N300 K304 C305 D306 P307 R308 H309 G310 K311 M317 D322 V323 V324 P325 K326 D327 A331 I332 A333 K336 T337 K338 R339 T340 I341 Q342 D345



• Molecule 54: Tubulin alpha chain

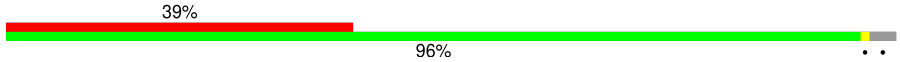
Chain WE:

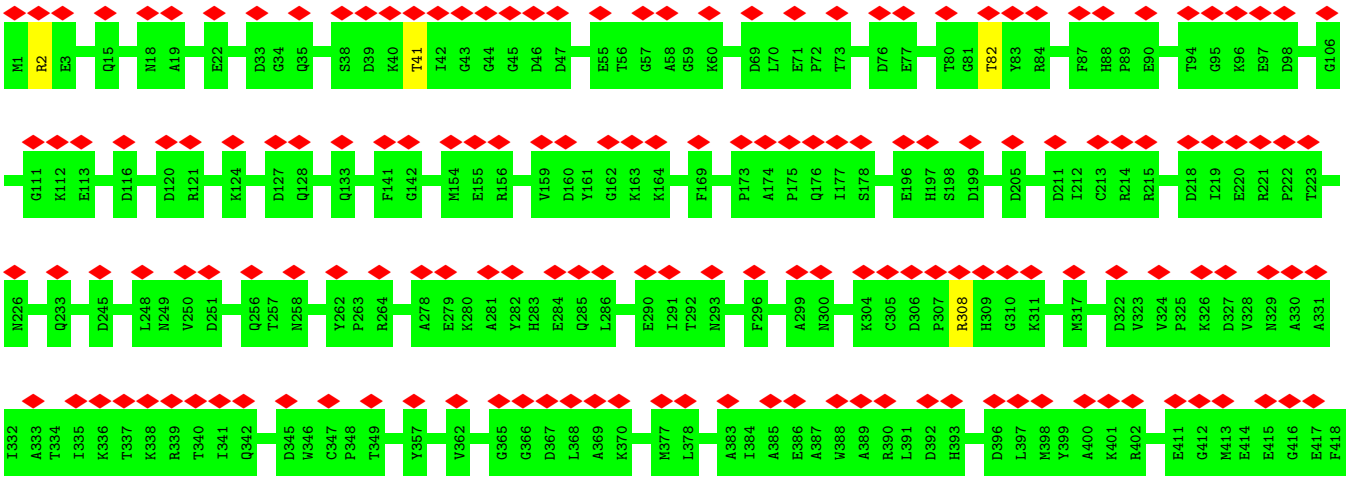


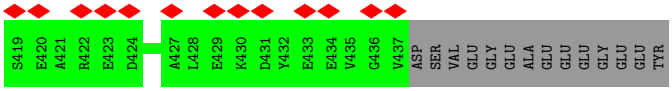


• Molecule 54: Tubulin alpha chain

Chain WG:

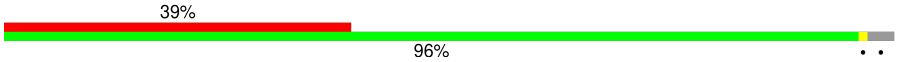


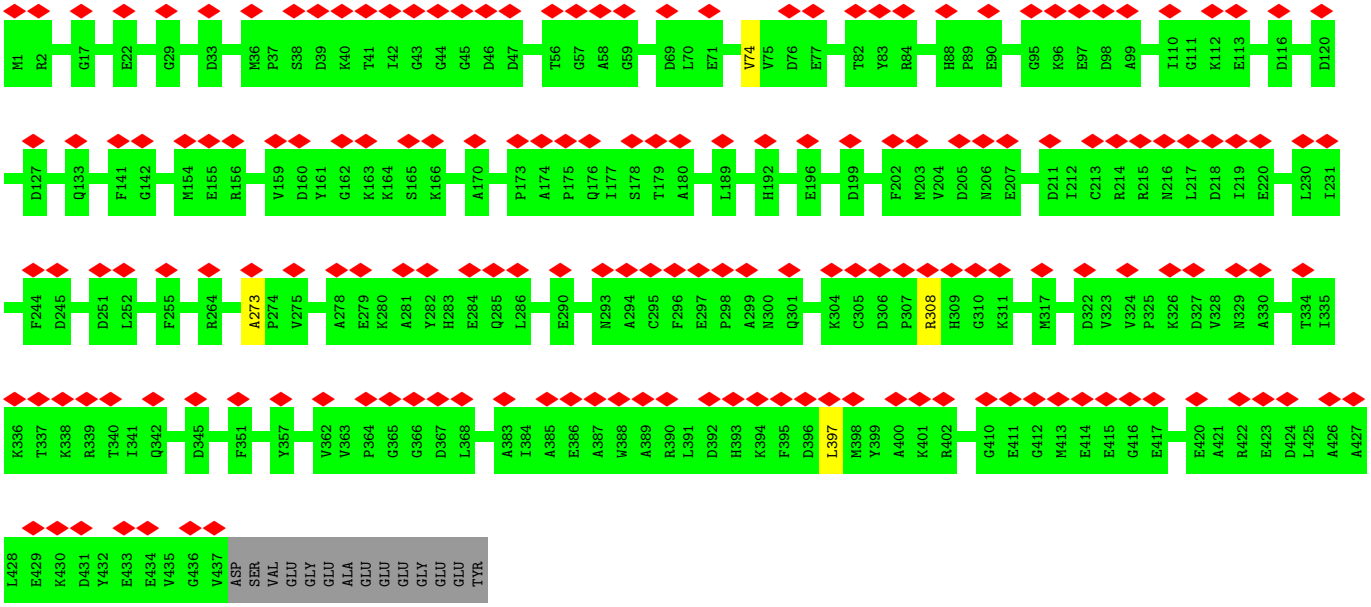




• Molecule 54: Tubulin alpha chain

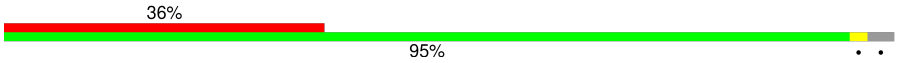
Chain WI:

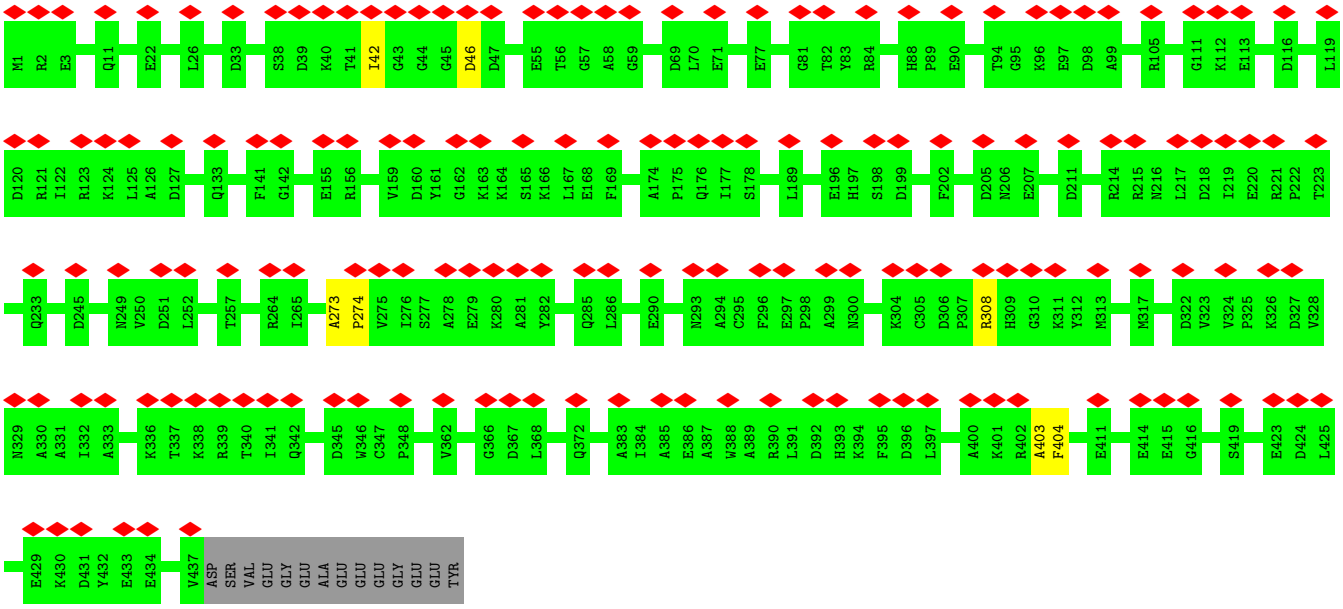




• Molecule 54: Tubulin alpha chain

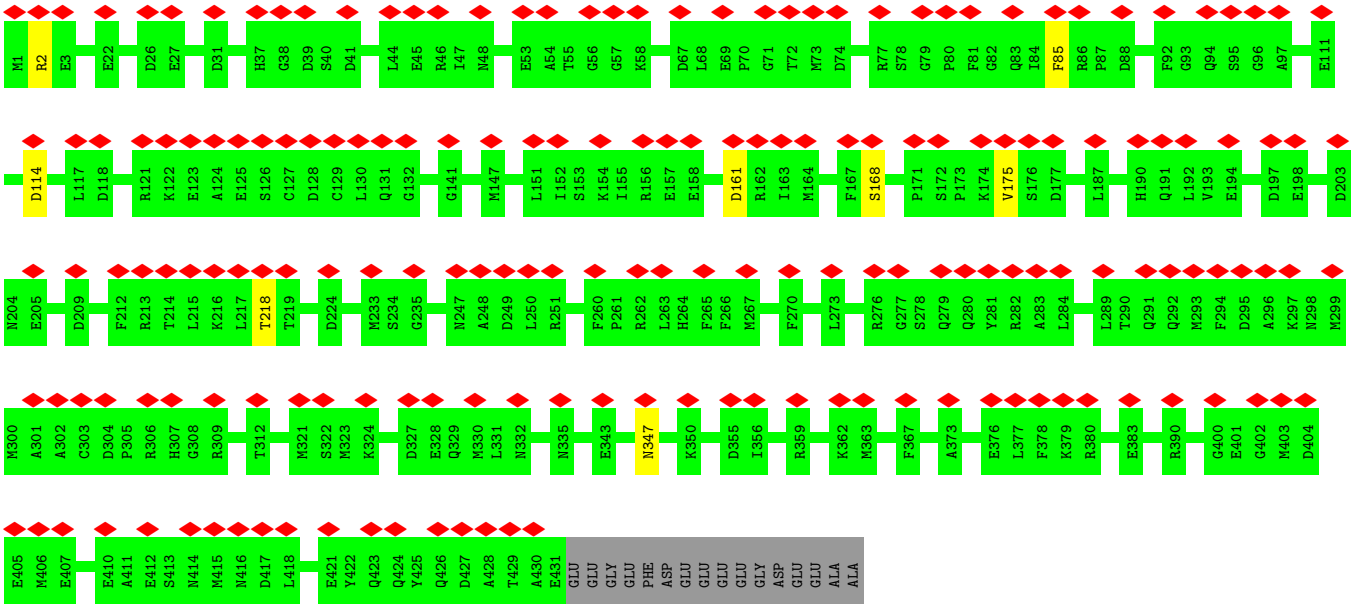
Chain WK:





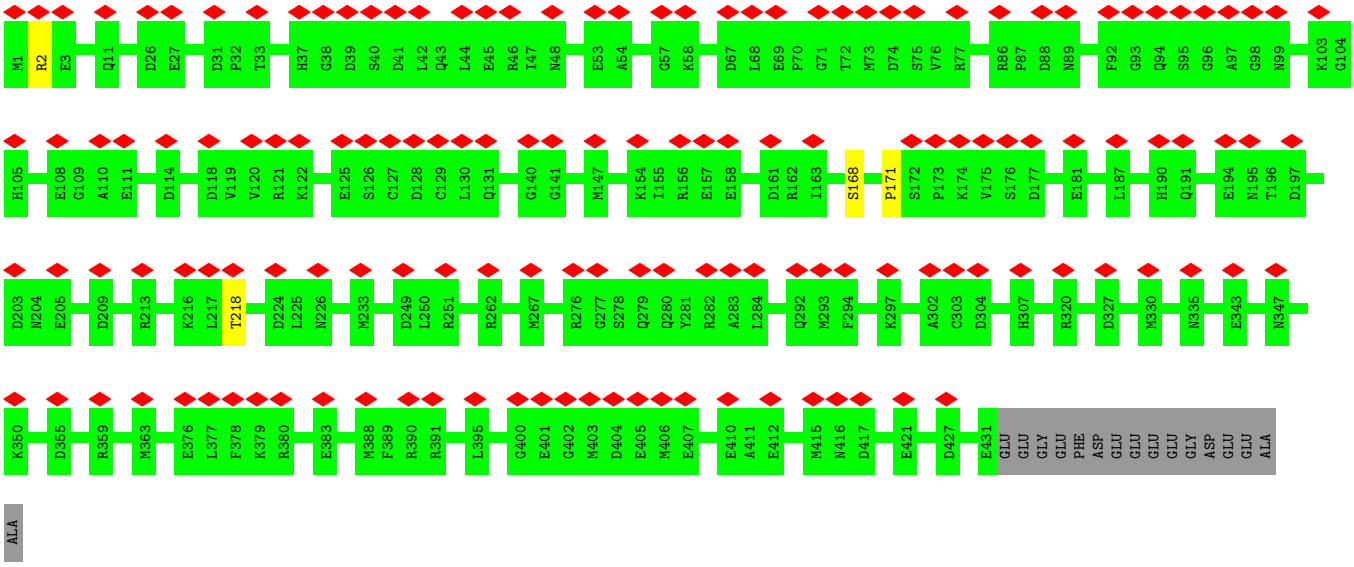
• Molecule 55: Tubulin beta chain

Chain AC: 40% 95%



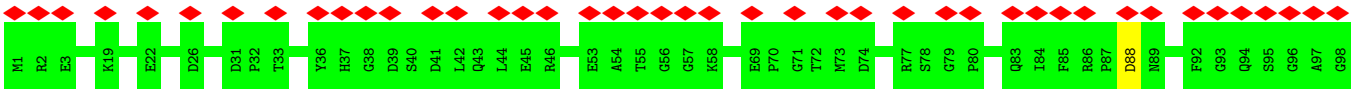
- Molecule 55: Tubulin beta chain

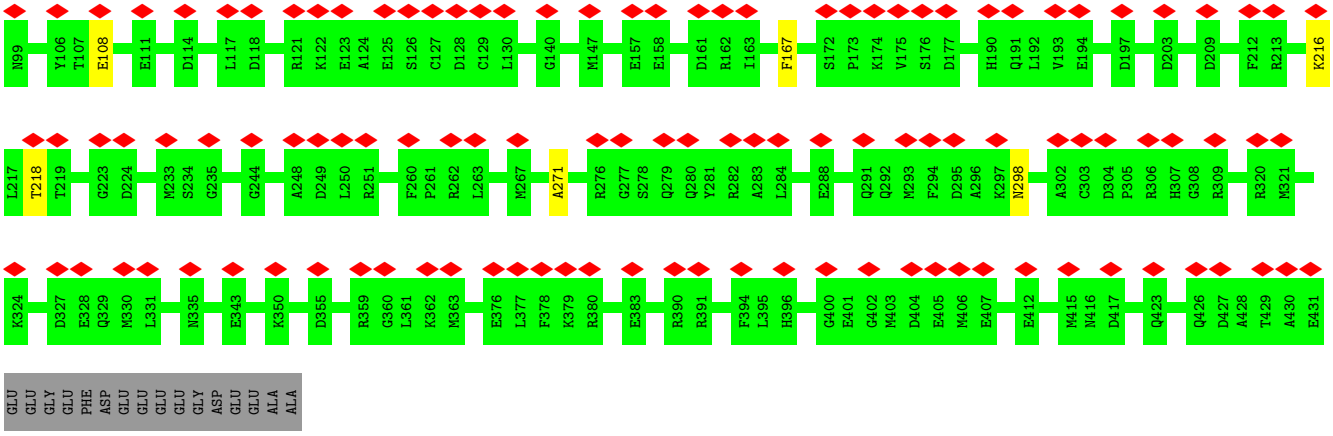
Chain AD: 32% 96%



- Molecule 55: Tubulin beta chain

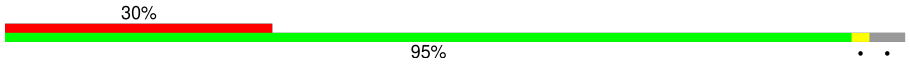
Chain AF: 35% 95%

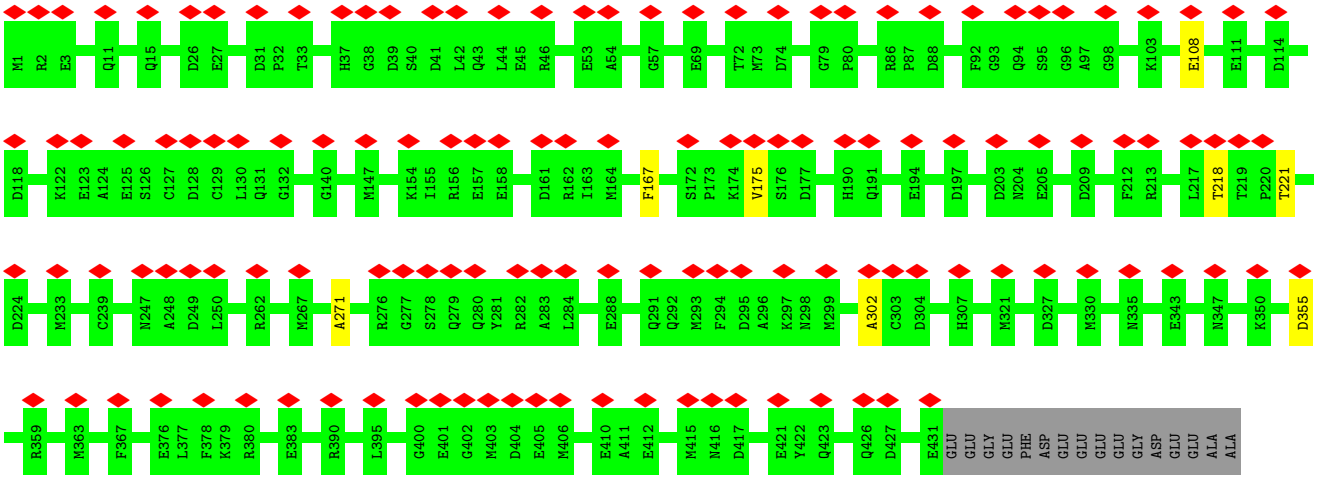




- Molecule 55: Tubulin beta chain

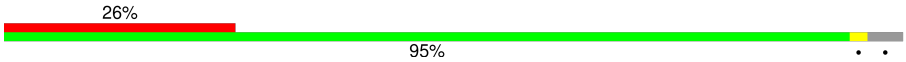
Chain AH:

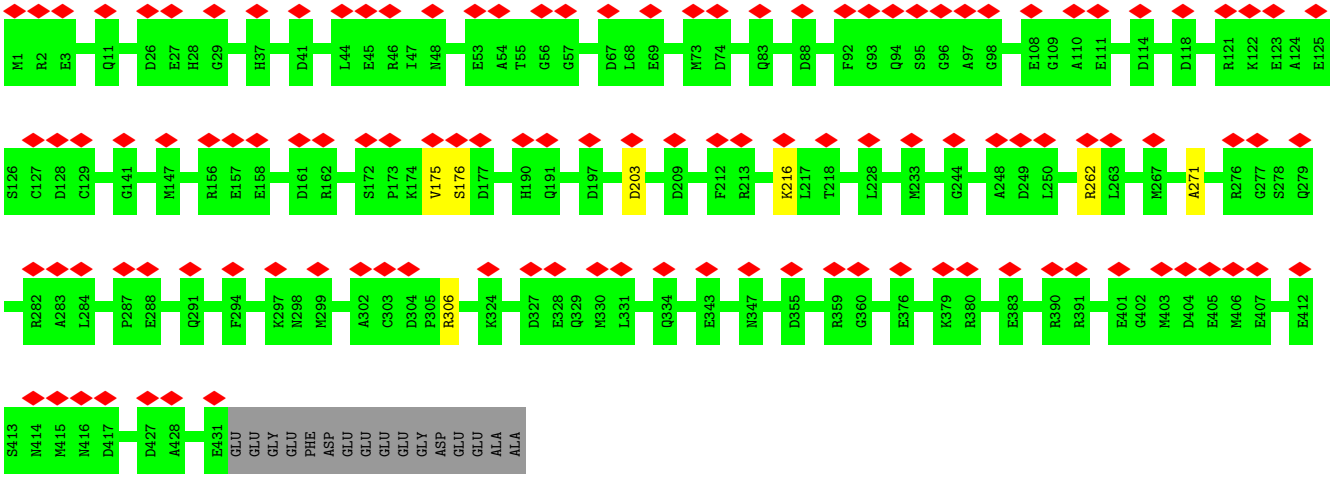




- Molecule 55: Tubulin beta chain

Chain AJ:





- Molecule 55: Tubulin beta chain

Chain AL: 31% 95%

M1 R2 E3 Q11 Q15 D26 E27 D31 P32 T33 H37 G38 D39 S40 D41 E45 A54 T55 G56 G57 D67 L68 E69 P70 G71 T72 M73 D74 R77 P80 Q83 I84 F85 R86 N89 G93 Q94 S95 G96 A97 G98 K103 Y106 T107 E108

G109 A110 E111 L112 V113 D114 L117 D118 R121 K122 E125 S126 C127 D128 C129 H137 G141 G146 M147 K154 I155 R156 E157 E158 D161 R162 P171 S172 P173 K174 V175 S176 D177 L187 H190 Q191 D197 D203 N204 E205 D209 F212 R213 T218

L225 T237 D249 L250 R251 K252 R262 L263 A271 R276 G277 S278 Q279 Q280 Y281 R282 A283 L284 T285 M293 F294 D295 A296 K297 N298 A301 A302 C303 D304 P305 R306 R318 G319 R320 M321 S322 E325 V326 D327 E328 L331 N332 N335 E343 N347

K350 D355 I356 R359 G360 L361 K362 E376 R380 E383 F389 R390 R391 G400 E401 G402 M403 D404 E405 M406 E407 E410 A411 E412 S413 N414 M415 N416 D417 D427 A428 E431 GLU GLU GLY GLU PHE ASP GLU GLU GLU GLU GLY ASP GLU GLU ALA ALA

- Molecule 55: Tubulin beta chain

Chain BC: 41% 95%

M1 R2 H6 Q11 I16 D26 D31 H37 G38 D39 S40 D41 E45 R46 E53 A54 T55 G56 G57 D67 L68 E69 P70 G71 T72 M73 D74 R77 S78 G79 R86 P87 D88 N89 G93 Q94 S95 G96 A97 G98 N99 N100 W101 A102 K103 G104 H105 Y106

T107 E108 G109 A110 E111 D114 L117 D118 R121 K122 E123 A124 E125 S126 C127 D128 C129 L130 Q131 G132 F133 G140 G141 G142 T143 G144 S145 G146 M147 L151 I152 S153 K154 I155 R156 E157 E158 Y159 P160 D161 R162 I163 F167 K174 V175 S176 D177 T178 V179 V180 E181 V189

E194 N195 T196 D197 E198 D203 N204 E205 Y208 D209 F212 R213 L217 T218 T219 P220 T221 Y222 G223 D224 M233 Q245 L246 N247 A248 D249 L250 R251 K252 F260 P261 R262 M267 Q279 Q280 Y281 R282 A283 L284 E288 Q291 Q292 M293 F294 D295 A296 K297

A302 C303 D304 P305 R306 H307 G308 R309 R318 G319 R320 M321 S322 M323 K324 E325 V326 D327 E328 Q329 M330 L331 N332 N335 S339 Y340 E343 V349 K350 D355 I356 R359 G360 L361 K362 M363 E376 K379 R380 E383 A387 R390 R391 K392 L395 H396

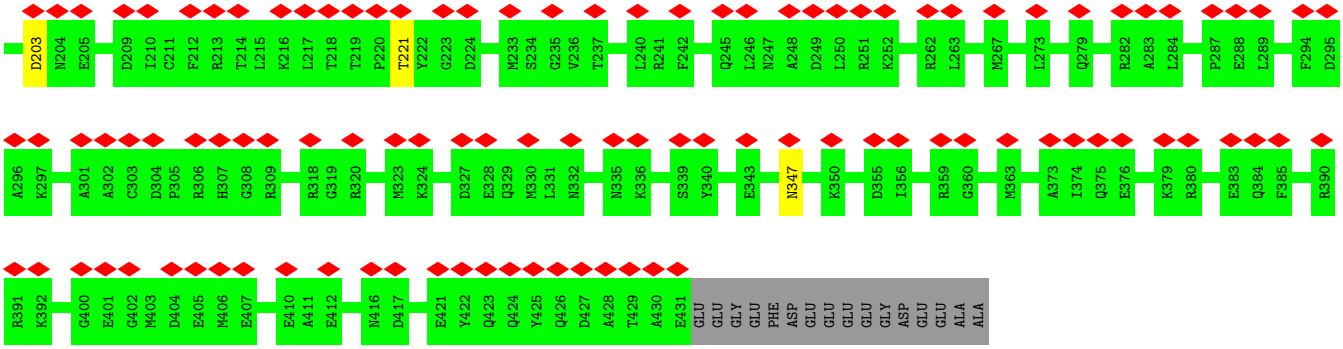
G400 E401 G402 M403 D404 E405 M406 E407 F408 T409 E410 A411 E412 M415 N416 D417 Q423 Q424 Y425 Q426 D427 A428 T429 A430 E431 GLU GLU GLY GLU PHE ASP GLU GLU GLU GLY ASP GLU GLU ALA ALA

- Molecule 55: Tubulin beta chain

Chain BD: 42% 95%

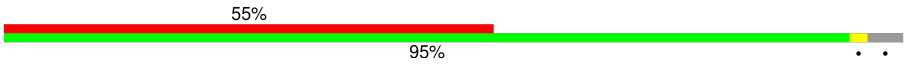
M1 R2 E3 H6 Q11 Q15 K19 E22 D26 G29 I30 D31 P32 T33 H37 G38 D39 S40 D41 L42 Q43 L44 E45 R46 E53 G56 G57 D67 L68 E69 P70 G71 D74 S75 G79 P80 F81 R86 P87 D88 N89 Q94 S95 G96 A97

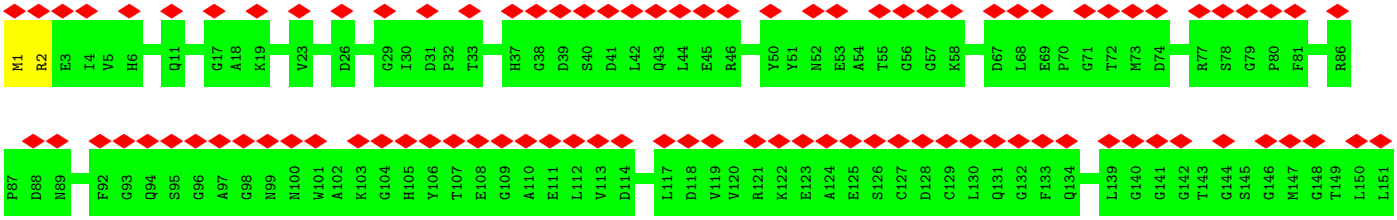
G98 N99 K103 E108 D114 D118 R121 K122 E123 A124 E125 S126 C127 D128 C129 L130 Q131 G132 F133 G140 G141 G142 S145 I152 R156 E157 E158 Y159 P160 D161 R162 I163 M164 N165 S172 P173 K174 V175 S176 D177 H190 Q191 L192 V193 E194 N195 T196 D197 E198

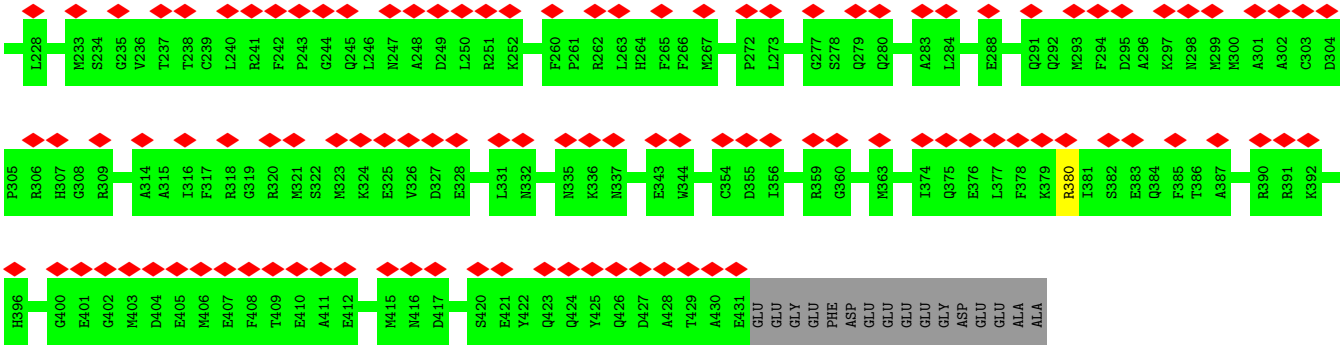


- Molecule 55: Tubulin beta chain

Chain BF:

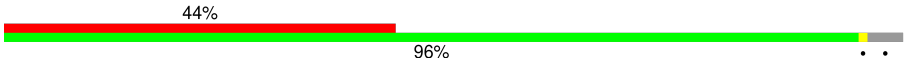


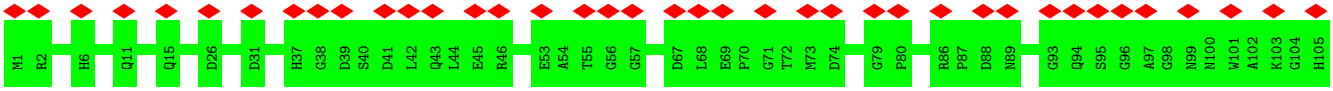


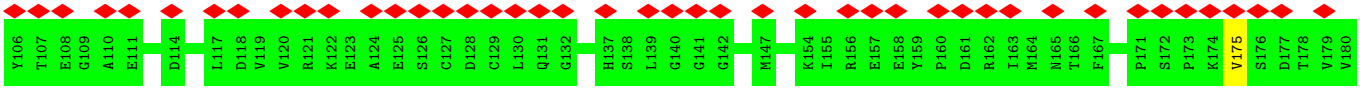


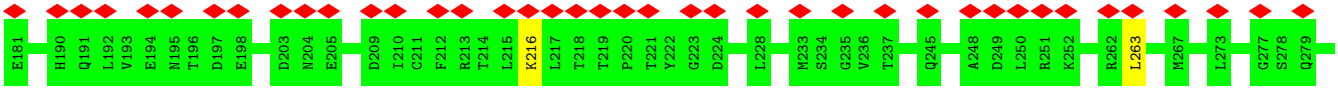
- Molecule 55: Tubulin beta chain

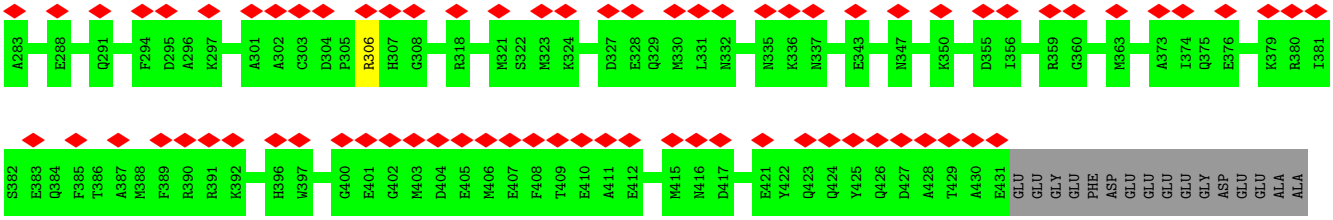
Chain BH:





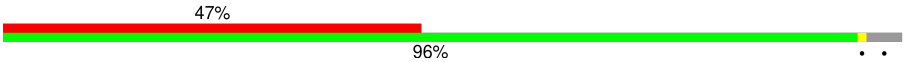






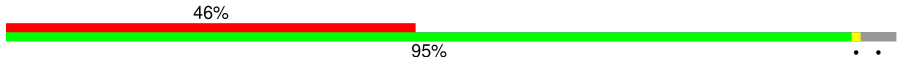
- Molecule 55: Tubulin beta chain

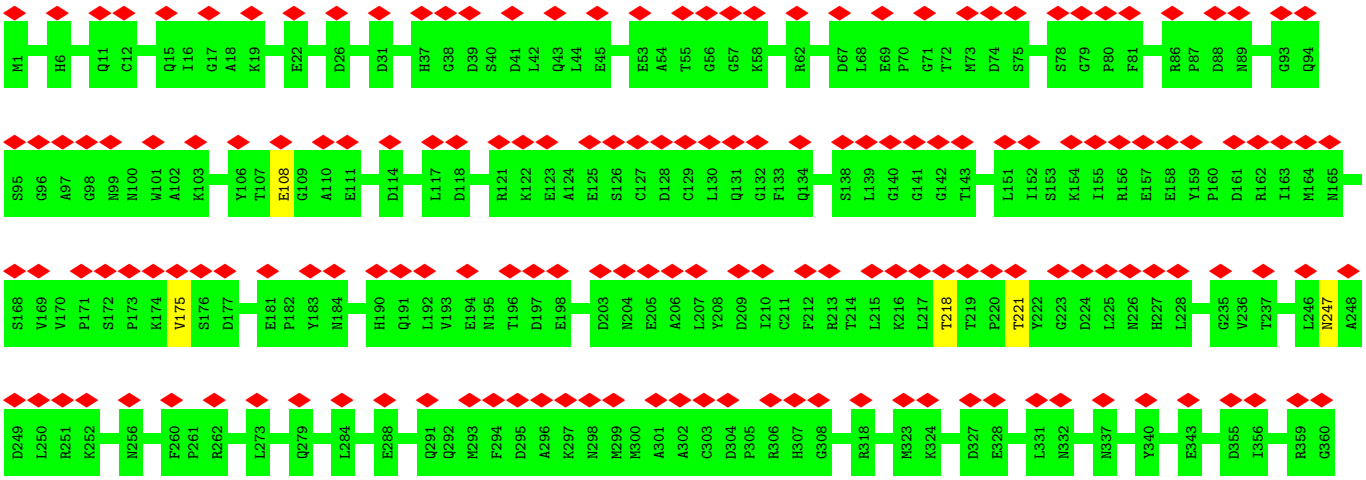
Chain BJ:

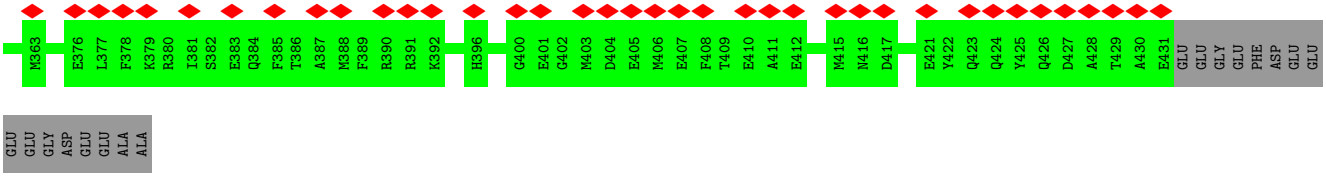


- Molecule 55: Tubulin beta chain

Chain BL:

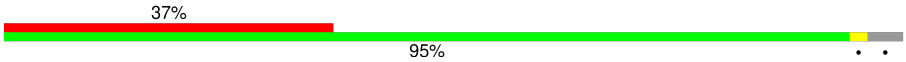


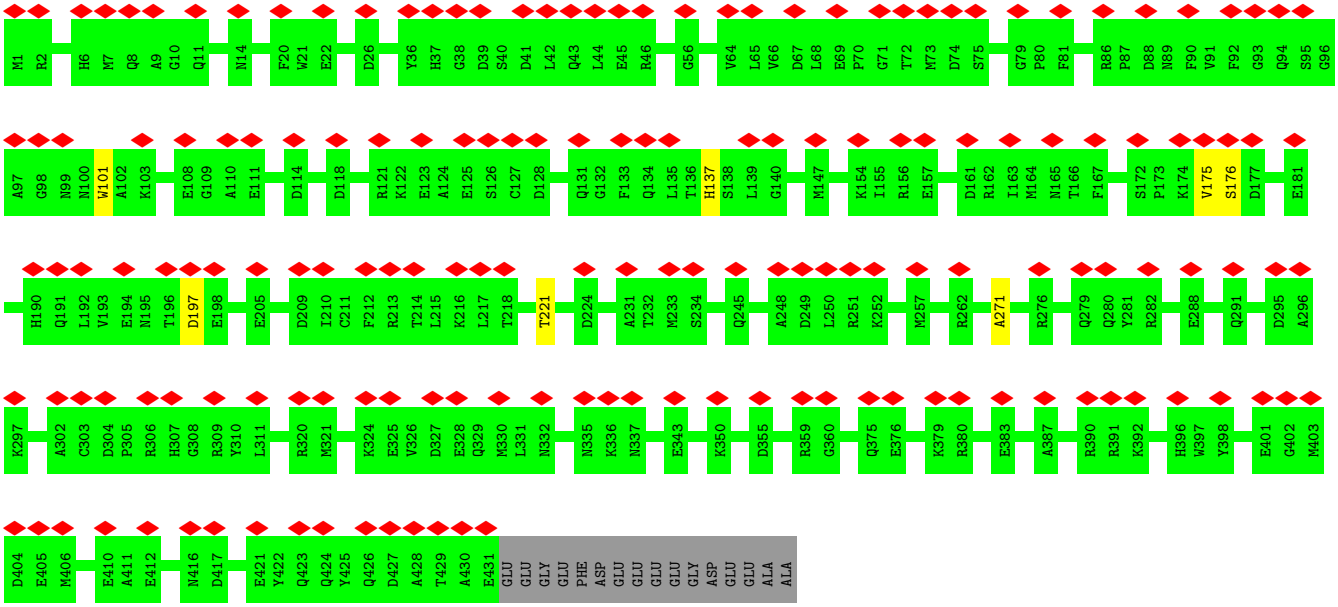




• Molecule 55: Tubulin beta chain

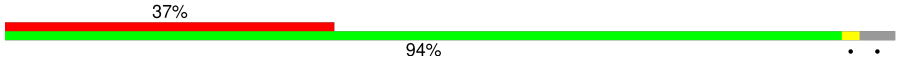
Chain CC:

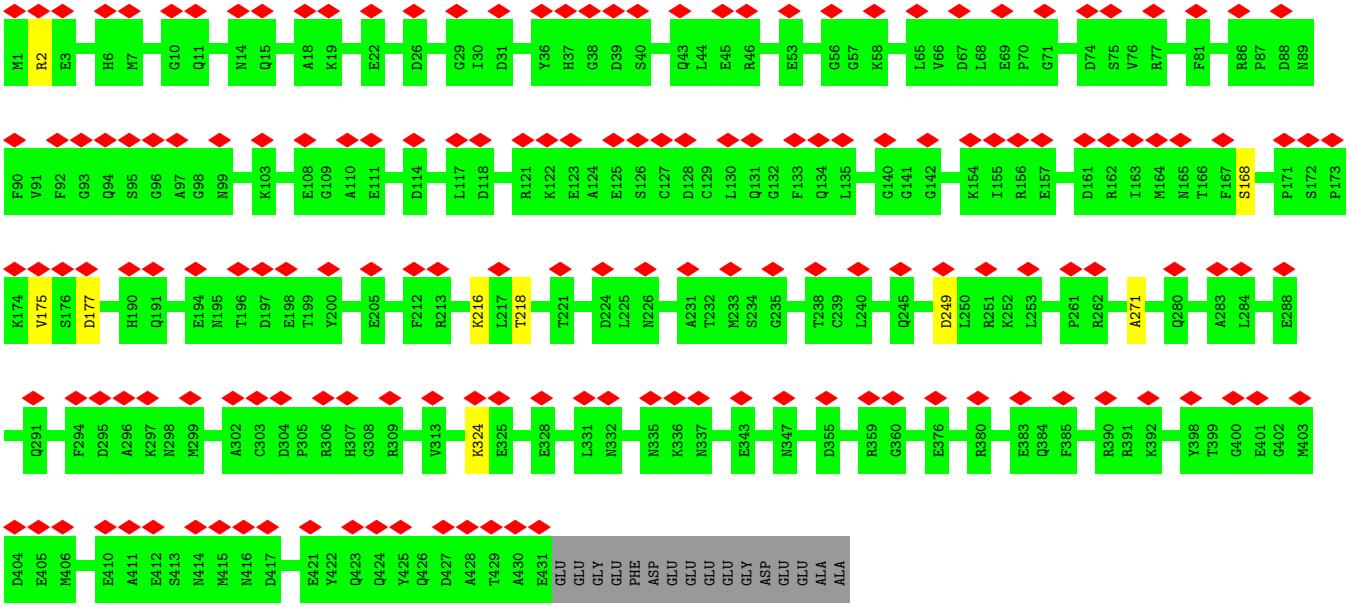




• Molecule 55: Tubulin beta chain

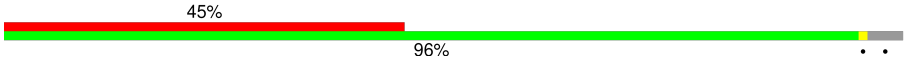
Chain CD:

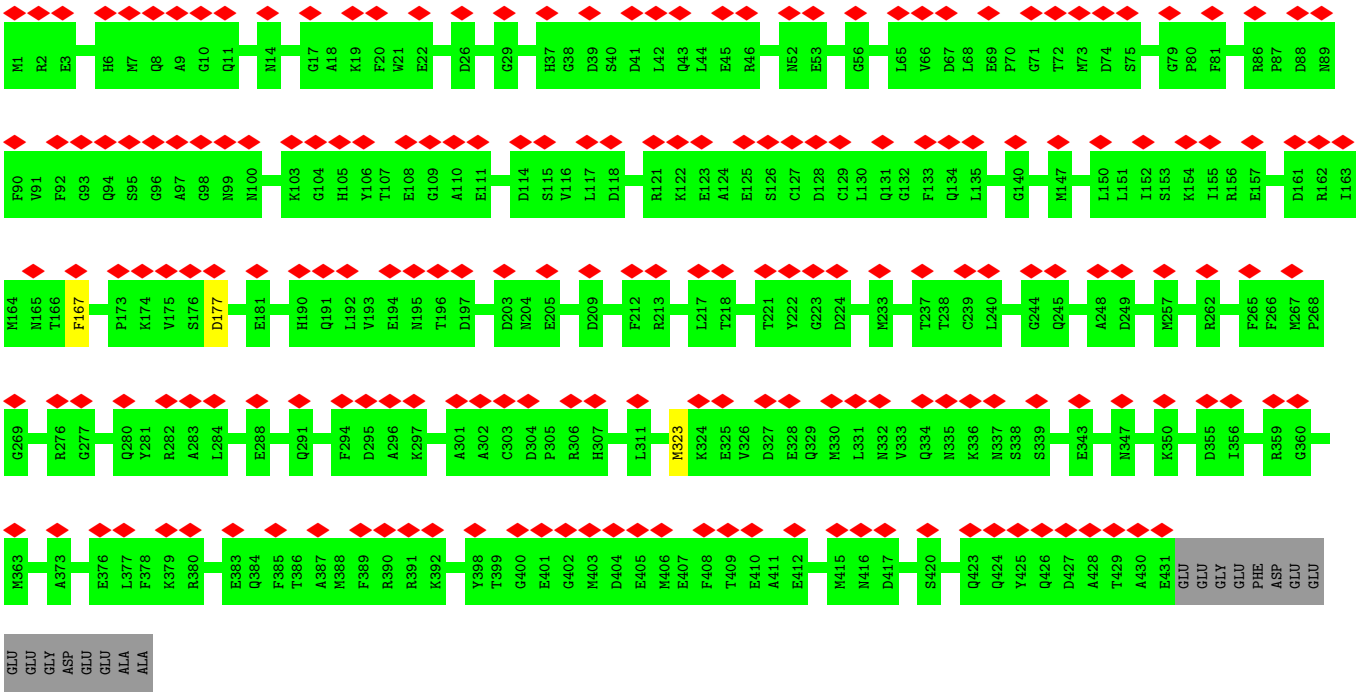




• Molecule 55: Tubulin beta chain

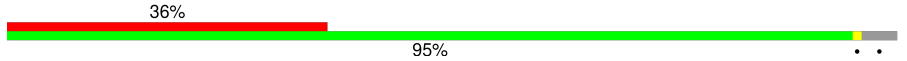
Chain CF:





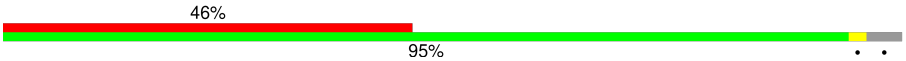
• Molecule 55: Tubulin beta chain

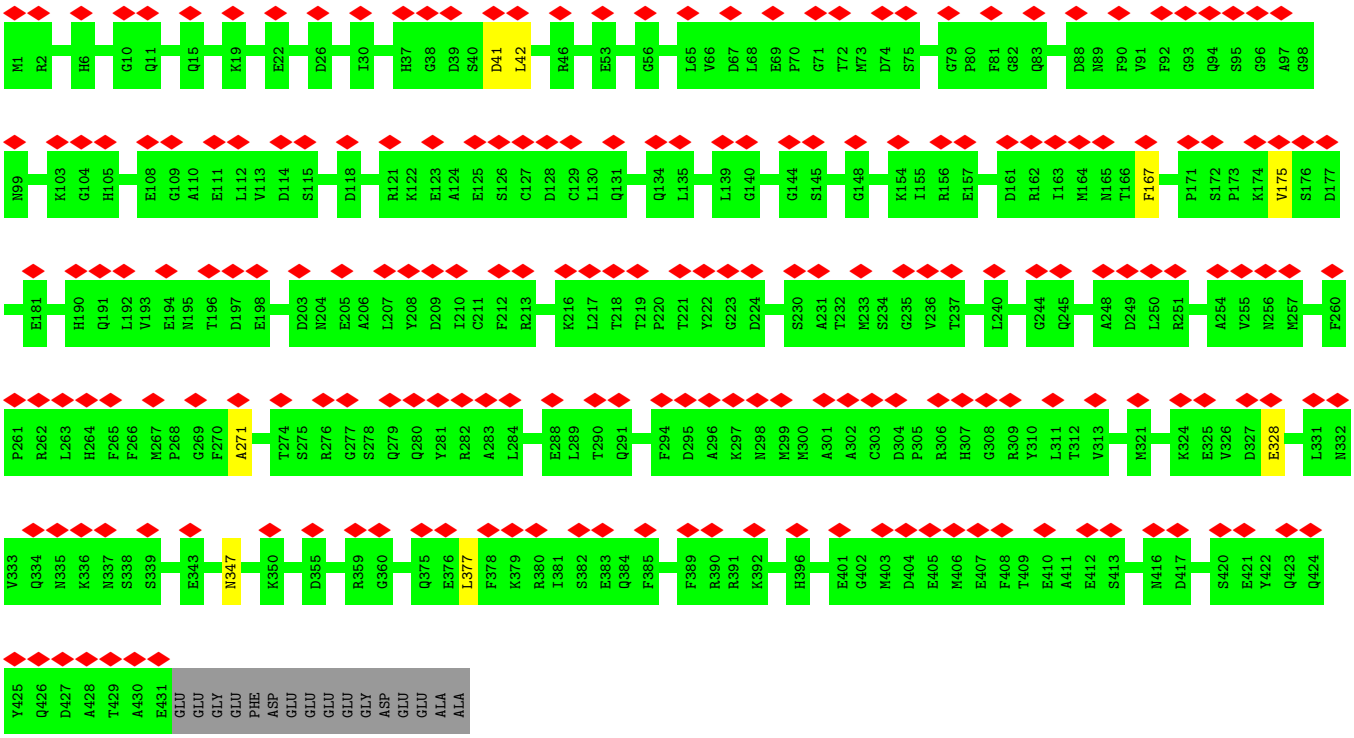
Chain CH:



• Molecule 55: Tubulin beta chain

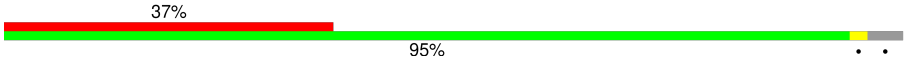
Chain CJ:

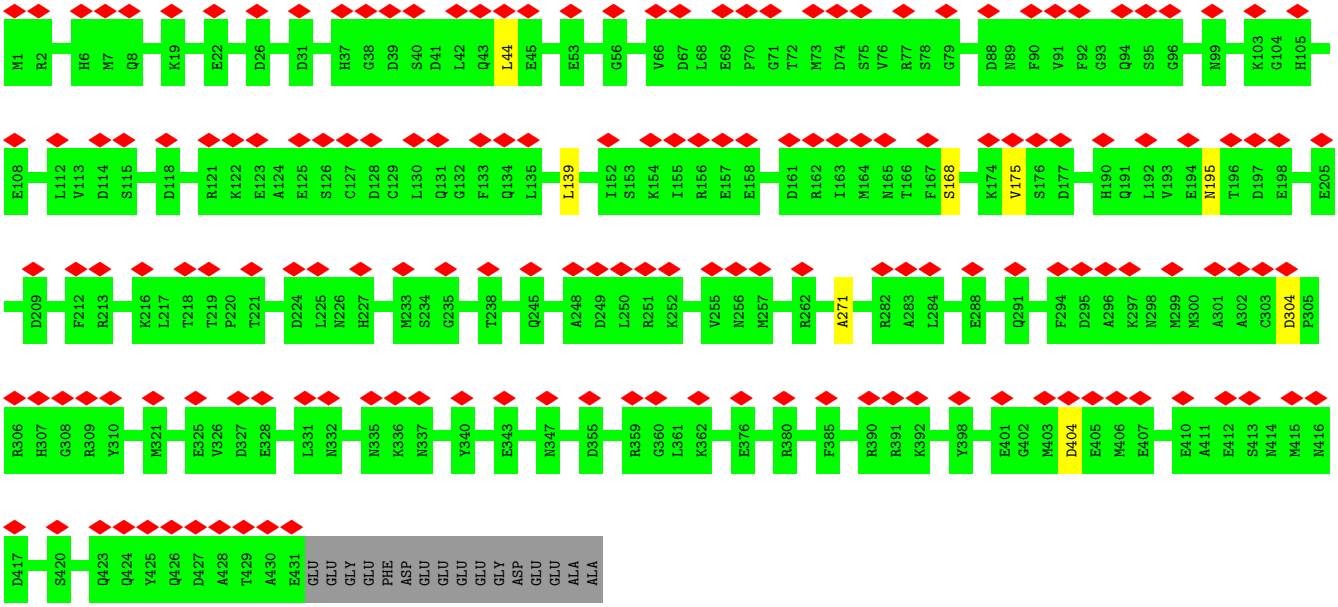




- Molecule 55: Tubulin beta chain

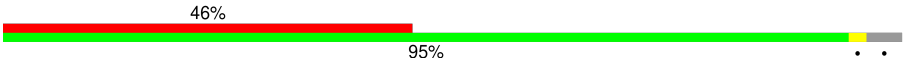
Chain CL:

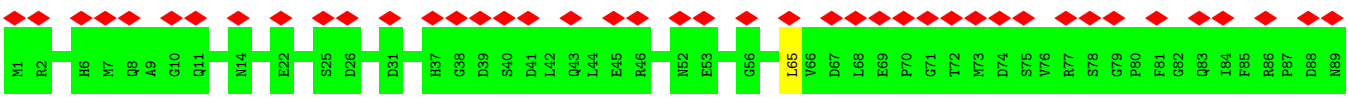


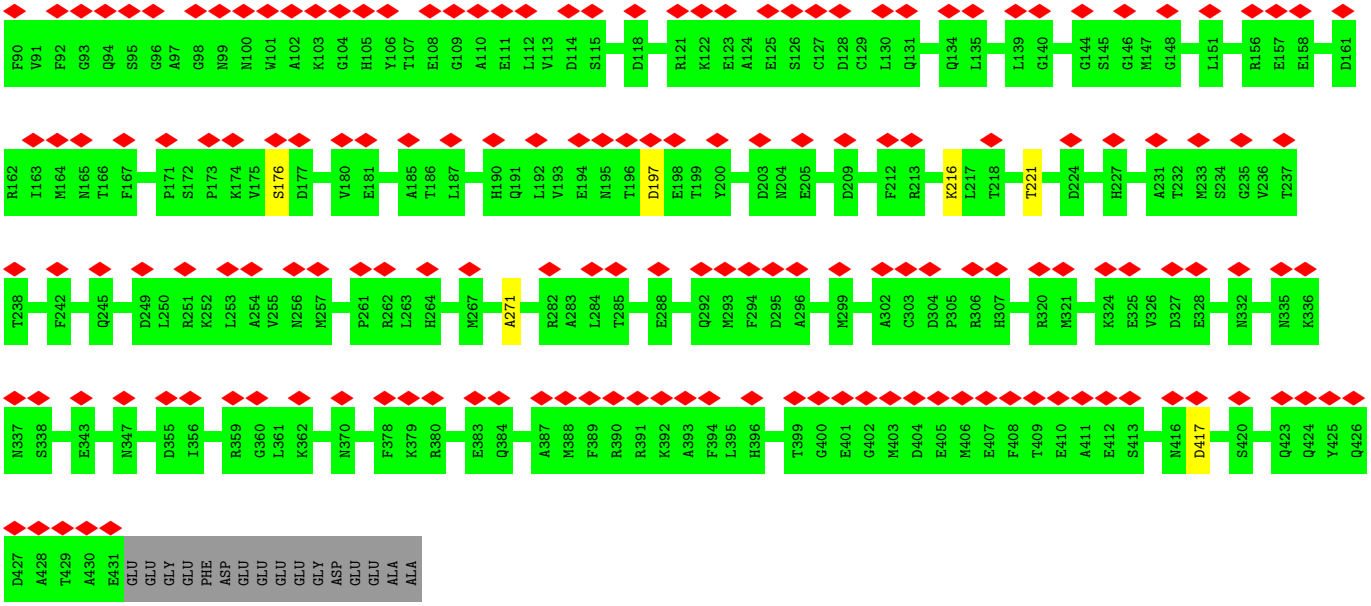


- Molecule 55: Tubulin beta chain

Chain DC:

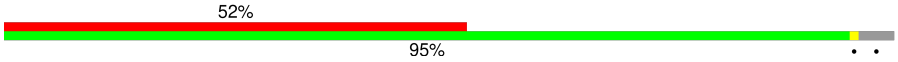


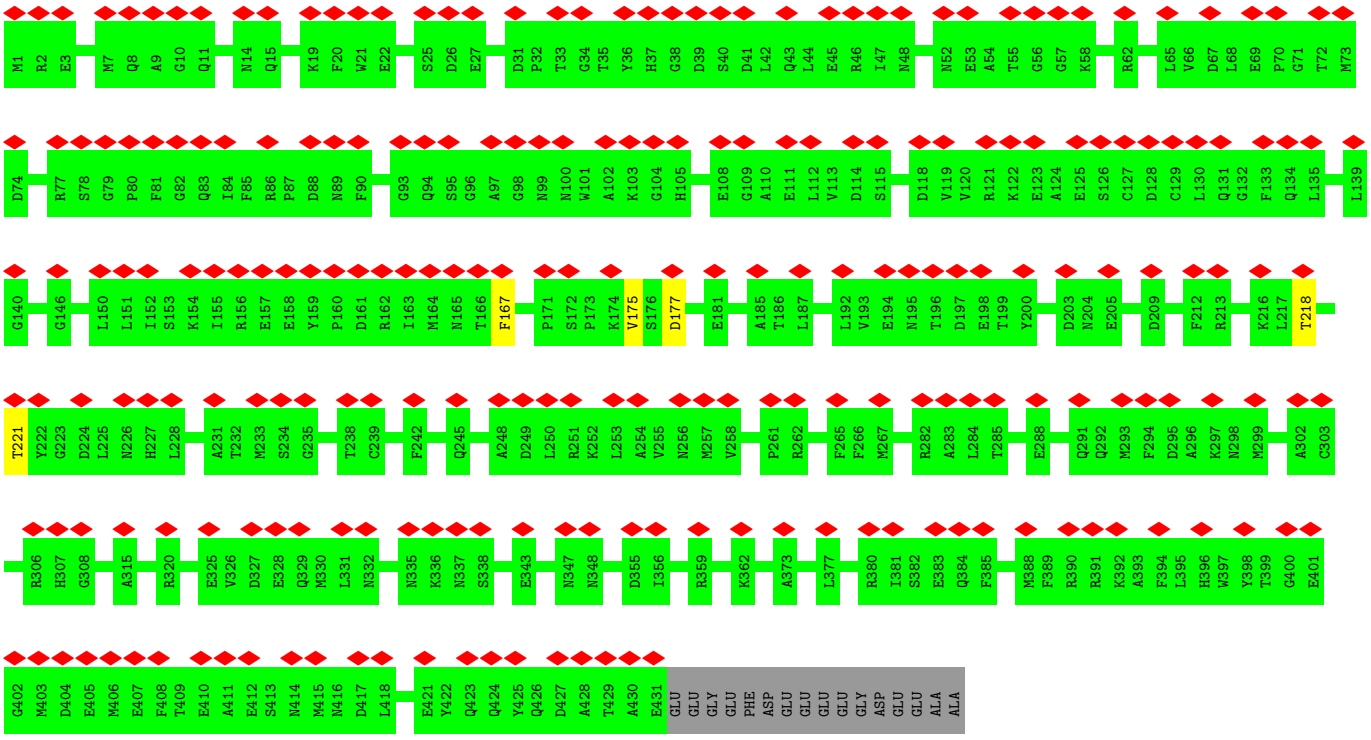




- Molecule 55: Tubulin beta chain

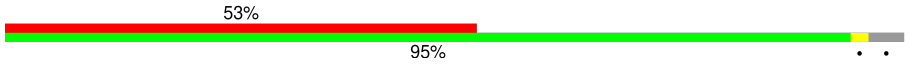
Chain DD:

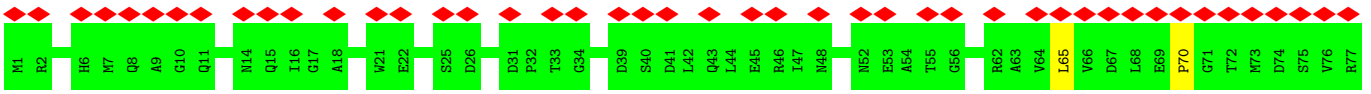




- Molecule 55: Tubulin beta chain

Chain DF:





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L139 G140 G141 G142 G148 L151 K154 I155 R156 E157 E158 Y159 P160 D161 R162 I163 M164 N165 T166 F167 S168 P171 S172 P173 K174 V175 S176 D177 E181 A185 T186 L187 S188 V189 H190 Q191 L192 V193 E194 N195 T196 D197 E198 T199 Y200 C201 I202 D203 N204 E205 A206 D209 I210

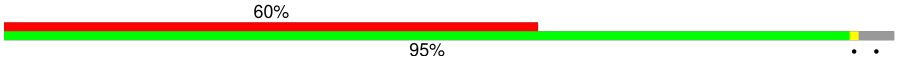
C211 F212 R213 K216 L217 T218 T221 Y222 G223 D224 L225 N226 H227 A231 T232 M233 T238 N247 A248 D249 L250 R251 K252 L253 A254 V255 N256 M257 P261 R262 L263 H264 F265 R276 Q280 Y281 R282 T285 E288 Q291 Q292 M293 F294 D295 A296 K297 N298 M299

A302 C303 D304 P305 R306 H307 G308 R309 Y310 L311 R318 G319 R320 M321 K324 E325 V326 D327 E328 N332 N335 K336 N337 S338 E343 N347 D355 R359 G360 L361 K362 I368 G369 N370 A373 E376 L377 F378 K379 R380 E383 A387 R390 R391 K392

L395 T399 G400 E401 G402 M403 D404 E405 M406 E407 F408 T409 E410 A411 E412 S413 N414 M415 N416 D417 L418 V419 S420 E421 Y422 Q423 Q424 Y425 Q426 D427 A428 T429 A430 E431 GLU GLU GLY GLU PHE ASP GLU GLU GLU GLU GLY ASP GLU GLU ALA ALA

- Molecule 55: Tubulin beta chain

Chain DH:



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R86 P87 D88 N89 F90 V91 F92 G93 Q94 S95 G96 A97 G98 N99 N100 W101 A102 K103 G104 H105 Y106 T107 E108 G109 A110 E111 L112 V113 D114 S115 V116 L117 D118 V119 V120 R121 K122 E123 A124 E125 S126 C127 D128 C129 L130 Q131 G132 F133 Q134 L135 T136 H137 S138 L139 G140 G141 G142 T143 G144 S145

G146 M147 G148 T149 L150 L151 I152 S153 K154 I155 R156 E157 E158 Y159 P160 D161 R162 I163 M164 N165 T166 F167 P171 S172 P173 K174 V175 S176 D177 T178 E181 A185 T186 L187 S188 V189 H190 Q191 L192 V193 E194 N195 T196 D197 E198 T199 Y200 D203 N204 E205 A206 L207 Y208 D209 F212

R213 K216 L217 T218 T221 Y222 G223 D224 L225 N226 H227 M233 S234 G235 T238 C239 N247 A248 D249 L250 R251 K252 L253 A254 V255 N256 M257 P261 R262 F265 F266 M267 P268 G269 F270 A271 G277 R282 A283 Q291 Q292 M293 F294 D295 A296 K297 A301 A302 C303

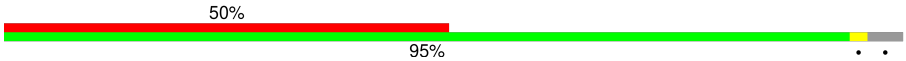
D304 P305 R306 H307 G308 R309 Y310 L311 A315 R320 M321 E325 V326 D327 E328 Q329 M330 L331 M332 N335 K336 N337 S338 F341 V342 E343 P346 M347 D355 R359 K362 I368 G369 N370 S371 T372 A373 I374 Q375 E376 L377 F378 K379 R380 I381 S382 E383 Q384 F385 T386

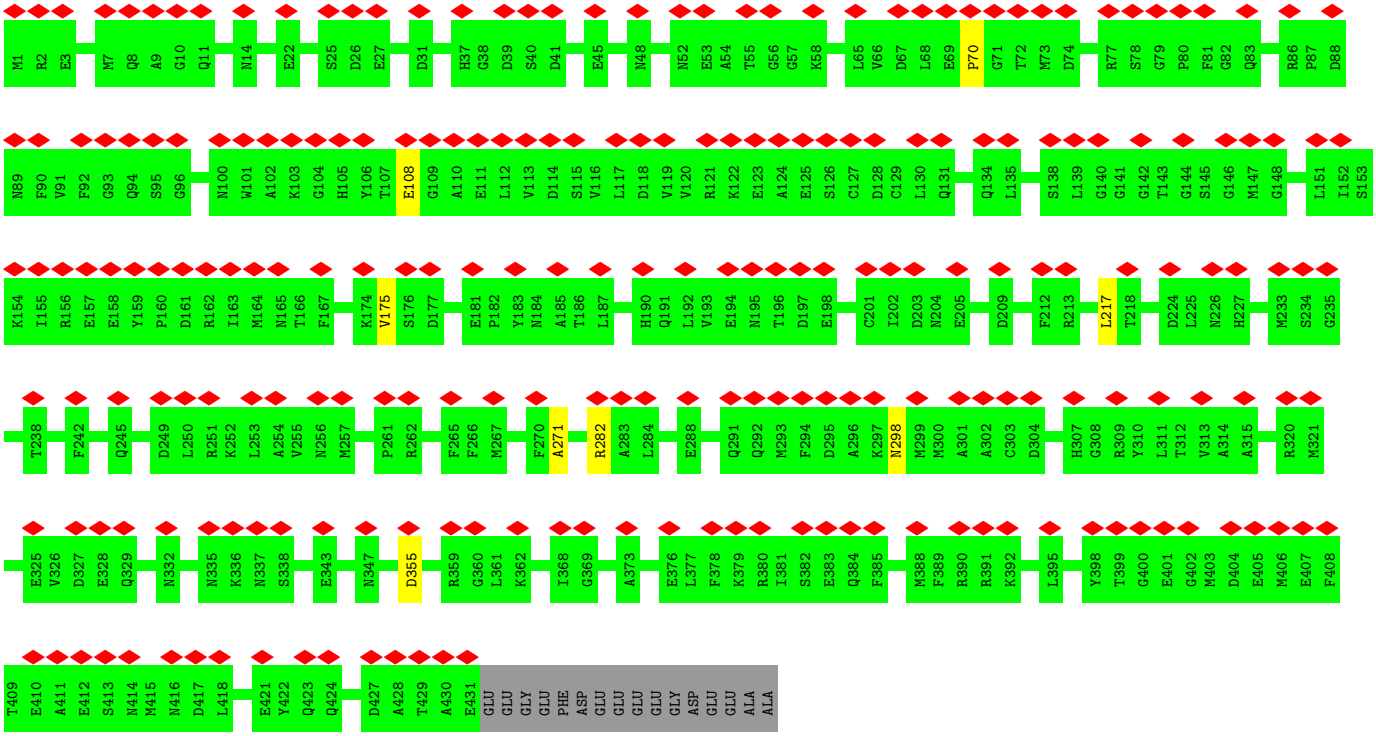
A387 M388 F389 R390 R391 K392 A393 F394 L395 H396 W397 Y398 T399 G400 E401 G402 M403 D404 E405 M406 E407 F408 T409 E410 A411 E412 S413 N414 M415 N416 D417 L418 V419 S420 E421 Y422 Q423 Q424 Y425 Q426 D427 A428 T429 A430 E431 GLU GLU GLY GLU PHE ASP GLU GLU GLU GLU GLY ASP GLU GLU ALA

ALA

- Molecule 55: Tubulin beta chain

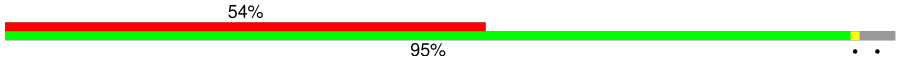
Chain DJ:

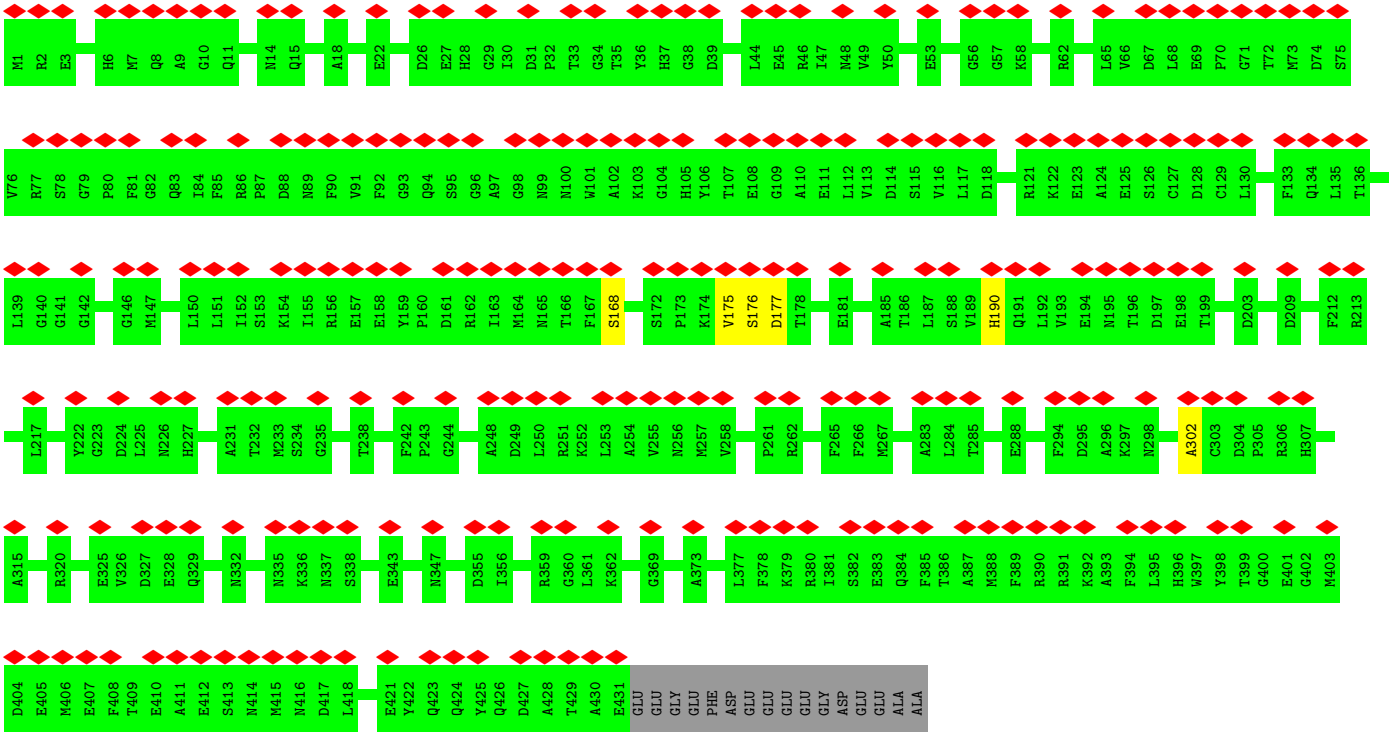




- Molecule 55: Tubulin beta chain

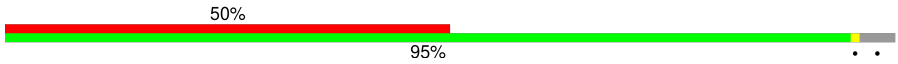
Chain DL:

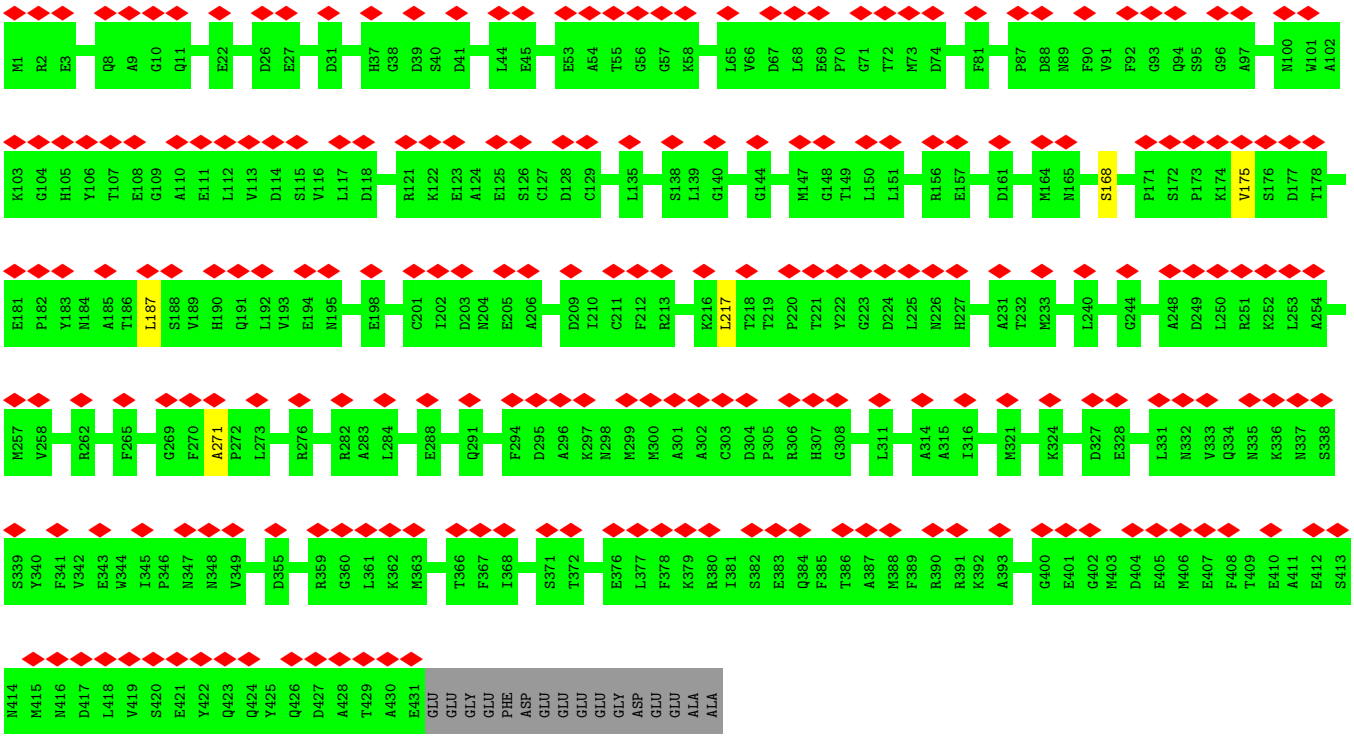




- Molecule 55: Tubulin beta chain

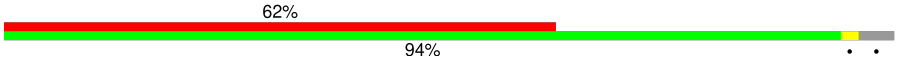
Chain EB:

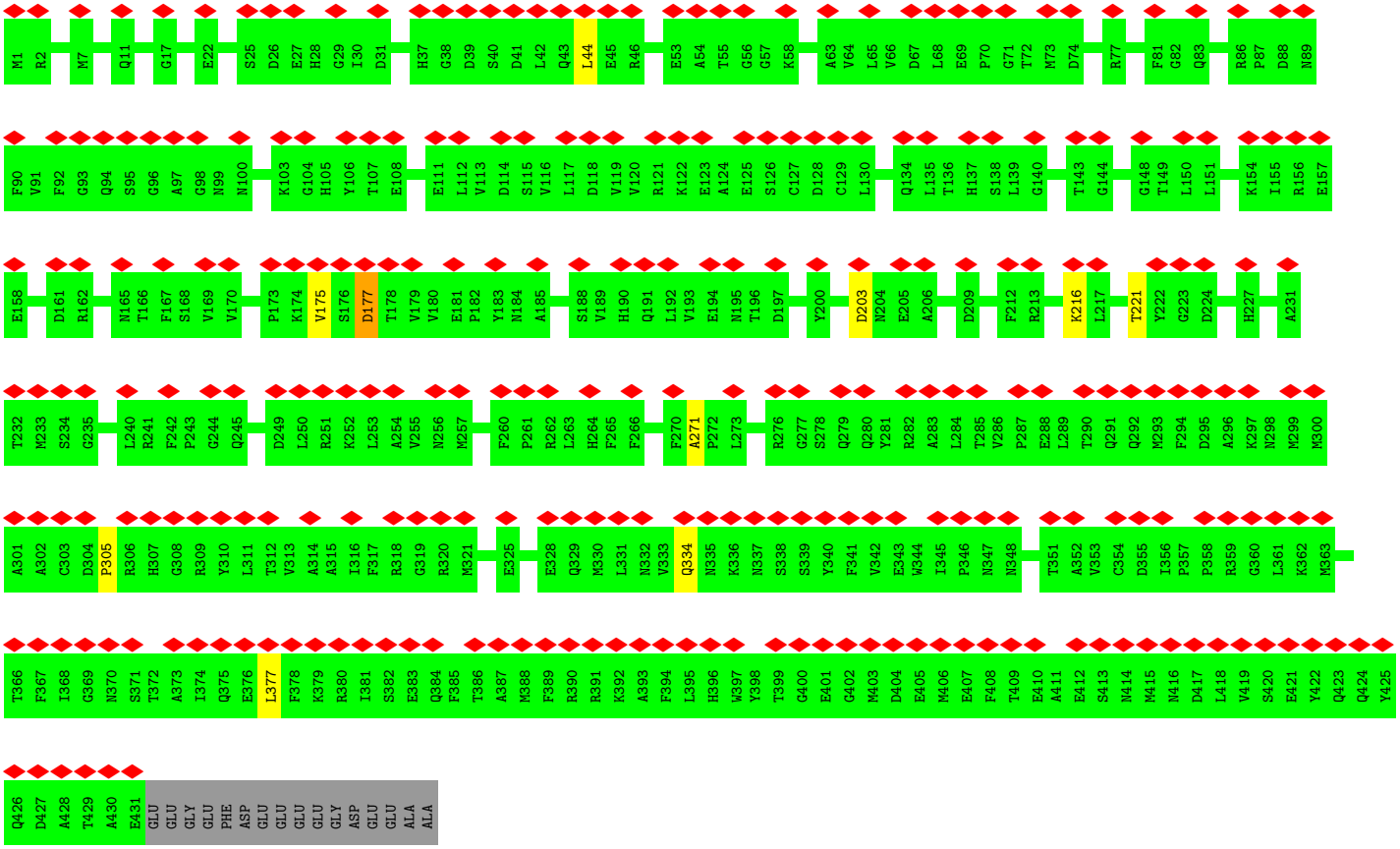




- Molecule 55: Tubulin beta chain

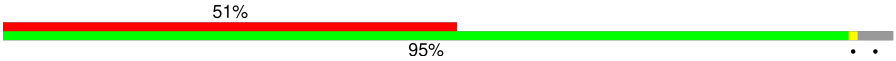
Chain ED:

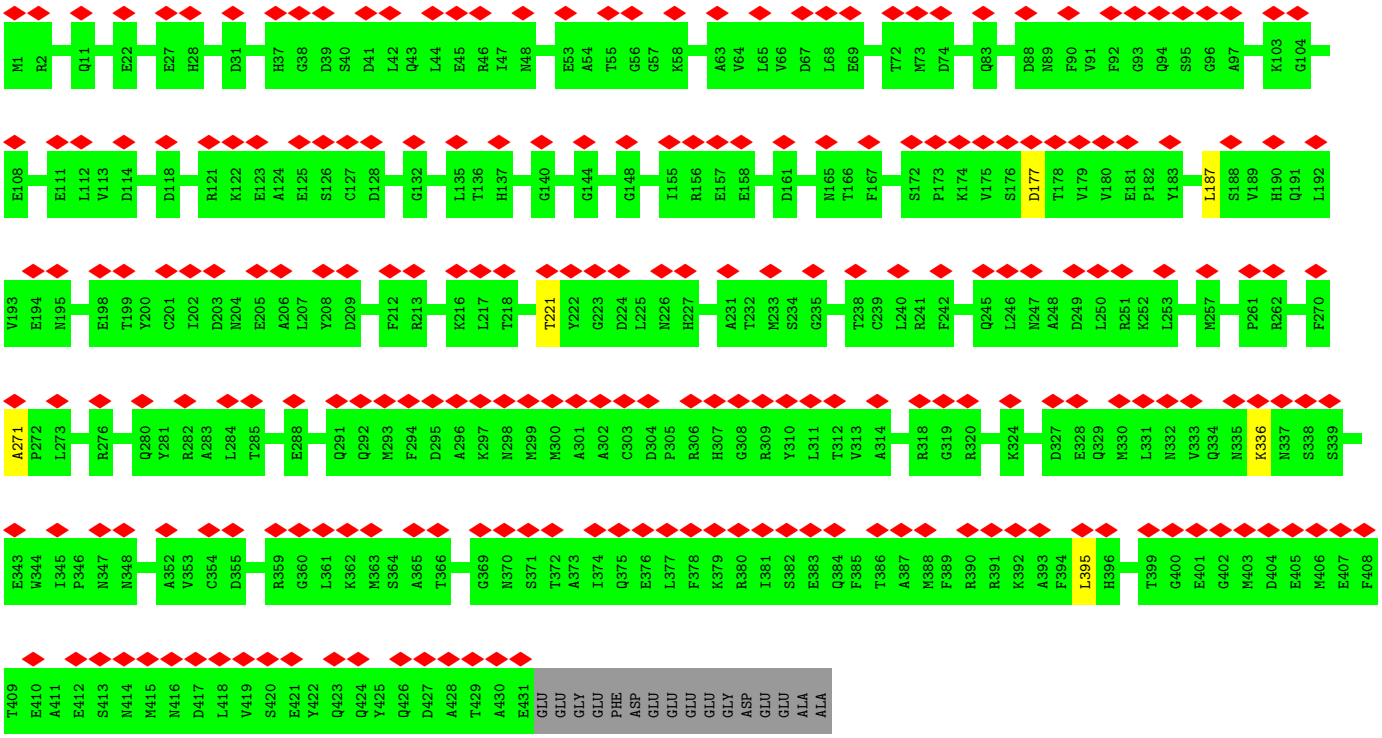




- Molecule 55: Tubulin beta chain

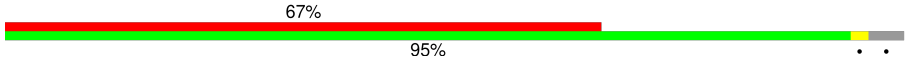
Chain EF:

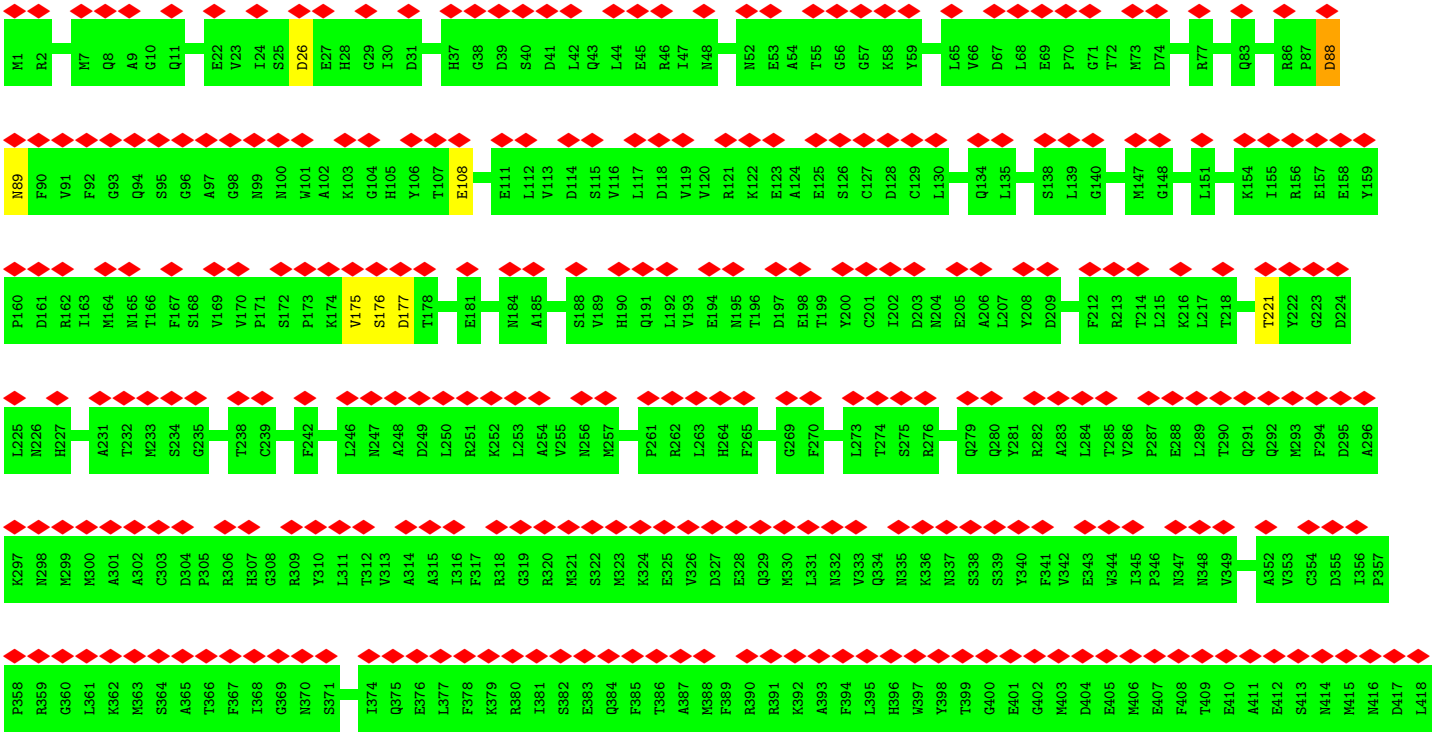


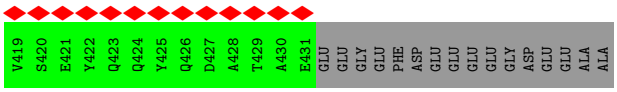


- Molecule 55: Tubulin beta chain

Chain EH:

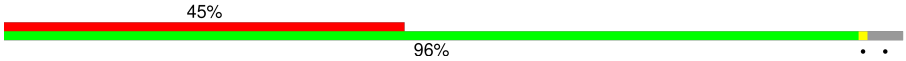


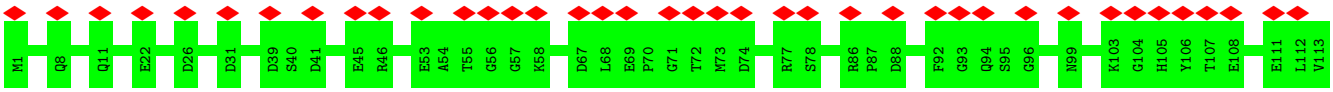


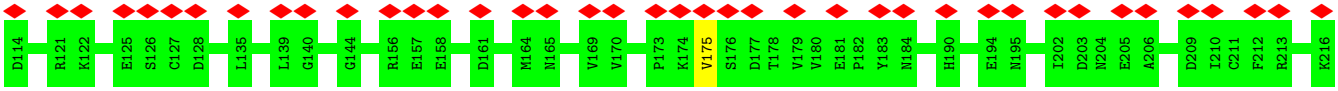


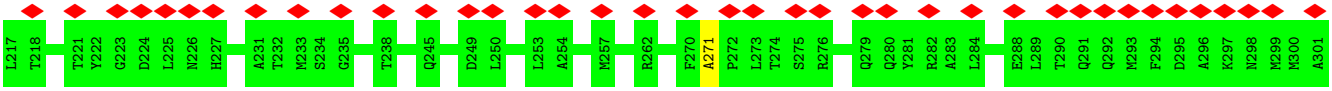
• Molecule 55: Tubulin beta chain

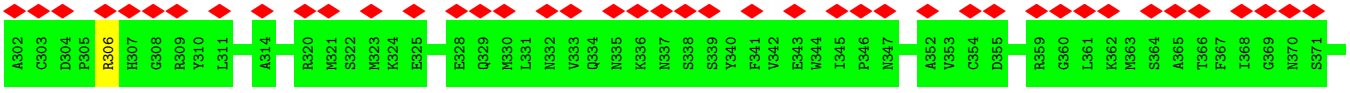
Chain EJ:

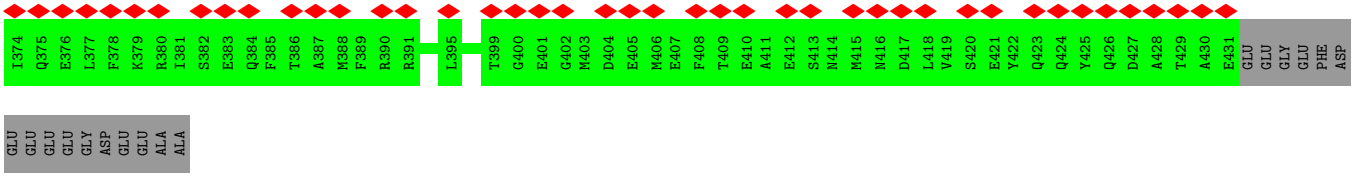






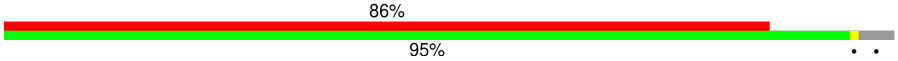


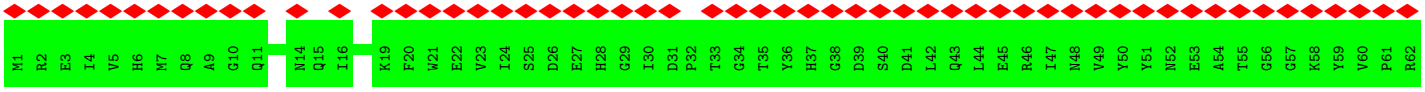


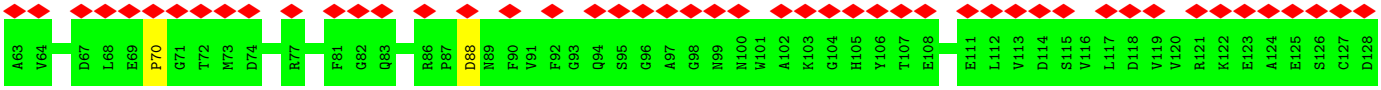


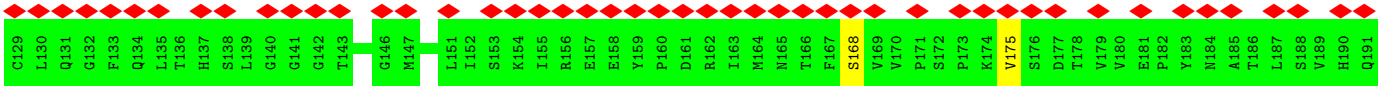
• Molecule 55: Tubulin beta chain

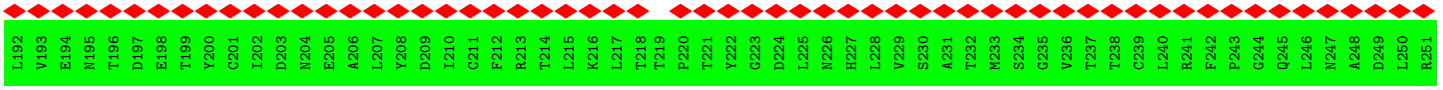
Chain EL:

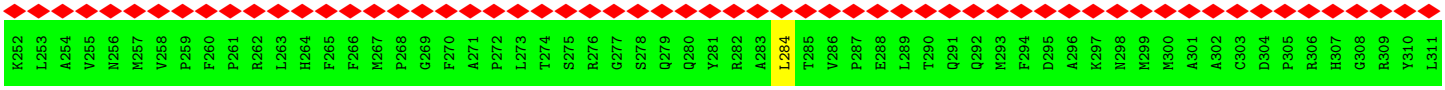


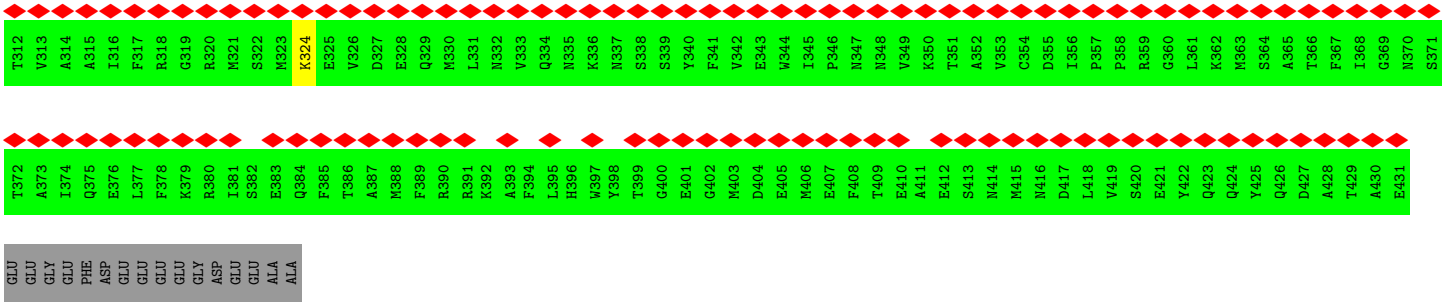






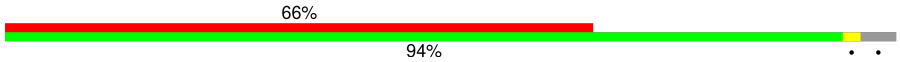


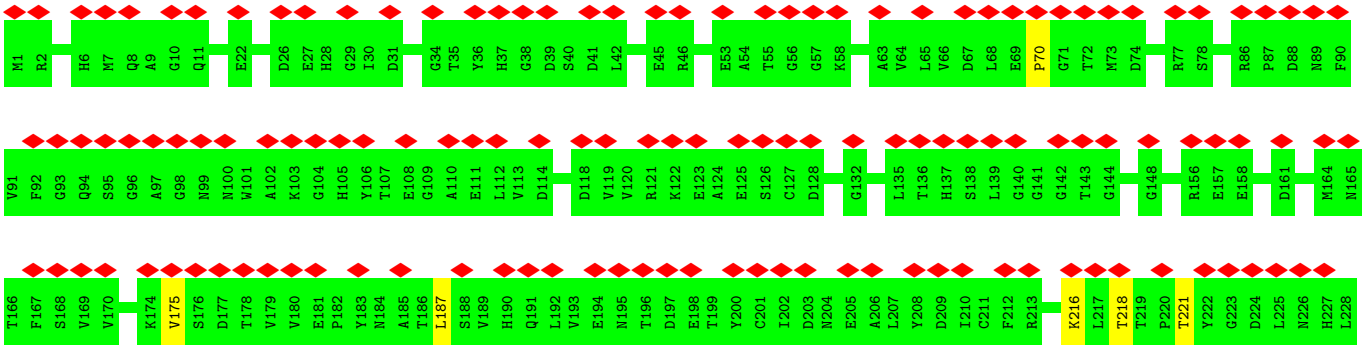


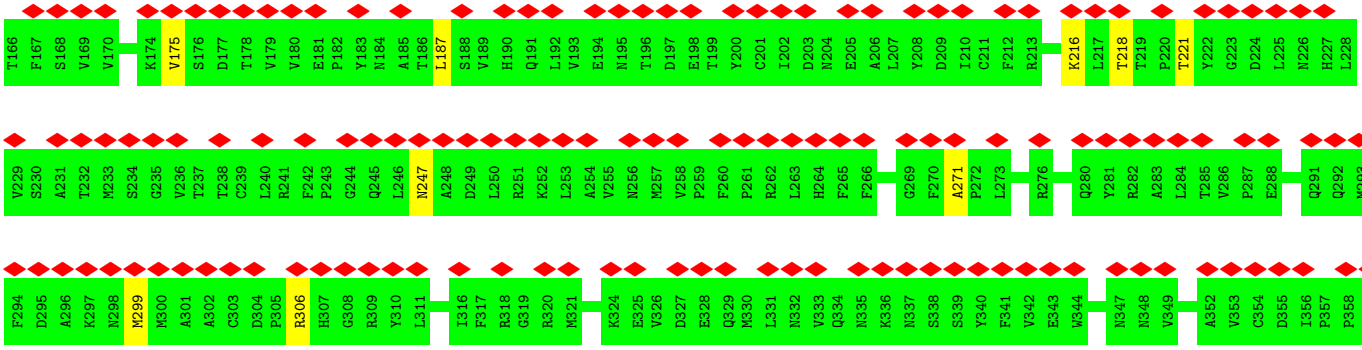


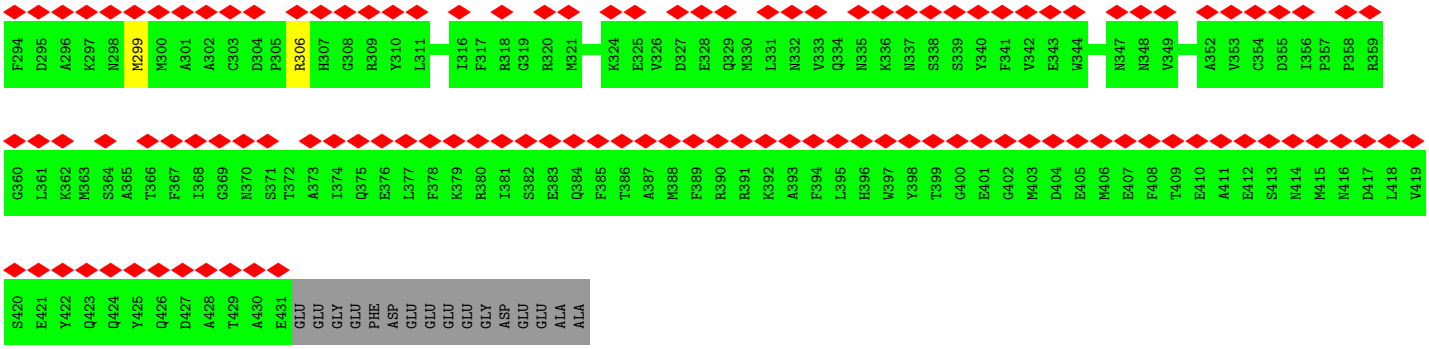
- Molecule 55: Tubulin beta chain

Chain EM:



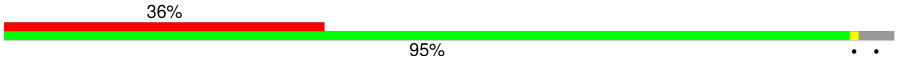


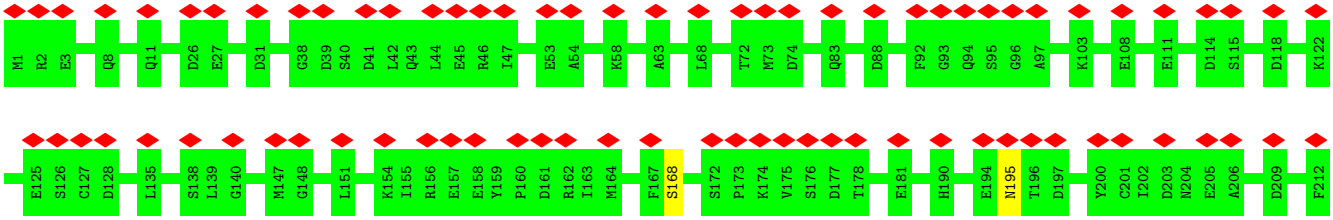


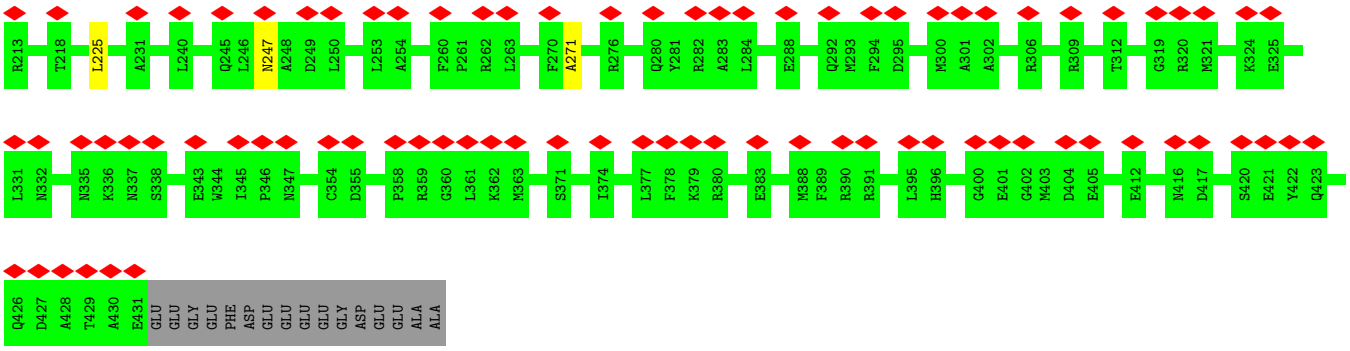


- Molecule 55: Tubulin beta chain

Chain FC:

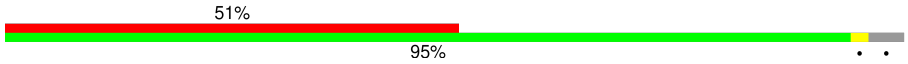


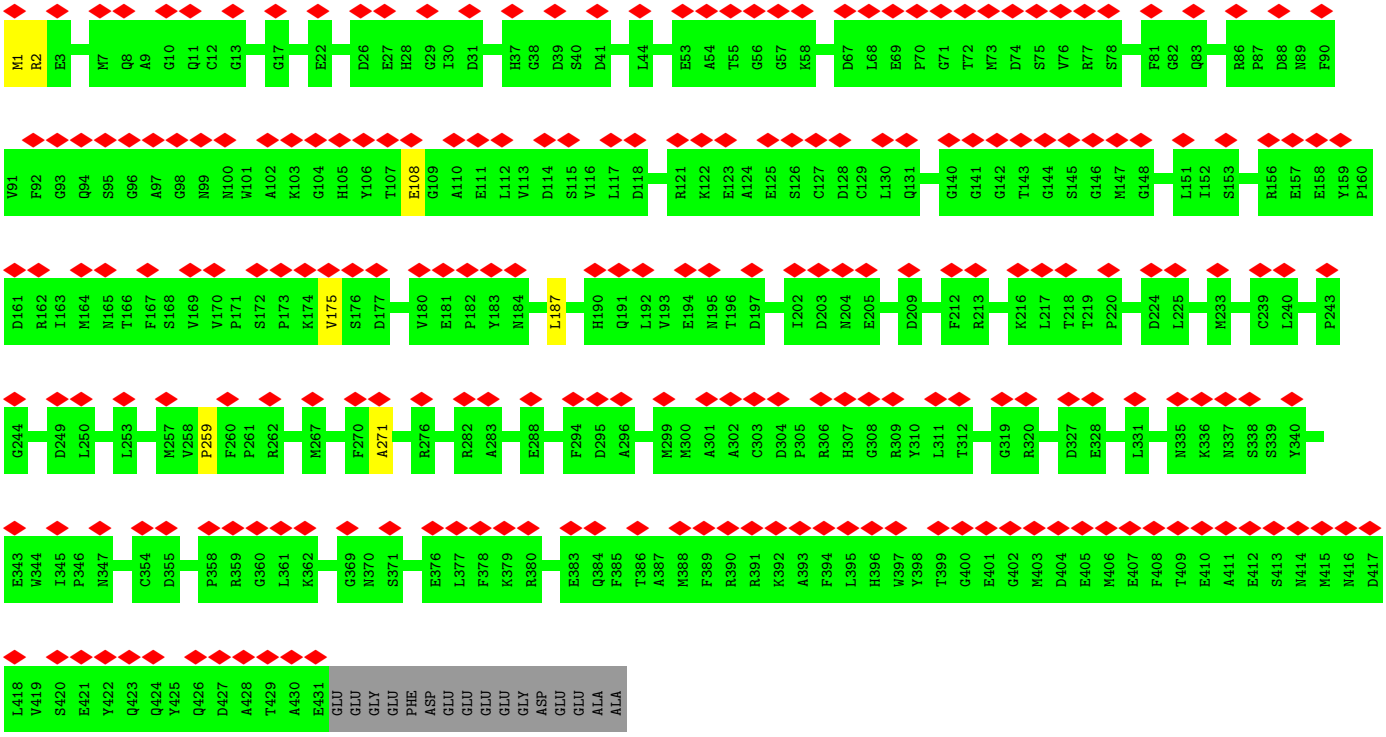




- Molecule 55: Tubulin beta chain

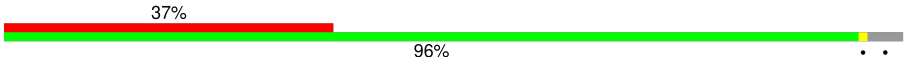
Chain FD:

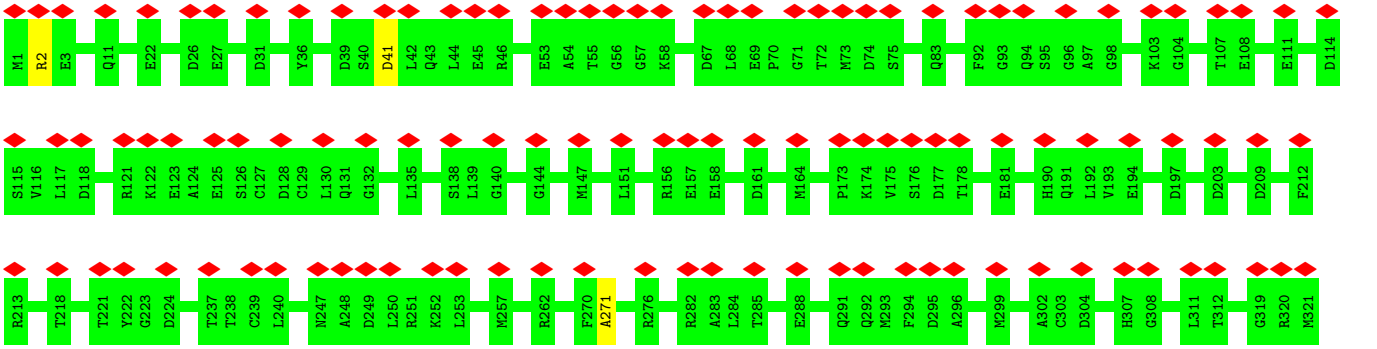


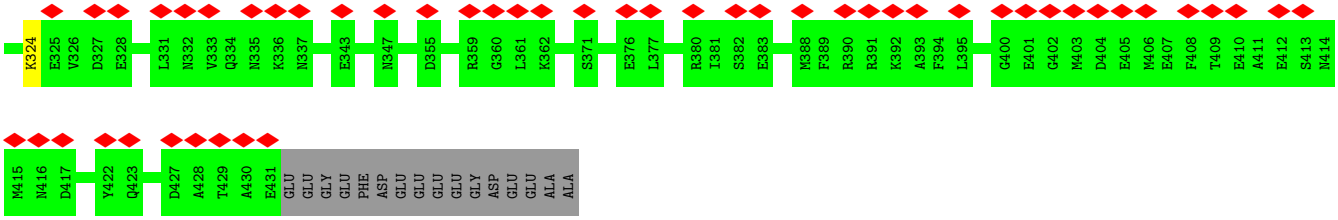


- Molecule 55: Tubulin beta chain

Chain FF:

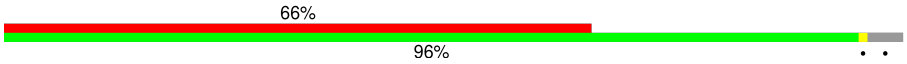


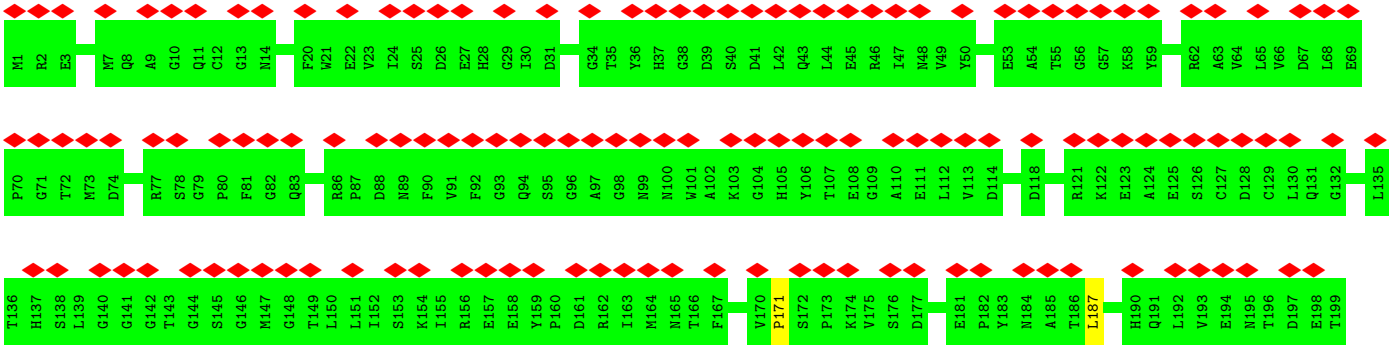


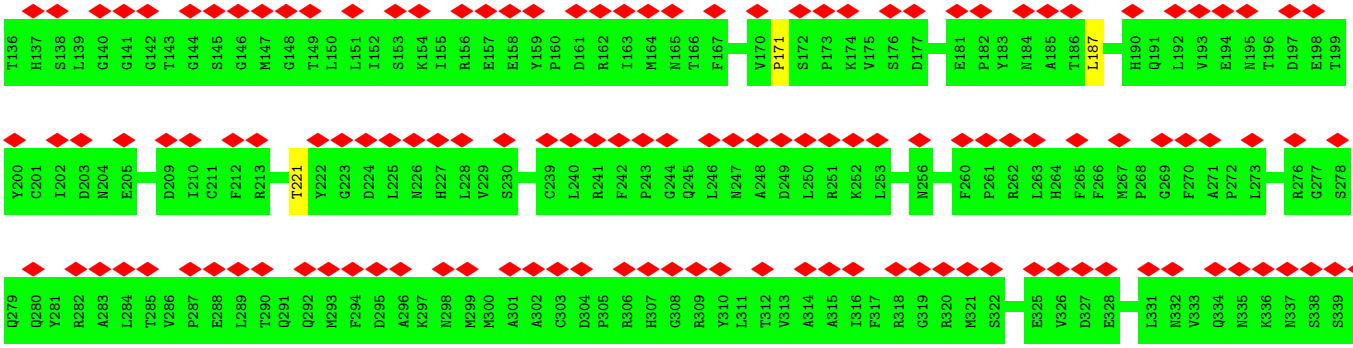


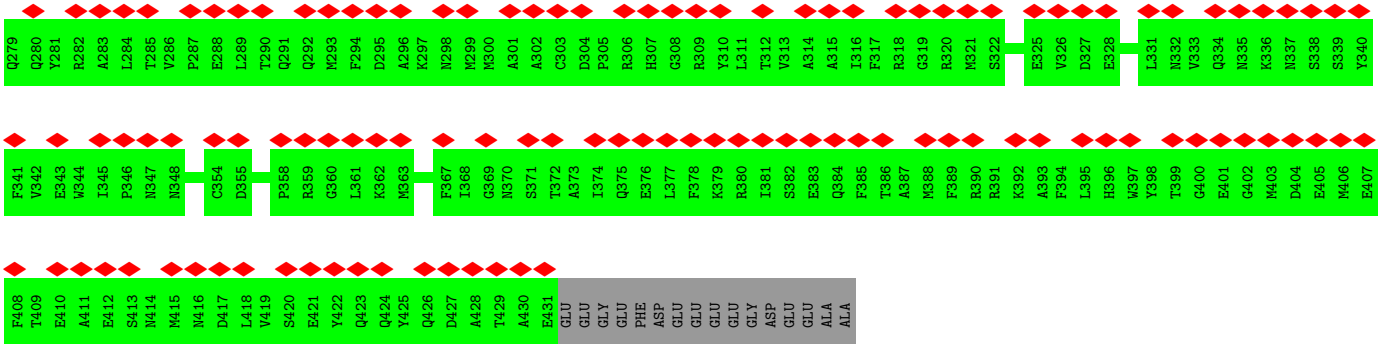
• Molecule 55: Tubulin beta chain

Chain FH:



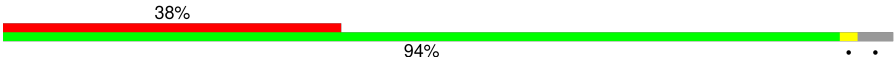


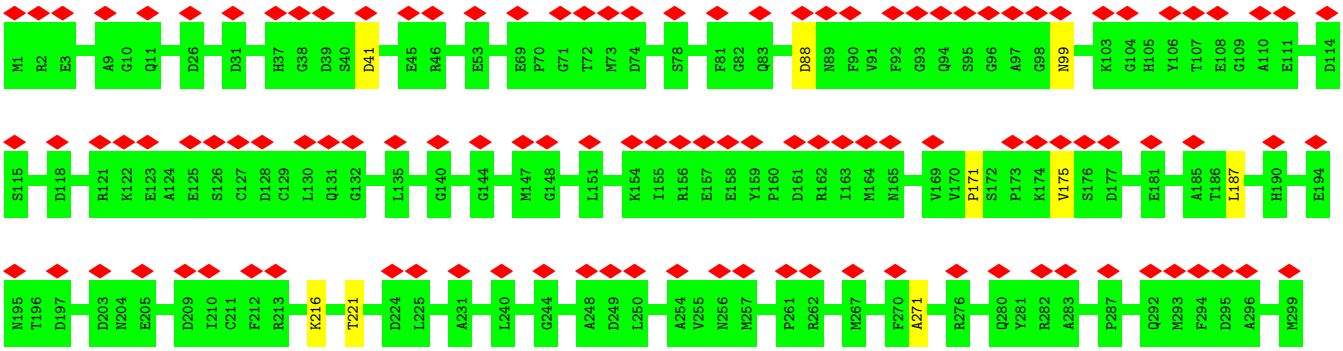


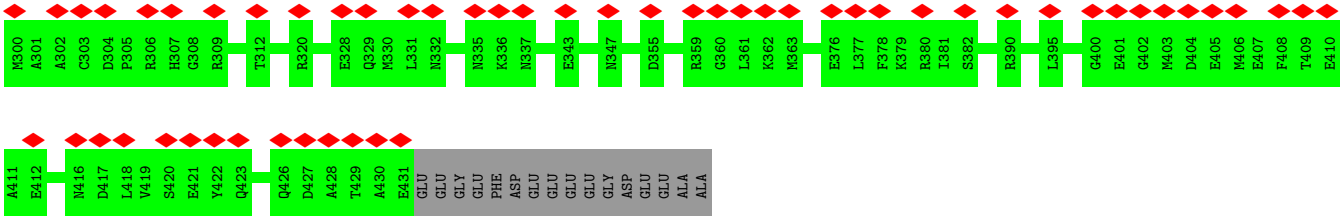


• Molecule 55: Tubulin beta chain

Chain FJ:

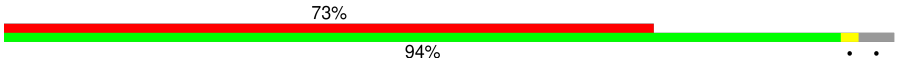


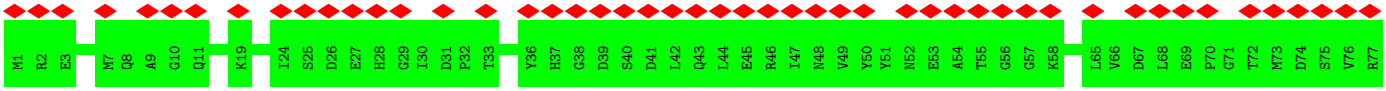


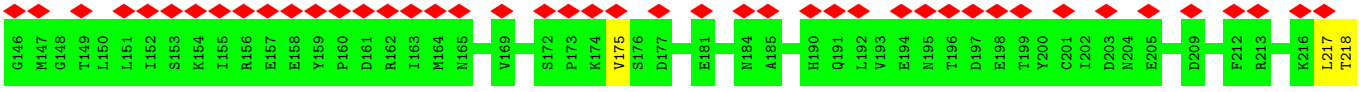


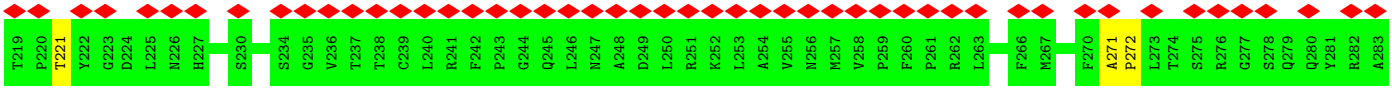
• Molecule 55: Tubulin beta chain

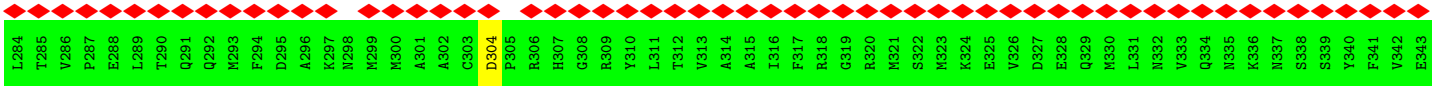
Chain FL:

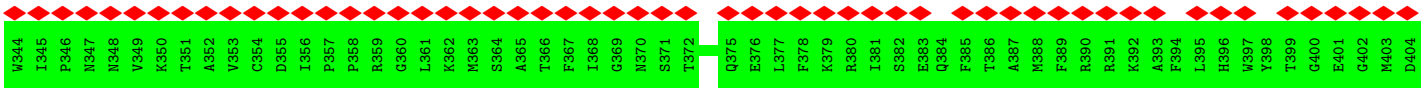


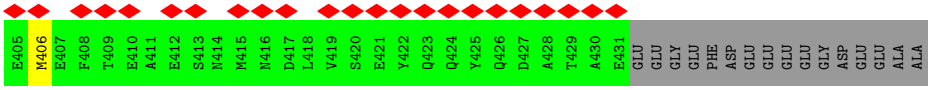






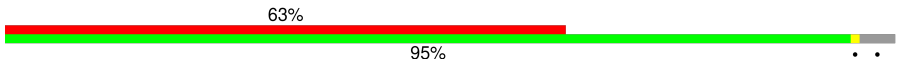


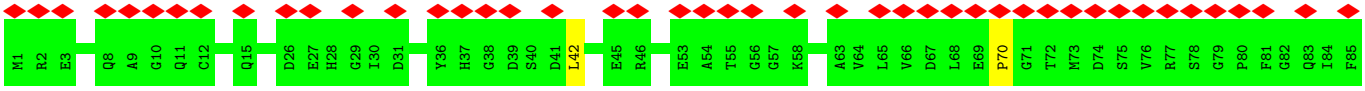


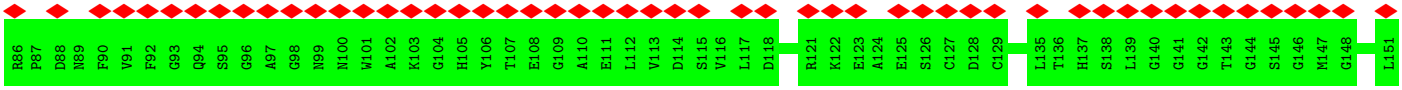


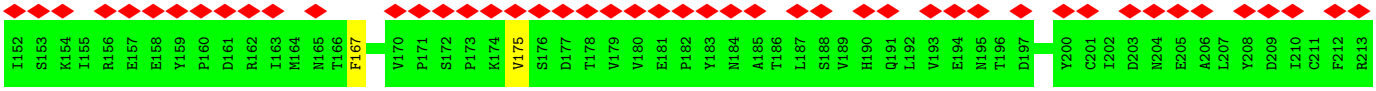
• Molecule 55: Tubulin beta chain

Chain FM:



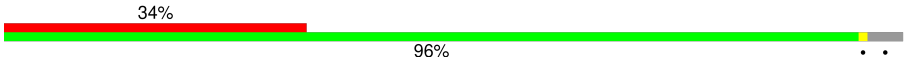


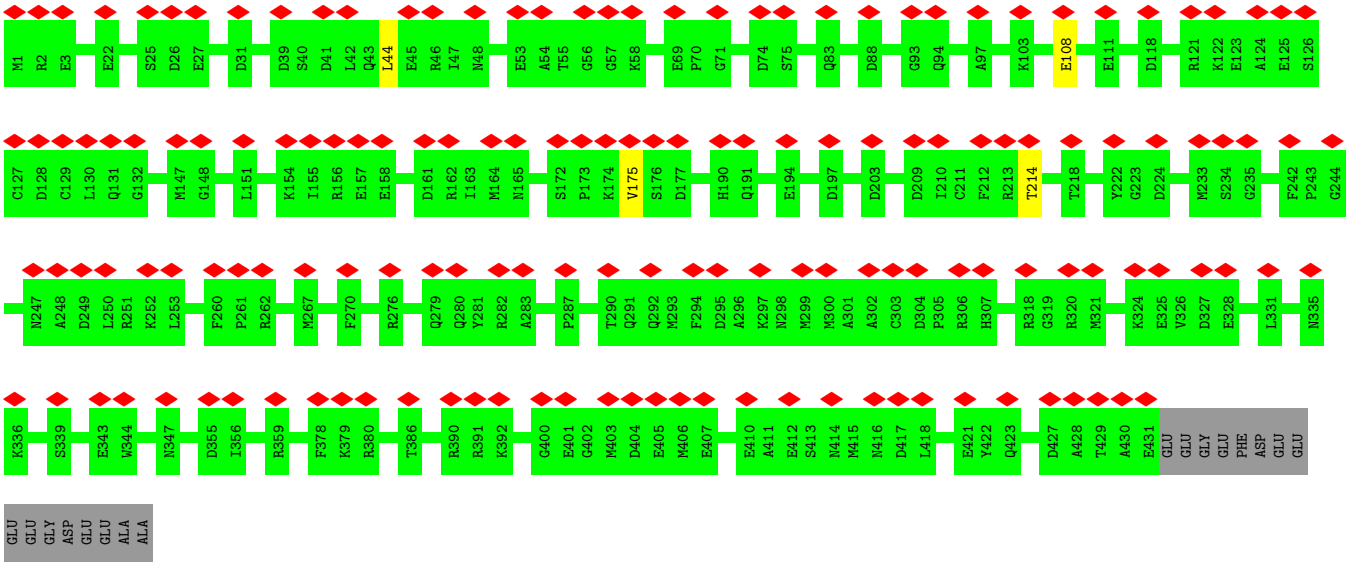




- Molecule 55: Tubulin beta chain

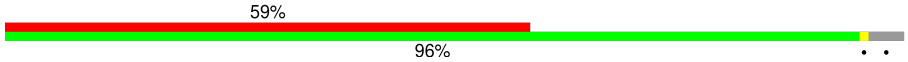
Chain GC:

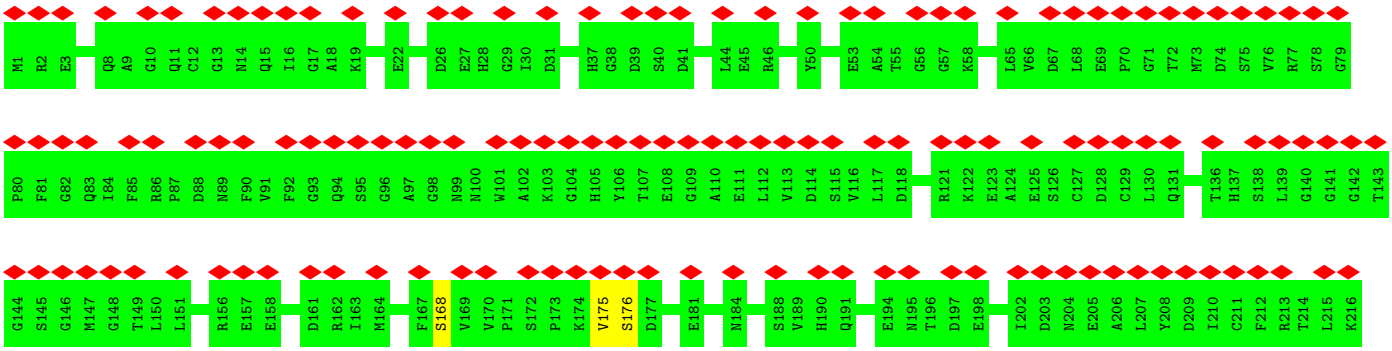


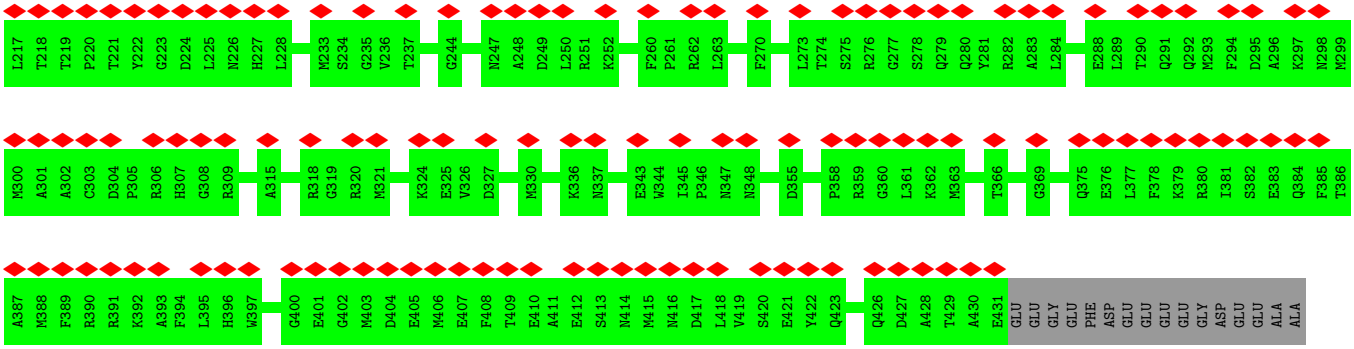


- Molecule 55: Tubulin beta chain

Chain GD:

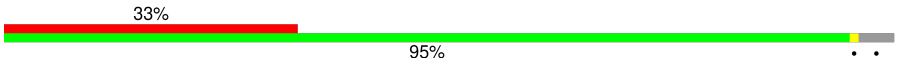


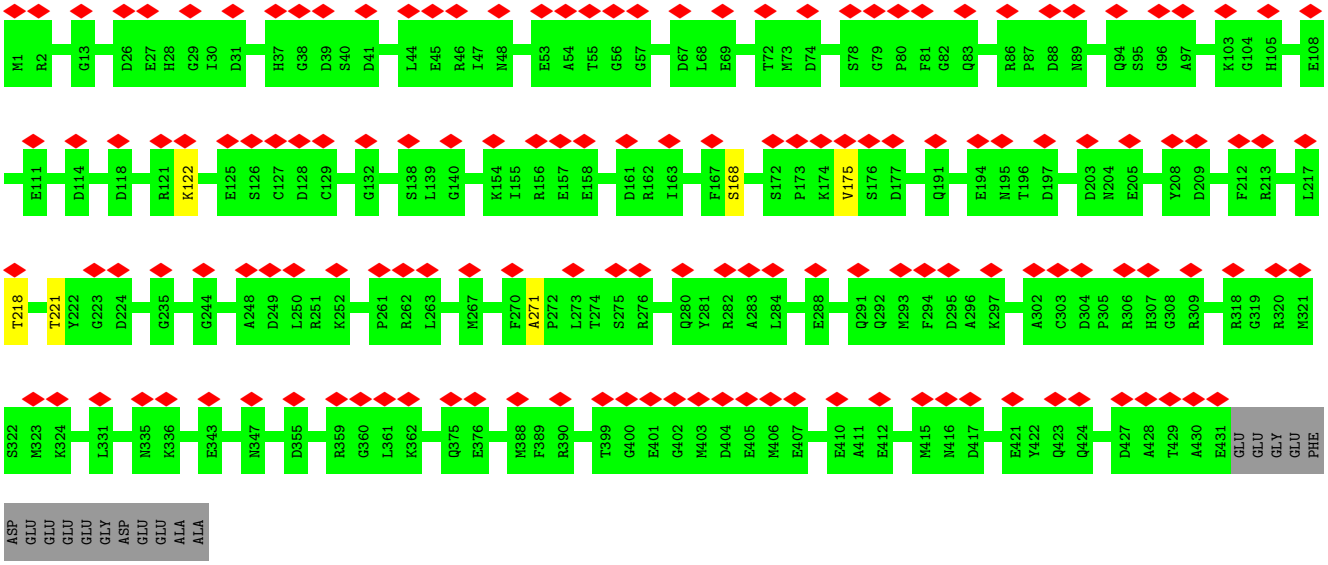




- Molecule 55: Tubulin beta chain

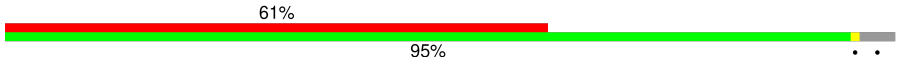
Chain GF:

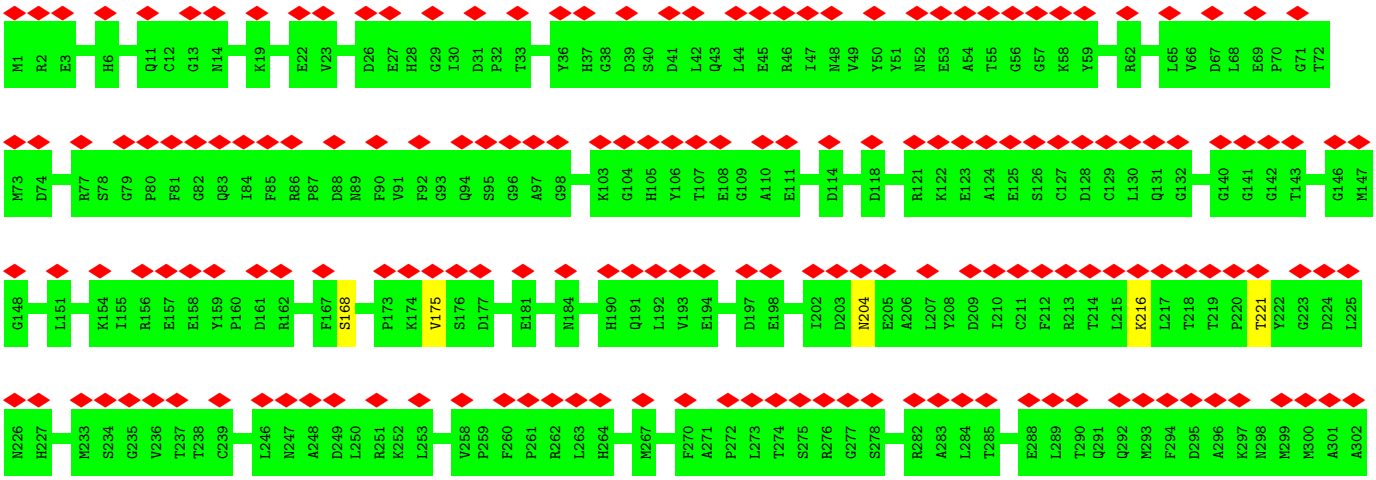


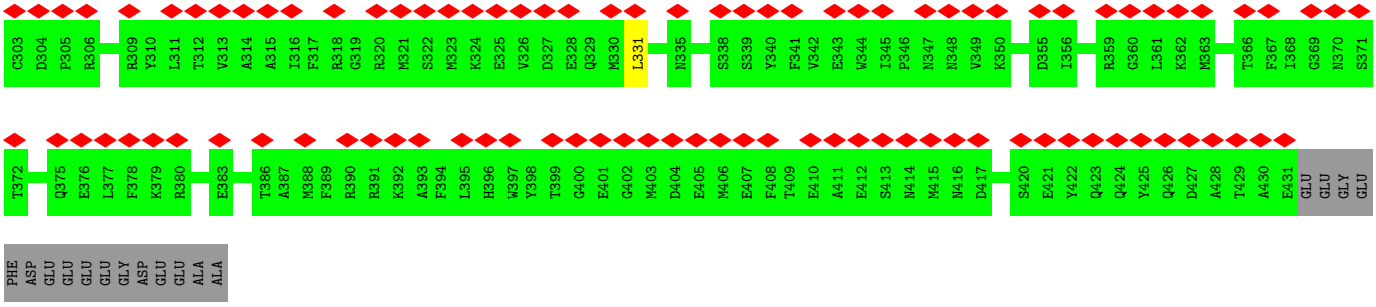


- Molecule 55: Tubulin beta chain

Chain GH:

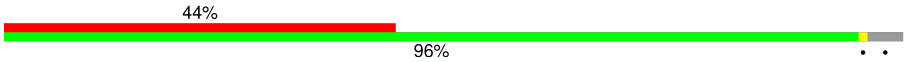






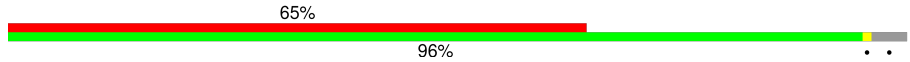
- Molecule 55: Tubulin beta chain

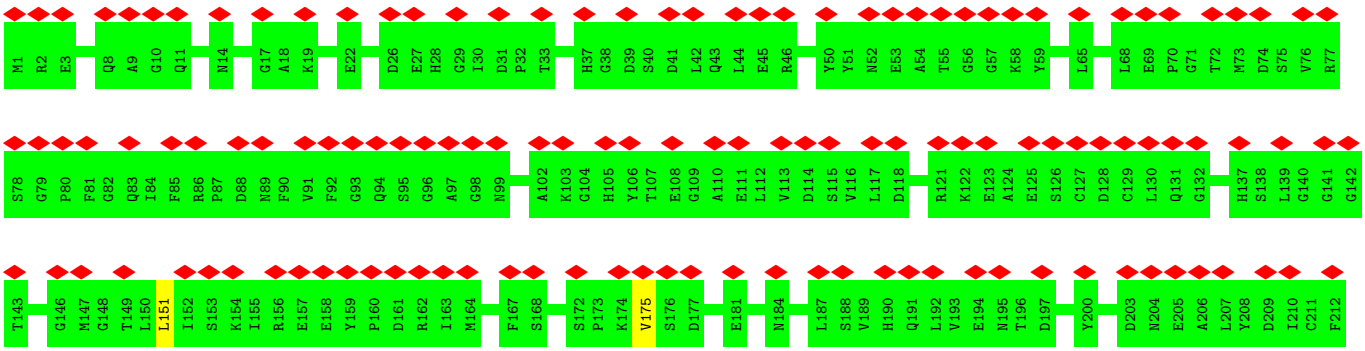
Chain GJ:

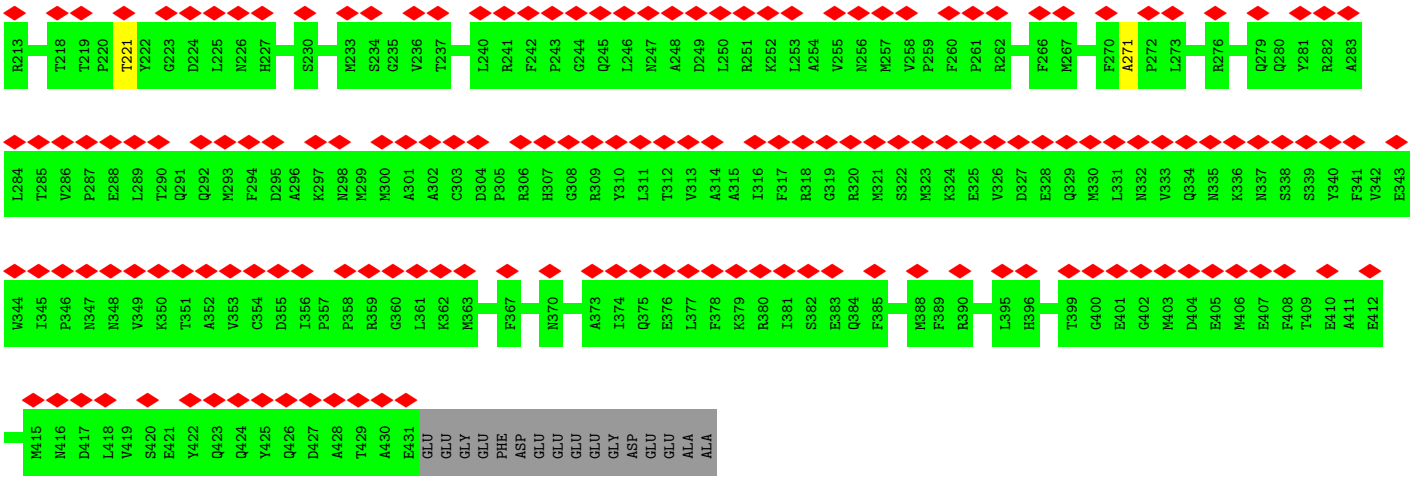


- Molecule 55: Tubulin beta chain

Chain GL:

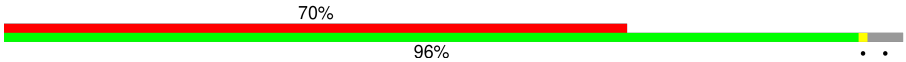


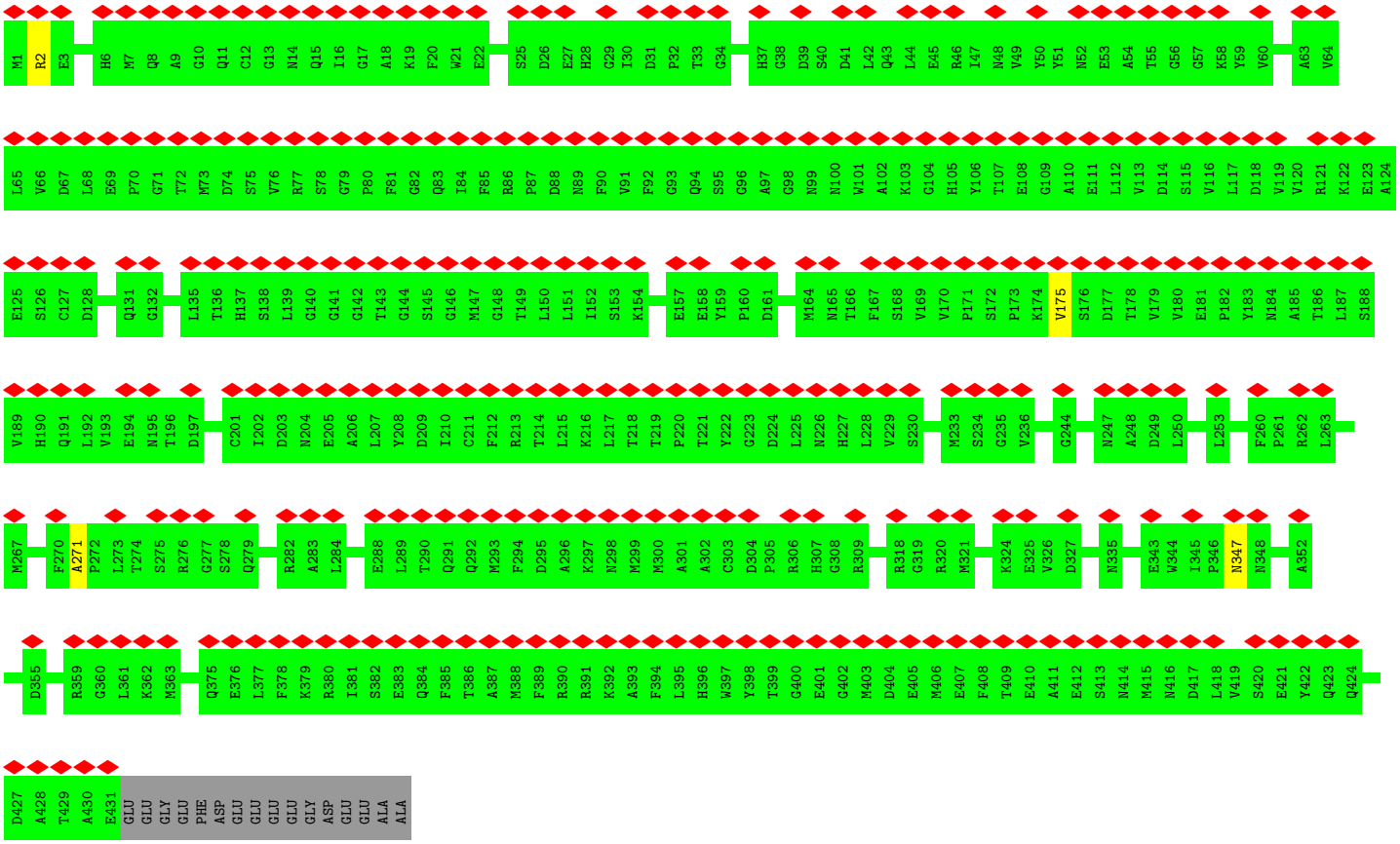




- Molecule 55: Tubulin beta chain

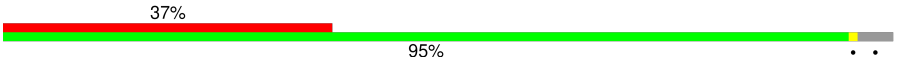
Chain GM:

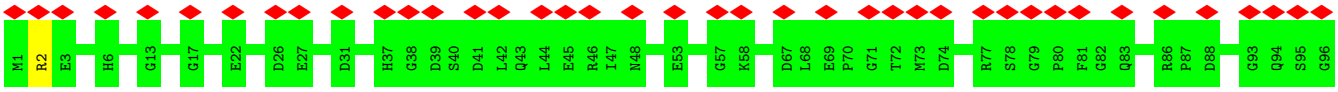


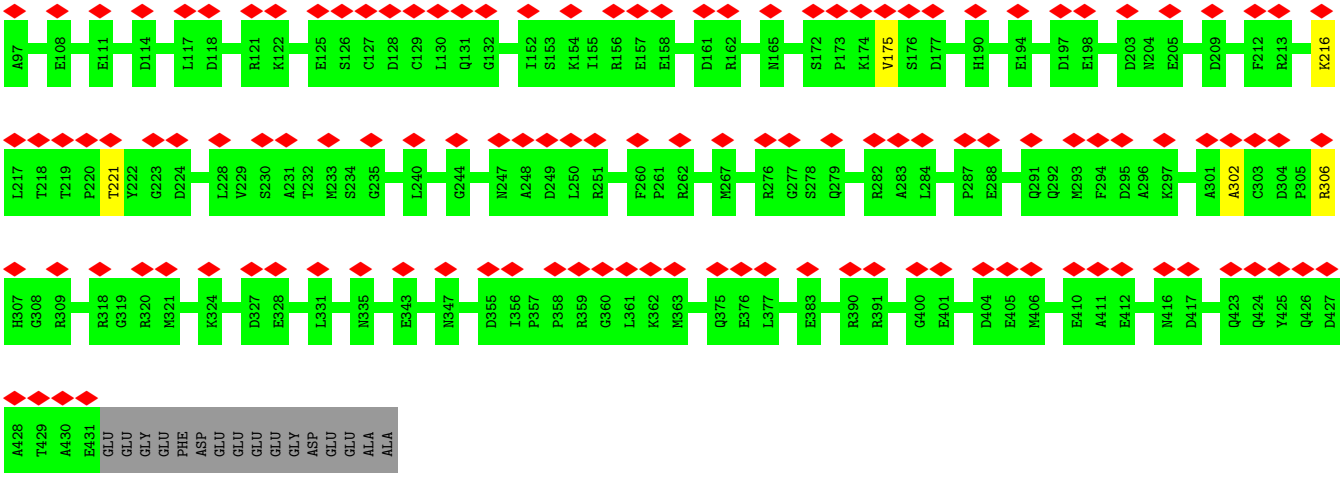


- Molecule 55: Tubulin beta chain

Chain HC:

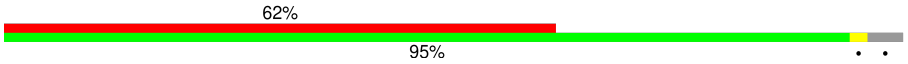


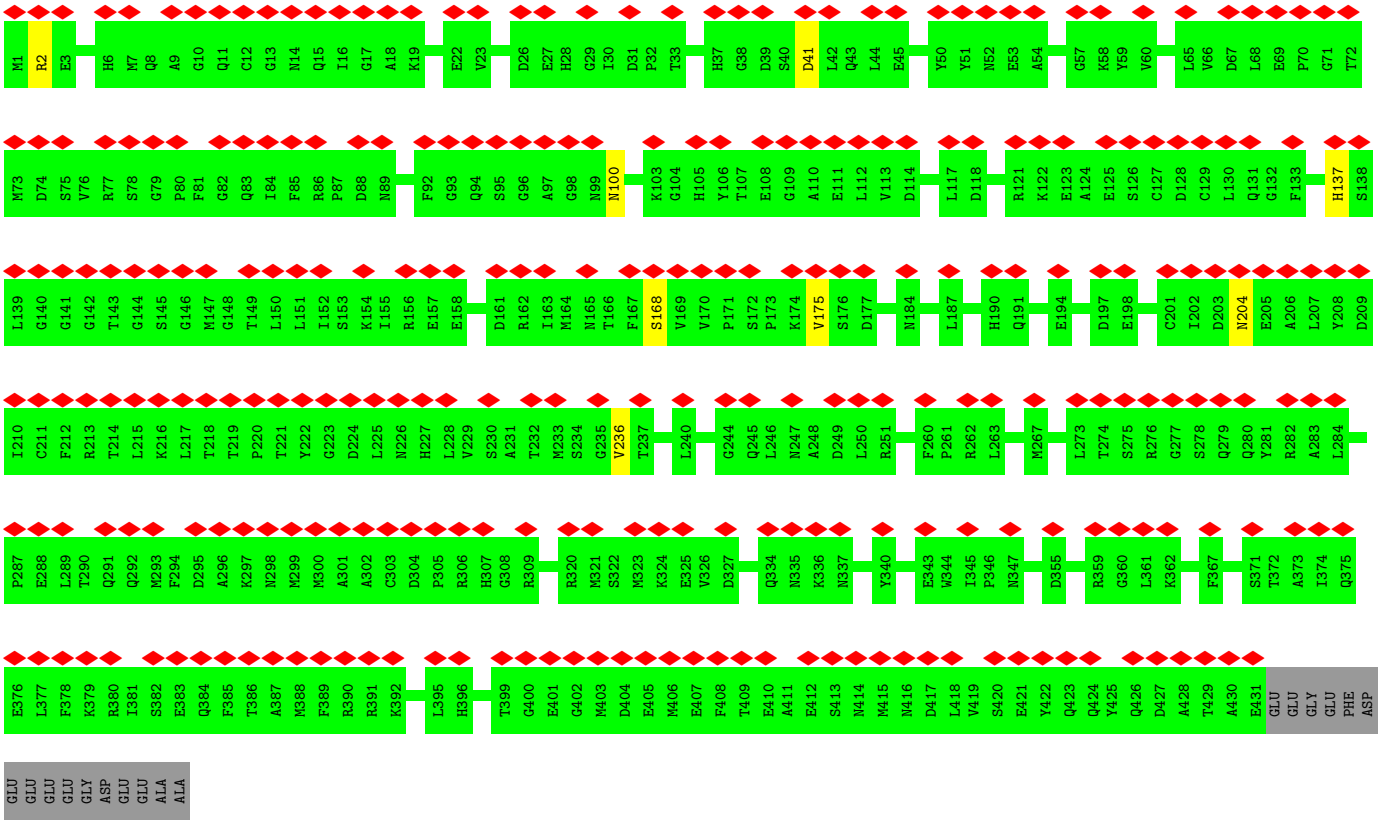




- Molecule 55: Tubulin beta chain

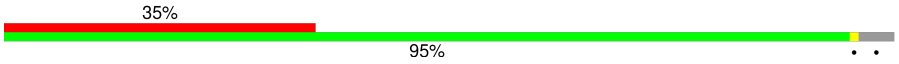
Chain HD:

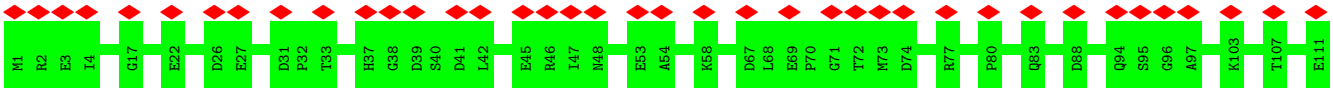


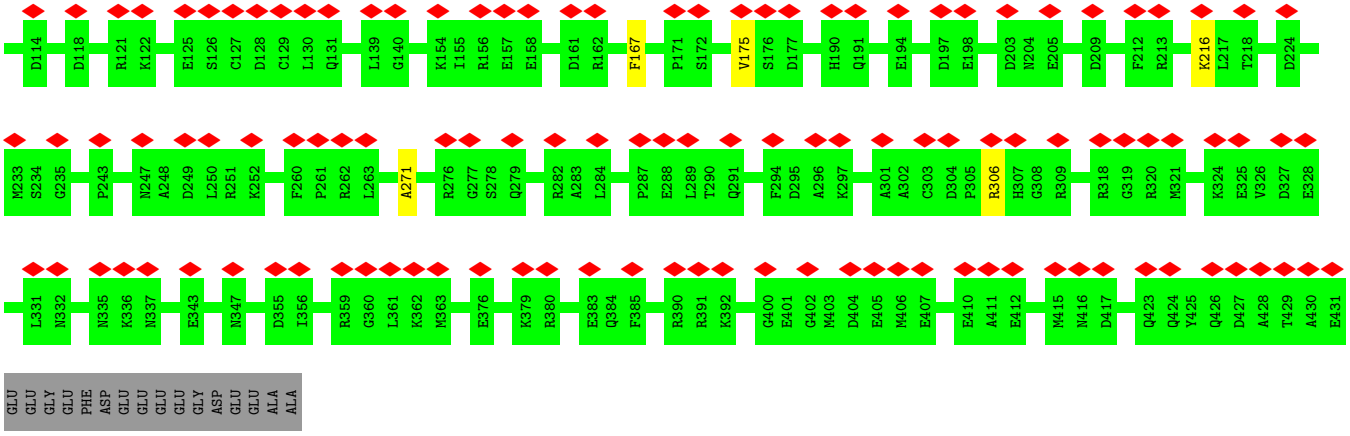


- Molecule 55: Tubulin beta chain

Chain HF:

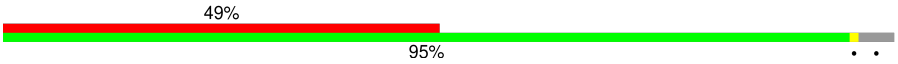


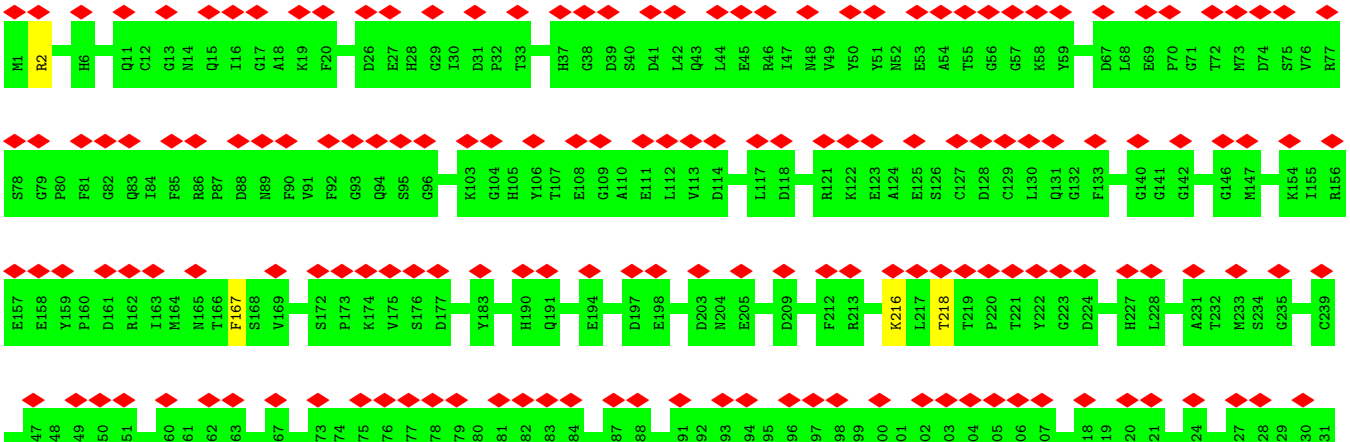


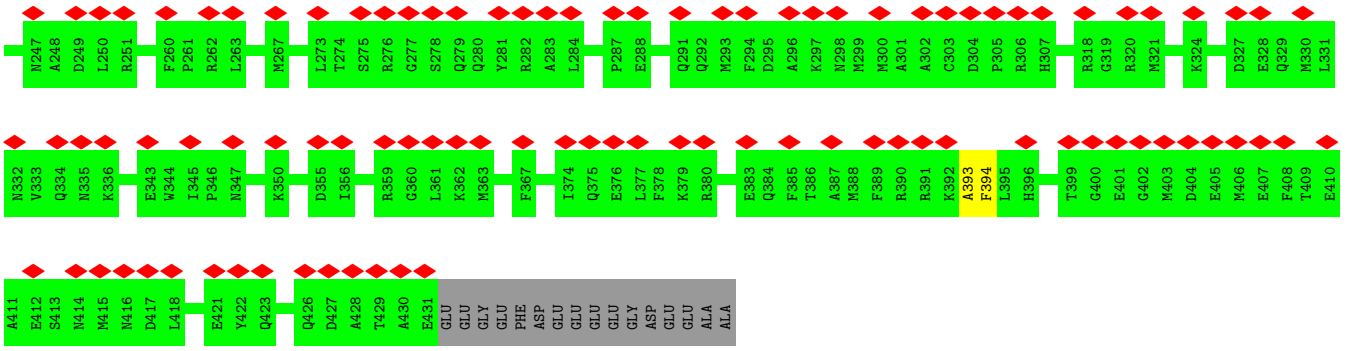


- Molecule 55: Tubulin beta chain

Chain HH:

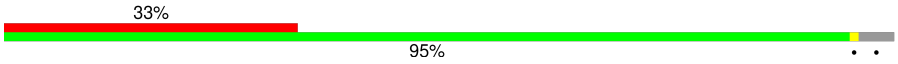


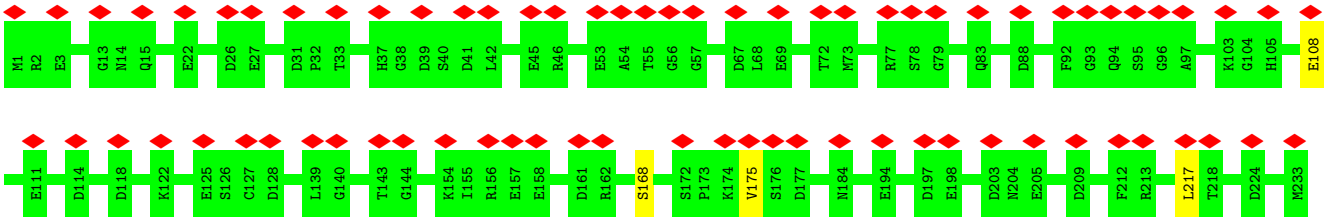


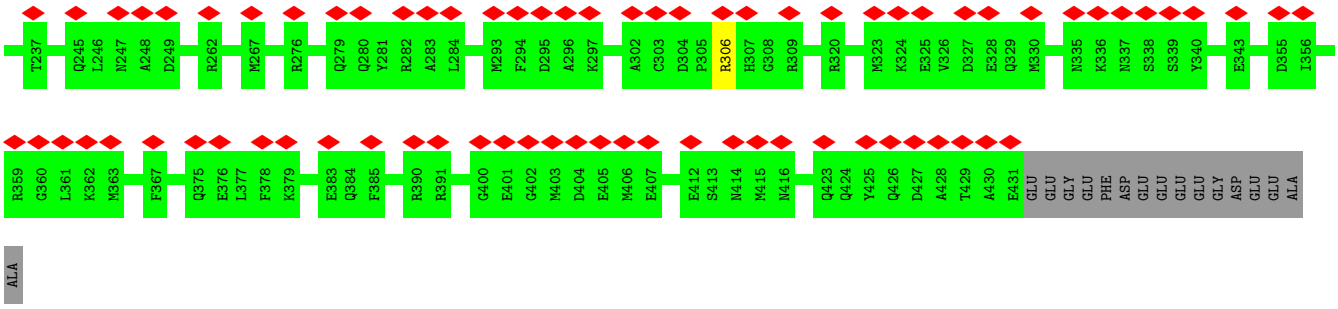


- Molecule 55: Tubulin beta chain

Chain HJ:

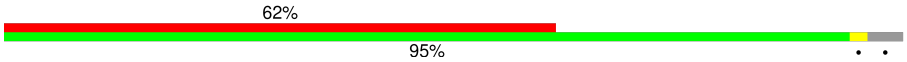


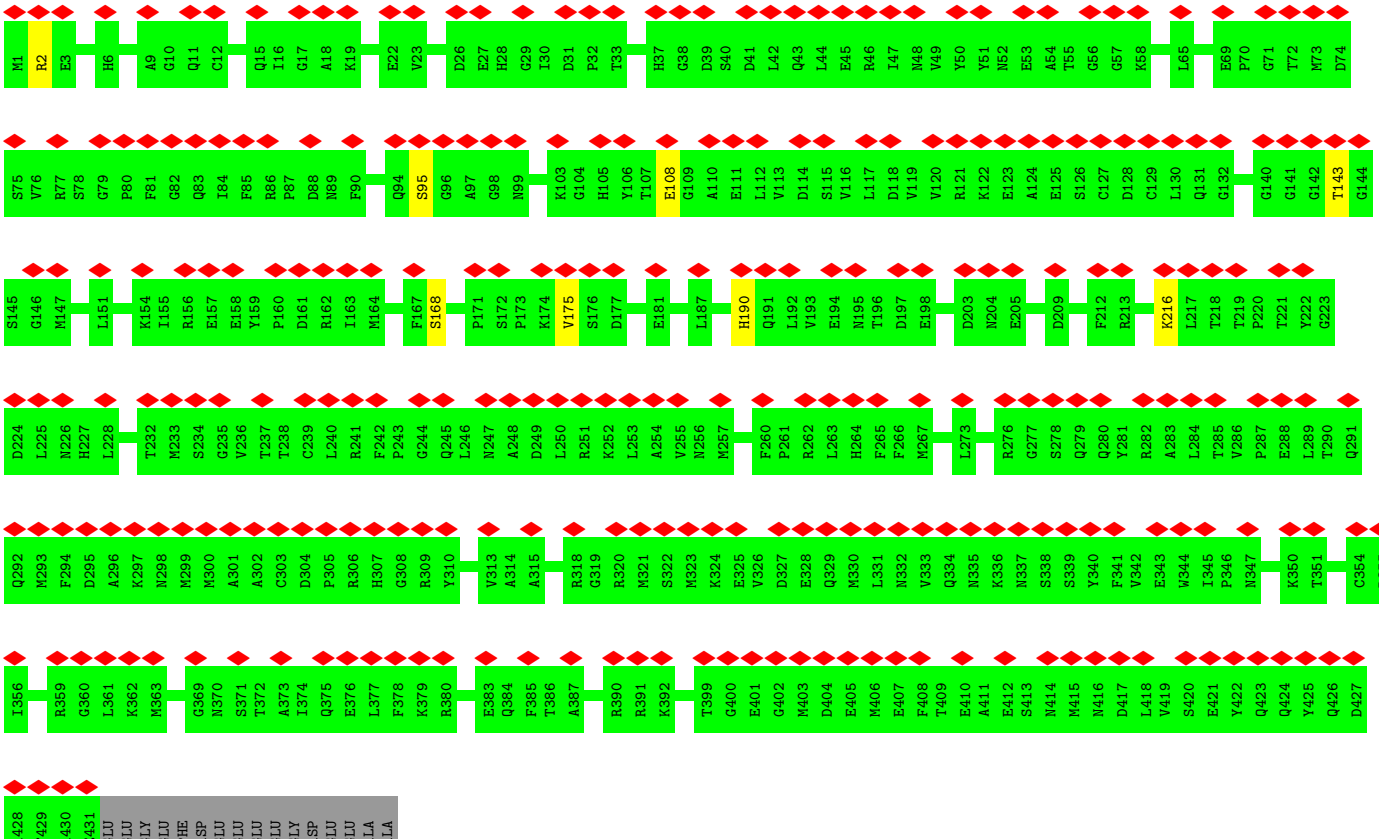




- Molecule 55: Tubulin beta chain

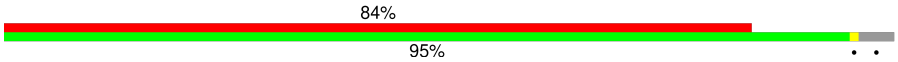
Chain HL:

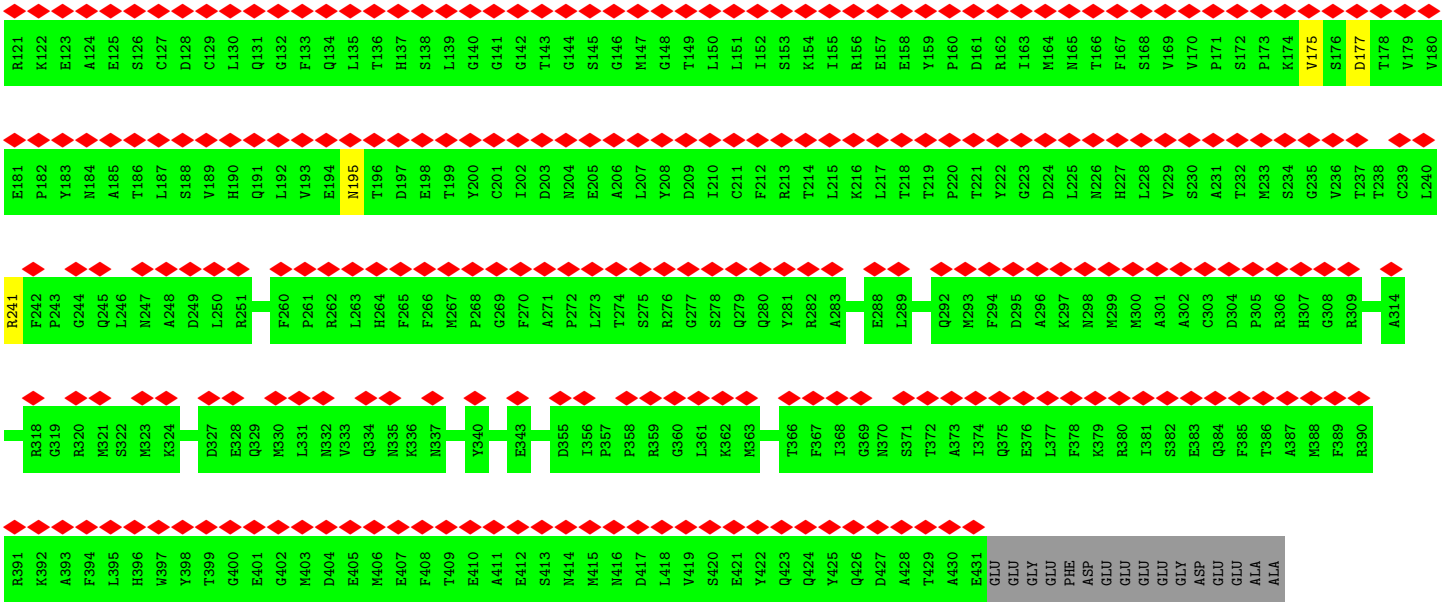




- Molecule 55: Tubulin beta chain

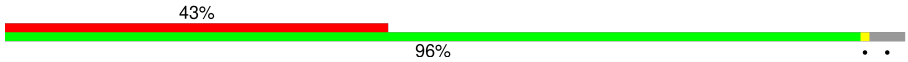
Chain HM:

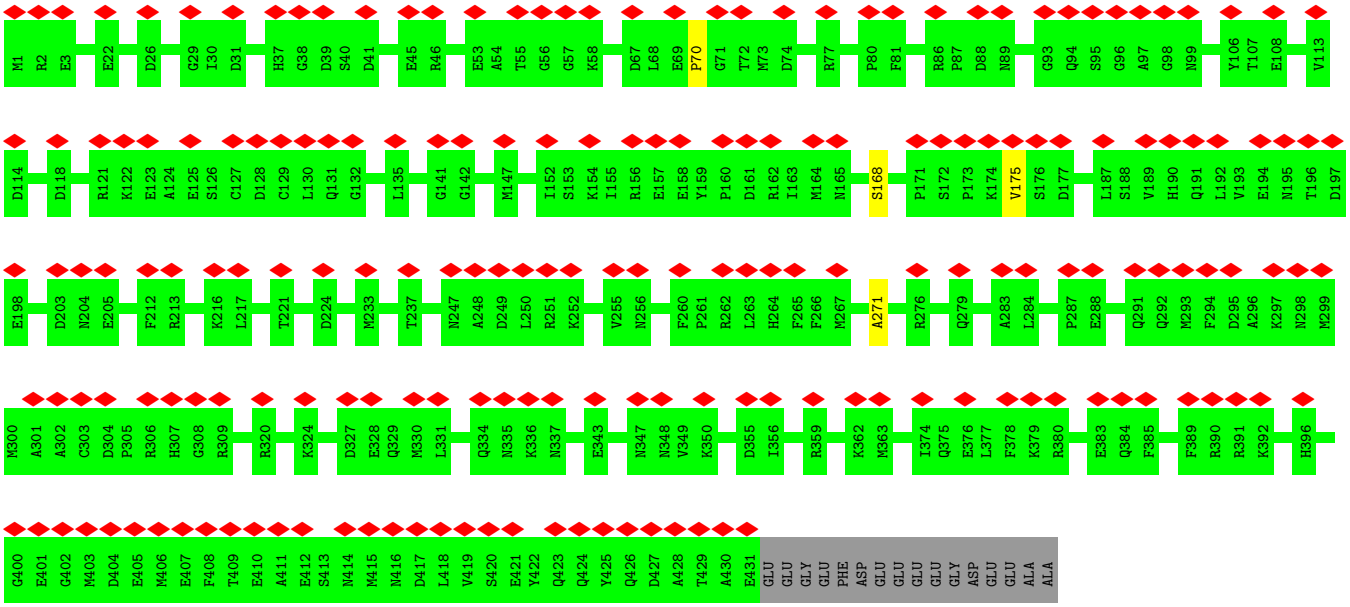




- Molecule 55: Tubulin beta chain

Chain IC:





- Molecule 55: Tubulin beta chain

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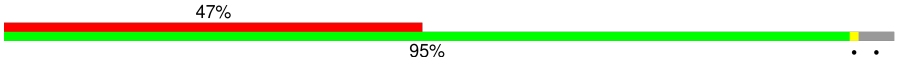
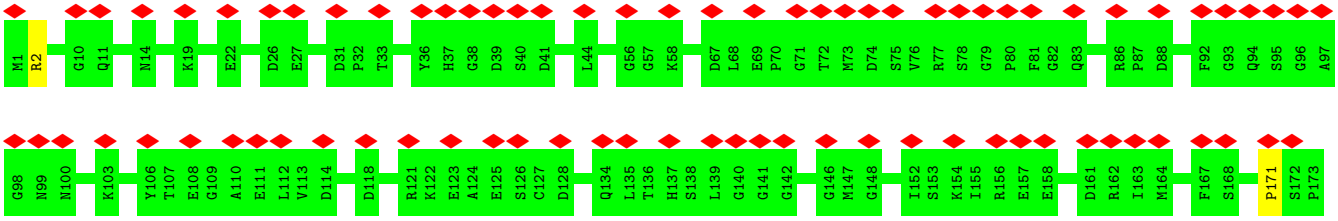
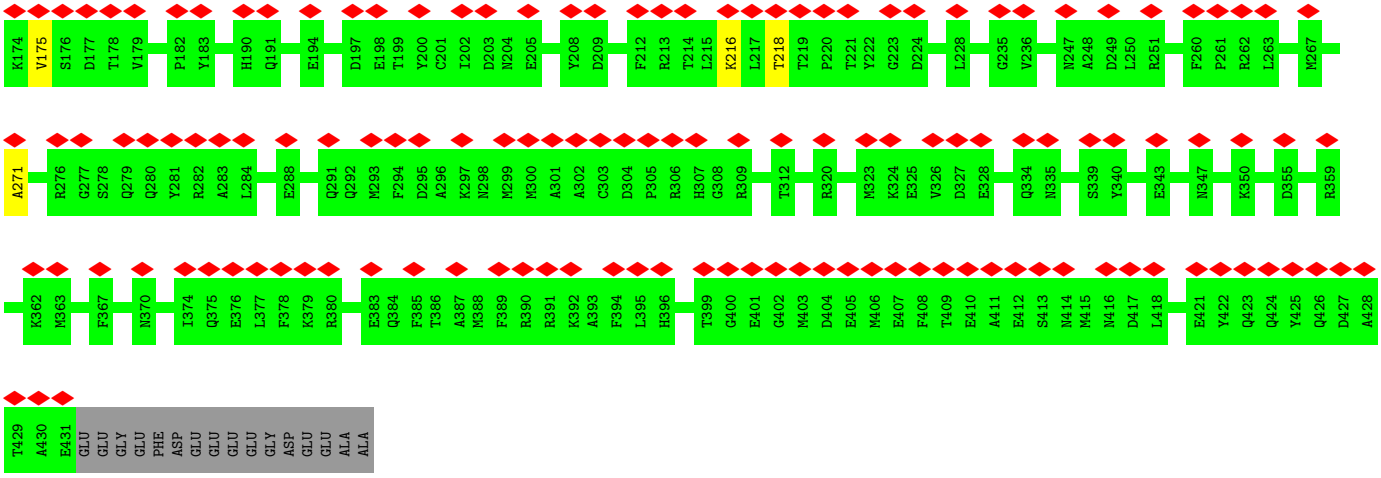
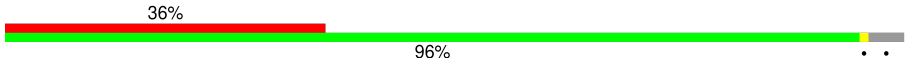


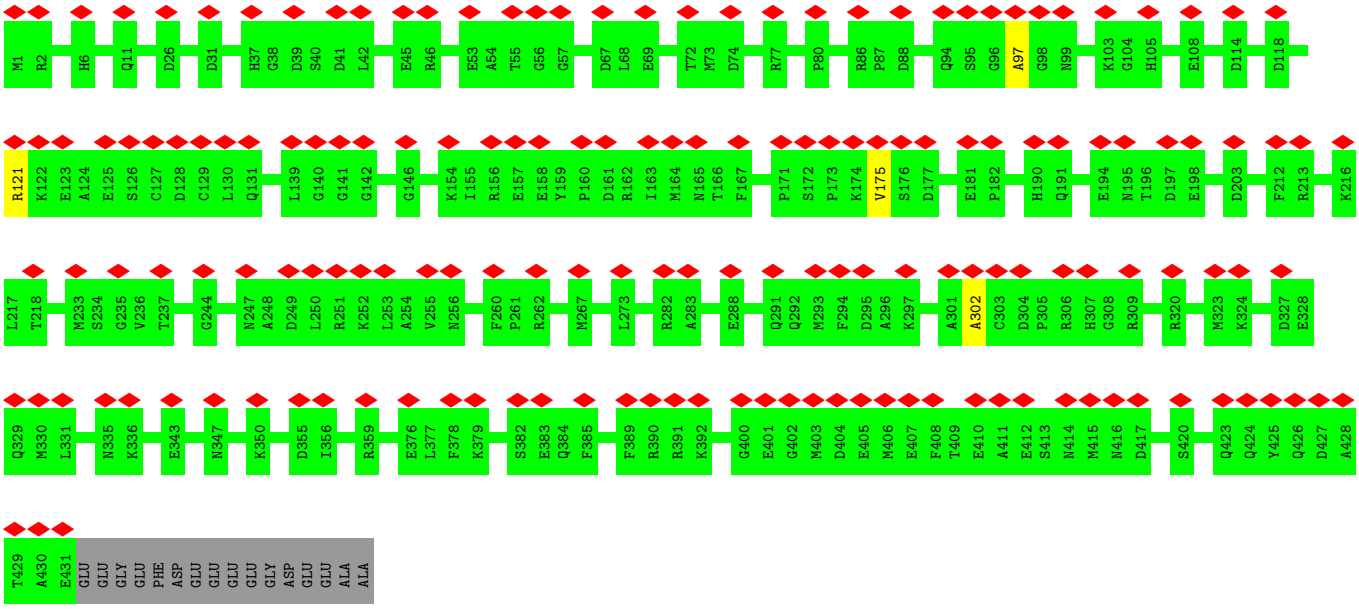




- Molecule 55: Tubulin beta chain

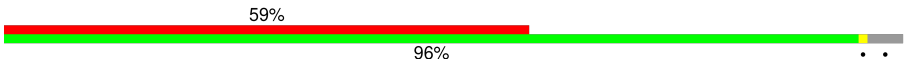
Chain IF:

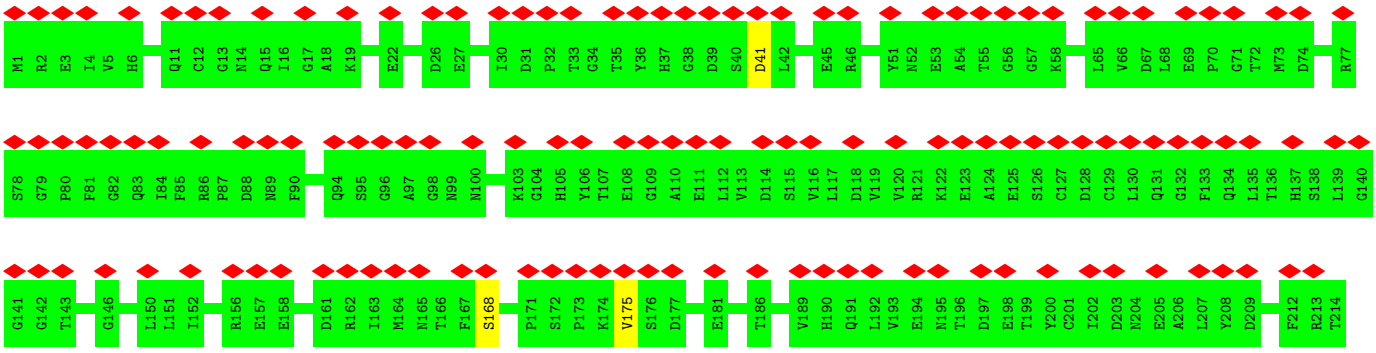


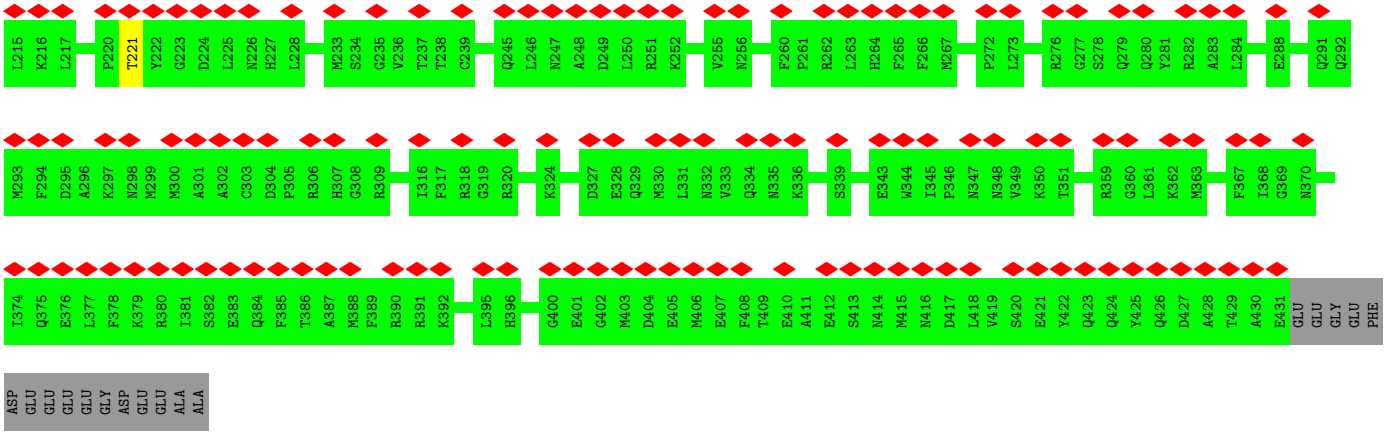


- Molecule 55: Tubulin beta chain

Chain IH:

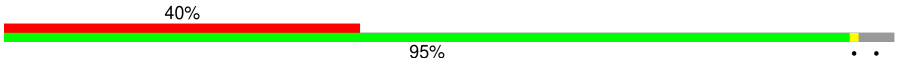


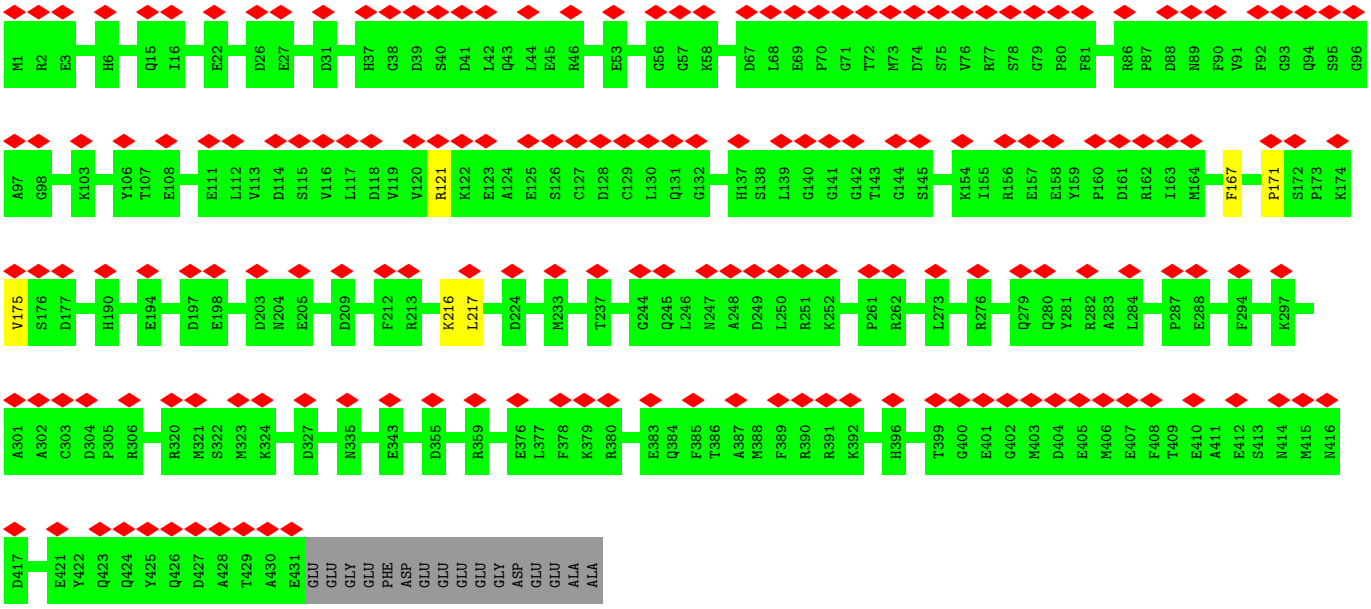




• Molecule 55: Tubulin beta chain

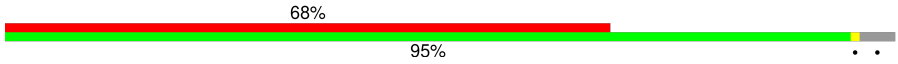
Chain IJ:

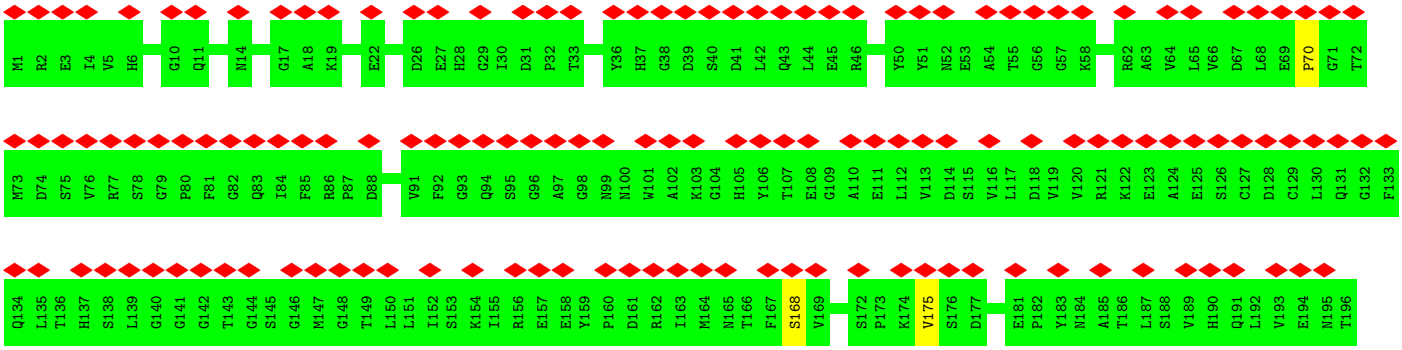


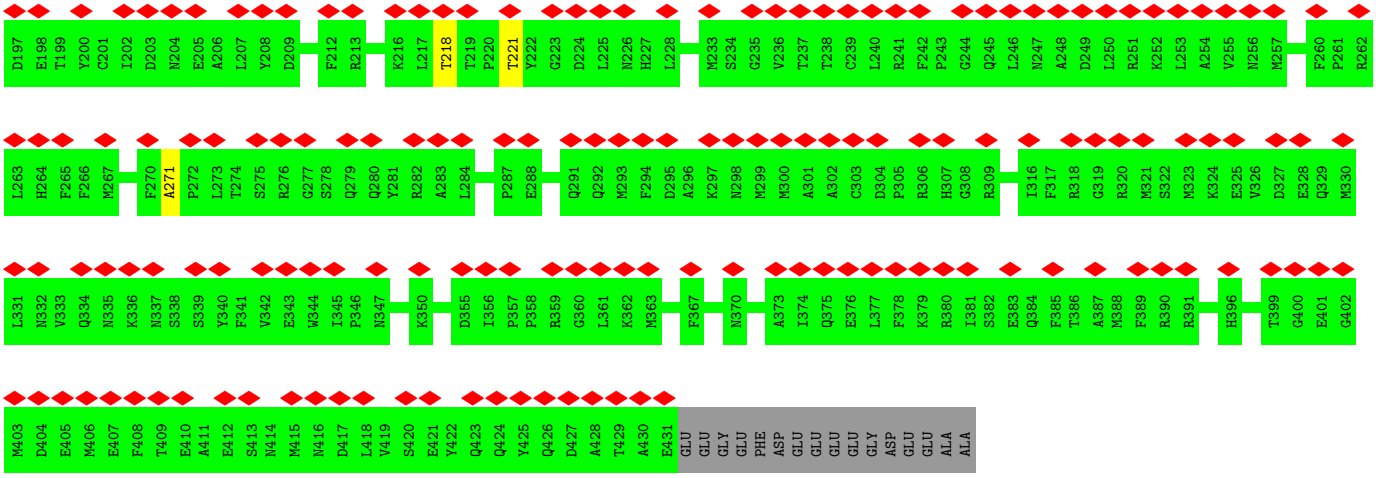


• Molecule 55: Tubulin beta chain

Chain IL:

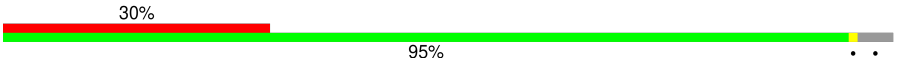


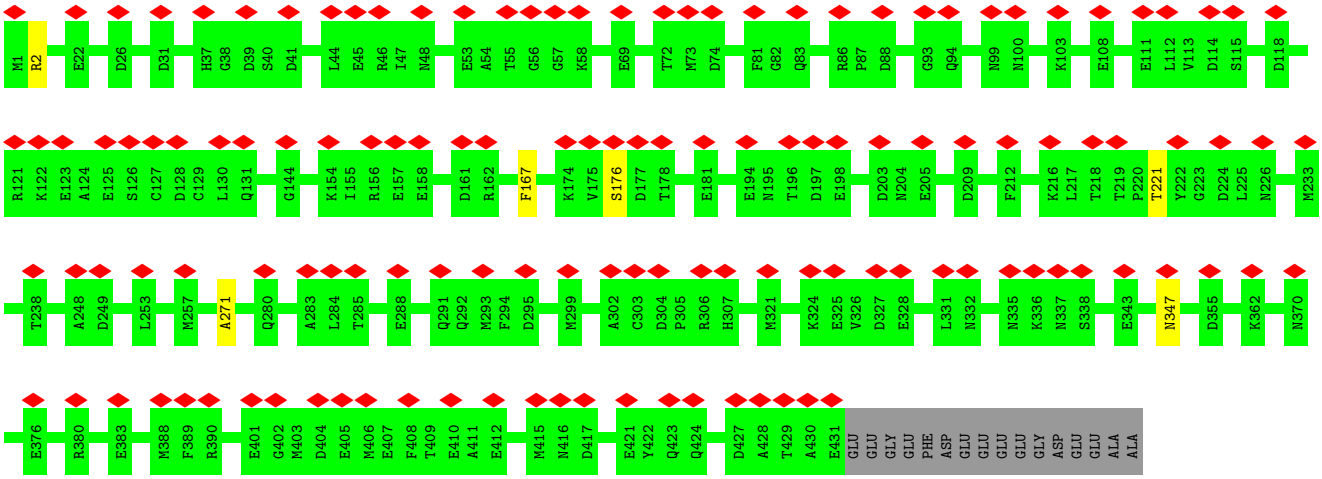




- Molecule 55: Tubulin beta chain

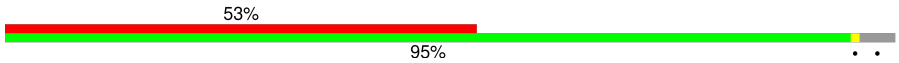
Chain JC:

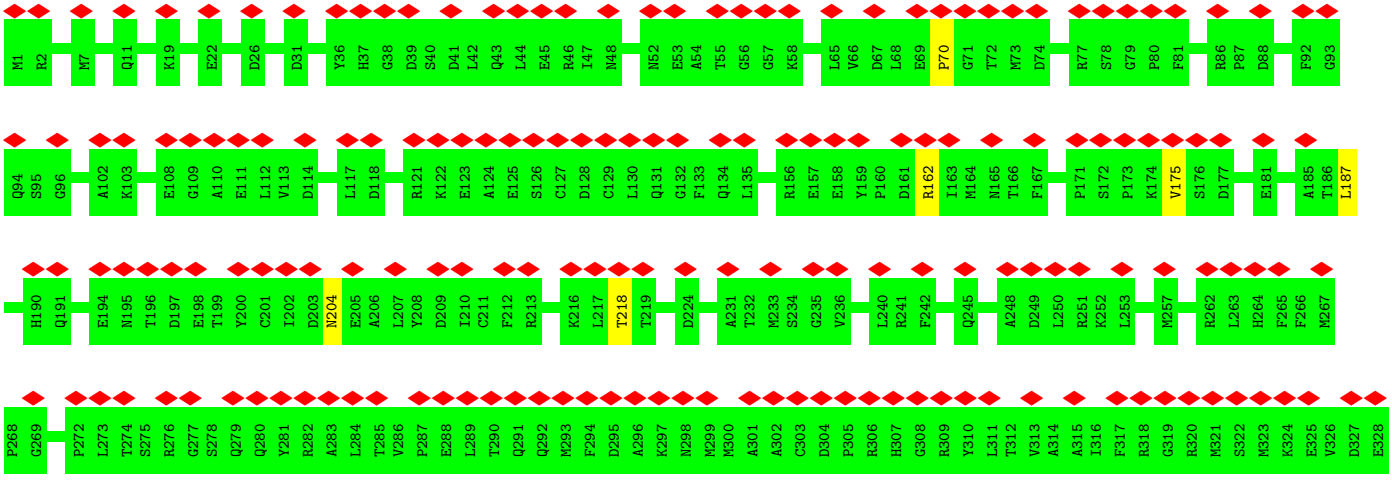


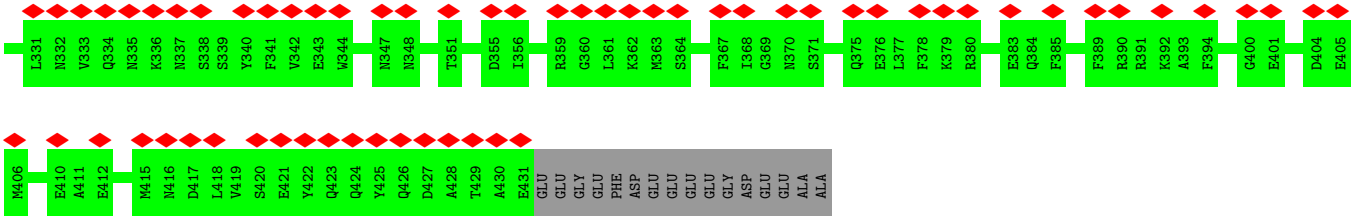


- Molecule 55: Tubulin beta chain

Chain JD:

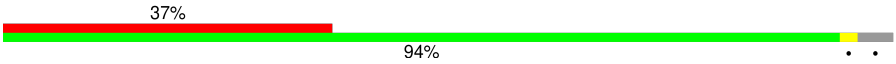


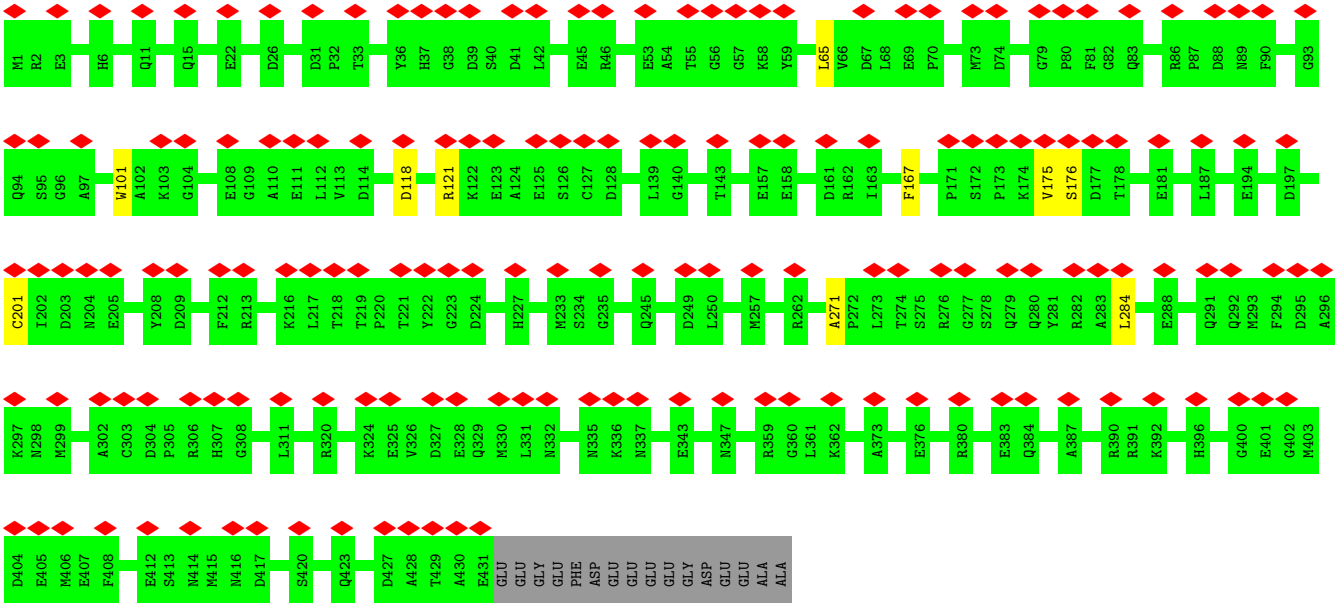




• Molecule 55: Tubulin beta chain

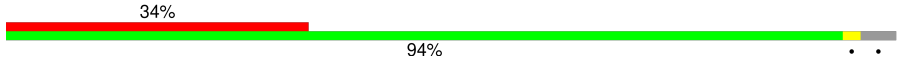
Chain JF:

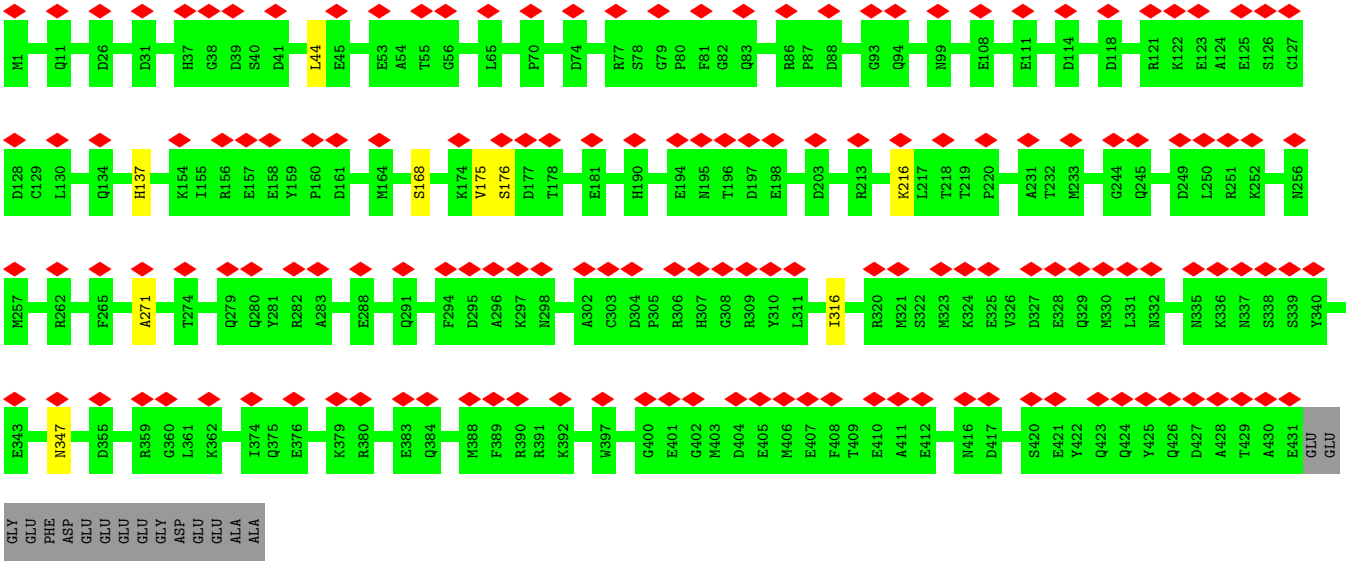




• Molecule 55: Tubulin beta chain

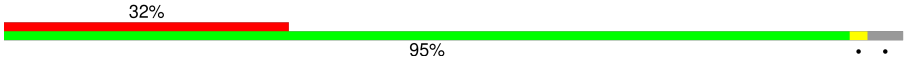
Chain JH:

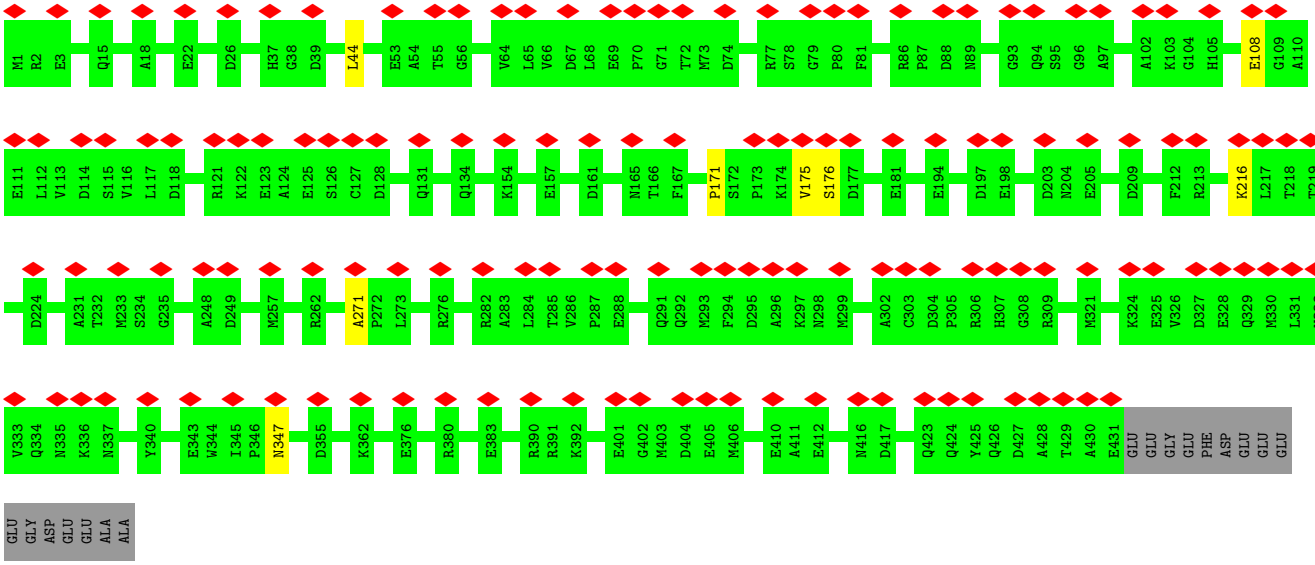




• Molecule 55: Tubulin beta chain

Chain JJ:





• Molecule 55: Tubulin beta chain

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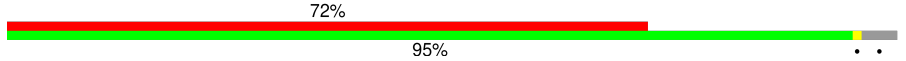
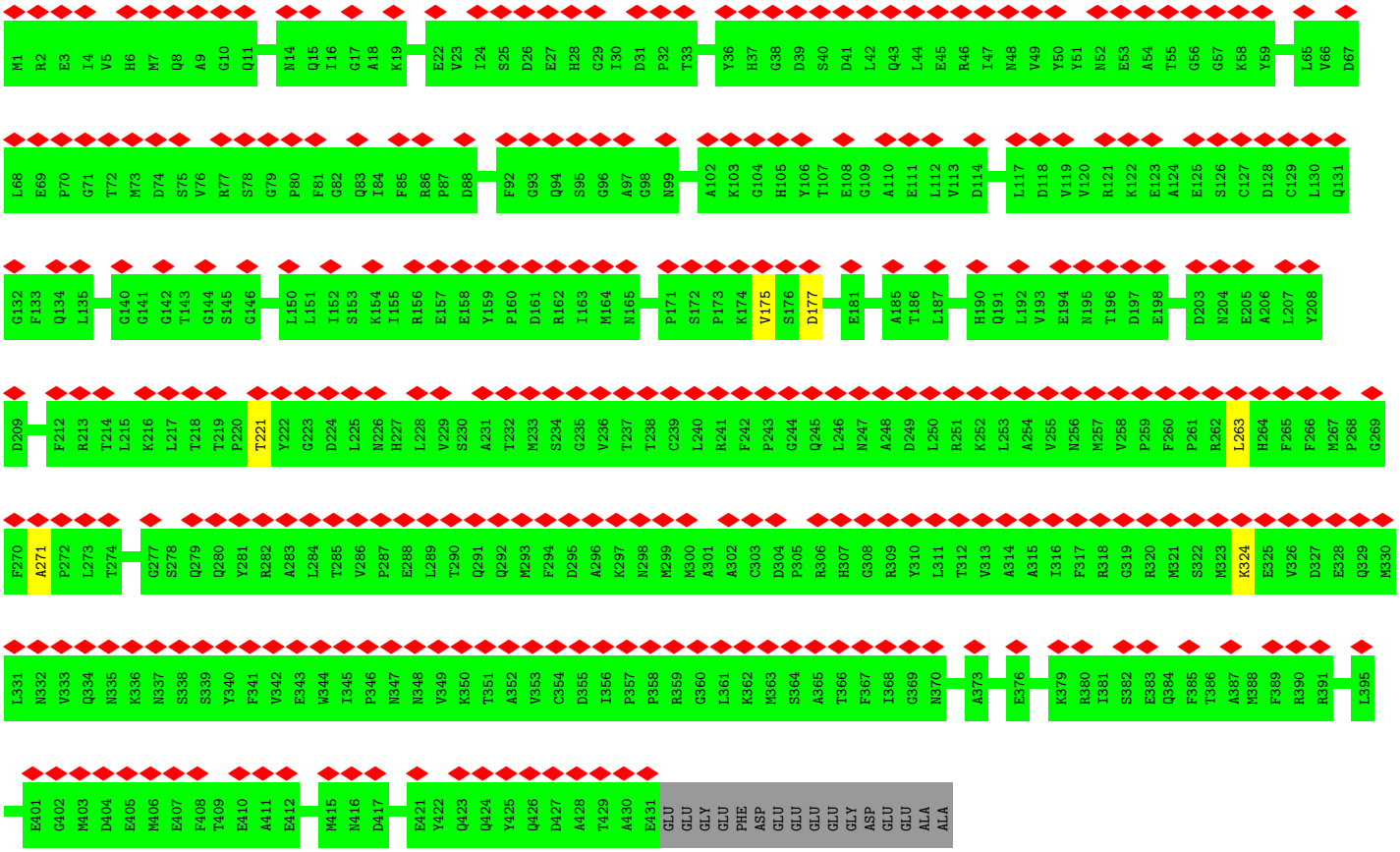
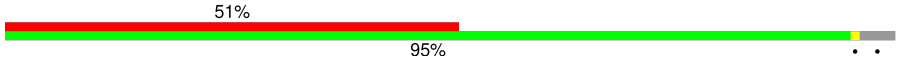
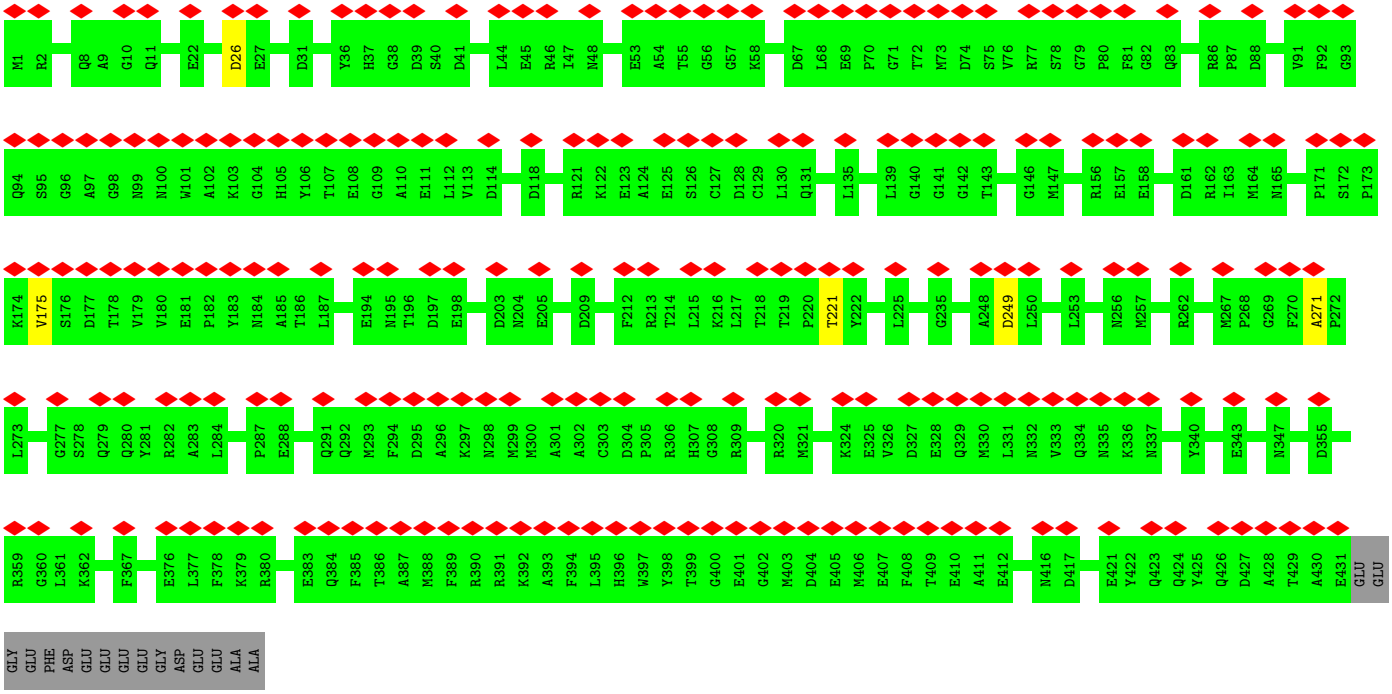




• Molecule 55: Tubulin beta chain

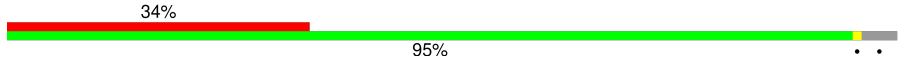
Chain JM:

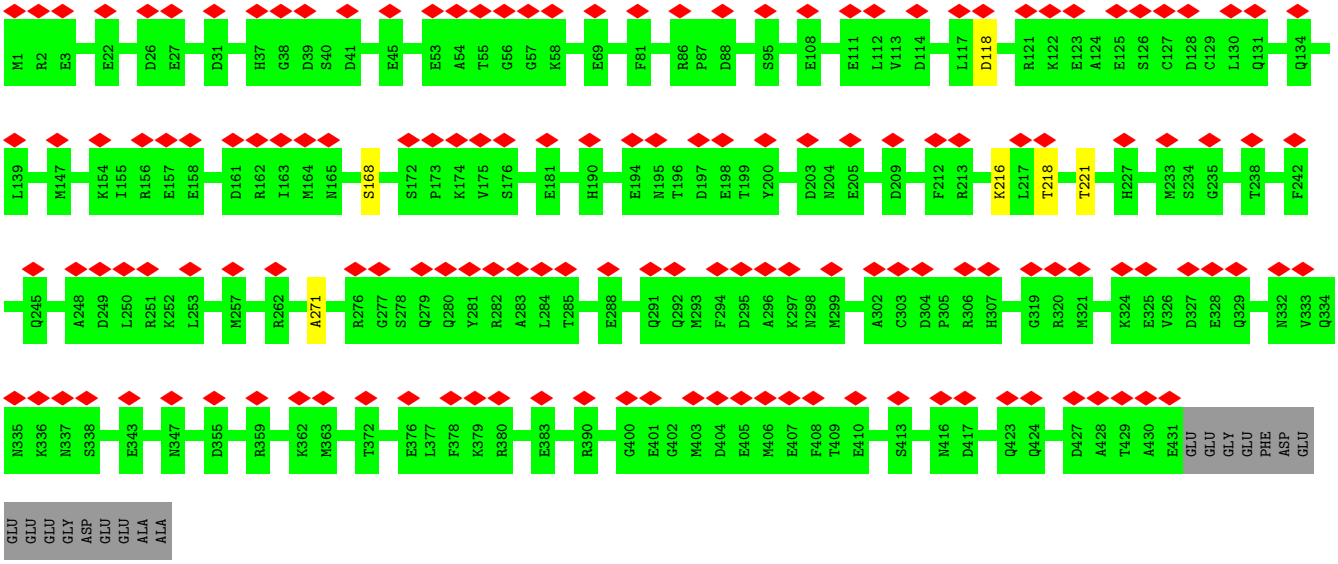




• Molecule 55: Tubulin beta chain

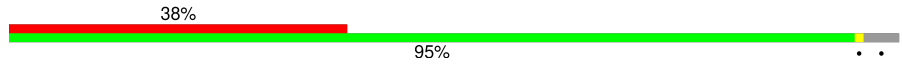
Chain KC:

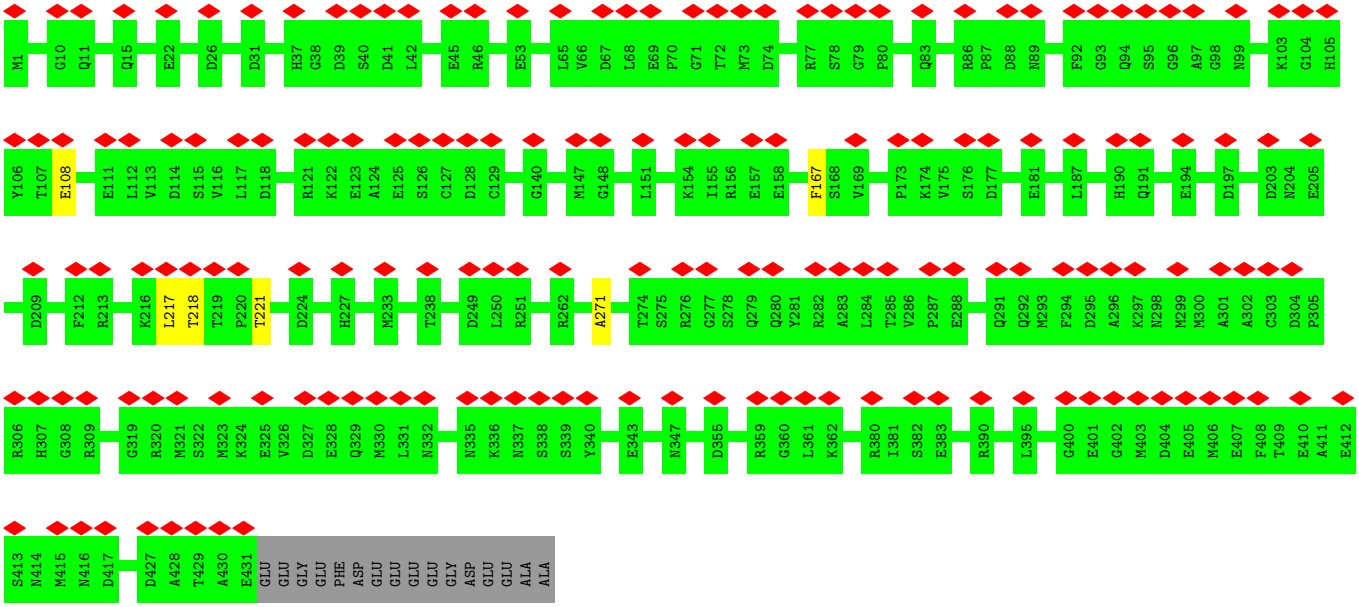




• Molecule 55: Tubulin beta chain

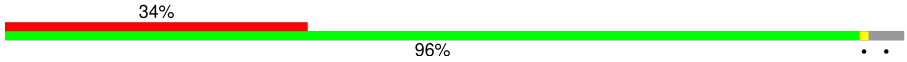
Chain KD:

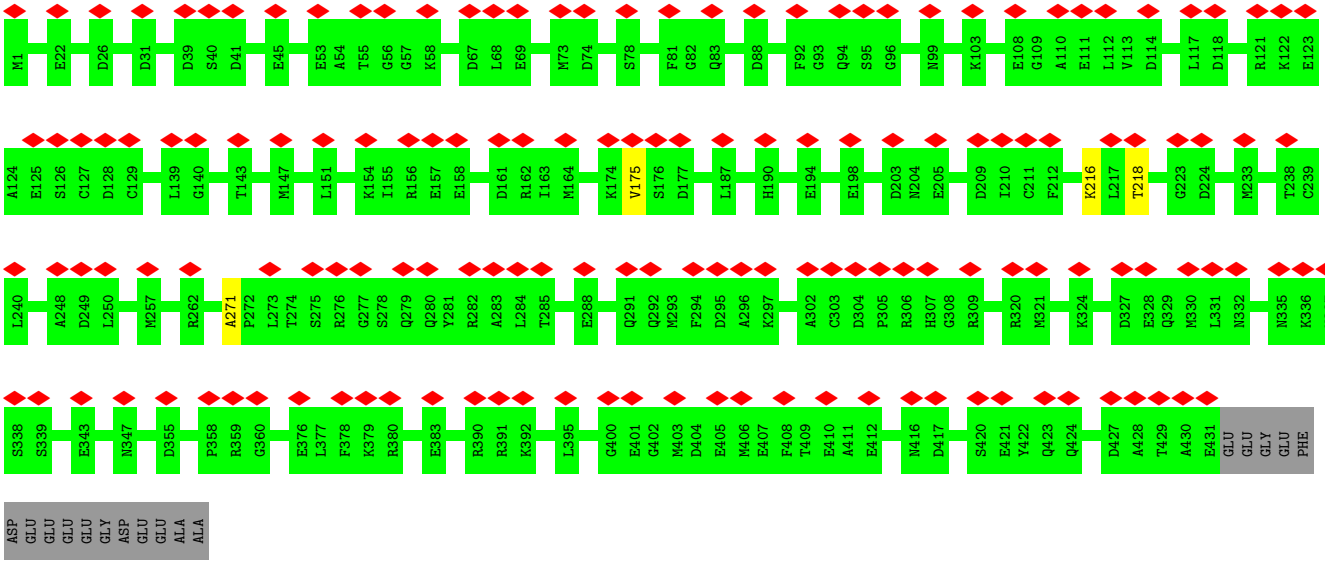




- Molecule 55: Tubulin beta chain

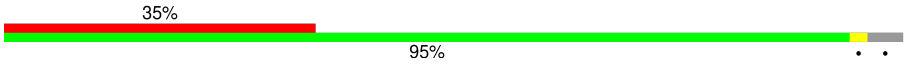
Chain KF:

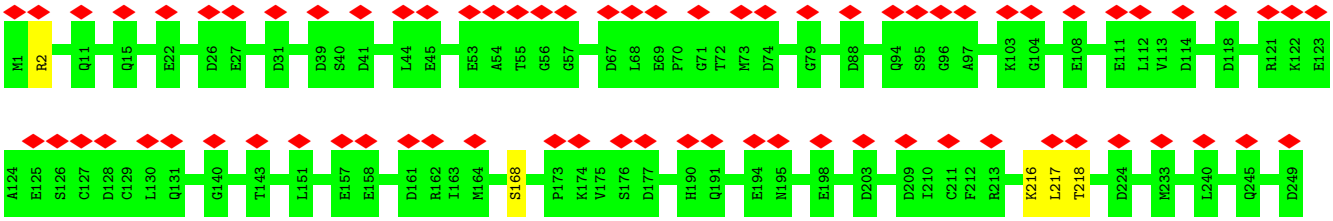


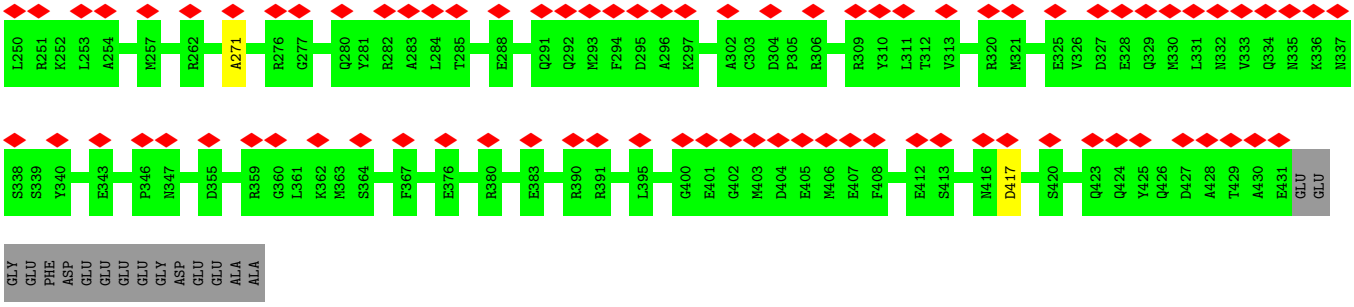


- Molecule 55: Tubulin beta chain

Chain KH:

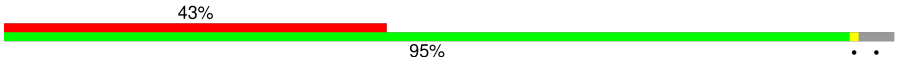


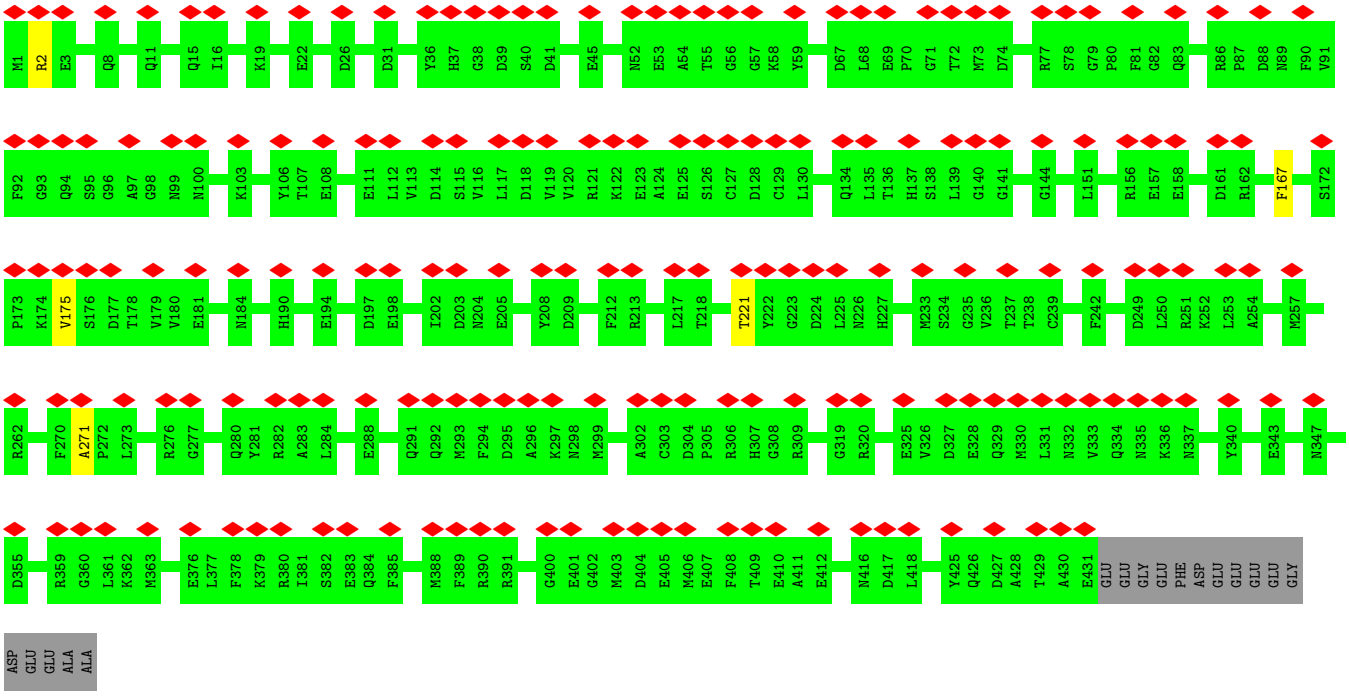




- Molecule 55: Tubulin beta chain

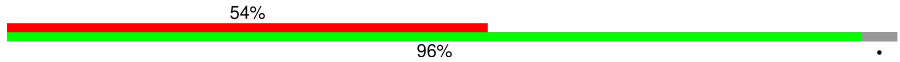
Chain KJ:

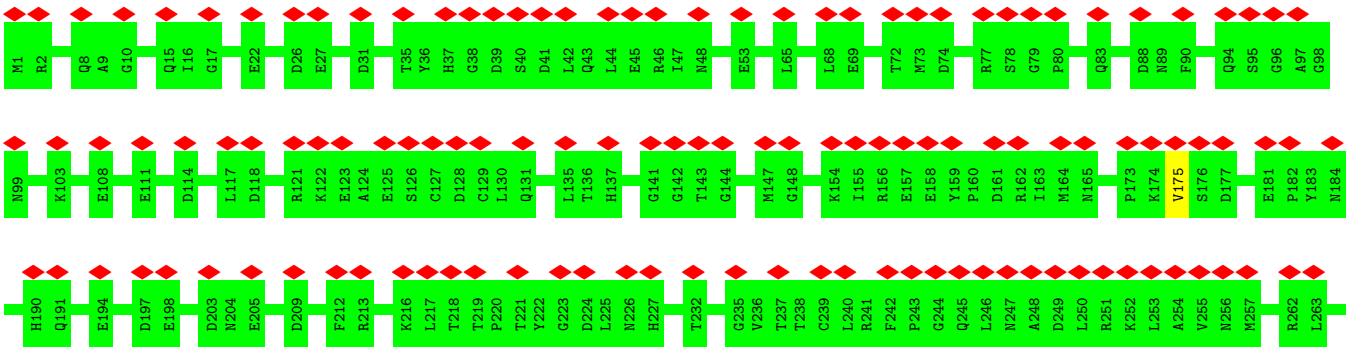


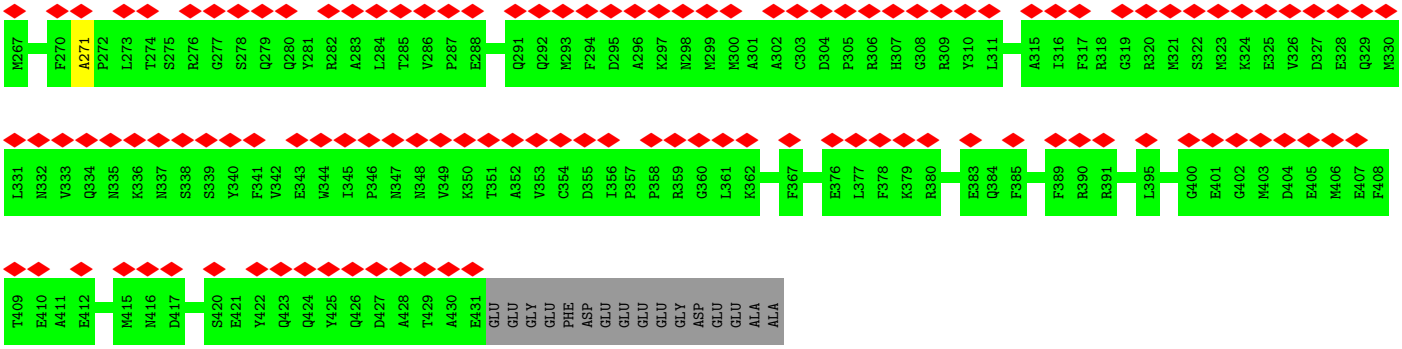


- Molecule 55: Tubulin beta chain

Chain KL:

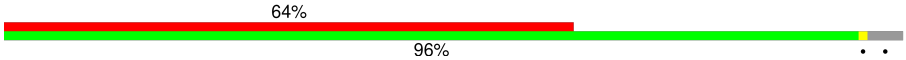


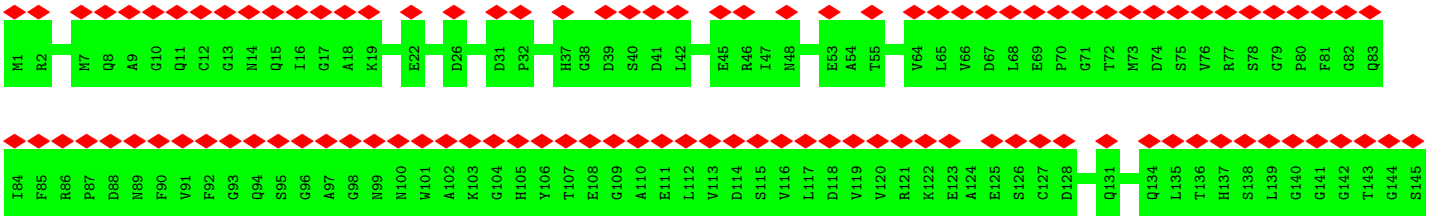




- Molecule 55: Tubulin beta chain

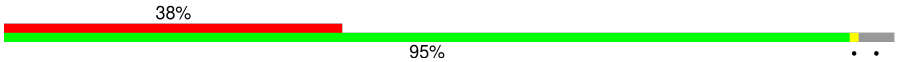
Chain KM:

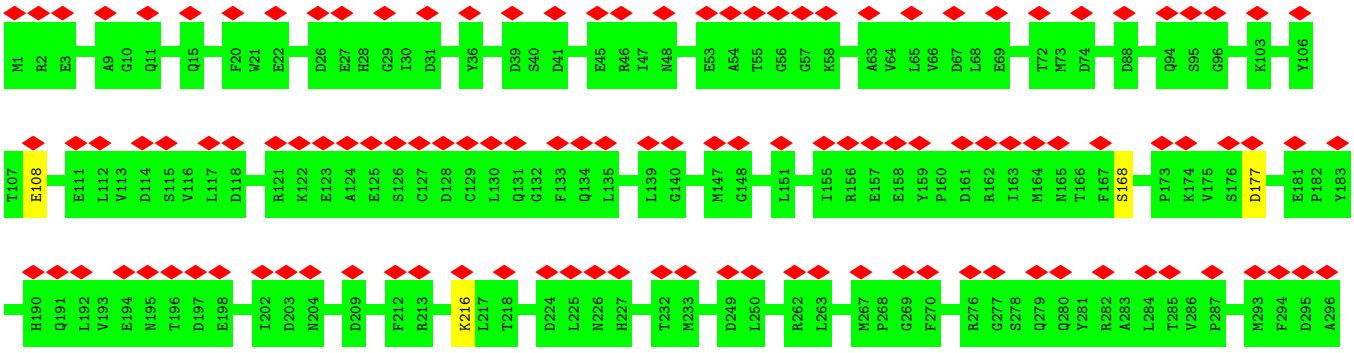


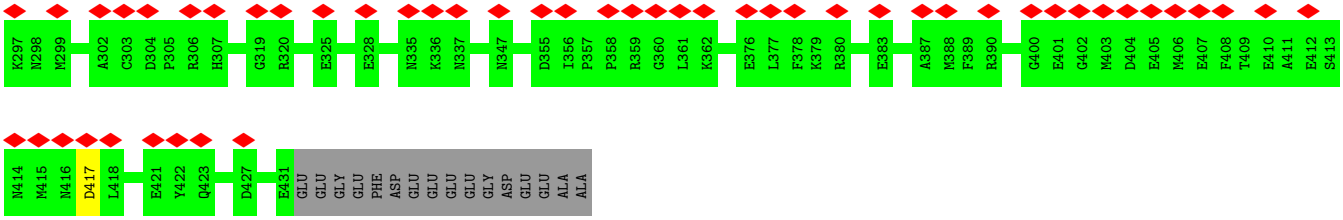


- Molecule 55: Tubulin beta chain

Chain LC:

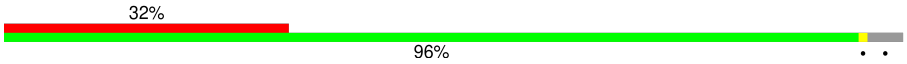


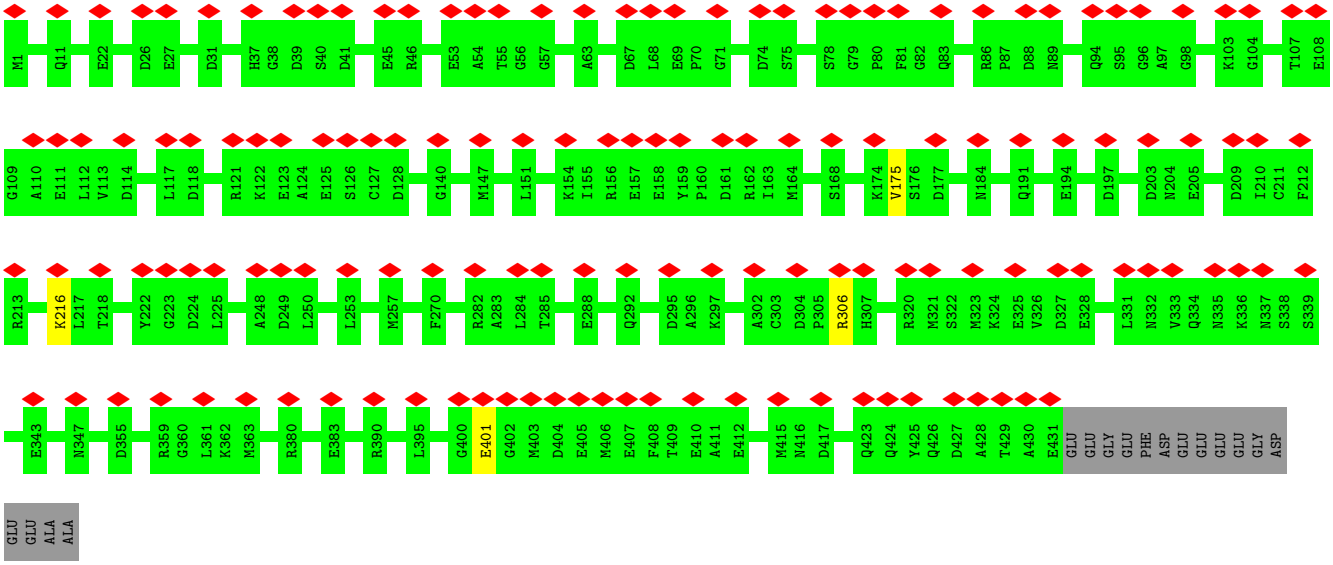




• Molecule 55: Tubulin beta chain

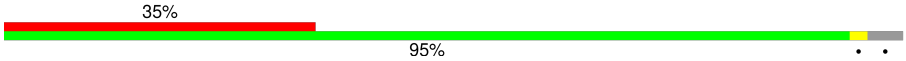
Chain LD:

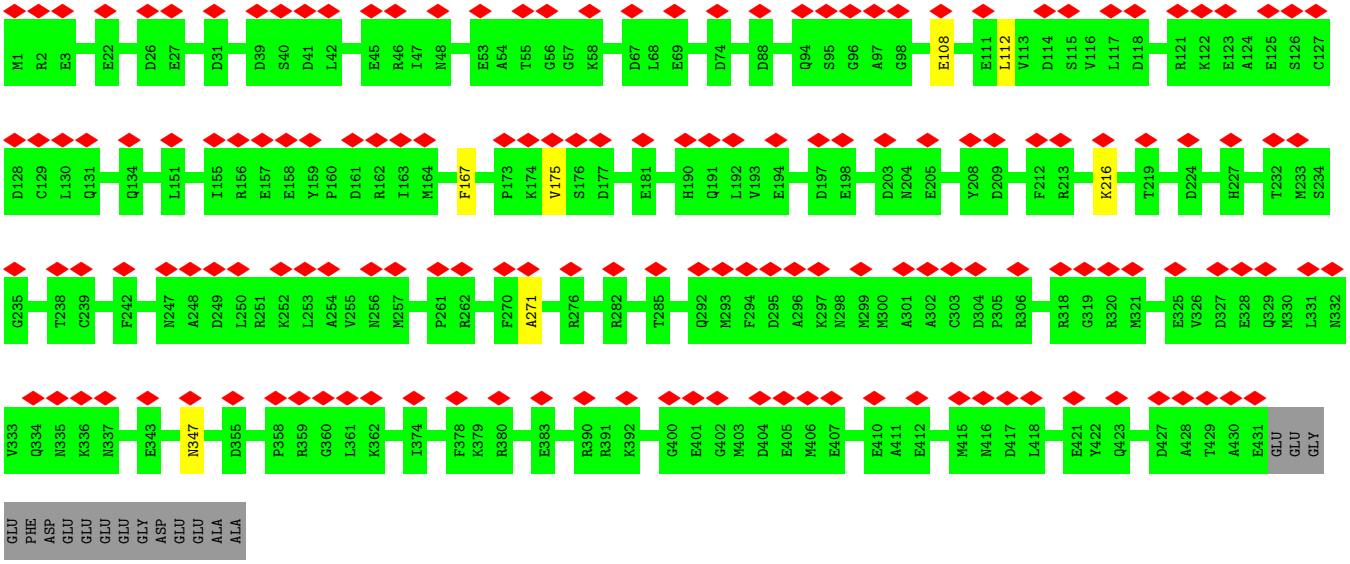




• Molecule 55: Tubulin beta chain

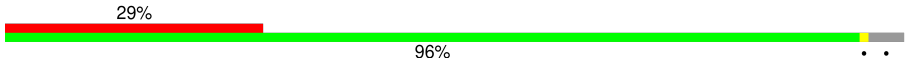
Chain LF:

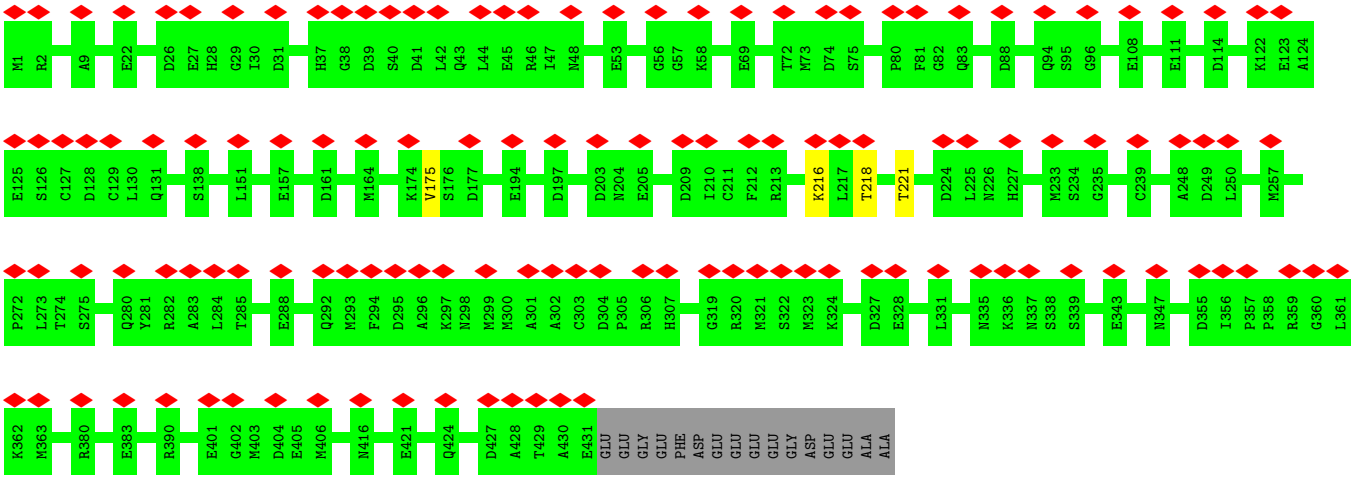




• Molecule 55: Tubulin beta chain

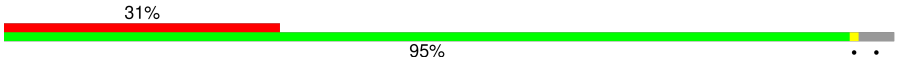
Chain LH:

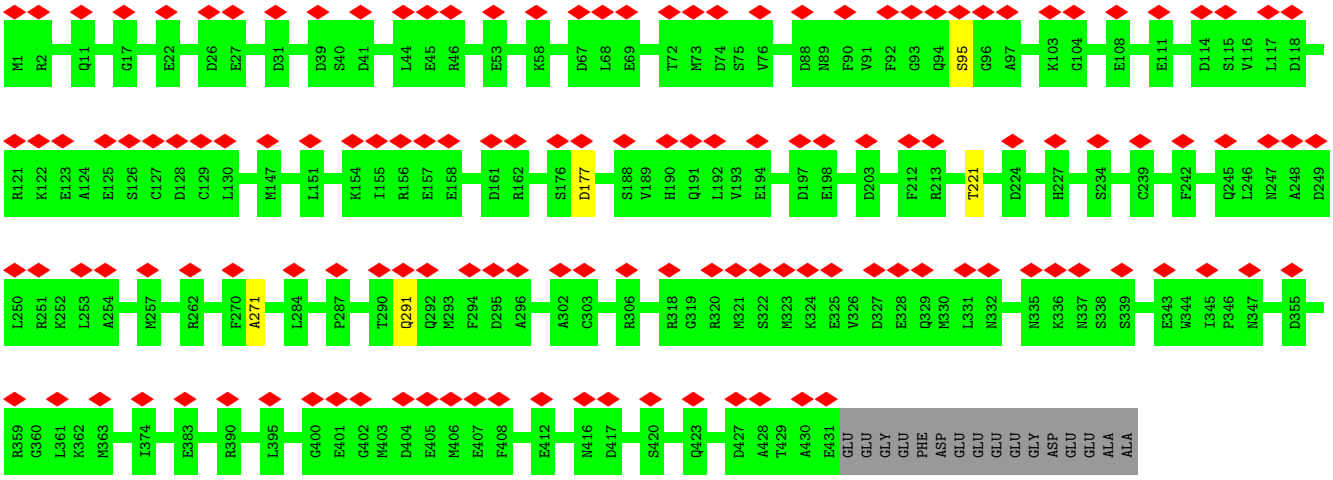




- Molecule 55: Tubulin beta chain

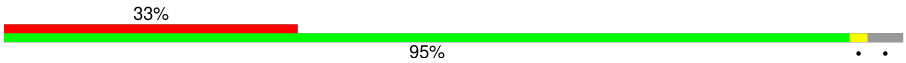
Chain LJ:

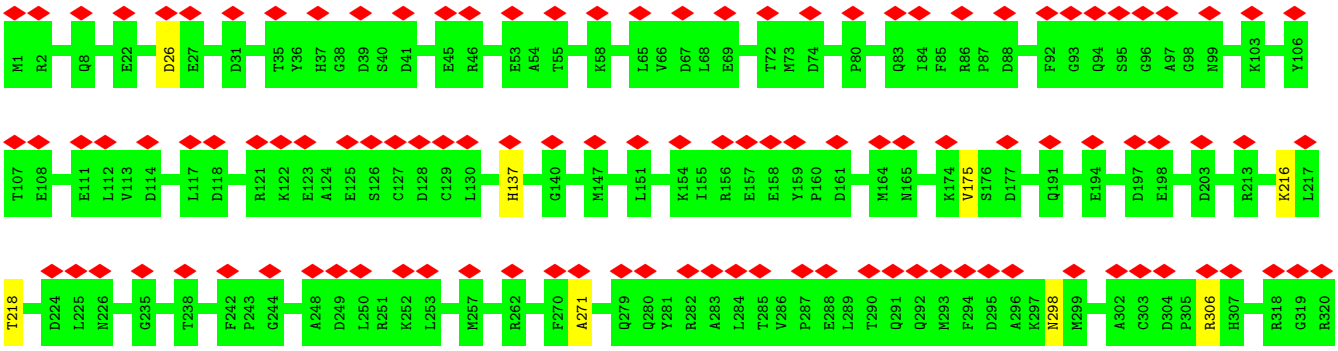


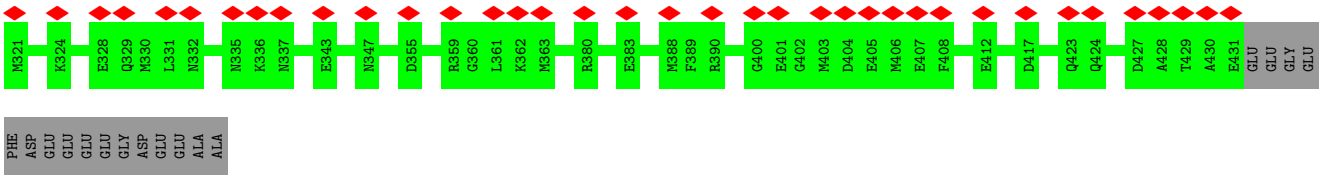


- Molecule 55: Tubulin beta chain

Chain LL:

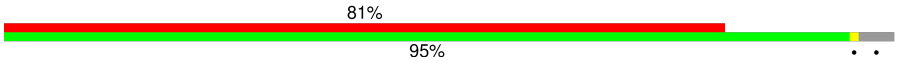


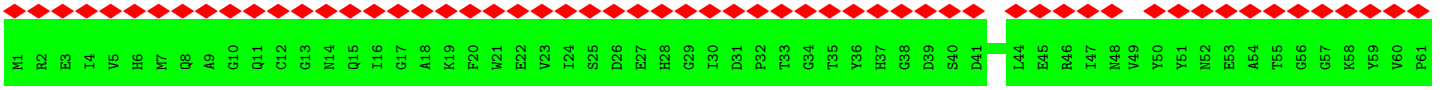


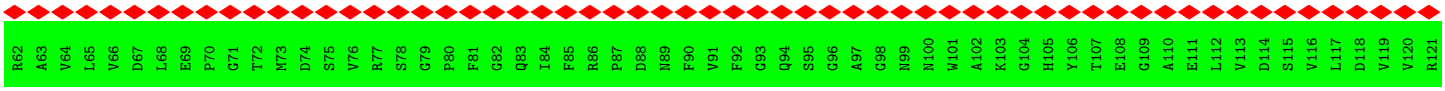


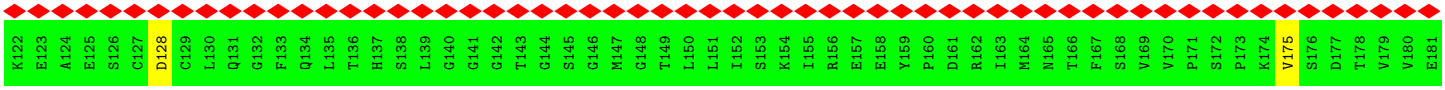
- Molecule 55: Tubulin beta chain

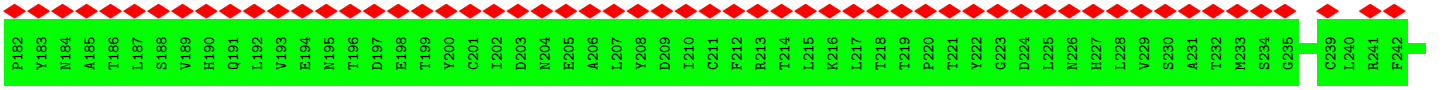
Chain LM:

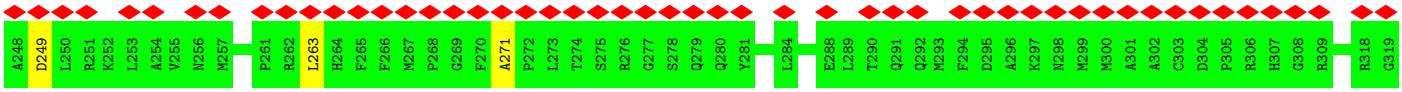


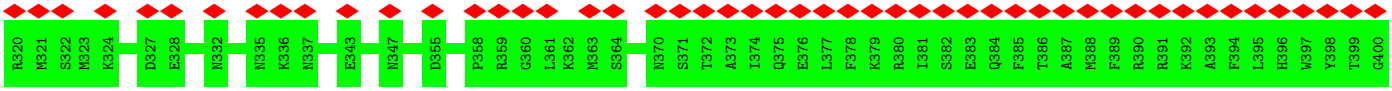


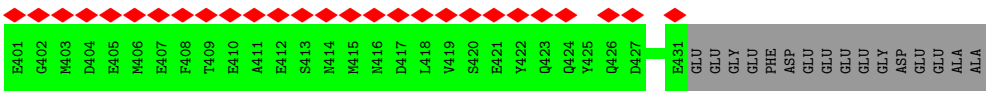






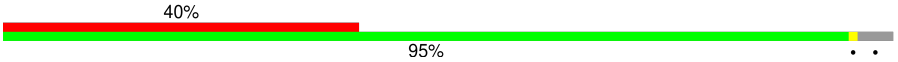


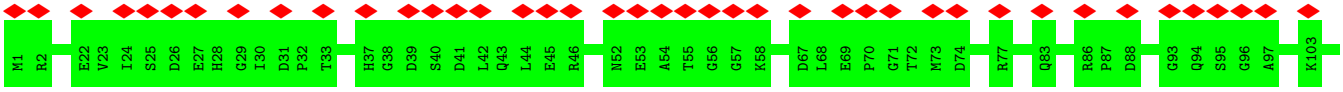


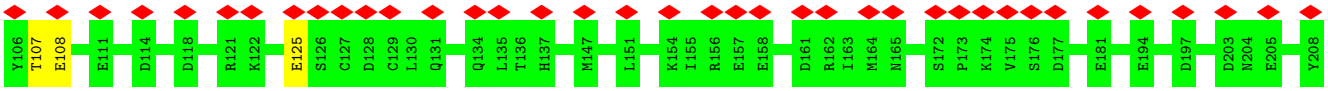


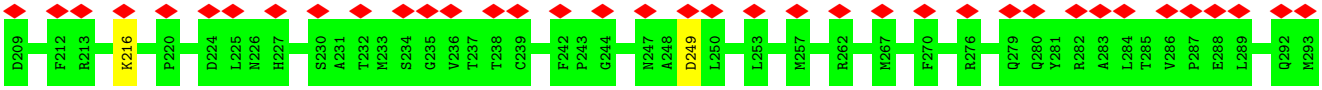
- Molecule 55: Tubulin beta chain

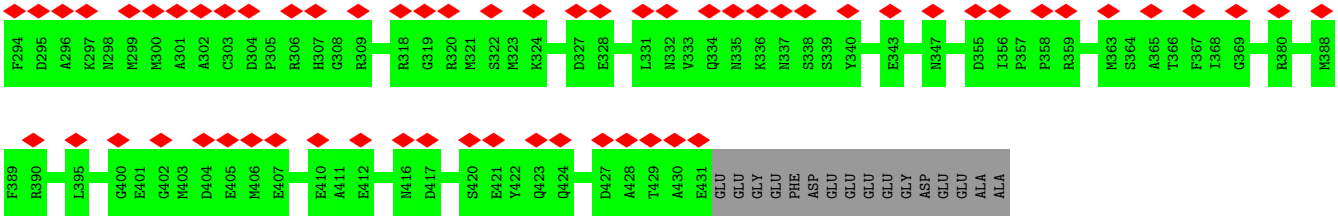
Chain MC:





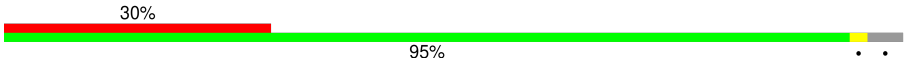


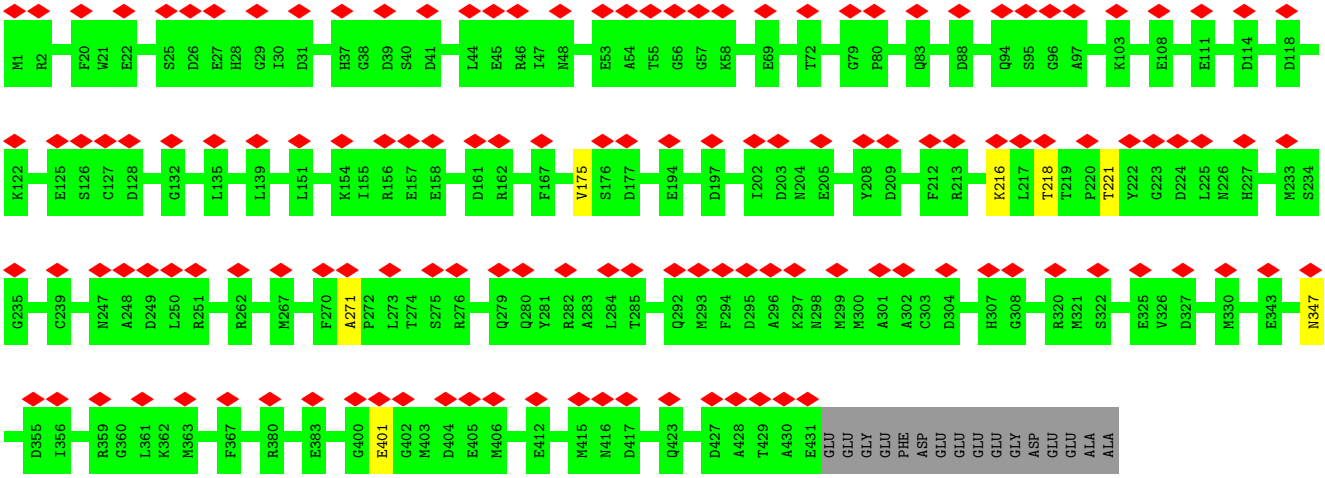




- Molecule 55: Tubulin beta chain

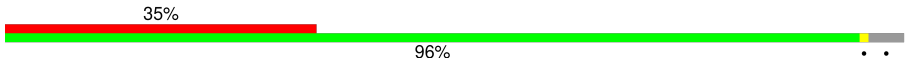
Chain MD:

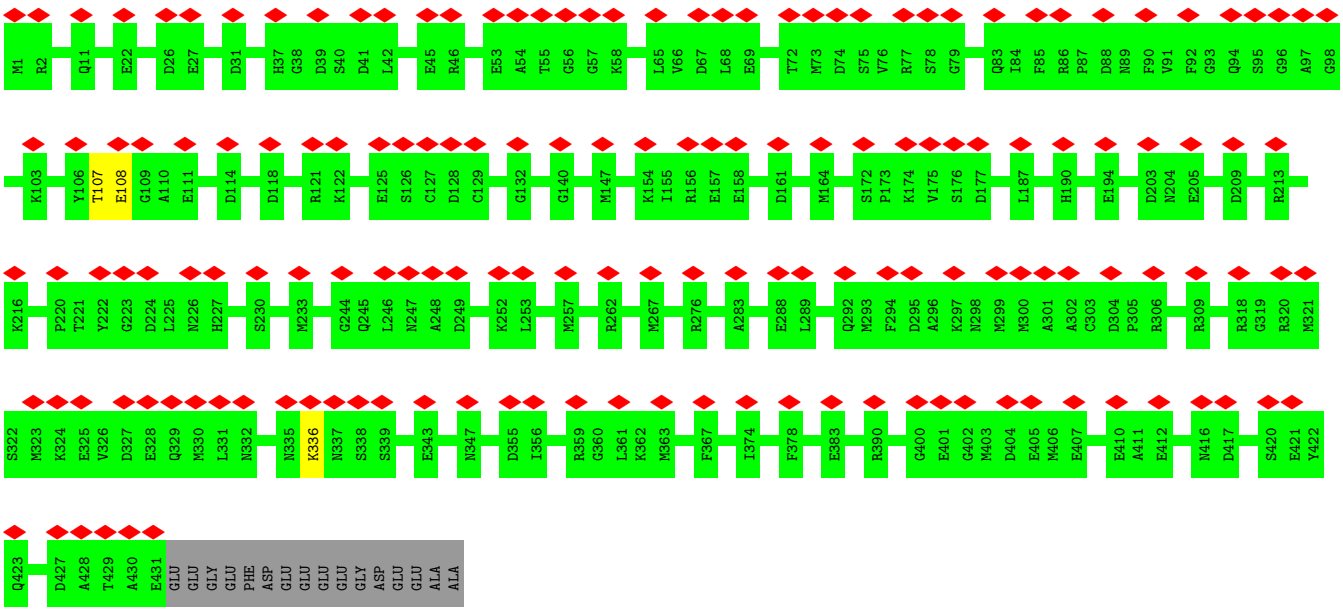




- Molecule 55: Tubulin beta chain

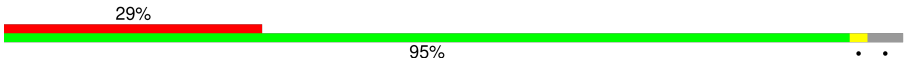
Chain MF:

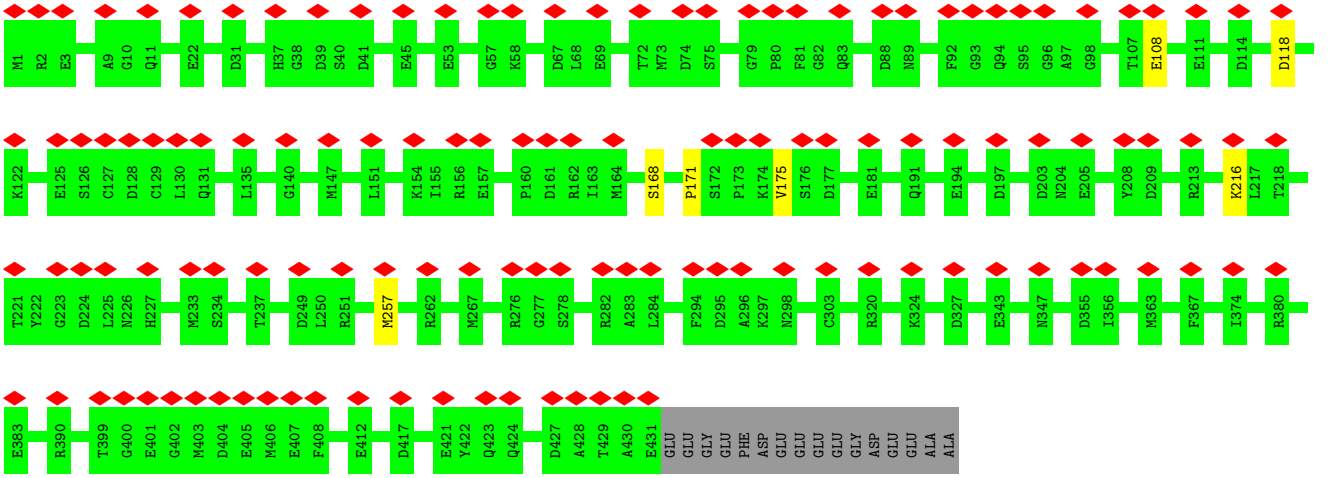




- Molecule 55: Tubulin beta chain

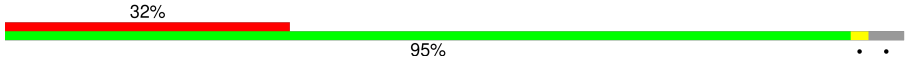
Chain MH:

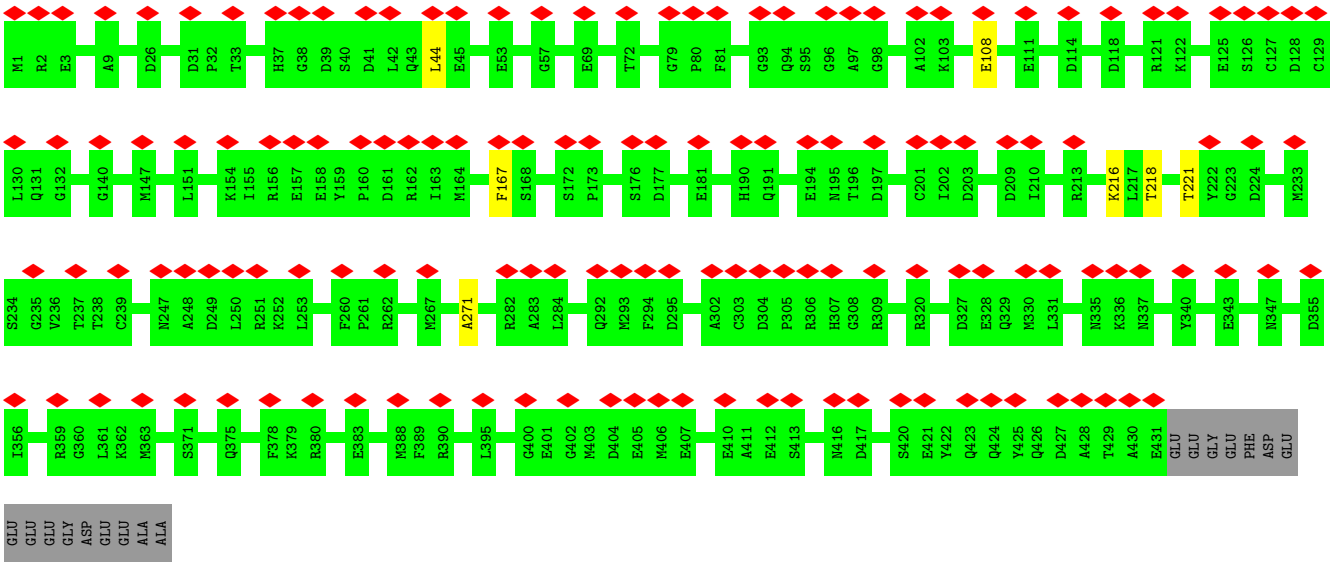




• Molecule 55: Tubulin beta chain

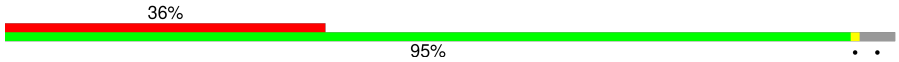
Chain MJ:

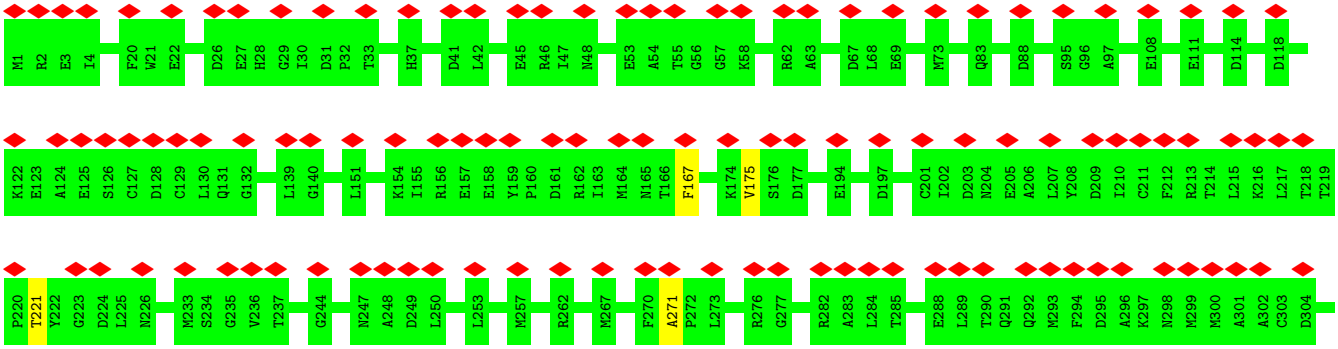


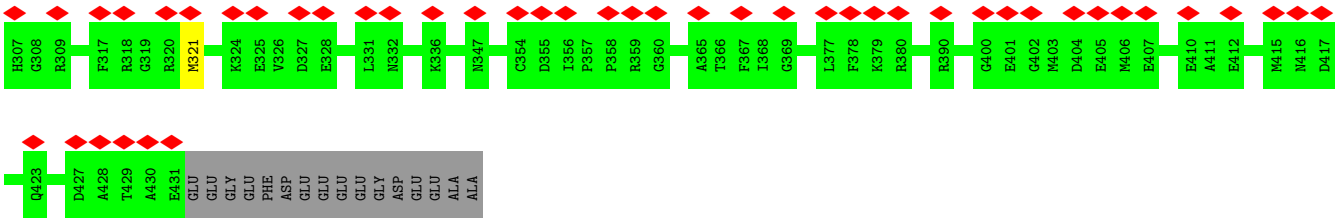


• Molecule 55: Tubulin beta chain

Chain MM:

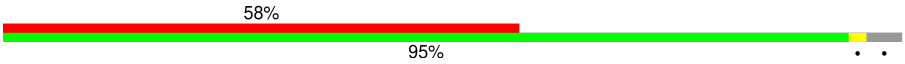


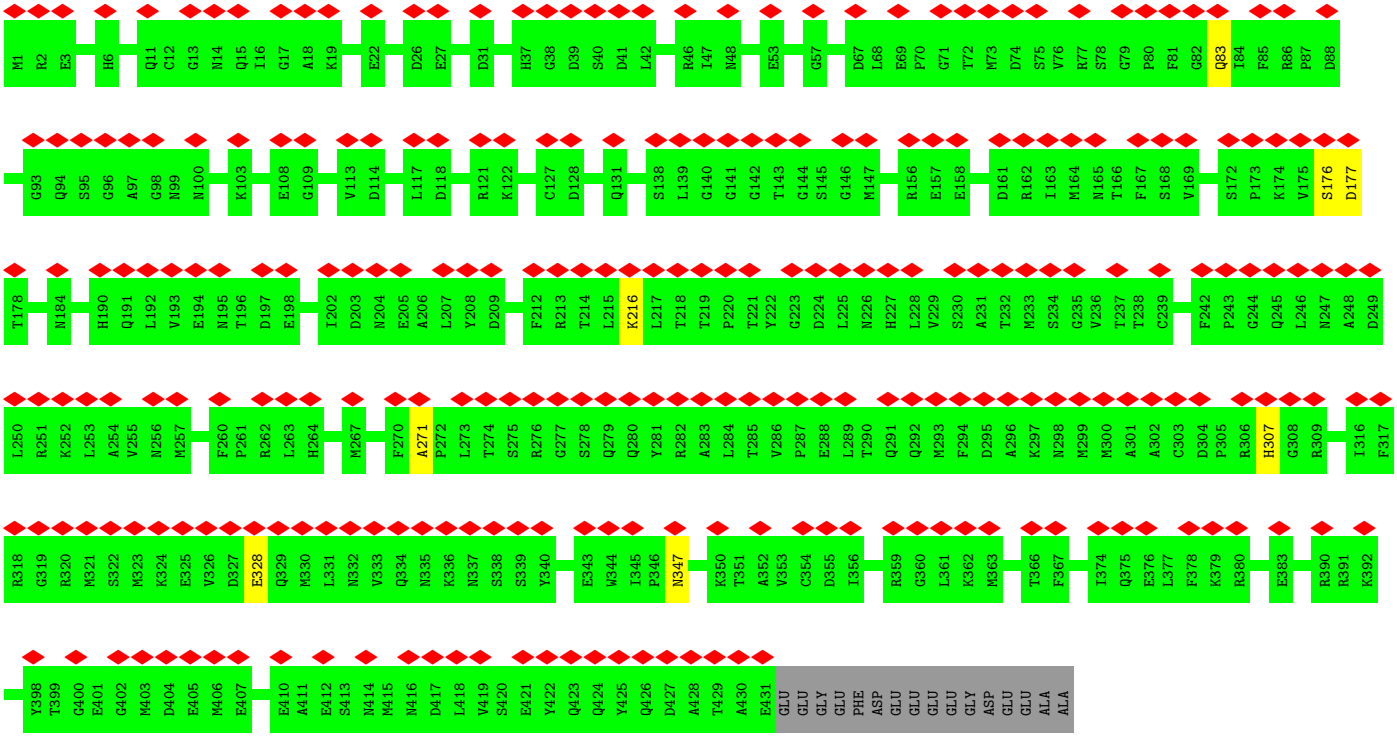




- Molecule 55: Tubulin beta chain

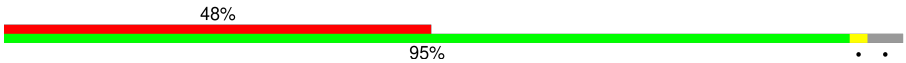
Chain NC:

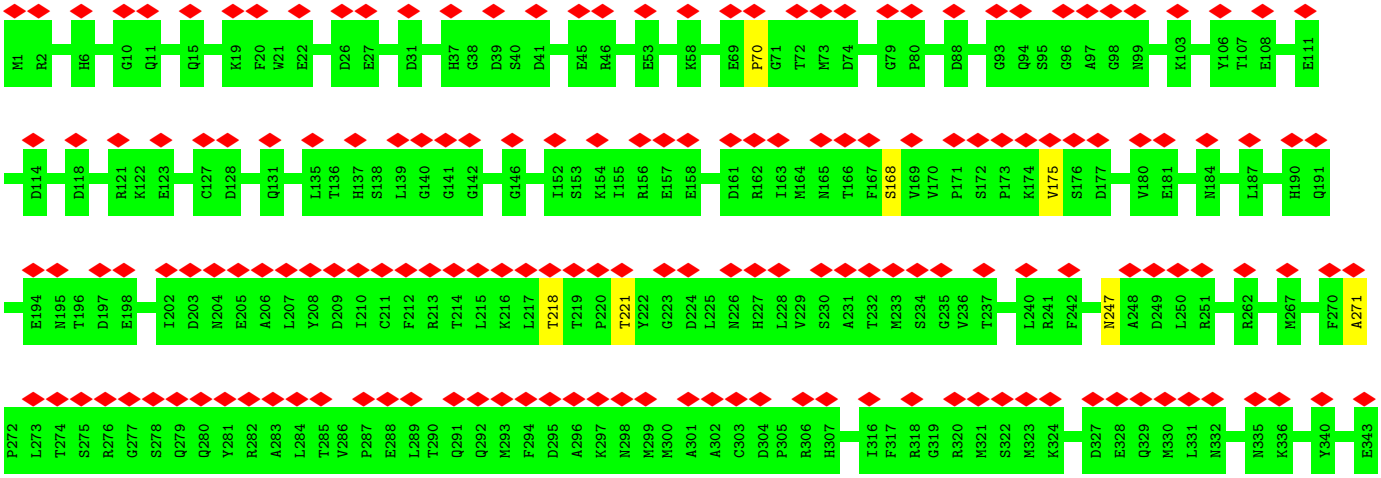


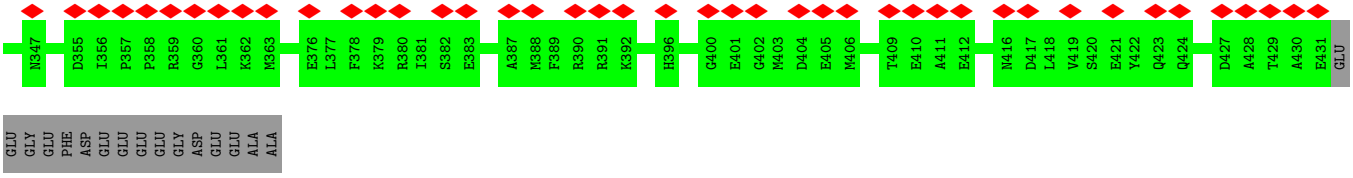


- Molecule 55: Tubulin beta chain

Chain ND:

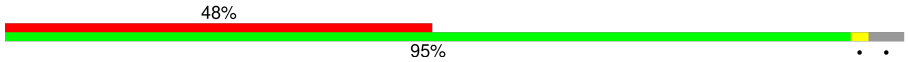


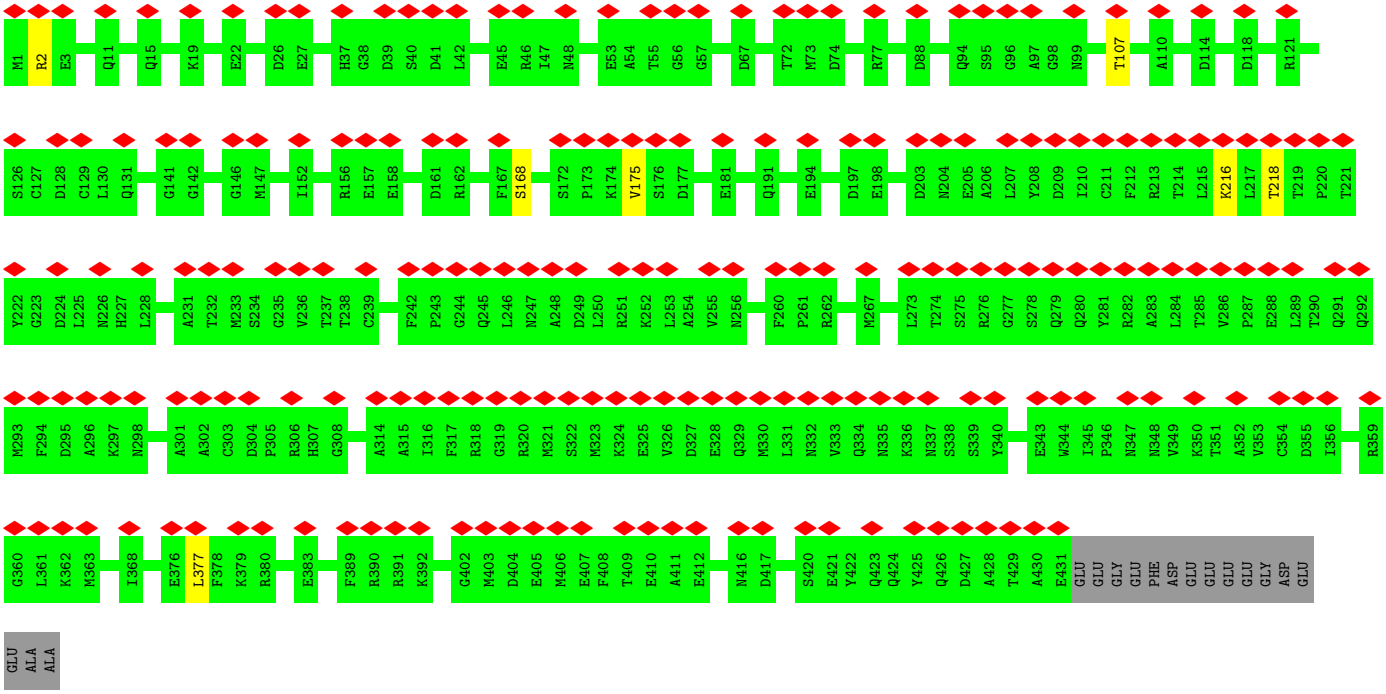




• Molecule 55: Tubulin beta chain

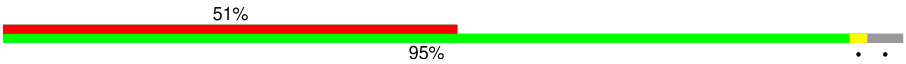
Chain NF:

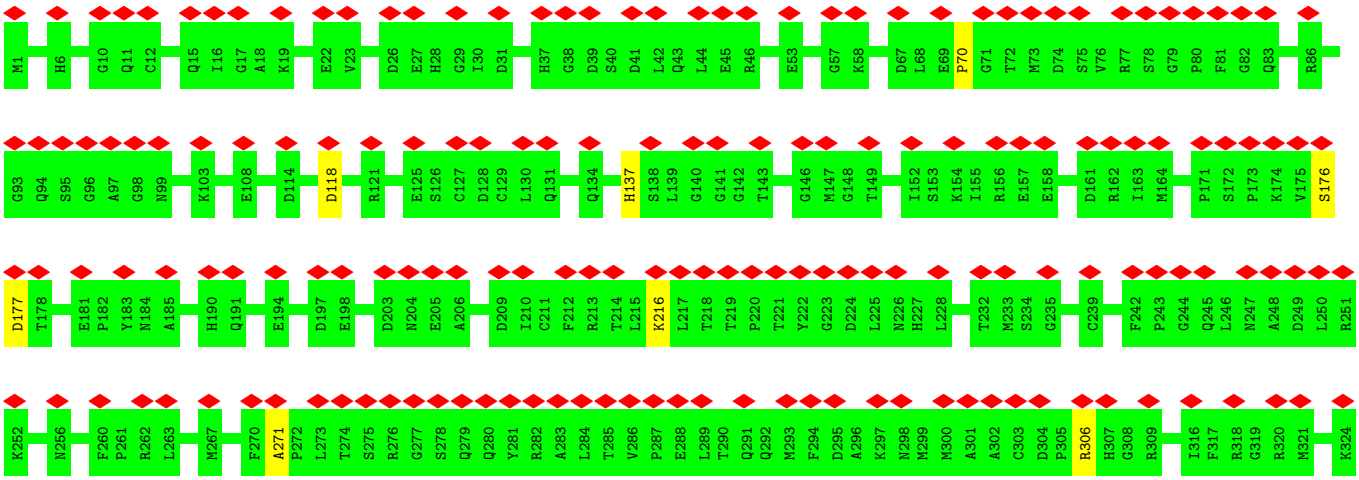


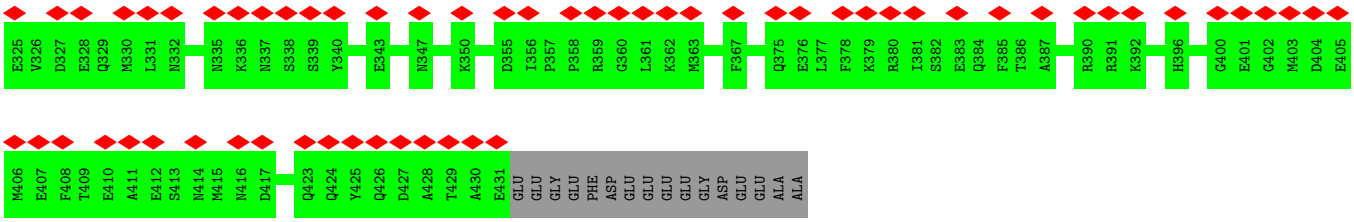


• Molecule 55: Tubulin beta chain

Chain NH:







• Molecule 55: Tubulin beta chain

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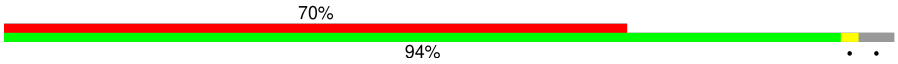

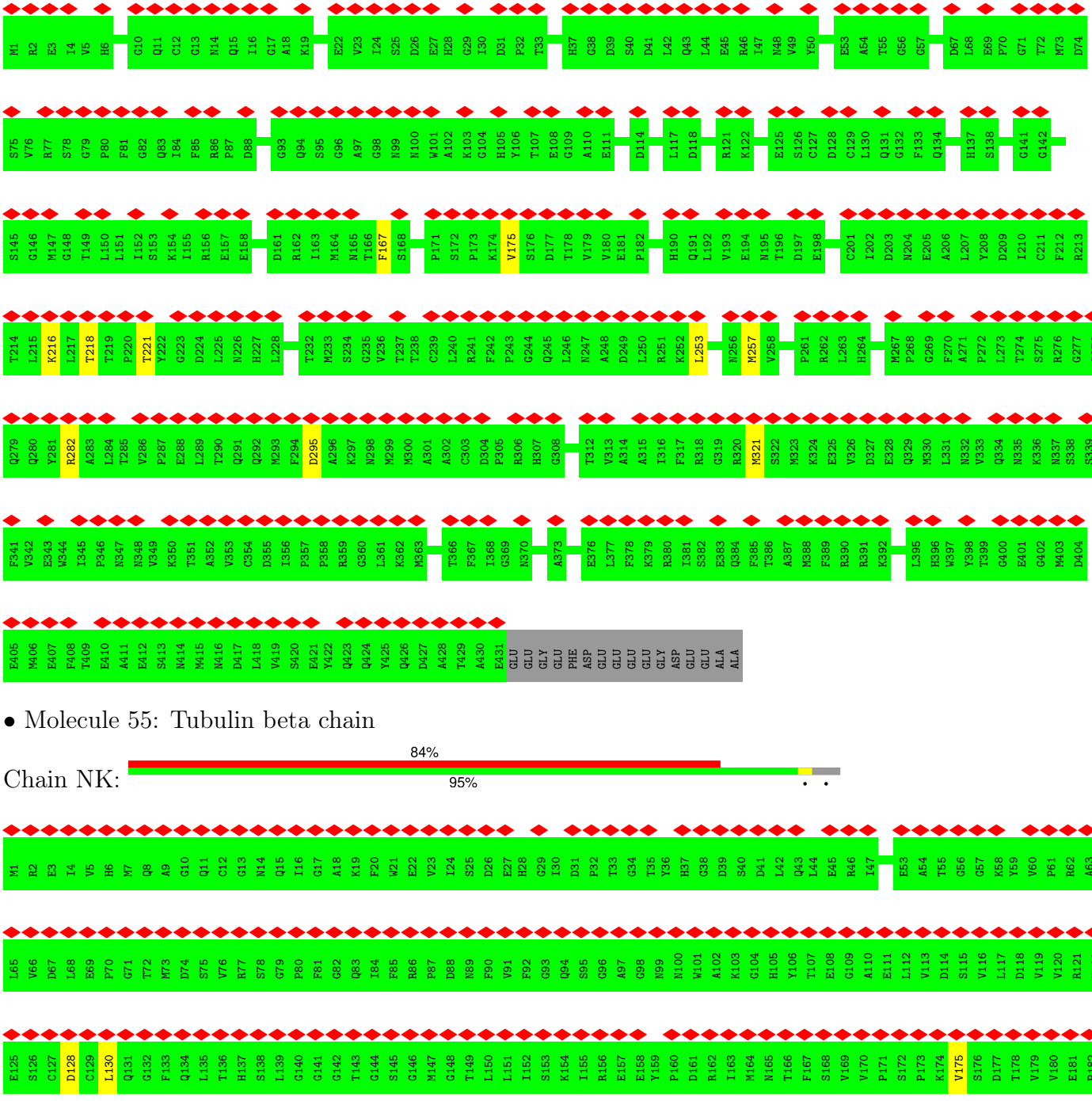

• Molecule 55: Tubulin beta chain

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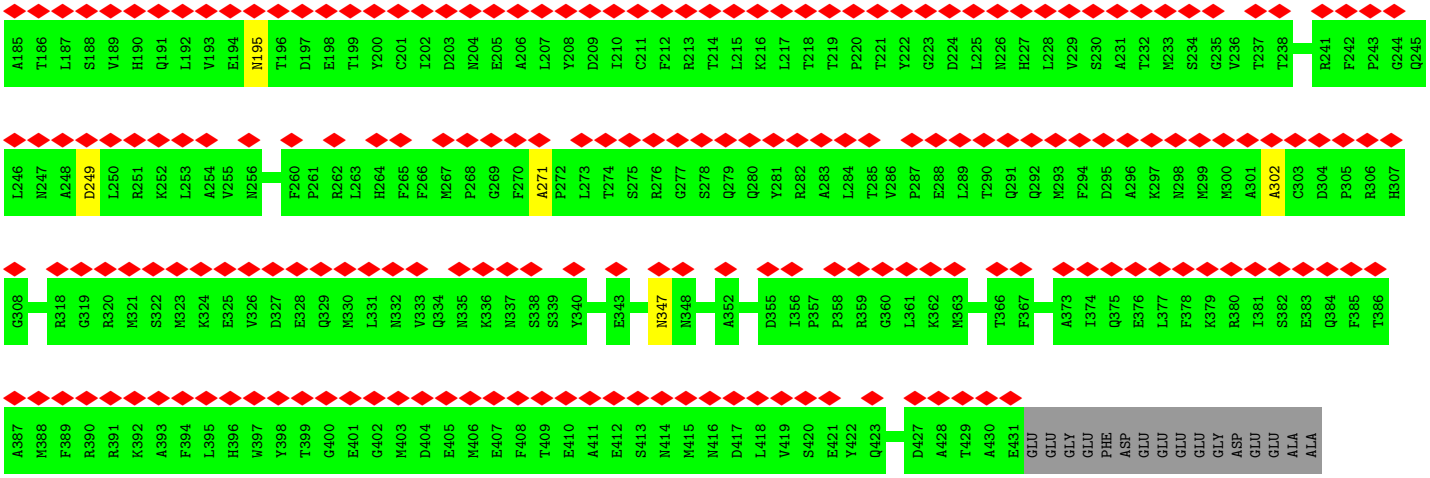
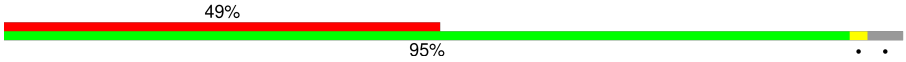
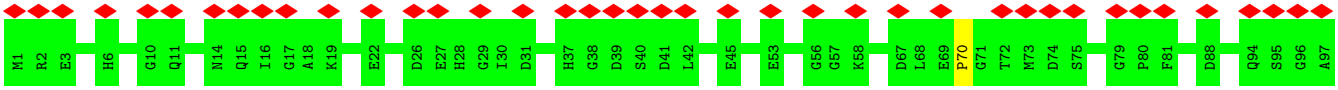
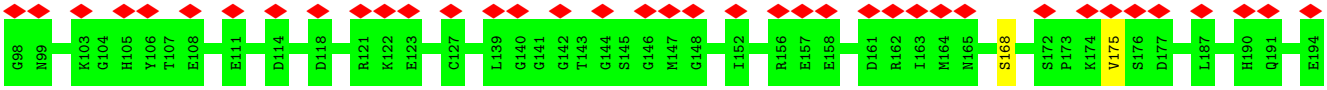


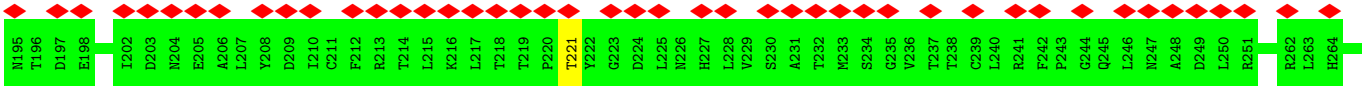
- Molecule 55: Tubulin beta chain

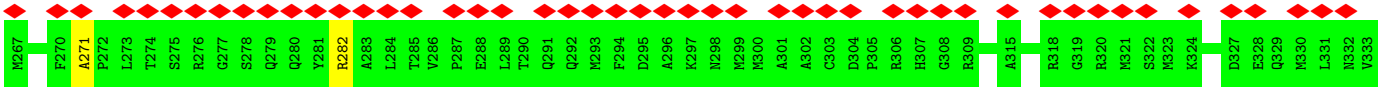
Chain NM:

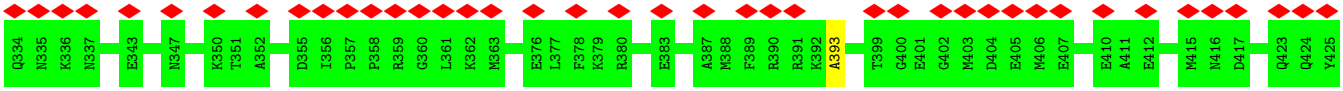


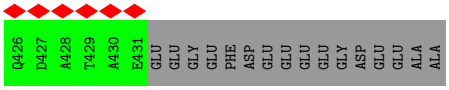






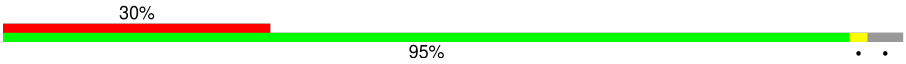


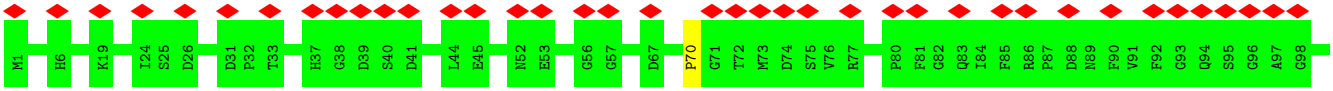


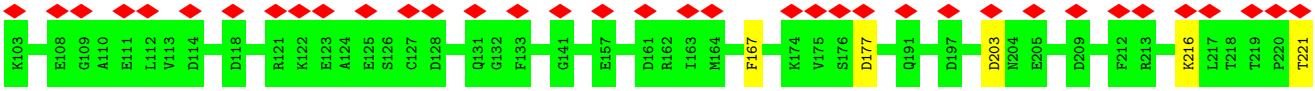


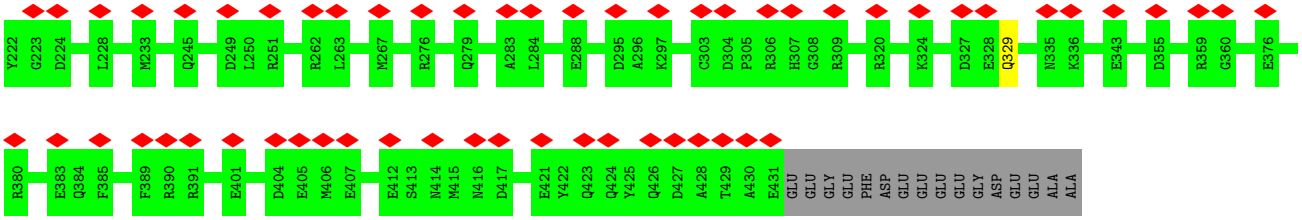
- Molecule 55: Tubulin beta chain

Chain OC:



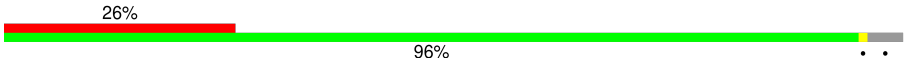


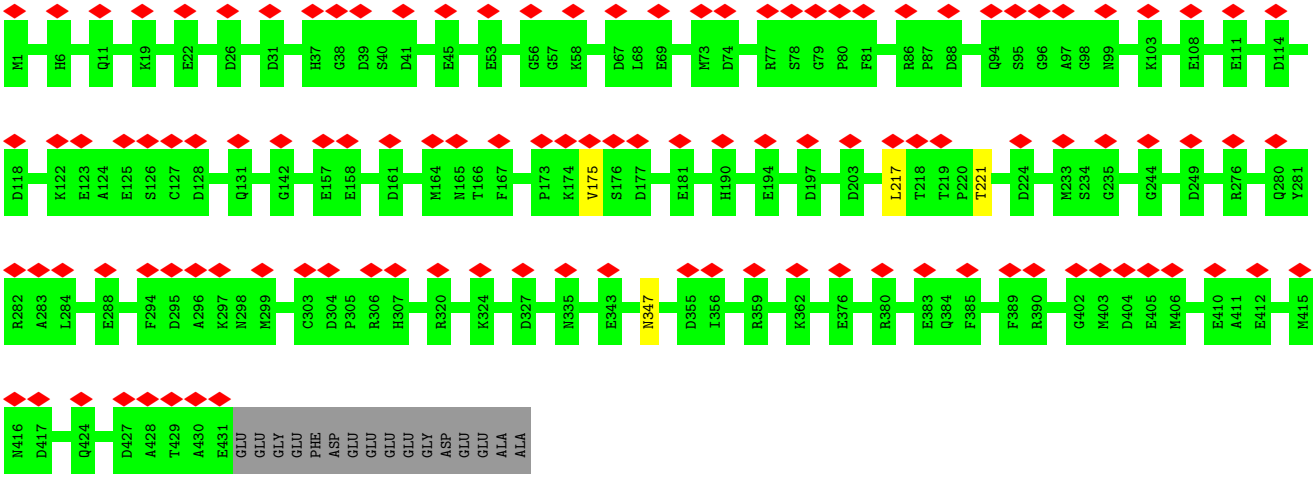




• Molecule 55: Tubulin beta chain

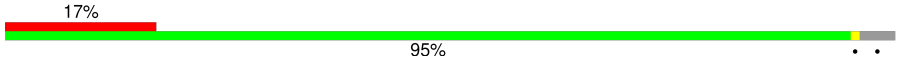
Chain OD:

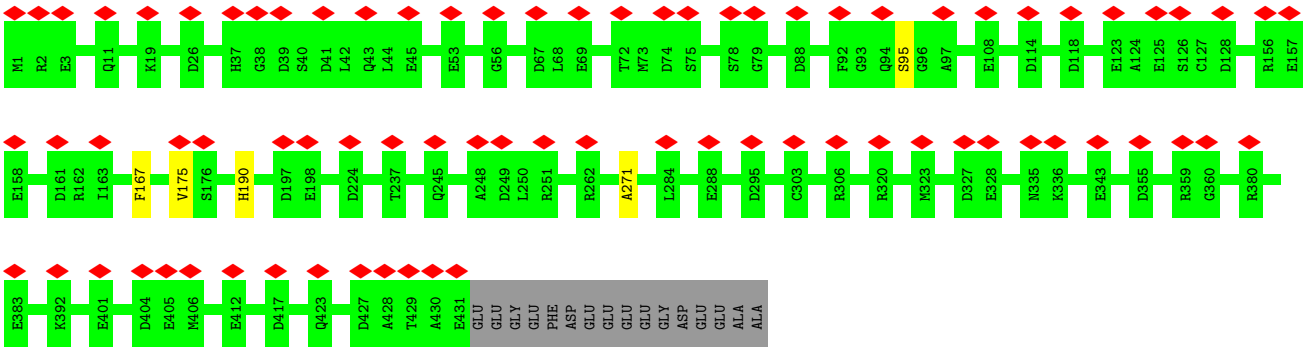




• Molecule 55: Tubulin beta chain

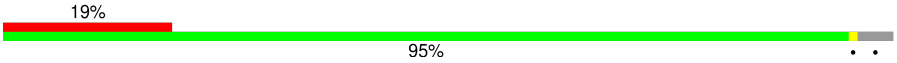
Chain OF:

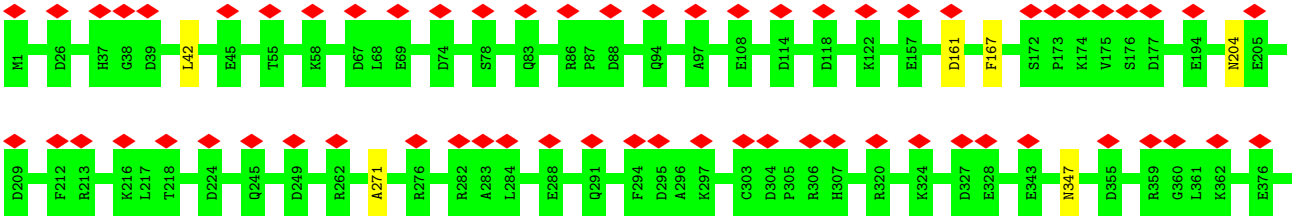


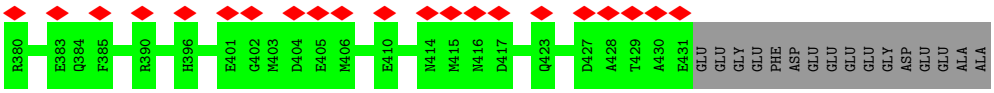


• Molecule 55: Tubulin beta chain

Chain OH:

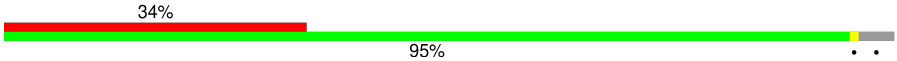


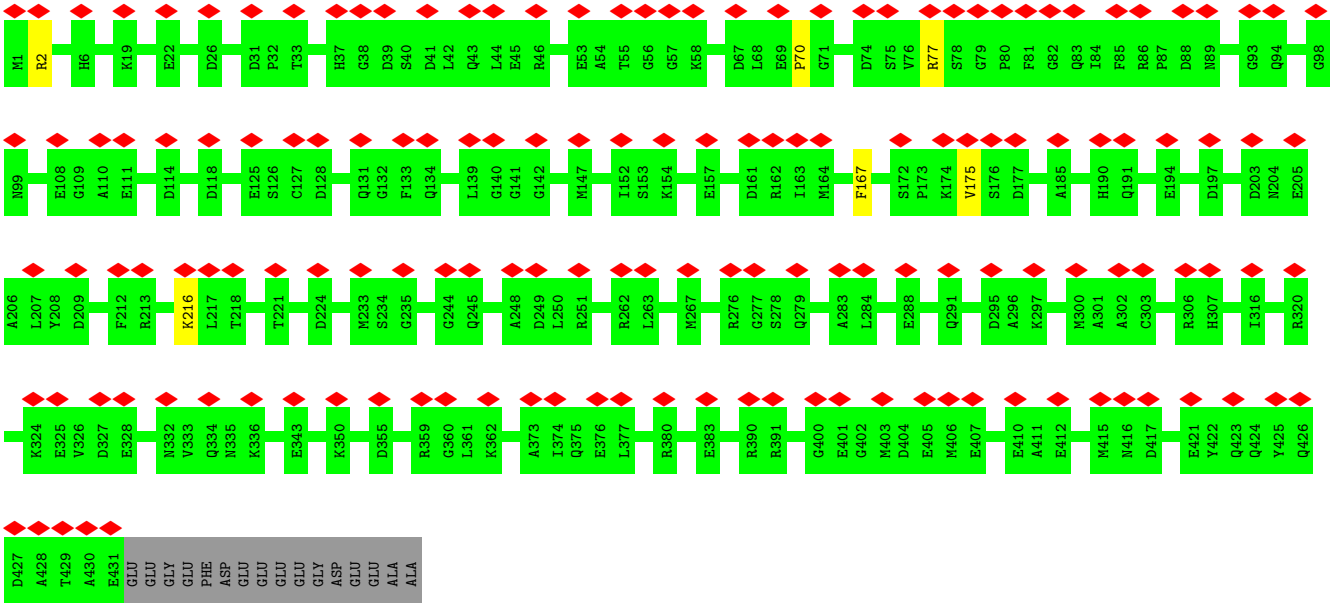




• Molecule 55: Tubulin beta chain

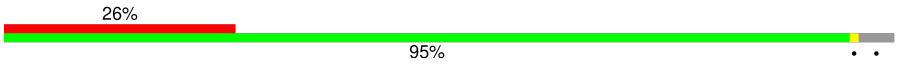
Chain OJ:

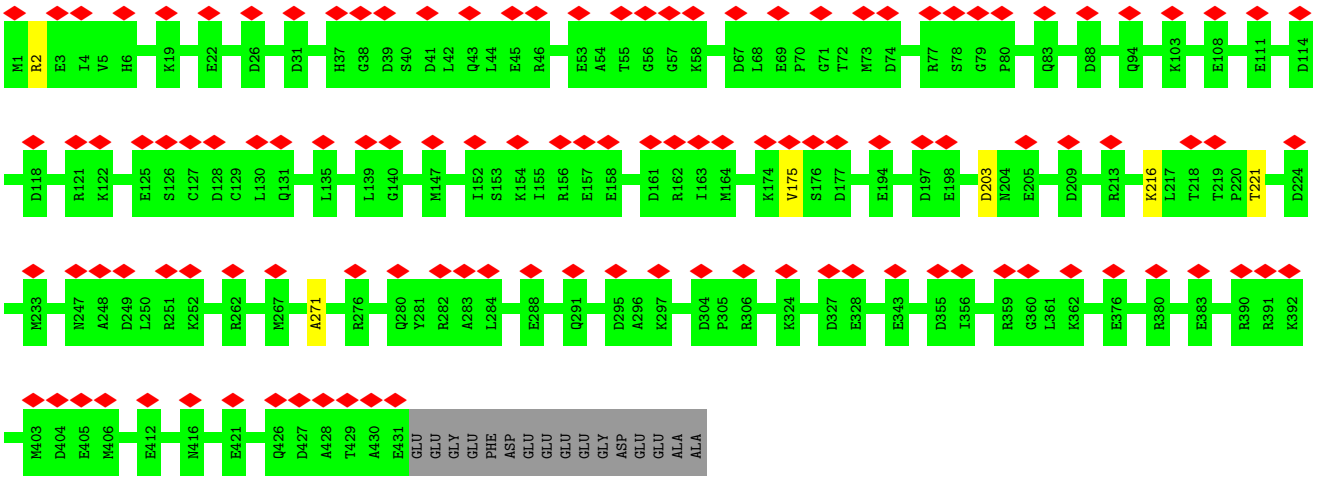




• Molecule 55: Tubulin beta chain

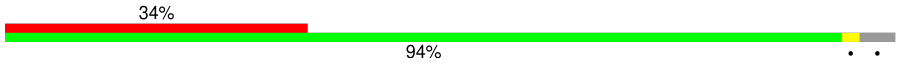
Chain OM:

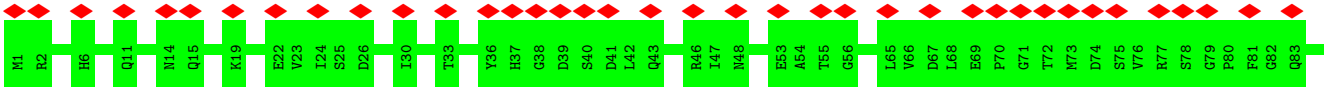


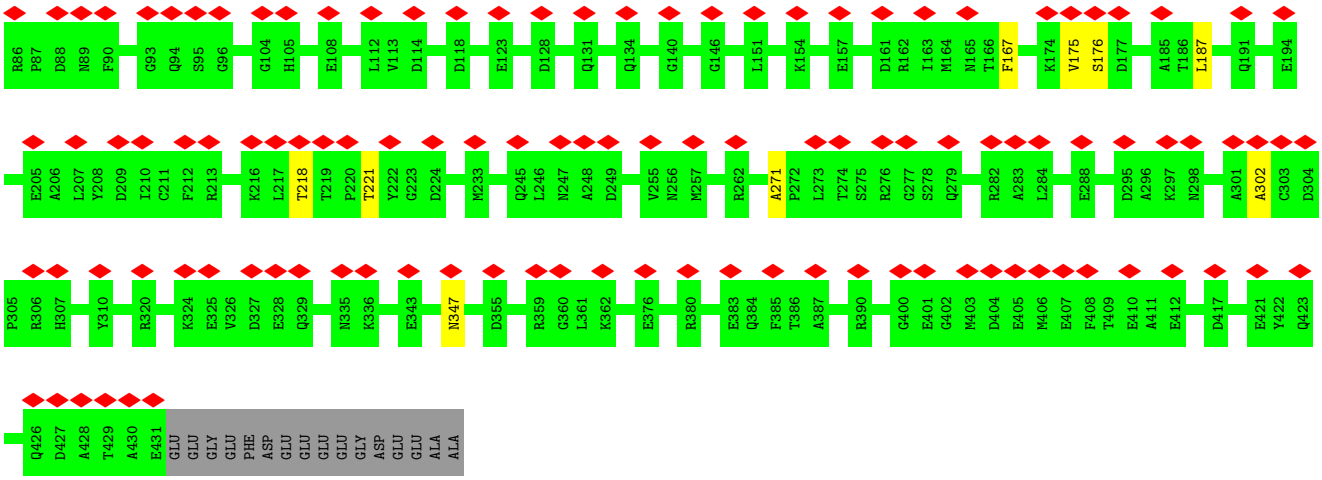


• Molecule 55: Tubulin beta chain

Chain PC:

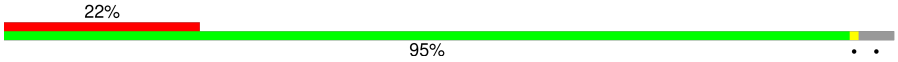


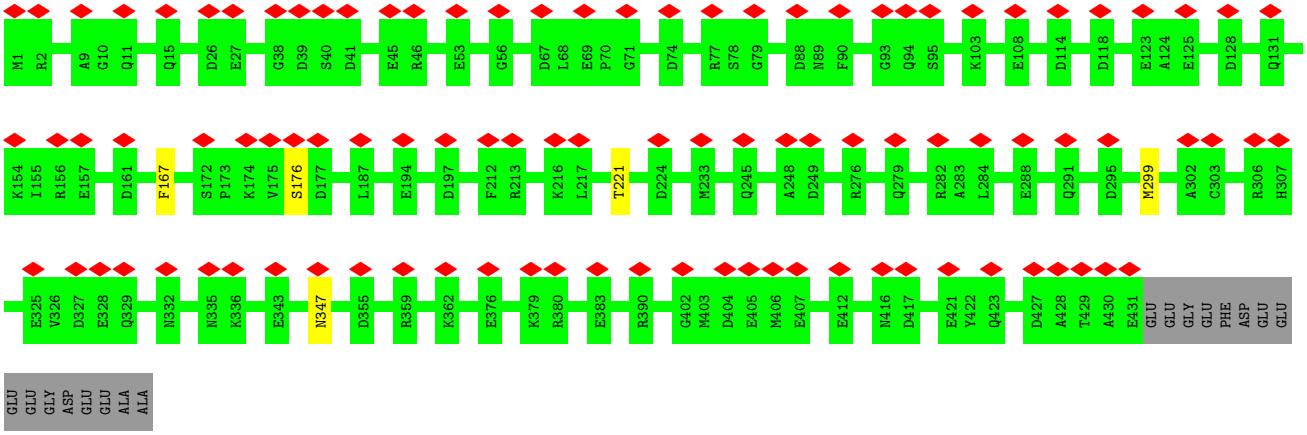




- Molecule 55: Tubulin beta chain

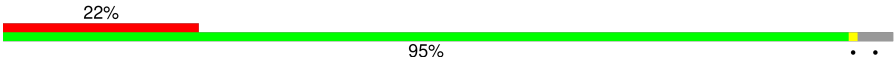
Chain PD:

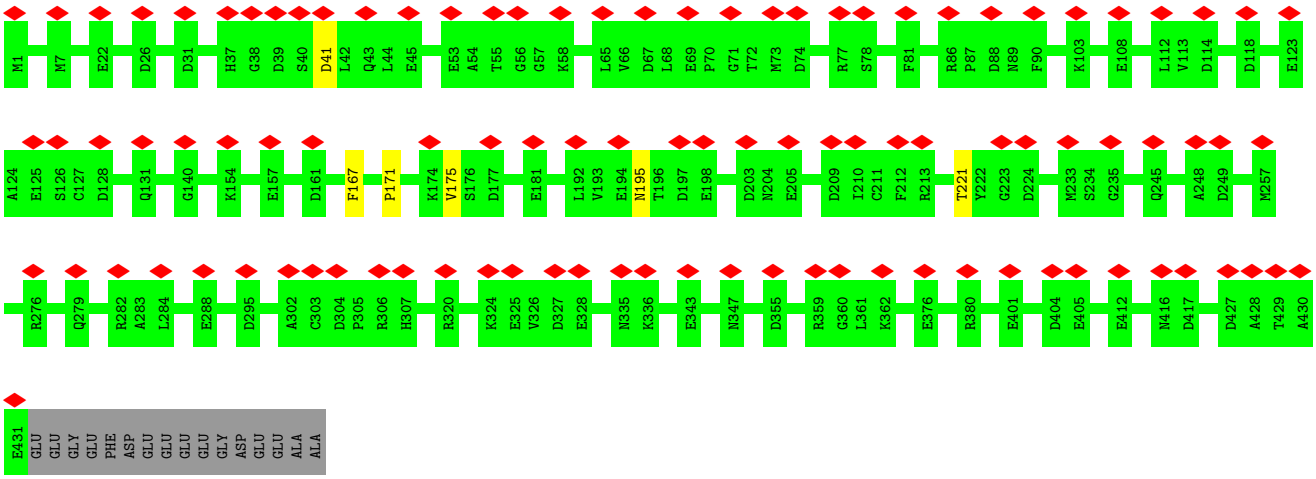




- Molecule 55: Tubulin beta chain

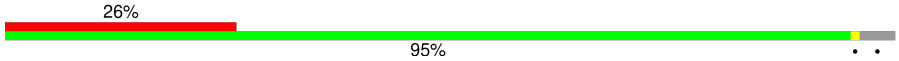
Chain PF:

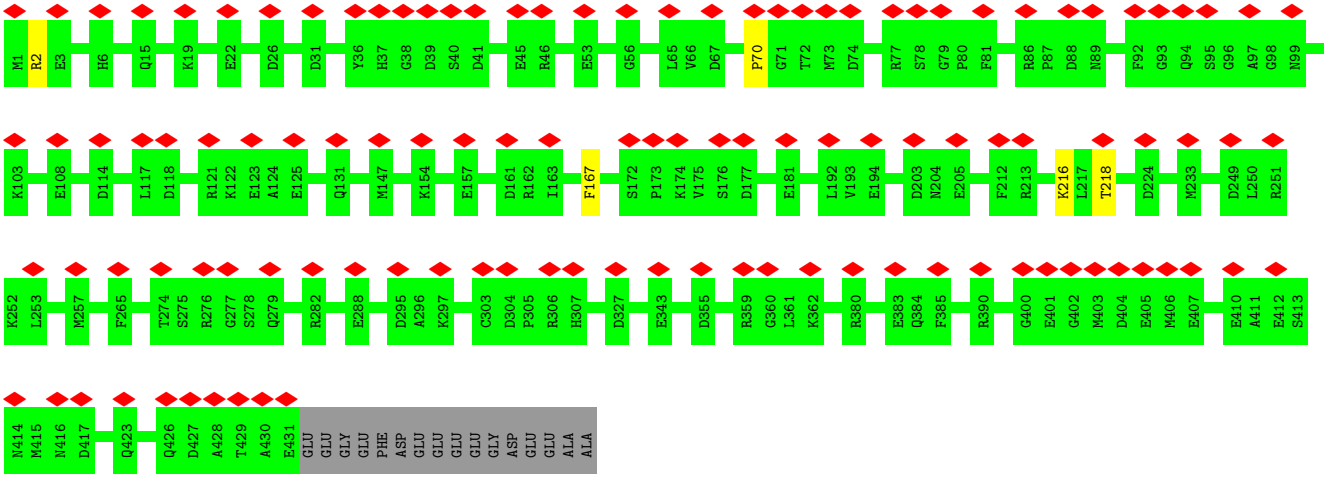




• Molecule 55: Tubulin beta chain

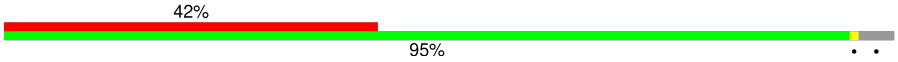
Chain PH:





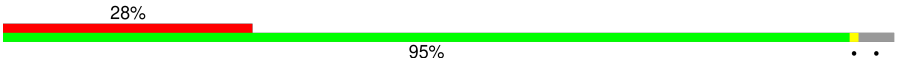
• Molecule 55: Tubulin beta chain

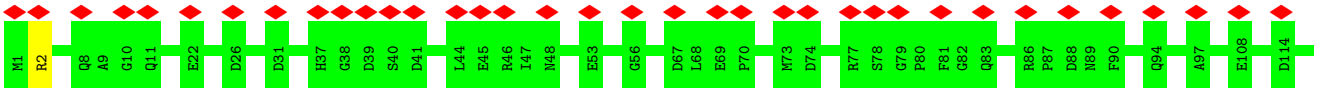
Chain PJ:

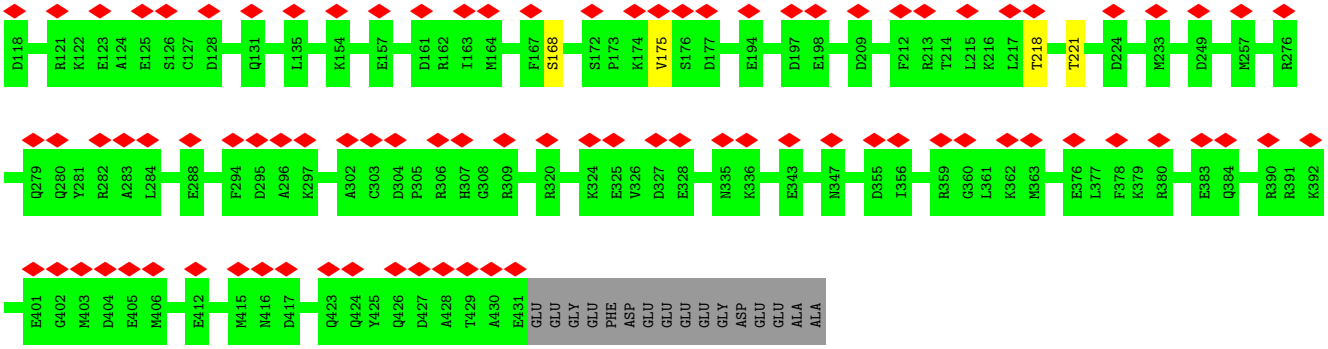


• Molecule 55: Tubulin beta chain

Chain PM:

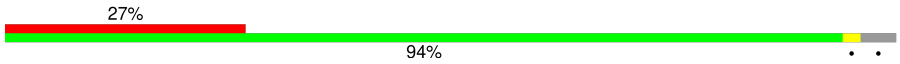


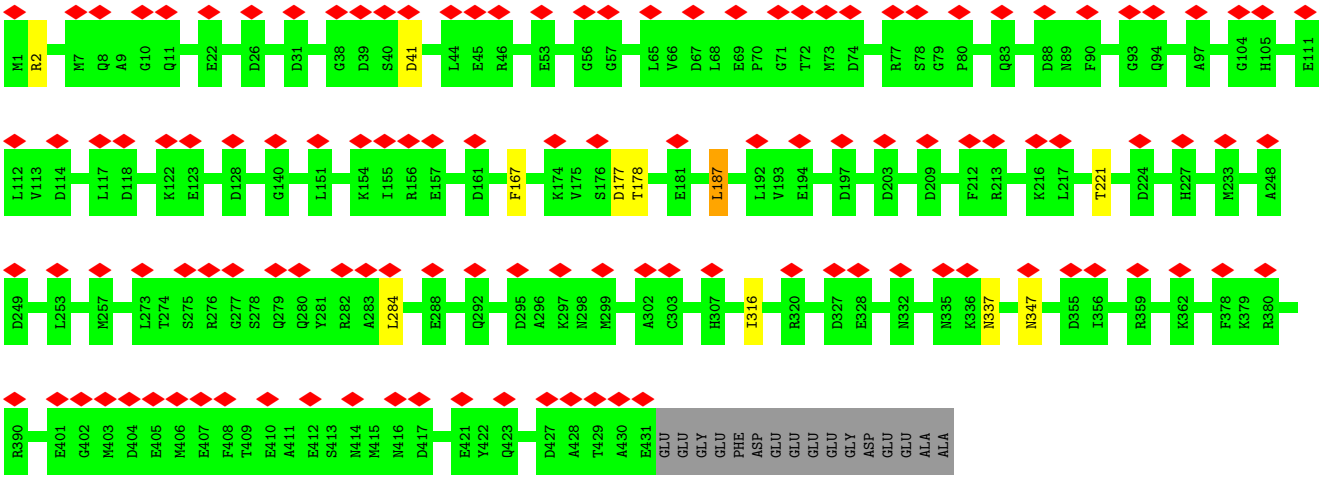




- Molecule 55: Tubulin beta chain

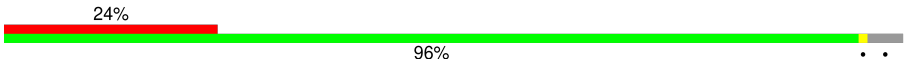
Chain QC:

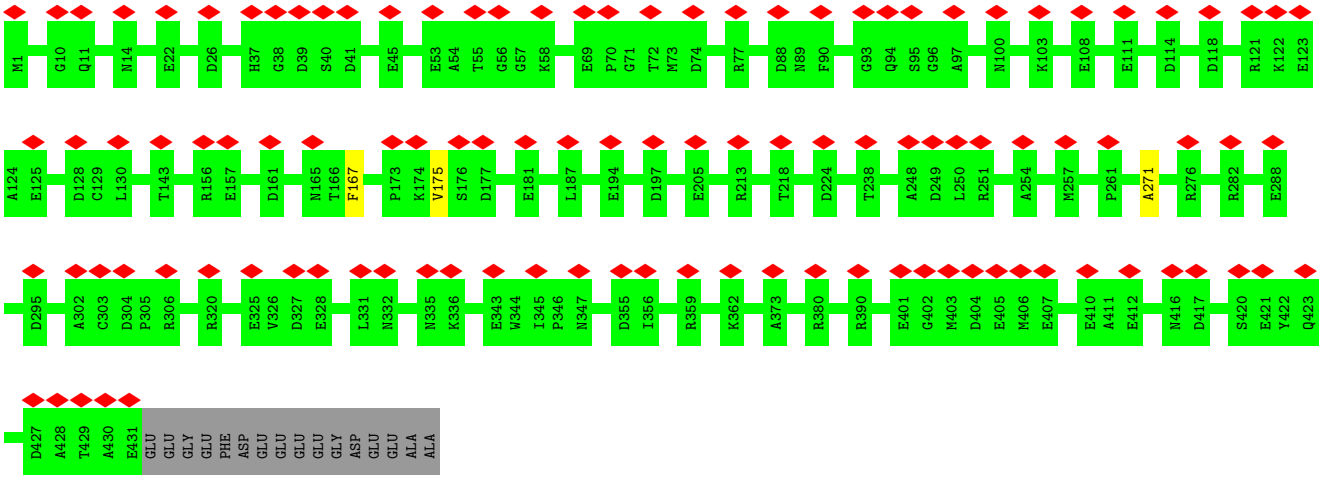




- Molecule 55: Tubulin beta chain

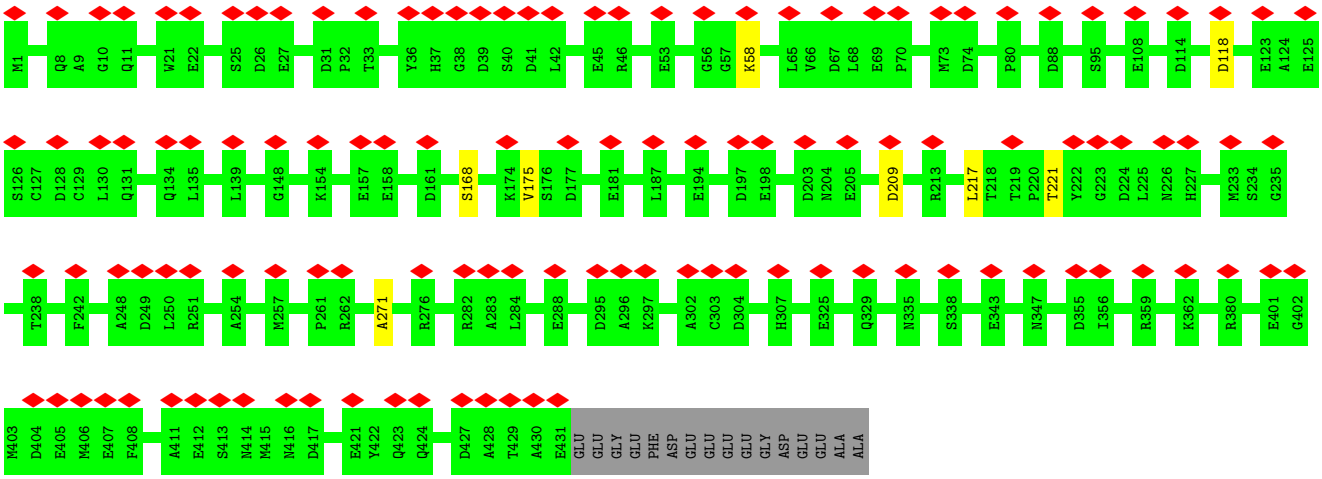
Chain QD:





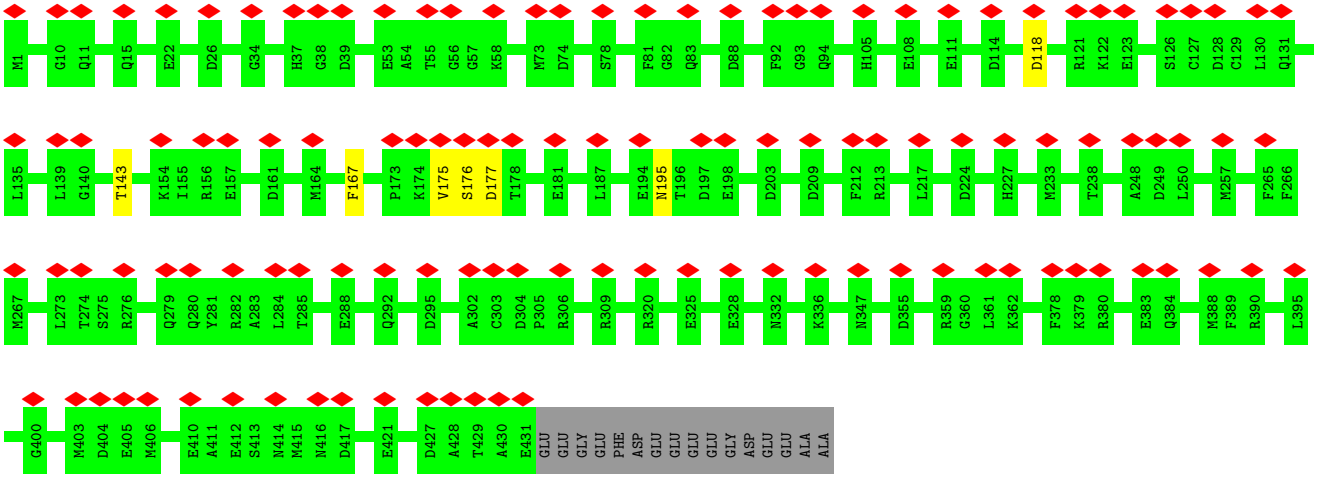
- Molecule 55: Tubulin beta chain

Chain QF: 27% 95%



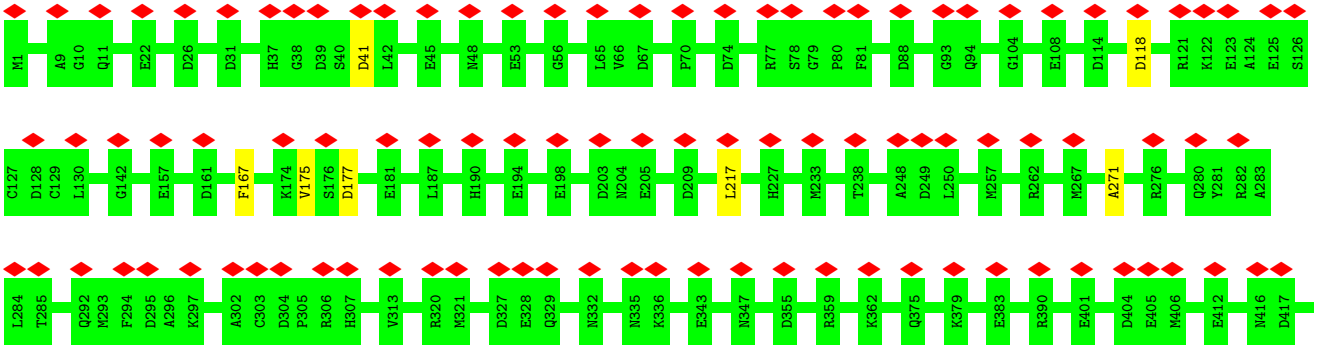
- Molecule 55: Tubulin beta chain

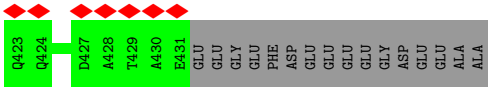
Chain QH: 27% 95%



- Molecule 55: Tubulin beta chain

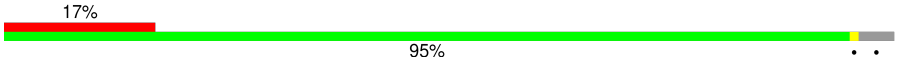
Chain QJ: 24% 95%

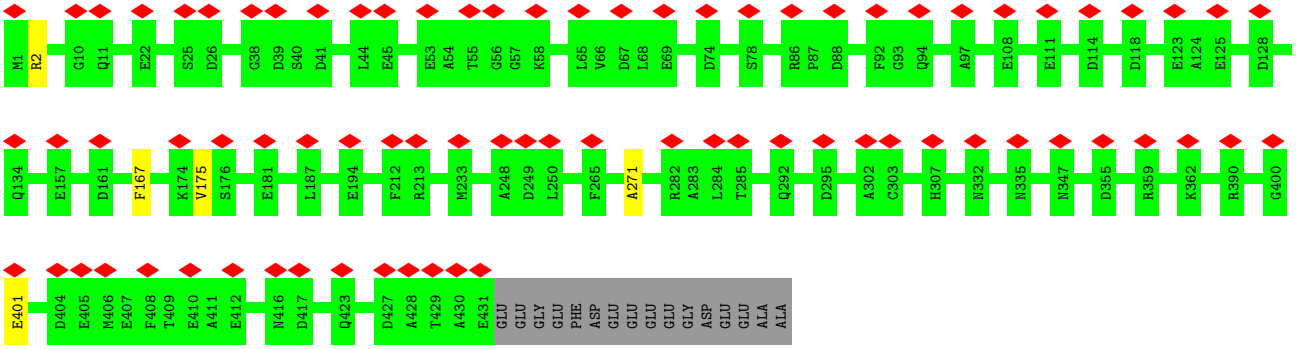




• Molecule 55: Tubulin beta chain

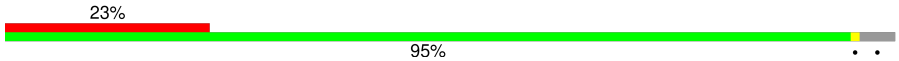
Chain QM:

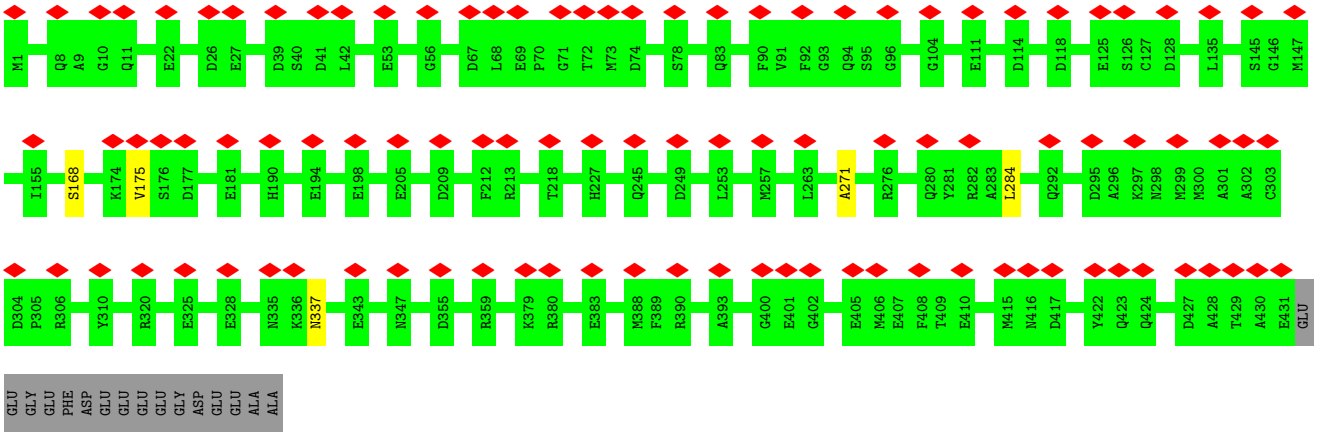




• Molecule 55: Tubulin beta chain

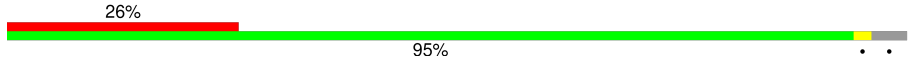
Chain RC:

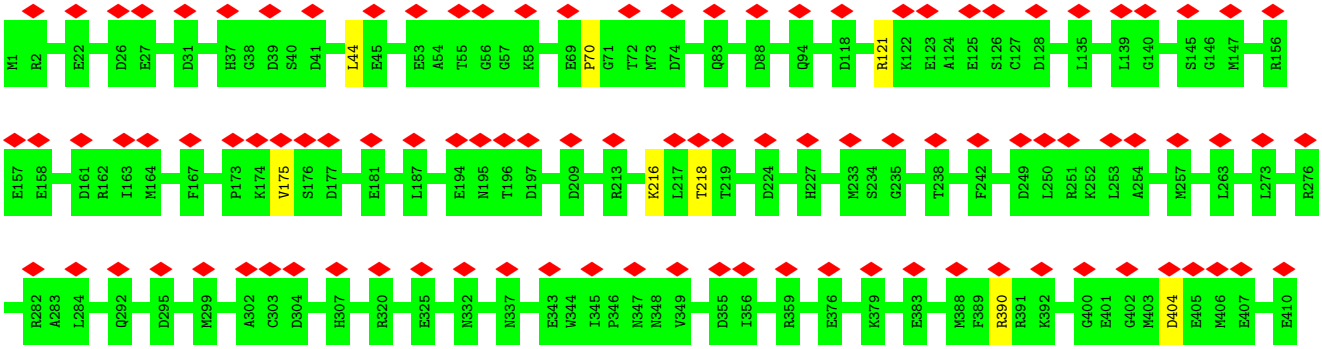


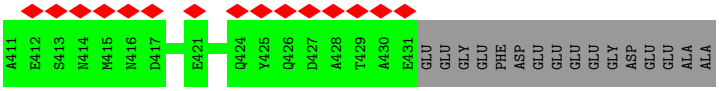


• Molecule 55: Tubulin beta chain

Chain RD:

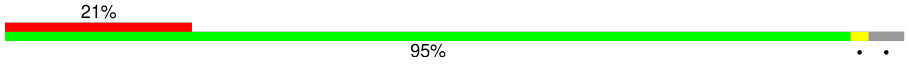


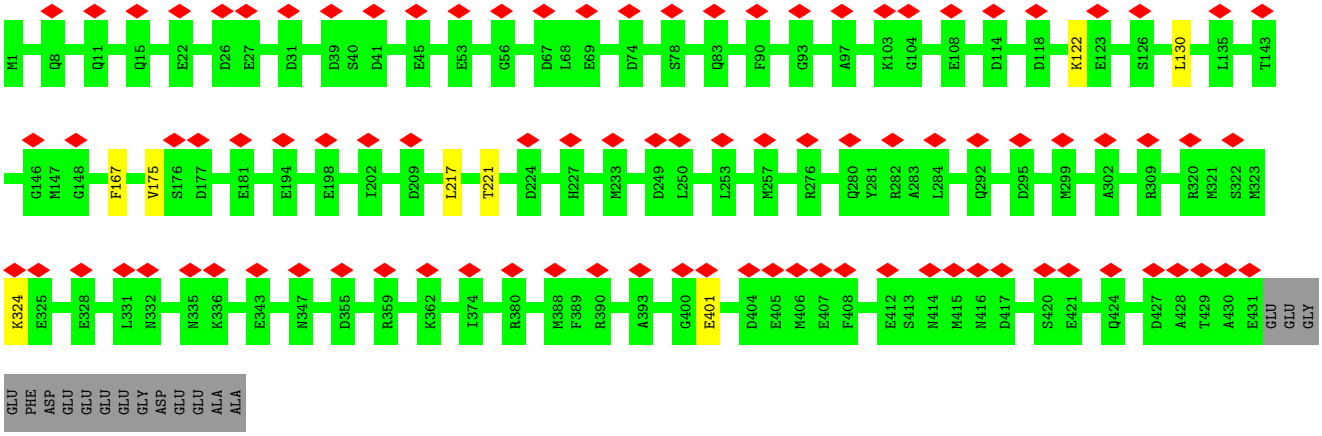




• Molecule 55: Tubulin beta chain

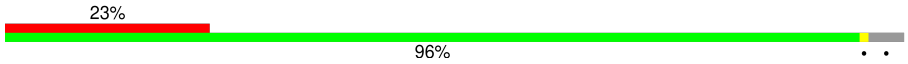
Chain RF:

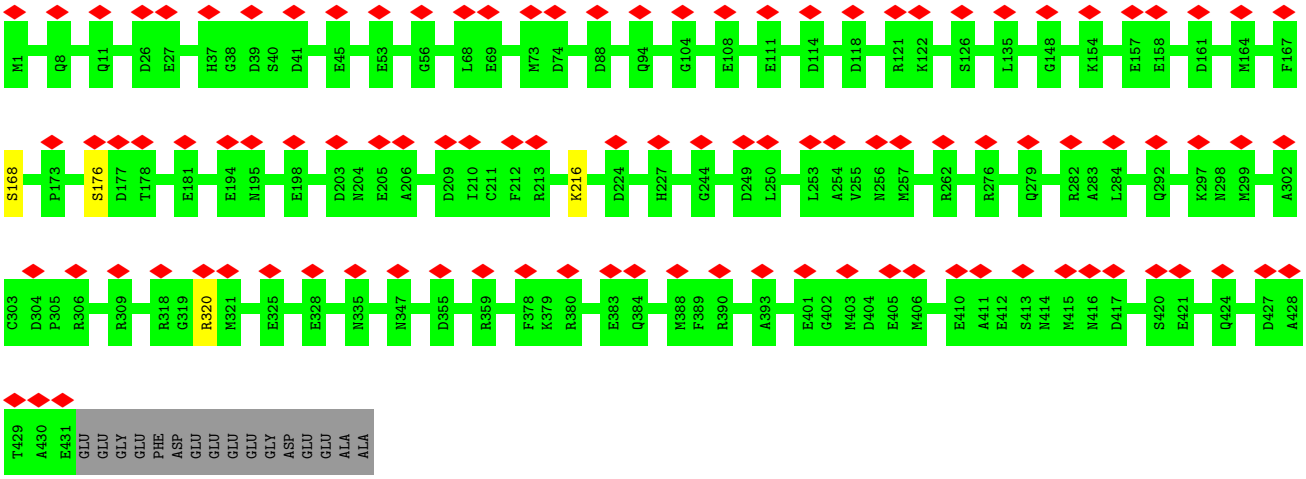




• Molecule 55: Tubulin beta chain

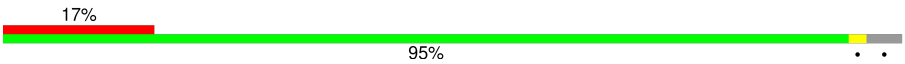
Chain RH:

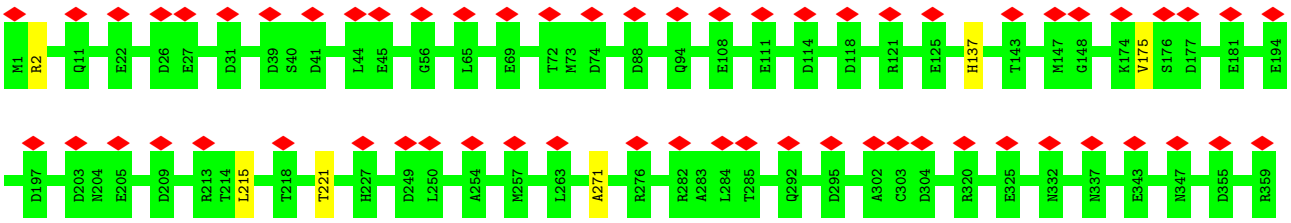


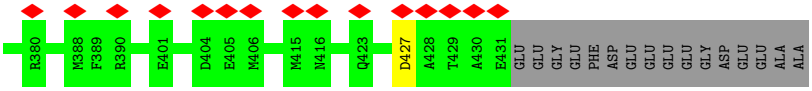


• Molecule 55: Tubulin beta chain

Chain RJ:

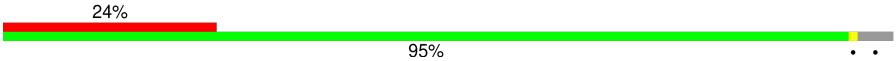


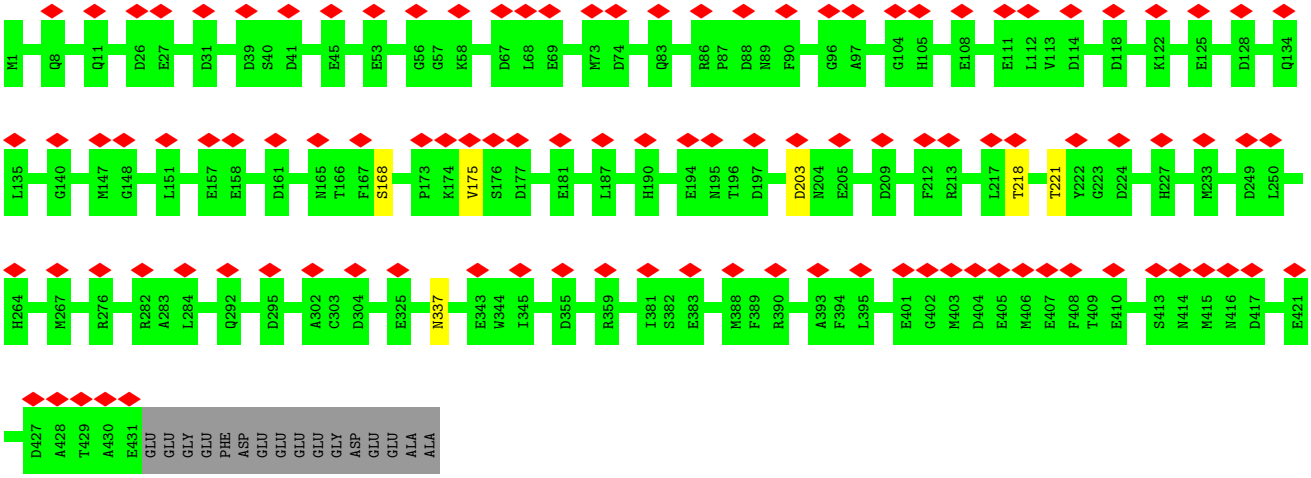




• Molecule 55: Tubulin beta chain

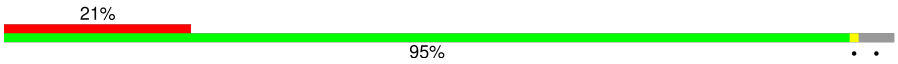
Chain RM:

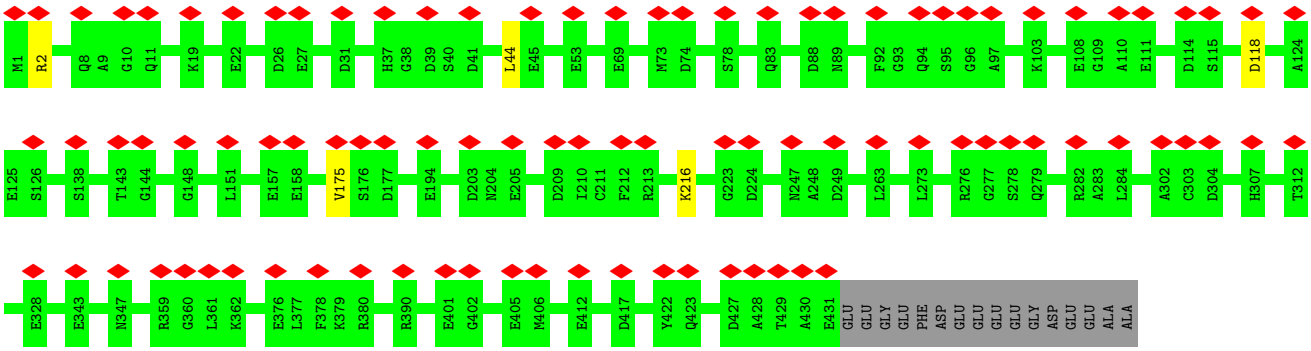




• Molecule 55: Tubulin beta chain

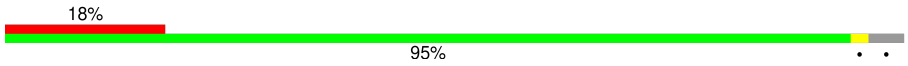
Chain SC:

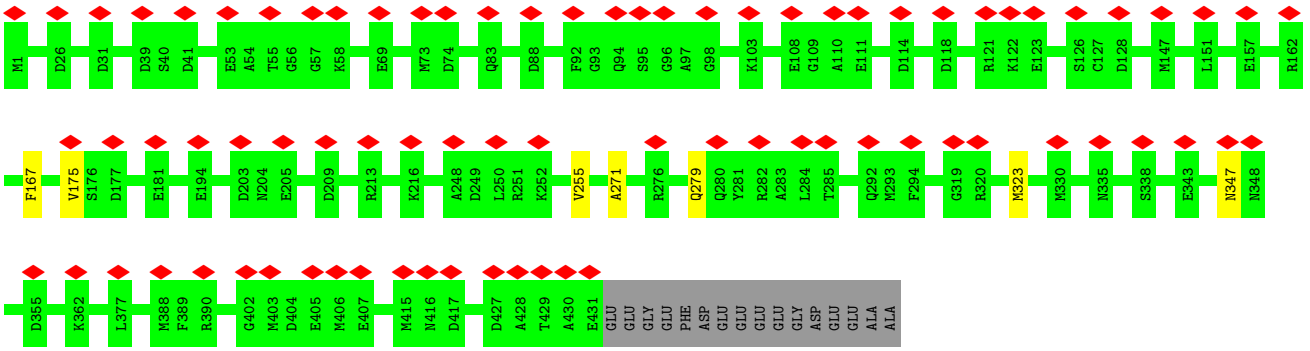




• Molecule 55: Tubulin beta chain

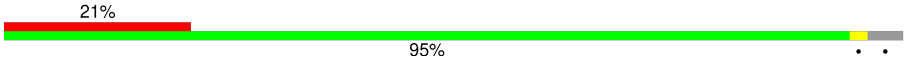
Chain SD:

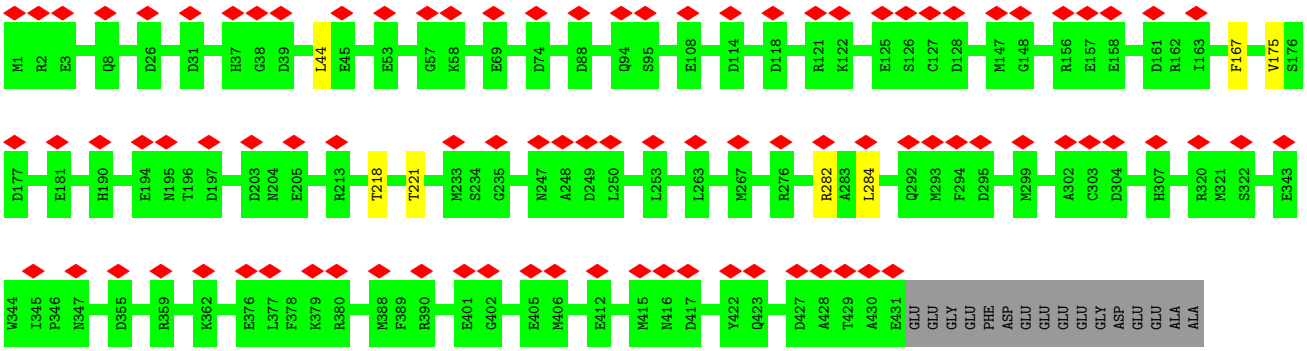




- Molecule 55: Tubulin beta chain

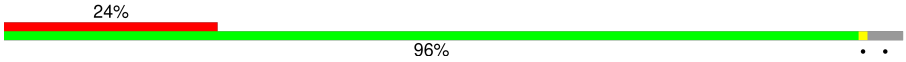
Chain SF:

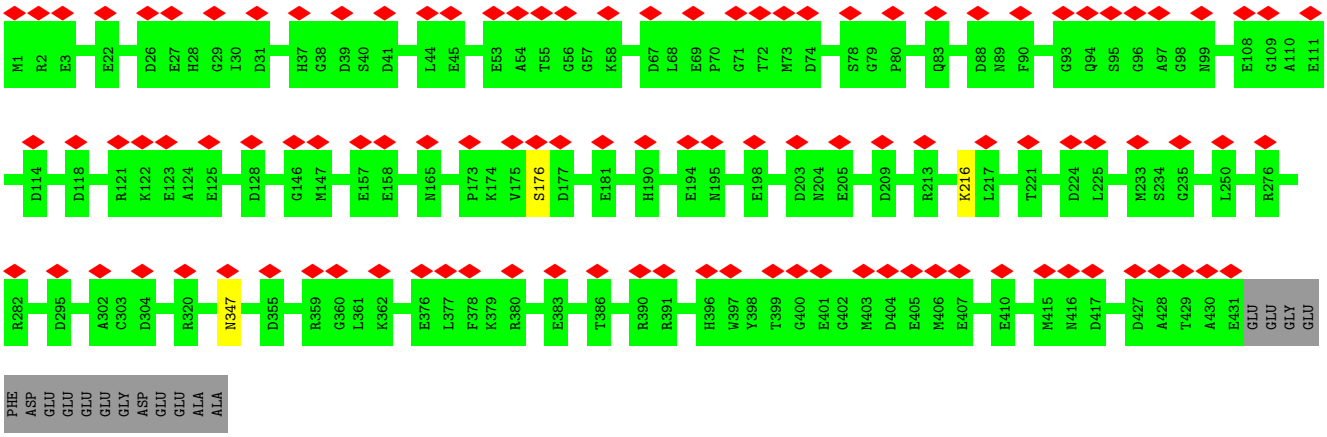




- Molecule 55: Tubulin beta chain

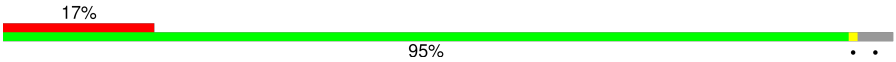
Chain SH:

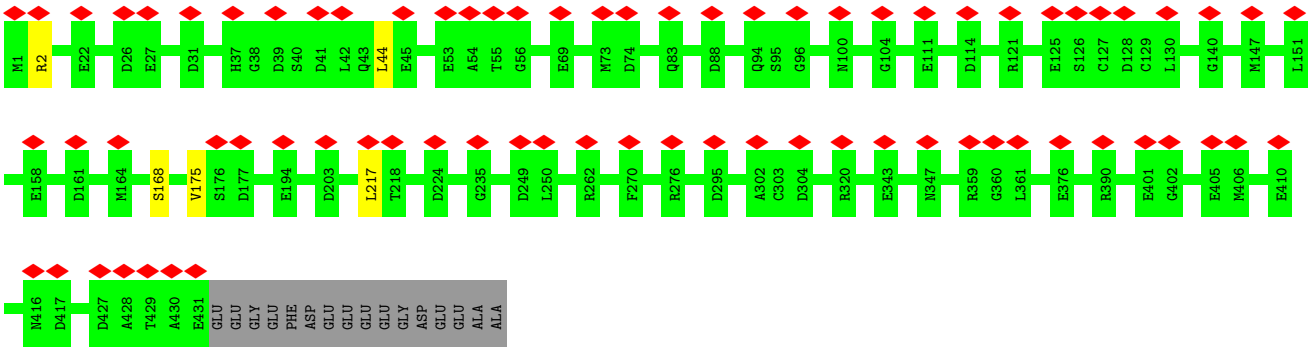




- Molecule 55: Tubulin beta chain

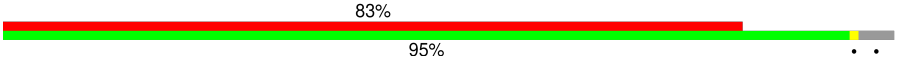
Chain SJ:

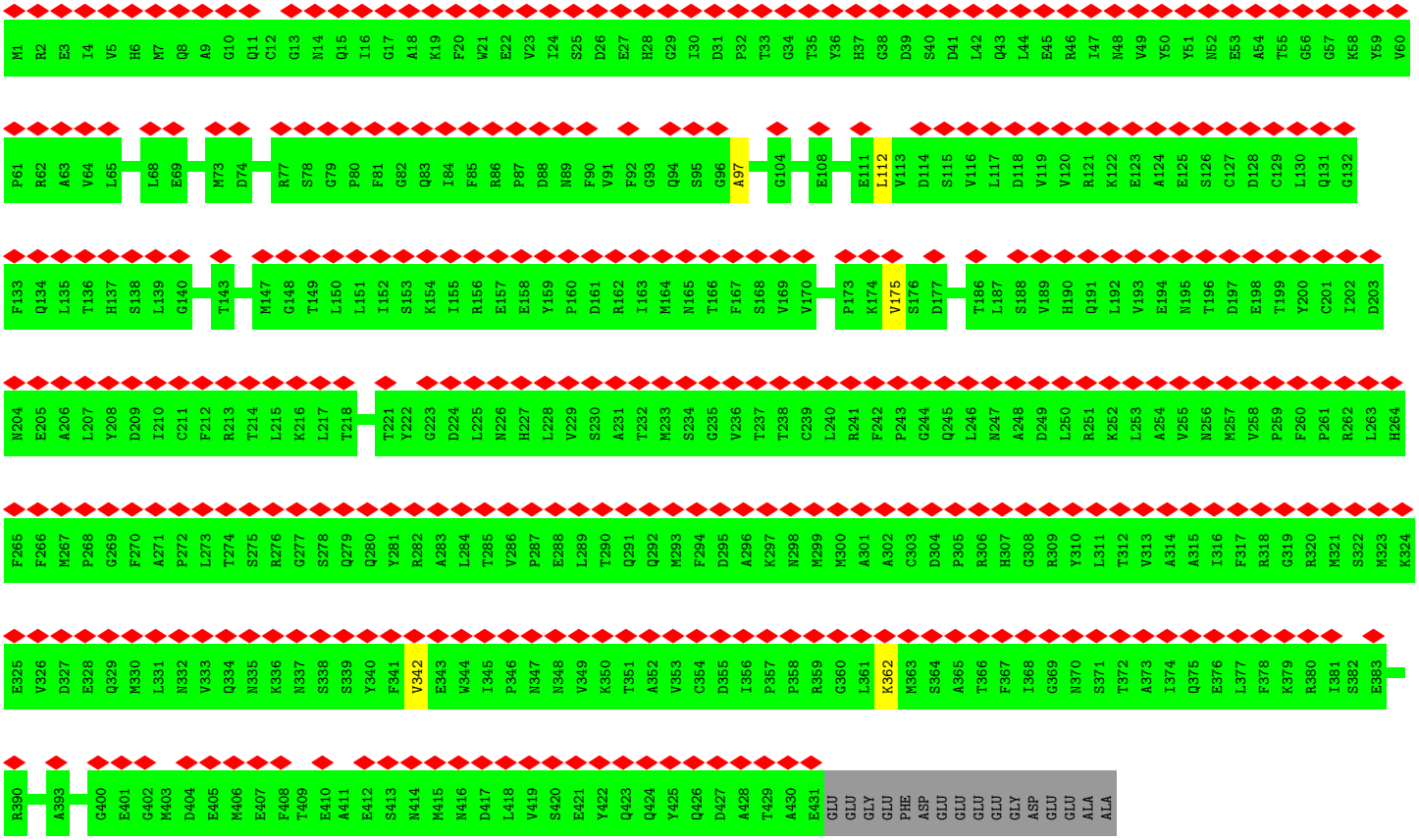




- Molecule 55: Tubulin beta chain

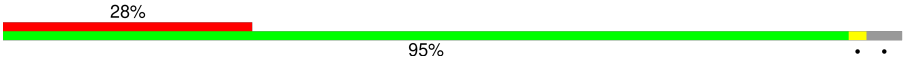
Chain SL:

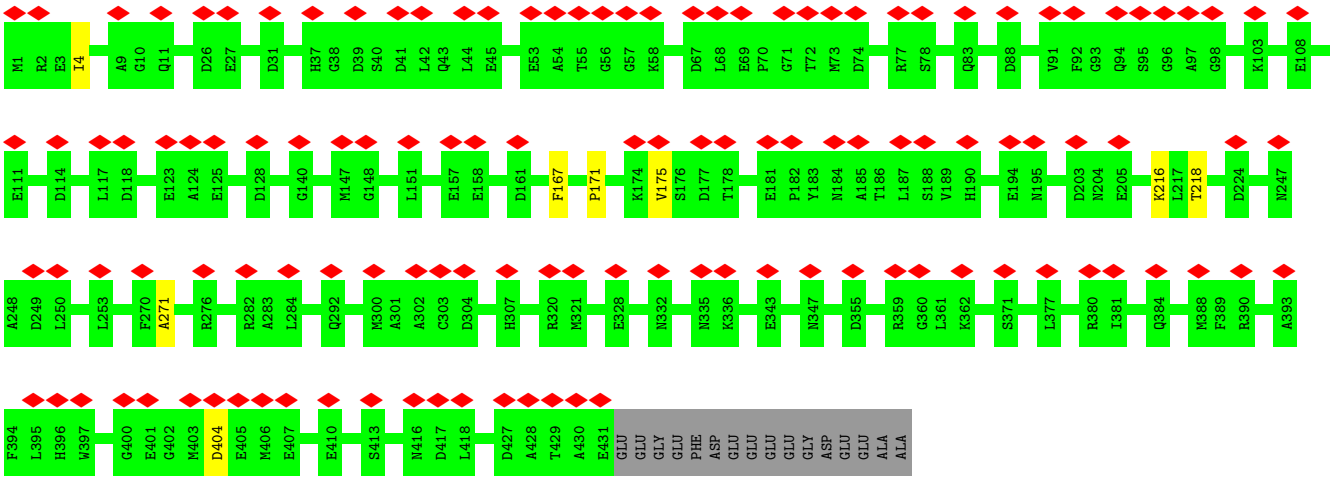




- Molecule 55: Tubulin beta chain

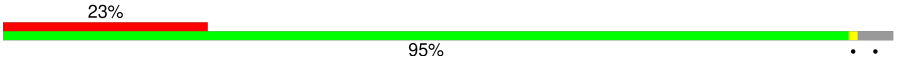
Chain SM:

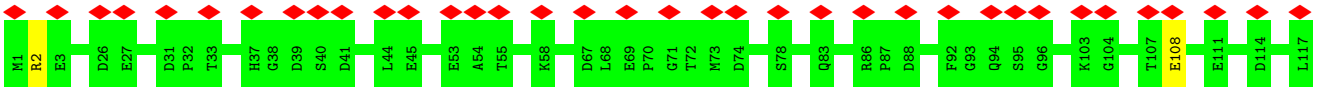


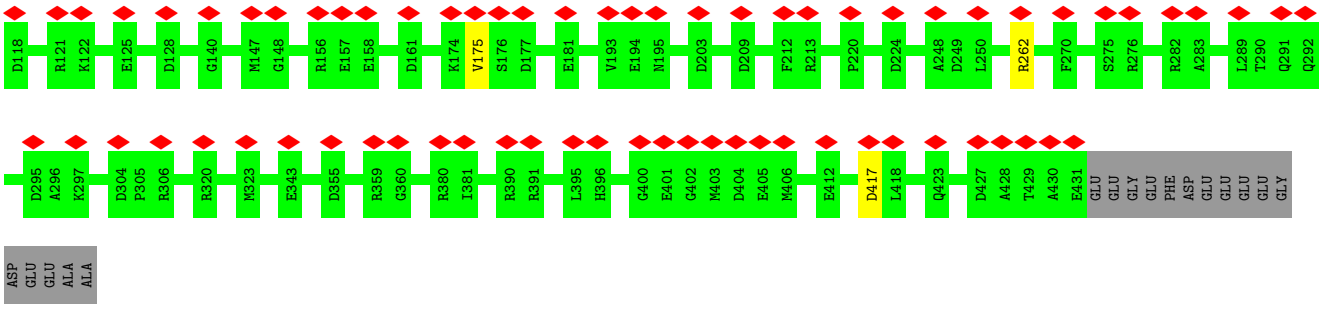


- Molecule 55: Tubulin beta chain

Chain TC:

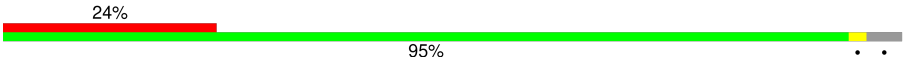


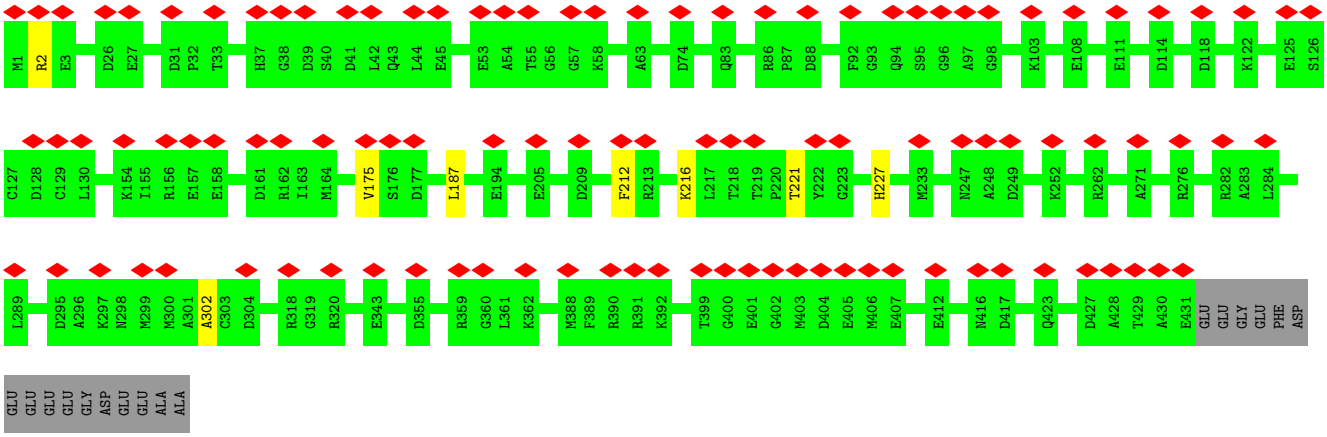




- Molecule 55: Tubulin beta chain

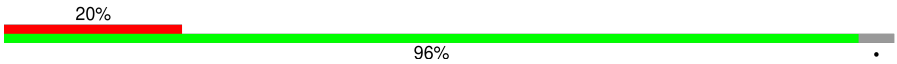
Chain TD:

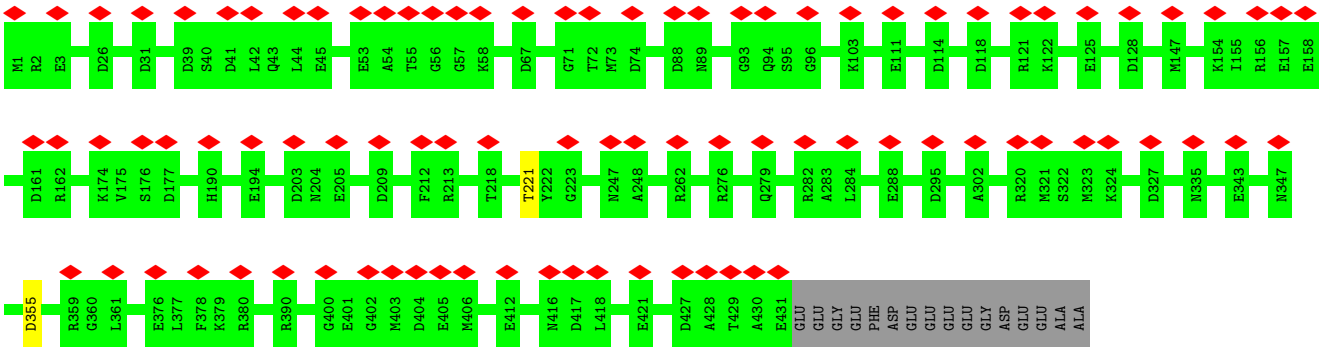




- Molecule 55: Tubulin beta chain

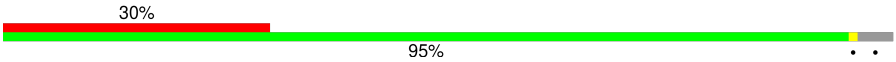
Chain TF:

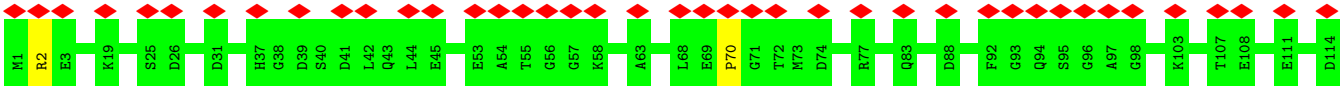


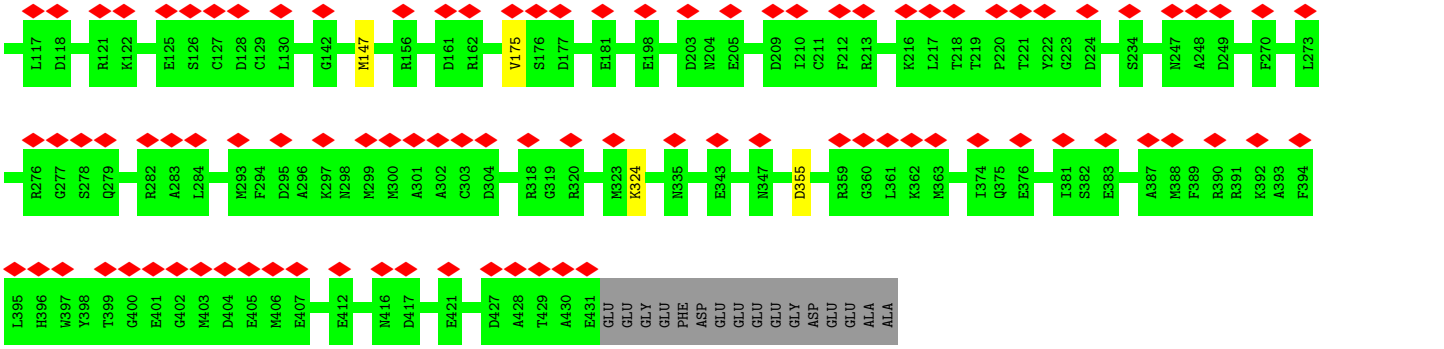


- Molecule 55: Tubulin beta chain

Chain TH:

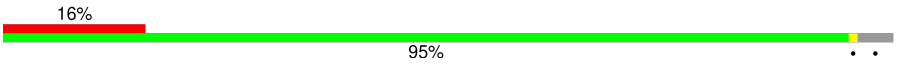


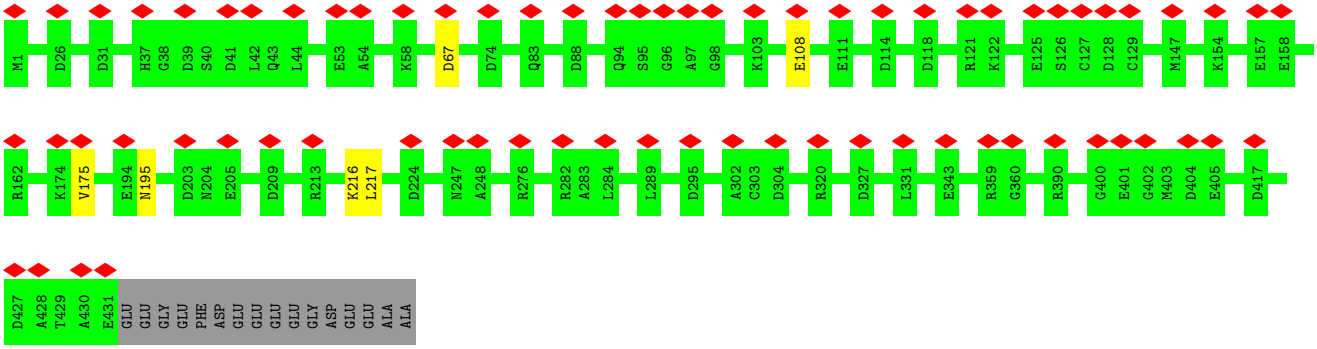




- Molecule 55: Tubulin beta chain

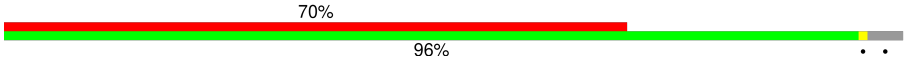
Chain TJ:

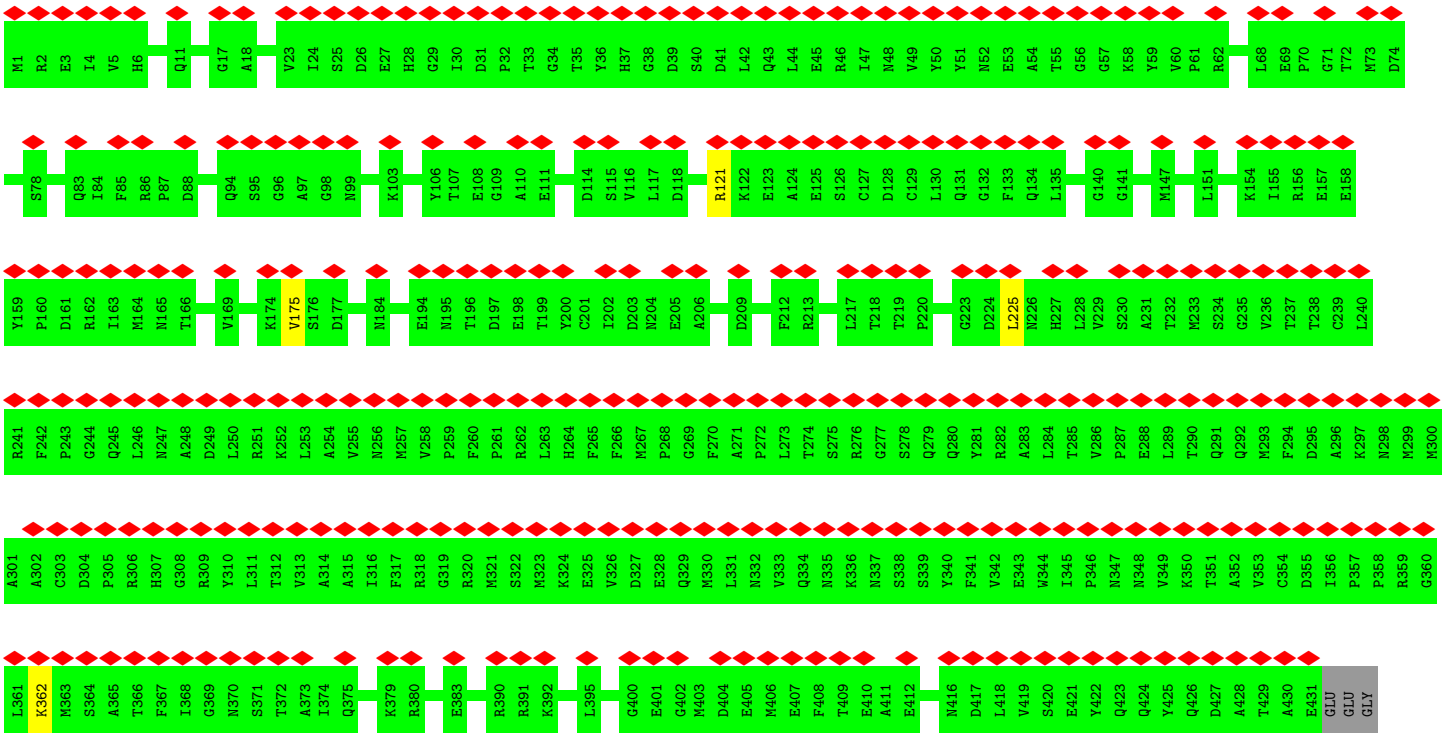




- Molecule 55: Tubulin beta chain

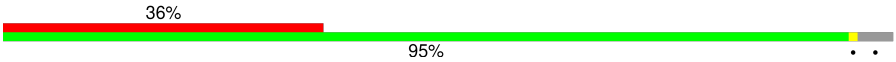
Chain TL:

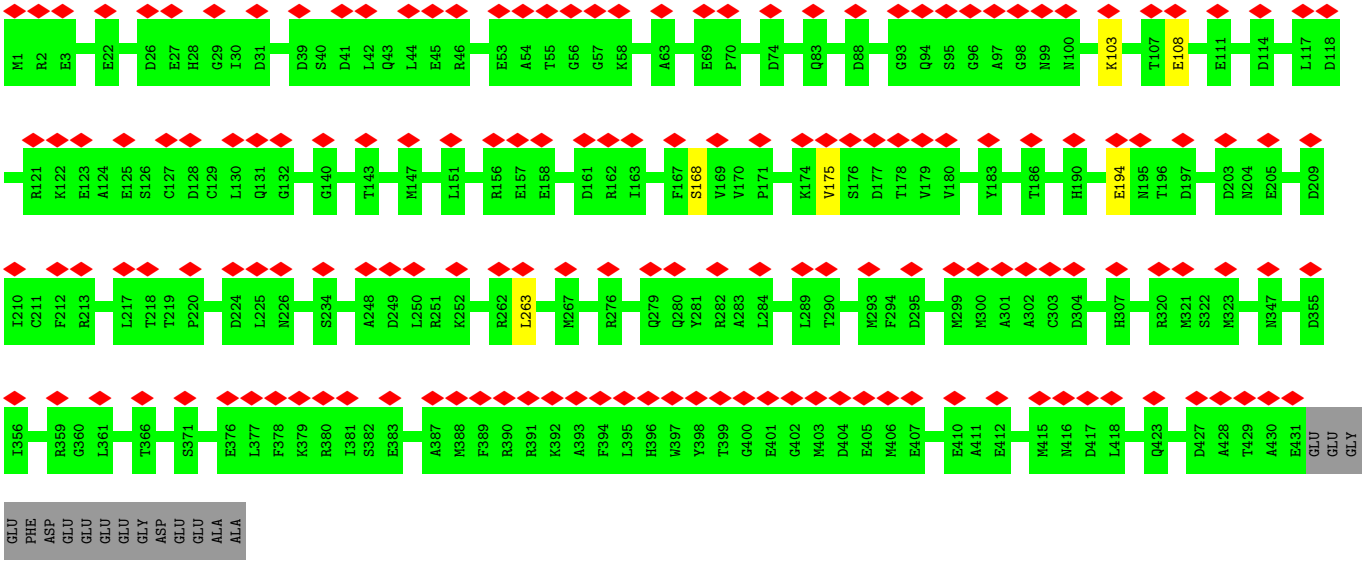




• Molecule 55: Tubulin beta chain

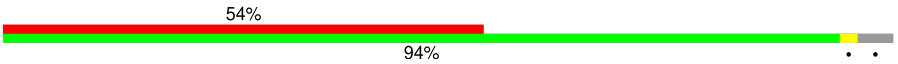
Chain TM:

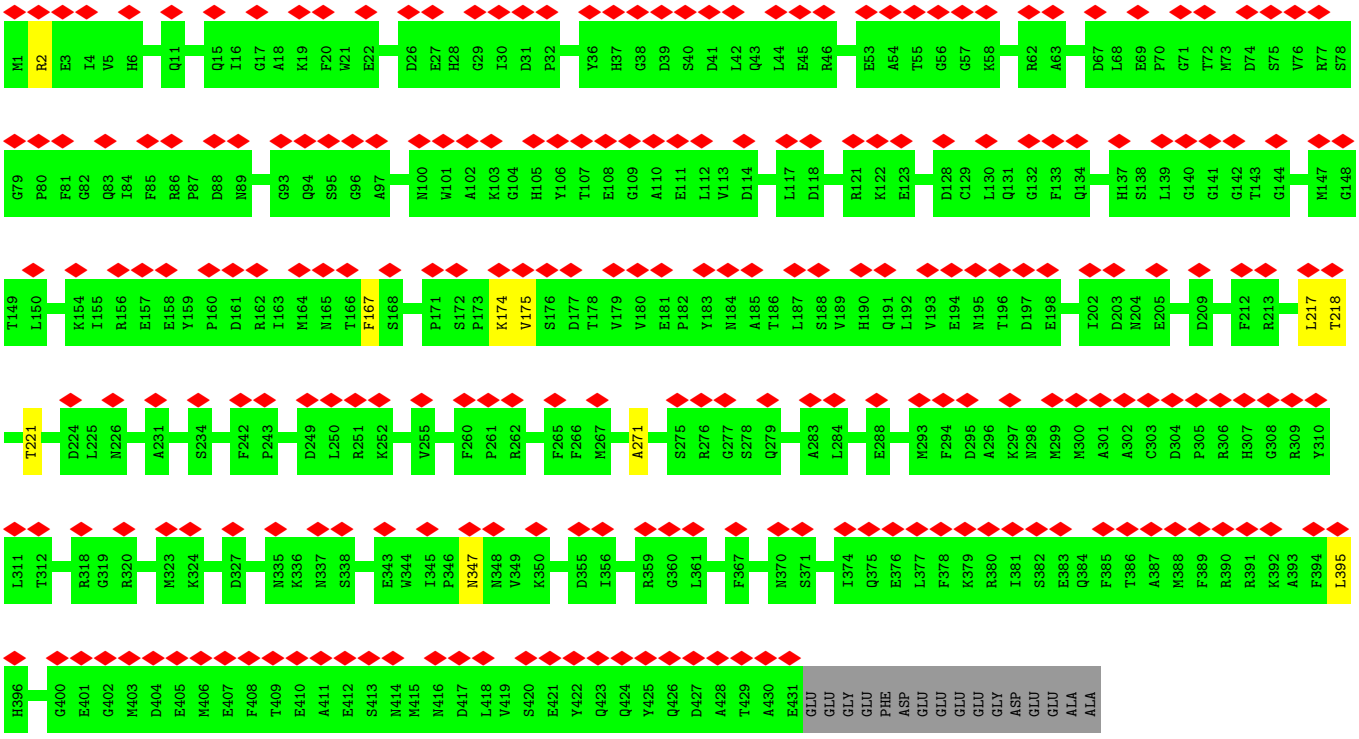




• Molecule 55: Tubulin beta chain

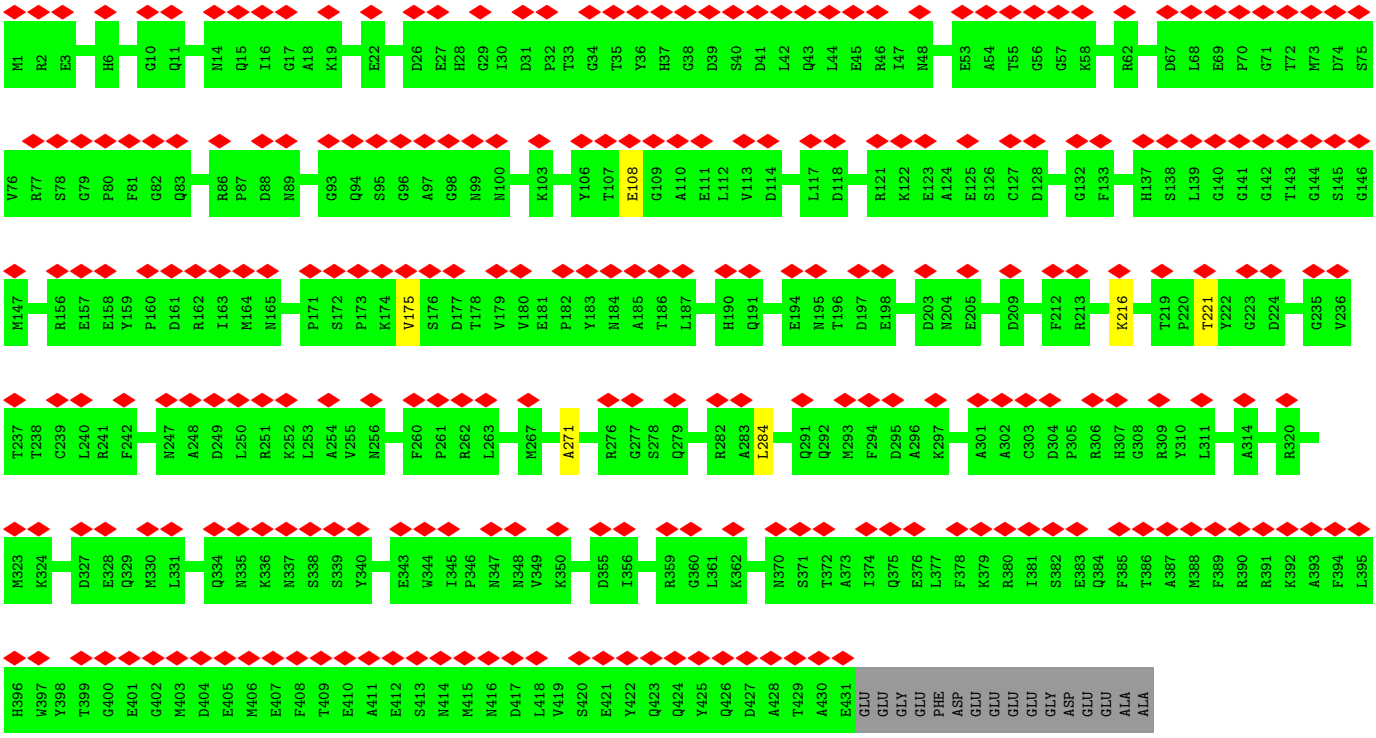
Chain UC:





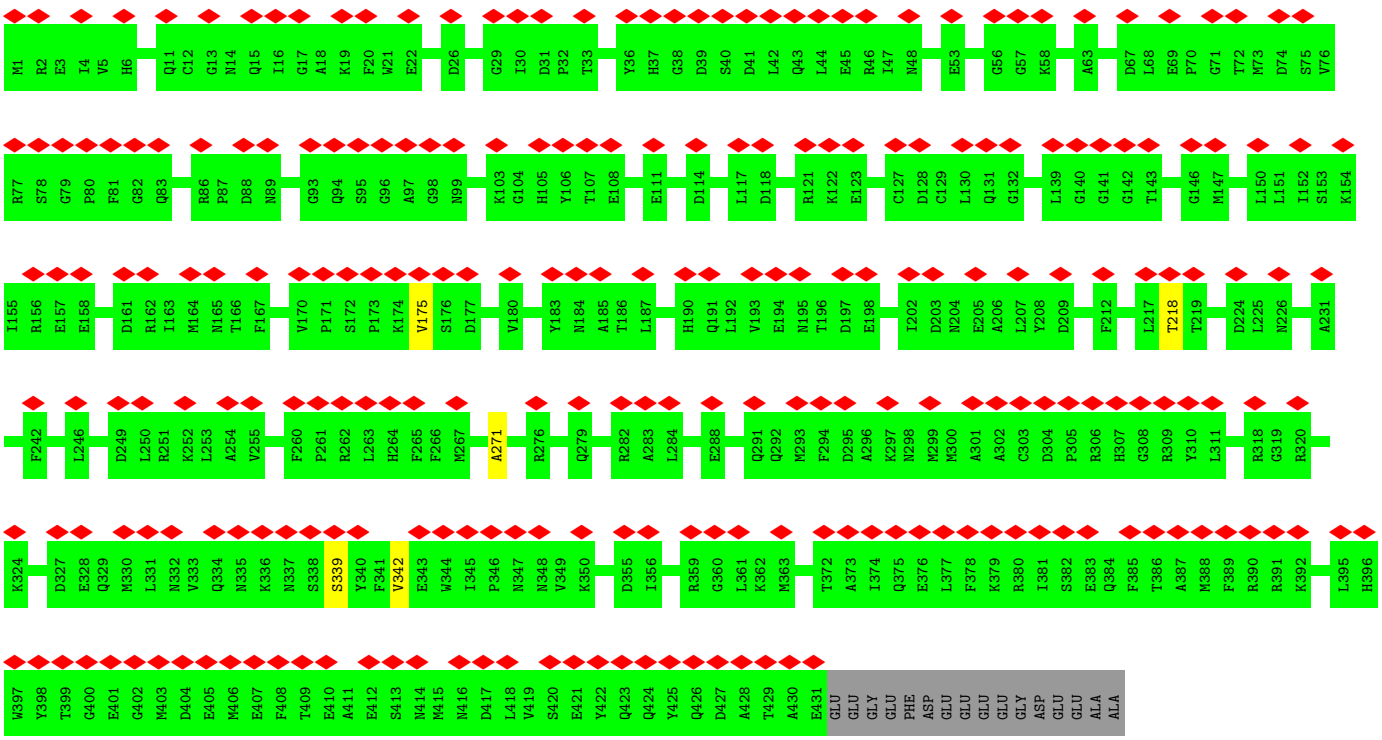
• Molecule 55: Tubulin beta chain

Chain UD: 57% 95%



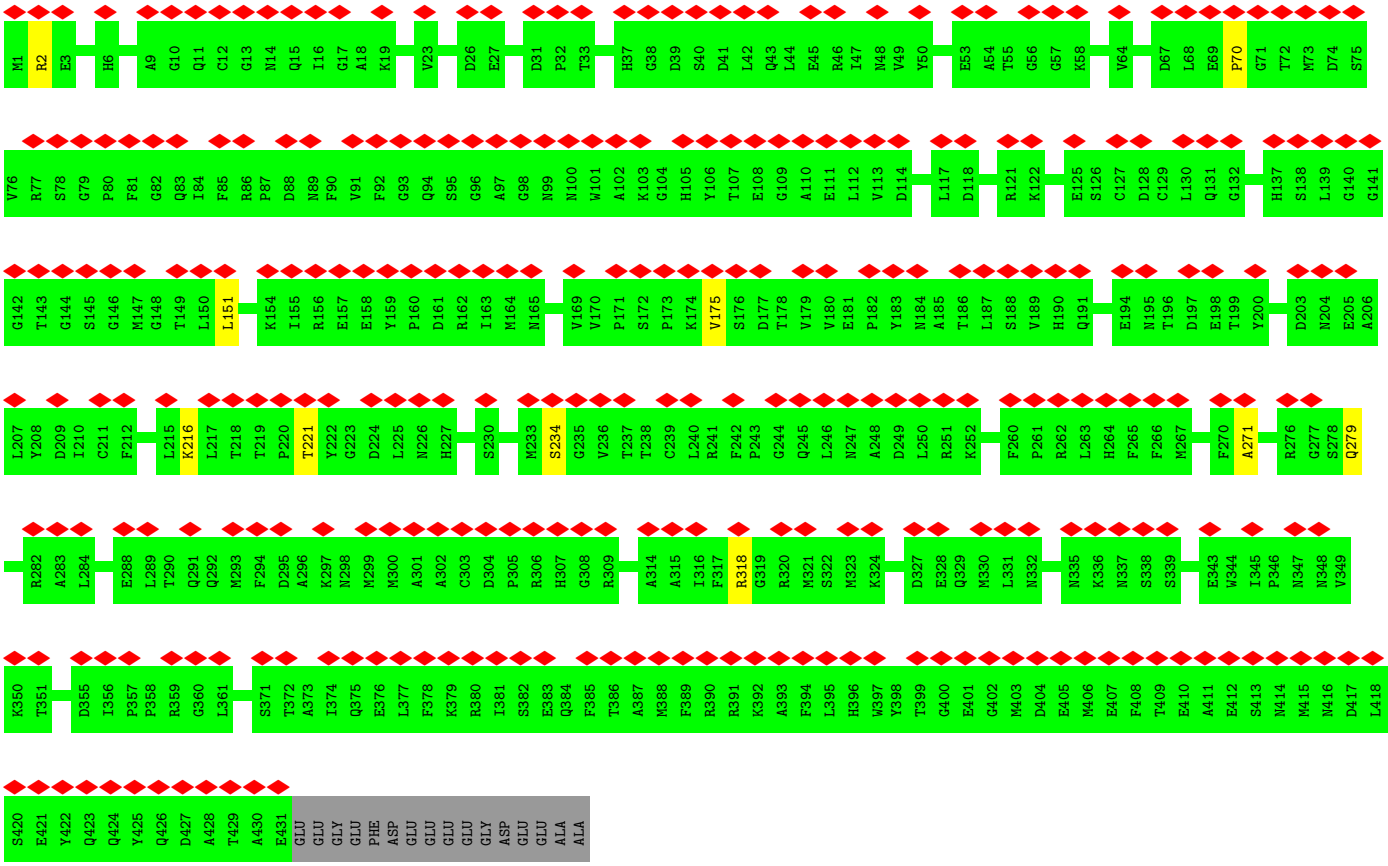
- Molecule 55: Tubulin beta chain

Chain UF: 54% 95%



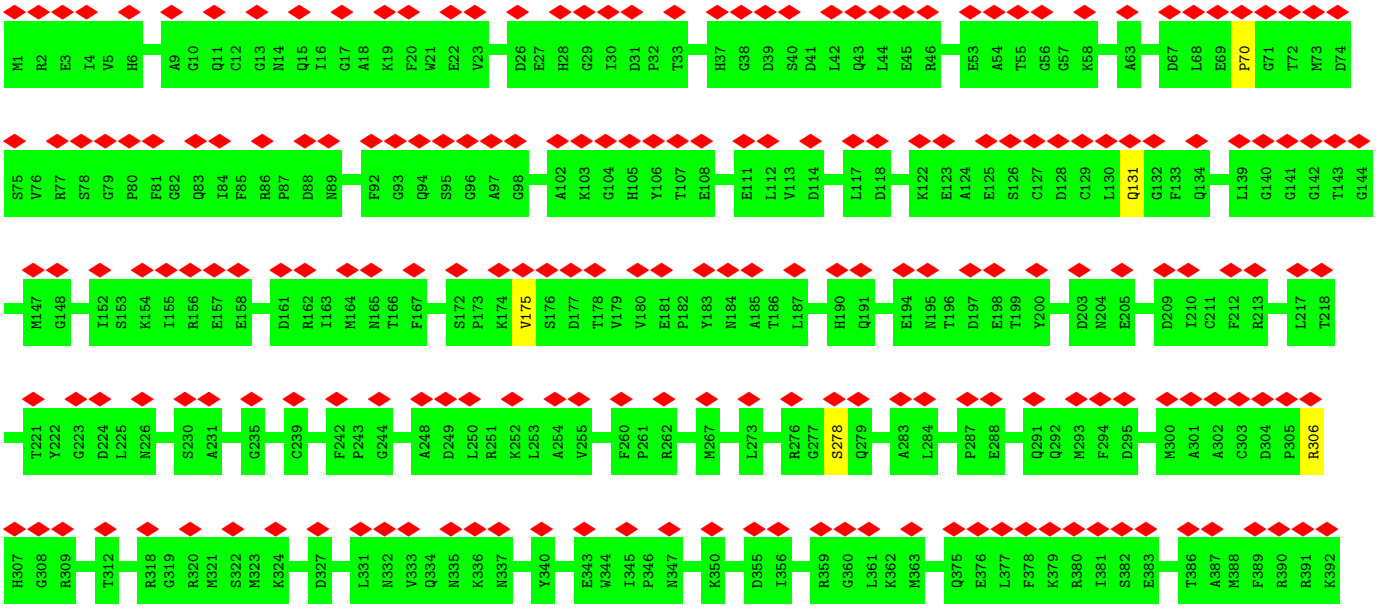
- Molecule 55: Tubulin beta chain

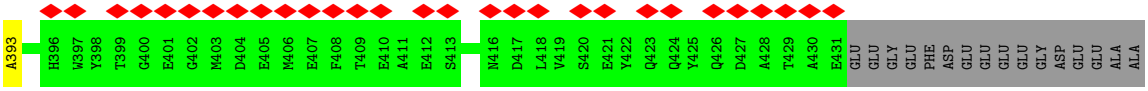
Chain UH: 66% 94%



- Molecule 55: Tubulin beta chain

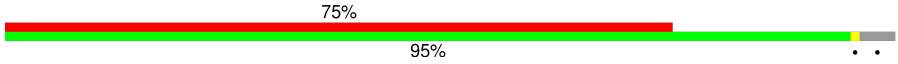
Chain UJ: 53% 95%

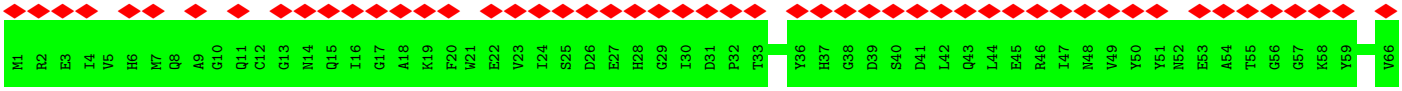


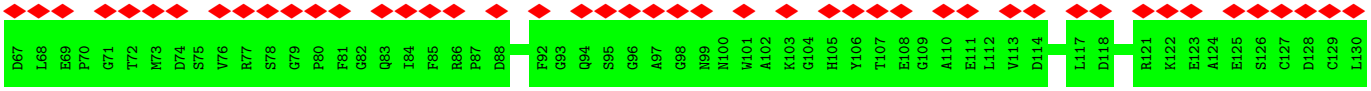


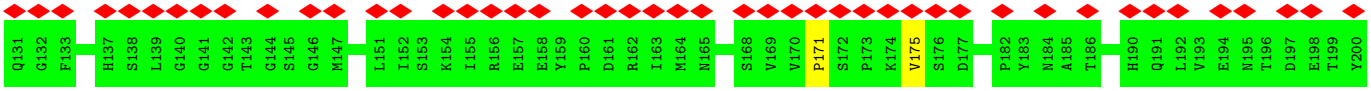
- Molecule 55: Tubulin beta chain

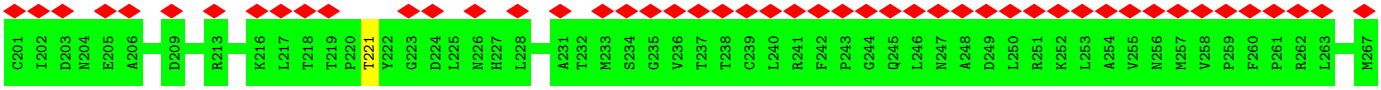
Chain UL:

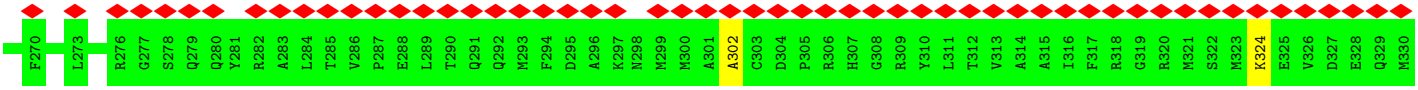


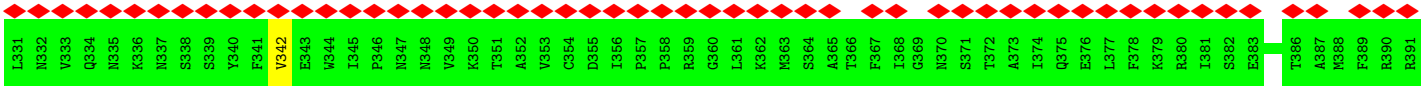


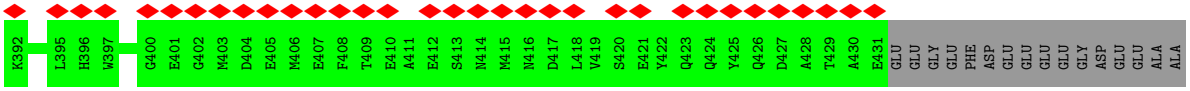






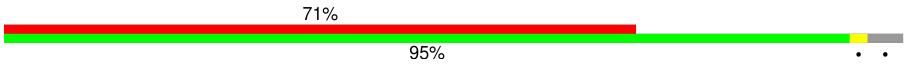


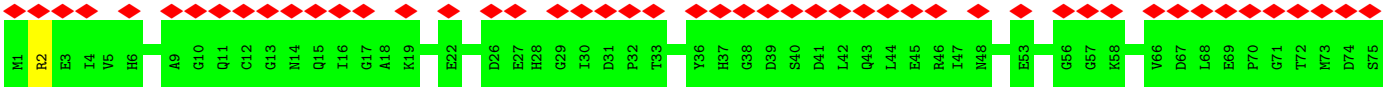


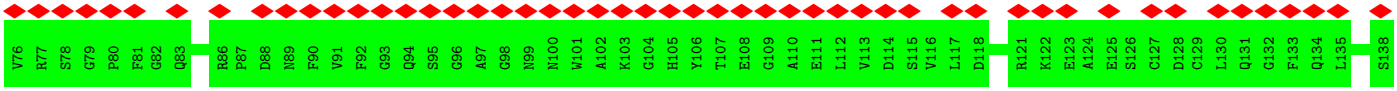


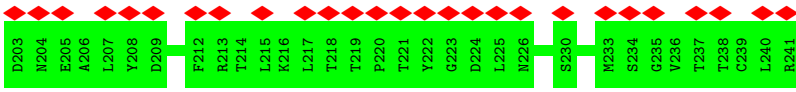
- Molecule 55: Tubulin beta chain

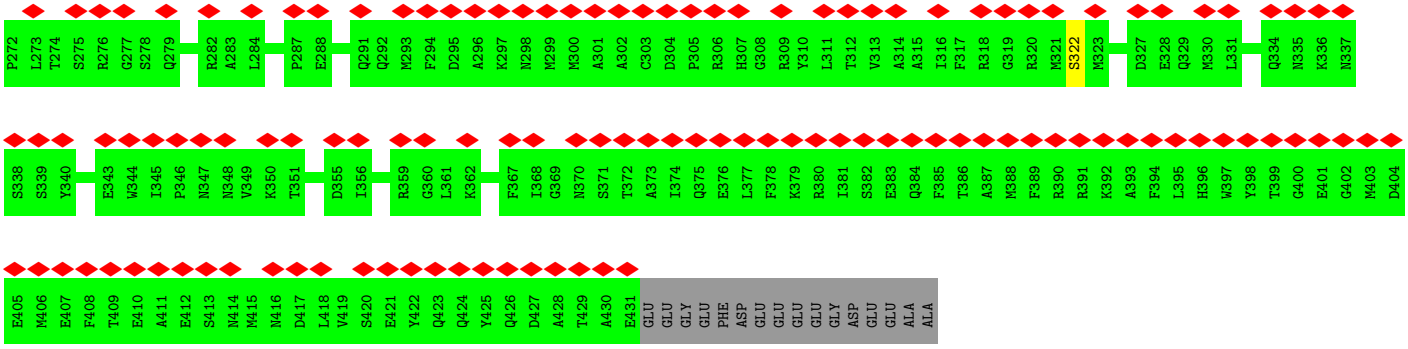
Chain UM:





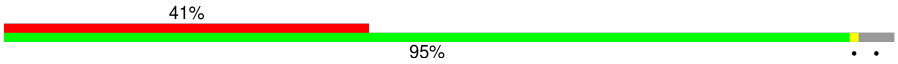


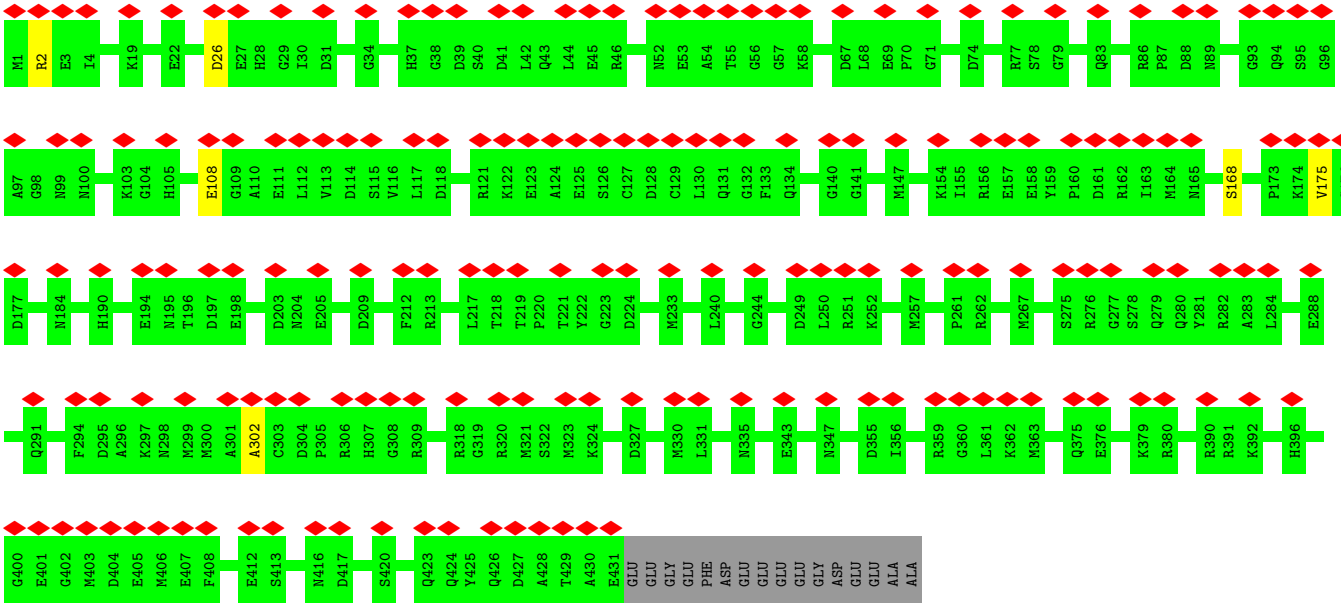




- Molecule 55: Tubulin beta chain

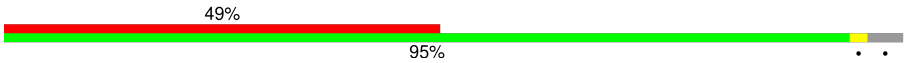
Chain VC:

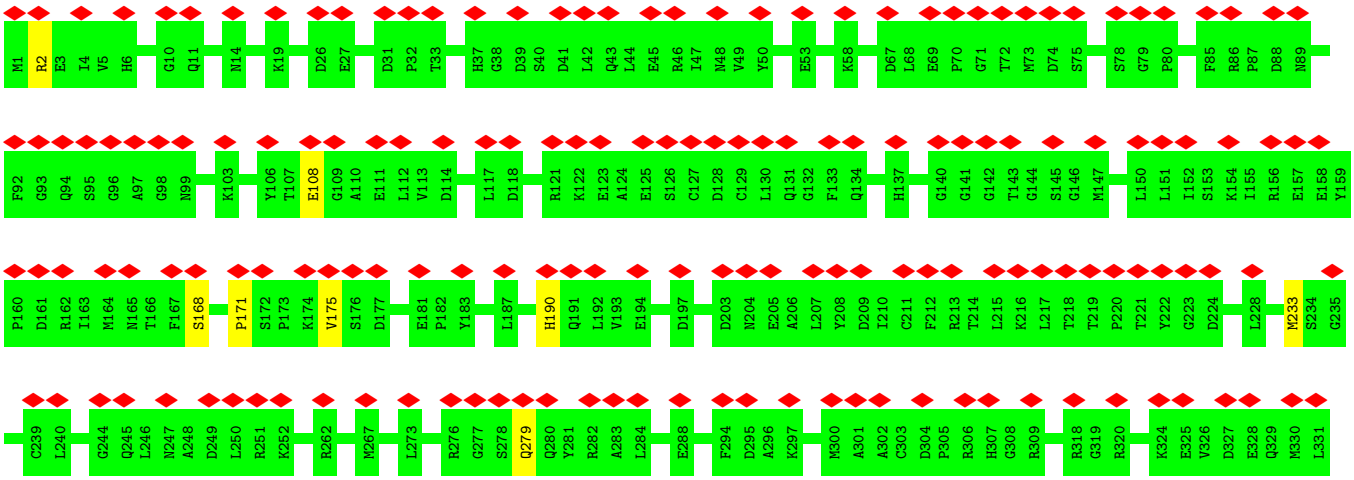


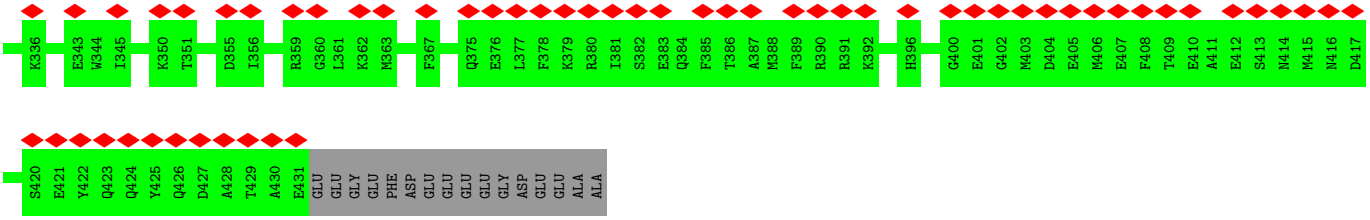


- Molecule 55: Tubulin beta chain

Chain VD:

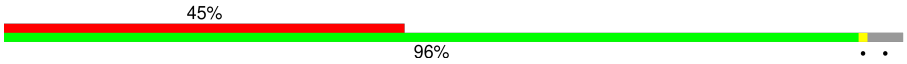


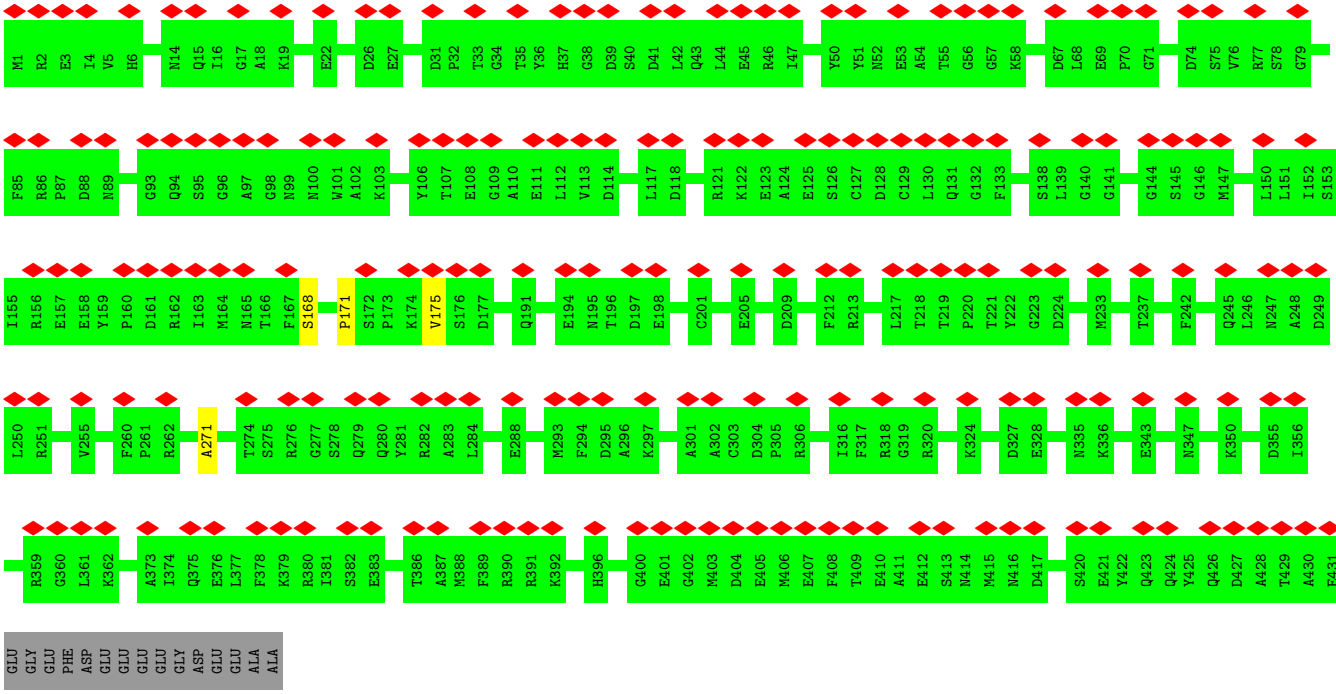




- Molecule 55: Tubulin beta chain

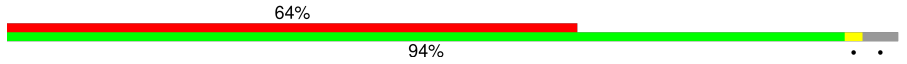
Chain VF:

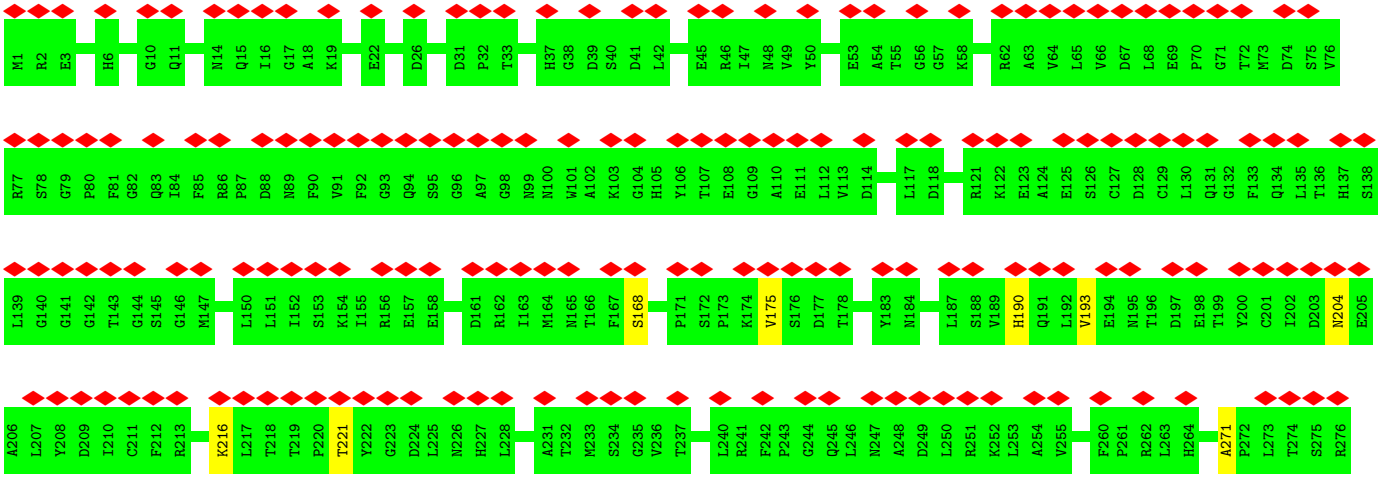


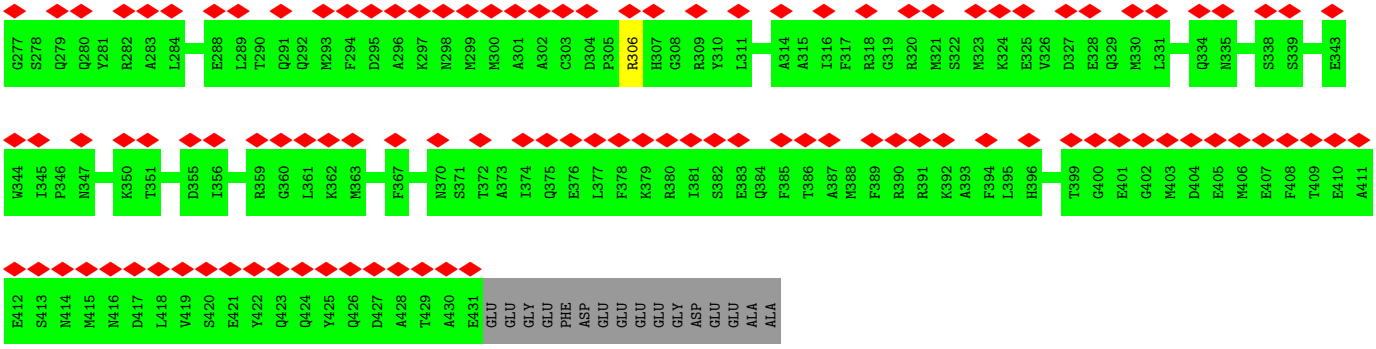


- Molecule 55: Tubulin beta chain

Chain VH:

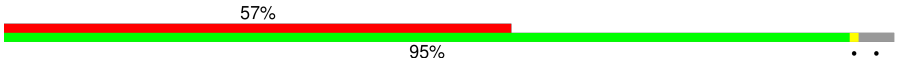


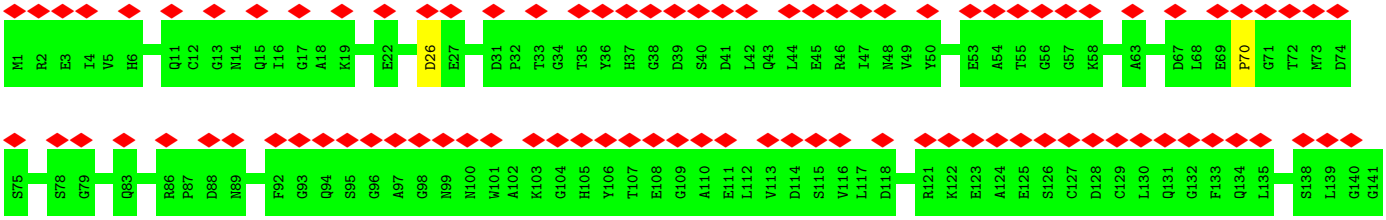




- Molecule 55: Tubulin beta chain

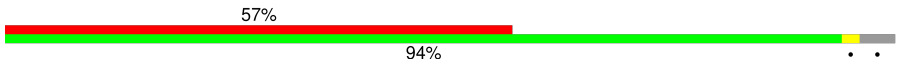
Chain VJ:

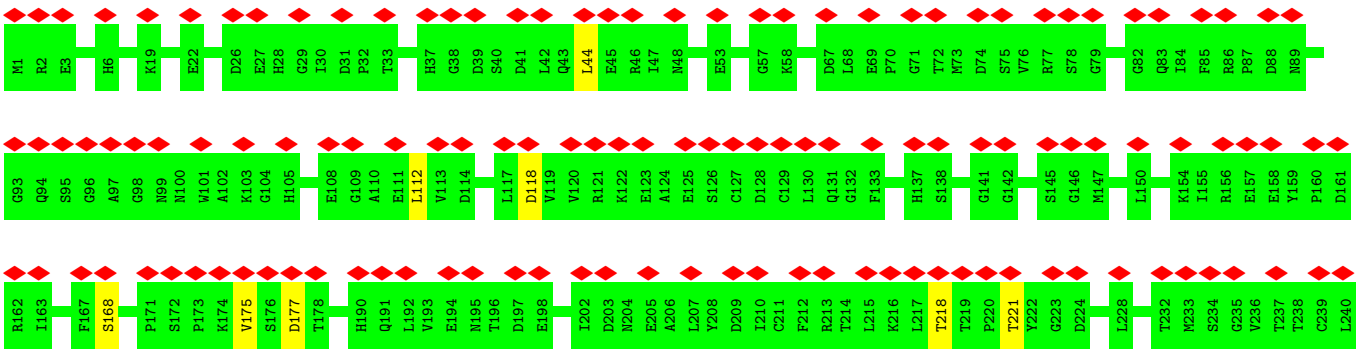


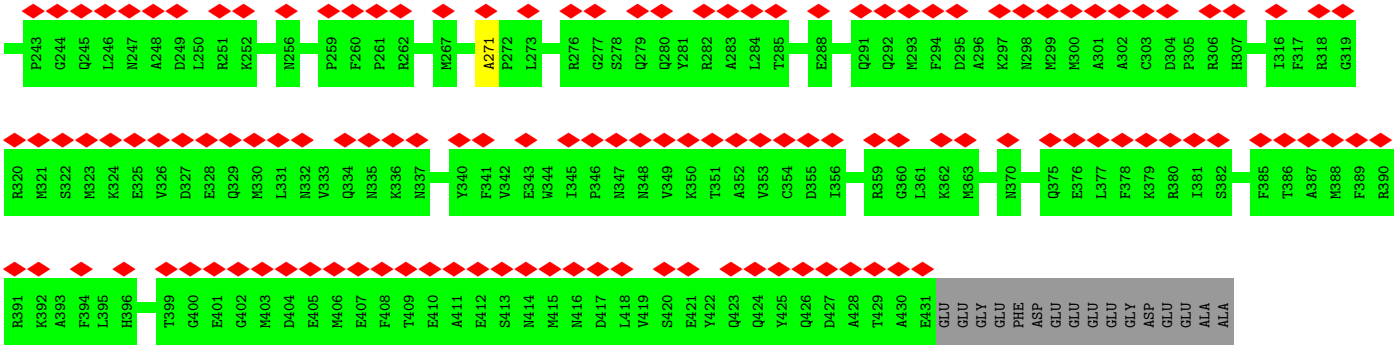


- Molecule 55: Tubulin beta chain

Chain VL:

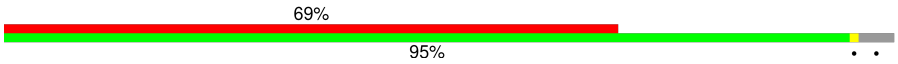


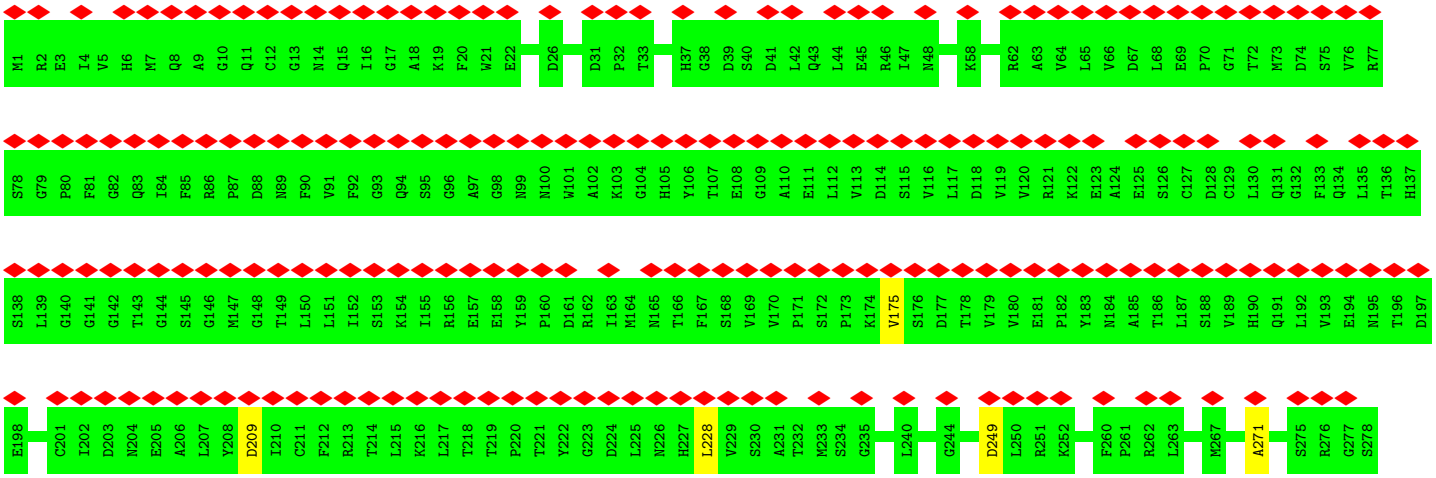




- Molecule 55: Tubulin beta chain

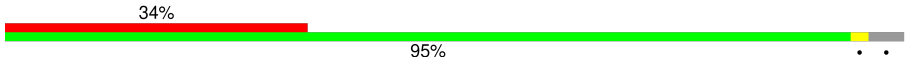
Chain VM:

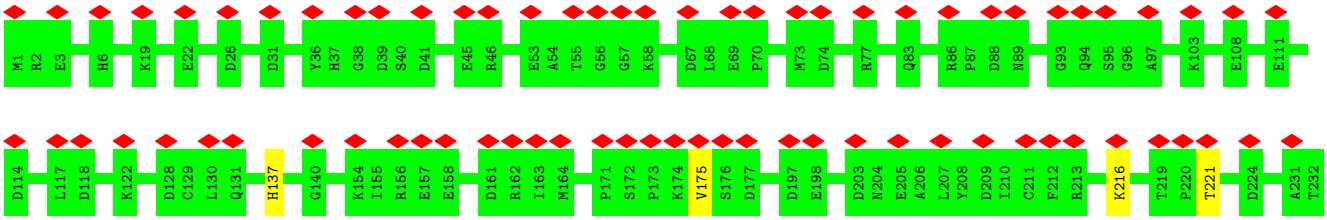


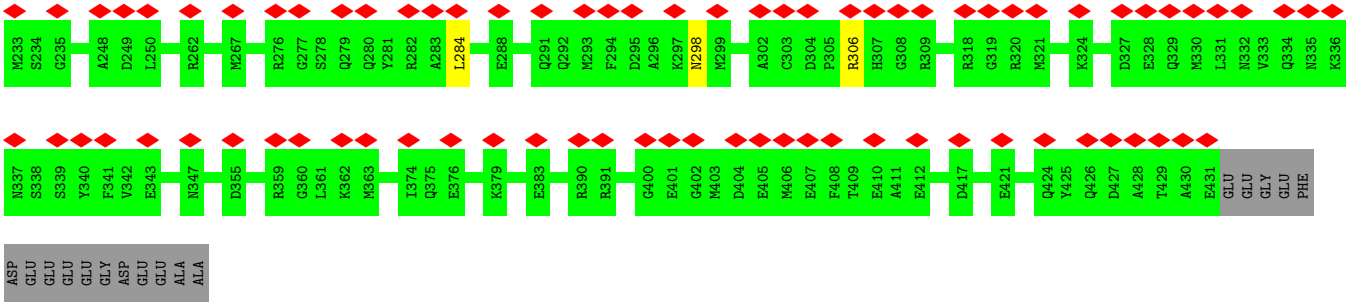


- Molecule 55: Tubulin beta chain

Chain WC:

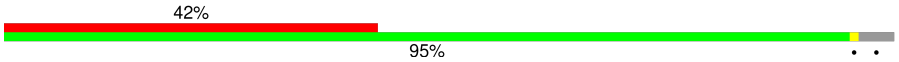


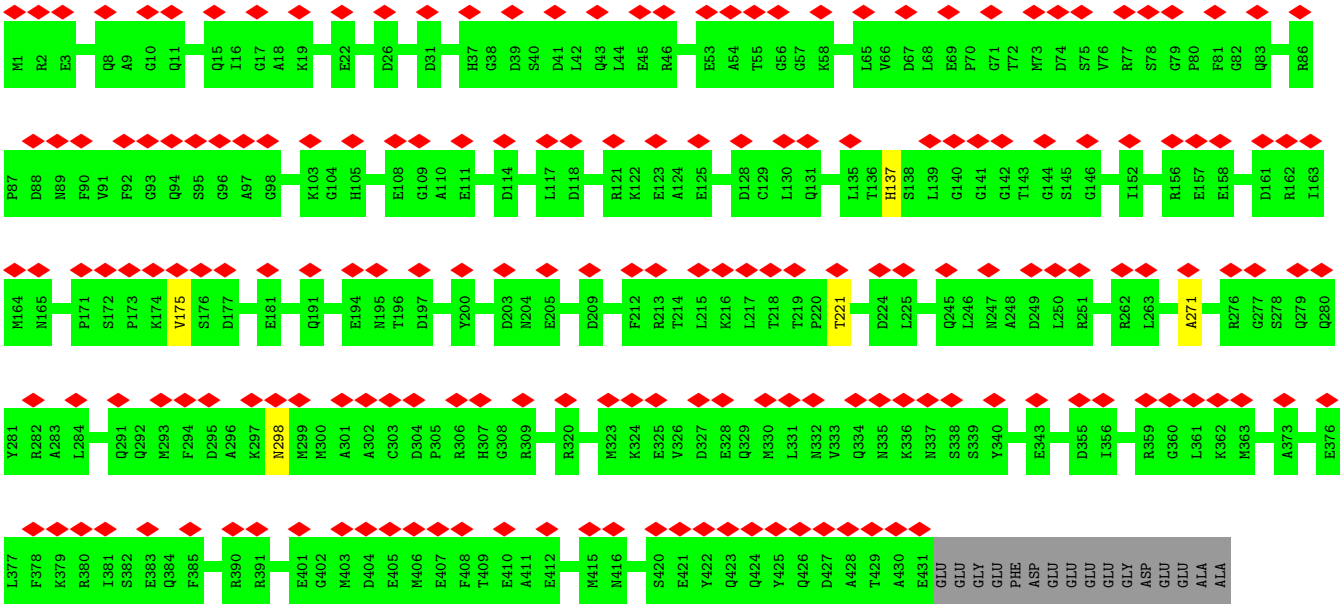




- Molecule 55: Tubulin beta chain

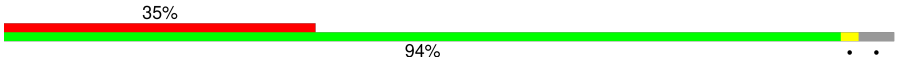
Chain WD:

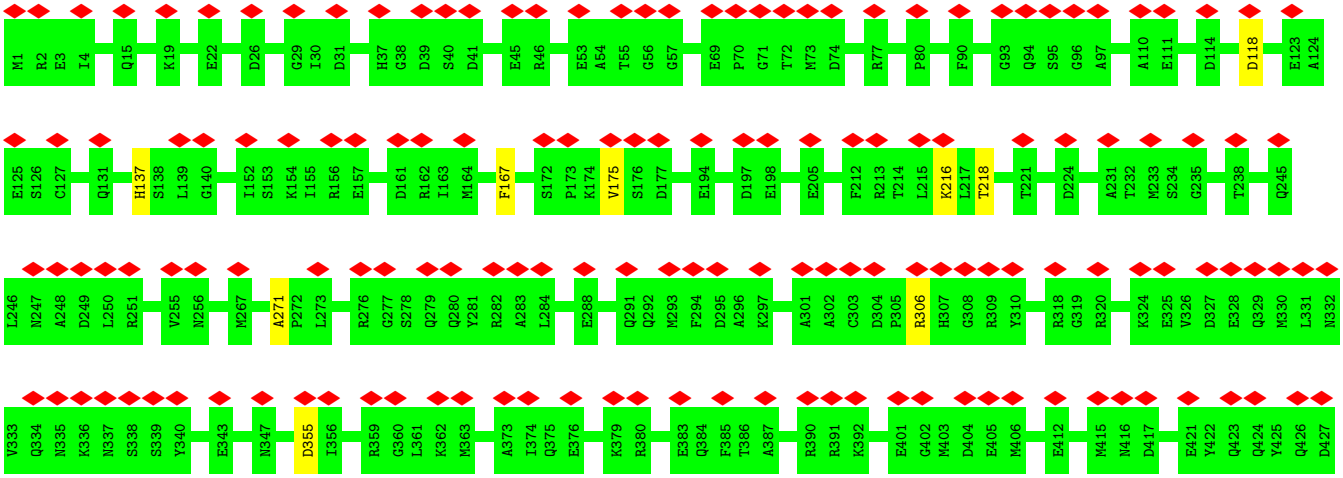


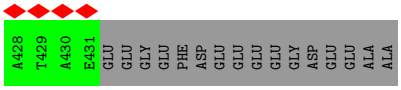


- Molecule 55: Tubulin beta chain

Chain WF:

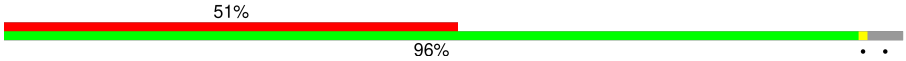


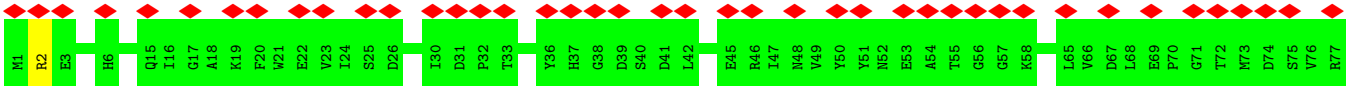


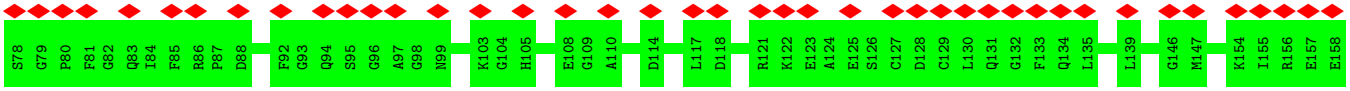


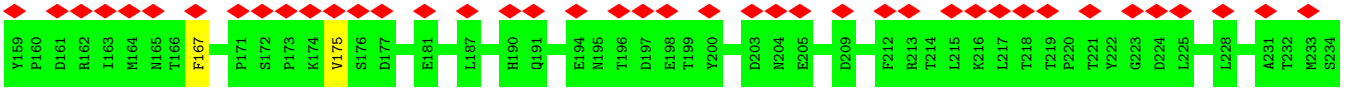
• Molecule 55: Tubulin beta chain

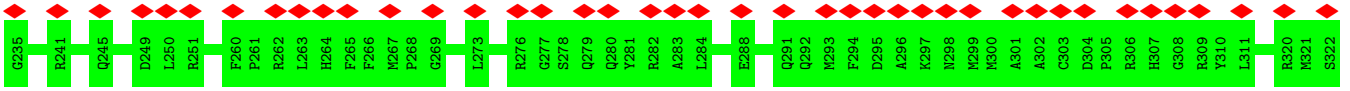
Chain WH:

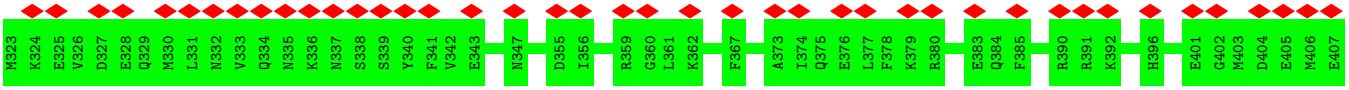


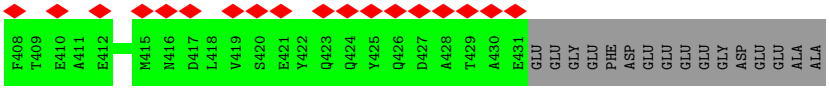






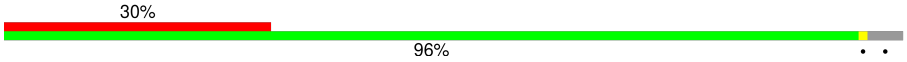


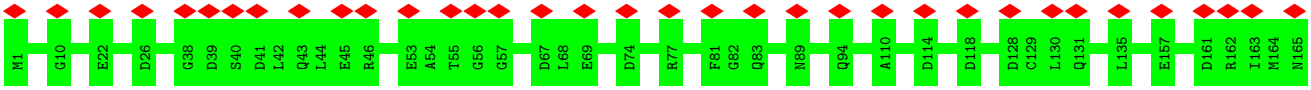


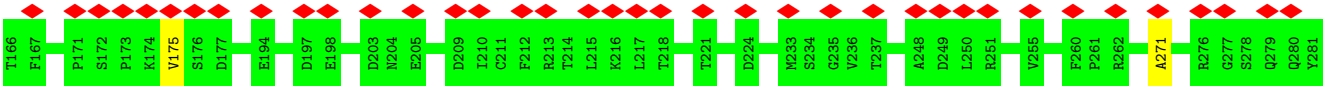


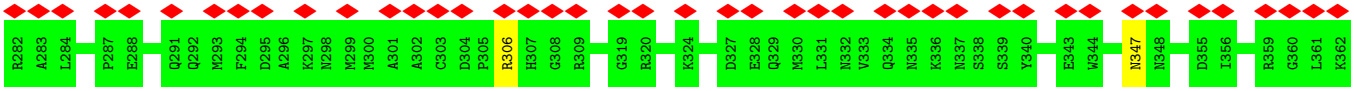
• Molecule 55: Tubulin beta chain

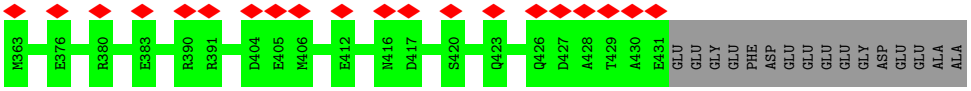
Chain WJ:





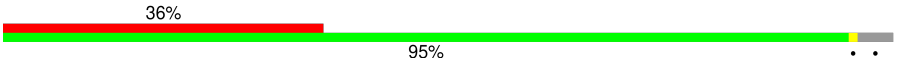


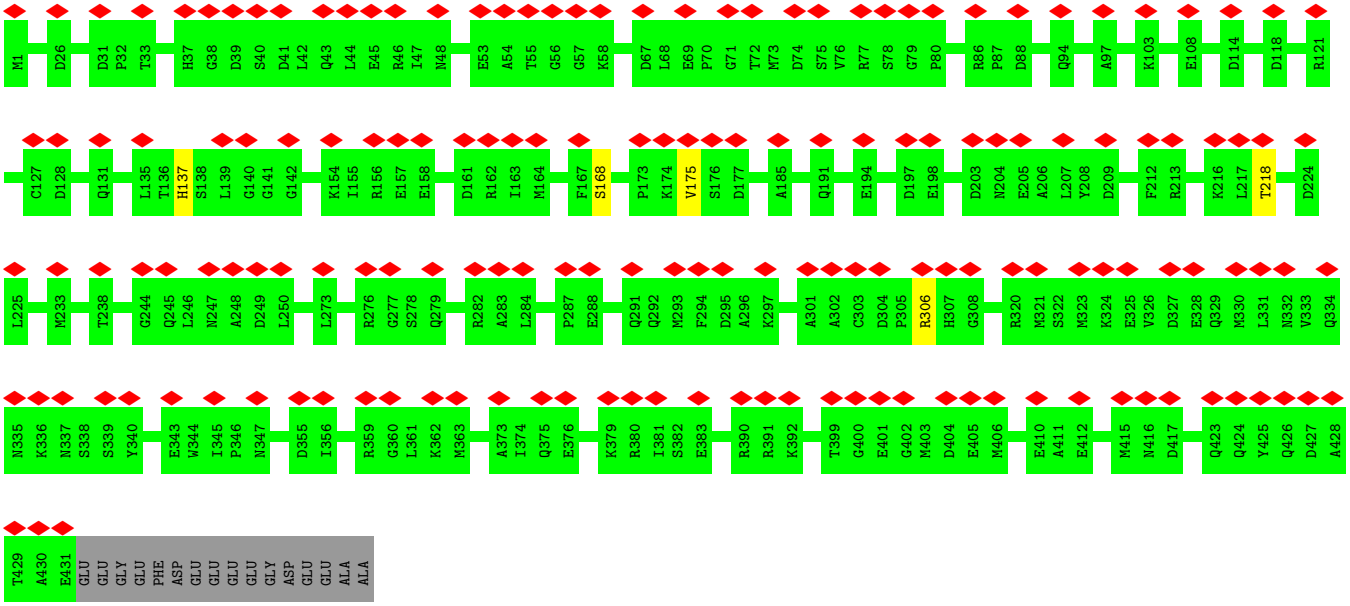




• Molecule 55: Tubulin beta chain

Chain WL:

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P32
T33
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G38
D39
S40
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L42
Q43
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N48
E53
A54
T55
G56
G57
K58
D67
L68
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P70
G71
T72
M73
D74
S75
V76
R77
S78
G79
P80
R86
P87
D88
Q94
A97
K103
E108
D114
D118
R121
C127
D128
Q131
L135
T136
H137
S138
L139
G140
G141
G142
K154
I155
R156
E157
E158
D161
R162
I163
M164
F167
S168
P173
K174
V175
S176
D177
A185
Q191
E194
D197
E198
D203
N204
E205
A206
L207
Y208
D209
F212
R213
K216
L217
T218
D224
L225
M233
T238
G244
Q245
L246
N247
A248
D249
L250
L273
R276
G277
S278
Q279
R282
A283
L284
P287
E288
Q291
Q292
M293
F294
D295
A296
K297
A301
A302
C303
D304
P305
R306
H307
G308
R320
M321
S322
M323
K324
E325
V326
D327
E328
Q329
M330
L331
N332
V333
Q334
N335
K336
N337
S338
S339
Y340
E343
W344
I345
P346
N347
D355
I356
R359
G360
L361
K362
M363
A373
I374
Q375
E376
K379
R380
I381
S382
E383
R390
R391
K392
T399
G400
E401
G402
M403
D404
E405
M406
E410
A411
E412
M415
N416
D417
Q423
Q424
Y425
Q426
D427
A428
T429
A430
E431
GLU
GLU
GLY
GLU
PHE
ASP
GLU
GLU
GLU
GLU
GLY
ASP
GLU
GLU
ALA
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127673	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 ($e^-/Å^2$)	34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	26.701	Depositor
Minimum map value	0.000	Depositor
Average map value	0.244	Depositor
Map value standard deviation	1.144	Depositor
Recommended contour level	6.63	Depositor
Map size (Å)	686.08, 686.08, 686.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	1A	0.32	0/330	0.83	1/440 (0.2%)
1	1B	0.30	0/2085	0.66	2/2806 (0.1%)
2	1E	0.31	0/3324	0.60	0/4478
2	1F	0.30	0/1298	0.57	0/1759
2	1G	0.28	0/2380	0.60	1/3191 (0.0%)
2	1H	0.30	0/3337	0.63	2/4495 (0.0%)
3	1K	0.28	0/1432	0.62	1/1926 (0.1%)
3	1L	0.30	0/1432	0.62	1/1926 (0.1%)
3	1M	0.29	0/1419	0.63	0/1910
3	1v	0.35	1/1737 (0.1%)	0.73	1/2324 (0.0%)
3	1w	0.31	0/736	0.69	1/981 (0.1%)
3	1x	0.30	0/2112	0.70	1/2824 (0.0%)
3	1y	0.35	1/1655 (0.1%)	0.68	0/2215
3	1z	0.31	0/736	0.68	1/981 (0.1%)
3	2a	0.24	0/457	0.61	0/609
4	1P	0.32	0/1665	0.64	0/2254
4	1Q	0.28	0/1154	0.63	0/1559
5	1T	0.29	0/1897	0.61	2/2561 (0.1%)
5	1U	0.30	0/927	0.61	0/1257
5	1V	0.32	0/1910	0.65	1/2578 (0.0%)
5	1W	0.29	0/889	0.62	0/1192
6	1Y	0.30	0/1033	0.66	0/1391
7	1a	0.32	0/1060	0.67	0/1434
7	1b	0.34	0/954	0.68	1/1297 (0.1%)
7	5E	0.30	0/1197	0.67	0/1627
7	5F	0.30	0/885	0.66	1/1197 (0.1%)
7	5G	0.31	0/1111	0.65	1/1512 (0.1%)
7	5H	0.31	0/922	0.70	1/1249 (0.1%)
7	5I	0.33	0/205	0.62	0/283
7	5J	0.30	0/1832	0.62	0/2482
7	5K	0.31	0/1046	0.66	0/1422
7	5L	0.30	0/985	0.62	0/1333

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	5M	0.26	0/115	0.51	0/157
7	5N	0.29	0/1915	0.63	0/2599
7	5O	0.32	0/122	0.62	0/169
8	1d	0.32	0/830	0.62	0/1125
9	1f	0.29	0/354	0.77	1/481 (0.2%)
9	1g	0.31	0/492	0.64	0/665
10	1i	0.27	0/314	0.64	0/422
10	1j	0.27	0/284	0.65	1/383 (0.3%)
10	9M	0.28	0/722	0.62	0/968
10	9N	0.27	0/722	0.58	0/968
10	9O	0.40	0/354	0.79	0/479
11	1l	0.29	0/307	0.63	0/415
11	1m	0.29	0/307	0.60	0/415
12	1o	0.33	0/255	0.80	0/338
12	1p	0.31	0/264	0.83	0/350
12	1q	0.27	0/387	0.77	0/515
12	1r	0.28	0/238	0.77	0/315
13	2A	0.30	0/2086	0.65	1/2797 (0.0%)
13	2B	0.31	0/2093	0.65	1/2807 (0.0%)
13	2C	0.31	0/2095	0.65	0/2809
13	2D	0.40	0/652	0.78	1/884 (0.1%)
14	2G	0.26	0/1920	0.59	0/2588
15	2J	0.29	0/884	0.61	0/1192
15	2K	0.29	0/884	0.60	0/1192
15	2L	0.28	0/884	0.62	0/1192
16	2O	0.35	0/989	0.63	0/1319
17	2R	0.32	0/1044	0.66	0/1382
17	2S	0.31	0/3277	0.62	0/4347
18	2V	0.28	0/2260	0.63	2/3067 (0.1%)
18	2W	0.28	0/2260	0.60	0/3067
19	3A	0.29	0/1582	0.63	1/2135 (0.0%)
19	3B	0.30	0/1582	0.66	1/2135 (0.0%)
19	3C	0.29	0/1526	0.69	1/2055 (0.0%)
19	3D	0.28	0/1492	0.66	1/2009 (0.0%)
19	3E	0.28	0/1574	0.65	0/2124
19	3F	0.29	0/1582	0.63	0/2135
19	3G	0.29	0/1574	0.61	0/2124
20	3J	0.29	0/4022	0.63	1/5441 (0.0%)
20	3K	0.31	0/559	0.74	1/752 (0.1%)
21	3N	0.40	0/2153	0.78	4/2863 (0.1%)
21	3O	0.34	0/2349	0.65	2/3126 (0.1%)
22	3R	0.30	0/1353	0.70	3/1833 (0.2%)
22	3S	0.30	0/1032	0.73	3/1397 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
22	3T	0.30	0/1353	0.68	2/1833 (0.1%)
23	3W	0.35	0/3244	0.72	3/4309 (0.1%)
23	3X	0.34	0/2677	0.63	0/3550
23	3Y	0.30	0/868	0.68	0/1153
23	3Z	0.28	0/1424	0.66	1/1897 (0.1%)
24	4A	0.28	0/4898	0.62	2/6616 (0.0%)
24	4B	0.28	0/4886	0.61	2/6600 (0.0%)
24	4C	0.29	0/4898	0.62	1/6616 (0.0%)
25	4F	0.33	0/2633	0.63	0/3500
25	4G	0.30	0/1775	0.66	1/2367 (0.0%)
26	4J	0.30	0/3050	0.63	2/4120 (0.0%)
26	4K	0.30	0/3039	0.65	0/4105
27	4N	0.31	0/1270	0.67	0/1714
27	4O	0.29	0/898	0.64	0/1212
27	4P	0.30	0/1252	0.65	0/1692
27	4Q	0.27	0/765	0.72	1/1035 (0.1%)
28	4T	0.26	0/1244	0.61	0/1666
28	4U	0.28	0/1244	0.66	1/1666 (0.1%)
28	4V	0.24	0/118	0.46	0/158
29	4Y	0.26	0/2480	0.56	0/3364
30	5A	0.28	0/274	0.59	0/369
30	5B	0.29	0/1705	0.62	0/2311
30	9Y	0.28	0/1118	0.68	1/1513 (0.1%)
30	9Z	0.32	0/811	0.66	0/1099
31	6A	0.29	0/1834	0.58	1/2479 (0.0%)
31	6B	0.33	0/1779	0.65	0/2406
31	6C	0.29	0/1811	0.58	1/2449 (0.0%)
31	6D	0.29	0/1826	0.56	0/2468
31	6E	0.28	0/1826	0.56	0/2468
31	6F	0.29	0/1826	0.57	0/2468
32	6I	0.28	0/653	0.60	0/887
32	6J	0.29	0/422	0.58	0/572
33	6M	0.27	0/3193	0.56	0/4326
33	6N	0.28	0/666	0.68	1/898 (0.1%)
34	6Q	0.29	0/1677	0.56	1/2275 (0.0%)
34	6R	0.33	0/624	0.58	0/853
35	6U	0.30	0/1260	0.63	1/1692 (0.1%)
35	6V	0.28	0/2304	0.57	0/3081
35	6W	0.29	0/2056	0.64	0/2743
35	6X	0.30	0/1041	0.65	0/1392
36	7A	0.29	0/6054	0.65	5/8189 (0.1%)
36	7B	0.28	0/3823	0.64	1/5163 (0.0%)
36	7C	0.28	0/4531	0.63	1/6118 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
36	7D	0.29	0/6046	0.65	4/8177 (0.0%)
37	7G	0.28	0/4421	0.61	0/5995
37	7H	0.30	0/4421	0.66	3/5995 (0.1%)
37	7I	0.29	0/5125	0.61	3/6942 (0.0%)
38	7M	0.28	0/2222	0.56	0/3012
38	7N	0.28	0/544	0.52	0/744
39	7Q	0.29	0/1234	0.67	1/1673 (0.1%)
39	7R	0.30	0/1167	0.67	1/1581 (0.1%)
40	7U	0.35	0/775	0.90	1/1052 (0.1%)
40	7V	0.35	0/472	0.78	0/645
41	7Y	0.29	0/1630	0.65	1/2209 (0.0%)
41	7Z	0.32	0/498	0.74	0/674
42	8A	0.28	0/1983	0.66	2/2694 (0.1%)
43	8D	0.25	0/3283	0.54	2/4406 (0.0%)
43	8E	0.29	0/1500	0.55	0/2013
43	8F	0.27	0/2155	0.54	0/2884
43	8G	0.28	0/3283	0.56	2/4406 (0.0%)
44	8J	0.26	0/3312	0.53	0/4461
44	8K	0.29	0/2646	0.55	0/3551
44	8L	0.27	0/3312	0.56	0/4461
44	8M	0.27	0/1064	0.55	0/1446
44	8N	0.29	0/145	0.63	0/195
45	8Q	0.24	0/182	0.50	0/245
45	8R	0.24	0/3268	0.54	1/4387 (0.0%)
45	8S	0.29	0/2497	0.58	2/3350 (0.1%)
45	8T	0.28	0/3268	0.58	0/4387
45	8U	0.29	0/962	0.58	0/1287
46	8X	0.28	0/902	0.68	0/1212
46	8Y	0.28	0/902	0.66	0/1212
46	8Z	0.28	0/902	0.71	2/1212 (0.2%)
47	9A	0.32	0/1747	0.71	3/2367 (0.1%)
48	9D	0.30	0/829	0.70	0/1110
49	9G	0.28	0/1270	0.57	0/1728
50	9J	0.26	0/847	0.60	0/1150
51	9R	0.26	0/1201	0.56	0/1631
52	9T	0.33	0/645	0.62	0/865
53	9V	0.34	0/196	0.74	0/266
53	9W	0.27	0/627	0.56	0/855
54	AA	0.29	0/3492	0.56	0/4742
54	AB	0.28	0/3492	0.54	0/4742
54	AE	0.29	0/3492	0.58	1/4742 (0.0%)
54	AG	0.28	0/3492	0.58	1/4742 (0.0%)
54	AI	0.29	0/3492	0.55	0/4742

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
54	AK	0.29	0/3492	0.58	0/4742
54	AM	0.28	0/3492	0.56	0/4742
54	BA	0.29	0/3492	0.60	2/4742 (0.0%)
54	BB	0.30	0/3492	0.59	0/4742
54	BE	0.30	0/3492	0.59	1/4742 (0.0%)
54	BG	0.29	0/3492	0.59	0/4742
54	BI	0.29	0/3492	0.59	1/4742 (0.0%)
54	BK	0.29	0/3492	0.60	1/4742 (0.0%)
54	BM	0.30	0/3492	0.59	0/4742
54	CA	0.29	0/3492	0.56	0/4742
54	CB	0.28	0/3492	0.59	1/4742 (0.0%)
54	CE	0.29	0/3492	0.59	1/4742 (0.0%)
54	CG	0.28	0/3492	0.58	0/4742
54	CI	0.30	0/3492	0.60	1/4742 (0.0%)
54	CK	0.29	0/3492	0.64	3/4742 (0.1%)
54	CM	0.31	0/3492	0.58	1/4742 (0.0%)
54	DA	0.29	0/3492	0.57	0/4742
54	DB	0.30	0/3492	0.58	0/4742
54	DE	0.29	0/3492	0.59	0/4742
54	DG	0.29	0/3492	0.63	3/4742 (0.1%)
54	DI	0.30	0/3492	0.58	1/4742 (0.0%)
54	DK	0.28	0/3492	0.56	0/4742
54	DM	0.29	0/3492	0.58	2/4742 (0.0%)
54	EA	0.39	0/3492	0.60	2/4742 (0.0%)
54	EC	0.29	0/3492	0.59	1/4742 (0.0%)
54	EE	0.28	0/3492	0.59	1/4742 (0.0%)
54	EG	0.30	0/3492	0.60	1/4742 (0.0%)
54	EI	0.30	0/3492	0.62	2/4742 (0.0%)
54	EK	0.30	0/3492	0.59	0/4742
54	FA	0.41	0/3492	0.60	1/4742 (0.0%)
54	FB	0.29	0/3492	0.61	2/4742 (0.0%)
54	FE	0.40	0/3492	0.62	1/4742 (0.0%)
54	FG	0.31	0/3492	0.62	3/4742 (0.1%)
54	FI	0.41	0/3492	0.63	0/4742
54	FK	0.29	0/3492	0.59	2/4742 (0.0%)
54	GA	0.30	0/3492	0.60	1/4742 (0.0%)
54	GB	0.30	0/3492	0.57	0/4742
54	GE	0.29	0/3492	0.57	0/4742
54	GG	0.29	0/3492	0.58	0/4742
54	GI	0.30	0/3492	0.59	1/4742 (0.0%)
54	GK	0.30	0/3492	0.61	2/4742 (0.0%)
54	HA	0.29	0/3492	0.59	1/4742 (0.0%)
54	HB	0.29	0/3492	0.57	1/4742 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
54	HE	0.28	0/3459	0.57	0/4697
54	HG	0.29	0/3483	0.57	2/4729 (0.0%)
54	HI	0.29	0/3492	0.56	0/4742
54	HK	0.29	0/3483	0.55	0/4729
54	IA	0.29	0/3492	0.58	1/4742 (0.0%)
54	IB	0.29	0/3475	0.56	0/4718
54	IE	0.31	0/3492	0.60	0/4742
54	IG	0.29	0/3492	0.57	1/4742 (0.0%)
54	II	0.29	0/3479	0.59	0/4723
54	IK	0.29	0/3492	0.56	0/4742
54	IM	0.28	0/3492	0.58	1/4742 (0.0%)
54	JA	0.29	0/3464	0.59	2/4703 (0.0%)
54	JB	0.28	0/3492	0.56	0/4742
54	JE	0.29	0/3492	0.57	1/4742 (0.0%)
54	JG	0.29	0/3492	0.57	0/4742
54	JI	0.30	0/3492	0.57	2/4742 (0.0%)
54	JK	0.28	0/3492	0.57	0/4742
54	KA	0.28	0/3492	0.55	0/4742
54	KB	0.31	0/3475	0.61	2/4718 (0.0%)
54	KE	0.30	0/3492	0.59	0/4742
54	KG	0.29	0/3492	0.60	1/4742 (0.0%)
54	KI	0.28	0/3492	0.56	0/4742
54	KK	0.29	0/3492	0.56	0/4742
54	LA	0.29	0/3492	0.54	1/4742 (0.0%)
54	LB	0.29	0/3492	0.59	1/4742 (0.0%)
54	LE	0.29	0/3492	0.57	2/4742 (0.0%)
54	LG	0.30	0/3492	0.58	1/4742 (0.0%)
54	LI	0.29	0/3492	0.55	0/4742
54	LK	0.29	0/3492	0.56	0/4742
54	MA	0.29	0/3492	0.56	0/4742
54	MB	0.29	0/3492	0.59	1/4742 (0.0%)
54	ME	0.29	0/3492	0.56	0/4742
54	MG	0.29	0/3492	0.57	0/4742
54	MI	0.30	0/3492	0.57	0/4742
54	MK	0.28	0/3492	0.57	1/4742 (0.0%)
54	ML	0.28	0/3492	0.55	0/4742
54	NA	0.30	0/3483	0.60	0/4729
54	NB	0.30	0/3492	0.60	0/4742
54	NE	0.29	0/3492	0.59	0/4742
54	NG	0.29	0/3492	0.60	2/4742 (0.0%)
54	NI	0.30	0/3475	0.61	1/4718 (0.0%)
54	NL	0.29	0/3468	0.59	0/4708
54	OA	0.30	0/3492	0.58	1/4742 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
54	OB	0.28	0/3475	0.57	0/4718
54	OE	0.30	0/3492	0.61	2/4742 (0.0%)
54	OG	0.30	0/3492	0.61	0/4742
54	OI	0.30	0/3492	0.59	0/4742
54	OK	0.29	0/3492	0.58	0/4742
54	OL	0.31	0/3492	0.59	0/4742
54	PA	0.29	0/3492	0.58	0/4742
54	PB	0.30	0/3492	0.58	1/4742 (0.0%)
54	PE	0.28	0/3492	0.55	0/4742
54	PG	0.30	0/3492	0.58	1/4742 (0.0%)
54	PI	0.30	0/3492	0.59	0/4742
54	PK	0.29	0/3492	0.61	1/4742 (0.0%)
54	PL	0.28	0/3492	0.59	0/4742
54	QA	0.29	0/3492	0.56	1/4742 (0.0%)
54	QB	0.29	0/3492	0.59	0/4742
54	QE	0.31	0/3492	0.58	0/4742
54	QG	0.31	0/3492	0.59	0/4742
54	QI	0.31	0/3492	0.60	0/4742
54	QK	0.29	0/3468	0.58	0/4708
54	QL	0.27	0/3487	0.58	1/4734 (0.0%)
54	RA	0.30	0/3492	0.59	2/4742 (0.0%)
54	RB	0.30	0/3492	0.61	2/4742 (0.0%)
54	RE	0.31	0/3492	0.65	5/4742 (0.1%)
54	RG	0.30	0/3492	0.59	1/4742 (0.0%)
54	RI	0.30	0/3492	0.61	0/4742
54	RK	0.30	0/3492	0.60	2/4742 (0.0%)
54	RL	0.29	0/3492	0.62	0/4742
54	SA	0.29	0/3492	0.62	4/4742 (0.1%)
54	SB	0.30	0/3492	0.59	1/4742 (0.0%)
54	SE	0.31	0/3492	0.59	1/4742 (0.0%)
54	SG	0.32	0/3492	0.62	0/4742
54	SI	0.31	0/3492	0.59	1/4742 (0.0%)
54	SK	0.29	0/3492	0.57	1/4742 (0.0%)
54	TA	0.29	0/3487	0.58	0/4734
54	TB	0.29	0/3487	0.58	0/4734
54	TE	0.31	0/3492	0.60	2/4742 (0.0%)
54	TG	0.30	0/3492	0.59	0/4742
54	TI	0.29	0/3492	0.60	2/4742 (0.0%)
54	TK	0.32	0/3492	0.64	1/4742 (0.0%)
54	UA	0.29	0/3487	0.60	1/4734 (0.0%)
54	UB	0.29	0/3472	0.59	2/4713 (0.0%)
54	UE	0.29	0/3492	0.59	0/4742
54	UG	0.28	0/3492	0.59	1/4742 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
54	UI	0.30	0/3492	0.62	2/4742 (0.0%)
54	UK	0.30	0/3492	0.61	1/4742 (0.0%)
54	VA	0.30	0/3492	0.62	1/4742 (0.0%)
54	VB	0.29	0/3492	0.59	0/4742
54	VE	0.30	0/3492	0.60	0/4742
54	VG	0.29	0/3483	0.63	2/4729 (0.0%)
54	VI	0.30	0/3492	0.60	1/4742 (0.0%)
54	VK	0.29	0/3492	0.60	2/4742 (0.0%)
54	WA	0.30	0/3492	0.62	1/4742 (0.0%)
54	WB	0.28	0/3487	0.58	0/4734
54	WE	0.30	0/3492	0.63	1/4742 (0.0%)
54	WG	0.30	0/3492	0.59	0/4742
54	WI	0.28	0/3492	0.59	1/4742 (0.0%)
54	WK	0.29	0/3492	0.56	1/4742 (0.0%)
55	AC	0.29	0/3458	0.60	2/4685 (0.0%)
55	AD	0.29	0/3458	0.60	1/4685 (0.0%)
55	AF	0.28	0/3458	0.59	1/4685 (0.0%)
55	AH	0.28	0/3458	0.59	0/4685
55	AJ	0.28	0/3458	0.58	1/4685 (0.0%)
55	AL	0.29	0/3458	0.58	0/4685
55	BC	0.30	0/3458	0.63	1/4685 (0.0%)
55	BD	0.30	0/3458	0.64	2/4685 (0.0%)
55	BF	0.30	0/3458	0.61	1/4685 (0.0%)
55	BH	0.33	0/3458	0.62	1/4685 (0.0%)
55	BJ	0.30	0/3458	0.62	1/4685 (0.0%)
55	BL	0.28	0/3458	0.60	0/4685
55	CC	0.30	0/3458	0.65	1/4685 (0.0%)
55	CD	0.30	0/3458	0.63	3/4685 (0.1%)
55	CF	0.29	0/3458	0.60	1/4685 (0.0%)
55	CH	0.30	0/3458	0.64	2/4685 (0.0%)
55	CJ	0.32	0/3458	0.67	4/4685 (0.1%)
55	CL	0.29	0/3458	0.62	4/4685 (0.1%)
55	DC	0.28	0/3458	0.61	3/4685 (0.1%)
55	DD	0.29	0/3458	0.60	1/4685 (0.0%)
55	DF	0.31	0/3458	0.61	1/4685 (0.0%)
55	DH	0.28	0/3458	0.61	2/4685 (0.0%)
55	DJ	0.28	0/3458	0.63	1/4685 (0.0%)
55	DL	0.30	0/3458	0.59	0/4685
55	EB	0.29	0/3458	0.62	2/4685 (0.0%)
55	ED	0.29	0/3458	0.65	6/4685 (0.1%)
55	EF	0.29	0/3458	0.62	3/4685 (0.1%)
55	EH	0.29	0/3458	0.65	2/4685 (0.0%)
55	EJ	0.29	0/3458	0.61	0/4685

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
55	EL	0.28	0/3458	0.63	2/4685 (0.0%)
55	EM	0.27	0/3458	0.60	2/4685 (0.0%)
55	FC	0.29	0/3458	0.64	1/4685 (0.0%)
55	FD	0.28	0/3458	0.59	1/4685 (0.0%)
55	FF	0.29	0/3458	0.62	2/4685 (0.0%)
55	FH	0.32	1/3458 (0.0%)	0.65	3/4685 (0.1%)
55	FJ	0.29	0/3458	0.64	4/4685 (0.1%)
55	FL	0.28	0/3458	0.63	3/4685 (0.1%)
55	FM	0.29	0/3458	0.60	1/4685 (0.0%)
55	GC	0.29	0/3458	0.60	1/4685 (0.0%)
55	GD	0.28	0/3458	0.58	0/4685
55	GF	0.28	0/3458	0.58	0/4685
55	GH	0.30	0/3458	0.59	1/4685 (0.0%)
55	GJ	0.31	0/3458	0.61	1/4685 (0.0%)
55	GL	0.28	0/3458	0.61	1/4685 (0.0%)
55	GM	0.28	0/3458	0.59	0/4685
55	HC	0.28	0/3458	0.57	0/4685
55	HD	0.29	0/3458	0.61	1/4685 (0.0%)
55	HF	0.28	0/3458	0.58	0/4685
55	HH	0.28	0/3458	0.57	0/4685
55	HJ	0.28	0/3458	0.57	0/4685
55	HL	0.29	0/3458	0.59	1/4685 (0.0%)
55	HM	0.27	0/3458	0.57	1/4685 (0.0%)
55	IC	0.28	0/3458	0.56	0/4685
55	ID	0.29	0/3458	0.60	1/4685 (0.0%)
55	IF	0.28	0/3458	0.56	0/4685
55	IH	0.28	0/3458	0.60	1/4685 (0.0%)
55	IJ	0.29	0/3458	0.59	1/4685 (0.0%)
55	IL	0.29	0/3458	0.61	0/4685
55	JC	0.29	0/3458	0.57	0/4685
55	JD	0.28	0/3458	0.60	1/4685 (0.0%)
55	JF	0.29	0/3458	0.62	3/4685 (0.1%)
55	JH	0.28	0/3458	0.59	1/4685 (0.0%)
55	JJ	0.28	0/3458	0.58	2/4685 (0.0%)
55	JL	0.29	0/3458	0.61	2/4685 (0.0%)
55	JM	0.29	0/3458	0.59	2/4685 (0.0%)
55	KC	0.29	0/3458	0.61	1/4685 (0.0%)
55	KD	0.29	0/3458	0.59	1/4685 (0.0%)
55	KF	0.28	0/3458	0.59	0/4685
55	KH	0.28	0/3458	0.60	2/4685 (0.0%)
55	KJ	0.28	0/3458	0.58	0/4685
55	KL	0.28	0/3458	0.61	0/4685
55	KM	0.28	0/3458	0.57	2/4685 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
55	LC	0.29	0/3458	0.59	2/4685 (0.0%)
55	LD	0.30	0/3458	0.57	0/4685
55	LF	0.29	0/3458	0.60	1/4685 (0.0%)
55	LH	0.28	0/3458	0.60	0/4685
55	LJ	0.30	0/3458	0.58	1/4685 (0.0%)
55	LL	0.30	0/3458	0.62	1/4685 (0.0%)
55	LM	0.28	0/3458	0.58	3/4685 (0.1%)
55	MC	0.29	0/3458	0.59	1/4685 (0.0%)
55	MD	0.29	0/3458	0.57	1/4685 (0.0%)
55	MF	0.28	0/3458	0.56	0/4685
55	MH	0.28	0/3458	0.58	2/4685 (0.0%)
55	MJ	0.28	0/3458	0.57	1/4685 (0.0%)
55	MM	0.29	0/3458	0.60	0/4685
55	NC	0.29	0/3458	0.63	3/4685 (0.1%)
55	ND	0.29	0/3458	0.59	0/4685
55	NF	0.29	0/3458	0.58	1/4685 (0.0%)
55	NH	0.28	0/3458	0.61	2/4685 (0.0%)
55	NJ	0.28	0/3458	0.60	2/4685 (0.0%)
55	NK	0.30	0/3458	0.65	3/4685 (0.1%)
55	NM	0.29	0/3458	0.61	0/4685
55	OC	0.29	0/3458	0.62	2/4685 (0.0%)
55	OD	0.29	0/3458	0.61	1/4685 (0.0%)
55	OF	0.30	0/3458	0.62	0/4685
55	OH	0.30	0/3458	0.63	2/4685 (0.0%)
55	OJ	0.29	0/3458	0.60	0/4685
55	OM	0.30	0/3458	0.61	1/4685 (0.0%)
55	PC	0.29	0/3458	0.63	1/4685 (0.0%)
55	PD	0.28	0/3458	0.59	1/4685 (0.0%)
55	PF	0.30	0/3458	0.63	2/4685 (0.0%)
55	PH	0.28	0/3458	0.57	0/4685
55	PJ	0.29	0/3458	0.60	1/4685 (0.0%)
55	PM	0.30	0/3458	0.58	0/4685
55	QC	0.30	0/3458	0.64	3/4685 (0.1%)
55	QD	0.30	0/3458	0.59	0/4685
55	QF	0.32	0/3458	0.66	3/4685 (0.1%)
55	QH	0.29	0/3458	0.64	2/4685 (0.0%)
55	QJ	0.31	0/3458	0.65	4/4685 (0.1%)
55	QM	0.29	0/3458	0.60	0/4685
55	RC	0.30	0/3458	0.64	1/4685 (0.0%)
55	RD	0.29	0/3458	0.63	2/4685 (0.0%)
55	RF	0.30	0/3458	0.62	3/4685 (0.1%)
55	RH	0.30	0/3458	0.63	0/4685
55	RJ	0.30	0/3458	0.63	2/4685 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
55	RM	0.31	0/3458	0.63	1/4685 (0.0%)
55	SC	0.30	0/3458	0.62	2/4685 (0.0%)
55	SD	0.30	0/3458	0.63	0/4685
55	SF	0.31	0/3458	0.63	2/4685 (0.0%)
55	SH	0.30	0/3458	0.61	0/4685
55	SJ	0.29	0/3458	0.62	1/4685 (0.0%)
55	SL	0.29	0/3458	0.63	1/4685 (0.0%)
55	SM	0.30	0/3458	0.64	3/4685 (0.1%)
55	TC	0.28	0/3458	0.59	1/4685 (0.0%)
55	TD	0.29	0/3458	0.62	1/4685 (0.0%)
55	TF	0.29	0/3458	0.62	0/4685
55	TH	0.29	0/3458	0.61	0/4685
55	TJ	0.30	0/3458	0.62	1/4685 (0.0%)
55	TL	0.28	0/3458	0.59	1/4685 (0.0%)
55	TM	0.30	1/3458 (0.0%)	0.61	1/4685 (0.0%)
55	UC	0.28	0/3458	0.61	2/4685 (0.0%)
55	UD	0.29	0/3458	0.61	1/4685 (0.0%)
55	UF	0.31	0/3458	0.67	0/4685
55	UH	0.31	0/3458	0.64	1/4685 (0.0%)
55	UJ	0.29	0/3458	0.62	0/4685
55	UL	0.30	0/3458	0.62	1/4685 (0.0%)
55	UM	0.30	0/3458	0.65	2/4685 (0.0%)
55	VC	0.30	0/3458	0.61	1/4685 (0.0%)
55	VD	0.30	0/3458	0.64	2/4685 (0.0%)
55	VF	0.31	0/3458	0.64	1/4685 (0.0%)
55	VH	0.31	0/3458	0.63	0/4685
55	VJ	0.29	0/3458	0.62	1/4685 (0.0%)
55	VL	0.29	0/3458	0.61	4/4685 (0.1%)
55	VM	0.30	0/3458	0.65	4/4685 (0.1%)
55	WC	0.30	0/3458	0.60	1/4685 (0.0%)
55	WD	0.30	0/3458	0.60	0/4685
55	WF	0.29	0/3458	0.60	1/4685 (0.0%)
55	WH	0.30	0/3458	0.62	0/4685
55	WJ	0.28	0/3458	0.59	0/4685
55	WL	0.29	0/3458	0.60	0/4685
All	All	0.29	4/1289690 (0.0%)	0.60	401/1747079 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1B	0	2
3	1v	0	1
3	1w	0	1
3	1y	0	1
3	2a	0	1
5	1V	0	1
6	1Y	0	1
7	1a	0	1
7	1b	0	2
7	5K	0	2
10	9O	0	1
12	1r	0	1
19	3B	0	1
20	3J	0	2
22	3S	0	1
23	3W	0	2
25	4G	0	1
26	4J	0	1
30	5B	0	1
30	9Z	0	2
31	6B	0	2
36	7A	0	1
36	7C	0	1
36	7D	0	1
37	7G	0	1
37	7H	0	1
37	7I	0	1
38	7M	0	2
40	7U	0	1
41	7Y	0	1
42	8A	0	1
43	8D	0	1
47	9A	0	1
48	9D	0	1
53	9V	0	2
54	AB	0	1
54	AE	0	1
54	AG	0	1
54	BA	0	1
54	BI	0	1
54	BK	0	1
54	CA	0	1
54	CB	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	CE	0	2
54	CI	0	1
54	CK	0	1
54	CM	0	1
54	DK	0	1
54	EG	0	2
54	EI	0	1
54	EK	0	1
54	FA	0	1
54	FB	0	2
54	FI	0	1
54	GB	0	1
54	HA	0	1
54	HB	0	1
54	HG	0	1
54	IA	0	1
54	IB	0	1
54	IG	0	2
54	II	0	1
54	IK	0	2
54	JA	0	1
54	JB	0	1
54	JE	0	1
54	JG	0	1
54	KB	0	1
54	KE	0	1
54	KG	0	1
54	KI	0	1
54	LA	0	1
54	MA	0	1
54	MB	0	1
54	MI	0	1
54	MK	0	1
54	NB	0	1
54	OE	0	2
54	OK	0	1
54	PA	0	1
54	PI	0	1
54	QB	0	2
54	QE	0	2
54	QI	0	1
54	QK	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	RA	0	1
54	RB	0	2
54	RE	0	1
54	RG	0	1
54	RI	0	1
54	RK	0	1
54	RL	0	2
54	SB	0	1
54	SE	0	1
54	SG	0	2
54	SI	0	1
54	TA	0	1
54	TB	0	2
54	TG	0	1
54	TI	0	1
54	TK	0	2
54	UB	0	1
54	UG	0	1
54	UI	0	1
54	UK	0	1
54	VB	0	1
54	VE	0	1
54	VG	0	1
54	WA	0	1
54	WB	0	1
54	WE	0	1
54	WI	0	1
54	WK	0	1
55	AC	0	1
55	AF	0	2
55	AH	0	2
55	AJ	0	1
55	AL	0	2
55	BC	0	3
55	CC	0	2
55	CD	0	1
55	CF	0	1
55	CH	0	1
55	CJ	0	2
55	CL	0	1
55	DC	0	1
55	DD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	DF	0	2
55	DH	0	3
55	DJ	0	2
55	DL	0	1
55	EB	0	1
55	ED	0	1
55	EF	0	1
55	EH	0	1
55	EJ	0	1
55	EL	0	1
55	EM	0	2
55	FC	0	1
55	FD	0	1
55	FF	0	1
55	FJ	0	1
55	FL	0	1
55	FM	0	2
55	GF	0	1
55	GL	0	1
55	GM	0	1
55	HC	0	1
55	HD	0	2
55	HF	0	2
55	HH	0	1
55	HM	0	1
55	IC	0	2
55	ID	0	1
55	IF	0	1
55	IJ	0	1
55	IL	0	1
55	JC	0	2
55	JD	0	1
55	JF	0	2
55	JH	0	2
55	JJ	0	1
55	JL	0	1
55	JM	0	1
55	KC	0	1
55	KD	0	2
55	KF	0	1
55	KH	0	1
55	KJ	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	KL	0	1
55	LD	0	1
55	LF	0	3
55	LJ	0	1
55	LL	0	2
55	LM	0	1
55	MC	0	2
55	MD	0	1
55	MF	0	1
55	MH	0	1
55	MJ	0	2
55	MM	0	2
55	NC	0	1
55	ND	0	2
55	NH	0	4
55	NJ	0	2
55	NK	0	2
55	NM	0	3
55	OC	0	2
55	OF	0	2
55	OH	0	2
55	OJ	0	2
55	OM	0	1
55	PC	0	3
55	PD	0	1
55	PF	0	1
55	PH	0	2
55	PJ	0	1
55	QC	0	2
55	QD	0	2
55	QF	0	2
55	QH	0	1
55	QJ	0	2
55	QM	0	3
55	RC	0	1
55	RF	0	3
55	RH	0	1
55	RJ	0	2
55	SD	0	4
55	SF	0	1
55	SJ	0	1
55	SM	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	TD	0	2
55	TH	0	1
55	TJ	0	1
55	UC	0	2
55	UD	0	1
55	UF	0	1
55	UH	0	3
55	UJ	0	2
55	UL	0	1
55	UM	0	2
55	VC	0	1
55	VF	0	1
55	VH	0	3
55	VJ	0	2
55	VL	0	1
55	VM	0	1
55	WC	0	1
55	WD	0	2
55	WF	0	4
55	WH	0	1
55	WJ	0	1
55	WL	0	1
All	All	0	323

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	FH	171	PRO	CG-CD	-7.52	1.25	1.50
3	1v	670	CYS	CB-SG	-6.48	1.71	1.82
3	1y	670	CYS	CB-SG	-5.45	1.73	1.81
55	TM	194	GLU	CA-CB	5.39	1.65	1.53

All (401) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3J	312	TYR	C-N-CD	-10.17	98.22	120.60
55	FH	171	PRO	N-CD-CG	-9.84	88.45	103.20
55	VD	171	PRO	C-N-CA	9.69	145.92	121.70
55	ED	177	ASP	CB-CG-OD1	9.50	126.85	118.30
55	QC	187	LEU	CA-CB-CG	9.37	136.85	115.30
55	RD	44	LEU	CA-CB-CG	8.81	135.57	115.30
3	1L	134	LEU	CA-CB-CG	8.25	134.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	FE	160	ASP	CB-CG-OD1	8.22	125.70	118.30
55	PC	187	LEU	CA-CB-CG	8.19	134.15	115.30
55	PF	171	PRO	C-N-CA	8.18	142.14	121.70
55	JL	177	ASP	CB-CG-OD1	8.15	125.64	118.30
54	FG	248	LEU	CA-CB-CG	8.14	134.03	115.30
55	FJ	171	PRO	C-N-CA	8.13	142.03	121.70
55	MH	171	PRO	C-N-CA	8.00	141.71	121.70
55	ED	305	PRO	CA-N-CD	-7.96	100.35	111.50
55	QC	284	LEU	CA-CB-CG	7.93	133.53	115.30
54	PG	120	ASP	CB-CG-OD2	7.89	125.40	118.30
55	VM	228	LEU	CA-CB-CG	7.86	133.38	115.30
55	TD	187	LEU	CA-CB-CG	7.86	133.38	115.30
55	SM	171	PRO	C-N-CA	7.79	141.19	121.70
21	3N	414	LEU	CA-CB-CG	7.78	133.19	115.30
55	GC	44	LEU	CA-CB-CG	7.74	133.11	115.30
3	1v	598	ASP	CB-CG-OD1	7.69	125.22	118.30
54	CB	47	ASP	CB-CG-OD2	7.68	125.21	118.30
55	JF	118	ASP	CB-CG-OD1	7.68	125.21	118.30
55	FM	42	LEU	CA-CB-CG	7.64	132.87	115.30
13	2A	99	LEU	CA-CB-CG	7.55	132.67	115.30
7	5H	210	ARG	C-N-CA	7.55	140.58	121.70
55	FL	217	LEU	CA-CB-CG	7.54	132.64	115.30
54	BA	227	LEU	CB-CG-CD2	7.49	123.73	111.00
1	1B	61	ASP	CB-CG-OD1	7.46	125.01	118.30
31	6A	93	ASP	CB-CG-OD2	7.43	124.99	118.30
54	FG	245	ASP	CB-CG-OD1	7.43	124.98	118.30
55	NK	128	ASP	CB-CG-OD1	7.42	124.98	118.30
55	DC	417	ASP	CB-CG-OD2	7.41	124.97	118.30
55	CH	209	ASP	CB-CG-OD1	7.38	124.95	118.30
54	KB	298	PRO	CA-N-CD	-7.37	101.19	111.50
55	OH	161	ASP	CB-CG-OD1	7.32	124.88	118.30
55	BD	203	ASP	CB-CG-OD1	7.29	124.86	118.30
26	4J	215	ASP	CB-CG-OD2	7.26	124.84	118.30
54	BA	160	ASP	CB-CG-OD1	7.25	124.83	118.30
55	VC	26	ASP	CB-CG-OD2	7.21	124.79	118.30
55	QC	41	ASP	CB-CG-OD2	7.20	124.78	118.30
55	CJ	41	ASP	CB-CG-OD1	7.17	124.76	118.30
54	RE	116	ASP	CB-CG-OD1	7.17	124.75	118.30
55	CC	197	ASP	CB-CG-OD1	7.16	124.74	118.30
55	ID	171	PRO	C-N-CA	7.16	139.59	121.70
40	7U	105	ASP	CB-CG-OD1	7.15	124.73	118.30
55	WF	118	ASP	CB-CG-OD1	7.15	124.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	QJ	177	ASP	CB-CG-OD1	7.09	124.68	118.30
55	JH	44	LEU	CA-CB-CG	7.09	131.61	115.30
54	CK	39	ASP	CB-CG-OD1	7.09	124.68	118.30
55	PF	41	ASP	CB-CG-OD1	7.08	124.67	118.30
55	OM	203	ASP	CB-CG-OD1	7.08	124.67	118.30
13	2B	222	ASP	CB-CG-OD1	7.06	124.65	118.30
55	FC	225	LEU	CA-CB-CG	7.04	131.48	115.30
54	VG	46	ASP	CB-CG-OD1	7.01	124.61	118.30
55	LL	26	ASP	CB-CG-OD1	6.99	124.59	118.30
55	RM	203	ASP	CB-CG-OD1	6.96	124.56	118.30
55	AD	171	PRO	C-N-CA	6.93	139.04	121.70
55	DD	177	ASP	CB-CG-OD1	6.93	124.54	118.30
41	7Y	132	ASP	CB-CG-OD1	6.91	124.52	118.30
55	ED	203	ASP	CB-CG-OD1	6.90	124.51	118.30
54	HG	251	ASP	CB-CG-OD1	6.84	124.45	118.30
54	NG	127	ASP	CB-CG-OD2	6.82	124.44	118.30
23	3Z	158	ASP	CB-CG-OD1	6.76	124.38	118.30
54	JE	273	ALA	C-N-CD	-6.75	105.76	120.60
55	FH	171	PRO	CA-N-CD	-6.71	102.10	111.50
54	MB	205	ASP	CB-CG-OD1	6.70	124.33	118.30
54	EE	431	ASP	CB-CG-OD2	6.70	124.33	118.30
55	UL	171	PRO	C-N-CA	6.70	138.44	121.70
55	UC	217	LEU	CA-CB-CG	6.68	130.67	115.30
55	CL	304	ASP	CB-CG-OD2	6.68	124.31	118.30
55	JD	187	LEU	CA-CB-CG	6.67	130.65	115.30
54	TK	364	PRO	CA-N-CD	-6.66	102.17	111.50
54	VK	252	LEU	CA-CB-CG	6.66	130.62	115.30
54	LG	205	ASP	CB-CG-OD1	6.65	124.28	118.30
24	4A	350	ASP	CB-CG-OD2	6.65	124.28	118.30
22	3R	166	ASP	CB-CG-OD2	6.64	124.28	118.30
2	1H	222	MET	CA-CB-CG	6.63	124.57	113.30
55	RJ	215	LEU	CA-CB-CG	6.61	130.51	115.30
54	JA	367	ASP	CB-CG-OD1	6.60	124.24	118.30
7	5F	171	ASP	CB-CG-OD2	6.60	124.24	118.30
54	WA	33	ASP	CB-CG-OD2	6.59	124.23	118.30
55	QJ	41	ASP	CB-CG-OD2	6.58	124.22	118.30
45	8R	243	ASP	CB-CG-OD2	6.57	124.21	118.30
55	NH	118	ASP	CB-CG-OD1	6.55	124.19	118.30
54	GI	397	LEU	CA-CB-CG	6.54	130.35	115.30
55	NH	177	ASP	CB-CG-OD1	6.54	124.19	118.30
54	SK	205	ASP	CB-CG-OD2	6.53	124.18	118.30
1	1B	257	LEU	CA-CB-CG	6.51	130.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	CL	44	LEU	CA-CB-CG	6.51	130.28	115.30
54	JA	245	ASP	CB-CG-OD1	6.50	124.16	118.30
54	HA	119	LEU	CA-CB-CG	6.44	130.12	115.30
55	CL	139	LEU	CA-CB-CG	6.43	130.09	115.30
22	3T	166	ASP	CB-CG-OD1	6.42	124.08	118.30
54	IA	205	ASP	CB-CG-OD1	6.42	124.07	118.30
54	PK	211	ASP	CB-CG-OD1	6.39	124.05	118.30
55	VM	417	ASP	CB-CG-OD2	6.38	124.05	118.30
22	3T	10	ASP	CB-CG-OD2	6.38	124.04	118.30
54	TE	322	ASP	CB-CG-OD2	6.37	124.03	118.30
5	1T	215	ASP	CB-CG-OD1	6.37	124.03	118.30
47	9A	128	LEU	CA-CB-CG	6.37	129.94	115.30
42	8A	180	LEU	CA-CB-CG	6.36	129.94	115.30
54	GA	397	LEU	CA-CB-CG	6.36	129.93	115.30
55	FL	112	LEU	CA-CB-CG	6.36	129.93	115.30
55	KH	417	ASP	CB-CG-OD1	6.32	123.99	118.30
55	NC	328	GLU	N-CA-CB	6.30	121.94	110.60
55	QJ	217	LEU	CA-CB-CG	6.27	129.73	115.30
28	4U	89	ASP	CB-CG-OD1	6.26	123.94	118.30
55	AJ	203	ASP	CB-CG-OD1	6.26	123.94	118.30
54	TE	218	ASP	CB-CG-OD1	6.25	123.92	118.30
54	HG	326	LYS	CB-CG-CD	-6.24	95.38	111.60
54	OE	1	MET	CB-CG-SD	-6.24	93.69	112.40
37	7H	475	PRO	CA-N-CD	-6.23	102.78	111.50
55	HL	108	GLU	CA-CB-CG	6.22	127.08	113.40
55	EH	177	ASP	CB-CG-OD1	6.21	123.89	118.30
55	JF	65	LEU	CB-CG-CD2	-6.21	100.44	111.00
3	1w	368	CYS	CA-CB-SG	-6.21	102.83	114.00
55	VD	233	MET	CA-CB-CG	6.19	123.83	113.30
23	3W	93	GLY	N-CA-C	6.18	128.56	113.10
36	7D	107	LEU	CA-CB-CG	6.18	129.52	115.30
47	9A	129	PRO	N-CD-CG	-6.18	93.93	103.20
55	AC	114	ASP	CB-CG-OD1	6.16	123.84	118.30
55	LF	112	LEU	CA-CB-CG	6.14	129.43	115.30
54	FK	205	ASP	CB-CG-OD2	6.14	123.83	118.30
54	UB	98	ASP	CB-CG-OD1	6.12	123.80	118.30
54	VG	424	ASP	CB-CG-OD2	6.11	123.80	118.30
54	DM	397	LEU	CA-CB-CG	6.10	129.33	115.30
55	SF	44	LEU	CA-CB-CG	6.10	129.32	115.30
54	AE	251	ASP	CB-CG-OD1	6.09	123.78	118.30
19	3C	138	ASP	CB-CG-OD2	6.09	123.78	118.30
55	CD	324	LYS	CD-CE-NZ	6.08	125.69	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	VA	396	ASP	CB-CG-OD2	6.08	123.77	118.30
5	1V	237	LEU	CA-CB-CG	6.07	129.26	115.30
45	8S	131	ASP	CB-CG-OD1	6.07	123.77	118.30
54	SA	86	LEU	CA-CB-CG	6.07	129.26	115.30
35	6U	272	ASP	CB-CG-OD2	6.07	123.76	118.30
54	RA	127	ASP	CB-CG-OD1	6.07	123.76	118.30
54	UB	265	ILE	CG1-CB-CG2	-6.07	98.05	111.40
54	EI	205	ASP	CB-CG-OD1	6.07	123.76	118.30
54	TI	245	ASP	CB-CG-OD1	6.06	123.76	118.30
55	QF	217	LEU	CA-CB-CG	6.06	129.24	115.30
55	AF	88	ASP	CB-CG-OD1	6.06	123.75	118.30
55	QF	118	ASP	CB-CG-OD2	6.06	123.75	118.30
54	UI	245	ASP	CB-CG-OD1	6.05	123.75	118.30
55	SM	404	ASP	CB-CG-OD2	6.05	123.75	118.30
55	BJ	31	ASP	CB-CG-OD1	6.04	123.74	118.30
55	GJ	203	ASP	CB-CG-OD2	6.02	123.72	118.30
55	CD	249	ASP	CB-CG-OD1	6.02	123.72	118.30
54	MK	205	ASP	CB-CG-OD1	6.02	123.72	118.30
43	8G	373	ASP	CB-CG-OD2	6.01	123.71	118.30
54	VK	98	ASP	CB-CG-OD1	6.01	123.71	118.30
55	FF	324	LYS	CD-CE-NZ	-6.01	97.89	111.70
54	SA	33	ASP	CB-CG-OD1	6.00	123.70	118.30
54	SA	413	MET	CA-CB-CG	6.00	123.51	113.30
55	SC	44	LEU	CA-CB-CG	6.00	129.09	115.30
36	7D	239	ASP	CB-CG-OD2	5.98	123.69	118.30
55	VL	44	LEU	CA-CB-CG	5.97	129.04	115.30
54	LE	205	ASP	CB-CG-OD1	5.96	123.66	118.30
54	OE	273	ALA	C-N-CD	-5.96	107.49	120.60
47	9A	114	ASP	CB-CG-OD2	5.96	123.66	118.30
55	FJ	88	ASP	CB-CG-OD1	5.95	123.66	118.30
55	NJ	295	ASP	CB-CG-OD1	5.94	123.65	118.30
39	7Q	105	ASP	CB-CG-OD2	5.94	123.64	118.30
26	4J	214	VAL	C-N-CA	5.93	136.52	121.70
55	UM	263	LEU	CA-CB-CG	5.93	128.93	115.30
19	3A	138	ASP	CB-CG-OD1	5.91	123.62	118.30
55	EL	88	ASP	CB-CG-OD2	5.91	123.61	118.30
37	7H	247	ASP	CB-CG-OD1	5.89	123.60	118.30
37	7I	13	ASP	CB-CG-OD2	5.89	123.60	118.30
45	8S	69	ASP	CB-CG-OD2	5.89	123.60	118.30
54	AG	218	ASP	CB-CG-OD1	5.88	123.59	118.30
55	CD	177	ASP	CB-CG-OD1	5.88	123.60	118.30
54	FA	116	ASP	CB-CG-OD1	5.88	123.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	EA	428	LEU	CA-CB-CG	5.88	128.81	115.30
55	SL	112	LEU	CA-CB-CG	5.87	128.81	115.30
54	PB	132	LEU	CA-CB-CG	5.87	128.79	115.30
54	DI	322	ASP	CB-CG-OD1	5.86	123.58	118.30
21	3N	414	LEU	CB-CG-CD1	5.86	120.96	111.00
55	OH	42	LEU	CA-CB-CG	5.85	128.75	115.30
54	RE	39	ASP	CB-CG-OD1	5.85	123.56	118.30
30	9Y	169	LEU	CA-CB-CG	5.84	128.74	115.30
54	DG	428	LEU	CA-CB-CG	5.84	128.74	115.30
55	DF	65	LEU	CB-CG-CD2	5.84	120.92	111.00
55	CL	404	ASP	CB-CG-OD1	5.84	123.55	118.30
55	LC	417	ASP	CB-CG-OD2	5.79	123.51	118.30
43	8D	196	ASP	CB-CG-OD1	5.79	123.51	118.30
54	CK	245	ASP	CB-CG-OD2	5.78	123.50	118.30
54	WI	397	LEU	CA-CB-CG	5.78	128.59	115.30
55	NC	177	ASP	CB-CG-OD1	5.77	123.49	118.30
55	GL	151	LEU	CA-CB-CG	5.74	128.51	115.30
54	HB	397	LEU	CA-CB-CG	5.74	128.51	115.30
54	RE	47	ASP	CB-CG-OD2	5.74	123.47	118.30
55	RD	404	ASP	CB-CG-OD1	5.74	123.46	118.30
55	TC	417	ASP	CB-CG-OD1	5.73	123.46	118.30
55	CJ	42	LEU	CA-CB-CG	5.73	128.47	115.30
55	JL	263	LEU	CA-CB-CG	5.73	128.47	115.30
55	LM	128	ASP	CB-CG-OD2	5.73	123.45	118.30
55	HM	44	LEU	CA-CB-CG	5.71	128.44	115.30
19	3D	127	ASP	CB-CG-OD2	5.71	123.44	118.30
54	FB	33	ASP	CB-CG-OD2	5.71	123.44	118.30
54	GK	189	LEU	CA-CB-CG	5.70	128.42	115.30
55	LM	249	ASP	CB-CG-OD2	5.70	123.43	118.30
55	FJ	41	ASP	CB-CG-OD1	5.70	123.43	118.30
36	7A	107	LEU	CA-CB-CG	5.70	128.40	115.30
55	VM	209	ASP	CB-CG-OD1	5.67	123.40	118.30
54	CM	317	MET	CA-CB-CG	5.66	122.92	113.30
54	EI	245	ASP	CB-CG-OD1	5.65	123.39	118.30
54	DG	66	VAL	CA-CB-CG1	5.65	119.38	110.90
55	FF	41	ASP	CB-CG-OD1	5.65	123.39	118.30
55	EB	217	LEU	CA-CB-CG	5.65	128.29	115.30
55	AC	161	ASP	CB-CG-OD1	5.64	123.38	118.30
55	EM	187	LEU	CA-CB-CG	5.63	128.25	115.30
54	IG	424	ASP	CB-CG-OD1	5.62	123.36	118.30
54	FB	120	ASP	CB-CG-OD2	5.62	123.35	118.30
54	FG	33	ASP	CB-CG-OD2	5.61	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1K	45	LEU	CA-CB-CG	5.60	128.18	115.30
55	KM	304	ASP	CB-CG-OD2	5.60	123.34	118.30
54	SI	116	ASP	CB-CG-OD1	5.60	123.34	118.30
24	4A	21	ASP	CB-CG-OD2	5.59	123.33	118.30
23	3W	97	VAL	C-N-CA	5.59	135.67	121.70
55	FD	187	LEU	CA-CB-CG	5.59	128.15	115.30
54	IM	33	ASP	CB-CG-OD2	5.58	123.33	118.30
55	OC	177	ASP	CB-CG-OD2	5.58	123.32	118.30
55	JJ	171	PRO	C-N-CA	5.58	135.65	121.70
55	CH	177	ASP	CB-CG-OD1	5.58	123.32	118.30
55	CJ	377	LEU	CA-CB-CG	5.57	128.12	115.30
55	JJ	44	LEU	CA-CB-CG	5.57	128.10	115.30
55	FH	187	LEU	CA-CB-CG	5.56	128.09	115.30
55	DC	65	LEU	CA-CB-CG	5.56	128.08	115.30
55	TJ	67	ASP	CB-CG-OD2	5.56	123.30	118.30
55	KH	217	LEU	CA-CB-CG	5.56	128.08	115.30
39	7R	124	LEU	CA-CB-CG	5.55	128.07	115.30
55	LM	263	LEU	CA-CB-CG	5.55	128.06	115.30
55	BD	31	ASP	CB-CG-OD1	5.55	123.29	118.30
10	1j	25	LEU	CA-CB-CG	5.54	128.06	115.30
37	7H	57	ASP	CB-CG-OD2	5.54	123.29	118.30
55	VL	118	ASP	CB-CG-OD1	5.54	123.29	118.30
54	BE	327	ASP	CB-CG-OD1	5.54	123.28	118.30
55	EF	395	LEU	CA-CB-CG	5.54	128.04	115.30
54	TI	218	ASP	CB-CG-OD1	5.54	123.28	118.30
55	VM	249	ASP	CB-CG-OD2	5.53	123.28	118.30
22	3S	84	ASP	CB-CG-OD1	5.53	123.27	118.30
54	KG	251	ASP	CB-CG-OD2	5.53	123.27	118.30
55	PJ	112	LEU	CA-CB-CG	5.52	128.00	115.30
54	BI	86	LEU	CA-CB-CG	5.52	127.99	115.30
22	3S	76	ASP	CB-CG-OD1	5.51	123.26	118.30
54	LA	251	ASP	CB-CG-OD2	5.51	123.26	118.30
34	6Q	294	LEU	CA-CB-CG	5.51	127.97	115.30
2	1H	84	ASP	CB-CG-OD1	5.51	123.26	118.30
55	ED	44	LEU	CA-CB-CG	5.51	127.96	115.30
55	UH	151	LEU	CA-CB-CG	5.50	127.96	115.30
54	DM	431	ASP	CB-CG-OD2	5.50	123.25	118.30
55	OC	203	ASP	CB-CG-OD2	5.50	123.25	118.30
55	DH	171	PRO	C-N-CA	5.49	135.42	121.70
54	CK	428	LEU	CA-CB-CG	5.48	127.90	115.30
54	RA	341	ILE	CG1-CB-CG2	-5.48	99.35	111.40
55	OD	217	LEU	CA-CB-CG	5.47	127.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	SA	245	ASP	CB-CG-OD2	5.47	123.22	118.30
55	VL	177	ASP	CB-CG-OD2	5.47	123.22	118.30
5	1T	112	PRO	CA-N-CD	-5.46	103.85	111.50
55	PD	299	MET	CB-CG-SD	-5.46	96.02	112.40
24	4B	21	ASP	CB-CG-OD1	5.46	123.21	118.30
55	FJ	187	LEU	CA-CB-CG	5.45	127.83	115.30
36	7A	129	LEU	CA-CB-CG	5.45	127.83	115.30
55	NK	249	ASP	CB-CG-OD2	5.44	123.20	118.30
22	3S	67	ASP	CB-CG-OD2	5.44	123.20	118.30
36	7A	142	ASP	CB-CG-OD2	5.44	123.20	118.30
55	IH	41	ASP	CB-CG-OD1	5.44	123.20	118.30
54	RK	341	ILE	CG1-CB-CG2	-5.44	99.44	111.40
55	KD	217	LEU	CA-CB-CG	5.43	127.78	115.30
55	JM	26	ASP	CB-CG-OD2	5.42	123.18	118.30
54	SB	203	MET	CB-CG-SD	5.42	128.66	112.40
36	7C	297	ILE	CG1-CB-CG2	-5.42	99.49	111.40
54	NG	116	ASP	CB-CG-OD2	5.42	123.17	118.30
55	HD	41	ASP	CB-CG-OD2	5.41	123.17	118.30
55	QH	118	ASP	CB-CG-OD1	5.41	123.17	118.30
54	RE	33	ASP	CB-CG-OD1	5.39	123.15	118.30
54	VI	160	ASP	CB-CG-OD1	5.39	123.15	118.30
54	QL	171	ILE	CG1-CB-CG2	-5.39	99.55	111.40
55	RJ	427	ASP	CB-CG-OD2	5.39	123.15	118.30
55	EF	187	LEU	CA-CB-CG	5.38	127.68	115.30
55	RF	122	LYS	CA-CB-CG	5.38	125.23	113.40
21	3N	413	ARG	CA-CB-CG	5.38	125.23	113.40
55	VF	171	PRO	C-N-CA	5.37	135.13	121.70
54	CE	47	ASP	CB-CG-OD1	5.37	123.13	118.30
2	1G	84	ASP	CB-CG-OD1	5.36	123.12	118.30
55	IJ	171	PRO	C-N-CA	5.36	135.10	121.70
55	RF	217	LEU	CA-CB-CG	5.36	127.63	115.30
37	7I	283	PRO	CA-N-CD	-5.36	104.00	111.50
55	NC	328	GLU	CA-CB-CG	5.35	125.18	113.40
54	WE	47	ASP	CB-CG-OD1	5.35	123.12	118.30
43	8D	132	LEU	CA-CB-CG	5.35	127.61	115.30
55	DH	295	ASP	CB-CG-OD2	5.34	123.10	118.30
55	MD	401	GLU	CA-CB-CG	5.33	125.14	113.40
55	NK	130	LEU	CA-CB-CG	5.33	127.57	115.30
54	BK	345	ASP	CB-CG-OD1	5.33	123.09	118.30
21	3O	269	ASP	CB-CG-OD2	5.32	123.09	118.30
54	RK	70	LEU	CA-CB-CG	5.32	127.55	115.30
55	NJ	253	LEU	CA-CB-CG	5.31	127.52	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	EG	36	MET	CB-CG-SD	5.31	128.34	112.40
55	JF	284	LEU	CA-CB-CG	5.31	127.51	115.30
54	UI	251	ASP	CB-CG-OD1	5.30	123.07	118.30
22	3R	32	MET	CA-CB-CG	5.29	122.30	113.30
33	6N	427	LEU	CA-CB-CG	5.29	127.47	115.30
54	JI	211	ASP	CB-CG-OD1	5.28	123.05	118.30
9	1f	36	ARG	CA-CB-CG	5.28	125.02	113.40
55	SM	4	ILE	CG1-CB-CG2	-5.28	99.78	111.40
55	VL	112	LEU	CA-CB-CG	5.28	127.44	115.30
54	EA	127	ASP	CB-CG-OD1	5.28	123.05	118.30
55	BC	151	LEU	CA-CB-CG	5.27	127.43	115.30
55	LJ	177	ASP	CB-CG-OD1	5.27	123.05	118.30
55	UD	284	LEU	CA-CB-CG	5.27	127.43	115.30
55	WC	284	LEU	CA-CB-CG	5.27	127.42	115.30
55	EB	187	LEU	CA-CB-CG	5.26	127.40	115.30
54	RE	127	ASP	CB-CG-OD2	5.26	123.03	118.30
46	8Z	72	VAL	CG1-CB-CG2	-5.25	102.50	110.90
55	EH	26	ASP	CB-CG-OD2	5.25	123.02	118.30
55	MJ	44	LEU	CA-CB-CG	5.25	127.37	115.30
19	3B	183	LEU	CA-CB-CG	5.25	127.37	115.30
24	4C	260	MET	CA-CB-CG	5.25	122.22	113.30
18	2V	266	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	1A	23	ASP	CB-CG-OD2	5.24	123.02	118.30
54	DG	218	ASP	CB-CG-OD1	5.24	123.01	118.30
54	FK	245	ASP	CB-CG-OD1	5.24	123.01	118.30
55	UC	395	LEU	CA-CB-CG	5.23	127.34	115.30
54	UK	218	ASP	CB-CG-OD1	5.23	123.01	118.30
54	CI	209	ILE	CG1-CB-CG2	-5.23	99.89	111.40
54	KB	326	LYS	CD-CE-NZ	-5.22	99.69	111.70
54	NI	120	ASP	CB-CG-OD1	5.22	122.99	118.30
55	FL	304	ASP	CB-CG-OD2	5.21	122.99	118.30
55	JM	249	ASP	CB-CG-OD2	5.21	122.99	118.30
55	QJ	118	ASP	CB-CG-OD1	5.21	122.99	118.30
55	SJ	217	LEU	CA-CB-CG	5.21	127.27	115.30
55	UM	192	LEU	CA-CB-CG	5.20	127.26	115.30
13	2D	131	THR	C-N-CA	5.20	134.70	121.70
54	GK	218	ASP	CB-CG-OD1	5.20	122.98	118.30
54	EC	217	LEU	CA-CB-CG	5.19	127.25	115.30
55	LC	177	ASP	CB-CG-OD1	5.19	122.97	118.30
54	JI	430	LYS	CD-CE-NZ	5.19	123.63	111.70
42	8A	22	ASP	CB-CG-OD1	5.18	122.97	118.30
55	CJ	328	GLU	CA-CB-CG	5.18	124.81	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2V	108	MET	CA-CB-CG	5.18	122.11	113.30
46	8Z	20	LEU	CA-CB-CG	5.18	127.21	115.30
55	RC	284	LEU	CA-CB-CG	5.18	127.21	115.30
24	4B	459	ILE	C-N-CA	5.16	134.60	121.70
55	MH	118	ASP	CB-CG-OD1	5.15	122.94	118.30
54	RB	76	ASP	CB-CG-OD2	5.15	122.94	118.30
27	4Q	180	LEU	CA-CB-CG	5.15	127.14	115.30
54	UG	218	ASP	CB-CG-OD1	5.15	122.93	118.30
55	MC	249	ASP	CB-CG-OD1	5.14	122.93	118.30
55	QF	209	ASP	CB-CG-OD1	5.14	122.93	118.30
54	RG	7	ILE	CG1-CB-CG2	-5.14	100.08	111.40
55	EM	299	MET	CB-CG-SD	-5.14	96.98	112.40
21	3N	397	GLU	CA-CB-CG	5.14	124.70	113.40
54	WK	46	ASP	CB-CG-OD1	5.14	122.92	118.30
55	BF	380	ARG	CB-CG-CD	5.13	124.95	111.60
54	LE	397	LEU	CA-CB-CG	5.13	127.11	115.30
55	BH	263	LEU	CA-CB-CG	5.13	127.11	115.30
55	GH	331	LEU	CA-CB-CG	5.13	127.11	115.30
55	EF	177	ASP	CB-CG-OD1	5.13	122.92	118.30
54	RB	275	VAL	CG1-CB-CG2	-5.13	102.70	110.90
36	7D	406	LEU	CA-CB-CG	5.12	127.06	115.30
25	4G	179	ASP	CB-CG-OD2	5.11	122.90	118.30
37	7I	142	LEU	CA-CB-CG	5.11	127.06	115.30
55	VJ	26	ASP	CB-CG-OD2	5.11	122.90	118.30
55	ED	377	LEU	CA-CB-CG	5.11	127.05	115.30
55	KM	225	LEU	CA-CB-CG	5.11	127.05	115.30
55	TM	263	LEU	CA-CB-CG	5.11	127.05	115.30
43	8G	359	LYS	CD-CE-NZ	-5.11	99.96	111.70
55	KC	118	ASP	CB-CG-OD1	5.10	122.89	118.30
31	6C	83	ASP	CB-CG-OD2	5.10	122.89	118.30
55	EL	284	LEU	CA-CB-CG	5.10	127.03	115.30
3	1z	413	ASP	CB-CG-OD1	5.08	122.87	118.30
54	OA	248	LEU	CA-CB-CG	5.08	126.98	115.30
54	SE	259	LEU	CA-CB-CG	5.08	126.98	115.30
36	7A	404	MET	CB-CG-SD	5.08	127.63	112.40
54	LB	23	LEU	CA-CB-CG	5.07	126.97	115.30
55	TL	225	LEU	CB-CG-CD1	-5.06	102.39	111.00
55	CF	177	ASP	CB-CG-OD1	5.06	122.85	118.30
55	SC	118	ASP	CB-CG-OD1	5.05	122.85	118.30
22	3R	33	PRO	C-N-CA	5.05	134.32	121.70
54	QA	132	LEU	CA-CB-CG	5.05	126.91	115.30
55	SF	284	LEU	CA-CB-CG	5.04	126.89	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	DC	197	ASP	CB-CG-OD2	5.04	122.83	118.30
55	QH	177	ASP	CB-CG-OD1	5.04	122.83	118.30
55	DJ	217	LEU	CA-CB-CG	5.03	126.88	115.30
3	1x	400	GLN	C-N-CA	5.03	134.28	121.70
7	1b	42	GLU	C-N-CA	-5.03	109.13	121.70
20	3K	51	GLU	CA-CB-CG	5.03	124.46	113.40
36	7B	578	ASP	CB-CG-OD1	5.02	122.82	118.30
55	RF	130	LEU	CB-CG-CD2	5.02	119.54	111.00
36	7A	534	ALA	C-N-CA	5.02	134.25	121.70
36	7D	407	LEU	CA-CB-CG	5.02	126.84	115.30
55	NF	377	LEU	CA-CB-CG	5.02	126.84	115.30
54	UA	218	ASP	CB-CG-OD1	5.02	122.82	118.30
23	3W	80	LEU	CA-CB-CG	5.01	126.83	115.30
55	ED	305	PRO	N-CD-CG	-5.01	95.69	103.20
21	3O	202	ASP	CB-CG-OD1	5.00	122.80	118.30
7	5G	94	PHE	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (323) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1B	189	ALA	Peptide
1	1B	296	MET	Peptide
5	1V	104	THR	Peptide
6	1Y	30	GLU	Peptide
7	1a	156	VAL	Peptide
7	1b	38	ILE	Peptide
7	1b	43	MET	Peptide
12	1r	3	GLN	Peptide
3	1v	669	GLN	Peptide
3	1w	400	GLN	Peptide
3	1y	669	GLN	Peptide
3	2a	670	CYS	Peptide
19	3B	95	ASP	Peptide
20	3J	304	ALA	Peptide
20	3J	312	TYR	Peptide
22	3S	116	PRO	Peptide
23	3W	97	VAL	Peptide
23	3W	98	LEU	Peptide
25	4G	27	MET	Peptide
26	4J	330	GLY	Peptide
30	5B	182	SER	Peptide

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Mol	Chain	Res	Type	Group
7	5K	71	VAL	Peptide
7	5K	72	THR	Peptide
31	6B	100	HIS	Peptide
31	6B	99	THR	Peptide
36	7A	534	ALA	Peptide
36	7C	406	LEU	Peptide
36	7D	4	PRO	Peptide
37	7G	59	LEU	Peptide
37	7H	344	ASP	Peptide
37	7I	344	ASP	Peptide
38	7M	232	ALA	Peptide
38	7M	246	GLU	Peptide
40	7U	188	LYS	Peptide
41	7Y	201	HIS	Peptide
42	8A	109	LYS	Peptide
43	8D	252	GLU	Peptide
47	9A	105	ILE	Peptide
48	9D	157	ASN	Peptide
10	9O	154	GLU	Peptide
53	9V	80	TRP	Peptide
53	9V	81	ARG	Sidechain
30	9Z	131	GLU	Peptide
30	9Z	60	HIS	Peptide
54	AB	273	ALA	Peptide
55	AC	85	PHE	Peptide
54	AE	254	GLU	Peptide
55	AF	167	PHE	Peptide
55	AF	271	ALA	Peptide
54	AG	273	ALA	Peptide
55	AH	167	PHE	Peptide
55	AH	271	ALA	Peptide
55	AJ	271	ALA	Peptide
55	AL	137	HIS	Peptide
55	AL	271	ALA	Peptide
54	BA	254	GLU	Peptide
55	BC	167	PHE	Peptide
55	BC	324	LYS	Peptide
55	BC	70	PRO	Peptide
54	BI	273	ALA	Peptide
54	BK	273	ALA	Peptide
54	CA	254	GLU	Peptide
54	CB	409	VAL	Peptide

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Mol	Chain	Res	Type	Group
55	CC	137	HIS	Peptide
55	CC	271	ALA	Peptide
55	CD	271	ALA	Peptide
54	CE	215	ARG	Sidechain
54	CE	273	ALA	Peptide
55	CF	167	PHE	Peptide
55	CH	271	ALA	Peptide
54	CI	100	ALA	Peptide
55	CJ	167	PHE	Peptide
55	CJ	271	ALA	Peptide
54	CK	273	ALA	Peptide
55	CL	271	ALA	Peptide
54	CM	273	ALA	Peptide
55	DC	271	ALA	Peptide
55	DD	167	PHE	Peptide
55	DF	137	HIS	Peptide
55	DF	70	PRO	Peptide
55	DH	137	HIS	Peptide
55	DH	167	PHE	Peptide
55	DH	271	ALA	Peptide
55	DJ	271	ALA	Peptide
55	DJ	70	PRO	Peptide
54	DK	141	PHE	Peptide
55	DL	302	ALA	Peptide
55	EB	271	ALA	Peptide
55	ED	271	ALA	Peptide
55	EF	271	ALA	Peptide
54	EG	273	ALA	Peptide
54	EG	357	TYR	Peptide
55	EH	88	ASP	Peptide
54	EI	273	ALA	Peptide
55	EJ	271	ALA	Peptide
54	EK	273	ALA	Peptide
55	EL	70	PRO	Peptide
55	EM	271	ALA	Peptide
55	EM	70	PRO	Peptide
54	FA	412	GLY	Peptide
54	FB	273	ALA	Peptide
54	FB	357	TYR	Peptide
55	FC	271	ALA	Peptide
55	FD	271	ALA	Peptide
55	FF	271	ALA	Peptide

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Mol	Chain	Res	Type	Group
54	FI	172	TYR	Peptide
55	FJ	271	ALA	Peptide
55	FL	271	ALA	Peptide
55	FM	167	PHE	Peptide
55	FM	70	PRO	Peptide
54	GB	303	VAL	Peptide
55	GF	271	ALA	Peptide
55	GL	271	ALA	Peptide
55	GM	271	ALA	Peptide
54	HA	159	VAL	Peptide
54	HB	273	ALA	Peptide
55	HC	302	ALA	Peptide
55	HD	137	HIS	Peptide
55	HD	236	VAL	Peptide
55	HF	167	PHE	Peptide
55	HF	271	ALA	Peptide
54	HG	273	ALA	Peptide
55	HH	167	PHE	Peptide
55	HM	195	ASN	Peptide
54	IA	243	ARG	Peptide
54	IB	273	ALA	Peptide
55	IC	271	ALA	Peptide
55	IC	70	PRO	Peptide
55	ID	271	ALA	Peptide
55	IF	302	ALA	Peptide
54	IG	160	ASP	Peptide
54	IG	273	ALA	Peptide
54	II	273	ALA	Peptide
55	IJ	167	PHE	Peptide
54	IK	273	ALA	Peptide
54	IK	316	CYS	Peptide
55	IL	271	ALA	Peptide
54	JA	273	ALA	Peptide
54	JB	273	ALA	Peptide
55	JC	167	PHE	Peptide
55	JC	271	ALA	Peptide
55	JD	70	PRO	Peptide
54	JE	273	ALA	Peptide
55	JF	167	PHE	Peptide
55	JF	271	ALA	Peptide
54	JG	273	ALA	Peptide
55	JH	137	HIS	Peptide

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Mol	Chain	Res	Type	Group
55	JH	271	ALA	Peptide
55	JJ	271	ALA	Peptide
55	JL	271	ALA	Peptide
55	JM	271	ALA	Peptide
54	KB	273	ALA	Peptide
55	KC	271	ALA	Peptide
55	KD	167	PHE	Peptide
55	KD	271	ALA	Peptide
54	KE	273	ALA	Peptide
55	KF	271	ALA	Peptide
54	KG	38	SER	Peptide
55	KH	271	ALA	Peptide
54	KI	1	MET	Peptide
55	KJ	167	PHE	Peptide
55	KJ	271	ALA	Peptide
55	KL	271	ALA	Peptide
54	LA	273	ALA	Peptide
55	LD	401	GLU	Peptide
55	LF	108	GLU	Peptide
55	LF	167	PHE	Peptide
55	LF	271	ALA	Peptide
55	LJ	271	ALA	Peptide
55	LL	137	HIS	Peptide
55	LL	271	ALA	Peptide
55	LM	271	ALA	Peptide
54	MA	273	ALA	Peptide
54	MB	339	ARG	Sidechain
55	MC	107	THR	Peptide
55	MC	125	GLU	Peptide
55	MD	271	ALA	Peptide
55	MF	107	THR	Peptide
55	MH	257	MET	Peptide
54	MI	273	ALA	Peptide
55	MJ	167	PHE	Peptide
55	MJ	271	ALA	Peptide
54	MK	273	ALA	Peptide
55	MM	167	PHE	Peptide
55	MM	271	ALA	Peptide
54	NB	273	ALA	Peptide
55	NC	271	ALA	Peptide
55	ND	271	ALA	Peptide
55	ND	70	PRO	Peptide

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Mol	Chain	Res	Type	Group
55	NH	137	HIS	Peptide
55	NH	216	LYS	Peptide
55	NH	271	ALA	Peptide
55	NH	70	PRO	Peptide
55	NJ	167	PHE	Peptide
55	NJ	257	MET	Peptide
55	NK	271	ALA	Peptide
55	NK	302	ALA	Peptide
55	NM	271	ALA	Peptide
55	NM	393	ALA	Peptide
55	NM	70	PRO	Peptide
55	OC	167	PHE	Peptide
55	OC	70	PRO	Peptide
54	OE	110	ILE	Peptide
54	OE	273	ALA	Peptide
55	OF	167	PHE	Peptide
55	OF	271	ALA	Peptide
55	OH	167	PHE	Peptide
55	OH	271	ALA	Peptide
55	OJ	167	PHE	Peptide
55	OJ	70	PRO	Peptide
54	OK	273	ALA	Peptide
55	OM	271	ALA	Peptide
54	PA	160	ASP	Peptide
55	PC	167	PHE	Peptide
55	PC	271	ALA	Peptide
55	PC	302	ALA	Peptide
55	PD	167	PHE	Peptide
55	PF	167	PHE	Peptide
55	PH	167	PHE	Peptide
55	PH	70	PRO	Peptide
54	PI	316	CYS	Peptide
55	PJ	167	PHE	Peptide
54	QB	202	PHE	Peptide
54	QB	273	ALA	Peptide
55	QC	167	PHE	Peptide
55	QC	187	LEU	Peptide
55	QD	167	PHE	Peptide
55	QD	271	ALA	Peptide
54	QE	273	ALA	Peptide
54	QE	403	ALA	Peptide
55	QF	271	ALA	Peptide

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Mol	Chain	Res	Type	Group
55	QF	58	LYS	Peptide
55	QH	167	PHE	Peptide
54	QI	273	ALA	Peptide
55	QJ	167	PHE	Peptide
55	QJ	271	ALA	Peptide
54	QK	216	ASN	Peptide
55	QM	167	PHE	Peptide
55	QM	271	ALA	Peptide
55	QM	401	GLU	Peptide
54	RA	273	ALA	Peptide
54	RB	141	PHE	Peptide
54	RB	273	ALA	Peptide
55	RC	271	ALA	Peptide
54	RE	273	ALA	Peptide
55	RF	167	PHE	Peptide
55	RF	324	LYS	Peptide
55	RF	401	GLU	Peptide
54	RG	273	ALA	Peptide
55	RH	320	ARG	Peptide
54	RI	273	ALA	Peptide
55	RJ	137	HIS	Peptide
55	RJ	271	ALA	Peptide
54	RK	273	ALA	Peptide
54	RL	273	ALA	Peptide
54	RL	72	PRO	Peptide
54	SB	42	ILE	Peptide
55	SD	167	PHE	Peptide
55	SD	255	VAL	Peptide
55	SD	271	ALA	Peptide
55	SD	323	MET	Peptide
54	SE	411	GLU	Peptide
55	SF	167	PHE	Peptide
54	SG	141	PHE	Peptide
54	SG	273	ALA	Peptide
54	SI	273	ALA	Peptide
55	SJ	44	LEU	Peptide
55	SM	167	PHE	Peptide
55	SM	271	ALA	Peptide
54	TA	31	GLN	Peptide
54	TB	273	ALA	Peptide
54	TB	285	GLN	Peptide
55	TD	212	PHE	Peptide

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Mol	Chain	Res	Type	Group
55	TD	302	ALA	Peptide
54	TG	160	ASP	Peptide
55	TH	70	PRO	Peptide
54	TI	273	ALA	Peptide
55	TJ	216	LYS	Peptide
54	TK	273	ALA	Peptide
54	TK	274	PRO	Peptide
54	UB	273	ALA	Peptide
55	UC	167	PHE	Peptide
55	UC	271	ALA	Peptide
55	UD	271	ALA	Peptide
55	UF	271	ALA	Peptide
54	UG	303	VAL	Peptide
55	UH	234	SER	Peptide
55	UH	271	ALA	Peptide
55	UH	70	PRO	Peptide
54	UI	273	ALA	Peptide
55	UJ	278	SER	Peptide
55	UJ	70	PRO	Peptide
54	UK	221	ARG	Sidechain
55	UL	302	ALA	Peptide
55	UM	271	ALA	Peptide
55	UM	322	SER	Peptide
54	VB	254	GLU	Peptide
55	VC	302	ALA	Peptide
54	VE	273	ALA	Peptide
55	VF	271	ALA	Peptide
54	VG	273	ALA	Peptide
55	VH	193	VAL	Peptide
55	VH	204	ASN	Peptide
55	VH	271	ALA	Peptide
55	VJ	167	PHE	Peptide
55	VJ	70	PRO	Peptide
55	VL	271	ALA	Peptide
55	VM	271	ALA	Peptide
54	WA	273	ALA	Peptide
54	WB	273	ALA	Peptide
55	WC	137	HIS	Peptide
55	WD	137	HIS	Peptide
55	WD	271	ALA	Peptide
54	WE	273	ALA	Peptide
55	WF	137	HIS	Peptide

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Mol	Chain	Res	Type	Group
55	WF	167	PHE	Peptide
55	WF	271	ALA	Peptide
55	WF	355	ASP	Peptide
55	WH	167	PHE	Peptide
54	WI	273	ALA	Peptide
55	WJ	271	ALA	Peptide
54	WK	273	ALA	Peptide
55	WL	137	HIS	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1A	40/309 (13%)	29 (72%)	9 (22%)	2 (5%)	1 12
1	1B	265/309 (86%)	219 (83%)	42 (16%)	4 (2%)	8 33
2	1E	415/448 (93%)	390 (94%)	22 (5%)	3 (1%)	19 50
2	1F	164/448 (37%)	149 (91%)	14 (8%)	1 (1%)	22 53
2	1G	290/448 (65%)	279 (96%)	10 (3%)	1 (0%)	37 66
2	1H	416/448 (93%)	379 (91%)	33 (8%)	4 (1%)	13 42
3	1K	173/696 (25%)	154 (89%)	16 (9%)	3 (2%)	7 31
3	1L	173/696 (25%)	156 (90%)	15 (9%)	2 (1%)	11 38
3	1M	173/696 (25%)	160 (92%)	12 (7%)	1 (1%)	22 53
3	1v	203/696 (29%)	181 (89%)	22 (11%)	0	100 100
3	1w	85/696 (12%)	76 (89%)	9 (11%)	0	100 100
3	1x	244/696 (35%)	220 (90%)	20 (8%)	4 (2%)	8 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1y	194/696 (28%)	181 (93%)	13 (7%)	0	100	100
3	1z	85/696 (12%)	83 (98%)	2 (2%)	0	100	100
3	2a	52/696 (8%)	45 (86%)	6 (12%)	1 (2%)	6	29
4	1P	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
4	1Q	136/204 (67%)	122 (90%)	14 (10%)	0	100	100
5	1T	220/429 (51%)	193 (88%)	25 (11%)	2 (1%)	14	44
5	1U	107/429 (25%)	97 (91%)	10 (9%)	0	100	100
5	1V	221/429 (52%)	190 (86%)	28 (13%)	3 (1%)	9	34
5	1W	103/429 (24%)	91 (88%)	10 (10%)	2 (2%)	6	29
6	1Y	115/139 (83%)	98 (85%)	17 (15%)	0	100	100
7	1a	132/251 (53%)	106 (80%)	23 (17%)	3 (2%)	5	26
7	1b	120/251 (48%)	95 (79%)	22 (18%)	3 (2%)	4	24
7	5E	152/251 (61%)	115 (76%)	35 (23%)	2 (1%)	10	36
7	5F	110/251 (44%)	89 (81%)	19 (17%)	2 (2%)	7	30
7	5G	140/251 (56%)	109 (78%)	29 (21%)	2 (1%)	9	34
7	5H	115/251 (46%)	90 (78%)	21 (18%)	4 (4%)	3	19
7	5I	25/251 (10%)	20 (80%)	4 (16%)	1 (4%)	2	16
7	5J	231/251 (92%)	189 (82%)	37 (16%)	5 (2%)	5	26
7	5K	132/251 (53%)	99 (75%)	30 (23%)	3 (2%)	5	26
7	5L	123/251 (49%)	99 (80%)	21 (17%)	3 (2%)	5	25
7	5M	12/251 (5%)	11 (92%)	0	1 (8%)	0	5
7	5N	242/251 (96%)	194 (80%)	44 (18%)	4 (2%)	7	31
7	5O	13/251 (5%)	9 (69%)	4 (31%)	0	100	100
8	1d	99/359 (28%)	91 (92%)	8 (8%)	0	100	100
9	1f	34/206 (16%)	28 (82%)	6 (18%)	0	100	100
9	1g	49/206 (24%)	43 (88%)	6 (12%)	0	100	100
10	1i	32/188 (17%)	29 (91%)	2 (6%)	1 (3%)	3	21
10	1j	29/188 (15%)	24 (83%)	4 (14%)	1 (3%)	3	19
10	9M	82/188 (44%)	67 (82%)	15 (18%)	0	100	100
10	9N	82/188 (44%)	71 (87%)	10 (12%)	1 (1%)	11	38
10	9O	39/188 (21%)	25 (64%)	11 (28%)	3 (8%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1l	37/176 (21%)	25 (68%)	12 (32%)	0	100	100
11	1m	37/176 (21%)	26 (70%)	11 (30%)	0	100	100
12	1o	27/142 (19%)	24 (89%)	1 (4%)	2 (7%)	1	6
12	1p	28/142 (20%)	27 (96%)	1 (4%)	0	100	100
12	1q	44/142 (31%)	40 (91%)	4 (9%)	0	100	100
12	1r	25/142 (18%)	23 (92%)	2 (8%)	0	100	100
13	2A	248/258 (96%)	216 (87%)	29 (12%)	3 (1%)	11	38
13	2B	249/258 (96%)	212 (85%)	30 (12%)	7 (3%)	4	22
13	2C	249/258 (96%)	209 (84%)	35 (14%)	5 (2%)	6	28
13	2D	77/258 (30%)	67 (87%)	8 (10%)	2 (3%)	4	23
14	2G	225/235 (96%)	187 (83%)	36 (16%)	2 (1%)	14	44
15	2J	105/141 (74%)	91 (87%)	14 (13%)	0	100	100
15	2K	105/141 (74%)	93 (89%)	10 (10%)	2 (2%)	6	29
15	2L	105/141 (74%)	95 (90%)	8 (8%)	2 (2%)	6	29
16	2O	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
17	2R	118/499 (24%)	112 (95%)	6 (5%)	0	100	100
17	2S	374/499 (75%)	366 (98%)	7 (2%)	1 (0%)	37	66
18	2V	282/292 (97%)	239 (85%)	38 (14%)	5 (2%)	7	30
18	2W	282/292 (97%)	243 (86%)	35 (12%)	4 (1%)	9	34
19	3A	185/195 (95%)	169 (91%)	16 (9%)	0	100	100
19	3B	185/195 (95%)	161 (87%)	24 (13%)	0	100	100
19	3C	176/195 (90%)	160 (91%)	16 (9%)	0	100	100
19	3D	170/195 (87%)	151 (89%)	18 (11%)	1 (1%)	22	53
19	3E	184/195 (94%)	163 (89%)	21 (11%)	0	100	100
19	3F	185/195 (95%)	170 (92%)	15 (8%)	0	100	100
19	3G	184/195 (94%)	168 (91%)	16 (9%)	0	100	100
20	3J	491/592 (83%)	400 (82%)	79 (16%)	12 (2%)	5	25
20	3K	68/592 (12%)	52 (76%)	14 (21%)	2 (3%)	3	22
21	3N	256/560 (46%)	245 (96%)	9 (4%)	2 (1%)	16	46
21	3O	276/560 (49%)	261 (95%)	12 (4%)	3 (1%)	12	40
22	3R	163/172 (95%)	130 (80%)	31 (19%)	2 (1%)	11	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	3S	125/172 (73%)	105 (84%)	19 (15%)	1 (1%)	16	46
22	3T	163/172 (95%)	137 (84%)	24 (15%)	2 (1%)	11	38
23	3W	382/541 (71%)	356 (93%)	22 (6%)	4 (1%)	13	42
23	3X	313/541 (58%)	311 (99%)	2 (1%)	0	100	100
23	3Y	102/541 (19%)	101 (99%)	1 (1%)	0	100	100
23	3Z	170/541 (31%)	160 (94%)	9 (5%)	1 (1%)	22	53
24	4A	615/635 (97%)	549 (89%)	65 (11%)	1 (0%)	44	71
24	4B	613/635 (96%)	564 (92%)	49 (8%)	0	100	100
24	4C	615/635 (97%)	551 (90%)	63 (10%)	1 (0%)	44	71
25	4F	311/516 (60%)	301 (97%)	10 (3%)	0	100	100
25	4G	204/516 (40%)	188 (92%)	12 (6%)	4 (2%)	6	28
26	4J	376/380 (99%)	319 (85%)	53 (14%)	4 (1%)	12	40
26	4K	374/380 (98%)	313 (84%)	56 (15%)	5 (1%)	10	36
27	4N	147/243 (60%)	130 (88%)	13 (9%)	4 (3%)	4	22
27	4O	104/243 (43%)	93 (89%)	9 (9%)	2 (2%)	6	29
27	4P	146/243 (60%)	131 (90%)	14 (10%)	1 (1%)	19	50
27	4Q	91/243 (37%)	74 (81%)	16 (18%)	1 (1%)	12	40
28	4T	141/231 (61%)	126 (89%)	11 (8%)	4 (3%)	4	22
28	4U	141/231 (61%)	128 (91%)	12 (8%)	1 (1%)	19	50
28	4V	12/231 (5%)	12 (100%)	0	0	100	100
29	4Y	298/302 (99%)	272 (91%)	23 (8%)	3 (1%)	13	42
30	5A	33/277 (12%)	28 (85%)	4 (12%)	1 (3%)	3	21
30	5B	209/277 (76%)	170 (81%)	34 (16%)	5 (2%)	5	25
30	9Y	136/277 (49%)	102 (75%)	28 (21%)	6 (4%)	2	14
30	9Z	97/277 (35%)	65 (67%)	29 (30%)	3 (3%)	3	21
31	6A	223/236 (94%)	213 (96%)	10 (4%)	0	100	100
31	6B	217/236 (92%)	194 (89%)	23 (11%)	0	100	100
31	6C	221/236 (94%)	208 (94%)	13 (6%)	0	100	100
31	6D	222/236 (94%)	204 (92%)	18 (8%)	0	100	100
31	6E	222/236 (94%)	213 (96%)	9 (4%)	0	100	100
31	6F	222/236 (94%)	204 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	6I	76/123 (62%)	65 (86%)	11 (14%)	0	100	100
32	6J	51/123 (42%)	46 (90%)	5 (10%)	0	100	100
33	6M	389/469 (83%)	370 (95%)	18 (5%)	1 (0%)	37	66
33	6N	78/469 (17%)	69 (88%)	9 (12%)	0	100	100
34	6Q	195/310 (63%)	182 (93%)	13 (7%)	0	100	100
34	6R	70/310 (23%)	59 (84%)	11 (16%)	0	100	100
35	6U	147/379 (39%)	143 (97%)	4 (3%)	0	100	100
35	6V	272/379 (72%)	256 (94%)	14 (5%)	2 (1%)	19	50
35	6W	241/379 (64%)	229 (95%)	9 (4%)	3 (1%)	11	38
35	6X	119/379 (31%)	111 (93%)	7 (6%)	1 (1%)	16	46
36	7A	721/744 (97%)	612 (85%)	96 (13%)	13 (2%)	7	30
36	7B	445/744 (60%)	372 (84%)	68 (15%)	5 (1%)	12	40
36	7C	533/744 (72%)	441 (83%)	81 (15%)	11 (2%)	5	27
36	7D	720/744 (97%)	621 (86%)	87 (12%)	12 (2%)	7	31
37	7G	525/645 (81%)	437 (83%)	77 (15%)	11 (2%)	5	27
37	7H	525/645 (81%)	432 (82%)	80 (15%)	13 (2%)	4	24
37	7I	610/645 (95%)	519 (85%)	79 (13%)	12 (2%)	6	28
38	7M	261/322 (81%)	239 (92%)	21 (8%)	1 (0%)	30	61
38	7N	66/322 (20%)	64 (97%)	2 (3%)	0	100	100
39	7Q	141/185 (76%)	118 (84%)	21 (15%)	2 (1%)	9	34
39	7R	138/185 (75%)	122 (88%)	16 (12%)	0	100	100
40	7U	91/200 (46%)	61 (67%)	25 (28%)	5 (6%)	1	10
40	7V	51/200 (26%)	44 (86%)	6 (12%)	1 (2%)	6	28
41	7Y	198/204 (97%)	162 (82%)	31 (16%)	5 (2%)	4	24
41	7Z	62/204 (30%)	40 (64%)	20 (32%)	2 (3%)	3	20
42	8A	241/268 (90%)	203 (84%)	35 (14%)	3 (1%)	11	38
43	8D	395/462 (86%)	383 (97%)	11 (3%)	1 (0%)	37	66
43	8E	174/462 (38%)	170 (98%)	3 (2%)	1 (1%)	22	53
43	8F	261/462 (56%)	252 (97%)	9 (3%)	0	100	100
43	8G	395/462 (86%)	379 (96%)	15 (4%)	1 (0%)	37	66
44	8J	401/430 (93%)	380 (95%)	19 (5%)	2 (0%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	8K	318/430 (74%)	307 (96%)	10 (3%)	1 (0%)	37	66
44	8L	401/430 (93%)	383 (96%)	16 (4%)	2 (0%)	25	56
44	8M	124/430 (29%)	112 (90%)	11 (9%)	1 (1%)	16	46
44	8N	15/430 (4%)	12 (80%)	2 (13%)	1 (7%)	1	7
45	8Q	19/402 (5%)	19 (100%)	0	0	100	100
45	8R	398/402 (99%)	386 (97%)	10 (2%)	2 (0%)	25	56
45	8S	300/402 (75%)	290 (97%)	8 (3%)	2 (1%)	19	50
45	8T	398/402 (99%)	384 (96%)	13 (3%)	1 (0%)	37	66
45	8U	118/402 (29%)	116 (98%)	2 (2%)	0	100	100
46	8X	102/119 (86%)	82 (80%)	20 (20%)	0	100	100
46	8Y	102/119 (86%)	84 (82%)	16 (16%)	2 (2%)	6	28
46	8Z	102/119 (86%)	85 (83%)	15 (15%)	2 (2%)	6	28
47	9A	205/220 (93%)	163 (80%)	37 (18%)	5 (2%)	5	25
48	9D	94/171 (55%)	79 (84%)	15 (16%)	0	100	100
49	9G	148/150 (99%)	133 (90%)	12 (8%)	3 (2%)	6	28
50	9J	99/179 (55%)	95 (96%)	3 (3%)	1 (1%)	13	42
51	9R	140/153 (92%)	120 (86%)	20 (14%)	0	100	100
52	9T	71/83 (86%)	62 (87%)	9 (13%)	0	100	100
53	9V	22/294 (8%)	17 (77%)	2 (9%)	3 (14%)	0	1
53	9W	68/294 (23%)	62 (91%)	6 (9%)	0	100	100
54	AA	435/451 (96%)	407 (94%)	26 (6%)	2 (0%)	25	56
54	AB	435/451 (96%)	406 (93%)	29 (7%)	0	100	100
54	AE	435/451 (96%)	402 (92%)	33 (8%)	0	100	100
54	AG	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	44	71
54	AI	435/451 (96%)	410 (94%)	25 (6%)	0	100	100
54	AK	435/451 (96%)	400 (92%)	35 (8%)	0	100	100
54	AM	435/451 (96%)	407 (94%)	28 (6%)	0	100	100
54	BA	435/451 (96%)	407 (94%)	27 (6%)	1 (0%)	44	71
54	BB	435/451 (96%)	409 (94%)	24 (6%)	2 (0%)	25	56
54	BE	435/451 (96%)	406 (93%)	29 (7%)	0	100	100
54	BG	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	44	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	BI	435/451 (96%)	407 (94%)	28 (6%)	0	100	100
54	BK	435/451 (96%)	401 (92%)	33 (8%)	1 (0%)	44	71
54	BM	435/451 (96%)	403 (93%)	31 (7%)	1 (0%)	44	71
54	CA	435/451 (96%)	402 (92%)	32 (7%)	1 (0%)	44	71
54	CB	435/451 (96%)	397 (91%)	37 (8%)	1 (0%)	44	71
54	CE	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	25	56
54	CG	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	44	71
54	CI	435/451 (96%)	409 (94%)	26 (6%)	0	100	100
54	CK	435/451 (96%)	399 (92%)	36 (8%)	0	100	100
54	CM	435/451 (96%)	402 (92%)	31 (7%)	2 (0%)	25	56
54	DA	435/451 (96%)	406 (93%)	29 (7%)	0	100	100
54	DB	435/451 (96%)	403 (93%)	32 (7%)	0	100	100
54	DE	435/451 (96%)	395 (91%)	39 (9%)	1 (0%)	44	71
54	DG	435/451 (96%)	385 (88%)	48 (11%)	2 (0%)	25	56
54	DI	435/451 (96%)	395 (91%)	39 (9%)	1 (0%)	44	71
54	DK	435/451 (96%)	395 (91%)	39 (9%)	1 (0%)	44	71
54	DM	435/451 (96%)	398 (92%)	36 (8%)	1 (0%)	44	71
54	EA	435/451 (96%)	367 (84%)	56 (13%)	12 (3%)	4	22
54	EC	435/451 (96%)	411 (94%)	23 (5%)	1 (0%)	44	71
54	EE	435/451 (96%)	402 (92%)	32 (7%)	1 (0%)	44	71
54	EG	435/451 (96%)	408 (94%)	27 (6%)	0	100	100
54	EI	435/451 (96%)	398 (92%)	35 (8%)	2 (0%)	25	56
54	EK	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	FA	435/451 (96%)	366 (84%)	57 (13%)	12 (3%)	4	22
54	FB	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	44	71
54	FE	435/451 (96%)	361 (83%)	60 (14%)	14 (3%)	3	20
54	FG	435/451 (96%)	397 (91%)	37 (8%)	1 (0%)	44	71
54	FI	435/451 (96%)	365 (84%)	59 (14%)	11 (2%)	4	24
54	FK	435/451 (96%)	392 (90%)	43 (10%)	0	100	100
54	GA	435/451 (96%)	393 (90%)	42 (10%)	0	100	100
54	GB	435/451 (96%)	400 (92%)	34 (8%)	1 (0%)	44	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	GE	435/451 (96%)	411 (94%)	23 (5%)	1 (0%)	44	71
54	GG	435/451 (96%)	408 (94%)	26 (6%)	1 (0%)	44	71
54	GI	435/451 (96%)	396 (91%)	39 (9%)	0	100	100
54	GK	435/451 (96%)	388 (89%)	45 (10%)	2 (0%)	25	56
54	HA	435/451 (96%)	402 (92%)	31 (7%)	2 (0%)	25	56
54	HB	435/451 (96%)	399 (92%)	36 (8%)	0	100	100
54	HE	428/451 (95%)	395 (92%)	31 (7%)	2 (0%)	25	56
54	HG	431/451 (96%)	400 (93%)	29 (7%)	2 (0%)	25	56
54	HI	435/451 (96%)	401 (92%)	33 (8%)	1 (0%)	44	71
54	HK	431/451 (96%)	404 (94%)	26 (6%)	1 (0%)	44	71
54	IA	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	44	71
54	IB	430/451 (95%)	400 (93%)	28 (6%)	2 (0%)	25	56
54	IE	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	IG	435/451 (96%)	402 (92%)	33 (8%)	0	100	100
54	II	431/451 (96%)	403 (94%)	28 (6%)	0	100	100
54	IK	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	25	56
54	IM	435/451 (96%)	392 (90%)	43 (10%)	0	100	100
54	JA	428/451 (95%)	397 (93%)	30 (7%)	1 (0%)	44	71
54	JB	435/451 (96%)	406 (93%)	28 (6%)	1 (0%)	44	71
54	JE	435/451 (96%)	410 (94%)	24 (6%)	1 (0%)	44	71
54	JG	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	JI	435/451 (96%)	401 (92%)	33 (8%)	1 (0%)	44	71
54	JK	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	44	71
54	KA	435/451 (96%)	416 (96%)	18 (4%)	1 (0%)	44	71
54	KB	430/451 (95%)	401 (93%)	29 (7%)	0	100	100
54	KE	435/451 (96%)	405 (93%)	29 (7%)	1 (0%)	44	71
54	KG	435/451 (96%)	404 (93%)	29 (7%)	2 (0%)	25	56
54	KI	435/451 (96%)	410 (94%)	25 (6%)	0	100	100
54	KK	435/451 (96%)	415 (95%)	20 (5%)	0	100	100
54	LA	435/451 (96%)	412 (95%)	23 (5%)	0	100	100
54	LB	435/451 (96%)	405 (93%)	29 (7%)	1 (0%)	44	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	LE	435/451 (96%)	414 (95%)	20 (5%)	1 (0%)	44	71
54	LG	435/451 (96%)	408 (94%)	25 (6%)	2 (0%)	25	56
54	LI	435/451 (96%)	414 (95%)	21 (5%)	0	100	100
54	LK	435/451 (96%)	416 (96%)	18 (4%)	1 (0%)	44	71
54	MA	435/451 (96%)	403 (93%)	30 (7%)	2 (0%)	25	56
54	MB	435/451 (96%)	412 (95%)	22 (5%)	1 (0%)	44	71
54	ME	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	44	71
54	MG	435/451 (96%)	412 (95%)	23 (5%)	0	100	100
54	MI	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	25	56
54	MK	435/451 (96%)	401 (92%)	34 (8%)	0	100	100
54	ML	435/451 (96%)	414 (95%)	21 (5%)	0	100	100
54	NA	431/451 (96%)	401 (93%)	28 (6%)	2 (0%)	25	56
54	NB	435/451 (96%)	387 (89%)	44 (10%)	4 (1%)	14	44
54	NE	435/451 (96%)	402 (92%)	32 (7%)	1 (0%)	44	71
54	NG	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	25	56
54	NI	430/451 (95%)	395 (92%)	34 (8%)	1 (0%)	44	71
54	NL	429/451 (95%)	389 (91%)	39 (9%)	1 (0%)	44	71
54	OA	435/451 (96%)	396 (91%)	38 (9%)	1 (0%)	44	71
54	OB	430/451 (95%)	405 (94%)	23 (5%)	2 (0%)	25	56
54	OE	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	25	56
54	OG	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	OI	435/451 (96%)	405 (93%)	28 (6%)	2 (0%)	25	56
54	OK	435/451 (96%)	402 (92%)	32 (7%)	1 (0%)	44	71
54	OL	435/451 (96%)	393 (90%)	42 (10%)	0	100	100
54	PA	435/451 (96%)	403 (93%)	31 (7%)	1 (0%)	44	71
54	PB	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	44	71
54	PE	435/451 (96%)	400 (92%)	33 (8%)	2 (0%)	25	56
54	PG	435/451 (96%)	402 (92%)	33 (8%)	0	100	100
54	PI	435/451 (96%)	398 (92%)	36 (8%)	1 (0%)	44	71
54	PK	435/451 (96%)	392 (90%)	40 (9%)	3 (1%)	19	50
54	PL	435/451 (96%)	403 (93%)	32 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	QA	435/451 (96%)	407 (94%)	25 (6%)	3 (1%)	19	50
54	QB	435/451 (96%)	392 (90%)	43 (10%)	0	100	100
54	QE	435/451 (96%)	390 (90%)	44 (10%)	1 (0%)	44	71
54	QG	435/451 (96%)	388 (89%)	45 (10%)	2 (0%)	25	56
54	QI	435/451 (96%)	398 (92%)	35 (8%)	2 (0%)	25	56
54	QK	429/451 (95%)	404 (94%)	24 (6%)	1 (0%)	44	71
54	QL	432/451 (96%)	389 (90%)	42 (10%)	1 (0%)	44	71
54	RA	435/451 (96%)	414 (95%)	18 (4%)	3 (1%)	19	50
54	RB	435/451 (96%)	391 (90%)	42 (10%)	2 (0%)	25	56
54	RE	435/451 (96%)	392 (90%)	41 (9%)	2 (0%)	25	56
54	RG	435/451 (96%)	395 (91%)	38 (9%)	2 (0%)	25	56
54	RI	435/451 (96%)	400 (92%)	35 (8%)	0	100	100
54	RK	435/451 (96%)	404 (93%)	30 (7%)	1 (0%)	44	71
54	RL	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	44	71
54	SA	435/451 (96%)	398 (92%)	37 (8%)	0	100	100
54	SB	435/451 (96%)	411 (94%)	23 (5%)	1 (0%)	44	71
54	SE	435/451 (96%)	402 (92%)	33 (8%)	0	100	100
54	SG	435/451 (96%)	409 (94%)	23 (5%)	3 (1%)	19	50
54	SI	435/451 (96%)	408 (94%)	26 (6%)	1 (0%)	44	71
54	SK	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	44	71
54	TA	432/451 (96%)	404 (94%)	28 (6%)	0	100	100
54	TB	432/451 (96%)	410 (95%)	21 (5%)	1 (0%)	44	71
54	TE	435/451 (96%)	406 (93%)	29 (7%)	0	100	100
54	TG	435/451 (96%)	402 (92%)	31 (7%)	2 (0%)	25	56
54	TI	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	TK	435/451 (96%)	399 (92%)	34 (8%)	2 (0%)	25	56
54	UA	432/451 (96%)	395 (91%)	37 (9%)	0	100	100
54	UB	430/451 (95%)	398 (93%)	32 (7%)	0	100	100
54	UE	435/451 (96%)	409 (94%)	26 (6%)	0	100	100
54	UG	435/451 (96%)	397 (91%)	38 (9%)	0	100	100
54	UI	435/451 (96%)	395 (91%)	39 (9%)	1 (0%)	44	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	UK	435/451 (96%)	394 (91%)	41 (9%)	0	100	100
54	VA	435/451 (96%)	399 (92%)	33 (8%)	3 (1%)	19	50
54	VB	435/451 (96%)	401 (92%)	34 (8%)	0	100	100
54	VE	435/451 (96%)	407 (94%)	26 (6%)	2 (0%)	25	56
54	VG	431/451 (96%)	395 (92%)	36 (8%)	0	100	100
54	VI	435/451 (96%)	399 (92%)	36 (8%)	0	100	100
54	VK	435/451 (96%)	407 (94%)	27 (6%)	1 (0%)	44	71
54	WA	435/451 (96%)	408 (94%)	26 (6%)	1 (0%)	44	71
54	WB	432/451 (96%)	397 (92%)	33 (8%)	2 (0%)	25	56
54	WE	435/451 (96%)	394 (91%)	40 (9%)	1 (0%)	44	71
54	WG	435/451 (96%)	400 (92%)	33 (8%)	2 (0%)	25	56
54	WI	435/451 (96%)	389 (89%)	45 (10%)	1 (0%)	44	71
54	WK	435/451 (96%)	392 (90%)	39 (9%)	4 (1%)	14	44
55	AC	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	19	50
55	AD	429/447 (96%)	398 (93%)	29 (7%)	2 (0%)	25	56
55	AF	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	19	50
55	AH	429/447 (96%)	391 (91%)	32 (8%)	6 (1%)	9	34
55	AJ	429/447 (96%)	395 (92%)	31 (7%)	3 (1%)	19	50
55	AL	429/447 (96%)	398 (93%)	30 (7%)	1 (0%)	44	71
55	BC	429/447 (96%)	394 (92%)	32 (8%)	3 (1%)	19	50
55	BD	429/447 (96%)	385 (90%)	42 (10%)	2 (0%)	25	56
55	BF	429/447 (96%)	388 (90%)	38 (9%)	3 (1%)	19	50
55	BH	429/447 (96%)	393 (92%)	34 (8%)	2 (0%)	25	56
55	BJ	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	25	56
55	BL	429/447 (96%)	392 (91%)	33 (8%)	4 (1%)	14	44
55	CC	429/447 (96%)	371 (86%)	54 (13%)	4 (1%)	14	44
55	CD	429/447 (96%)	385 (90%)	40 (9%)	4 (1%)	14	44
55	CF	429/447 (96%)	390 (91%)	38 (9%)	1 (0%)	44	71
55	CH	429/447 (96%)	390 (91%)	37 (9%)	2 (0%)	25	56
55	CJ	429/447 (96%)	382 (89%)	45 (10%)	2 (0%)	25	56
55	CL	429/447 (96%)	386 (90%)	41 (10%)	2 (0%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	DC	429/447 (96%)	391 (91%)	35 (8%)	3 (1%)	19	50
55	DD	429/447 (96%)	386 (90%)	40 (9%)	3 (1%)	19	50
55	DF	429/447 (96%)	380 (89%)	44 (10%)	5 (1%)	11	38
55	DH	429/447 (96%)	393 (92%)	35 (8%)	1 (0%)	44	71
55	DJ	429/447 (96%)	389 (91%)	36 (8%)	4 (1%)	14	44
55	DL	429/447 (96%)	389 (91%)	36 (8%)	4 (1%)	14	44
55	EB	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	25	56
55	ED	429/447 (96%)	383 (89%)	42 (10%)	4 (1%)	14	44
55	EF	429/447 (96%)	394 (92%)	34 (8%)	1 (0%)	44	71
55	EH	429/447 (96%)	387 (90%)	36 (8%)	6 (1%)	9	34
55	EJ	429/447 (96%)	389 (91%)	39 (9%)	1 (0%)	44	71
55	EL	429/447 (96%)	389 (91%)	38 (9%)	2 (0%)	25	56
55	EM	429/447 (96%)	385 (90%)	40 (9%)	4 (1%)	14	44
55	FC	429/447 (96%)	386 (90%)	42 (10%)	1 (0%)	44	71
55	FD	429/447 (96%)	394 (92%)	32 (8%)	3 (1%)	19	50
55	FF	429/447 (96%)	403 (94%)	26 (6%)	0	100	100
55	FH	429/447 (96%)	384 (90%)	44 (10%)	1 (0%)	44	71
55	FJ	429/447 (96%)	390 (91%)	35 (8%)	4 (1%)	14	44
55	FL	429/447 (96%)	384 (90%)	40 (9%)	5 (1%)	11	38
55	FM	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	25	56
55	GC	429/447 (96%)	382 (89%)	44 (10%)	3 (1%)	19	50
55	GD	429/447 (96%)	376 (88%)	50 (12%)	3 (1%)	19	50
55	GF	429/447 (96%)	386 (90%)	39 (9%)	4 (1%)	14	44
55	GH	429/447 (96%)	391 (91%)	34 (8%)	4 (1%)	14	44
55	GJ	429/447 (96%)	393 (92%)	33 (8%)	3 (1%)	19	50
55	GL	429/447 (96%)	390 (91%)	37 (9%)	2 (0%)	25	56
55	GM	429/447 (96%)	399 (93%)	29 (7%)	1 (0%)	44	71
55	HC	429/447 (96%)	398 (93%)	28 (6%)	3 (1%)	19	50
55	HD	429/447 (96%)	382 (89%)	45 (10%)	2 (0%)	25	56
55	HF	429/447 (96%)	395 (92%)	32 (8%)	2 (0%)	25	56
55	HH	429/447 (96%)	393 (92%)	32 (8%)	4 (1%)	14	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	HJ	429/447 (96%)	398 (93%)	27 (6%)	4 (1%)	14	44
55	HL	429/447 (96%)	384 (90%)	40 (9%)	5 (1%)	11	38
55	HM	429/447 (96%)	393 (92%)	33 (8%)	3 (1%)	19	50
55	IC	429/447 (96%)	385 (90%)	42 (10%)	2 (0%)	25	56
55	ID	429/447 (96%)	390 (91%)	36 (8%)	3 (1%)	19	50
55	IF	429/447 (96%)	393 (92%)	34 (8%)	2 (0%)	25	56
55	IH	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	19	50
55	IJ	429/447 (96%)	386 (90%)	40 (9%)	3 (1%)	19	50
55	IL	429/447 (96%)	385 (90%)	39 (9%)	5 (1%)	11	38
55	JC	429/447 (96%)	407 (95%)	20 (5%)	2 (0%)	25	56
55	JD	429/447 (96%)	391 (91%)	36 (8%)	2 (0%)	25	56
55	JF	429/447 (96%)	385 (90%)	40 (9%)	4 (1%)	14	44
55	JH	429/447 (96%)	379 (88%)	45 (10%)	5 (1%)	11	38
55	JJ	429/447 (96%)	393 (92%)	32 (8%)	4 (1%)	14	44
55	JL	429/447 (96%)	382 (89%)	45 (10%)	2 (0%)	25	56
55	JM	429/447 (96%)	400 (93%)	27 (6%)	2 (0%)	25	56
55	KC	429/447 (96%)	389 (91%)	36 (8%)	4 (1%)	14	44
55	KD	429/447 (96%)	388 (90%)	38 (9%)	3 (1%)	19	50
55	KF	429/447 (96%)	399 (93%)	27 (6%)	3 (1%)	19	50
55	KH	429/447 (96%)	398 (93%)	28 (6%)	3 (1%)	19	50
55	KJ	429/447 (96%)	390 (91%)	37 (9%)	2 (0%)	25	56
55	KL	429/447 (96%)	386 (90%)	42 (10%)	1 (0%)	44	71
55	KM	429/447 (96%)	409 (95%)	19 (4%)	1 (0%)	44	71
55	LC	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	19	50
55	LD	429/447 (96%)	397 (92%)	30 (7%)	2 (0%)	25	56
55	LF	429/447 (96%)	395 (92%)	32 (8%)	2 (0%)	25	56
55	LH	429/447 (96%)	388 (90%)	37 (9%)	4 (1%)	14	44
55	LJ	429/447 (96%)	397 (92%)	30 (7%)	2 (0%)	25	56
55	LL	429/447 (96%)	392 (91%)	34 (8%)	3 (1%)	19	50
55	LM	429/447 (96%)	397 (92%)	31 (7%)	1 (0%)	44	71
55	MC	429/447 (96%)	392 (91%)	35 (8%)	2 (0%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	MD	429/447 (96%)	402 (94%)	23 (5%)	4 (1%)	14	44
55	MF	429/447 (96%)	407 (95%)	21 (5%)	1 (0%)	44	71
55	MH	429/447 (96%)	385 (90%)	40 (9%)	4 (1%)	14	44
55	MJ	429/447 (96%)	395 (92%)	30 (7%)	4 (1%)	14	44
55	MM	429/447 (96%)	389 (91%)	38 (9%)	2 (0%)	25	56
55	NC	429/447 (96%)	383 (89%)	44 (10%)	2 (0%)	25	56
55	ND	429/447 (96%)	391 (91%)	33 (8%)	5 (1%)	11	38
55	NF	429/447 (96%)	388 (90%)	36 (8%)	5 (1%)	11	38
55	NH	429/447 (96%)	386 (90%)	42 (10%)	1 (0%)	44	71
55	NJ	429/447 (96%)	381 (89%)	44 (10%)	4 (1%)	14	44
55	NK	429/447 (96%)	388 (90%)	40 (9%)	1 (0%)	44	71
55	NM	429/447 (96%)	381 (89%)	45 (10%)	3 (1%)	19	50
55	OC	429/447 (96%)	391 (91%)	36 (8%)	2 (0%)	25	56
55	OD	429/447 (96%)	386 (90%)	41 (10%)	2 (0%)	25	56
55	OF	429/447 (96%)	395 (92%)	32 (8%)	2 (0%)	25	56
55	OH	429/447 (96%)	391 (91%)	38 (9%)	0	100	100
55	OJ	429/447 (96%)	392 (91%)	34 (8%)	3 (1%)	19	50
55	OM	429/447 (96%)	393 (92%)	33 (8%)	3 (1%)	19	50
55	PC	429/447 (96%)	389 (91%)	36 (8%)	4 (1%)	14	44
55	PD	429/447 (96%)	396 (92%)	31 (7%)	2 (0%)	25	56
55	PF	429/447 (96%)	389 (91%)	38 (9%)	2 (0%)	25	56
55	PH	429/447 (96%)	391 (91%)	36 (8%)	2 (0%)	25	56
55	PJ	429/447 (96%)	377 (88%)	49 (11%)	3 (1%)	19	50
55	PM	429/447 (96%)	387 (90%)	38 (9%)	4 (1%)	14	44
55	QC	429/447 (96%)	386 (90%)	39 (9%)	4 (1%)	14	44
55	QD	429/447 (96%)	391 (91%)	37 (9%)	1 (0%)	44	71
55	QF	429/447 (96%)	383 (89%)	43 (10%)	3 (1%)	19	50
55	QH	429/447 (96%)	388 (90%)	38 (9%)	3 (1%)	19	50
55	QJ	429/447 (96%)	379 (88%)	49 (11%)	1 (0%)	44	71
55	QM	429/447 (96%)	393 (92%)	35 (8%)	1 (0%)	44	71
55	RC	429/447 (96%)	383 (89%)	44 (10%)	2 (0%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	RD	429/447 (96%)	395 (92%)	30 (7%)	4 (1%)	14	44
55	RF	429/447 (96%)	391 (91%)	36 (8%)	2 (0%)	25	56
55	RH	429/447 (96%)	388 (90%)	38 (9%)	3 (1%)	19	50
55	RJ	429/447 (96%)	381 (89%)	46 (11%)	2 (0%)	25	56
55	RM	429/447 (96%)	396 (92%)	29 (7%)	4 (1%)	14	44
55	SC	429/447 (96%)	396 (92%)	31 (7%)	2 (0%)	25	56
55	SD	429/447 (96%)	380 (89%)	48 (11%)	1 (0%)	44	71
55	SF	429/447 (96%)	405 (94%)	21 (5%)	3 (1%)	19	50
55	SH	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	25	56
55	SJ	429/447 (96%)	389 (91%)	38 (9%)	2 (0%)	25	56
55	SL	429/447 (96%)	384 (90%)	42 (10%)	3 (1%)	19	50
55	SM	429/447 (96%)	390 (91%)	36 (8%)	3 (1%)	19	50
55	TC	429/447 (96%)	386 (90%)	40 (9%)	3 (1%)	19	50
55	TD	429/447 (96%)	384 (90%)	42 (10%)	3 (1%)	19	50
55	TF	429/447 (96%)	395 (92%)	32 (8%)	2 (0%)	25	56
55	TH	429/447 (96%)	385 (90%)	41 (10%)	3 (1%)	19	50
55	TJ	429/447 (96%)	386 (90%)	39 (9%)	4 (1%)	14	44
55	TL	429/447 (96%)	381 (89%)	47 (11%)	1 (0%)	44	71
55	TM	429/447 (96%)	384 (90%)	42 (10%)	3 (1%)	19	50
55	UC	429/447 (96%)	380 (89%)	46 (11%)	3 (1%)	19	50
55	UD	429/447 (96%)	392 (91%)	33 (8%)	4 (1%)	14	44
55	UF	429/447 (96%)	379 (88%)	46 (11%)	4 (1%)	14	44
55	UH	429/447 (96%)	380 (89%)	45 (10%)	4 (1%)	14	44
55	UJ	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	25	56
55	UL	429/447 (96%)	381 (89%)	45 (10%)	3 (1%)	19	50
55	UM	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	25	56
55	VC	429/447 (96%)	378 (88%)	48 (11%)	3 (1%)	19	50
55	VD	429/447 (96%)	386 (90%)	39 (9%)	4 (1%)	14	44
55	VF	429/447 (96%)	388 (90%)	39 (9%)	2 (0%)	25	56
55	VH	429/447 (96%)	372 (87%)	53 (12%)	4 (1%)	14	44
55	VJ	429/447 (96%)	384 (90%)	44 (10%)	1 (0%)	44	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	VL	429/447 (96%)	377 (88%)	48 (11%)	4 (1%)	14	44
55	VM	429/447 (96%)	397 (92%)	31 (7%)	1 (0%)	44	71
55	WC	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	19	50
55	WD	429/447 (96%)	392 (91%)	35 (8%)	2 (0%)	25	56
55	WF	429/447 (96%)	390 (91%)	36 (8%)	3 (1%)	19	50
55	WH	429/447 (96%)	394 (92%)	34 (8%)	1 (0%)	44	71
55	WJ	429/447 (96%)	405 (94%)	23 (5%)	1 (0%)	44	71
55	WL	429/447 (96%)	390 (91%)	36 (8%)	3 (1%)	19	50
All	All	159050/186788 (85%)	144743 (91%)	13391 (8%)	916 (1%)	24	53

All (916) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1E	132	ARG
2	1E	359	GLU
2	1F	51	ASP
2	1H	222	MET
3	1L	68	ASN
3	1M	16	LYS
7	1a	156	VAL
7	1a	247	ILE
7	1b	16	ALA
10	1i	5	PHE
10	1j	30	LYS
3	1x	445	ARG
13	2B	142	SER
13	2B	253	ILE
13	2C	132	VAL
13	2D	132	VAL
13	2D	156	GLU
17	2S	269	GLU
18	2V	70	VAL
18	2V	227	CYS
3	2a	669	GLN
20	3J	160	THR
20	3J	212	VAL
20	3J	224	ASP
20	3J	313	PRO
20	3J	516	ILE

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Mol	Chain	Res	Type
21	3O	47	VAL
22	3R	34	TYR
23	3W	81	ILE
25	4G	30	LYS
26	4J	172	ILE
26	4J	290	LYS
26	4K	63	LEU
28	4T	94	TYR
28	4U	26	ASP
30	5B	94	HIS
30	5B	146	MET
7	5E	137	ASN
7	5F	247	ILE
7	5G	95	LYS
7	5H	160	ARG
7	5K	73	ARG
7	5L	247	ILE
7	5N	247	ILE
36	7A	108	GLU
36	7A	130	ILE
36	7A	316	ILE
36	7A	504	LEU
36	7B	445	VAL
36	7C	108	GLU
36	7C	316	ILE
36	7C	445	VAL
36	7D	108	GLU
36	7D	316	ILE
37	7G	41	ILE
37	7G	131	HIS
37	7G	363	ILE
37	7H	7	PRO
37	7H	363	ILE
38	7M	231	ARG
40	7U	110	GLU
40	7U	189	VAL
41	7Y	36	ALA
41	7Y	59	ILE
41	7Y	147	VAL
41	7Y	202	PRO
41	7Z	10	LEU
42	8A	48	PRO

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Mol	Chain	Res	Type
43	8E	265	VAL
45	8R	207	ILE
45	8S	204	VAL
45	8T	208	GLU
47	9A	134	GLU
47	9A	202	THR
10	9O	161	ASP
53	9V	88	PRO
30	9Y	140	HIS
30	9Y	273	VAL
30	9Z	123	PRO
30	9Z	131	GLU
54	AA	219	ILE
54	AA	281	ALA
55	AH	175	VAL
55	AH	355	ASP
55	AJ	175	VAL
55	AL	175	VAL
55	BC	175	VAL
55	BD	175	VAL
55	BF	175	VAL
55	BF	221	THR
55	BH	175	VAL
55	BJ	175	VAL
55	BL	175	VAL
54	CA	109	THR
54	CB	74	VAL
55	CD	175	VAL
55	CD	218	THR
55	CF	323	MET
54	CG	278	ALA
55	CJ	175	VAL
54	CM	161	TYR
55	DC	221	THR
55	DD	175	VAL
54	DE	74	VAL
55	DF	176	SER
54	DG	74	VAL
55	DH	175	VAL
55	DJ	175	VAL
55	DJ	355	ASP
55	DL	176	SER

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Mol	Chain	Res	Type
54	EA	261	PRO
54	EA	348	PRO
54	EC	42	ILE
55	ED	175	VAL
55	ED	177	ASP
54	EE	74	VAL
55	EF	221	THR
55	EH	89	ASN
55	EH	221	THR
54	EI	74	VAL
55	EJ	175	VAL
55	EL	175	VAL
55	EM	175	VAL
55	EM	218	THR
55	EM	221	THR
54	FA	74	VAL
54	FA	240	ALA
55	FD	175	VAL
54	FE	74	VAL
55	FH	221	THR
55	FJ	175	VAL
55	FJ	221	THR
55	FL	221	THR
55	FM	175	VAL
55	FM	221	THR
55	GD	176	SER
55	GF	218	THR
55	GF	221	THR
55	GH	221	THR
55	HD	175	VAL
54	HE	219	ILE
54	HG	48	SER
55	HH	218	THR
55	HJ	175	VAL
54	HK	82	THR
55	HL	175	VAL
55	ID	175	VAL
55	IJ	175	VAL
55	IL	175	VAL
55	IL	221	THR
54	JA	281	ALA
54	JB	42	ILE

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Mol	Chain	Res	Type
55	JC	221	THR
55	JD	175	VAL
55	JD	218	THR
55	JH	176	SER
54	JI	278	ALA
55	JJ	175	VAL
55	JL	175	VAL
55	KC	218	THR
54	KE	339	ARG
55	KF	175	VAL
55	KJ	175	VAL
55	KM	175	VAL
54	LE	82	THR
55	LF	175	VAL
55	LH	175	VAL
55	LH	218	THR
55	LH	221	THR
55	LJ	221	THR
54	LK	74	VAL
55	LL	218	THR
54	MA	74	VAL
54	MB	39	ASP
55	MH	175	VAL
54	MI	252	LEU
55	MJ	108	GLU
55	MJ	221	THR
55	MM	175	VAL
54	NB	281	ALA
55	ND	175	VAL
55	ND	221	THR
55	NF	175	VAL
54	NG	161	TYR
54	NI	281	ALA
55	NJ	175	VAL
55	NK	175	VAL
55	NM	175	VAL
55	NM	221	THR
55	OD	175	VAL
55	OJ	175	VAL
54	OK	240	ALA
55	OM	175	VAL
54	PA	40	LYS

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Mol	Chain	Res	Type
54	PB	278	ALA
55	PC	176	SER
55	PD	176	SER
55	PD	221	THR
55	PF	175	VAL
55	PF	221	THR
54	PI	161	TYR
55	PJ	175	VAL
54	PK	74	VAL
54	PK	82	THR
55	PM	175	VAL
55	PM	221	THR
55	QC	221	THR
55	QD	175	VAL
54	QE	39	ASP
55	QF	175	VAL
54	QG	48	SER
54	QG	73	THR
55	QH	176	SER
54	QI	73	THR
55	QJ	175	VAL
54	QK	219	ILE
54	QL	82	THR
55	QM	175	VAL
54	RB	74	VAL
55	RC	175	VAL
55	RD	175	VAL
54	RE	40	LYS
55	RF	175	VAL
54	RG	74	VAL
55	RJ	175	VAL
55	RM	175	VAL
55	SC	175	VAL
55	SD	175	VAL
55	SF	218	THR
54	SG	340	THR
55	SJ	175	VAL
55	SL	342	VAL
55	SM	175	VAL
55	TC	262	ARG
55	TD	175	VAL
55	TF	221	THR

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Mol	Chain	Res	Type
55	TH	175	VAL
55	TJ	175	VAL
55	TL	175	VAL
55	TM	175	VAL
55	UC	175	VAL
55	UC	221	THR
55	UD	175	VAL
55	UF	175	VAL
55	UF	339	SER
55	UF	342	VAL
55	UH	175	VAL
55	UH	279	GLN
55	UJ	175	VAL
55	UL	175	VAL
55	UL	342	VAL
55	VC	175	VAL
55	VD	175	VAL
55	VD	279	GLN
55	VF	175	VAL
55	VH	175	VAL
55	VJ	175	VAL
55	VL	175	VAL
54	WA	82	THR
55	WD	175	VAL
54	WE	275	VAL
55	WF	218	THR
55	WH	175	VAL
54	WI	74	VAL
1	1A	23	ASP
1	1B	114	LEU
1	1B	155	THR
2	1E	247	ASN
2	1G	132	ARG
5	1V	238	LYS
12	1o	27	MET
12	1o	28	THR
3	1x	401	PHE
13	2A	93	LYS
13	2B	20	VAL
13	2B	98	PRO
13	2C	20	VAL
15	2K	42	ILE

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Mol	Chain	Res	Type
18	2W	70	VAL
20	3J	83	VAL
20	3K	51	GLU
20	3K	83	VAL
21	3O	108	ILE
22	3R	138	LYS
22	3S	138	LYS
23	3W	112	THR
26	4J	44	LYS
27	4N	170	ASN
27	4O	173	ILE
29	4Y	36	ALA
30	5A	42	ARG
30	5B	98	THR
7	5H	247	ILE
7	5J	101	SER
35	6V	124	PRO
35	6V	262	SER
35	6W	40	VAL
35	6X	40	VAL
36	7A	473	ILE
36	7B	473	ILE
36	7B	632	ASN
36	7C	130	ILE
36	7D	130	ILE
36	7D	473	ILE
36	7D	709	VAL
37	7G	269	VAL
37	7H	269	VAL
37	7I	41	ILE
37	7I	143	ILE
37	7I	269	VAL
39	7Q	99	VAL
40	7U	141	GLU
40	7V	35	VAL
49	9G	33	SER
50	9J	172	THR
10	9N	112	SER
10	9O	160	ASN
55	AF	216	LYS
55	AF	218	THR
55	AH	108	GLU

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Mol	Chain	Res	Type
55	AH	218	THR
55	AH	221	THR
55	AH	302	ALA
54	BB	42	ILE
55	BC	108	GLU
55	BC	218	THR
55	BD	221	THR
55	BJ	218	THR
55	BL	218	THR
55	BL	221	THR
54	BM	46	ASP
55	CC	176	SER
55	CD	168	SER
54	CE	72	PRO
55	CJ	347	ASN
54	CM	264	ARG
55	DD	221	THR
55	DF	108	GLU
55	DF	336	LYS
54	DI	42	ILE
54	EA	263	PRO
54	EA	299	ALA
54	EA	300	ASN
55	EB	175	VAL
55	ED	221	THR
55	EH	108	GLU
55	EH	176	SER
54	FA	241	SER
54	FA	283	HIS
54	FE	145	THR
54	FE	283	HIS
54	FE	351	PHE
54	FG	82	THR
54	FI	261	PRO
54	FI	300	ASN
54	FI	332	ILE
54	FI	348	PRO
55	FJ	99	ASN
55	FL	95	SER
55	GC	108	GLU
55	GC	214	THR
55	GH	216	LYS

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Mol	Chain	Res	Type
55	GJ	175	VAL
55	GJ	216	LYS
55	GJ	218	THR
54	HE	82	THR
55	HF	216	LYS
55	HH	216	LYS
54	HI	82	THR
55	HJ	108	GLU
55	HJ	217	LEU
55	HL	95	SER
55	HL	143	THR
55	HM	175	VAL
55	HM	177	ASP
54	IA	161	TYR
54	IB	40	LYS
55	ID	218	THR
55	IH	168	SER
55	IH	221	THR
54	IK	41	THR
55	IL	218	THR
54	JE	109	THR
55	JF	176	SER
55	JF	201	CYS
55	JM	175	VAL
55	KD	108	GLU
55	KD	221	THR
55	KF	218	THR
54	KG	37	PRO
55	KH	218	THR
54	LB	82	THR
55	LC	216	LYS
55	LD	175	VAL
55	LJ	95	SER
55	LL	175	VAL
55	LL	216	LYS
54	MA	82	THR
55	MC	108	GLU
55	MC	216	LYS
55	MD	218	THR
55	MF	108	GLU
55	MH	108	GLU
55	MH	168	SER

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Mol	Chain	Res	Type
55	MH	216	LYS
54	MI	38	SER
55	MJ	218	THR
54	NA	41	THR
55	ND	218	THR
54	NE	110	ILE
55	NF	107	THR
55	NF	216	LYS
55	NF	218	THR
55	NJ	221	THR
54	NL	110	ILE
54	OA	110	ILE
54	OB	110	ILE
55	OD	221	THR
55	OF	95	SER
55	OJ	77	ARG
55	OJ	216	LYS
55	OM	221	THR
55	PC	218	THR
55	PC	221	THR
55	PH	218	THR
54	QA	72	PRO
54	QA	73	THR
55	QF	221	THR
54	RA	82	THR
54	RB	48	SER
55	RD	218	THR
54	RG	42	ILE
55	RH	176	SER
55	RM	221	THR
55	SF	221	THR
55	SL	175	VAL
55	SM	218	THR
55	TC	175	VAL
55	TF	355	ASP
55	TJ	108	GLU
55	TJ	195	ASN
55	TM	108	GLU
55	UD	108	GLU
55	UD	221	THR
55	UF	218	THR
55	UH	216	LYS

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Mol	Chain	Res	Type
54	UI	41	THR
54	VA	82	THR
55	VD	108	GLU
54	VE	220	GLU
55	VL	221	THR
55	WC	175	VAL
55	WC	221	THR
54	WG	41	THR
54	WG	82	THR
54	WK	42	ILE
55	WL	175	VAL
55	WL	218	THR
2	1H	360	THR
5	1T	147	LYS
5	1V	147	LYS
5	1V	272	GLU
5	1W	147	LYS
5	1W	177	LYS
7	1a	172	LEU
7	1b	73	ARG
7	1b	77	ASP
3	1x	449	PHE
13	2B	156	GLU
13	2C	156	GLU
14	2G	101	LYS
15	2L	8	ASN
18	2W	284	LYS
25	4G	8	ARG
26	4J	232	ARG
26	4K	44	LYS
26	4K	83	ASP
26	4K	356	ASN
27	4N	102	ASP
27	4O	170	ASN
7	5F	184	VAL
7	5H	157	TYR
7	5I	6	TYR
7	5K	9	THR
36	7A	383	ASN
37	7G	143	ILE
37	7G	355	TYR
37	7G	458	ILE

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Mol	Chain	Res	Type
37	7H	143	ILE
37	7H	402	LYS
37	7H	458	ILE
37	7I	35	ALA
37	7I	402	LYS
40	7U	162	ILE
41	7Y	8	ARG
44	8J	3	ILE
44	8L	3	ILE
45	8R	204	VAL
47	9A	164	PHE
49	9G	7	THR
53	9V	92	ARG
30	9Y	153	ARG
30	9Y	200	LYS
55	AC	168	SER
55	AD	218	THR
55	AJ	176	SER
54	BB	48	SER
55	BF	218	THR
55	CH	216	LYS
55	DF	168	SER
55	DJ	108	GLU
55	DJ	282	ARG
54	DK	38	SER
55	DL	168	SER
54	EA	247	ALA
54	EA	286	LEU
55	ED	216	LYS
55	EL	168	SER
54	FA	239	THR
54	FA	261	PRO
54	FA	351	PHE
54	FB	274	PRO
54	FE	265	ILE
54	FE	273	ALA
54	FE	322	ASP
54	FI	257	THR
55	FJ	216	LYS
54	GB	38	SER
55	GD	168	SER
54	GE	42	ILE

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Mol	Chain	Res	Type
54	GG	41	THR
54	GK	109	THR
55	GL	175	VAL
54	HA	82	THR
55	HD	168	SER
55	IC	168	SER
55	ID	216	LYS
55	IL	168	SER
55	JC	176	SER
55	JH	175	VAL
55	JJ	216	LYS
55	JL	221	THR
55	KC	168	SER
54	KG	41	THR
55	KH	168	SER
55	KJ	221	THR
55	KL	175	VAL
55	LC	168	SER
54	LG	40	LYS
55	LH	216	LYS
55	MD	175	VAL
55	MD	216	LYS
55	MJ	216	LYS
55	MM	221	THR
54	NB	145	THR
55	NC	176	SER
55	NF	168	SER
55	NJ	218	THR
55	NM	168	SER
55	OC	216	LYS
54	OI	82	THR
55	OM	216	LYS
54	PE	39	ASP
54	PE	41	THR
55	PJ	216	LYS
54	QA	278	ALA
55	QC	177	ASP
55	QH	143	THR
54	QI	40	LYS
54	RA	274	PRO
55	RD	216	LYS
55	RH	216	LYS

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Mol	Chain	Res	Type
55	RJ	221	THR
54	RL	38	SER
55	SC	216	LYS
55	SH	216	LYS
54	SK	39	ASP
55	SM	216	LYS
54	TB	274	PRO
55	TD	216	LYS
55	TD	221	THR
55	TH	147	MET
55	TH	355	ASP
54	TK	274	PRO
55	UH	221	THR
55	UM	168	SER
55	UM	175	VAL
55	VC	168	SER
55	VH	221	THR
55	VL	168	SER
55	VL	218	THR
54	WB	274	PRO
55	WC	216	LYS
55	WF	175	VAL
55	WF	216	LYS
55	WL	168	SER
1	1B	139	ILE
2	1H	261	THR
3	1K	3	GLU
3	1L	6	SER
5	1T	419	ARG
13	2C	217	LEU
14	2G	227	ARG
21	3N	491	VAL
21	3O	109	ARG
23	3W	151	GLN
23	3Z	81	ILE
27	4N	169	MET
28	4T	88	VAL
28	4T	129	TYR
30	5B	210	ILE
7	5J	157	TYR
7	5J	180	SER
7	5J	184	VAL

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Mol	Chain	Res	Type
7	5L	184	VAL
7	5M	247	ILE
7	5N	157	TYR
7	5N	184	VAL
33	6M	170	ALA
35	6W	124	PRO
36	7A	542	ILE
36	7C	473	ILE
36	7C	505	TYR
36	7D	380	ALA
37	7G	430	LYS
37	7I	430	LYS
37	7I	448	PHE
39	7Q	160	VAL
41	7Z	59	ILE
44	8M	3	ILE
45	8S	6	LYS
10	9O	166	PHE
30	9Y	210	ILE
55	AC	175	VAL
55	AD	168	SER
55	BH	216	LYS
54	BK	109	THR
55	CC	101	TRP
55	CC	175	VAL
55	CC	221	THR
55	CH	217	LEU
55	CL	168	SER
55	DC	176	SER
55	DF	175	VAL
55	DL	175	VAL
55	EH	175	VAL
54	EI	274	PRO
54	FA	256	GLN
54	FA	279	GLU
55	FC	168	SER
55	FD	259	PRO
54	FE	275	VAL
54	FE	312	TYR
54	FE	340	THR
54	FE	341	ILE
54	FI	258	ASN

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Mol	Chain	Res	Type
54	FI	286	LEU
55	FL	218	THR
55	GD	175	VAL
55	GF	168	SER
55	GM	175	VAL
55	HC	216	LYS
54	HG	274	PRO
55	HJ	168	SER
55	HL	216	LYS
55	IJ	216	LYS
55	JF	175	VAL
55	JH	168	SER
55	JM	221	THR
55	LM	175	VAL
55	MD	221	THR
54	NB	274	PRO
55	ND	168	SER
55	PC	175	VAL
54	PK	219	ILE
55	PM	168	SER
55	QC	178	THR
55	QF	168	SER
55	QH	175	VAL
54	RA	161	TYR
55	RC	168	SER
55	RF	221	THR
55	RH	168	SER
55	RM	168	SER
55	SF	175	VAL
55	SJ	168	SER
55	TJ	217	LEU
55	TM	168	SER
55	VD	168	SER
55	VF	168	SER
55	VM	175	VAL
55	WJ	175	VAL
54	WK	403	ALA
2	1H	51	ASP
3	1K	19	THR
13	2A	253	ILE
18	2V	190	VAL
18	2V	284	LYS

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Mol	Chain	Res	Type
18	2W	190	VAL
20	3J	196	ARG
20	3J	206	PHE
20	3J	562	VAL
21	3N	528	VAL
25	4G	35	HIS
26	4K	331	PRO
27	4N	168	ASN
27	4Q	168	ASN
28	4T	98	SER
29	4Y	10	VAL
7	5G	101	SER
7	5H	184	VAL
7	5J	247	ILE
35	6W	127	VAL
36	7A	184	ILE
36	7C	184	ILE
36	7D	184	ILE
36	7D	504	LEU
37	7G	197	ALA
37	7G	457	ILE
37	7H	35	ALA
37	7H	430	LYS
37	7I	197	ALA
42	8A	29	GLN
43	8G	265	VAL
44	8L	328	PRO
46	8Y	110	LYS
46	8Z	73	GLU
47	9A	152	TYR
49	9G	2	SER
53	9V	89	PRO
55	AC	218	THR
55	AJ	216	LYS
55	BL	108	GLU
54	CE	73	THR
55	CL	175	VAL
55	DC	216	LYS
54	DM	40	LYS
54	EA	273	ALA
55	EB	168	SER
55	EH	88	ASP

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Mol	Chain	Res	Type
54	FA	259	LEU
54	FE	261	PRO
54	FE	348	PRO
54	FI	273	ALA
54	FI	298	PRO
55	FL	175	VAL
55	GF	175	VAL
55	HH	393	ALA
54	IB	163	LYS
55	IJ	217	LEU
54	IK	274	PRO
55	JF	101	TRP
55	JJ	176	SER
54	JK	42	ILE
55	KD	218	THR
55	KF	216	LYS
55	LC	108	GLU
55	LD	216	LYS
54	ME	46	ASP
55	NC	216	LYS
55	ND	247	ASN
54	NG	58	ALA
55	NH	176	SER
55	NJ	216	LYS
54	OE	220	GLU
54	OE	274	PRO
55	OF	175	VAL
55	PJ	218	THR
54	RE	160	ASP
54	RK	109	THR
55	RM	218	THR
55	SH	176	SER
54	SI	274	PRO
55	SL	97	ALA
55	TC	108	GLU
55	UJ	393	ALA
55	VH	168	SER
54	WB	261	PRO
55	WD	221	THR
54	WK	404	PHE
1	1A	35	GLU
3	1K	15	HIS

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Mol	Chain	Res	Type
3	1x	450	ASN
13	2C	188	MET
15	2K	38	PHE
18	2W	146	THR
20	3J	97	ALA
20	3J	109	SER
20	3J	111	LYS
23	3W	153	ASN
29	4Y	191	GLN
30	5B	255	TYR
7	5E	9	THR
7	5L	157	TYR
7	5N	20	THR
36	7A	505	TYR
36	7A	513	HIS
36	7B	437	LEU
36	7B	505	TYR
36	7D	505	TYR
37	7I	367	THR
43	8D	265	VAL
44	8J	328	PRO
44	8K	328	PRO
46	8Z	110	LYS
47	9A	181	THR
55	AF	108	GLU
54	AG	65	ALA
54	BA	46	ASP
55	CD	216	LYS
55	DD	218	THR
55	DL	177	ASP
54	EA	265	ILE
55	EM	216	LYS
55	FD	108	GLU
54	FE	281	ALA
55	GC	175	VAL
55	GH	168	SER
54	GK	37	PRO
55	GL	221	THR
55	HC	221	THR
55	HH	394	PHE
55	HL	168	SER
55	HM	241	ARG

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Mol	Chain	Res	Type
55	IF	97	ALA
55	IH	175	VAL
55	JH	216	LYS
55	JJ	108	GLU
55	KC	216	LYS
55	KC	221	THR
55	KH	216	LYS
55	LF	216	LYS
54	OB	40	LYS
55	OC	221	THR
54	OI	41	THR
55	PH	216	LYS
55	PM	218	THR
55	QC	316	ILE
54	SB	278	ALA
54	TG	243	ARG
55	UC	218	THR
55	UD	216	LYS
55	UL	221	THR
54	VA	42	ILE
54	VA	74	VAL
55	VC	108	GLU
55	VH	216	LYS
24	4A	121	VAL
36	7A	54	GLN
44	8N	328	PRO
54	FI	275	VAL
55	FL	272	PRO
55	GH	175	VAL
55	HC	175	VAL
55	IF	175	VAL
54	NB	110	ILE
54	SG	42	ILE
13	2A	20	VAL
13	2B	132	VAL
15	2L	42	ILE
37	7I	458	ILE
30	9Y	134	HIS
54	EA	298	PRO
54	FA	265	ILE
54	TK	110	ILE
54	WK	274	PRO

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Mol	Chain	Res	Type
13	2B	92	PRO
18	2V	236	VAL
19	3D	178	PRO
22	3T	121	GLU
25	4G	28	PRO
37	7H	377	LEU
40	7U	134	ILE
54	DG	66	VAL
54	FI	110	ILE
55	HF	175	VAL
55	IC	175	VAL
55	IL	70	PRO
54	LG	110	ILE
55	RD	70	PRO
54	TG	110	ILE
54	VE	274	PRO
22	3T	33	PRO
7	5K	108	GLY
36	7A	186	ALA
36	7A	389	PRO
36	7C	6	LEU
36	7C	54	GLN
36	7C	186	ALA
36	7C	389	PRO
36	7D	54	GLN
37	7G	377	LEU
37	7H	197	ALA
37	7H	457	ILE
37	7H	478	PRO
37	7I	457	ILE
42	8A	55	GLY
30	9Z	52	PRO
54	BG	261	PRO
54	EA	274	PRO
54	EA	328	VAL
54	FA	348	PRO
54	HA	110	ILE
55	JH	316	ILE
54	KA	110	ILE
54	VK	110	ILE
1	1B	97	PRO
24	4C	121	VAL

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Mol	Chain	Res	Type
27	4P	89	VAL
36	7D	186	ALA
36	7D	389	PRO
37	7H	470	MET
37	7I	470	MET
46	8Y	73	GLU
54	NA	110	ILE
54	SG	274	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	34/253 (13%)	34 (100%)	0	100	100
1	1B	221/253 (87%)	221 (100%)	0	100	100
2	1E	350/374 (94%)	349 (100%)	1 (0%)	91	94
2	1F	140/374 (37%)	139 (99%)	1 (1%)	81	88
2	1G	248/374 (66%)	247 (100%)	1 (0%)	89	93
2	1H	352/374 (94%)	350 (99%)	2 (1%)	84	90
3	1K	159/612 (26%)	159 (100%)	0	100	100
3	1L	159/612 (26%)	158 (99%)	1 (1%)	84	90
3	1M	155/612 (25%)	155 (100%)	0	100	100
3	1v	187/612 (31%)	187 (100%)	0	100	100
3	1w	81/612 (13%)	81 (100%)	0	100	100
3	1x	226/612 (37%)	225 (100%)	1 (0%)	89	93
3	1y	178/612 (29%)	178 (100%)	0	100	100
3	1z	81/612 (13%)	80 (99%)	1 (1%)	67	80
3	2a	50/612 (8%)	50 (100%)	0	100	100
4	1P	175/183 (96%)	175 (100%)	0	100	100
4	1Q	121/183 (66%)	120 (99%)	1 (1%)	79	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	1T	199/383 (52%)	198 (100%)	1 (0%)	86	91
5	1U	97/383 (25%)	97 (100%)	0	100	100
5	1V	201/383 (52%)	201 (100%)	0	100	100
5	1W	95/383 (25%)	95 (100%)	0	100	100
6	1Y	112/126 (89%)	112 (100%)	0	100	100
7	1a	118/213 (55%)	118 (100%)	0	100	100
7	1b	99/213 (46%)	99 (100%)	0	100	100
7	5E	127/213 (60%)	127 (100%)	0	100	100
7	5F	99/213 (46%)	99 (100%)	0	100	100
7	5G	117/213 (55%)	117 (100%)	0	100	100
7	5H	103/213 (48%)	103 (100%)	0	100	100
7	5I	22/213 (10%)	21 (96%)	1 (4%)	23	52
7	5J	197/213 (92%)	197 (100%)	0	100	100
7	5K	109/213 (51%)	108 (99%)	1 (1%)	75	85
7	5L	110/213 (52%)	109 (99%)	1 (1%)	75	85
7	5M	14/213 (7%)	14 (100%)	0	100	100
7	5N	206/213 (97%)	206 (100%)	0	100	100
7	5O	12/213 (6%)	12 (100%)	0	100	100
8	1d	92/311 (30%)	90 (98%)	2 (2%)	47	69
9	1f	33/180 (18%)	33 (100%)	0	100	100
9	1g	48/180 (27%)	48 (100%)	0	100	100
10	1i	31/164 (19%)	31 (100%)	0	100	100
10	1j	28/164 (17%)	28 (100%)	0	100	100
10	9M	76/164 (46%)	76 (100%)	0	100	100
10	9N	76/164 (46%)	76 (100%)	0	100	100
10	9O	37/164 (23%)	37 (100%)	0	100	100
11	1l	33/153 (22%)	33 (100%)	0	100	100
11	1m	33/153 (22%)	32 (97%)	1 (3%)	36	62
12	1o	26/129 (20%)	26 (100%)	0	100	100
12	1p	27/129 (21%)	27 (100%)	0	100	100
12	1q	41/129 (32%)	40 (98%)	1 (2%)	44	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	1r	24/129 (19%)	24 (100%)	0	100	100
13	2A	226/233 (97%)	226 (100%)	0	100	100
13	2B	226/233 (97%)	224 (99%)	2 (1%)	75	85
13	2C	227/233 (97%)	227 (100%)	0	100	100
13	2D	69/233 (30%)	69 (100%)	0	100	100
14	2G	199/205 (97%)	199 (100%)	0	100	100
15	2J	93/122 (76%)	93 (100%)	0	100	100
15	2K	93/122 (76%)	93 (100%)	0	100	100
15	2L	93/122 (76%)	93 (100%)	0	100	100
16	2O	99/100 (99%)	99 (100%)	0	100	100
17	2R	108/457 (24%)	108 (100%)	0	100	100
17	2S	347/457 (76%)	346 (100%)	1 (0%)	91	94
18	2V	252/259 (97%)	251 (100%)	1 (0%)	89	93
18	2W	252/259 (97%)	252 (100%)	0	100	100
19	3A	174/180 (97%)	174 (100%)	0	100	100
19	3B	174/180 (97%)	173 (99%)	1 (1%)	84	90
19	3C	167/180 (93%)	167 (100%)	0	100	100
19	3D	164/180 (91%)	164 (100%)	0	100	100
19	3E	173/180 (96%)	173 (100%)	0	100	100
19	3F	174/180 (97%)	174 (100%)	0	100	100
19	3G	173/180 (96%)	172 (99%)	1 (1%)	84	90
20	3J	429/509 (84%)	421 (98%)	8 (2%)	52	72
20	3K	61/509 (12%)	60 (98%)	1 (2%)	58	76
21	3N	222/478 (46%)	219 (99%)	3 (1%)	62	78
21	3O	240/478 (50%)	234 (98%)	6 (2%)	42	67
22	3R	147/154 (96%)	146 (99%)	1 (1%)	81	88
22	3S	112/154 (73%)	112 (100%)	0	100	100
22	3T	147/154 (96%)	147 (100%)	0	100	100
23	3W	342/480 (71%)	337 (98%)	5 (2%)	60	77
23	3X	278/480 (58%)	276 (99%)	2 (1%)	81	88
23	3Y	89/480 (18%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	3Z	153/480 (32%)	152 (99%)	1 (1%)	81	88
24	4A	532/546 (97%)	532 (100%)	0	100	100
24	4B	530/546 (97%)	528 (100%)	2 (0%)	89	93
24	4C	532/546 (97%)	531 (100%)	1 (0%)	92	95
25	4F	266/454 (59%)	266 (100%)	0	100	100
25	4G	191/454 (42%)	191 (100%)	0	100	100
26	4J	325/327 (99%)	324 (100%)	1 (0%)	91	94
26	4K	324/327 (99%)	324 (100%)	0	100	100
27	4N	132/212 (62%)	132 (100%)	0	100	100
27	4O	92/212 (43%)	92 (100%)	0	100	100
27	4P	129/212 (61%)	129 (100%)	0	100	100
27	4Q	75/212 (35%)	74 (99%)	1 (1%)	65	79
28	4T	133/209 (64%)	133 (100%)	0	100	100
28	4U	133/209 (64%)	132 (99%)	1 (1%)	79	87
28	4V	12/209 (6%)	12 (100%)	0	100	100
29	4Y	265/267 (99%)	265 (100%)	0	100	100
30	5A	26/237 (11%)	26 (100%)	0	100	100
30	5B	182/237 (77%)	180 (99%)	2 (1%)	70	82
30	9Y	122/237 (52%)	120 (98%)	2 (2%)	58	76
30	9Z	82/237 (35%)	82 (100%)	0	100	100
31	6A	195/204 (96%)	194 (100%)	1 (0%)	86	91
31	6B	188/204 (92%)	187 (100%)	1 (0%)	86	91
31	6C	192/204 (94%)	192 (100%)	0	100	100
31	6D	194/204 (95%)	194 (100%)	0	100	100
31	6E	194/204 (95%)	193 (100%)	1 (0%)	86	91
31	6F	194/204 (95%)	194 (100%)	0	100	100
32	6I	70/106 (66%)	69 (99%)	1 (1%)	62	78
32	6J	46/106 (43%)	46 (100%)	0	100	100
33	6M	343/410 (84%)	343 (100%)	0	100	100
33	6N	69/410 (17%)	69 (100%)	0	100	100
34	6Q	183/275 (66%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	6R	67/275 (24%)	67 (100%)	0	100	100
35	6U	132/338 (39%)	131 (99%)	1 (1%)	79	87
35	6V	240/338 (71%)	238 (99%)	2 (1%)	79	87
35	6W	219/338 (65%)	219 (100%)	0	100	100
35	6X	112/338 (33%)	112 (100%)	0	100	100
36	7A	644/660 (98%)	642 (100%)	2 (0%)	91	94
36	7B	410/660 (62%)	408 (100%)	2 (0%)	86	91
36	7C	480/660 (73%)	478 (100%)	2 (0%)	89	93
36	7D	643/660 (97%)	643 (100%)	0	100	100
37	7G	477/577 (83%)	476 (100%)	1 (0%)	92	95
37	7H	477/577 (83%)	474 (99%)	3 (1%)	84	90
37	7I	553/577 (96%)	550 (100%)	3 (0%)	86	91
38	7M	230/283 (81%)	229 (100%)	1 (0%)	89	93
38	7N	62/283 (22%)	62 (100%)	0	100	100
39	7Q	127/160 (79%)	127 (100%)	0	100	100
39	7R	119/160 (74%)	119 (100%)	0	100	100
40	7U	87/183 (48%)	86 (99%)	1 (1%)	70	82
40	7V	49/183 (27%)	48 (98%)	1 (2%)	50	71
41	7Y	179/183 (98%)	179 (100%)	0	100	100
41	7Z	55/183 (30%)	55 (100%)	0	100	100
42	8A	210/231 (91%)	209 (100%)	1 (0%)	86	91
43	8D	364/412 (88%)	364 (100%)	0	100	100
43	8E	164/412 (40%)	164 (100%)	0	100	100
43	8F	242/412 (59%)	241 (100%)	1 (0%)	89	93
43	8G	364/412 (88%)	364 (100%)	0	100	100
44	8J	364/389 (94%)	364 (100%)	0	100	100
44	8K	287/389 (74%)	287 (100%)	0	100	100
44	8L	364/389 (94%)	364 (100%)	0	100	100
44	8M	122/389 (31%)	122 (100%)	0	100	100
44	8N	16/389 (4%)	16 (100%)	0	100	100
45	8Q	18/365 (5%)	18 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	8R	363/365 (100%)	361 (99%)	2 (1%)	84	90
45	8S	278/365 (76%)	277 (100%)	1 (0%)	89	93
45	8T	363/365 (100%)	362 (100%)	1 (0%)	91	94
45	8U	108/365 (30%)	108 (100%)	0	100	100
46	8X	99/111 (89%)	99 (100%)	0	100	100
46	8Y	99/111 (89%)	99 (100%)	0	100	100
46	8Z	99/111 (89%)	98 (99%)	1 (1%)	73	84
47	9A	187/200 (94%)	187 (100%)	0	100	100
48	9D	87/149 (58%)	87 (100%)	0	100	100
49	9G	138/139 (99%)	137 (99%)	1 (1%)	81	88
50	9J	91/157 (58%)	91 (100%)	0	100	100
51	9R	130/139 (94%)	130 (100%)	0	100	100
52	9T	70/77 (91%)	70 (100%)	0	100	100
53	9V	19/250 (8%)	19 (100%)	0	100	100
53	9W	64/250 (26%)	64 (100%)	0	100	100
54	AA	365/376 (97%)	365 (100%)	0	100	100
54	AB	365/376 (97%)	365 (100%)	0	100	100
54	AE	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	AG	365/376 (97%)	365 (100%)	0	100	100
54	AI	365/376 (97%)	365 (100%)	0	100	100
54	AK	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	AM	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	BA	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	BB	365/376 (97%)	365 (100%)	0	100	100
54	BE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	BG	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	BI	365/376 (97%)	365 (100%)	0	100	100
54	BK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	BM	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	CA	365/376 (97%)	365 (100%)	0	100	100
54	CB	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	CE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	CG	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	CI	365/376 (97%)	365 (100%)	0	100	100
54	CK	365/376 (97%)	365 (100%)	0	100	100
54	CM	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	DA	365/376 (97%)	365 (100%)	0	100	100
54	DB	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	DE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	DG	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	DI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	DK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	DM	365/376 (97%)	365 (100%)	0	100	100
54	EA	365/376 (97%)	332 (91%)	33 (9%)	8	27
54	EC	365/376 (97%)	365 (100%)	0	100	100
54	EE	365/376 (97%)	365 (100%)	0	100	100
54	EG	365/376 (97%)	365 (100%)	0	100	100
54	EI	365/376 (97%)	365 (100%)	0	100	100
54	EK	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	FA	365/376 (97%)	329 (90%)	36 (10%)	6	24
54	FB	365/376 (97%)	365 (100%)	0	100	100
54	FE	365/376 (97%)	322 (88%)	43 (12%)	4	17
54	FG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	FI	365/376 (97%)	339 (93%)	26 (7%)	12	37
54	FK	365/376 (97%)	365 (100%)	0	100	100
54	GA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	GB	365/376 (97%)	365 (100%)	0	100	100
54	GE	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	GG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	GI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	GK	365/376 (97%)	365 (100%)	0	100	100
54	HA	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	HB	365/376 (97%)	365 (100%)	0	100	100
54	HE	362/376 (96%)	361 (100%)	1 (0%)	91	94
54	HG	365/376 (97%)	362 (99%)	3 (1%)	79	87
54	HI	365/376 (97%)	365 (100%)	0	100	100
54	HK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	IA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	IB	364/376 (97%)	364 (100%)	0	100	100
54	IE	365/376 (97%)	365 (100%)	0	100	100
54	IG	365/376 (97%)	365 (100%)	0	100	100
54	II	364/376 (97%)	364 (100%)	0	100	100
54	IK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	IM	365/376 (97%)	362 (99%)	3 (1%)	79	87
54	JA	363/376 (96%)	363 (100%)	0	100	100
54	JB	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	JE	365/376 (97%)	365 (100%)	0	100	100
54	JG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	JI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	JK	365/376 (97%)	365 (100%)	0	100	100
54	KA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	KB	364/376 (97%)	362 (100%)	2 (0%)	86	91
54	KE	365/376 (97%)	365 (100%)	0	100	100
54	KG	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	KI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	KK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	LA	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	LB	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	LE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	LG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	LI	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	LK	365/376 (97%)	365 (100%)	0	100	100
54	MA	365/376 (97%)	364 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	MB	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	ME	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	MG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	MI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	MK	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	ML	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	NA	365/376 (97%)	365 (100%)	0	100	100
54	NB	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	NE	365/376 (97%)	365 (100%)	0	100	100
54	NG	365/376 (97%)	365 (100%)	0	100	100
54	NI	364/376 (97%)	363 (100%)	1 (0%)	91	94
54	NL	363/376 (96%)	363 (100%)	0	100	100
54	OA	365/376 (97%)	365 (100%)	0	100	100
54	OB	364/376 (97%)	362 (100%)	2 (0%)	86	91
54	OE	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	OG	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	OI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	OK	365/376 (97%)	365 (100%)	0	100	100
54	OL	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	PA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	PB	365/376 (97%)	365 (100%)	0	100	100
54	PE	365/376 (97%)	365 (100%)	0	100	100
54	PG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	PI	365/376 (97%)	365 (100%)	0	100	100
54	PK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	PL	365/376 (97%)	365 (100%)	0	100	100
54	QA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	QB	365/376 (97%)	365 (100%)	0	100	100
54	QE	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	QG	365/376 (97%)	361 (99%)	4 (1%)	70	82
54	QI	365/376 (97%)	363 (100%)	2 (0%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	QK	363/376 (96%)	362 (100%)	1 (0%)	91	94
54	QL	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	RA	365/376 (97%)	365 (100%)	0	100	100
54	RB	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	RE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	RG	365/376 (97%)	365 (100%)	0	100	100
54	RI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	RK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	RL	365/376 (97%)	365 (100%)	0	100	100
54	SA	365/376 (97%)	365 (100%)	0	100	100
54	SB	365/376 (97%)	365 (100%)	0	100	100
54	SE	365/376 (97%)	365 (100%)	0	100	100
54	SG	365/376 (97%)	365 (100%)	0	100	100
54	SI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	SK	365/376 (97%)	365 (100%)	0	100	100
54	TA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	TB	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	TE	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	TG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	TI	365/376 (97%)	365 (100%)	0	100	100
54	TK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	UA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	UB	363/376 (96%)	362 (100%)	1 (0%)	91	94
54	UE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	UG	365/376 (97%)	365 (100%)	0	100	100
54	UI	365/376 (97%)	365 (100%)	0	100	100
54	UK	365/376 (97%)	365 (100%)	0	100	100
54	VA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	VB	365/376 (97%)	365 (100%)	0	100	100
54	VE	365/376 (97%)	365 (100%)	0	100	100
54	VG	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	VI	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	VK	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	WA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	WB	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	WE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	WG	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	WI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	WK	365/376 (97%)	364 (100%)	1 (0%)	91	94
55	AC	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	AD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	AF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	AH	369/381 (97%)	369 (100%)	0	100	100
55	AJ	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	AL	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	BC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	BD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	BF	369/381 (97%)	366 (99%)	3 (1%)	79	87
55	BH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	BJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	BL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	CC	369/381 (97%)	369 (100%)	0	100	100
55	CD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	CF	369/381 (97%)	369 (100%)	0	100	100
55	CH	369/381 (97%)	369 (100%)	0	100	100
55	CJ	369/381 (97%)	369 (100%)	0	100	100
55	CL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	DC	369/381 (97%)	369 (100%)	0	100	100
55	DD	369/381 (97%)	369 (100%)	0	100	100
55	DF	369/381 (97%)	369 (100%)	0	100	100
55	DH	369/381 (97%)	369 (100%)	0	100	100
55	DJ	369/381 (97%)	368 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	DL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	EB	369/381 (97%)	369 (100%)	0	100	100
55	ED	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	EF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	EH	369/381 (97%)	369 (100%)	0	100	100
55	EJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	EL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	EM	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	FC	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	FD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	FF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	FH	369/381 (97%)	369 (100%)	0	100	100
55	FJ	369/381 (97%)	369 (100%)	0	100	100
55	FL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	FM	369/381 (97%)	369 (100%)	0	100	100
55	GC	369/381 (97%)	369 (100%)	0	100	100
55	GD	369/381 (97%)	369 (100%)	0	100	100
55	GF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	GH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	GJ	369/381 (97%)	369 (100%)	0	100	100
55	GL	369/381 (97%)	369 (100%)	0	100	100
55	GM	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	HC	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	HD	369/381 (97%)	366 (99%)	3 (1%)	79	87
55	HF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	HH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	HJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	HL	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	HM	369/381 (97%)	369 (100%)	0	100	100
55	IC	369/381 (97%)	369 (100%)	0	100	100
55	ID	369/381 (97%)	368 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	IF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	IH	369/381 (97%)	369 (100%)	0	100	100
55	IJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	IL	369/381 (97%)	369 (100%)	0	100	100
55	JC	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	JD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	JF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	JH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	JJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	JL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	JM	369/381 (97%)	369 (100%)	0	100	100
55	KC	369/381 (97%)	369 (100%)	0	100	100
55	KD	369/381 (97%)	369 (100%)	0	100	100
55	KF	369/381 (97%)	369 (100%)	0	100	100
55	KH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	KJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	KL	369/381 (97%)	369 (100%)	0	100	100
55	KM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	LC	369/381 (97%)	369 (100%)	0	100	100
55	LD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	LF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	LH	369/381 (97%)	369 (100%)	0	100	100
55	LJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	LL	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	LM	369/381 (97%)	369 (100%)	0	100	100
55	MC	369/381 (97%)	369 (100%)	0	100	100
55	MD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	MF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	MH	369/381 (97%)	369 (100%)	0	100	100
55	MJ	369/381 (97%)	369 (100%)	0	100	100
55	MM	369/381 (97%)	368 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	NC	369/381 (97%)	366 (99%)	3 (1%)	79	87
55	ND	369/381 (97%)	369 (100%)	0	100	100
55	NF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	NH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	NJ	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	NK	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	NM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	OC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	OD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	OF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	OH	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	OJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	OM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	PC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	PD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	PF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	PH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	PJ	369/381 (97%)	369 (100%)	0	100	100
55	PM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	QC	369/381 (97%)	366 (99%)	3 (1%)	79	87
55	QD	369/381 (97%)	369 (100%)	0	100	100
55	QF	369/381 (97%)	369 (100%)	0	100	100
55	QH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	QJ	369/381 (97%)	369 (100%)	0	100	100
55	QM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	RC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	RD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	RF	369/381 (97%)	369 (100%)	0	100	100
55	RH	369/381 (97%)	369 (100%)	0	100	100
55	RJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	RM	369/381 (97%)	368 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	SC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	SD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	SF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	SH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	SJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	SL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	SM	369/381 (97%)	369 (100%)	0	100	100
55	TC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	TD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	TF	369/381 (97%)	369 (100%)	0	100	100
55	TH	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	TJ	369/381 (97%)	369 (100%)	0	100	100
55	TL	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	TM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	UC	369/381 (97%)	366 (99%)	3 (1%)	79	87
55	UD	369/381 (97%)	369 (100%)	0	100	100
55	UF	369/381 (97%)	369 (100%)	0	100	100
55	UH	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	UJ	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	UL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	UM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	VC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	VD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	VF	369/381 (97%)	369 (100%)	0	100	100
55	VH	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	VJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	VL	369/381 (97%)	369 (100%)	0	100	100
55	VM	369/381 (97%)	369 (100%)	0	100	100
55	WC	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	WD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	WF	369/381 (97%)	368 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	WH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	WJ	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	WL	369/381 (97%)	368 (100%)	1 (0%)	91	94
All	All	136639/159445 (86%)	136150 (100%)	489 (0%)	88	93

All (489) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1E	301	ARG
2	1F	73	ARG
2	1G	147	HIS
2	1H	388	ARG
2	1H	442	ARG
3	1L	136	ARG
4	1Q	197	ARG
5	1T	405	ARG
8	1d	311	LYS
8	1d	324	ARG
11	1m	155	ASN
12	1q	118	GLN
3	1x	607	ARG
3	1z	443	LYS
13	2B	94	ARG
13	2B	249	LYS
17	2S	357	GLN
18	2V	136	GLN
19	3B	170	ARG
19	3G	124	ARG
20	3J	151	ARG
20	3J	200	ARG
20	3J	201	LYS
20	3J	202	THR
20	3J	212	VAL
20	3J	213	ASP
20	3J	215	GLU
20	3J	514	LYS
20	3K	38	ASN
21	3N	383	ARG
21	3N	400	ARG
21	3N	413	ARG
21	3O	107	LYS

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Mol	Chain	Res	Type
21	3O	109	ARG
21	3O	110	GLU
21	3O	111	GLU
21	3O	112	LYS
21	3O	113	GLU
22	3R	51	ASN
23	3W	150	ARG
23	3W	151	GLN
23	3W	152	LYS
23	3W	153	ASN
23	3W	365	ARG
23	3X	374	LYS
23	3X	534	ARG
23	3Z	178	GLN
24	4B	26	MET
24	4B	462	ARG
24	4C	349	ASN
26	4J	146	LYS
27	4Q	159	LYS
28	4U	63	ARG
30	5B	115	LYS
30	5B	224	MET
7	5I	2	ASN
7	5K	73	ARG
7	5L	202	ASN
31	6A	13	ARG
31	6B	27	LYS
31	6E	194	GLN
32	6I	67	LYS
35	6U	232	ARG
35	6V	233	ARG
35	6V	293	ARG
36	7A	532	LYS
36	7A	611	LYS
36	7B	210	ARG
36	7B	385	ARG
36	7C	9	ASN
36	7C	279	ARG
37	7G	375	MET
37	7H	17	ARG
37	7H	72	LYS
37	7H	375	MET

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Mol	Chain	Res	Type
37	7I	211	LYS
37	7I	576	ASN
37	7I	640	LYS
38	7M	131	ARG
40	7U	109	ARG
40	7V	65	ARG
42	8A	26	ARG
43	8F	436	ASN
45	8R	189	ARG
45	8R	398	ASN
45	8S	189	ARG
45	8T	277	LYS
46	8Z	101	LYS
49	9G	96	ASN
30	9Y	155	ARG
30	9Y	224	MET
55	AC	2	ARG
55	AC	347	ASN
55	AD	2	ARG
54	AE	84	ARG
55	AF	298	ASN
55	AJ	262	ARG
55	AJ	306	ARG
54	AK	2	ARG
54	AK	308	ARG
55	AL	298	ASN
55	AL	306	ARG
54	AM	308	ARG
54	BA	2	ARG
54	BA	339	ARG
55	BC	306	ARG
55	BD	2	ARG
55	BD	347	ASN
54	BE	2	ARG
54	BE	373	ARG
55	BF	1	MET
55	BF	2	ARG
55	BF	174	LYS
54	BG	2	ARG
54	BG	243	ARG
55	BH	306	ARG
55	BJ	2	ARG

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Mol	Chain	Res	Type
54	BK	243	ARG
55	BL	247	ASN
54	BM	2	ARG
54	BM	258	ASN
55	CD	2	ARG
54	CE	215	ARG
54	CE	339	ARG
54	CG	300	ASN
54	CG	309	HIS
55	CL	195	ASN
54	CM	2	ARG
54	DB	101	ASN
54	DB	373	ARG
54	DE	101	ASN
54	DE	128	GLN
54	DG	233	GLN
54	DG	300	ASN
54	DI	40	LYS
55	DJ	298	ASN
54	DK	339	ARG
55	DL	190	HIS
54	EA	244	PHE
54	EA	245	ASP
54	EA	248	LEU
54	EA	249	ASN
54	EA	250	VAL
54	EA	256	GLN
54	EA	258	ASN
54	EA	260	VAL
54	EA	264	ARG
54	EA	269	LEU
54	EA	272	TYR
54	EA	277	SER
54	EA	279	GLU
54	EA	280	LYS
54	EA	286	LEU
54	EA	287	SER
54	EA	302	MET
54	EA	306	ASP
54	EA	311	LYS
54	EA	317	MET
54	EA	320	ARG

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Mol	Chain	Res	Type
54	EA	322	ASP
54	EA	324	VAL
54	EA	326	LYS
54	EA	329	ASN
54	EA	334	THR
54	EA	335	ILE
54	EA	339	ARG
54	EA	340	THR
54	EA	344	VAL
54	EA	349	THR
54	EA	355	ILE
54	EA	358	GLN
55	ED	334	GLN
55	EF	336	LYS
55	EJ	306	ARG
54	EK	2	ARG
54	EK	35	GLN
55	EL	324	LYS
55	EM	247	ASN
55	EM	306	ARG
54	FA	128	GLN
54	FA	243	ARG
54	FA	248	LEU
54	FA	250	VAL
54	FA	251	ASP
54	FA	253	THR
54	FA	264	ARG
54	FA	265	ILE
54	FA	269	LEU
54	FA	275	VAL
54	FA	276	ILE
54	FA	280	LYS
54	FA	282	TYR
54	FA	283	HIS
54	FA	284	GLU
54	FA	286	LEU
54	FA	291	ILE
54	FA	295	CYS
54	FA	303	VAL
54	FA	306	ASP
54	FA	311	LYS
54	FA	317	MET

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Mol	Chain	Res	Type
54	FA	318	LEU
54	FA	322	ASP
54	FA	323	VAL
54	FA	326	LYS
54	FA	327	ASP
54	FA	334	THR
54	FA	336	LYS
54	FA	338	LYS
54	FA	339	ARG
54	FA	342	GLN
54	FA	344	VAL
54	FA	345	ASP
54	FA	351	PHE
54	FA	353	VAL
55	FC	195	ASN
55	FC	247	ASN
55	FD	1	MET
55	FD	2	ARG
54	FE	2	ARG
54	FE	112	LYS
54	FE	236	SER
54	FE	237	SER
54	FE	241	SER
54	FE	242	LEU
54	FE	244	PHE
54	FE	249	ASN
54	FE	251	ASP
54	FE	252	LEU
54	FE	255	PHE
54	FE	256	GLN
54	FE	257	THR
54	FE	264	ARG
54	FE	265	ILE
54	FE	269	LEU
54	FE	271	THR
54	FE	275	VAL
54	FE	276	ILE
54	FE	280	LYS
54	FE	283	HIS
54	FE	285	GLN
54	FE	300	ASN
54	FE	302	MET

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Mol	Chain	Res	Type
54	FE	311	LYS
54	FE	313	MET
54	FE	320	ARG
54	FE	324	VAL
54	FE	326	LYS
54	FE	327	ASP
54	FE	328	VAL
54	FE	332	ILE
54	FE	334	THR
54	FE	336	LYS
54	FE	338	LYS
54	FE	339	ARG
54	FE	340	THR
54	FE	341	ILE
54	FE	342	GLN
54	FE	344	VAL
54	FE	351	PHE
54	FE	352	LYS
54	FE	361	THR
55	FF	2	ARG
54	FG	326	LYS
54	FI	251	ASP
54	FI	255	PHE
54	FI	256	GLN
54	FI	264	ARG
54	FI	265	ILE
54	FI	266	HIS
54	FI	272	TYR
54	FI	276	ILE
54	FI	280	LYS
54	FI	284	GLU
54	FI	285	GLN
54	FI	291	ILE
54	FI	293	ASN
54	FI	297	GLU
54	FI	300	ASN
54	FI	302	MET
54	FI	311	LYS
54	FI	313	MET
54	FI	319	TYR
54	FI	324	VAL
54	FI	327	ASP

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Mol	Chain	Res	Type
54	FI	334	THR
54	FI	338	LYS
54	FI	340	THR
54	FI	341	ILE
54	FI	362	VAL
55	FL	406	MET
54	GA	18	ASN
54	GE	2	ARG
55	GF	122	LYS
54	GG	2	ARG
55	GH	204	ASN
54	GI	2	ARG
55	GM	2	ARG
55	GM	347	ASN
55	HC	2	ARG
55	HC	306	ARG
55	HD	2	ARG
55	HD	100	ASN
55	HD	204	ASN
54	HE	133	GLN
55	HF	306	ARG
54	HG	2	ARG
54	HG	50	ASN
54	HG	221	ARG
55	HH	2	ARG
55	HJ	306	ARG
54	HK	308	ARG
55	HL	2	ARG
55	HL	190	HIS
54	IA	2	ARG
55	ID	2	ARG
55	IF	121	ARG
55	IJ	121	ARG
54	IK	133	GLN
54	IM	18	ASN
54	IM	243	ARG
54	IM	308	ARG
54	JB	2	ARG
55	JC	2	ARG
55	JC	347	ASN
55	JD	162	ARG
55	JD	204	ASN

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Mol	Chain	Res	Type
55	JF	121	ARG
54	JG	308	ARG
55	JH	347	ASN
54	JI	50	ASN
55	JJ	347	ASN
55	JL	324	LYS
54	KA	2	ARG
54	KB	2	ARG
54	KB	221	ARG
54	KG	2	ARG
54	KG	373	ARG
55	KH	2	ARG
54	KI	2	ARG
55	KJ	2	ARG
54	KK	308	ARG
55	KM	347	ASN
54	LA	2	ARG
54	LA	79	ARG
54	LB	308	ARG
55	LD	306	ARG
54	LE	308	ARG
54	LE	373	ARG
55	LF	347	ASN
54	LG	308	ARG
54	LI	326	LYS
54	LI	422	ARG
55	LJ	291	GLN
55	LL	298	ASN
55	LL	306	ARG
54	MA	326	LYS
54	MB	112	LYS
55	MD	347	ASN
54	ME	2	ARG
54	ME	308	ARG
55	MF	336	LYS
54	MG	2	ARG
54	MI	2	ARG
54	MK	243	ARG
54	MK	373	ARG
54	ML	221	ARG
55	MM	321	MET
54	NB	356	ASN

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Mol	Chain	Res	Type
55	NC	83	GLN
55	NC	307	HIS
55	NC	347	ASN
55	NF	2	ARG
55	NH	306	ARG
54	NI	40	LYS
55	NJ	282	ARG
55	NJ	321	MET
55	NK	195	ASN
55	NK	347	ASN
55	NM	282	ARG
54	OB	308	ARG
54	OB	370	LYS
55	OC	329	GLN
55	OD	347	ASN
54	OE	2	ARG
55	OF	190	HIS
54	OG	18	ASN
54	OG	221	ARG
55	OH	204	ASN
55	OH	347	ASN
54	OI	372	GLN
55	OJ	2	ARG
54	OL	2	ARG
55	OM	2	ARG
54	PA	326	LYS
55	PC	347	ASN
55	PD	347	ASN
55	PF	195	ASN
54	PG	2	ARG
55	PH	2	ARG
54	PK	285	GLN
55	PM	2	ARG
54	QA	2	ARG
55	QC	2	ARG
55	QC	337	ASN
55	QC	347	ASN
54	QE	102	ASN
54	QG	2	ARG
54	QG	40	LYS
54	QG	339	ARG
54	QG	373	ARG

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Mol	Chain	Res	Type
55	QH	195	ASN
54	QI	2	ARG
54	QI	84	ARG
54	QK	258	ASN
54	QL	2	ARG
55	QM	2	ARG
54	RB	79	ARG
55	RC	337	ASN
55	RD	121	ARG
55	RD	390	ARG
54	RE	40	LYS
54	RE	308	ARG
54	RI	339	ARG
55	RJ	2	ARG
54	RK	2	ARG
55	RM	337	ASN
55	SC	2	ARG
55	SD	279	GLN
55	SD	347	ASN
55	SF	282	ARG
55	SH	347	ASN
54	SI	112	LYS
55	SJ	2	ARG
55	SL	362	LYS
54	TA	358	GLN
54	TB	2	ARG
54	TB	326	LYS
55	TC	2	ARG
55	TD	2	ARG
55	TD	227	HIS
54	TE	2	ARG
54	TG	2	ARG
55	TH	2	ARG
55	TH	324	LYS
54	TK	163	LYS
55	TL	121	ARG
55	TL	362	LYS
55	TM	103	LYS
54	UA	401	LYS
54	UB	308	ARG
55	UC	2	ARG
55	UC	174	LYS

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Mol	Chain	Res	Type
55	UC	347	ASN
54	UE	18	ASN
54	UE	215	ARG
55	UH	2	ARG
55	UH	318	ARG
55	UJ	131	GLN
55	UJ	306	ARG
55	UL	324	LYS
55	UM	2	ARG
54	VA	373	ARG
55	VC	2	ARG
55	VD	2	ARG
55	VD	190	HIS
55	VH	190	HIS
55	VH	306	ARG
54	VI	221	ARG
54	VI	373	ARG
55	VJ	213	ARG
54	VK	206	ASN
54	VK	300	ASN
54	WA	308	ARG
54	WB	308	ARG
55	WC	298	ASN
55	WC	306	ARG
55	WD	298	ASN
54	WE	163	LYS
54	WE	308	ARG
55	WF	306	ARG
54	WG	2	ARG
54	WG	308	ARG
55	WH	2	ARG
54	WI	308	ARG
55	WJ	306	ARG
55	WJ	347	ASN
54	WK	308	ARG
55	WL	306	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (400) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	14	GLN
1	1B	180	GLN

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Mol	Chain	Res	Type
2	1E	296	GLN
3	1M	139	GLN
5	1T	398	HIS
5	1T	416	ASN
5	1T	422	ASN
5	1V	230	GLN
11	1m	155	ASN
12	1r	3	GLN
3	1y	478	GLN
13	2A	72	GLN
13	2A	250	HIS
14	2G	28	ASN
15	2K	9	GLN
15	2K	12	GLN
15	2L	9	GLN
18	2V	206	GLN
19	3A	131	GLN
19	3B	159	ASN
19	3C	109	GLN
19	3F	131	GLN
20	3J	205	ASN
20	3J	207	HIS
21	3N	322	GLN
21	3O	143	GLN
23	3W	151	GLN
23	3W	153	ASN
23	3W	388	ASN
23	3W	448	GLN
23	3X	432	GLN
23	3Z	178	GLN
24	4C	349	ASN
25	4F	454	GLN
26	4K	355	HIS
27	4N	168	ASN
27	4O	80	ASN
7	5E	39	ASN
7	5F	248	GLN
7	5H	240	GLN
7	5K	45	GLN
7	5N	136	ASN
31	6C	194	GLN
31	6E	171	GLN

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Mol	Chain	Res	Type
34	6Q	51	GLN
36	7B	555	GLN
36	7B	556	HIS
36	7D	171	GLN
36	7D	555	GLN
36	7D	556	HIS
37	7G	261	GLN
37	7G	353	GLN
37	7I	261	GLN
39	7Q	148	GLN
43	8F	400	GLN
43	8F	436	ASN
43	8G	178	GLN
44	8M	207	ASN
45	8R	398	ASN
45	8S	389	GLN
47	9A	201	ASN
54	AA	11	GLN
55	AC	8	GLN
55	AC	134	GLN
55	AD	37	HIS
55	AD	347	ASN
54	AE	101	ASN
54	AE	206	ASN
55	AF	256	ASN
55	AF	298	ASN
55	AF	334	GLN
54	AG	11	GLN
55	AH	6	HIS
55	AH	134	GLN
55	AH	190	HIS
55	AH	347	ASN
55	AL	334	GLN
54	AM	35	GLN
55	BC	131	GLN
54	BG	91	GLN
54	BG	285	GLN
54	BI	8	HIS
55	BJ	6	HIS
55	BJ	134	GLN
54	BM	329	ASN
54	CB	85	GLN

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Mol	Chain	Res	Type
54	CB	128	GLN
55	CC	165	ASN
55	CD	347	ASN
55	CF	134	GLN
54	CG	285	GLN
55	CH	204	ASN
55	CJ	8	GLN
55	CL	14	ASN
55	CL	134	GLN
55	DC	14	ASN
55	DC	165	ASN
55	DD	134	GLN
55	DD	256	ASN
54	DE	128	GLN
54	DI	11	GLN
55	DJ	11	GLN
55	DJ	14	ASN
55	DL	14	ASN
55	DL	204	ASN
54	DM	101	ASN
54	EA	249	ASN
54	EA	372	GLN
54	EE	256	GLN
55	EF	6	HIS
55	EF	134	GLN
55	EF	195	ASN
54	EG	91	GLN
54	EG	101	ASN
54	EI	35	GLN
55	EJ	8	GLN
55	EJ	14	ASN
54	FA	309	HIS
54	FA	329	ASN
54	FB	258	ASN
54	FE	249	ASN
54	FE	256	GLN
54	FE	293	ASN
54	FE	329	ASN
55	FF	375	GLN
55	FF	426	GLN
54	FG	293	ASN
54	FI	11	GLN

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Mol	Chain	Res	Type
54	FI	28	HIS
54	FI	206	ASN
54	FI	266	HIS
54	FI	285	GLN
54	FI	300	ASN
54	FI	309	HIS
54	FI	356	ASN
55	FJ	94	GLN
55	FJ	334	GLN
55	FJ	347	ASN
55	FJ	348	ASN
55	FL	8	GLN
55	FL	99	ASN
55	FL	137	HIS
55	FL	375	GLN
55	FL	423	GLN
55	FL	426	GLN
55	FM	6	HIS
55	FM	134	GLN
54	GA	8	HIS
54	GA	18	ASN
54	GA	258	ASN
55	GC	48	ASN
55	GC	256	ASN
55	GD	334	GLN
55	GF	14	ASN
55	GF	99	ASN
55	GF	256	ASN
55	GH	99	ASN
55	GJ	204	ASN
54	GK	101	ASN
55	GL	134	GLN
55	GM	15	GLN
55	GM	204	ASN
55	GM	348	ASN
54	HB	11	GLN
55	HD	100	ASN
54	HE	128	GLN
54	HE	283	HIS
55	HF	298	ASN
54	HI	101	ASN
55	HL	375	GLN

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Mol	Chain	Res	Type
55	HL	423	GLN
55	HL	426	GLN
55	HM	292	GLN
55	HM	298	ASN
54	IA	258	ASN
54	IA	329	ASN
54	IB	11	GLN
54	IB	285	GLN
55	IC	99	ASN
55	IC	337	ASN
55	ID	298	ASN
55	IJ	100	ASN
54	IK	133	GLN
55	IL	165	ASN
55	IL	329	GLN
54	IM	88	HIS
54	IM	356	ASN
54	JA	101	ASN
54	JA	128	GLN
54	JA	206	ASN
54	JA	329	ASN
54	JB	11	GLN
54	JB	101	ASN
54	JB	206	ASN
54	JB	356	ASN
55	JD	334	GLN
54	JE	11	GLN
54	JE	15	GLN
55	JF	14	ASN
55	JF	247	ASN
54	JG	11	GLN
55	JH	99	ASN
55	JH	298	ASN
55	JL	137	HIS
55	JL	226	ASN
55	JM	6	HIS
55	JM	134	GLN
55	JM	204	ASN
55	JM	256	ASN
54	KA	50	ASN
54	KA	285	GLN
54	KB	101	ASN

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Mol	Chain	Res	Type
55	KD	334	GLN
54	KG	206	ASN
55	KJ	100	ASN
55	KL	131	GLN
55	KM	184	ASN
54	LB	101	ASN
55	LC	134	GLN
55	LD	334	GLN
54	LG	35	GLN
55	LH	347	ASN
54	LI	35	GLN
54	LI	226	ASN
55	LJ	8	GLN
55	LJ	134	GLN
55	LJ	414	ASN
54	LK	197	HIS
54	MA	91	GLN
54	MB	206	ASN
55	MC	204	ASN
55	MF	190	HIS
55	MF	334	GLN
55	MJ	8	GLN
55	MJ	134	GLN
55	MJ	256	ASN
55	MJ	347	ASN
54	MK	101	ASN
54	MK	329	ASN
55	MM	337	ASN
54	NA	258	ASN
54	NB	128	GLN
55	NC	6	HIS
55	NC	347	ASN
55	ND	94	GLN
55	ND	256	ASN
54	NE	101	ASN
54	NE	176	GLN
55	NF	334	GLN
55	NH	6	HIS
55	NH	134	GLN
55	NH	298	ASN
55	NH	334	GLN
54	NI	356	ASN

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Mol	Chain	Res	Type
55	NJ	165	ASN
55	NK	334	GLN
54	NL	101	ASN
54	OA	11	GLN
55	OC	329	GLN
55	OD	337	ASN
55	OD	347	ASN
54	OE	258	ASN
55	OF	99	ASN
55	OF	256	ASN
54	OG	206	ASN
55	OH	8	GLN
55	OH	204	ASN
55	OH	256	ASN
55	OJ	99	ASN
55	OJ	347	ASN
54	OK	356	ASN
55	OM	375	GLN
55	OM	426	GLN
55	PC	347	ASN
55	PD	89	ASN
55	PD	131	GLN
55	PD	256	ASN
54	PE	101	ASN
54	PE	197	HIS
55	PH	99	ASN
54	PK	101	ASN
54	PK	300	ASN
55	PM	14	ASN
55	PM	131	GLN
55	PM	134	GLN
55	PM	334	GLN
54	QA	128	GLN
55	QD	11	GLN
54	QE	11	GLN
54	QE	102	ASN
54	QE	258	ASN
55	QF	100	ASN
55	QF	347	ASN
54	QG	372	GLN
55	QH	337	ASN
54	QI	133	GLN

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Mol	Chain	Res	Type
55	QJ	191	GLN
55	QJ	298	ASN
55	QJ	334	GLN
55	QJ	347	ASN
54	QK	128	GLN
54	QK	133	GLN
55	QM	11	GLN
54	RA	11	GLN
54	RA	139	HIS
55	RC	256	ASN
55	RC	334	GLN
55	RC	426	GLN
55	RD	131	GLN
55	RD	396	HIS
54	RE	15	GLN
54	RE	356	ASN
55	RF	94	GLN
55	RF	334	GLN
55	RH	37	HIS
55	RH	256	ASN
54	RI	101	ASN
55	RJ	100	ASN
55	RJ	227	HIS
55	RJ	334	GLN
54	RL	28	HIS
55	RM	99	ASN
55	RM	247	ASN
54	SA	35	GLN
54	SB	11	GLN
55	SC	426	GLN
55	SD	184	ASN
55	SD	256	ASN
54	SE	101	ASN
54	SE	102	ASN
55	SF	256	ASN
55	SF	291	GLN
54	SG	11	GLN
54	SG	256	GLN
54	SG	293	ASN
55	SH	347	ASN
54	SI	11	GLN
55	SJ	298	ASN

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Mol	Chain	Res	Type
55	SJ	334	GLN
54	SK	258	ASN
55	SL	8	GLN
55	SL	204	ASN
55	SL	292	GLN
55	SL	298	ASN
54	TA	139	HIS
54	TA	226	ASN
54	TA	293	ASN
54	TB	226	ASN
54	TB	258	ASN
55	TC	292	GLN
55	TC	334	GLN
55	TD	334	GLN
54	TE	206	ASN
55	TH	8	GLN
55	TH	256	ASN
55	TH	334	GLN
54	TI	35	GLN
55	TJ	99	ASN
54	TK	8	HIS
54	TK	139	HIS
54	TK	293	ASN
55	TL	396	HIS
55	TM	256	ASN
55	TM	416	ASN
54	UA	8	HIS
54	UA	372	GLN
55	UC	334	GLN
55	UD	416	ASN
54	UE	8	HIS
54	UE	128	GLN
54	UG	293	ASN
55	UH	14	ASN
54	UI	372	GLN
55	UJ	279	GLN
55	UJ	416	ASN
55	UM	329	GLN
54	VA	256	GLN
55	VC	134	GLN
55	VD	337	ASN
54	VE	101	ASN

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Mol	Chain	Res	Type
54	VG	28	HIS
54	VG	101	ASN
55	VH	347	ASN
54	VK	101	ASN
55	VL	134	GLN
55	VL	226	ASN
55	VM	279	GLN
54	WA	285	GLN
55	WD	8	GLN
55	WD	165	ASN
54	WG	15	GLN
55	WH	94	GLN
55	WH	334	GLN
55	WH	426	GLN
54	WI	102	ASN
55	WJ	256	ASN
54	WK	206	ASN
54	WK	285	GLN
55	WL	8	GLN
55	WL	14	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 446 ligands modelled in this entry, 148 are monoatomic - leaving 298 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	$\#\|Z\| > 2$
56	GTP	IB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	5 (14%)
56	GTP	PE	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	3 (8%)
56	GTP	KB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	LB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	OM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	3 (10%)
58	GDP	PH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	FG	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.31	4 (11%)
58	GDP	AL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	WB	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	3 (8%)
58	GDP	JC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.10	3 (10%)
58	GDP	EB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	GJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
56	GTP	NA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	QH	501	-	25,30,30	1.03	1 (4%)	30,47,47	1.05	2 (6%)
56	GTP	IK	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	SM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	OI	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.25	4 (11%)
58	GDP	IF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	1 (3%)
56	GTP	BB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.25	3 (8%)
56	GTP	JI	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	JK	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	RI	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.31	5 (14%)
56	GTP	CG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
56	GTP	OG	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	GK	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	UB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	TF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	LF	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.11	2 (6%)
58	GDP	LL	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
56	GTP	UA	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	GC	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	TE	501	57	29,34,34	1.19	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
58	GDP	HL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	1 (3%)
56	GTP	DM	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	SC	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	3 (10%)
58	GDP	OF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	PL	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	DE	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	HC	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.06	2 (6%)
58	GDP	OD	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.19	3 (10%)
58	GDP	UL	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	3 (10%)
56	GTP	LK	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	UK	501	57	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	PG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	CH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
56	GTP	KA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	UI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.30	5 (14%)
58	GDP	HM	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	OH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	SH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	QG	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	WL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	DF	501	-	25,30,30	0.95	2 (8%)	30,47,47	1.00	1 (3%)
58	GDP	EF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
58	GDP	BH	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	TK	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.25	4 (11%)
58	GDP	CJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	KJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.11	2 (6%)
56	GTP	IE	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	DB	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	QA	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	TD	501	-	25,30,30	0.92	0	30,47,47	1.10	2 (6%)
58	GDP	FL	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	GI	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	3 (8%)
58	GDP	CL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	VF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	LC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
58	GDP	DH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	3 (10%)
58	GDP	VL	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.03	1 (3%)
56	GTP	BK	501	57	29,34,34	1.26	3 (10%)	35,54,54	1.31	6 (17%)
56	GTP	QK	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.31	4 (11%)
56	GTP	NB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	PC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	GH	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.16	3 (10%)
56	GTP	NG	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	CA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	3 (8%)
56	GTP	BI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	LA	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	TB	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	GD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	MF	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	1 (3%)
58	GDP	MM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	2 (6%)
58	GDP	NJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
58	GDP	NC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.14	2 (6%)
58	GDP	UD	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.21	3 (10%)
56	GTP	IA	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	DD	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.04	1 (3%)
56	GTP	GB	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	OJ	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	QM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
56	GTP	GE	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.26	4 (11%)
58	GDP	VM	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.13	2 (6%)
56	GTP	RG	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	QE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	CK	501	-	29,34,34	1.28	4 (13%)	35,54,54	1.27	5 (14%)
56	GTP	VA	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	JL	501	-	25,30,30	0.98	1 (4%)	30,47,47	0.98	1 (3%)
56	GTP	BE	501	57	29,34,34	1.17	2 (6%)	35,54,54	1.36	5 (14%)
58	GDP	GF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	CE	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	3 (8%)
56	GTP	HE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.32	4 (11%)
58	GDP	MC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	GTP	OE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	ED	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.15	2 (6%)
56	GTP	EK	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	ML	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	5 (14%)
56	GTP	NE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	JM	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	BJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	CD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	GG	501	57	29,34,34	1.19	2 (6%)	35,54,54	1.29	3 (8%)
56	GTP	VB	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	QB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	4 (11%)
56	GTP	WI	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	RM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.18	3 (10%)
56	GTP	FB	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.32	4 (11%)
56	GTP	RK	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	EA	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.35	5 (14%)
56	GTP	TI	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.23	4 (11%)
58	GDP	BF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
58	GDP	IH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	AD	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.10	3 (10%)
58	GDP	CF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	ND	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
56	GTP	WG	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.30	5 (14%)
56	GTP	RL	501	57	29,34,34	1.26	3 (10%)	35,54,54	1.33	5 (14%)
58	GDP	AF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
58	GDP	IJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	QF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	3 (10%)
58	GDP	RD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	RC	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
56	GTP	AG	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.25	4 (11%)
56	GTP	AM	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
58	GDP	KH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	MJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	SI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
56	GTP	SA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
56	GTP	FE	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	WA	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	5 (14%)
58	GDP	NH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	3 (10%)
56	GTP	RE	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	CI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	JB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	OA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	AC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	FJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	IL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	DG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
56	GTP	MA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.33	5 (14%)
58	GDP	MH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	EI	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	PI	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	PK	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	FC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
58	GDP	HF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	RF	501	-	25,30,30	0.92	1 (4%)	30,47,47	1.04	1 (3%)
56	GTP	SB	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	JH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.05	2 (6%)
56	GTP	JE	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	KE	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	5 (14%)
56	GTP	VE	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	HG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	PJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	TM	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.11	2 (6%)
56	GTP	AI	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.31	5 (14%)
56	GTP	IM	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	HK	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	DJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.19	3 (10%)
58	GDP	KM	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	SK	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	DL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	1 (3%)
56	GTP	DA	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.27	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	GTP	IG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	VI	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	VK	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	VJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
56	GTP	JA	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	WJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
56	GTP	AA	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	UH	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.05	2 (6%)
58	GDP	KC	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	VH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.18	3 (10%)
58	GDP	NF	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.10	2 (6%)
58	GDP	TC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	HI	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	KL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	JG	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	NL	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	EJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	BA	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	LE	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.31	3 (8%)
58	GDP	CC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	TL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	AB	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	LM	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	LI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	HB	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	LD	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	QC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	SJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	PD	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.12	2 (6%)
58	GDP	TH	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.12	2 (6%)
56	GTP	FA	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	PM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	HD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	VG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	5 (14%)
58	GDP	JD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	GDP	JF	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	3 (10%)
58	GDP	DC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	KI	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	BL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	BG	501	57	29,34,34	1.28	3 (10%)	35,54,54	1.32	5 (14%)
56	GTP	BM	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.30	5 (14%)
56	GTP	WE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
58	GDP	NM	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	AK	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
58	GDP	FD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	MI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.25	3 (8%)
56	GTP	EG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	AH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
58	GDP	QD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	2 (6%)
58	GDP	SF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.16	3 (10%)
56	GTP	II	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	TA	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	OB	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	QI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	5 (14%)
56	GTP	ME	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	UC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
58	GDP	BD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.11	3 (10%)
56	GTP	PB	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	3 (8%)
56	GTP	MK	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	3 (8%)
56	GTP	SE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	MG	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	EH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	3 (10%)
58	GDP	AJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
58	GDP	WF	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	KK	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	FM	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.13	2 (6%)
58	GDP	RJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	EM	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	KD	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	UF	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	GTP	RA	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	SL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	VD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.17	4 (13%)
56	GTP	PA	501	57	29,34,34	1.27	2 (6%)	35,54,54	1.30	5 (14%)
58	GDP	WC	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	DK	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.32	5 (14%)
56	GTP	UE	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.32	4 (11%)
58	GDP	WD	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.13	3 (10%)
56	GTP	NI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	UJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
58	GDP	VC	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	HH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
56	GTP	CB	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.31	4 (11%)
56	GTP	SG	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	UM	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.14	3 (10%)
58	GDP	FF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.12	2 (6%)
56	GTP	CM	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.26	4 (11%)
58	GDP	IC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.15	3 (10%)
56	GTP	WK	501	57	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	OC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	EE	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	OK	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	LG	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	5 (14%)
58	GDP	ID	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	KG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	4 (11%)
56	GTP	OL	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	EL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	2 (6%)
58	GDP	BC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	FI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.33	4 (11%)
58	GDP	GL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	2 (6%)
56	GTP	HA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	UG	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	KF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	NK	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	TJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	GTP	EC	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	GM	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	AE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	HJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	MB	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.31	4 (11%)
56	GTP	GA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.25	3 (8%)
58	GDP	LJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	PF	501	-	25,30,30	0.86	0	30,47,47	1.51	5 (16%)
56	GTP	QL	501	57	29,34,34	1.28	5 (17%)	35,54,54	1.31	4 (11%)
56	GTP	RB	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	RH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	3 (10%)
56	GTP	FK	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	SD	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	1 (3%)
58	GDP	QJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.05	3 (10%)
56	GTP	DI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	3 (8%)
58	GDP	WH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
58	GDP	MD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	LH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	TG	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	JJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
58	GDP	FH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	2 (6%)

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
56	GTP	IB	501	57	-	5/18/38/38	0/3/3/3
56	GTP	PE	501	57	-	3/18/38/38	0/3/3/3
56	GTP	KB	501	57	-	2/18/38/38	0/3/3/3
56	GTP	LB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	OM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	PH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	FG	501	57	-	5/18/38/38	0/3/3/3
58	GDP	AL	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	WB	501	57	-	7/18/38/38	0/3/3/3
58	GDP	JC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	EB	501	-	-	1/12/32/32	0/3/3/3
58	GDP	GJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	NA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	QH	501	-	-	5/12/32/32	0/3/3/3
56	GTP	IK	501	57	-	4/18/38/38	0/3/3/3
58	GDP	SM	501	-	-	1/12/32/32	0/3/3/3
56	GTP	OI	501	57	-	4/18/38/38	0/3/3/3
58	GDP	IF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	BB	501	57	-	4/18/38/38	0/3/3/3
56	GTP	JI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	JK	501	57	-	8/18/38/38	0/3/3/3
56	GTP	RI	501	57	-	5/18/38/38	0/3/3/3
56	GTP	CG	501	57	-	4/18/38/38	0/3/3/3
56	GTP	OG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	GK	501	57	-	4/18/38/38	0/3/3/3
56	GTP	UB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	TF	501	-	-	1/12/32/32	0/3/3/3
58	GDP	LF	501	-	-	3/12/32/32	0/3/3/3
58	GDP	LL	501	-	-	1/12/32/32	0/3/3/3
56	GTP	UA	501	57	-	8/18/38/38	0/3/3/3
58	GDP	GC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	TE	501	57	-	4/18/38/38	0/3/3/3
58	GDP	HL	501	-	-	3/12/32/32	0/3/3/3
56	GTP	DM	501	57	-	3/18/38/38	0/3/3/3
58	GDP	SC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	OF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	PL	501	57	-	3/18/38/38	0/3/3/3
56	GTP	DE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	HC	501	-	-	5/12/32/32	0/3/3/3
58	GDP	OD	501	-	-	4/12/32/32	0/3/3/3
58	GDP	UL	501	-	-	3/12/32/32	0/3/3/3
56	GTP	LK	501	57	-	8/18/38/38	0/3/3/3
56	GTP	UK	501	57	-	9/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	PG	501	57	-	7/18/38/38	0/3/3/3
58	GDP	CH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	KA	501	57	-	2/18/38/38	0/3/3/3
56	GTP	UI	501	57	-	3/18/38/38	0/3/3/3
58	GDP	HM	501	-	-	1/12/32/32	0/3/3/3
58	GDP	OH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	SH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	QG	501	57	-	6/18/38/38	0/3/3/3
58	GDP	WL	501	-	-	1/12/32/32	0/3/3/3
58	GDP	DF	501	-	-	1/12/32/32	0/3/3/3
58	GDP	EF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	BH	501	-	-	1/12/32/32	0/3/3/3
56	GTP	TK	501	57	-	4/18/38/38	0/3/3/3
58	GDP	CJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	KJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	IE	501	57	-	6/18/38/38	0/3/3/3
56	GTP	DB	501	57	-	1/18/38/38	0/3/3/3
56	GTP	QA	501	57	-	6/18/38/38	0/3/3/3
58	GDP	TD	501	-	-	3/12/32/32	0/3/3/3
58	GDP	FL	501	-	-	2/12/32/32	0/3/3/3
56	GTP	GI	501	57	-	3/18/38/38	0/3/3/3
58	GDP	CL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	VF	501	-	-	1/12/32/32	0/3/3/3
58	GDP	LC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	DH	501	-	-	1/12/32/32	0/3/3/3
58	GDP	VL	501	-	-	5/12/32/32	0/3/3/3
56	GTP	BK	501	57	-	5/18/38/38	0/3/3/3
56	GTP	QK	501	57	-	3/18/38/38	0/3/3/3
56	GTP	NB	501	57	-	10/18/38/38	0/3/3/3
58	GDP	PC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	GH	501	-	-	1/12/32/32	0/3/3/3
56	GTP	NG	501	57	-	7/18/38/38	0/3/3/3
56	GTP	CA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	BI	501	57	-	7/18/38/38	0/3/3/3
56	GTP	LA	501	57	-	7/18/38/38	0/3/3/3
56	GTP	TB	501	57	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	GD	501	-	-	1/12/32/32	0/3/3/3
58	GDP	MF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	MM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	NJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	NC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	UD	501	-	-	3/12/32/32	0/3/3/3
56	GTP	IA	501	57	-	2/18/38/38	0/3/3/3
58	GDP	DD	501	-	-	3/12/32/32	0/3/3/3
56	GTP	GB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	OJ	501	-	-	1/12/32/32	0/3/3/3
58	GDP	QM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	GE	501	57	-	2/18/38/38	0/3/3/3
58	GDP	VM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	RG	501	57	-	2/18/38/38	0/3/3/3
56	GTP	QE	501	57	-	2/18/38/38	0/3/3/3
56	GTP	CK	501	-	-	7/18/38/38	0/3/3/3
56	GTP	VA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	JL	501	-	-	3/12/32/32	0/3/3/3
56	GTP	BE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	GF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	CE	501	57	-	3/18/38/38	0/3/3/3
56	GTP	HE	501	57	-	6/18/38/38	0/3/3/3
58	GDP	MC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	OE	501	57	-	7/18/38/38	0/3/3/3
58	GDP	ED	501	-	-	2/12/32/32	0/3/3/3
56	GTP	EK	501	57	-	2/18/38/38	0/3/3/3
56	GTP	ML	501	57	-	3/18/38/38	0/3/3/3
56	GTP	NE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	JM	501	-	-	1/12/32/32	0/3/3/3
58	GDP	BJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	CD	501	-	-	3/12/32/32	0/3/3/3
56	GTP	GG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	VB	501	57	-	6/18/38/38	0/3/3/3
56	GTP	QB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	WI	501	57	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	RM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	FB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	RK	501	57	-	3/18/38/38	0/3/3/3
56	GTP	EA	501	57	-	2/18/38/38	0/3/3/3
56	GTP	TI	501	57	-	7/18/38/38	0/3/3/3
58	GDP	BF	501	-	-	1/12/32/32	0/3/3/3
58	GDP	IH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	AD	501	-	-	5/12/32/32	0/3/3/3
58	GDP	CF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	ND	501	-	-	1/12/32/32	0/3/3/3
56	GTP	WG	501	57	-	2/18/38/38	0/3/3/3
56	GTP	RL	501	57	-	8/18/38/38	0/3/3/3
58	GDP	AF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	IJ	501	-	-	1/12/32/32	0/3/3/3
58	GDP	QF	501	-	-	4/12/32/32	0/3/3/3
58	GDP	RD	501	-	-	2/12/32/32	0/3/3/3
58	GDP	RC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	AG	501	57	-	4/18/38/38	0/3/3/3
56	GTP	AM	501	57	-	6/18/38/38	0/3/3/3
58	GDP	KH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	MJ	501	-	-	3/12/32/32	0/3/3/3
56	GTP	SI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	SA	501	57	-	4/18/38/38	0/3/3/3
56	GTP	FE	501	57	-	8/18/38/38	0/3/3/3
56	GTP	WA	501	57	-	1/18/38/38	0/3/3/3
58	GDP	NH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	RE	501	57	-	3/18/38/38	0/3/3/3
56	GTP	CI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	JB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	OA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	AC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	FJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	IL	501	-	-	2/12/32/32	0/3/3/3
56	GTP	DG	501	57	-	5/18/38/38	0/3/3/3
56	GTP	MA	501	57	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	MH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	EI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	PI	501	57	-	3/18/38/38	0/3/3/3
56	GTP	PK	501	57	-	1/18/38/38	0/3/3/3
58	GDP	FC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	HF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	RF	501	-	-	5/12/32/32	0/3/3/3
56	GTP	SB	501	57	-	1/18/38/38	0/3/3/3
58	GDP	JH	501	-	-	1/12/32/32	0/3/3/3
56	GTP	JE	501	57	-	3/18/38/38	0/3/3/3
56	GTP	KE	501	57	-	2/18/38/38	0/3/3/3
56	GTP	VE	501	57	-	4/18/38/38	0/3/3/3
56	GTP	HG	501	57	-	3/18/38/38	0/3/3/3
58	GDP	PJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	TM	501	-	-	1/12/32/32	0/3/3/3
56	GTP	AI	501	57	-	3/18/38/38	0/3/3/3
56	GTP	IM	501	57	-	7/18/38/38	0/3/3/3
56	GTP	HK	501	57	-	10/18/38/38	0/3/3/3
58	GDP	DJ	501	-	-	4/12/32/32	0/3/3/3
58	GDP	KM	501	-	-	1/12/32/32	0/3/3/3
56	GTP	SK	501	57	-	3/18/38/38	0/3/3/3
58	GDP	DL	501	-	-	1/12/32/32	0/3/3/3
56	GTP	DA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	IG	501	57	-	6/18/38/38	0/3/3/3
56	GTP	VI	501	57	-	3/18/38/38	0/3/3/3
56	GTP	VK	501	57	-	7/18/38/38	0/3/3/3
58	GDP	VJ	501	-	-	1/12/32/32	0/3/3/3
56	GTP	JA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	WJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	AA	501	57	-	7/18/38/38	0/3/3/3
58	GDP	UH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	KC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	VH	501	-	-	3/12/32/32	0/3/3/3
58	GDP	NF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	TC	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	HI	501	57	-	6/18/38/38	0/3/3/3
58	GDP	KL	501	-	-	2/12/32/32	0/3/3/3
56	GTP	JG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	NL	501	57	-	4/18/38/38	0/3/3/3
58	GDP	EJ	501	-	-	1/12/32/32	0/3/3/3
56	GTP	BA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	LE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	CC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	TL	501	-	-	2/12/32/32	0/3/3/3
56	GTP	AB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	LM	501	-	-	1/12/32/32	0/3/3/3
56	GTP	LI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	HB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	LD	501	-	-	2/12/32/32	0/3/3/3
58	GDP	QC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	SJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	PD	501	-	-	1/12/32/32	0/3/3/3
58	GDP	TH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	FA	501	57	-	4/18/38/38	0/3/3/3
58	GDP	PM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	HD	501	-	-	2/12/32/32	0/3/3/3
56	GTP	VG	501	57	-	4/18/38/38	0/3/3/3
58	GDP	JD	501	-	-	2/12/32/32	0/3/3/3
58	GDP	JF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	DC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	KI	501	57	-	1/18/38/38	0/3/3/3
58	GDP	BL	501	-	-	2/12/32/32	0/3/3/3
56	GTP	BG	501	57	-	8/18/38/38	0/3/3/3
56	GTP	BM	501	57	-	9/18/38/38	0/3/3/3
56	GTP	WE	501	57	-	4/18/38/38	0/3/3/3
58	GDP	NM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	AK	501	57	-	5/18/38/38	0/3/3/3
58	GDP	FD	501	-	-	1/12/32/32	0/3/3/3
56	GTP	MI	501	57	-	3/18/38/38	0/3/3/3
56	GTP	EG	501	57	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	AH	501	-	-	3/12/32/32	0/3/3/3
58	GDP	QD	501	-	-	1/12/32/32	0/3/3/3
58	GDP	SF	501	-	-	3/12/32/32	0/3/3/3
56	GTP	II	501	57	-	8/18/38/38	0/3/3/3
56	GTP	TA	501	57	-	8/18/38/38	0/3/3/3
56	GTP	OB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	QI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	ME	501	57	-	6/18/38/38	0/3/3/3
58	GDP	UC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	BD	501	-	-	3/12/32/32	0/3/3/3
56	GTP	PB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	MK	501	57	-	6/18/38/38	0/3/3/3
56	GTP	SE	501	57	-	6/18/38/38	0/3/3/3
56	GTP	MG	501	57	-	3/18/38/38	0/3/3/3
58	GDP	EH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	AJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	WF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	KK	501	57	-	4/18/38/38	0/3/3/3
58	GDP	FM	501	-	-	1/12/32/32	0/3/3/3
58	GDP	RJ	501	-	-	1/12/32/32	0/3/3/3
58	GDP	EM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	KD	501	-	-	2/12/32/32	0/3/3/3
58	GDP	UF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	RA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	SL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	VD	501	-	-	1/12/32/32	0/3/3/3
56	GTP	PA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	WC	501	-	-	1/12/32/32	0/3/3/3
56	GTP	DK	501	57	-	5/18/38/38	0/3/3/3
56	GTP	UE	501	57	-	4/18/38/38	0/3/3/3
58	GDP	WD	501	-	-	1/12/32/32	0/3/3/3
56	GTP	NI	501	57	-	6/18/38/38	0/3/3/3
58	GDP	UJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	VC	501	-	-	1/12/32/32	0/3/3/3
58	GDP	HH	501	-	-	1/12/32/32	0/3/3/3
56	GTP	CB	501	57	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	SG	501	57	-	7/18/38/38	0/3/3/3
58	GDP	UM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	FF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	CM	501	57	-	4/18/38/38	0/3/3/3
58	GDP	IC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	WK	501	57	-	6/18/38/38	0/3/3/3
58	GDP	OC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	EE	501	57	-	1/18/38/38	0/3/3/3
56	GTP	OK	501	57	-	6/18/38/38	0/3/3/3
56	GTP	LG	501	57	-	3/18/38/38	0/3/3/3
58	GDP	ID	501	-	-	2/12/32/32	0/3/3/3
56	GTP	KG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	OL	501	57	-	7/18/38/38	0/3/3/3
58	GDP	EL	501	-	-	1/12/32/32	0/3/3/3
58	GDP	BC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	FI	501	57	-	3/18/38/38	0/3/3/3
58	GDP	GL	501	-	-	1/12/32/32	0/3/3/3
56	GTP	HA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	UG	501	57	-	6/18/38/38	0/3/3/3
58	GDP	KF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	NK	501	-	-	1/12/32/32	0/3/3/3
58	GDP	TJ	501	-	-	1/12/32/32	0/3/3/3
56	GTP	EC	501	57	-	3/18/38/38	0/3/3/3
58	GDP	GM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	AE	501	57	-	6/18/38/38	0/3/3/3
58	GDP	HJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	MB	501	57	-	5/18/38/38	0/3/3/3
56	GTP	GA	501	57	-	6/18/38/38	0/3/3/3
58	GDP	LJ	501	-	-	4/12/32/32	0/3/3/3
58	GDP	PF	501	-	-	1/12/32/32	0/3/3/3
56	GTP	QL	501	57	-	9/18/38/38	0/3/3/3
56	GTP	RB	501	57	-	6/18/38/38	0/3/3/3
58	GDP	RH	501	-	-	1/12/32/32	0/3/3/3
56	GTP	FK	501	57	-	7/18/38/38	0/3/3/3
58	GDP	SD	501	-	-	4/12/32/32	0/3/3/3
58	GDP	QJ	501	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	DI	501	57	-	2/18/38/38	0/3/3/3
58	GDP	WH	501	-	-	1/12/32/32	0/3/3/3
58	GDP	MD	501	-	-	1/12/32/32	0/3/3/3
58	GDP	LH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	TG	501	57	-	6/18/38/38	0/3/3/3
58	GDP	JJ	501	-	-	3/12/32/32	0/3/3/3
58	GDP	FH	501	-	-	3/12/32/32	0/3/3/3

All (453) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	PA	501	GTP	C5-C6	-4.53	1.38	1.47
56	RE	501	GTP	C5-C6	-4.42	1.38	1.47
56	RG	501	GTP	C5-C6	-4.31	1.38	1.47
56	EE	501	GTP	C5-C6	-4.30	1.38	1.47
56	KG	501	GTP	C5-C6	-4.30	1.38	1.47
56	EA	501	GTP	C5-C6	-4.30	1.38	1.47
56	OK	501	GTP	C5-C6	-4.29	1.39	1.47
56	TA	501	GTP	C5-C6	-4.29	1.39	1.47
56	SK	501	GTP	C5-C6	-4.29	1.39	1.47
56	QB	501	GTP	C5-C6	-4.29	1.39	1.47
56	GE	501	GTP	C5-C6	-4.29	1.39	1.47
56	RK	501	GTP	C5-C6	-4.29	1.39	1.47
56	RA	501	GTP	C5-C6	-4.28	1.39	1.47
56	PI	501	GTP	C5-C6	-4.28	1.39	1.47
56	IB	501	GTP	C5-C6	-4.28	1.39	1.47
56	HB	501	GTP	C5-C6	-4.28	1.39	1.47
56	TE	501	GTP	C5-C6	-4.28	1.39	1.47
56	QA	501	GTP	C5-C6	-4.27	1.39	1.47
56	WI	501	GTP	C5-C6	-4.27	1.39	1.47
56	AG	501	GTP	C5-C6	-4.26	1.39	1.47
56	AK	501	GTP	C5-C6	-4.26	1.39	1.47
56	BA	501	GTP	C5-C6	-4.26	1.39	1.47
56	LK	501	GTP	C5-C6	-4.26	1.39	1.47
56	QI	501	GTP	C5-C6	-4.26	1.39	1.47
56	TI	501	GTP	C5-C6	-4.26	1.39	1.47
56	EI	501	GTP	C5-C6	-4.25	1.39	1.47
56	KK	501	GTP	C5-C6	-4.25	1.39	1.47
56	SB	501	GTP	C5-C6	-4.25	1.39	1.47
56	KB	501	GTP	C5-C6	-4.25	1.39	1.47
56	WG	501	GTP	C5-C6	-4.25	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	FI	501	GTP	C5-C6	-4.24	1.39	1.47
56	KI	501	GTP	C5-C6	-4.24	1.39	1.47
56	IK	501	GTP	C5-C6	-4.24	1.39	1.47
56	DB	501	GTP	C5-C6	-4.24	1.39	1.47
56	SE	501	GTP	C5-C6	-4.24	1.39	1.47
56	EC	501	GTP	C5-C6	-4.24	1.39	1.47
56	MG	501	GTP	C5-C6	-4.23	1.39	1.47
56	SI	501	GTP	C5-C6	-4.23	1.39	1.47
56	GB	501	GTP	C5-C6	-4.23	1.39	1.47
56	RI	501	GTP	C5-C6	-4.23	1.39	1.47
56	WA	501	GTP	C5-C6	-4.23	1.39	1.47
56	AB	501	GTP	C5-C6	-4.23	1.39	1.47
56	TB	501	GTP	C5-C6	-4.23	1.39	1.47
56	FA	501	GTP	C5-C6	-4.23	1.39	1.47
56	PL	501	GTP	C5-C6	-4.23	1.39	1.47
56	IA	501	GTP	C5-C6	-4.23	1.39	1.47
56	LI	501	GTP	C5-C6	-4.23	1.39	1.47
56	QG	501	GTP	C5-C6	-4.23	1.39	1.47
56	MK	501	GTP	C5-C6	-4.23	1.39	1.47
56	LG	501	GTP	C5-C6	-4.23	1.39	1.47
56	EK	501	GTP	C5-C6	-4.23	1.39	1.47
56	JK	501	GTP	C5-C6	-4.23	1.39	1.47
56	SG	501	GTP	C5-C6	-4.23	1.39	1.47
56	MA	501	GTP	C5-C6	-4.22	1.39	1.47
56	HE	501	GTP	C5-C6	-4.22	1.39	1.47
56	QK	501	GTP	C5-C6	-4.22	1.39	1.47
56	JA	501	GTP	C5-C6	-4.22	1.39	1.47
56	JG	501	GTP	C5-C6	-4.22	1.39	1.47
56	CB	501	GTP	C5-C6	-4.22	1.39	1.47
56	TK	501	GTP	C5-C6	-4.22	1.39	1.47
56	ME	501	GTP	C5-C6	-4.22	1.39	1.47
56	JE	501	GTP	C5-C6	-4.22	1.39	1.47
56	KE	501	GTP	C5-C6	-4.22	1.39	1.47
56	ML	501	GTP	C5-C6	-4.22	1.39	1.47
56	VB	501	GTP	C5-C6	-4.21	1.39	1.47
56	DI	501	GTP	C5-C6	-4.21	1.39	1.47
56	JI	501	GTP	C5-C6	-4.21	1.39	1.47
56	BM	501	GTP	C5-C6	-4.21	1.39	1.47
56	VE	501	GTP	C5-C6	-4.21	1.39	1.47
56	UK	501	GTP	C5-C6	-4.21	1.39	1.47
56	VG	501	GTP	C5-C6	-4.21	1.39	1.47
56	FE	501	GTP	C5-C6	-4.21	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	AE	501	GTP	C5-C6	-4.20	1.39	1.47
56	SA	501	GTP	C5-C6	-4.20	1.39	1.47
56	BI	501	GTP	C5-C6	-4.20	1.39	1.47
56	RB	501	GTP	C5-C6	-4.20	1.39	1.47
56	LB	501	GTP	C5-C6	-4.20	1.39	1.47
56	CG	501	GTP	C5-C6	-4.20	1.39	1.47
56	NG	501	GTP	C5-C6	-4.20	1.39	1.47
56	AM	501	GTP	C5-C6	-4.20	1.39	1.47
56	HG	501	GTP	C5-C6	-4.20	1.39	1.47
56	OG	501	GTP	C5-C6	-4.20	1.39	1.47
56	JB	501	GTP	C5-C6	-4.19	1.39	1.47
56	OA	501	GTP	C5-C6	-4.19	1.39	1.47
56	EG	501	GTP	C5-C6	-4.19	1.39	1.47
56	FK	501	GTP	C5-C6	-4.19	1.39	1.47
56	QE	501	GTP	C5-C6	-4.19	1.39	1.47
56	NL	501	GTP	C5-C6	-4.19	1.39	1.47
56	HK	501	GTP	C5-C6	-4.19	1.39	1.47
56	AI	501	GTP	C5-C6	-4.19	1.39	1.47
56	HA	501	GTP	C5-C6	-4.19	1.39	1.47
56	NI	501	GTP	C5-C6	-4.19	1.39	1.47
56	UG	501	GTP	C5-C6	-4.19	1.39	1.47
56	DE	501	GTP	C5-C6	-4.19	1.39	1.47
56	DA	501	GTP	C5-C6	-4.19	1.39	1.47
56	IG	501	GTP	C5-C6	-4.18	1.39	1.47
56	GK	501	GTP	C5-C6	-4.18	1.39	1.47
56	MI	501	GTP	C5-C6	-4.18	1.39	1.47
56	HI	501	GTP	C5-C6	-4.18	1.39	1.47
56	PK	501	GTP	C5-C6	-4.18	1.39	1.47
56	NE	501	GTP	C5-C6	-4.18	1.39	1.47
56	NA	501	GTP	C5-C6	-4.18	1.39	1.47
56	OB	501	GTP	C5-C6	-4.17	1.39	1.47
56	VK	501	GTP	C5-C6	-4.17	1.39	1.47
56	II	501	GTP	C5-C6	-4.17	1.39	1.47
56	FG	501	GTP	C5-C6	-4.17	1.39	1.47
56	UE	501	GTP	C5-C6	-4.17	1.39	1.47
56	MB	501	GTP	C5-C6	-4.17	1.39	1.47
56	BB	501	GTP	C5-C6	-4.17	1.39	1.47
56	IM	501	GTP	C5-C6	-4.17	1.39	1.47
56	WE	501	GTP	C5-C6	-4.17	1.39	1.47
56	GG	501	GTP	C5-C6	-4.17	1.39	1.47
56	UB	501	GTP	C5-C6	-4.17	1.39	1.47
56	VA	501	GTP	C5-C6	-4.17	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	FB	501	GTP	C5-C6	-4.16	1.39	1.47
56	VI	501	GTP	C5-C6	-4.16	1.39	1.47
56	LA	501	GTP	C5-C6	-4.16	1.39	1.47
56	DM	501	GTP	C5-C6	-4.16	1.39	1.47
56	KA	501	GTP	C5-C6	-4.16	1.39	1.47
56	WK	501	GTP	C5-C6	-4.16	1.39	1.47
56	CK	501	GTP	C5-C6	-4.16	1.39	1.47
56	DG	501	GTP	C5-C6	-4.16	1.39	1.47
56	LE	501	GTP	C5-C6	-4.16	1.39	1.47
56	OI	501	GTP	C5-C6	-4.15	1.39	1.47
56	BE	501	GTP	C5-C6	-4.15	1.39	1.47
56	TG	501	GTP	C5-C6	-4.15	1.39	1.47
56	OE	501	GTP	C5-C6	-4.15	1.39	1.47
56	AA	501	GTP	C5-C6	-4.14	1.39	1.47
56	BG	501	GTP	C5-C6	-4.14	1.39	1.47
56	UI	501	GTP	C5-C6	-4.14	1.39	1.47
56	OL	501	GTP	C5-C6	-4.14	1.39	1.47
56	CM	501	GTP	C5-C6	-4.14	1.39	1.47
56	PG	501	GTP	C5-C6	-4.14	1.39	1.47
56	CI	501	GTP	C5-C6	-4.14	1.39	1.47
56	NB	501	GTP	C5-C6	-4.13	1.39	1.47
56	CA	501	GTP	C5-C6	-4.13	1.39	1.47
56	PE	501	GTP	C5-C6	-4.13	1.39	1.47
56	WB	501	GTP	C5-C6	-4.12	1.39	1.47
56	IE	501	GTP	C5-C6	-4.12	1.39	1.47
56	RL	501	GTP	C5-C6	-4.12	1.39	1.47
56	QL	501	GTP	C5-C6	-4.11	1.39	1.47
56	CE	501	GTP	C5-C6	-4.11	1.39	1.47
56	PB	501	GTP	C5-C6	-4.11	1.39	1.47
56	UA	501	GTP	C5-C6	-4.10	1.39	1.47
56	GI	501	GTP	C5-C6	-4.09	1.39	1.47
56	DK	501	GTP	C5-C6	-4.09	1.39	1.47
56	BK	501	GTP	C5-C6	-4.09	1.39	1.47
56	GA	501	GTP	C5-C6	-4.08	1.39	1.47
58	AD	501	GDP	C6-N1	-2.70	1.33	1.37
58	HC	501	GDP	C6-N1	-2.68	1.33	1.37
58	VL	501	GDP	C6-N1	-2.67	1.33	1.37
58	DD	501	GDP	C6-N1	-2.64	1.33	1.37
58	JL	501	GDP	C6-N1	-2.61	1.33	1.37
58	CF	501	GDP	C6-N1	-2.55	1.33	1.37
58	NF	501	GDP	C6-N1	-2.53	1.33	1.37
58	QF	501	GDP	C6-N1	-2.51	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	TH	501	GDP	C6-N1	-2.51	1.34	1.37
58	FL	501	GDP	C6-N1	-2.49	1.34	1.37
58	WD	501	GDP	C6-N1	-2.47	1.34	1.37
58	NJ	501	GDP	C6-N1	-2.47	1.34	1.37
58	EM	501	GDP	C6-N1	-2.46	1.34	1.37
58	BF	501	GDP	C6-N1	-2.45	1.34	1.37
58	SJ	501	GDP	C6-N1	-2.45	1.34	1.37
58	RC	501	GDP	C6-N1	-2.45	1.34	1.37
58	LH	501	GDP	C6-N1	-2.44	1.34	1.37
58	LL	501	GDP	C6-N1	-2.44	1.34	1.37
58	SC	501	GDP	C6-N1	-2.43	1.34	1.37
58	FF	501	GDP	C6-N1	-2.43	1.34	1.37
58	WF	501	GDP	C6-N1	-2.43	1.34	1.37
58	RM	501	GDP	C6-N1	-2.42	1.34	1.37
58	RD	501	GDP	C6-N1	-2.42	1.34	1.37
58	UF	501	GDP	C6-N1	-2.42	1.34	1.37
58	OH	501	GDP	C6-N1	-2.42	1.34	1.37
58	AJ	501	GDP	C6-N1	-2.41	1.34	1.37
58	UH	501	GDP	C6-N1	-2.41	1.34	1.37
58	IL	501	GDP	C6-N1	-2.41	1.34	1.37
58	AC	501	GDP	C6-N1	-2.41	1.34	1.37
58	RH	501	GDP	C6-N1	-2.41	1.34	1.37
58	JH	501	GDP	C6-N1	-2.41	1.34	1.37
58	GF	501	GDP	C6-N1	-2.40	1.34	1.37
58	EL	501	GDP	C6-N1	-2.40	1.34	1.37
58	IJ	501	GDP	C6-N1	-2.40	1.34	1.37
58	PD	501	GDP	C6-N1	-2.40	1.34	1.37
58	PM	501	GDP	C6-N1	-2.40	1.34	1.37
58	RJ	501	GDP	C6-N1	-2.40	1.34	1.37
58	BC	501	GDP	C6-N1	-2.40	1.34	1.37
58	FM	501	GDP	C6-N1	-2.40	1.34	1.37
58	UC	501	GDP	C6-N1	-2.39	1.34	1.37
58	HL	501	GDP	C6-N1	-2.39	1.34	1.37
58	SL	501	GDP	C6-N1	-2.39	1.34	1.37
58	LC	501	GDP	C6-N1	-2.39	1.34	1.37
58	NC	501	GDP	C6-N1	-2.39	1.34	1.37
58	AF	501	GDP	C6-N1	-2.39	1.34	1.37
58	MH	501	GDP	C6-N1	-2.38	1.34	1.37
58	DJ	501	GDP	C6-N1	-2.38	1.34	1.37
58	MC	501	GDP	C6-N1	-2.38	1.34	1.37
58	CD	501	GDP	C6-N1	-2.38	1.34	1.37
58	GD	501	GDP	C6-N1	-2.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	GH	501	GDP	C6-N1	-2.38	1.34	1.37
58	PC	501	GDP	C6-N1	-2.38	1.34	1.37
58	QC	501	GDP	C6-N1	-2.38	1.34	1.37
58	EB	501	GDP	C6-N1	-2.38	1.34	1.37
58	KF	501	GDP	C6-N1	-2.38	1.34	1.37
58	KC	501	GDP	C6-N1	-2.38	1.34	1.37
58	LJ	501	GDP	C6-N1	-2.38	1.34	1.37
58	JC	501	GDP	C6-N1	-2.37	1.34	1.37
58	BL	501	GDP	C6-N1	-2.37	1.34	1.37
58	AL	501	GDP	C6-N1	-2.37	1.34	1.37
58	MF	501	GDP	C6-N1	-2.37	1.34	1.37
58	LF	501	GDP	C6-N1	-2.37	1.34	1.37
58	NM	501	GDP	C6-N1	-2.37	1.34	1.37
58	JM	501	GDP	C6-N1	-2.36	1.34	1.37
58	TF	501	GDP	C6-N1	-2.36	1.34	1.37
58	IF	501	GDP	C6-N1	-2.36	1.34	1.37
58	MJ	501	GDP	C6-N1	-2.36	1.34	1.37
58	NH	501	GDP	C6-N1	-2.36	1.34	1.37
58	TC	501	GDP	C6-N1	-2.36	1.34	1.37
58	KJ	501	GDP	C6-N1	-2.36	1.34	1.37
58	OJ	501	GDP	C6-N1	-2.36	1.34	1.37
58	CJ	501	GDP	C6-N1	-2.36	1.34	1.37
58	VF	501	GDP	C6-N1	-2.36	1.34	1.37
58	DL	501	GDP	C6-N1	-2.35	1.34	1.37
58	MD	501	GDP	C6-N1	-2.35	1.34	1.37
58	SH	501	GDP	C6-N1	-2.35	1.34	1.37
58	UL	501	GDP	C6-N1	-2.35	1.34	1.37
58	VD	501	GDP	C6-N1	-2.35	1.34	1.37
58	QM	501	GDP	C6-N1	-2.35	1.34	1.37
58	JJ	501	GDP	C6-N1	-2.35	1.34	1.37
58	PH	501	GDP	C6-N1	-2.35	1.34	1.37
58	QJ	501	GDP	C6-N1	-2.35	1.34	1.37
58	UJ	501	GDP	C6-N1	-2.35	1.34	1.37
58	KL	501	GDP	C6-N1	-2.35	1.34	1.37
58	KH	501	GDP	C6-N1	-2.35	1.34	1.37
58	FD	501	GDP	C6-N1	-2.35	1.34	1.37
58	GC	501	GDP	C6-N1	-2.35	1.34	1.37
58	VJ	501	GDP	C6-N1	-2.35	1.34	1.37
58	DH	501	GDP	C6-N1	-2.35	1.34	1.37
58	JD	501	GDP	C6-N1	-2.34	1.34	1.37
58	HH	501	GDP	C6-N1	-2.34	1.34	1.37
58	HJ	501	GDP	C6-N1	-2.34	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	FH	501	GDP	C6-N1	-2.34	1.34	1.37
58	IC	501	GDP	C6-N1	-2.34	1.34	1.37
58	VM	501	GDP	C6-N1	-2.34	1.34	1.37
58	TL	501	GDP	C6-N1	-2.34	1.34	1.37
58	IH	501	GDP	C6-N1	-2.34	1.34	1.37
56	RL	501	GTP	PB-O3B	2.34	1.62	1.59
58	GJ	501	GDP	C6-N1	-2.33	1.34	1.37
58	OF	501	GDP	C6-N1	-2.33	1.34	1.37
58	FC	501	GDP	C6-N1	-2.33	1.34	1.37
58	QD	501	GDP	C6-N1	-2.33	1.34	1.37
58	ID	501	GDP	C6-N1	-2.33	1.34	1.37
56	BK	501	GTP	PB-O3B	2.33	1.62	1.59
58	DC	501	GDP	C6-N1	-2.33	1.34	1.37
58	JF	501	GDP	C6-N1	-2.33	1.34	1.37
58	QH	501	GDP	C6-N1	-2.33	1.34	1.37
58	KD	501	GDP	C6-N1	-2.33	1.34	1.37
58	WC	501	GDP	C6-N1	-2.33	1.34	1.37
58	ND	501	GDP	C6-N1	-2.33	1.34	1.37
58	OC	501	GDP	C6-N1	-2.33	1.34	1.37
58	BJ	501	GDP	C6-N1	-2.32	1.34	1.37
56	BG	501	GTP	PA-O3A	2.32	1.62	1.59
58	PJ	501	GDP	C6-N1	-2.32	1.34	1.37
58	VC	501	GDP	C6-N1	-2.32	1.34	1.37
58	EJ	501	GDP	C6-N1	-2.32	1.34	1.37
58	WH	501	GDP	C6-N1	-2.32	1.34	1.37
58	EF	501	GDP	C6-N1	-2.32	1.34	1.37
58	WJ	501	GDP	C6-N1	-2.32	1.34	1.37
58	AH	501	GDP	C6-N1	-2.32	1.34	1.37
58	LD	501	GDP	C6-N1	-2.31	1.34	1.37
58	HF	501	GDP	C6-N1	-2.31	1.34	1.37
58	MM	501	GDP	C6-N1	-2.31	1.34	1.37
58	GL	501	GDP	C6-N1	-2.31	1.34	1.37
58	OM	501	GDP	C6-N1	-2.31	1.34	1.37
58	EH	501	GDP	C6-N1	-2.30	1.34	1.37
58	SM	501	GDP	C6-N1	-2.30	1.34	1.37
58	HD	501	GDP	C6-N1	-2.30	1.34	1.37
58	TM	501	GDP	C6-N1	-2.30	1.34	1.37
58	CC	501	GDP	C6-N1	-2.30	1.34	1.37
58	BD	501	GDP	C6-N1	-2.30	1.34	1.37
58	NK	501	GDP	C6-N1	-2.30	1.34	1.37
58	WL	501	GDP	C6-N1	-2.30	1.34	1.37
58	OD	501	GDP	C6-N1	-2.29	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	TJ	501	GDP	C6-N1	-2.29	1.34	1.37
58	BH	501	GDP	C6-N1	-2.29	1.34	1.37
58	ED	501	GDP	C6-N1	-2.29	1.34	1.37
58	GM	501	GDP	C6-N1	-2.28	1.34	1.37
58	CL	501	GDP	C6-N1	-2.28	1.34	1.37
58	FJ	501	GDP	C6-N1	-2.28	1.34	1.37
58	CH	501	GDP	C6-N1	-2.27	1.34	1.37
58	SD	501	GDP	C6-N1	-2.27	1.34	1.37
58	LM	501	GDP	C6-N1	-2.27	1.34	1.37
56	TG	501	GTP	C2-N3	2.27	1.38	1.33
58	VH	501	GDP	C6-N1	-2.27	1.34	1.37
58	UM	501	GDP	C6-N1	-2.26	1.34	1.37
58	SF	501	GDP	C6-N1	-2.26	1.34	1.37
56	CK	501	GTP	C2-N3	2.26	1.38	1.33
56	RL	501	GTP	C2-N3	2.24	1.38	1.33
56	BK	501	GTP	C2-N3	2.24	1.38	1.33
56	TA	501	GTP	C2-N3	2.23	1.38	1.33
58	KM	501	GDP	C6-N1	-2.23	1.34	1.37
56	LA	501	GTP	C2-N3	2.20	1.38	1.33
56	IA	501	GTP	C2-N3	2.20	1.38	1.33
58	HM	501	GDP	C6-N1	-2.19	1.34	1.37
56	GB	501	GTP	C2-N3	2.19	1.38	1.33
56	PL	501	GTP	C2-N3	2.19	1.38	1.33
56	UA	501	GTP	C2-N3	2.19	1.38	1.33
56	PI	501	GTP	C2-N3	2.19	1.38	1.33
56	ML	501	GTP	C2-N3	2.18	1.38	1.33
56	TI	501	GTP	C2-N3	2.18	1.38	1.33
56	PK	501	GTP	C2-N3	2.18	1.38	1.33
56	SK	501	GTP	C2-N3	2.18	1.38	1.33
56	TB	501	GTP	C2-N3	2.17	1.38	1.33
56	NB	501	GTP	C2-N3	2.17	1.38	1.33
56	QL	501	GTP	PA-O3A	2.17	1.61	1.59
56	FI	501	GTP	C2-N3	2.16	1.38	1.33
56	MA	501	GTP	C2-N3	2.16	1.38	1.33
56	AE	501	GTP	C2-N3	2.16	1.38	1.33
56	IM	501	GTP	C2-N3	2.16	1.38	1.33
56	GE	501	GTP	C2-N3	2.16	1.38	1.33
56	HI	501	GTP	C2-N3	2.16	1.38	1.33
56	AK	501	GTP	C2-N3	2.15	1.38	1.33
56	FB	501	GTP	C2-N3	2.15	1.38	1.33
56	GI	501	GTP	C2-N3	2.15	1.38	1.33
56	QL	501	GTP	C2-N3	2.15	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	SG	501	GTP	C2-N3	2.15	1.38	1.33
56	BI	501	GTP	C2-N3	2.15	1.38	1.33
56	KA	501	GTP	C2-N3	2.15	1.38	1.33
56	OA	501	GTP	C2-N3	2.15	1.38	1.33
56	OG	501	GTP	C2-N3	2.15	1.38	1.33
56	BG	501	GTP	C2-N3	2.15	1.38	1.33
56	UI	501	GTP	C2-N3	2.15	1.38	1.33
56	IE	501	GTP	C2-N3	2.15	1.38	1.33
56	UE	501	GTP	C2-N3	2.15	1.38	1.33
56	IK	501	GTP	C2-N3	2.14	1.38	1.33
56	VA	501	GTP	C2-N3	2.14	1.38	1.33
56	HA	501	GTP	C2-N3	2.14	1.38	1.33
56	BA	501	GTP	C2-N3	2.14	1.38	1.33
56	EC	501	GTP	C2-N3	2.14	1.38	1.33
56	EK	501	GTP	C2-N3	2.14	1.38	1.33
56	OB	501	GTP	C2-N3	2.14	1.38	1.33
56	GA	501	GTP	C2-N3	2.14	1.38	1.33
56	DK	501	GTP	C2-N3	2.14	1.38	1.33
56	HB	501	GTP	C2-N3	2.14	1.38	1.33
56	OI	501	GTP	C2-N3	2.14	1.38	1.33
56	SI	501	GTP	C2-N3	2.14	1.38	1.33
56	II	501	GTP	C2-N3	2.14	1.38	1.33
56	NE	501	GTP	C2-N3	2.14	1.38	1.33
56	FG	501	GTP	C2-N3	2.14	1.38	1.33
56	QK	501	GTP	C2-N3	2.14	1.38	1.33
56	CM	501	GTP	C2-N3	2.14	1.38	1.33
56	AG	501	GTP	C2-N3	2.14	1.38	1.33
56	GG	501	GTP	C2-N3	2.14	1.38	1.33
56	NG	501	GTP	C2-N3	2.14	1.38	1.33
56	RA	501	GTP	C2-N3	2.13	1.38	1.33
56	AM	501	GTP	C2-N3	2.13	1.38	1.33
56	EA	501	GTP	C2-N3	2.13	1.38	1.33
56	IB	501	GTP	C2-N3	2.13	1.38	1.33
56	WK	501	GTP	C2-N3	2.13	1.38	1.33
56	JB	501	GTP	C2-N3	2.13	1.38	1.33
56	OL	501	GTP	C2-N3	2.13	1.38	1.33
56	SB	501	GTP	C2-N3	2.13	1.38	1.33
56	CA	501	GTP	C2-N3	2.13	1.38	1.33
56	NA	501	GTP	C2-N3	2.13	1.38	1.33
56	PB	501	GTP	C2-N3	2.13	1.38	1.33
56	VI	501	GTP	C2-N3	2.13	1.38	1.33
56	JG	501	GTP	C2-N3	2.13	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	SA	501	GTP	C2-N3	2.13	1.38	1.33
56	FA	501	GTP	C2-N3	2.13	1.38	1.33
56	OE	501	GTP	C2-N3	2.13	1.38	1.33
56	TK	501	GTP	C2-N3	2.13	1.38	1.33
56	WG	501	GTP	C2-N3	2.13	1.38	1.33
56	PG	501	GTP	C2-N3	2.13	1.38	1.33
56	HE	501	GTP	C2-N3	2.13	1.38	1.33
56	FE	501	GTP	C2-N3	2.12	1.38	1.33
56	JE	501	GTP	C2-N3	2.12	1.38	1.33
56	RE	501	GTP	C2-N3	2.12	1.38	1.33
56	VE	501	GTP	C2-N3	2.12	1.38	1.33
56	PA	501	GTP	C2-N3	2.12	1.38	1.33
56	CB	501	GTP	C2-N3	2.12	1.38	1.33
56	RI	501	GTP	C2-N3	2.12	1.38	1.33
56	CK	501	GTP	PB-O3B	2.12	1.61	1.59
56	QI	501	GTP	C2-N3	2.12	1.38	1.33
56	WI	501	GTP	C2-N3	2.12	1.38	1.33
56	VK	501	GTP	C2-N3	2.12	1.38	1.33
56	GK	501	GTP	C2-N3	2.12	1.38	1.33
56	PE	501	GTP	C2-N3	2.12	1.38	1.33
56	NL	501	GTP	C2-N3	2.12	1.38	1.33
56	HG	501	GTP	C2-N3	2.12	1.38	1.33
56	AA	501	GTP	C2-N3	2.12	1.38	1.33
56	LB	501	GTP	C2-N3	2.12	1.38	1.33
56	KK	501	GTP	C2-N3	2.12	1.38	1.33
56	VB	501	GTP	C2-N3	2.12	1.38	1.33
56	DI	501	GTP	C2-N3	2.12	1.38	1.33
56	SE	501	GTP	C2-N3	2.12	1.38	1.33
56	EI	501	GTP	C2-N3	2.12	1.38	1.33
56	CI	501	GTP	C2-N3	2.11	1.38	1.33
56	WB	501	GTP	C2-N3	2.11	1.38	1.33
56	EG	501	GTP	C2-N3	2.11	1.38	1.33
56	JA	501	GTP	C2-N3	2.11	1.38	1.33
56	BB	501	GTP	C2-N3	2.11	1.38	1.33
56	NI	501	GTP	C2-N3	2.11	1.38	1.33
56	WA	501	GTP	C2-N3	2.11	1.38	1.33
56	LI	501	GTP	C2-N3	2.11	1.38	1.33
56	AB	501	GTP	C2-N3	2.11	1.38	1.33
56	JK	501	GTP	C2-N3	2.11	1.38	1.33
56	UB	501	GTP	C2-N3	2.11	1.38	1.33
56	LG	501	GTP	C2-N3	2.11	1.38	1.33
56	MG	501	GTP	C2-N3	2.11	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	WE	501	GTP	C2-N3	2.11	1.38	1.33
56	LK	501	GTP	C2-N3	2.11	1.38	1.33
56	RK	501	GTP	C2-N3	2.10	1.38	1.33
56	KB	501	GTP	C2-N3	2.10	1.38	1.33
56	FK	501	GTP	C2-N3	2.10	1.38	1.33
56	RG	501	GTP	C2-N3	2.10	1.38	1.33
56	DG	501	GTP	C2-N3	2.10	1.38	1.33
56	DA	501	GTP	C2-N3	2.10	1.38	1.33
56	AI	501	GTP	C2-N3	2.10	1.38	1.33
56	IG	501	GTP	C2-N3	2.09	1.38	1.33
56	TE	501	GTP	C2-N3	2.09	1.38	1.33
56	ME	501	GTP	C2-N3	2.09	1.38	1.33
56	KI	501	GTP	C2-N3	2.09	1.38	1.33
56	BM	501	GTP	C2-N3	2.09	1.38	1.33
56	VG	501	GTP	C2-N3	2.09	1.38	1.33
56	QG	501	GTP	C2-N3	2.09	1.38	1.33
56	QE	501	GTP	C2-N3	2.09	1.38	1.33
56	KE	501	GTP	C2-N3	2.09	1.38	1.33
56	UG	501	GTP	C2-N3	2.08	1.38	1.33
56	CK	501	GTP	PA-O3A	2.08	1.61	1.59
56	QA	501	GTP	C2-N3	2.08	1.38	1.33
56	HK	501	GTP	C2-N3	2.08	1.38	1.33
56	UK	501	GTP	C2-N3	2.08	1.38	1.33
56	DE	501	GTP	C2-N3	2.08	1.38	1.33
56	EE	501	GTP	C2-N3	2.08	1.38	1.33
56	MK	501	GTP	C2-N3	2.08	1.38	1.33
56	KG	501	GTP	C2-N3	2.08	1.38	1.33
56	JI	501	GTP	C2-N3	2.08	1.38	1.33
56	QB	501	GTP	C2-N3	2.08	1.38	1.33
56	RB	501	GTP	C2-N3	2.08	1.38	1.33
56	LE	501	GTP	C2-N3	2.07	1.38	1.33
58	RF	501	GDP	C6-N1	-2.07	1.34	1.37
58	DF	501	GDP	C6-N1	-2.07	1.34	1.37
56	MI	501	GTP	C2-N3	2.07	1.38	1.33
56	DM	501	GTP	C2-N3	2.07	1.38	1.33
56	QL	501	GTP	PB-O3A	2.06	1.61	1.59
56	MB	501	GTP	C2-N3	2.06	1.38	1.33
56	DB	501	GTP	C2-N3	2.06	1.38	1.33
56	CG	501	GTP	C2-N3	2.06	1.38	1.33
56	CE	501	GTP	C2-N3	2.06	1.38	1.33
56	OK	501	GTP	C2-N3	2.05	1.38	1.33
56	BE	501	GTP	C2-N3	2.03	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	UD	501	GDP	C6-N1	-2.03	1.34	1.37
58	DF	501	GDP	O4'-C1'	2.01	1.43	1.40
56	QL	501	GTP	PB-O3B	2.00	1.61	1.59

All (919) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	PF	501	GDP	O6-C6-C5	-3.81	116.77	124.32
56	TG	501	GTP	C8-N7-C5	3.74	108.92	102.55
56	SE	501	GTP	C8-N7-C5	3.73	108.89	102.55
56	GK	501	GTP	C8-N7-C5	3.72	108.88	102.55
56	CE	501	GTP	C8-N7-C5	3.72	108.88	102.55
56	LE	501	GTP	C8-N7-C5	3.72	108.88	102.55
56	GG	501	GTP	C8-N7-C5	3.71	108.87	102.55
56	II	501	GTP	C8-N7-C5	3.71	108.87	102.55
56	LA	501	GTP	C8-N7-C5	3.71	108.87	102.55
56	PE	501	GTP	C8-N7-C5	3.71	108.86	102.55
56	AB	501	GTP	C8-N7-C5	3.70	108.85	102.55
56	FG	501	GTP	C8-N7-C5	3.70	108.85	102.55
56	HE	501	GTP	C8-N7-C5	3.69	108.84	102.55
56	UB	501	GTP	C8-N7-C5	3.69	108.84	102.55
56	UK	501	GTP	C8-N7-C5	3.69	108.84	102.55
56	UA	501	GTP	C8-N7-C5	3.69	108.83	102.55
56	OA	501	GTP	C8-N7-C5	3.69	108.83	102.55
56	OE	501	GTP	C8-N7-C5	3.69	108.83	102.55
56	HK	501	GTP	C8-N7-C5	3.68	108.82	102.55
56	IE	501	GTP	C8-N7-C5	3.68	108.82	102.55
56	FK	501	GTP	C8-N7-C5	3.68	108.82	102.55
56	WK	501	GTP	C8-N7-C5	3.68	108.81	102.55
56	TK	501	GTP	C8-N7-C5	3.68	108.81	102.55
56	HG	501	GTP	C8-N7-C5	3.67	108.80	102.55
56	OL	501	GTP	C8-N7-C5	3.67	108.80	102.55
56	VI	501	GTP	C8-N7-C5	3.67	108.80	102.55
56	AA	501	GTP	C8-N7-C5	3.67	108.80	102.55
56	EC	501	GTP	C8-N7-C5	3.67	108.80	102.55
56	PB	501	GTP	C8-N7-C5	3.67	108.79	102.55
56	DA	501	GTP	C8-N7-C5	3.67	108.79	102.55
56	JI	501	GTP	C8-N7-C5	3.67	108.79	102.55
56	WB	501	GTP	C8-N7-C5	3.67	108.79	102.55
56	GI	501	GTP	C8-N7-C5	3.66	108.78	102.55
56	HI	501	GTP	C8-N7-C5	3.66	108.78	102.55
56	IM	501	GTP	C8-N7-C5	3.66	108.78	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	NI	501	GTP	C8-N7-C5	3.66	108.78	102.55
56	VK	501	GTP	C8-N7-C5	3.66	108.78	102.55
56	DE	501	GTP	C8-N7-C5	3.66	108.78	102.55
56	TE	501	GTP	C8-N7-C5	3.66	108.78	102.55
56	CA	501	GTP	C8-N7-C5	3.66	108.78	102.55
56	SK	501	GTP	C8-N7-C5	3.66	108.78	102.55
56	GA	501	GTP	C8-N7-C5	3.66	108.77	102.55
56	VA	501	GTP	C8-N7-C5	3.65	108.77	102.55
56	LK	501	GTP	C8-N7-C5	3.65	108.77	102.55
56	SA	501	GTP	C8-N7-C5	3.65	108.77	102.55
56	BE	501	GTP	C8-N7-C5	3.65	108.77	102.55
56	FA	501	GTP	C8-N7-C5	3.65	108.76	102.55
56	FB	501	GTP	C8-N7-C5	3.65	108.76	102.55
56	IG	501	GTP	C8-N7-C5	3.65	108.76	102.55
56	NB	501	GTP	C8-N7-C5	3.64	108.75	102.55
56	DB	501	GTP	C8-N7-C5	3.64	108.75	102.55
56	CM	501	GTP	C8-N7-C5	3.64	108.75	102.55
56	AE	501	GTP	C8-N7-C5	3.64	108.75	102.55
56	JE	501	GTP	C8-N7-C5	3.64	108.75	102.55
56	ME	501	GTP	C8-N7-C5	3.64	108.75	102.55
56	JB	501	GTP	C8-N7-C5	3.64	108.75	102.55
56	DK	501	GTP	C8-N7-C5	3.64	108.75	102.55
56	MI	501	GTP	C8-N7-C5	3.64	108.75	102.55
56	SG	501	GTP	C8-N7-C5	3.64	108.75	102.55
56	KB	501	GTP	C8-N7-C5	3.64	108.74	102.55
56	OG	501	GTP	C8-N7-C5	3.64	108.74	102.55
56	VE	501	GTP	C8-N7-C5	3.64	108.74	102.55
56	BI	501	GTP	C8-N7-C5	3.64	108.74	102.55
56	MG	501	GTP	C8-N7-C5	3.64	108.74	102.55
56	AI	501	GTP	C8-N7-C5	3.63	108.73	102.55
56	AK	501	GTP	C8-N7-C5	3.63	108.73	102.55
56	KA	501	GTP	C8-N7-C5	3.63	108.73	102.55
56	KG	501	GTP	C8-N7-C5	3.63	108.73	102.55
56	MB	501	GTP	C8-N7-C5	3.63	108.73	102.55
56	FI	501	GTP	C8-N7-C5	3.63	108.73	102.55
56	BB	501	GTP	C8-N7-C5	3.63	108.73	102.55
56	QB	501	GTP	C8-N7-C5	3.63	108.73	102.55
56	FE	501	GTP	C8-N7-C5	3.63	108.73	102.55
56	PG	501	GTP	C8-N7-C5	3.63	108.72	102.55
56	PK	501	GTP	C8-N7-C5	3.63	108.72	102.55
56	QG	501	GTP	C8-N7-C5	3.63	108.72	102.55
56	RI	501	GTP	C8-N7-C5	3.63	108.72	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	CI	501	GTP	C8-N7-C5	3.63	108.72	102.55
56	EG	501	GTP	C8-N7-C5	3.62	108.72	102.55
56	QI	501	GTP	C8-N7-C5	3.62	108.72	102.55
56	LI	501	GTP	C8-N7-C5	3.62	108.72	102.55
56	ML	501	GTP	C8-N7-C5	3.62	108.72	102.55
56	OI	501	GTP	C8-N7-C5	3.62	108.72	102.55
56	RB	501	GTP	C8-N7-C5	3.62	108.72	102.55
56	DI	501	GTP	C8-N7-C5	3.62	108.71	102.55
56	OB	501	GTP	C8-N7-C5	3.62	108.71	102.55
56	DM	501	GTP	C8-N7-C5	3.62	108.71	102.55
56	BK	501	GTP	C8-N7-C5	3.62	108.71	102.55
56	EK	501	GTP	C8-N7-C5	3.62	108.71	102.55
56	QA	501	GTP	C8-N7-C5	3.62	108.71	102.55
56	BM	501	GTP	C8-N7-C5	3.62	108.71	102.55
56	UG	501	GTP	C8-N7-C5	3.62	108.71	102.55
56	WE	501	GTP	C8-N7-C5	3.62	108.71	102.55
56	NA	501	GTP	C8-N7-C5	3.62	108.70	102.55
56	PI	501	GTP	C8-N7-C5	3.62	108.70	102.55
56	VB	501	GTP	C8-N7-C5	3.62	108.70	102.55
56	HA	501	GTP	C8-N7-C5	3.61	108.70	102.55
56	MK	501	GTP	C8-N7-C5	3.61	108.70	102.55
56	JA	501	GTP	C8-N7-C5	3.61	108.70	102.55
56	QE	501	GTP	C8-N7-C5	3.61	108.70	102.55
56	TB	501	GTP	C8-N7-C5	3.61	108.70	102.55
56	KE	501	GTP	C8-N7-C5	3.61	108.70	102.55
56	NL	501	GTP	C8-N7-C5	3.61	108.70	102.55
56	BG	501	GTP	C8-N7-C5	3.61	108.69	102.55
56	AM	501	GTP	C8-N7-C5	3.61	108.69	102.55
56	BA	501	GTP	C8-N7-C5	3.61	108.69	102.55
56	GB	501	GTP	C8-N7-C5	3.61	108.69	102.55
56	QK	501	GTP	C8-N7-C5	3.61	108.69	102.55
56	TA	501	GTP	C8-N7-C5	3.61	108.69	102.55
56	TI	501	GTP	C8-N7-C5	3.60	108.68	102.55
56	KI	501	GTP	C8-N7-C5	3.60	108.68	102.55
56	WI	501	GTP	C8-N7-C5	3.60	108.68	102.55
56	UE	501	GTP	C8-N7-C5	3.60	108.68	102.55
56	CG	501	GTP	C8-N7-C5	3.60	108.67	102.55
56	HB	501	GTP	C8-N7-C5	3.60	108.67	102.55
56	NE	501	GTP	C8-N7-C5	3.59	108.67	102.55
56	IB	501	GTP	C8-N7-C5	3.59	108.66	102.55
56	IK	501	GTP	C8-N7-C5	3.59	108.66	102.55
56	CB	501	GTP	C8-N7-C5	3.59	108.66	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	EI	501	GTP	C8-N7-C5	3.59	108.66	102.55
56	JK	501	GTP	C8-N7-C5	3.59	108.66	102.55
56	KK	501	GTP	C8-N7-C5	3.59	108.66	102.55
56	LB	501	GTP	C8-N7-C5	3.58	108.65	102.55
56	MA	501	GTP	C8-N7-C5	3.58	108.65	102.55
56	LG	501	GTP	C8-N7-C5	3.58	108.65	102.55
56	AG	501	GTP	C8-N7-C5	3.58	108.65	102.55
56	WA	501	GTP	C8-N7-C5	3.58	108.64	102.55
56	RA	501	GTP	C8-N7-C5	3.58	108.64	102.55
56	QL	501	GTP	C8-N7-C5	3.58	108.64	102.55
56	UI	501	GTP	C8-N7-C5	3.58	108.64	102.55
56	JG	501	GTP	C8-N7-C5	3.57	108.63	102.55
56	GE	501	GTP	C8-N7-C5	3.57	108.63	102.55
56	SB	501	GTP	C8-N7-C5	3.57	108.62	102.55
56	SI	501	GTP	C8-N7-C5	3.56	108.62	102.55
56	PL	501	GTP	C8-N7-C5	3.56	108.61	102.55
56	IA	501	GTP	C8-N7-C5	3.56	108.61	102.55
56	VG	501	GTP	C8-N7-C5	3.56	108.61	102.55
56	EA	501	GTP	C8-N7-C5	3.56	108.61	102.55
56	RK	501	GTP	C8-N7-C5	3.55	108.60	102.55
56	RG	501	GTP	C8-N7-C5	3.55	108.60	102.55
56	CK	501	GTP	C8-N7-C5	3.55	108.59	102.55
56	DG	501	GTP	C8-N7-C5	3.55	108.59	102.55
56	WG	501	GTP	C8-N7-C5	3.55	108.58	102.55
56	RL	501	GTP	C8-N7-C5	3.53	108.56	102.55
56	NG	501	GTP	C8-N7-C5	3.53	108.56	102.55
56	OK	501	GTP	C8-N7-C5	3.53	108.55	102.55
56	EE	501	GTP	C8-N7-C5	3.52	108.55	102.55
56	RE	501	GTP	C8-N7-C5	3.49	108.49	102.55
56	PA	501	GTP	C8-N7-C5	3.39	108.32	102.55
56	TG	501	GTP	C2-N1-C6	-3.15	119.35	125.11
56	EE	501	GTP	C5-C6-N1	3.13	120.05	114.07
56	CB	501	GTP	C5-C6-N1	3.11	120.00	114.07
56	BE	501	GTP	C2-N1-C6	-3.08	119.47	125.11
56	PB	501	GTP	C5-C6-N1	3.08	119.94	114.07
56	OL	501	GTP	C5-C6-N1	3.07	119.93	114.07
56	BE	501	GTP	C5-C6-N1	3.06	119.92	114.07
56	FB	501	GTP	C5-C6-N1	3.06	119.91	114.07
56	LE	501	GTP	C5-C6-N1	3.05	119.90	114.07
56	IA	501	GTP	C5-C6-N1	3.05	119.89	114.07
56	EG	501	GTP	C5-C6-N1	3.04	119.88	114.07
56	SG	501	GTP	C5-C6-N1	3.04	119.87	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	EC	501	GTP	C5-C6-N1	3.04	119.87	114.07
56	CE	501	GTP	C5-C6-N1	3.04	119.86	114.07
56	RG	501	GTP	C5-C6-N1	3.03	119.86	114.07
56	OA	501	GTP	C5-C6-N1	3.03	119.84	114.07
56	GB	501	GTP	C5-C6-N1	3.03	119.84	114.07
56	SG	501	GTP	C2-N1-C6	-3.02	119.58	125.11
56	WB	501	GTP	C5-C6-N1	3.02	119.84	114.07
56	PI	501	GTP	C2-N1-C6	-3.02	119.58	125.11
56	RL	501	GTP	C5-C6-N1	3.02	119.83	114.07
56	KK	501	GTP	C5-C6-N1	3.02	119.83	114.07
56	FA	501	GTP	C2-N1-C6	-3.02	119.59	125.11
56	QG	501	GTP	C2-N1-C6	-3.02	119.59	125.11
56	JA	501	GTP	C5-C6-N1	3.02	119.82	114.07
56	FA	501	GTP	C5-C6-N1	3.01	119.82	114.07
56	TB	501	GTP	C5-C6-N1	3.01	119.82	114.07
56	JB	501	GTP	C5-C6-N1	3.01	119.82	114.07
56	BM	501	GTP	C2-N1-C6	-3.01	119.59	125.11
56	BI	501	GTP	C5-C6-N1	3.01	119.81	114.07
56	IB	501	GTP	C5-C6-N1	3.01	119.81	114.07
56	PE	501	GTP	C5-C6-N1	3.01	119.81	114.07
56	PL	501	GTP	C5-C6-N1	3.01	119.81	114.07
56	RG	501	GTP	C2-N1-C6	-3.01	119.60	125.11
56	OE	501	GTP	C5-C6-N1	3.01	119.81	114.07
56	LK	501	GTP	C5-C6-N1	3.01	119.81	114.07
56	PB	501	GTP	C2-N1-C6	-3.01	119.60	125.11
56	MG	501	GTP	C5-C6-N1	3.01	119.81	114.07
56	NG	501	GTP	C2-N1-C6	-3.01	119.61	125.11
56	OA	501	GTP	C2-N1-C6	-3.01	119.61	125.11
56	KB	501	GTP	C5-C6-N1	3.00	119.80	114.07
56	HE	501	GTP	C5-C6-N1	3.00	119.80	114.07
56	SB	501	GTP	C5-C6-N1	3.00	119.80	114.07
56	OI	501	GTP	C2-N1-C6	-3.00	119.61	125.11
56	VB	501	GTP	C2-N1-C6	-3.00	119.61	125.11
56	KA	501	GTP	C5-C6-N1	3.00	119.80	114.07
56	HK	501	GTP	C5-C6-N1	3.00	119.80	114.07
58	PC	501	GDP	C8-N7-C5	3.00	107.66	102.55
56	JB	501	GTP	C2-N1-C6	-3.00	119.62	125.11
56	UE	501	GTP	C2-N1-C6	-3.00	119.62	125.11
56	HB	501	GTP	C2-N1-C6	-3.00	119.62	125.11
56	TK	501	GTP	C5-C6-N1	3.00	119.79	114.07
56	TB	501	GTP	C2-N1-C6	-3.00	119.62	125.11
56	IE	501	GTP	C5-C6-N1	3.00	119.79	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	EB	501	GDP	C8-N7-C5	3.00	107.65	102.55
56	OL	501	GTP	C2-N1-C6	-2.99	119.63	125.11
56	KA	501	GTP	C2-N1-C6	-2.99	119.63	125.11
56	AB	501	GTP	C2-N1-C6	-2.99	119.63	125.11
56	NB	501	GTP	C5-C6-N1	2.99	119.78	114.07
56	WE	501	GTP	C5-C6-N1	2.99	119.78	114.07
56	GK	501	GTP	C5-C6-N1	2.99	119.78	114.07
56	VK	501	GTP	C5-C6-N1	2.99	119.78	114.07
56	UE	501	GTP	C5-C6-N1	2.99	119.78	114.07
56	EA	501	GTP	C2-N1-C6	-2.99	119.64	125.11
56	OE	501	GTP	C2-N1-C6	-2.99	119.64	125.11
56	DA	501	GTP	C5-C6-N1	2.99	119.78	114.07
56	SA	501	GTP	C5-C6-N1	2.99	119.78	114.07
56	SK	501	GTP	C5-C6-N1	2.99	119.78	114.07
56	AI	501	GTP	C5-C6-N1	2.99	119.78	114.07
56	BI	501	GTP	C2-N1-C6	-2.99	119.64	125.11
56	JG	501	GTP	C5-C6-N1	2.99	119.77	114.07
56	SI	501	GTP	C5-C6-N1	2.99	119.77	114.07
56	QL	501	GTP	C2-N1-C6	-2.99	119.64	125.11
56	IA	501	GTP	C2-N1-C6	-2.99	119.64	125.11
56	OI	501	GTP	C5-C6-N1	2.99	119.77	114.07
56	LA	501	GTP	C5-C6-N1	2.99	119.77	114.07
56	JG	501	GTP	C2-N1-C6	-2.99	119.64	125.11
56	QL	501	GTP	C5-C6-N1	2.99	119.77	114.07
56	DE	501	GTP	C5-C6-N1	2.98	119.77	114.07
56	PI	501	GTP	C5-C6-N1	2.98	119.76	114.07
58	WD	501	GDP	C8-N7-C5	2.98	107.63	102.55
56	FB	501	GTP	C2-N1-C6	-2.98	119.65	125.11
56	WI	501	GTP	C2-N1-C6	-2.98	119.65	125.11
56	MK	501	GTP	C5-C6-N1	2.98	119.76	114.07
56	RB	501	GTP	C5-C6-N1	2.98	119.76	114.07
56	DI	501	GTP	C2-N1-C6	-2.98	119.65	125.11
56	BG	501	GTP	C5-C6-N1	2.98	119.76	114.07
56	TK	501	GTP	C2-N1-C6	-2.98	119.66	125.11
56	DB	501	GTP	C5-C6-N1	2.98	119.76	114.07
56	CA	501	GTP	C5-C6-N1	2.98	119.75	114.07
56	HB	501	GTP	C5-C6-N1	2.98	119.75	114.07
56	VK	501	GTP	C2-N1-C6	-2.98	119.66	125.11
56	IE	501	GTP	C2-N1-C6	-2.98	119.66	125.11
56	OK	501	GTP	C2-N1-C6	-2.98	119.66	125.11
56	SE	501	GTP	C5-C6-N1	2.98	119.75	114.07
56	JA	501	GTP	C2-N1-C6	-2.98	119.66	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	EG	501	GTP	C2-N1-C6	-2.98	119.66	125.11
56	JE	501	GTP	C5-C6-N1	2.98	119.75	114.07
56	WK	501	GTP	C5-C6-N1	2.98	119.75	114.07
56	IK	501	GTP	C2-N1-C6	-2.98	119.66	125.11
56	AM	501	GTP	C5-C6-N1	2.98	119.75	114.07
56	FI	501	GTP	C5-C6-N1	2.98	119.75	114.07
56	LE	501	GTP	C2-N1-C6	-2.98	119.66	125.11
56	QA	501	GTP	C5-C6-N1	2.98	119.75	114.07
56	NE	501	GTP	C2-N1-C6	-2.97	119.67	125.11
56	WG	501	GTP	C5-C6-N1	2.97	119.75	114.07
56	NE	501	GTP	C5-C6-N1	2.97	119.74	114.07
56	BG	501	GTP	C2-N1-C6	-2.97	119.67	125.11
56	RE	501	GTP	C5-C6-N1	2.97	119.74	114.07
56	BA	501	GTP	C2-N1-C6	-2.97	119.67	125.11
56	KG	501	GTP	C5-C6-N1	2.97	119.74	114.07
56	TG	501	GTP	C5-C6-N1	2.97	119.74	114.07
56	VA	501	GTP	C2-N1-C6	-2.97	119.67	125.11
56	FK	501	GTP	C5-C6-N1	2.97	119.74	114.07
56	PK	501	GTP	C5-C6-N1	2.97	119.74	114.07
56	WK	501	GTP	C2-N1-C6	-2.97	119.68	125.11
56	QG	501	GTP	C5-C6-N1	2.97	119.73	114.07
56	RI	501	GTP	C5-C6-N1	2.97	119.73	114.07
58	IC	501	GDP	C8-N7-C5	2.97	107.60	102.55
56	PL	501	GTP	C2-N1-C6	-2.97	119.68	125.11
56	SK	501	GTP	C2-N1-C6	-2.97	119.68	125.11
56	IK	501	GTP	C5-C6-N1	2.97	119.73	114.07
56	MB	501	GTP	C5-C6-N1	2.97	119.73	114.07
58	VC	501	GDP	C8-N7-C5	2.97	107.60	102.55
56	NG	501	GTP	C5-C6-N1	2.97	119.73	114.07
56	EK	501	GTP	C5-C6-N1	2.97	119.73	114.07
56	QK	501	GTP	C5-C6-N1	2.97	119.73	114.07
56	UA	501	GTP	C5-C6-N1	2.97	119.73	114.07
56	IM	501	GTP	C2-N1-C6	-2.97	119.68	125.11
56	VA	501	GTP	C5-C6-N1	2.96	119.73	114.07
56	CE	501	GTP	C2-N1-C6	-2.96	119.68	125.11
56	CM	501	GTP	C2-N1-C6	-2.96	119.68	125.11
56	GG	501	GTP	C5-C6-N1	2.96	119.72	114.07
56	TA	501	GTP	C5-C6-N1	2.96	119.72	114.07
56	TE	501	GTP	C5-C6-N1	2.96	119.72	114.07
56	KI	501	GTP	C5-C6-N1	2.96	119.72	114.07
56	BB	501	GTP	C5-C6-N1	2.96	119.72	114.07
56	FG	501	GTP	C5-C6-N1	2.96	119.72	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	EK	501	GTP	C2-N1-C6	-2.96	119.69	125.11
56	WE	501	GTP	C2-N1-C6	-2.96	119.69	125.11
58	FL	501	GDP	C8-N7-C5	2.96	107.59	102.55
56	PG	501	GTP	C5-C6-N1	2.96	119.72	114.07
56	EE	501	GTP	C2-N1-C6	-2.96	119.69	125.11
56	OB	501	GTP	C2-N1-C6	-2.96	119.69	125.11
56	II	501	GTP	C2-N1-C6	-2.96	119.69	125.11
56	UA	501	GTP	C2-N1-C6	-2.96	119.69	125.11
56	AB	501	GTP	C5-C6-N1	2.96	119.72	114.07
56	HI	501	GTP	C5-C6-N1	2.96	119.72	114.07
56	EI	501	GTP	C5-C6-N1	2.96	119.72	114.07
56	IB	501	GTP	C2-N1-C6	-2.96	119.69	125.11
56	ME	501	GTP	C5-C6-N1	2.96	119.72	114.07
56	EC	501	GTP	C2-N1-C6	-2.96	119.69	125.11
56	NA	501	GTP	C5-C6-N1	2.96	119.71	114.07
56	RA	501	GTP	C5-C6-N1	2.96	119.71	114.07
56	PG	501	GTP	C2-N1-C6	-2.96	119.70	125.11
56	HA	501	GTP	C5-C6-N1	2.96	119.71	114.07
56	II	501	GTP	C5-C6-N1	2.96	119.71	114.07
56	VE	501	GTP	C5-C6-N1	2.96	119.71	114.07
56	AK	501	GTP	C5-C6-N1	2.96	119.71	114.07
56	DG	501	GTP	C5-C6-N1	2.96	119.71	114.07
56	MA	501	GTP	C5-C6-N1	2.96	119.71	114.07
56	OG	501	GTP	C5-C6-N1	2.96	119.71	114.07
56	DK	501	GTP	C2-N1-C6	-2.95	119.70	125.11
56	UB	501	GTP	C2-N1-C6	-2.95	119.70	125.11
56	SB	501	GTP	C2-N1-C6	-2.95	119.70	125.11
56	FI	501	GTP	C2-N1-C6	-2.95	119.70	125.11
56	VE	501	GTP	C2-N1-C6	-2.95	119.70	125.11
56	GE	501	GTP	C5-C6-N1	2.95	119.70	114.07
56	AA	501	GTP	C2-N1-C6	-2.95	119.71	125.11
56	JK	501	GTP	C2-N1-C6	-2.95	119.71	125.11
58	EL	501	GDP	C8-N7-C5	2.95	107.58	102.55
56	JE	501	GTP	C2-N1-C6	-2.95	119.71	125.11
56	LB	501	GTP	C5-C6-N1	2.95	119.70	114.07
56	HE	501	GTP	C2-N1-C6	-2.95	119.71	125.11
56	MG	501	GTP	C2-N1-C6	-2.95	119.71	125.11
56	IM	501	GTP	C5-C6-N1	2.95	119.70	114.07
56	GB	501	GTP	C2-N1-C6	-2.95	119.71	125.11
56	OG	501	GTP	C2-N1-C6	-2.95	119.71	125.11
56	BA	501	GTP	C5-C6-N1	2.95	119.69	114.07
56	CM	501	GTP	C5-C6-N1	2.95	119.69	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	NI	501	GTP	C5-C6-N1	2.95	119.69	114.07
56	DG	501	GTP	C2-N1-C6	-2.95	119.72	125.11
56	AA	501	GTP	C5-C6-N1	2.95	119.69	114.07
56	UB	501	GTP	C5-C6-N1	2.95	119.69	114.07
56	CI	501	GTP	C5-C6-N1	2.95	119.69	114.07
56	JI	501	GTP	C5-C6-N1	2.95	119.69	114.07
56	HI	501	GTP	C2-N1-C6	-2.95	119.72	125.11
56	VI	501	GTP	C2-N1-C6	-2.95	119.72	125.11
56	RK	501	GTP	C5-C6-N1	2.95	119.69	114.07
56	KK	501	GTP	C2-N1-C6	-2.94	119.72	125.11
58	FF	501	GDP	C8-N7-C5	2.94	107.56	102.55
56	BB	501	GTP	C2-N1-C6	-2.94	119.72	125.11
58	EM	501	GDP	C8-N7-C5	2.94	107.56	102.55
56	AK	501	GTP	C2-N1-C6	-2.94	119.72	125.11
56	VB	501	GTP	C5-C6-N1	2.94	119.69	114.07
58	ID	501	GDP	C8-N7-C5	2.94	107.56	102.55
56	HG	501	GTP	C5-C6-N1	2.94	119.68	114.07
56	LG	501	GTP	C5-C6-N1	2.94	119.68	114.07
56	WB	501	GTP	C2-N1-C6	-2.94	119.72	125.11
56	IG	501	GTP	C2-N1-C6	-2.94	119.73	125.11
56	DI	501	GTP	C5-C6-N1	2.94	119.68	114.07
56	TA	501	GTP	C2-N1-C6	-2.94	119.73	125.11
56	MA	501	GTP	C2-N1-C6	-2.94	119.73	125.11
56	FE	501	GTP	C5-C6-N1	2.94	119.68	114.07
56	LI	501	GTP	C5-C6-N1	2.94	119.68	114.07
56	ML	501	GTP	C5-C6-N1	2.94	119.68	114.07
58	OM	501	GDP	C8-N7-C5	2.94	107.55	102.55
56	PE	501	GTP	C2-N1-C6	-2.94	119.73	125.11
56	OB	501	GTP	C5-C6-N1	2.94	119.67	114.07
56	LA	501	GTP	C2-N1-C6	-2.94	119.73	125.11
56	LK	501	GTP	C2-N1-C6	-2.94	119.73	125.11
56	PK	501	GTP	C2-N1-C6	-2.94	119.73	125.11
56	VI	501	GTP	C5-C6-N1	2.94	119.67	114.07
58	BF	501	GDP	C8-N7-C5	2.94	107.55	102.55
56	AG	501	GTP	C2-N1-C6	-2.94	119.74	125.11
56	HA	501	GTP	C2-N1-C6	-2.93	119.74	125.11
56	NI	501	GTP	C2-N1-C6	-2.93	119.74	125.11
56	NL	501	GTP	C2-N1-C6	-2.93	119.74	125.11
56	WI	501	GTP	C5-C6-N1	2.93	119.67	114.07
56	WG	501	GTP	C2-N1-C6	-2.93	119.74	125.11
56	NL	501	GTP	C5-C6-N1	2.93	119.67	114.07
56	JK	501	GTP	C5-C6-N1	2.93	119.67	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	LC	501	GDP	C8-N7-C5	2.93	107.54	102.55
56	MI	501	GTP	C5-C6-N1	2.93	119.66	114.07
56	AI	501	GTP	C2-N1-C6	-2.93	119.74	125.11
56	CB	501	GTP	C2-N1-C6	-2.93	119.74	125.11
56	DM	501	GTP	C5-C6-N1	2.93	119.66	114.07
56	UK	501	GTP	C5-C6-N1	2.93	119.66	114.07
56	RA	501	GTP	C2-N1-C6	-2.93	119.75	125.11
56	EA	501	GTP	C5-C6-N1	2.93	119.66	114.07
56	DE	501	GTP	C2-N1-C6	-2.93	119.75	125.11
56	QI	501	GTP	C2-N1-C6	-2.93	119.75	125.11
56	RI	501	GTP	C2-N1-C6	-2.93	119.75	125.11
56	AE	501	GTP	C5-C6-N1	2.93	119.66	114.07
56	BM	501	GTP	C5-C6-N1	2.93	119.66	114.07
56	DB	501	GTP	C2-N1-C6	-2.93	119.75	125.11
56	LG	501	GTP	C2-N1-C6	-2.93	119.75	125.11
56	MB	501	GTP	C2-N1-C6	-2.93	119.75	125.11
56	SE	501	GTP	C2-N1-C6	-2.93	119.75	125.11
58	BD	501	GDP	C8-N7-C5	2.93	107.53	102.55
58	PD	501	GDP	C8-N7-C5	2.93	107.53	102.55
56	BK	501	GTP	C5-C6-N1	2.93	119.66	114.07
56	SI	501	GTP	C2-N1-C6	-2.93	119.75	125.11
58	EF	501	GDP	C8-N7-C5	2.93	107.53	102.55
56	CK	501	GTP	C2-N1-C6	-2.93	119.75	125.11
56	NB	501	GTP	C2-N1-C6	-2.93	119.75	125.11
56	IG	501	GTP	C5-C6-N1	2.93	119.65	114.07
56	RB	501	GTP	C2-N1-C6	-2.93	119.75	125.11
56	QA	501	GTP	C2-N1-C6	-2.92	119.76	125.11
56	OK	501	GTP	C5-C6-N1	2.92	119.65	114.07
56	CA	501	GTP	C2-N1-C6	-2.92	119.76	125.11
56	FK	501	GTP	C2-N1-C6	-2.92	119.76	125.11
58	QD	501	GDP	C8-N7-C5	2.92	107.53	102.55
58	UC	501	GDP	C8-N7-C5	2.92	107.53	102.55
56	BK	501	GTP	C2-N1-C6	-2.92	119.76	125.11
56	HK	501	GTP	C2-N1-C6	-2.92	119.76	125.11
56	LB	501	GTP	C2-N1-C6	-2.92	119.76	125.11
56	WA	501	GTP	C2-N1-C6	-2.92	119.76	125.11
56	FG	501	GTP	C2-N1-C6	-2.92	119.76	125.11
56	NA	501	GTP	C2-N1-C6	-2.92	119.76	125.11
56	AM	501	GTP	C2-N1-C6	-2.92	119.77	125.11
58	TH	501	GDP	C8-N7-C5	2.92	107.52	102.55
56	KE	501	GTP	C5-C6-N1	2.92	119.64	114.07
56	HG	501	GTP	C2-N1-C6	-2.92	119.77	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	GL	501	GDP	C8-N7-C5	2.92	107.51	102.55
56	AG	501	GTP	C5-C6-N1	2.92	119.63	114.07
56	CG	501	GTP	C2-N1-C6	-2.92	119.77	125.11
58	LL	501	GDP	C8-N7-C5	2.91	107.51	102.55
58	NC	501	GDP	C8-N7-C5	2.91	107.51	102.55
58	TL	501	GDP	C8-N7-C5	2.91	107.51	102.55
58	UL	501	GDP	C8-N7-C5	2.91	107.51	102.55
56	EI	501	GTP	C2-N1-C6	-2.91	119.78	125.11
58	CJ	501	GDP	C8-N7-C5	2.91	107.51	102.55
56	FE	501	GTP	C2-N1-C6	-2.91	119.78	125.11
56	GG	501	GTP	C2-N1-C6	-2.91	119.78	125.11
56	JI	501	GTP	C2-N1-C6	-2.91	119.78	125.11
58	SL	501	GDP	C8-N7-C5	2.91	107.51	102.55
58	JC	501	GDP	C8-N7-C5	2.91	107.50	102.55
56	CI	501	GTP	C2-N1-C6	-2.91	119.78	125.11
56	MK	501	GTP	C2-N1-C6	-2.91	119.78	125.11
56	RK	501	GTP	C2-N1-C6	-2.91	119.78	125.11
56	GK	501	GTP	C2-N1-C6	-2.91	119.78	125.11
56	ML	501	GTP	C2-N1-C6	-2.91	119.78	125.11
58	AJ	501	GDP	C8-N7-C5	2.91	107.50	102.55
56	KI	501	GTP	C2-N1-C6	-2.91	119.79	125.11
56	VG	501	GTP	C5-C6-N1	2.91	119.61	114.07
58	BH	501	GDP	C8-N7-C5	2.90	107.50	102.55
58	NH	501	GDP	C8-N7-C5	2.90	107.50	102.55
56	GE	501	GTP	C2-N1-C6	-2.90	119.79	125.11
56	AE	501	GTP	C2-N1-C6	-2.90	119.79	125.11
58	FC	501	GDP	C8-N7-C5	2.90	107.49	102.55
56	LI	501	GTP	C2-N1-C6	-2.90	119.80	125.11
56	UG	501	GTP	C5-C6-N1	2.90	119.61	114.07
56	CK	501	GTP	C5-C6-N1	2.90	119.61	114.07
58	WC	501	GDP	C8-N7-C5	2.90	107.49	102.55
58	UH	501	GDP	C8-N7-C5	2.90	107.49	102.55
58	LH	501	GDP	C8-N7-C5	2.90	107.49	102.55
58	NF	501	GDP	C8-N7-C5	2.90	107.49	102.55
56	QB	501	GTP	C5-C6-N1	2.90	119.60	114.07
58	UJ	501	GDP	C8-N7-C5	2.90	107.49	102.55
56	ME	501	GTP	C2-N1-C6	-2.90	119.80	125.11
58	DH	501	GDP	C8-N7-C5	2.90	107.48	102.55
58	JF	501	GDP	C8-N7-C5	2.90	107.48	102.55
56	UG	501	GTP	C2-N1-C6	-2.90	119.80	125.11
58	DL	501	GDP	C8-N7-C5	2.90	107.48	102.55
58	FJ	501	GDP	C8-N7-C5	2.90	107.48	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	VH	501	GDP	C8-N7-C5	2.90	107.48	102.55
56	GI	501	GTP	C5-C6-N1	2.90	119.60	114.07
56	WA	501	GTP	C5-C6-N1	2.90	119.60	114.07
58	BJ	501	GDP	C8-N7-C5	2.89	107.48	102.55
58	LJ	501	GDP	C8-N7-C5	2.89	107.48	102.55
58	HH	501	GDP	C8-N7-C5	2.89	107.47	102.55
58	UM	501	GDP	C8-N7-C5	2.89	107.47	102.55
56	DA	501	GTP	C2-N1-C6	-2.89	119.81	125.11
56	KG	501	GTP	C2-N1-C6	-2.89	119.81	125.11
58	KD	501	GDP	C8-N7-C5	2.89	107.47	102.55
56	UK	501	GTP	C2-N1-C6	-2.89	119.82	125.11
56	KE	501	GTP	C2-N1-C6	-2.89	119.82	125.11
56	RE	501	GTP	C2-N1-C6	-2.89	119.82	125.11
56	DK	501	GTP	C5-C6-N1	2.89	119.58	114.07
56	QE	501	GTP	C5-C6-N1	2.89	119.58	114.07
56	GI	501	GTP	C2-N1-C6	-2.89	119.82	125.11
56	QK	501	GTP	C2-N1-C6	-2.89	119.82	125.11
56	UI	501	GTP	C2-N1-C6	-2.89	119.82	125.11
58	GD	501	GDP	C8-N7-C5	2.89	107.47	102.55
58	ND	501	GDP	C8-N7-C5	2.89	107.47	102.55
58	JJ	501	GDP	C8-N7-C5	2.89	107.46	102.55
58	KM	501	GDP	C8-N7-C5	2.88	107.46	102.55
58	NK	501	GDP	C8-N7-C5	2.88	107.46	102.55
56	TE	501	GTP	C2-N1-C6	-2.88	119.83	125.11
58	WH	501	GDP	C8-N7-C5	2.88	107.46	102.55
58	HJ	501	GDP	C8-N7-C5	2.88	107.46	102.55
56	KB	501	GTP	C2-N1-C6	-2.88	119.83	125.11
58	FH	501	GDP	C8-N7-C5	2.88	107.45	102.55
56	DM	501	GTP	C2-N1-C6	-2.88	119.84	125.11
56	GA	501	GTP	C5-C6-N1	2.88	119.56	114.07
58	GM	501	GDP	C8-N7-C5	2.88	107.45	102.55
58	CH	501	GDP	C8-N7-C5	2.88	107.45	102.55
58	AF	501	GDP	C8-N7-C5	2.88	107.45	102.55
58	IJ	501	GDP	C8-N7-C5	2.88	107.45	102.55
56	TI	501	GTP	C2-N1-C6	-2.88	119.84	125.11
58	QC	501	GDP	C8-N7-C5	2.88	107.44	102.55
58	HF	501	GDP	C8-N7-C5	2.88	107.44	102.55
58	HL	501	GDP	C8-N7-C5	2.88	107.44	102.55
58	JD	501	GDP	C8-N7-C5	2.87	107.44	102.55
58	OF	501	GDP	C8-N7-C5	2.87	107.44	102.55
56	VG	501	GTP	C2-N1-C6	-2.87	119.85	125.11
58	EJ	501	GDP	C8-N7-C5	2.87	107.44	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	QM	501	GDP	C8-N7-C5	2.87	107.44	102.55
58	IL	501	GDP	C8-N7-C5	2.87	107.43	102.55
58	LF	501	GDP	C8-N7-C5	2.87	107.43	102.55
58	PM	501	GDP	C8-N7-C5	2.87	107.43	102.55
56	MI	501	GTP	C2-N1-C6	-2.87	119.86	125.11
56	UI	501	GTP	C5-C6-N1	2.87	119.54	114.07
58	TM	501	GDP	C8-N7-C5	2.87	107.43	102.55
58	CC	501	GDP	C8-N7-C5	2.87	107.43	102.55
58	UF	501	GDP	C8-N7-C5	2.87	107.43	102.55
58	SM	501	GDP	C8-N7-C5	2.87	107.43	102.55
58	WF	501	GDP	C8-N7-C5	2.86	107.42	102.55
58	FD	501	GDP	C8-N7-C5	2.86	107.42	102.55
56	SA	501	GTP	C2-N1-C6	-2.86	119.87	125.11
56	QE	501	GTP	C2-N1-C6	-2.86	119.87	125.11
58	OC	501	GDP	C8-N7-C5	2.86	107.42	102.55
58	SD	501	GDP	C8-N7-C5	2.86	107.42	102.55
56	TI	501	GTP	C5-C6-N1	2.86	119.53	114.07
58	TF	501	GDP	C8-N7-C5	2.86	107.42	102.55
58	VF	501	GDP	C8-N7-C5	2.86	107.41	102.55
56	PA	501	GTP	C2-N1-C6	-2.86	119.88	125.11
58	EH	501	GDP	C8-N7-C5	2.85	107.41	102.55
58	MH	501	GDP	C8-N7-C5	2.85	107.41	102.55
56	QB	501	GTP	C2-N1-C6	-2.85	119.89	125.11
58	KJ	501	GDP	C8-N7-C5	2.85	107.40	102.55
58	MD	501	GDP	C8-N7-C5	2.85	107.40	102.55
58	NJ	501	GDP	C8-N7-C5	2.85	107.40	102.55
58	CF	501	GDP	C8-N7-C5	2.85	107.40	102.55
58	IH	501	GDP	C8-N7-C5	2.85	107.40	102.55
58	LM	501	GDP	C8-N7-C5	2.85	107.40	102.55
56	GA	501	GTP	C2-N1-C6	-2.85	119.89	125.11
58	VJ	501	GDP	C8-N7-C5	2.85	107.40	102.55
58	WL	501	GDP	C8-N7-C5	2.85	107.40	102.55
58	DC	501	GDP	C8-N7-C5	2.85	107.40	102.55
58	HD	501	GDP	C8-N7-C5	2.85	107.40	102.55
58	SF	501	GDP	C8-N7-C5	2.85	107.40	102.55
58	JM	501	GDP	C8-N7-C5	2.85	107.39	102.55
58	RJ	501	GDP	C8-N7-C5	2.85	107.39	102.55
58	PF	501	GDP	C2-N1-C6	-2.85	119.90	125.11
58	GF	501	GDP	C8-N7-C5	2.84	107.39	102.55
58	RC	501	GDP	C8-N7-C5	2.84	107.39	102.55
58	SH	501	GDP	C8-N7-C5	2.84	107.39	102.55
58	IF	501	GDP	C8-N7-C5	2.84	107.39	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	KL	501	GDP	C8-N7-C5	2.84	107.39	102.55
58	BC	501	GDP	C8-N7-C5	2.84	107.39	102.55
58	BL	501	GDP	C8-N7-C5	2.84	107.39	102.55
58	LD	501	GDP	C8-N7-C5	2.84	107.39	102.55
58	MM	501	GDP	C8-N7-C5	2.84	107.39	102.55
58	QJ	501	GDP	C8-N7-C5	2.84	107.39	102.55
58	SJ	501	GDP	C8-N7-C5	2.84	107.39	102.55
58	AC	501	GDP	C8-N7-C5	2.84	107.38	102.55
58	GC	501	GDP	C8-N7-C5	2.84	107.38	102.55
58	PH	501	GDP	C8-N7-C5	2.84	107.38	102.55
58	RH	501	GDP	C8-N7-C5	2.84	107.38	102.55
58	AH	501	GDP	C8-N7-C5	2.84	107.38	102.55
58	TC	501	GDP	C8-N7-C5	2.84	107.38	102.55
58	HM	501	GDP	C8-N7-C5	2.84	107.38	102.55
58	TJ	501	GDP	C8-N7-C5	2.84	107.38	102.55
56	RL	501	GTP	C2-N1-C6	-2.83	119.92	125.11
56	CG	501	GTP	C5-C6-N1	2.83	119.47	114.07
58	KF	501	GDP	C8-N7-C5	2.83	107.37	102.55
58	PJ	501	GDP	C8-N7-C5	2.83	107.37	102.55
58	MJ	501	GDP	C8-N7-C5	2.83	107.37	102.55
58	WJ	501	GDP	C8-N7-C5	2.83	107.37	102.55
58	AL	501	GDP	C8-N7-C5	2.83	107.37	102.55
58	NM	501	GDP	C8-N7-C5	2.83	107.36	102.55
58	KC	501	GDP	C8-N7-C5	2.83	107.36	102.55
58	KH	501	GDP	C8-N7-C5	2.82	107.35	102.55
58	GJ	501	GDP	C8-N7-C5	2.82	107.34	102.55
58	OJ	501	GDP	C8-N7-C5	2.82	107.34	102.55
58	OH	501	GDP	C8-N7-C5	2.81	107.34	102.55
56	PA	501	GTP	C5-C6-N1	2.81	119.44	114.07
58	CD	501	GDP	C8-N7-C5	2.81	107.33	102.55
58	ED	501	GDP	C8-N7-C5	2.81	107.33	102.55
58	MF	501	GDP	C8-N7-C5	2.81	107.33	102.55
58	RD	501	GDP	C8-N7-C5	2.81	107.33	102.55
58	MC	501	GDP	C8-N7-C5	2.80	107.32	102.55
58	PF	501	GDP	O6-C6-N1	2.80	123.94	120.62
58	GH	501	GDP	C4'-O4'-C1'	2.80	112.49	109.92
58	DJ	501	GDP	C8-N7-C5	2.80	107.31	102.55
58	RM	501	GDP	C8-N7-C5	2.79	107.30	102.55
58	OD	501	GDP	C8-N7-C5	2.79	107.30	102.55
58	SC	501	GDP	C8-N7-C5	2.78	107.29	102.55
58	FM	501	GDP	C8-N7-C5	2.78	107.27	102.55
58	JH	501	GDP	C8-N7-C5	2.77	107.26	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	CL	501	GDP	C8-N7-C5	2.76	107.26	102.55
56	QI	501	GTP	C5-C6-N1	2.76	119.34	114.07
58	VD	501	GDP	C8-N7-C5	2.75	107.23	102.55
56	BM	501	GTP	O3G-PG-O3B	2.74	113.82	104.64
58	TD	501	GDP	C8-N7-C5	2.74	107.21	102.55
58	PF	501	GDP	C5-C6-N1	2.73	119.27	114.07
58	GH	501	GDP	C8-N7-C5	2.73	107.19	102.55
58	VM	501	GDP	C8-N7-C5	2.69	107.13	102.55
58	RF	501	GDP	C8-N7-C5	2.64	107.04	102.55
58	UD	501	GDP	C8-N7-C5	2.60	106.98	102.55
58	PF	501	GDP	C8-N7-C5	2.58	106.94	102.55
56	MA	501	GTP	C4'-O4'-C1'	2.58	112.28	109.92
58	DF	501	GDP	C8-N7-C5	2.57	106.92	102.55
56	BG	501	GTP	O3G-PG-O3B	2.55	113.19	104.64
56	EA	501	GTP	C4'-O4'-C1'	2.53	112.24	109.92
58	UD	501	GDP	O4'-C1'-N9	-2.50	105.43	108.75
58	DD	501	GDP	C8-N7-C5	2.50	106.81	102.55
58	HC	501	GDP	C8-N7-C5	2.49	106.80	102.55
56	BE	501	GTP	C4'-O4'-C1'	2.49	112.21	109.92
58	QH	501	GDP	C5-C6-N1	2.47	118.79	114.07
56	RL	501	GTP	O3G-PG-O3B	2.47	112.92	104.64
56	RL	501	GTP	C4'-O4'-C1'	2.44	112.16	109.92
58	VD	501	GDP	C2'-C3'-C4'	2.42	107.28	102.61
56	DK	501	GTP	C4'-O4'-C1'	2.41	112.13	109.92
58	JL	501	GDP	C8-N7-C5	2.41	106.65	102.55
58	IC	501	GDP	C4'-O4'-C1'	2.40	112.12	109.92
58	VD	501	GDP	C5-C6-N1	2.38	118.61	114.07
56	RE	501	GTP	O6-C6-C5	-2.36	119.64	124.32
56	PA	501	GTP	C4'-O4'-C1'	2.36	112.09	109.92
56	QI	501	GTP	O6-C6-C5	-2.36	119.65	124.32
58	QF	501	GDP	C8-N7-C5	2.35	106.55	102.55
56	EA	501	GTP	O6-C6-C5	-2.34	119.67	124.32
58	VH	501	GDP	C4'-O4'-C1'	2.34	112.07	109.92
56	BK	501	GTP	O3G-PG-O3B	2.32	112.40	104.64
56	SK	501	GTP	O6-C6-C5	-2.29	119.77	124.32
58	QF	501	GDP	C4'-O4'-C1'	2.29	112.03	109.92
58	AD	501	GDP	C8-N7-C5	2.25	106.38	102.55
56	BK	501	GTP	C4'-O4'-C1'	2.25	111.98	109.92
58	CF	501	GDP	C5-C6-N1	2.25	118.36	114.07
58	UD	501	GDP	C5-C6-N1	2.24	118.34	114.07
56	UE	501	GTP	O6-C6-C5	-2.24	119.89	124.32
58	JC	501	GDP	C5-C6-N1	2.23	118.33	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	EI	501	GTP	O6-C6-C5	-2.23	119.91	124.32
58	AD	501	GDP	C2'-C3'-C4'	2.23	106.91	102.61
56	JG	501	GTP	O6-C6-C5	-2.23	119.91	124.32
58	VM	501	GDP	C4'-O4'-C1'	2.22	111.96	109.92
58	RM	501	GDP	C5-C6-N1	2.22	118.30	114.07
56	QI	501	GTP	C4'-O4'-C1'	2.22	111.95	109.92
56	TK	501	GTP	O6-C6-C5	-2.22	119.93	124.32
58	TD	501	GDP	O6-C6-C5	-2.21	119.93	124.32
56	EE	501	GTP	O6-C6-C5	-2.21	119.94	124.32
58	NF	501	GDP	C5-C6-N1	2.21	118.29	114.07
56	TG	501	GTP	O6-C6-C5	-2.21	119.94	124.32
58	LL	501	GDP	C5-C6-N1	2.21	118.28	114.07
56	MA	501	GTP	O6-C6-C5	-2.21	119.95	124.32
56	LK	501	GTP	O6-C6-C5	-2.20	119.95	124.32
58	RM	501	GDP	C2'-C3'-C4'	2.20	106.86	102.61
58	EM	501	GDP	C5-C6-N1	2.20	118.27	114.07
58	FM	501	GDP	C5-C6-N1	2.19	118.26	114.07
56	UI	501	GTP	C4'-O4'-C1'	2.19	111.93	109.92
56	SA	501	GTP	O6-C6-C5	-2.19	119.97	124.32
56	QL	501	GTP	O6-C6-C5	-2.19	119.98	124.32
56	MG	501	GTP	O6-C6-C5	-2.19	119.98	124.32
56	FA	501	GTP	O6-C6-C5	-2.19	119.98	124.32
56	SB	501	GTP	O6-C6-C5	-2.19	119.98	124.32
56	SE	501	GTP	O6-C6-C5	-2.19	119.98	124.32
56	JE	501	GTP	O6-C6-C5	-2.19	119.98	124.32
58	DJ	501	GDP	C4'-O4'-C1'	2.18	111.93	109.92
56	IB	501	GTP	O6-C6-C5	-2.18	119.99	124.32
56	TB	501	GTP	O6-C6-C5	-2.18	119.99	124.32
56	RI	501	GTP	O6-C6-C5	-2.18	120.00	124.32
58	HC	501	GDP	C2'-C3'-C4'	2.18	106.82	102.61
56	LI	501	GTP	O6-C6-C5	-2.18	120.00	124.32
56	RK	501	GTP	O6-C6-C5	-2.17	120.01	124.32
56	PI	501	GTP	O6-C6-C5	-2.17	120.01	124.32
58	FH	501	GDP	C5-C6-N1	2.17	118.21	114.07
56	EK	501	GTP	O6-C6-C5	-2.17	120.02	124.32
58	OD	501	GDP	C4'-O4'-C1'	2.17	111.91	109.92
58	UM	501	GDP	C4'-O4'-C1'	2.17	111.91	109.92
56	AB	501	GTP	O6-C6-C5	-2.17	120.02	124.32
56	NG	501	GTP	O6-C6-C5	-2.17	120.02	124.32
58	GL	501	GDP	C5-C6-N1	2.17	118.20	114.07
58	UL	501	GDP	C2'-C3'-C4'	2.17	106.80	102.61
56	JK	501	GTP	O6-C6-C5	-2.17	120.03	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	RD	501	GDP	C5-C6-N1	2.17	118.20	114.07
56	AM	501	GTP	O6-C6-C5	-2.16	120.03	124.32
58	PM	501	GDP	C5-C6-N1	2.16	118.19	114.07
56	RA	501	GTP	O6-C6-C5	-2.16	120.04	124.32
58	LC	501	GDP	C5-C6-N1	2.16	118.19	114.07
56	HA	501	GTP	O6-C6-C5	-2.16	120.04	124.32
56	HB	501	GTP	O6-C6-C5	-2.16	120.04	124.32
56	BE	501	GTP	O6-C6-C5	-2.15	120.05	124.32
56	SI	501	GTP	O6-C6-C5	-2.15	120.05	124.32
56	FI	501	GTP	O6-C6-C5	-2.15	120.05	124.32
56	KI	501	GTP	O6-C6-C5	-2.15	120.05	124.32
56	BA	501	GTP	O6-C6-C5	-2.15	120.06	124.32
56	LG	501	GTP	O6-C6-C5	-2.15	120.06	124.32
58	CJ	501	GDP	C5-C6-N1	2.15	118.17	114.07
56	VG	501	GTP	C4'-O4'-C1'	2.15	111.89	109.92
58	VL	501	GDP	C8-N7-C5	2.15	106.21	102.55
56	TE	501	GTP	O6-C6-C5	-2.15	120.06	124.32
56	ML	501	GTP	C4'-O4'-C1'	2.14	111.89	109.92
58	QH	501	GDP	O2B-PB-O3A	2.14	111.83	104.64
56	FE	501	GTP	O6-C6-C5	-2.14	120.07	124.32
58	FL	501	GDP	C5-C6-N1	2.14	118.16	114.07
56	WI	501	GTP	O6-C6-C5	-2.14	120.07	124.32
58	OJ	501	GDP	C5-C6-N1	2.14	118.16	114.07
58	TF	501	GDP	C5-C6-N1	2.14	118.16	114.07
56	AK	501	GTP	O6-C6-C5	-2.14	120.08	124.32
56	BI	501	GTP	O6-C6-C5	-2.14	120.08	124.32
56	NL	501	GTP	O6-C6-C5	-2.14	120.08	124.32
56	RB	501	GTP	O6-C6-C5	-2.14	120.08	124.32
56	TI	501	GTP	O6-C6-C5	-2.14	120.08	124.32
58	EH	501	GDP	C2'-C3'-C4'	2.14	106.74	102.61
58	BL	501	GDP	C5-C6-N1	2.14	118.15	114.07
56	IG	501	GTP	O6-C6-C5	-2.14	120.08	124.32
56	HG	501	GTP	O6-C6-C5	-2.14	120.08	124.32
56	CB	501	GTP	O6-C6-C5	-2.13	120.09	124.32
56	VA	501	GTP	O6-C6-C5	-2.13	120.09	124.32
56	KG	501	GTP	O6-C6-C5	-2.13	120.09	124.32
56	WG	501	GTP	O6-C6-C5	-2.13	120.09	124.32
58	EB	501	GDP	C5-C6-N1	2.13	118.14	114.07
58	ID	501	GDP	C5-C6-N1	2.13	118.14	114.07
56	PL	501	GTP	O6-C6-C5	-2.13	120.09	124.32
56	SG	501	GTP	O6-C6-C5	-2.13	120.10	124.32
56	CK	501	GTP	O6-C6-C5	-2.13	120.10	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	EC	501	GTP	O6-C6-C5	-2.13	120.10	124.32
58	EJ	501	GDP	C5-C6-N1	2.13	118.13	114.07
56	QA	501	GTP	O6-C6-C5	-2.13	120.10	124.32
56	FG	501	GTP	O6-C6-C5	-2.13	120.10	124.32
58	WD	501	GDP	C5-C6-N1	2.13	118.13	114.07
56	KE	501	GTP	O6-C6-C5	-2.13	120.10	124.32
56	HI	501	GTP	O6-C6-C5	-2.13	120.10	124.32
56	LB	501	GTP	O6-C6-C5	-2.13	120.10	124.32
56	QK	501	GTP	O6-C6-C5	-2.13	120.10	124.32
56	NE	501	GTP	O6-C6-C5	-2.13	120.10	124.32
56	IM	501	GTP	O6-C6-C5	-2.13	120.11	124.32
58	BF	501	GDP	C5-C6-N1	2.13	118.12	114.07
56	MB	501	GTP	O6-C6-C5	-2.12	120.11	124.32
56	UG	501	GTP	O6-C6-C5	-2.12	120.11	124.32
58	GJ	501	GDP	C5-C6-N1	2.12	118.12	114.07
58	LH	501	GDP	C5-C6-N1	2.12	118.12	114.07
58	EH	501	GDP	C5-C6-N1	2.12	118.12	114.07
58	UH	501	GDP	C5-C6-N1	2.12	118.12	114.07
58	JC	501	GDP	C2'-C3'-C4'	2.12	106.71	102.61
56	UK	501	GTP	O6-C6-C5	-2.12	120.12	124.32
56	AE	501	GTP	O6-C6-C5	-2.12	120.12	124.32
56	LA	501	GTP	O6-C6-C5	-2.12	120.12	124.32
56	WA	501	GTP	O6-C6-C5	-2.12	120.12	124.32
56	RG	501	GTP	O6-C6-C5	-2.12	120.12	124.32
56	AA	501	GTP	O6-C6-C5	-2.12	120.12	124.32
56	OK	501	GTP	O6-C6-C5	-2.12	120.13	124.32
58	PH	501	GDP	C5-C6-N1	2.12	118.11	114.07
58	ED	501	GDP	C5-C6-N1	2.12	118.11	114.07
58	IL	501	GDP	C5-C6-N1	2.11	118.10	114.07
56	AG	501	GTP	O6-C6-C5	-2.11	120.13	124.32
56	JB	501	GTP	O6-C6-C5	-2.11	120.13	124.32
56	DM	501	GTP	O6-C6-C5	-2.11	120.14	124.32
58	WJ	501	GDP	C5-C6-N1	2.11	118.10	114.07
56	BM	501	GTP	O6-C6-C5	-2.11	120.14	124.32
58	OM	501	GDP	C5-C6-N1	2.11	118.09	114.07
56	IK	501	GTP	O6-C6-C5	-2.11	120.14	124.32
58	TJ	501	GDP	C5-C6-N1	2.11	118.09	114.07
58	BD	501	GDP	C5-C6-N1	2.10	118.08	114.07
56	II	501	GTP	O6-C6-C5	-2.10	120.15	124.32
58	BJ	501	GDP	C5-C6-N1	2.10	118.08	114.07
56	JA	501	GTP	O6-C6-C5	-2.10	120.15	124.32
58	RJ	501	GDP	C5-C6-N1	2.10	118.08	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	VB	501	GTP	O6-C6-C5	-2.10	120.15	124.32
58	BD	501	GDP	C2'-C3'-C4'	2.10	106.67	102.61
58	AF	501	GDP	C5-C6-N1	2.10	118.08	114.07
56	UA	501	GTP	O6-C6-C5	-2.10	120.16	124.32
58	SJ	501	GDP	C5-C6-N1	2.10	118.08	114.07
58	EL	501	GDP	C5-C6-N1	2.10	118.08	114.07
58	IH	501	GDP	C5-C6-N1	2.10	118.08	114.07
58	LF	501	GDP	C5-C6-N1	2.10	118.08	114.07
56	WK	501	GTP	O6-C6-C5	-2.10	120.16	124.32
58	VF	501	GDP	C5-C6-N1	2.10	118.07	114.07
56	FK	501	GTP	O6-C6-C5	-2.10	120.16	124.32
56	GE	501	GTP	O6-C6-C5	-2.10	120.16	124.32
56	DA	501	GTP	O6-C6-C5	-2.10	120.16	124.32
58	HH	501	GDP	C5-C6-N1	2.10	118.07	114.07
56	UI	501	GTP	O6-C6-C5	-2.10	120.17	124.32
58	RC	501	GDP	C5-C6-N1	2.10	118.07	114.07
58	NC	501	GDP	C5-C6-N1	2.09	118.07	114.07
58	FJ	501	GDP	C5-C6-N1	2.09	118.06	114.07
58	JF	501	GDP	C2'-C3'-C4'	2.09	106.66	102.61
56	IA	501	GTP	O6-C6-C5	-2.09	120.17	124.32
58	IJ	501	GDP	C5-C6-N1	2.09	118.06	114.07
56	AI	501	GTP	C4'-O4'-C1'	2.09	111.84	109.92
56	TA	501	GTP	O6-C6-C5	-2.09	120.17	124.32
58	TL	501	GDP	C5-C6-N1	2.09	118.06	114.07
58	UF	501	GDP	C5-C6-N1	2.09	118.06	114.07
58	AJ	501	GDP	C5-C6-N1	2.09	118.06	114.07
58	WC	501	GDP	C5-C6-N1	2.09	118.06	114.07
58	DH	501	GDP	C5-C6-N1	2.09	118.06	114.07
56	KA	501	GTP	O6-C6-C5	-2.09	120.18	124.32
56	VE	501	GTP	O6-C6-C5	-2.09	120.18	124.32
58	AC	501	GDP	C5-C6-N1	2.09	118.05	114.07
58	JF	501	GDP	C5-C6-N1	2.09	118.05	114.07
56	VK	501	GTP	O6-C6-C5	-2.09	120.18	124.32
58	MH	501	GDP	C5-C6-N1	2.09	118.05	114.07
56	ML	501	GTP	O6-C6-C5	-2.09	120.18	124.32
58	ND	501	GDP	C5-C6-N1	2.09	118.05	114.07
58	GF	501	GDP	C5-C6-N1	2.09	118.05	114.07
58	VC	501	GDP	C5-C6-N1	2.08	118.05	114.07
56	DK	501	GTP	O6-C6-C5	-2.08	120.19	124.32
56	VG	501	GTP	O6-C6-C5	-2.08	120.19	124.32
58	WH	501	GDP	C5-C6-N1	2.08	118.05	114.07
56	QB	501	GTP	O6-C6-C5	-2.08	120.19	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	QE	501	GTP	O6-C6-C5	-2.08	120.19	124.32
58	GD	501	GDP	C5-C6-N1	2.08	118.04	114.07
58	SF	501	GDP	C4'-O4'-C1'	2.08	111.83	109.92
58	QM	501	GDP	C5-C6-N1	2.08	118.04	114.07
58	TC	501	GDP	C5-C6-N1	2.08	118.04	114.07
58	NM	501	GDP	C5-C6-N1	2.08	118.04	114.07
56	KK	501	GTP	O6-C6-C5	-2.08	120.19	124.32
58	TH	501	GDP	C5-C6-N1	2.08	118.04	114.07
58	FC	501	GDP	C5-C6-N1	2.08	118.04	114.07
58	SC	501	GDP	C5-C6-N1	2.08	118.04	114.07
58	KC	501	GDP	C5-C6-N1	2.08	118.04	114.07
58	VJ	501	GDP	C5-C6-N1	2.08	118.03	114.07
56	ME	501	GTP	O6-C6-C5	-2.08	120.20	124.32
58	OH	501	GDP	C5-C6-N1	2.08	118.03	114.07
58	JH	501	GDP	C5-C6-N1	2.08	118.03	114.07
58	NH	501	GDP	C5-C6-N1	2.08	118.03	114.07
56	DE	501	GTP	O6-C6-C5	-2.08	120.20	124.32
56	UB	501	GTP	O6-C6-C5	-2.08	120.20	124.32
58	JD	501	GDP	C5-C6-N1	2.08	118.03	114.07
58	KF	501	GDP	C5-C6-N1	2.07	118.03	114.07
56	DG	501	GTP	O6-C6-C5	-2.07	120.21	124.32
58	FD	501	GDP	C5-C6-N1	2.07	118.03	114.07
58	PD	501	GDP	C5-C6-N1	2.07	118.02	114.07
56	RI	501	GTP	O2A-PA-O3A	2.07	112.87	107.27
58	AD	501	GDP	C5-C6-N1	2.07	118.02	114.07
58	GC	501	GDP	C5-C6-N1	2.07	118.02	114.07
58	QC	501	GDP	C5-C6-N1	2.07	118.02	114.07
56	PA	501	GTP	O6-C6-C5	-2.07	120.22	124.32
58	WL	501	GDP	C2'-C3'-C4'	2.07	106.61	102.61
56	WG	501	GTP	C4'-O4'-C1'	2.07	111.82	109.92
58	RH	501	GDP	C4'-O4'-C1'	2.07	111.82	109.92
58	OC	501	GDP	C5-C6-N1	2.07	118.02	114.07
58	RH	501	GDP	C5-C6-N1	2.07	118.02	114.07
58	UC	501	GDP	C5-C6-N1	2.07	118.02	114.07
56	KB	501	GTP	O6-C6-C5	-2.07	120.22	124.32
58	DC	501	GDP	C5-C6-N1	2.07	118.02	114.07
58	CD	501	GDP	C5-C6-N1	2.07	118.02	114.07
58	KD	501	GDP	C5-C6-N1	2.07	118.02	114.07
58	BH	501	GDP	C5-C6-N1	2.07	118.01	114.07
58	HD	501	GDP	C5-C6-N1	2.07	118.01	114.07
58	OF	501	GDP	C5-C6-N1	2.07	118.01	114.07
58	VH	501	GDP	C5-C6-N1	2.07	118.01	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	MM	501	GDP	C5-C6-N1	2.07	118.01	114.07
58	CH	501	GDP	C5-C6-N1	2.06	118.01	114.07
58	HJ	501	GDP	C5-C6-N1	2.06	118.01	114.07
58	HF	501	GDP	C5-C6-N1	2.06	118.00	114.07
58	SM	501	GDP	C5-C6-N1	2.06	118.00	114.07
56	IB	501	GTP	C4'-O4'-C1'	2.06	111.81	109.92
56	CI	501	GTP	O6-C6-C5	-2.06	120.23	124.32
58	KL	501	GDP	C5-C6-N1	2.06	118.00	114.07
58	AL	501	GDP	C5-C6-N1	2.06	118.00	114.07
56	GB	501	GTP	O6-C6-C5	-2.06	120.24	124.32
56	OE	501	GTP	O6-C6-C5	-2.06	120.24	124.32
56	WA	501	GTP	C4'-O4'-C1'	2.06	111.81	109.92
56	EG	501	GTP	O6-C6-C5	-2.06	120.24	124.32
56	GK	501	GTP	O6-C6-C5	-2.06	120.24	124.32
58	FF	501	GDP	C5-C6-N1	2.06	118.00	114.07
58	EF	501	GDP	C5-C6-N1	2.06	117.99	114.07
58	QD	501	GDP	C5-C6-N1	2.06	117.99	114.07
56	OL	501	GTP	O6-C6-C5	-2.06	120.24	124.32
58	SH	501	GDP	C5-C6-N1	2.06	117.99	114.07
56	HE	501	GTP	O6-C6-C5	-2.06	120.25	124.32
58	VD	501	GDP	O6-C6-C5	-2.05	120.25	124.32
58	JM	501	GDP	C5-C6-N1	2.05	117.99	114.07
58	NJ	501	GDP	C5-C6-N1	2.05	117.99	114.07
58	UJ	501	GDP	C5-C6-N1	2.05	117.99	114.07
58	LD	501	GDP	C5-C6-N1	2.05	117.99	114.07
58	QJ	501	GDP	C2'-C3'-C4'	2.05	106.58	102.61
56	PG	501	GTP	O6-C6-C5	-2.05	120.25	124.32
58	CC	501	GDP	C5-C6-N1	2.05	117.99	114.07
58	KJ	501	GDP	C5-C6-N1	2.05	117.99	114.07
56	IE	501	GTP	O6-C6-C5	-2.05	120.25	124.32
58	MC	501	GDP	C5-C6-N1	2.05	117.98	114.07
58	LM	501	GDP	C5-C6-N1	2.05	117.98	114.07
58	BC	501	GDP	C5-C6-N1	2.05	117.98	114.07
58	MJ	501	GDP	C5-C6-N1	2.05	117.98	114.07
58	CL	501	GDP	C5-C6-N1	2.05	117.98	114.07
58	TM	501	GDP	C5-C6-N1	2.05	117.98	114.07
56	OI	501	GTP	O6-C6-C5	-2.05	120.26	124.32
58	OD	501	GDP	C5-C6-N1	2.05	117.97	114.07
58	MD	501	GDP	C5-C6-N1	2.05	117.97	114.07
58	SF	501	GDP	C5-C6-N1	2.05	117.97	114.07
56	BG	501	GTP	O6-C6-C5	-2.04	120.27	124.32
56	AI	501	GTP	O6-C6-C5	-2.04	120.27	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	NK	501	GDP	C5-C6-N1	2.04	117.97	114.07
56	NB	501	GTP	O6-C6-C5	-2.04	120.28	124.32
58	JJ	501	GDP	C5-C6-N1	2.04	117.96	114.07
58	IC	501	GDP	C5-C6-N1	2.04	117.96	114.07
56	OG	501	GTP	O6-C6-C5	-2.04	120.28	124.32
58	OM	501	GDP	C2'-C3'-C4'	2.04	106.55	102.61
56	QG	501	GTP	O6-C6-C5	-2.04	120.28	124.32
58	PJ	501	GDP	C5-C6-N1	2.04	117.95	114.07
58	AH	501	GDP	C5-C6-N1	2.03	117.95	114.07
58	QJ	501	GDP	C5-C6-N1	2.03	117.95	114.07
56	VI	501	GTP	O6-C6-C5	-2.03	120.30	124.32
56	HK	501	GTP	O4'-C1'-N9	2.03	111.44	108.75
56	FB	501	GTP	O6-C6-C5	-2.03	120.30	124.32
56	PK	501	GTP	O6-C6-C5	-2.03	120.30	124.32
56	WE	501	GTP	O6-C6-C5	-2.03	120.30	124.32
58	UM	501	GDP	C5-C6-N1	2.03	117.94	114.07
58	LJ	501	GDP	C5-C6-N1	2.03	117.94	114.07
56	NI	501	GTP	O6-C6-C5	-2.03	120.30	124.32
58	KH	501	GDP	C5-C6-N1	2.03	117.93	114.07
58	GM	501	GDP	C5-C6-N1	2.02	117.93	114.07
58	UL	501	GDP	C5-C6-N1	2.02	117.93	114.07
58	WF	501	GDP	C5-C6-N1	2.02	117.93	114.07
56	KE	501	GTP	C4'-O4'-C1'	2.02	111.78	109.92
56	CK	501	GTP	O3G-PG-O3B	2.02	111.42	104.64
58	SL	501	GDP	C5-C6-N1	2.02	117.93	114.07
58	KM	501	GDP	C5-C6-N1	2.02	117.93	114.07
58	GH	501	GDP	C5-C6-N1	2.02	117.92	114.07
56	NA	501	GTP	O6-C6-C5	-2.02	120.32	124.32
58	HM	501	GDP	C5-C6-N1	2.02	117.92	114.07
56	BK	501	GTP	O6-C6-C5	-2.02	120.32	124.32
56	OA	501	GTP	O6-C6-C5	-2.02	120.32	124.32
56	JI	501	GTP	O6-C6-C5	-2.02	120.32	124.32
58	QF	501	GDP	C5-C6-N1	2.02	117.92	114.07
58	DH	501	GDP	C2'-C3'-C4'	2.02	106.50	102.61
58	SC	501	GDP	C4'-O4'-C1'	2.02	111.77	109.92
56	OB	501	GTP	O6-C6-C5	-2.01	120.33	124.32
58	DJ	501	GDP	C5-C6-N1	2.01	117.91	114.07
56	CM	501	GTP	O6-C6-C5	-2.01	120.33	124.32
56	CG	501	GTP	O6-C6-C5	-2.01	120.34	124.32
58	WD	501	GDP	C2'-C3'-C4'	2.01	106.49	102.61
58	PC	501	GDP	C5-C6-N1	2.01	117.90	114.07
56	DB	501	GTP	O6-C6-C5	-2.00	120.35	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	LG	501	GTP	C4'-O4'-C1'	2.00	111.76	109.92
58	NH	501	GDP	C2'-C3'-C4'	2.00	106.47	102.61

There are no chirality outliers.

All (937) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	AA	501	GTP	C5'-O5'-PA-O3A
56	AA	501	GTP	C5'-O5'-PA-O1A
56	AA	501	GTP	C5'-O5'-PA-O2A
56	AB	501	GTP	C5'-O5'-PA-O3A
56	AE	501	GTP	C5'-O5'-PA-O3A
56	AE	501	GTP	C5'-O5'-PA-O1A
56	AE	501	GTP	C5'-O5'-PA-O2A
56	AG	501	GTP	C5'-O5'-PA-O3A
56	AG	501	GTP	C5'-O5'-PA-O1A
56	AG	501	GTP	C5'-O5'-PA-O2A
56	AI	501	GTP	C5'-O5'-PA-O3A
56	AI	501	GTP	C5'-O5'-PA-O2A
56	AK	501	GTP	C5'-O5'-PA-O3A
56	AK	501	GTP	C5'-O5'-PA-O1A
56	AM	501	GTP	C5'-O5'-PA-O3A
56	AM	501	GTP	C5'-O5'-PA-O1A
56	AM	501	GTP	C5'-O5'-PA-O2A
56	BA	501	GTP	C5'-O5'-PA-O3A
56	BA	501	GTP	C5'-O5'-PA-O2A
56	BB	501	GTP	C5'-O5'-PA-O3A
56	BB	501	GTP	C5'-O5'-PA-O2A
56	BE	501	GTP	C5'-O5'-PA-O3A
56	BE	501	GTP	C5'-O5'-PA-O2A
56	BG	501	GTP	C5'-O5'-PA-O3A
56	BG	501	GTP	C5'-O5'-PA-O1A
56	BI	501	GTP	C5'-O5'-PA-O3A
56	BI	501	GTP	C5'-O5'-PA-O1A
56	BI	501	GTP	C5'-O5'-PA-O2A
56	BK	501	GTP	PB-O3B-PG-O2G
56	BK	501	GTP	C5'-O5'-PA-O3A
56	BM	501	GTP	C5'-O5'-PA-O3A
56	BM	501	GTP	C5'-O5'-PA-O1A
56	BM	501	GTP	C5'-O5'-PA-O2A
56	CA	501	GTP	C5'-O5'-PA-O3A
56	CA	501	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
56	CB	501	GTP	C5'-O5'-PA-O3A
56	CE	501	GTP	C5'-O5'-PA-O3A
56	CE	501	GTP	C5'-O5'-PA-O2A
56	CG	501	GTP	C5'-O5'-PA-O3A
56	CG	501	GTP	C5'-O5'-PA-O1A
56	CG	501	GTP	C5'-O5'-PA-O2A
56	CI	501	GTP	C5'-O5'-PA-O3A
56	CK	501	GTP	C5'-O5'-PA-O3A
56	CK	501	GTP	C5'-O5'-PA-O2A
56	CM	501	GTP	C5'-O5'-PA-O3A
56	CM	501	GTP	C5'-O5'-PA-O1A
56	CM	501	GTP	C5'-O5'-PA-O2A
56	DA	501	GTP	C5'-O5'-PA-O3A
56	DA	501	GTP	C5'-O5'-PA-O2A
56	DE	501	GTP	C5'-O5'-PA-O3A
56	DG	501	GTP	C5'-O5'-PA-O3A
56	DG	501	GTP	C5'-O5'-PA-O2A
56	DK	501	GTP	C5'-O5'-PA-O3A
56	DK	501	GTP	C5'-O5'-PA-O2A
56	DM	501	GTP	C5'-O5'-PA-O3A
56	DM	501	GTP	C5'-O5'-PA-O2A
56	EA	501	GTP	C5'-O5'-PA-O3A
56	EC	501	GTP	C5'-O5'-PA-O3A
56	EC	501	GTP	C5'-O5'-PA-O2A
56	EG	501	GTP	C5'-O5'-PA-O3A
56	EG	501	GTP	C5'-O5'-PA-O2A
56	EI	501	GTP	C5'-O5'-PA-O3A
56	FA	501	GTP	PB-O3B-PG-O3G
56	FA	501	GTP	C5'-O5'-PA-O3A
56	FA	501	GTP	C5'-O5'-PA-O2A
56	FB	501	GTP	C5'-O5'-PA-O3A
56	FB	501	GTP	C5'-O5'-PA-O2A
56	FE	501	GTP	C5'-O5'-PA-O3A
56	FE	501	GTP	C5'-O5'-PA-O1A
56	FE	501	GTP	C5'-O5'-PA-O2A
56	FG	501	GTP	C5'-O5'-PA-O3A
56	FG	501	GTP	C5'-O5'-PA-O1A
56	FG	501	GTP	C5'-O5'-PA-O2A
56	FI	501	GTP	C5'-O5'-PA-O3A
56	FI	501	GTP	C5'-O5'-PA-O2A
56	FK	501	GTP	C5'-O5'-PA-O3A
56	FK	501	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
56	FK	501	GTP	C5'-O5'-PA-O2A
56	GA	501	GTP	C5'-O5'-PA-O3A
56	GA	501	GTP	C5'-O5'-PA-O1A
56	GA	501	GTP	C5'-O5'-PA-O2A
56	GB	501	GTP	C5'-O5'-PA-O3A
56	GB	501	GTP	C5'-O5'-PA-O2A
56	GE	501	GTP	C5'-O5'-PA-O3A
56	GG	501	GTP	C5'-O5'-PA-O3A
56	GG	501	GTP	C5'-O5'-PA-O2A
56	GI	501	GTP	C5'-O5'-PA-O3A
56	GI	501	GTP	C5'-O5'-PA-O2A
56	GK	501	GTP	C5'-O5'-PA-O3A
56	GK	501	GTP	C5'-O5'-PA-O1A
56	GK	501	GTP	C5'-O5'-PA-O2A
56	HA	501	GTP	C5'-O5'-PA-O3A
56	HB	501	GTP	C5'-O5'-PA-O3A
56	HB	501	GTP	C5'-O5'-PA-O2A
56	HE	501	GTP	C5'-O5'-PA-O3A
56	HE	501	GTP	C5'-O5'-PA-O1A
56	HE	501	GTP	C5'-O5'-PA-O2A
56	HG	501	GTP	C5'-O5'-PA-O3A
56	HG	501	GTP	C5'-O5'-PA-O2A
56	HI	501	GTP	C5'-O5'-PA-O3A
56	HI	501	GTP	C5'-O5'-PA-O1A
56	HI	501	GTP	C5'-O5'-PA-O2A
56	HK	501	GTP	C5'-O5'-PA-O3A
56	HK	501	GTP	C5'-O5'-PA-O1A
56	IA	501	GTP	C5'-O5'-PA-O3A
56	IB	501	GTP	PB-O3B-PG-O2G
56	IB	501	GTP	C5'-O5'-PA-O3A
56	IB	501	GTP	C5'-O5'-PA-O2A
56	IE	501	GTP	C5'-O5'-PA-O3A
56	IE	501	GTP	C5'-O5'-PA-O1A
56	IE	501	GTP	C5'-O5'-PA-O2A
56	IG	501	GTP	C5'-O5'-PA-O3A
56	IG	501	GTP	C5'-O5'-PA-O1A
56	IG	501	GTP	C5'-O5'-PA-O2A
56	II	501	GTP	C5'-O5'-PA-O3A
56	II	501	GTP	C5'-O5'-PA-O1A
56	II	501	GTP	C5'-O5'-PA-O2A
56	IK	501	GTP	C5'-O5'-PA-O3A
56	IK	501	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
56	IM	501	GTP	C5'-O5'-PA-O3A
56	IM	501	GTP	C5'-O5'-PA-O1A
56	IM	501	GTP	C5'-O5'-PA-O2A
56	JA	501	GTP	C5'-O5'-PA-O3A
56	JA	501	GTP	C5'-O5'-PA-O2A
56	JB	501	GTP	C5'-O5'-PA-O3A
56	JB	501	GTP	C5'-O5'-PA-O2A
56	JE	501	GTP	C5'-O5'-PA-O3A
56	JE	501	GTP	C5'-O5'-PA-O2A
56	JG	501	GTP	C5'-O5'-PA-O3A
56	JI	501	GTP	C5'-O5'-PA-O3A
56	JK	501	GTP	C5'-O5'-PA-O3A
56	JK	501	GTP	C5'-O5'-PA-O1A
56	JK	501	GTP	C5'-O5'-PA-O2A
56	KA	501	GTP	C5'-O5'-PA-O3A
56	KB	501	GTP	C5'-O5'-PA-O3A
56	KE	501	GTP	C5'-O5'-PA-O3A
56	KG	501	GTP	C5'-O5'-PA-O3A
56	KG	501	GTP	C5'-O5'-PA-O2A
56	KK	501	GTP	C5'-O5'-PA-O3A
56	KK	501	GTP	C5'-O5'-PA-O1A
56	KK	501	GTP	C5'-O5'-PA-O2A
56	LA	501	GTP	C5'-O5'-PA-O3A
56	LA	501	GTP	C5'-O5'-PA-O1A
56	LA	501	GTP	C5'-O5'-PA-O2A
56	LB	501	GTP	C5'-O5'-PA-O3A
56	LB	501	GTP	C5'-O5'-PA-O2A
56	LE	501	GTP	C5'-O5'-PA-O3A
56	LE	501	GTP	C5'-O5'-PA-O2A
56	LG	501	GTP	C5'-O5'-PA-O3A
56	LG	501	GTP	C5'-O5'-PA-O2A
56	LK	501	GTP	C5'-O5'-PA-O3A
56	LK	501	GTP	C5'-O5'-PA-O1A
56	LK	501	GTP	C5'-O5'-PA-O2A
56	MA	501	GTP	C5'-O5'-PA-O3A
56	MB	501	GTP	C5'-O5'-PA-O3A
56	MB	501	GTP	C5'-O5'-PA-O1A
56	MB	501	GTP	C5'-O5'-PA-O2A
56	ME	501	GTP	C5'-O5'-PA-O3A
56	ME	501	GTP	C5'-O5'-PA-O1A
56	ME	501	GTP	C5'-O5'-PA-O2A
56	MG	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
56	MG	501	GTP	C5'-O5'-PA-O2A
56	MI	501	GTP	C5'-O5'-PA-O3A
56	MI	501	GTP	C5'-O5'-PA-O2A
56	MK	501	GTP	C5'-O5'-PA-O3A
56	MK	501	GTP	C5'-O5'-PA-O1A
56	MK	501	GTP	C5'-O5'-PA-O2A
56	ML	501	GTP	C5'-O5'-PA-O3A
56	ML	501	GTP	C5'-O5'-PA-O2A
56	NA	501	GTP	C5'-O5'-PA-O3A
56	NA	501	GTP	C5'-O5'-PA-O2A
56	NB	501	GTP	C5'-O5'-PA-O3A
56	NB	501	GTP	C5'-O5'-PA-O1A
56	NB	501	GTP	C5'-O5'-PA-O2A
56	NE	501	GTP	C5'-O5'-PA-O3A
56	NE	501	GTP	C5'-O5'-PA-O2A
56	NG	501	GTP	C5'-O5'-PA-O3A
56	NG	501	GTP	C5'-O5'-PA-O1A
56	NG	501	GTP	C5'-O5'-PA-O2A
56	NI	501	GTP	C5'-O5'-PA-O3A
56	NI	501	GTP	C5'-O5'-PA-O1A
56	NI	501	GTP	C5'-O5'-PA-O2A
56	NL	501	GTP	C5'-O5'-PA-O3A
56	NL	501	GTP	C5'-O5'-PA-O1A
56	NL	501	GTP	C5'-O5'-PA-O2A
56	OA	501	GTP	C5'-O5'-PA-O3A
56	OA	501	GTP	C5'-O5'-PA-O2A
56	OB	501	GTP	C5'-O5'-PA-O3A
56	OB	501	GTP	C5'-O5'-PA-O2A
56	OE	501	GTP	C5'-O5'-PA-O3A
56	OE	501	GTP	C5'-O5'-PA-O1A
56	OE	501	GTP	C5'-O5'-PA-O2A
56	OG	501	GTP	C5'-O5'-PA-O3A
56	OG	501	GTP	C5'-O5'-PA-O2A
56	OI	501	GTP	C5'-O5'-PA-O3A
56	OI	501	GTP	C5'-O5'-PA-O1A
56	OI	501	GTP	C5'-O5'-PA-O2A
56	OK	501	GTP	C5'-O5'-PA-O3A
56	OK	501	GTP	C5'-O5'-PA-O2A
56	OL	501	GTP	C5'-O5'-PA-O3A
56	OL	501	GTP	C5'-O5'-PA-O1A
56	OL	501	GTP	C5'-O5'-PA-O2A
56	PA	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
56	PA	501	GTP	C5'-O5'-PA-O2A
56	PB	501	GTP	C5'-O5'-PA-O3A
56	PB	501	GTP	C5'-O5'-PA-O2A
56	PE	501	GTP	C5'-O5'-PA-O3A
56	PE	501	GTP	C5'-O5'-PA-O2A
56	PG	501	GTP	C5'-O5'-PA-O3A
56	PG	501	GTP	C5'-O5'-PA-O1A
56	PG	501	GTP	C5'-O5'-PA-O2A
56	PI	501	GTP	C5'-O5'-PA-O3A
56	PI	501	GTP	C5'-O5'-PA-O2A
56	PL	501	GTP	C5'-O5'-PA-O3A
56	PL	501	GTP	C5'-O5'-PA-O2A
56	QA	501	GTP	C5'-O5'-PA-O3A
56	QA	501	GTP	C5'-O5'-PA-O1A
56	QA	501	GTP	C5'-O5'-PA-O2A
56	QG	501	GTP	C5'-O5'-PA-O3A
56	QG	501	GTP	C5'-O5'-PA-O1A
56	QG	501	GTP	C5'-O5'-PA-O2A
56	QI	501	GTP	C5'-O5'-PA-O3A
56	QK	501	GTP	C5'-O5'-PA-O3A
56	QL	501	GTP	C5'-O5'-PA-O3A
56	QL	501	GTP	C5'-O5'-PA-O1A
56	QL	501	GTP	C5'-O5'-PA-O2A
56	RA	501	GTP	C5'-O5'-PA-O3A
56	RB	501	GTP	C5'-O5'-PA-O3A
56	RB	501	GTP	C5'-O5'-PA-O1A
56	RB	501	GTP	C5'-O5'-PA-O2A
56	RE	501	GTP	C5'-O5'-PA-O3A
56	RI	501	GTP	C5'-O5'-PA-O3A
56	RI	501	GTP	C5'-O5'-PA-O2A
56	RK	501	GTP	C5'-O5'-PA-O3A
56	RL	501	GTP	C5'-O5'-PA-O3A
56	RL	501	GTP	C5'-O5'-PA-O2A
56	SA	501	GTP	C5'-O5'-PA-O3A
56	SA	501	GTP	C5'-O5'-PA-O2A
56	SE	501	GTP	C5'-O5'-PA-O3A
56	SE	501	GTP	C5'-O5'-PA-O1A
56	SE	501	GTP	C5'-O5'-PA-O2A
56	SG	501	GTP	C5'-O5'-PA-O3A
56	SG	501	GTP	C5'-O5'-PA-O1A
56	SG	501	GTP	C5'-O5'-PA-O2A
56	SI	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
56	SK	501	GTP	C5'-O5'-PA-O3A
56	SK	501	GTP	C5'-O5'-PA-O2A
56	TA	501	GTP	C5'-O5'-PA-O3A
56	TA	501	GTP	C5'-O5'-PA-O1A
56	TA	501	GTP	C5'-O5'-PA-O2A
56	TB	501	GTP	C5'-O5'-PA-O3A
56	TB	501	GTP	C5'-O5'-PA-O1A
56	TB	501	GTP	C5'-O5'-PA-O2A
56	TE	501	GTP	C5'-O5'-PA-O3A
56	TE	501	GTP	C5'-O5'-PA-O1A
56	TE	501	GTP	C5'-O5'-PA-O2A
56	TG	501	GTP	C5'-O5'-PA-O3A
56	TG	501	GTP	C5'-O5'-PA-O1A
56	TG	501	GTP	C5'-O5'-PA-O2A
56	TI	501	GTP	C5'-O5'-PA-O3A
56	TI	501	GTP	C5'-O5'-PA-O1A
56	TI	501	GTP	O4'-C4'-C5'-O5'
56	TK	501	GTP	C5'-O5'-PA-O3A
56	TK	501	GTP	C5'-O5'-PA-O1A
56	TK	501	GTP	C5'-O5'-PA-O2A
56	UA	501	GTP	C5'-O5'-PA-O3A
56	UA	501	GTP	C5'-O5'-PA-O1A
56	UA	501	GTP	C5'-O5'-PA-O2A
56	UB	501	GTP	C5'-O5'-PA-O3A
56	UB	501	GTP	C5'-O5'-PA-O2A
56	UE	501	GTP	C5'-O5'-PA-O3A
56	UE	501	GTP	C5'-O5'-PA-O1A
56	UE	501	GTP	C5'-O5'-PA-O2A
56	UG	501	GTP	C5'-O5'-PA-O3A
56	UG	501	GTP	C5'-O5'-PA-O1A
56	UG	501	GTP	C5'-O5'-PA-O2A
56	UI	501	GTP	C5'-O5'-PA-O3A
56	UI	501	GTP	C5'-O5'-PA-O2A
56	UK	501	GTP	C5'-O5'-PA-O3A
56	UK	501	GTP	C5'-O5'-PA-O1A
56	UK	501	GTP	C5'-O5'-PA-O2A
56	VA	501	GTP	C5'-O5'-PA-O3A
56	VA	501	GTP	C5'-O5'-PA-O2A
56	VB	501	GTP	C5'-O5'-PA-O3A
56	VB	501	GTP	C5'-O5'-PA-O1A
56	VB	501	GTP	C5'-O5'-PA-O2A
56	VE	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
56	VE	501	GTP	C5'-O5'-PA-O2A
56	VG	501	GTP	C5'-O5'-PA-O3A
56	VG	501	GTP	C5'-O5'-PA-O2A
56	VI	501	GTP	C5'-O5'-PA-O3A
56	VI	501	GTP	C5'-O5'-PA-O2A
56	VK	501	GTP	C5'-O5'-PA-O3A
56	VK	501	GTP	C5'-O5'-PA-O1A
56	VK	501	GTP	C5'-O5'-PA-O2A
56	WB	501	GTP	C5'-O5'-PA-O3A
56	WB	501	GTP	C5'-O5'-PA-O1A
56	WB	501	GTP	C5'-O5'-PA-O2A
56	WE	501	GTP	C5'-O5'-PA-O3A
56	WE	501	GTP	C5'-O5'-PA-O2A
56	WG	501	GTP	C5'-O5'-PA-O3A
56	WI	501	GTP	C5'-O5'-PA-O3A
56	WI	501	GTP	C5'-O5'-PA-O2A
56	WK	501	GTP	C5'-O5'-PA-O3A
56	WK	501	GTP	C5'-O5'-PA-O1A
56	WK	501	GTP	C5'-O5'-PA-O2A
58	AC	501	GDP	C5'-O5'-PA-O3A
58	AD	501	GDP	C5'-O5'-PA-O3A
58	AD	501	GDP	C5'-O5'-PA-O1A
58	AD	501	GDP	C5'-O5'-PA-O2A
58	AD	501	GDP	O4'-C4'-C5'-O5'
58	AF	501	GDP	C5'-O5'-PA-O3A
58	AH	501	GDP	C5'-O5'-PA-O3A
58	AH	501	GDP	C5'-O5'-PA-O2A
58	AJ	501	GDP	C5'-O5'-PA-O3A
58	AJ	501	GDP	C5'-O5'-PA-O1A
58	AL	501	GDP	C5'-O5'-PA-O3A
58	AL	501	GDP	C5'-O5'-PA-O1A
58	BC	501	GDP	C5'-O5'-PA-O3A
58	BC	501	GDP	C5'-O5'-PA-O1A
58	BD	501	GDP	C5'-O5'-PA-O3A
58	BD	501	GDP	C5'-O5'-PA-O1A
58	BD	501	GDP	C5'-O5'-PA-O2A
58	BF	501	GDP	C5'-O5'-PA-O1A
58	BH	501	GDP	C5'-O5'-PA-O1A
58	BJ	501	GDP	C5'-O5'-PA-O3A
58	BJ	501	GDP	C5'-O5'-PA-O1A
58	BL	501	GDP	C5'-O5'-PA-O3A
58	BL	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
58	CC	501	GDP	C5'-O5'-PA-O3A
58	CC	501	GDP	C5'-O5'-PA-O1A
58	CD	501	GDP	C5'-O5'-PA-O3A
58	CD	501	GDP	C5'-O5'-PA-O2A
58	CF	501	GDP	C5'-O5'-PA-O3A
58	CF	501	GDP	C5'-O5'-PA-O1A
58	CH	501	GDP	C5'-O5'-PA-O3A
58	CH	501	GDP	C5'-O5'-PA-O1A
58	CJ	501	GDP	C5'-O5'-PA-O3A
58	CJ	501	GDP	C5'-O5'-PA-O1A
58	CL	501	GDP	C5'-O5'-PA-O3A
58	DC	501	GDP	C5'-O5'-PA-O3A
58	DC	501	GDP	C5'-O5'-PA-O1A
58	DD	501	GDP	C5'-O5'-PA-O1A
58	DF	501	GDP	C5'-O5'-PA-O1A
58	DH	501	GDP	C5'-O5'-PA-O1A
58	DJ	501	GDP	C5'-O5'-PA-O3A
58	EB	501	GDP	C5'-O5'-PA-O1A
58	ED	501	GDP	C5'-O5'-PA-O3A
58	EF	501	GDP	C5'-O5'-PA-O3A
58	EF	501	GDP	C5'-O5'-PA-O1A
58	EH	501	GDP	C5'-O5'-PA-O3A
58	EJ	501	GDP	C5'-O5'-PA-O1A
58	EM	501	GDP	C5'-O5'-PA-O3A
58	EM	501	GDP	C5'-O5'-PA-O1A
58	FC	501	GDP	C5'-O5'-PA-O3A
58	FC	501	GDP	C5'-O5'-PA-O1A
58	FF	501	GDP	C5'-O5'-PA-O3A
58	FF	501	GDP	C5'-O5'-PA-O1A
58	FH	501	GDP	C5'-O5'-PA-O3A
58	FH	501	GDP	C5'-O5'-PA-O1A
58	FH	501	GDP	C5'-O5'-PA-O2A
58	FJ	501	GDP	C5'-O5'-PA-O3A
58	FJ	501	GDP	C5'-O5'-PA-O1A
58	FL	501	GDP	C5'-O5'-PA-O3A
58	FL	501	GDP	C5'-O5'-PA-O1A
58	GC	501	GDP	C5'-O5'-PA-O3A
58	GC	501	GDP	C5'-O5'-PA-O1A
58	GF	501	GDP	C5'-O5'-PA-O3A
58	GH	501	GDP	C5'-O5'-PA-O1A
58	GJ	501	GDP	C5'-O5'-PA-O3A
58	GJ	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
58	GM	501	GDP	C5'-O5'-PA-O1A
58	HC	501	GDP	C5'-O5'-PA-O3A
58	HC	501	GDP	C5'-O5'-PA-O1A
58	HC	501	GDP	C5'-O5'-PA-O2A
58	HD	501	GDP	C5'-O5'-PA-O3A
58	HD	501	GDP	C5'-O5'-PA-O1A
58	HF	501	GDP	C5'-O5'-PA-O1A
58	HH	501	GDP	C5'-O5'-PA-O1A
58	HJ	501	GDP	C5'-O5'-PA-O1A
58	HL	501	GDP	C5'-O5'-PA-O3A
58	HL	501	GDP	C5'-O5'-PA-O1A
58	HM	501	GDP	C5'-O5'-PA-O1A
58	IC	501	GDP	C5'-O5'-PA-O3A
58	IC	501	GDP	C5'-O5'-PA-O1A
58	ID	501	GDP	C5'-O5'-PA-O3A
58	ID	501	GDP	C5'-O5'-PA-O1A
58	IF	501	GDP	C5'-O5'-PA-O3A
58	IH	501	GDP	C5'-O5'-PA-O3A
58	IJ	501	GDP	C5'-O5'-PA-O1A
58	IL	501	GDP	C5'-O5'-PA-O3A
58	IL	501	GDP	C5'-O5'-PA-O1A
58	JC	501	GDP	C5'-O5'-PA-O3A
58	JC	501	GDP	C5'-O5'-PA-O1A
58	JD	501	GDP	C5'-O5'-PA-O3A
58	JF	501	GDP	C5'-O5'-PA-O3A
58	JF	501	GDP	C5'-O5'-PA-O1A
58	JJ	501	GDP	C5'-O5'-PA-O3A
58	JL	501	GDP	C5'-O5'-PA-O1A
58	JL	501	GDP	O4'-C4'-C5'-O5'
58	JL	501	GDP	C3'-C4'-C5'-O5'
58	JM	501	GDP	C5'-O5'-PA-O1A
58	KC	501	GDP	C5'-O5'-PA-O3A
58	KC	501	GDP	C5'-O5'-PA-O1A
58	KD	501	GDP	C5'-O5'-PA-O3A
58	KF	501	GDP	C5'-O5'-PA-O3A
58	KH	501	GDP	C5'-O5'-PA-O3A
58	KJ	501	GDP	C5'-O5'-PA-O3A
58	KJ	501	GDP	C5'-O5'-PA-O1A
58	KL	501	GDP	C5'-O5'-PA-O3A
58	KL	501	GDP	C5'-O5'-PA-O1A
58	KM	501	GDP	C5'-O5'-PA-O1A
58	LC	501	GDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
58	LC	501	GDP	C5'-O5'-PA-O1A
58	LD	501	GDP	C5'-O5'-PA-O3A
58	LF	501	GDP	C5'-O5'-PA-O3A
58	LF	501	GDP	C5'-O5'-PA-O1A
58	LH	501	GDP	C5'-O5'-PA-O3A
58	LJ	501	GDP	C5'-O5'-PA-O3A
58	LJ	501	GDP	C5'-O5'-PA-O1A
58	LL	501	GDP	C5'-O5'-PA-O1A
58	MC	501	GDP	C5'-O5'-PA-O3A
58	MC	501	GDP	C5'-O5'-PA-O1A
58	MD	501	GDP	C5'-O5'-PA-O1A
58	MF	501	GDP	C5'-O5'-PA-O3A
58	MH	501	GDP	C5'-O5'-PA-O3A
58	MH	501	GDP	C5'-O5'-PA-O1A
58	MJ	501	GDP	C5'-O5'-PA-O3A
58	MM	501	GDP	C5'-O5'-PA-O3A
58	MM	501	GDP	C5'-O5'-PA-O1A
58	NC	501	GDP	C5'-O5'-PA-O3A
58	NC	501	GDP	C5'-O5'-PA-O1A
58	ND	501	GDP	C5'-O5'-PA-O1A
58	NF	501	GDP	C5'-O5'-PA-O3A
58	NF	501	GDP	C5'-O5'-PA-O1A
58	NH	501	GDP	C5'-O5'-PA-O3A
58	NH	501	GDP	C5'-O5'-PA-O1A
58	NJ	501	GDP	C5'-O5'-PA-O3A
58	NJ	501	GDP	C5'-O5'-PA-O1A
58	NK	501	GDP	C5'-O5'-PA-O1A
58	NM	501	GDP	C5'-O5'-PA-O1A
58	OC	501	GDP	C5'-O5'-PA-O3A
58	OD	501	GDP	C5'-O5'-PA-O3A
58	OF	501	GDP	C5'-O5'-PA-O3A
58	OH	501	GDP	C5'-O5'-PA-O3A
58	OJ	501	GDP	C5'-O5'-PA-O1A
58	OM	501	GDP	C5'-O5'-PA-O3A
58	OM	501	GDP	C5'-O5'-PA-O1A
58	PC	501	GDP	C5'-O5'-PA-O3A
58	PC	501	GDP	C5'-O5'-PA-O1A
58	PH	501	GDP	C5'-O5'-PA-O3A
58	PH	501	GDP	C5'-O5'-PA-O1A
58	PJ	501	GDP	C5'-O5'-PA-O3A
58	PJ	501	GDP	C5'-O5'-PA-O1A
58	PM	501	GDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
58	PM	501	GDP	C5'-O5'-PA-O1A
58	QC	501	GDP	C5'-O5'-PA-O3A
58	QC	501	GDP	C5'-O5'-PA-O1A
58	QD	501	GDP	C5'-O5'-PA-O1A
58	QF	501	GDP	C5'-O5'-PA-O3A
58	QF	501	GDP	C5'-O5'-PA-O2A
58	QH	501	GDP	PA-O3A-PB-O2B
58	QH	501	GDP	C5'-O5'-PA-O3A
58	QH	501	GDP	C5'-O5'-PA-O1A
58	QJ	501	GDP	C5'-O5'-PA-O1A
58	QM	501	GDP	C5'-O5'-PA-O3A
58	QM	501	GDP	C5'-O5'-PA-O1A
58	RC	501	GDP	C5'-O5'-PA-O3A
58	RC	501	GDP	C5'-O5'-PA-O1A
58	RD	501	GDP	C5'-O5'-PA-O3A
58	RF	501	GDP	C5'-O5'-PA-O3A
58	RF	501	GDP	C5'-O5'-PA-O1A
58	RF	501	GDP	C5'-O5'-PA-O2A
58	RJ	501	GDP	C5'-O5'-PA-O1A
58	RM	501	GDP	C5'-O5'-PA-O3A
58	RM	501	GDP	C5'-O5'-PA-O1A
58	SC	501	GDP	C5'-O5'-PA-O3A
58	SF	501	GDP	C5'-O5'-PA-O3A
58	SH	501	GDP	C5'-O5'-PA-O3A
58	SH	501	GDP	C5'-O5'-PA-O1A
58	SJ	501	GDP	C5'-O5'-PA-O3A
58	SJ	501	GDP	C5'-O5'-PA-O1A
58	SL	501	GDP	C5'-O5'-PA-O3A
58	SL	501	GDP	C5'-O5'-PA-O1A
58	SM	501	GDP	C5'-O5'-PA-O1A
58	TC	501	GDP	C5'-O5'-PA-O3A
58	TC	501	GDP	C5'-O5'-PA-O1A
58	TD	501	GDP	C5'-O5'-PA-O1A
58	TD	501	GDP	O4'-C4'-C5'-O5'
58	TF	501	GDP	C5'-O5'-PA-O1A
58	TH	501	GDP	C5'-O5'-PA-O3A
58	TH	501	GDP	C5'-O5'-PA-O1A
58	TJ	501	GDP	C5'-O5'-PA-O1A
58	TL	501	GDP	C5'-O5'-PA-O3A
58	TL	501	GDP	C5'-O5'-PA-O1A
58	TM	501	GDP	C5'-O5'-PA-O1A
58	UC	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
58	UD	501	GDP	O4'-C4'-C5'-O5'
58	UF	501	GDP	C5'-O5'-PA-O3A
58	UF	501	GDP	C5'-O5'-PA-O1A
58	UH	501	GDP	C5'-O5'-PA-O3A
58	UH	501	GDP	C5'-O5'-PA-O1A
58	UJ	501	GDP	C5'-O5'-PA-O3A
58	UJ	501	GDP	C5'-O5'-PA-O1A
58	UL	501	GDP	C5'-O5'-PA-O3A
58	UL	501	GDP	C5'-O5'-PA-O1A
58	UL	501	GDP	C5'-O5'-PA-O2A
58	VC	501	GDP	C5'-O5'-PA-O1A
58	VD	501	GDP	C5'-O5'-PA-O1A
58	VF	501	GDP	C5'-O5'-PA-O1A
58	VH	501	GDP	C5'-O5'-PA-O1A
58	VH	501	GDP	O4'-C4'-C5'-O5'
58	VJ	501	GDP	C5'-O5'-PA-O1A
58	VL	501	GDP	C5'-O5'-PA-O3A
58	VL	501	GDP	C5'-O5'-PA-O2A
58	VM	501	GDP	C5'-O5'-PA-O1A
58	WC	501	GDP	C5'-O5'-PA-O1A
58	WD	501	GDP	C5'-O5'-PA-O1A
58	WF	501	GDP	C5'-O5'-PA-O3A
58	WF	501	GDP	C5'-O5'-PA-O1A
58	WH	501	GDP	C5'-O5'-PA-O1A
58	WJ	501	GDP	C5'-O5'-PA-O3A
58	WL	501	GDP	C5'-O5'-PA-O1A
56	AA	501	GTP	O4'-C4'-C5'-O5'
56	AA	501	GTP	C3'-C4'-C5'-O5'
56	BG	501	GTP	C3'-C4'-C5'-O5'
56	BM	501	GTP	O4'-C4'-C5'-O5'
56	BM	501	GTP	C3'-C4'-C5'-O5'
56	HK	501	GTP	O4'-C4'-C5'-O5'
56	HK	501	GTP	C3'-C4'-C5'-O5'
56	II	501	GTP	C3'-C4'-C5'-O5'
56	JK	501	GTP	O4'-C4'-C5'-O5'
56	JK	501	GTP	C3'-C4'-C5'-O5'
56	NB	501	GTP	O4'-C4'-C5'-O5'
56	NI	501	GTP	O4'-C4'-C5'-O5'
56	SE	501	GTP	O4'-C4'-C5'-O5'
56	SE	501	GTP	C3'-C4'-C5'-O5'
56	TG	501	GTP	O4'-C4'-C5'-O5'
56	TG	501	GTP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
56	TI	501	GTP	C3'-C4'-C5'-O5'
56	UG	501	GTP	O4'-C4'-C5'-O5'
56	UG	501	GTP	C3'-C4'-C5'-O5'
56	UK	501	GTP	O4'-C4'-C5'-O5'
56	UK	501	GTP	C3'-C4'-C5'-O5'
58	AD	501	GDP	C3'-C4'-C5'-O5'
58	DD	501	GDP	O4'-C4'-C5'-O5'
58	DD	501	GDP	C3'-C4'-C5'-O5'
58	RF	501	GDP	O4'-C4'-C5'-O5'
58	RF	501	GDP	C3'-C4'-C5'-O5'
58	TD	501	GDP	C3'-C4'-C5'-O5'
58	UD	501	GDP	C3'-C4'-C5'-O5'
58	VH	501	GDP	C3'-C4'-C5'-O5'
56	RL	501	GTP	C4'-C5'-O5'-PA
56	BG	501	GTP	O4'-C4'-C5'-O5'
56	IE	501	GTP	O4'-C4'-C5'-O5'
56	IE	501	GTP	C3'-C4'-C5'-O5'
56	II	501	GTP	O4'-C4'-C5'-O5'
56	NB	501	GTP	C3'-C4'-C5'-O5'
56	NG	501	GTP	O4'-C4'-C5'-O5'
56	NG	501	GTP	C3'-C4'-C5'-O5'
56	NI	501	GTP	C3'-C4'-C5'-O5'
56	OE	501	GTP	O4'-C4'-C5'-O5'
56	OE	501	GTP	C3'-C4'-C5'-O5'
56	OK	501	GTP	O4'-C4'-C5'-O5'
56	PG	501	GTP	O4'-C4'-C5'-O5'
56	PG	501	GTP	C3'-C4'-C5'-O5'
58	DJ	501	GDP	O4'-C4'-C5'-O5'
58	DJ	501	GDP	C3'-C4'-C5'-O5'
58	HC	501	GDP	O4'-C4'-C5'-O5'
58	HC	501	GDP	C3'-C4'-C5'-O5'
56	BK	501	GTP	C4'-C5'-O5'-PA
56	GK	501	GTP	C4'-C5'-O5'-PA
56	IB	501	GTP	C4'-C5'-O5'-PA
56	OK	501	GTP	C3'-C4'-C5'-O5'
56	TB	501	GTP	C3'-C4'-C5'-O5'
56	EG	501	GTP	C4'-C5'-O5'-PA
56	HA	501	GTP	C4'-C5'-O5'-PA
56	JI	501	GTP	C4'-C5'-O5'-PA
56	KB	501	GTP	C4'-C5'-O5'-PA
56	RK	501	GTP	C4'-C5'-O5'-PA
56	VG	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
56	WE	501	GTP	C4'-C5'-O5'-PA
56	BI	501	GTP	C3'-C4'-C5'-O5'
56	HE	501	GTP	C3'-C4'-C5'-O5'
56	IM	501	GTP	C3'-C4'-C5'-O5'
56	OL	501	GTP	C3'-C4'-C5'-O5'
56	TB	501	GTP	O4'-C4'-C5'-O5'
56	EI	501	GTP	C4'-C5'-O5'-PA
56	OL	501	GTP	O4'-C4'-C5'-O5'
56	SG	501	GTP	C3'-C4'-C5'-O5'
56	UA	501	GTP	C3'-C4'-C5'-O5'
58	OD	501	GDP	C3'-C4'-C5'-O5'
58	SD	501	GDP	C3'-C4'-C5'-O5'
56	CA	501	GTP	C4'-C5'-O5'-PA
56	DE	501	GTP	C4'-C5'-O5'-PA
56	FB	501	GTP	C4'-C5'-O5'-PA
56	GE	501	GTP	C4'-C5'-O5'-PA
56	KA	501	GTP	C4'-C5'-O5'-PA
56	LE	501	GTP	C4'-C5'-O5'-PA
56	LG	501	GTP	C4'-C5'-O5'-PA
56	QB	501	GTP	C4'-C5'-O5'-PA
56	QK	501	GTP	C4'-C5'-O5'-PA
56	RA	501	GTP	C4'-C5'-O5'-PA
56	UE	501	GTP	C4'-C5'-O5'-PA
56	WG	501	GTP	C4'-C5'-O5'-PA
56	BI	501	GTP	O4'-C4'-C5'-O5'
56	HE	501	GTP	O4'-C4'-C5'-O5'
56	MK	501	GTP	C3'-C4'-C5'-O5'
56	RL	501	GTP	C3'-C4'-C5'-O5'
56	TA	501	GTP	C3'-C4'-C5'-O5'
58	LJ	501	GDP	C3'-C4'-C5'-O5'
56	GG	501	GTP	C4'-C5'-O5'-PA
56	IK	501	GTP	C4'-C5'-O5'-PA
56	KG	501	GTP	C4'-C5'-O5'-PA
56	PL	501	GTP	C4'-C5'-O5'-PA
56	QE	501	GTP	C4'-C5'-O5'-PA
56	WA	501	GTP	C4'-C5'-O5'-PA
56	FK	501	GTP	C3'-C4'-C5'-O5'
56	IM	501	GTP	O4'-C4'-C5'-O5'
56	QL	501	GTP	C3'-C4'-C5'-O5'
56	VB	501	GTP	C3'-C4'-C5'-O5'
56	WB	501	GTP	C3'-C4'-C5'-O5'
56	HI	501	GTP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
56	II	501	GTP	PB-O3A-PA-O1A
56	OL	501	GTP	PB-O3A-PA-O1A
56	QL	501	GTP	PB-O3A-PA-O1A
56	AB	501	GTP	C4'-C5'-O5'-PA
56	AI	501	GTP	C4'-C5'-O5'-PA
56	BA	501	GTP	C4'-C5'-O5'-PA
56	BB	501	GTP	C4'-C5'-O5'-PA
56	BE	501	GTP	C4'-C5'-O5'-PA
56	CB	501	GTP	C4'-C5'-O5'-PA
56	CE	501	GTP	C4'-C5'-O5'-PA
56	CI	501	GTP	C4'-C5'-O5'-PA
56	DA	501	GTP	C4'-C5'-O5'-PA
56	DM	501	GTP	C4'-C5'-O5'-PA
56	EA	501	GTP	C4'-C5'-O5'-PA
56	EE	501	GTP	C4'-C5'-O5'-PA
56	EK	501	GTP	C4'-C5'-O5'-PA
56	GB	501	GTP	C4'-C5'-O5'-PA
56	JA	501	GTP	C4'-C5'-O5'-PA
56	JB	501	GTP	C4'-C5'-O5'-PA
56	JE	501	GTP	C4'-C5'-O5'-PA
56	JG	501	GTP	C4'-C5'-O5'-PA
56	KE	501	GTP	C4'-C5'-O5'-PA
56	LB	501	GTP	C4'-C5'-O5'-PA
56	MA	501	GTP	C4'-C5'-O5'-PA
56	ML	501	GTP	C4'-C5'-O5'-PA
56	NA	501	GTP	C4'-C5'-O5'-PA
56	OB	501	GTP	C4'-C5'-O5'-PA
56	OG	501	GTP	C4'-C5'-O5'-PA
56	PB	501	GTP	C4'-C5'-O5'-PA
56	RE	501	GTP	C4'-C5'-O5'-PA
56	RG	501	GTP	C4'-C5'-O5'-PA
56	UI	501	GTP	C4'-C5'-O5'-PA
56	VA	501	GTP	C4'-C5'-O5'-PA
56	VI	501	GTP	C4'-C5'-O5'-PA
56	SG	501	GTP	O4'-C4'-C5'-O5'
56	DI	501	GTP	C4'-C5'-O5'-PA
56	EC	501	GTP	C4'-C5'-O5'-PA
56	HG	501	GTP	C4'-C5'-O5'-PA
56	IA	501	GTP	C4'-C5'-O5'-PA
56	KI	501	GTP	C4'-C5'-O5'-PA
56	LI	501	GTP	C4'-C5'-O5'-PA
56	MG	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
56	NE	501	GTP	C4'-C5'-O5'-PA
56	OA	501	GTP	C4'-C5'-O5'-PA
56	PI	501	GTP	C4'-C5'-O5'-PA
56	SB	501	GTP	C4'-C5'-O5'-PA
56	TE	501	GTP	C4'-C5'-O5'-PA
56	TK	501	GTP	C4'-C5'-O5'-PA
56	TA	501	GTP	O4'-C4'-C5'-O5'
56	UA	501	GTP	O4'-C4'-C5'-O5'
56	CK	501	GTP	PB-O3A-PA-O5'
56	FI	501	GTP	C4'-C5'-O5'-PA
58	VL	501	GDP	C3'-C4'-C5'-O5'
56	HK	501	GTP	PB-O3B-PG-O1G
56	RL	501	GTP	PB-O3B-PG-O1G
58	GM	501	GDP	PA-O3A-PB-O1B
56	BB	501	GTP	PB-O3B-PG-O2G
56	BM	501	GTP	PB-O3B-PG-O3G
56	QL	501	GTP	PB-O3B-PG-O3G
56	WI	501	GTP	PB-O3B-PG-O2G
56	CK	501	GTP	C3'-C4'-C5'-O5'
56	DG	501	GTP	C3'-C4'-C5'-O5'
56	QE	501	GTP	C3'-C4'-C5'-O5'
56	RK	501	GTP	C3'-C4'-C5'-O5'
56	VK	501	GTP	C3'-C4'-C5'-O5'
58	SD	501	GDP	O4'-C4'-C5'-O5'
56	CK	501	GTP	C4'-C5'-O5'-PA
56	GA	501	GTP	C4'-C5'-O5'-PA
56	QA	501	GTP	C4'-C5'-O5'-PA
56	QG	501	GTP	C4'-C5'-O5'-PA
56	WB	501	GTP	C4'-C5'-O5'-PA
56	CK	501	GTP	PA-O3A-PB-O2B
56	FE	501	GTP	PB-O3A-PA-O1A
56	FG	501	GTP	PB-O3A-PA-O2A
56	FK	501	GTP	PB-O3A-PA-O2A
56	MB	501	GTP	PB-O3A-PA-O2A
56	OE	501	GTP	PB-O3A-PA-O1A
56	OK	501	GTP	PA-O3A-PB-O2B
56	QA	501	GTP	PB-O3A-PA-O1A
56	UK	501	GTP	PB-O3A-PA-O1A
56	VK	501	GTP	PB-O3A-PA-O1A
56	WB	501	GTP	PB-O3A-PA-O1A
56	WK	501	GTP	PB-O3A-PA-O1A
56	FE	501	GTP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
56	WE	501	GTP	C3'-C4'-C5'-O5'
58	OD	501	GDP	O4'-C4'-C5'-O5'
56	AE	501	GTP	C4'-C5'-O5'-PA
56	BI	501	GTP	C4'-C5'-O5'-PA
56	FE	501	GTP	C4'-C5'-O5'-PA
56	FG	501	GTP	C4'-C5'-O5'-PA
56	FK	501	GTP	C4'-C5'-O5'-PA
56	HB	501	GTP	C4'-C5'-O5'-PA
56	HI	501	GTP	C4'-C5'-O5'-PA
56	IM	501	GTP	C4'-C5'-O5'-PA
56	LA	501	GTP	C4'-C5'-O5'-PA
56	MI	501	GTP	C4'-C5'-O5'-PA
56	MK	501	GTP	C4'-C5'-O5'-PA
56	NB	501	GTP	C4'-C5'-O5'-PA
56	NI	501	GTP	C4'-C5'-O5'-PA
56	NL	501	GTP	C4'-C5'-O5'-PA
56	OK	501	GTP	C4'-C5'-O5'-PA
56	PA	501	GTP	C4'-C5'-O5'-PA
56	RI	501	GTP	C4'-C5'-O5'-PA
56	SA	501	GTP	C4'-C5'-O5'-PA
56	SG	501	GTP	C4'-C5'-O5'-PA
56	TI	501	GTP	C4'-C5'-O5'-PA
56	UK	501	GTP	C4'-C5'-O5'-PA
56	VB	501	GTP	C4'-C5'-O5'-PA
56	VK	501	GTP	C4'-C5'-O5'-PA
56	WK	501	GTP	C4'-C5'-O5'-PA
56	MK	501	GTP	O4'-C4'-C5'-O5'
56	QL	501	GTP	O4'-C4'-C5'-O5'
56	VB	501	GTP	O4'-C4'-C5'-O5'
56	WB	501	GTP	O4'-C4'-C5'-O5'
58	LJ	501	GDP	O4'-C4'-C5'-O5'
56	AB	501	GTP	C5'-O5'-PA-O2A
56	AK	501	GTP	C5'-O5'-PA-O2A
56	BG	501	GTP	C5'-O5'-PA-O2A
56	BK	501	GTP	C5'-O5'-PA-O2A
56	DE	501	GTP	C5'-O5'-PA-O2A
56	DI	501	GTP	C5'-O5'-PA-O3A
56	EK	501	GTP	C5'-O5'-PA-O3A
56	HK	501	GTP	C5'-O5'-PA-O2A
56	JG	501	GTP	C5'-O5'-PA-O2A
56	LI	501	GTP	C5'-O5'-PA-O3A
56	QB	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
56	QK	501	GTP	C5'-O5'-PA-O2A
56	RA	501	GTP	C5'-O5'-PA-O2A
56	TI	501	GTP	C5'-O5'-PA-O2A
58	AC	501	GDP	C5'-O5'-PA-O1A
58	AF	501	GDP	C5'-O5'-PA-O1A
58	AH	501	GDP	C5'-O5'-PA-O1A
58	CD	501	GDP	C5'-O5'-PA-O1A
58	CL	501	GDP	C5'-O5'-PA-O1A
58	DJ	501	GDP	C5'-O5'-PA-O1A
58	DL	501	GDP	C5'-O5'-PA-O1A
58	ED	501	GDP	C5'-O5'-PA-O1A
58	EH	501	GDP	C5'-O5'-PA-O1A
58	EL	501	GDP	C5'-O5'-PA-O1A
58	FD	501	GDP	C5'-O5'-PA-O1A
58	FM	501	GDP	C5'-O5'-PA-O1A
58	GD	501	GDP	C5'-O5'-PA-O1A
58	GF	501	GDP	C5'-O5'-PA-O1A
58	GL	501	GDP	C5'-O5'-PA-O1A
58	HF	501	GDP	C5'-O5'-PA-O3A
58	HJ	501	GDP	C5'-O5'-PA-O3A
58	IF	501	GDP	C5'-O5'-PA-O1A
58	IH	501	GDP	C5'-O5'-PA-O1A
58	JD	501	GDP	C5'-O5'-PA-O1A
58	JH	501	GDP	C5'-O5'-PA-O1A
58	JJ	501	GDP	C5'-O5'-PA-O1A
58	KD	501	GDP	C5'-O5'-PA-O1A
58	KF	501	GDP	C5'-O5'-PA-O1A
58	KH	501	GDP	C5'-O5'-PA-O1A
58	LD	501	GDP	C5'-O5'-PA-O1A
58	LH	501	GDP	C5'-O5'-PA-O1A
58	LM	501	GDP	C5'-O5'-PA-O1A
58	MF	501	GDP	C5'-O5'-PA-O1A
58	MJ	501	GDP	C5'-O5'-PA-O1A
58	NM	501	GDP	C5'-O5'-PA-O3A
58	OC	501	GDP	C5'-O5'-PA-O1A
58	OD	501	GDP	C5'-O5'-PA-O1A
58	OF	501	GDP	C5'-O5'-PA-O1A
58	OH	501	GDP	C5'-O5'-PA-O1A
58	PD	501	GDP	C5'-O5'-PA-O1A
58	PF	501	GDP	C5'-O5'-PA-O1A
58	QF	501	GDP	C5'-O5'-PA-O1A
58	RD	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
58	RH	501	GDP	C5'-O5'-PA-O1A
58	SC	501	GDP	C5'-O5'-PA-O1A
58	SD	501	GDP	C5'-O5'-PA-O1A
58	SF	501	GDP	C5'-O5'-PA-O1A
58	UC	501	GDP	C5'-O5'-PA-O3A
58	UM	501	GDP	C5'-O5'-PA-O1A
58	VL	501	GDP	C5'-O5'-PA-O1A
58	WJ	501	GDP	C5'-O5'-PA-O1A
56	AA	501	GTP	C4'-C5'-O5'-PA
56	AG	501	GTP	C4'-C5'-O5'-PA
56	AM	501	GTP	C4'-C5'-O5'-PA
56	BG	501	GTP	C4'-C5'-O5'-PA
56	CG	501	GTP	C4'-C5'-O5'-PA
56	DB	501	GTP	C4'-C5'-O5'-PA
56	DG	501	GTP	C4'-C5'-O5'-PA
56	DK	501	GTP	C4'-C5'-O5'-PA
56	FA	501	GTP	C4'-C5'-O5'-PA
56	GI	501	GTP	C4'-C5'-O5'-PA
56	HE	501	GTP	C4'-C5'-O5'-PA
56	HK	501	GTP	C4'-C5'-O5'-PA
56	IE	501	GTP	C4'-C5'-O5'-PA
56	IG	501	GTP	C4'-C5'-O5'-PA
56	JK	501	GTP	C4'-C5'-O5'-PA
56	KK	501	GTP	C4'-C5'-O5'-PA
56	MB	501	GTP	C4'-C5'-O5'-PA
56	ME	501	GTP	C4'-C5'-O5'-PA
56	NG	501	GTP	C4'-C5'-O5'-PA
56	OE	501	GTP	C4'-C5'-O5'-PA
56	OI	501	GTP	C4'-C5'-O5'-PA
56	OL	501	GTP	C4'-C5'-O5'-PA
56	PE	501	GTP	C4'-C5'-O5'-PA
56	PG	501	GTP	C4'-C5'-O5'-PA
56	PK	501	GTP	C4'-C5'-O5'-PA
56	QI	501	GTP	C4'-C5'-O5'-PA
56	QL	501	GTP	C4'-C5'-O5'-PA
56	RB	501	GTP	C4'-C5'-O5'-PA
56	SE	501	GTP	C4'-C5'-O5'-PA
56	SI	501	GTP	C4'-C5'-O5'-PA
56	TA	501	GTP	C4'-C5'-O5'-PA
56	UA	501	GTP	C4'-C5'-O5'-PA
56	UB	501	GTP	C4'-C5'-O5'-PA
56	UG	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
56	VE	501	GTP	C4'-C5'-O5'-PA
56	WI	501	GTP	C4'-C5'-O5'-PA
58	QH	501	GDP	C4'-C5'-O5'-PA
56	BK	501	GTP	C3'-C4'-C5'-O5'
56	LK	501	GTP	C3'-C4'-C5'-O5'
56	BM	501	GTP	C4'-C5'-O5'-PA
56	SK	501	GTP	C4'-C5'-O5'-PA
56	TB	501	GTP	C4'-C5'-O5'-PA
56	TG	501	GTP	C4'-C5'-O5'-PA
56	BG	501	GTP	PA-O3A-PB-O2B
56	DK	501	GTP	PA-O3A-PB-O2B
56	HK	501	GTP	PB-O3A-PA-O1A
56	IG	501	GTP	PB-O3A-PA-O2A
56	JK	501	GTP	PA-O3A-PB-O2B
56	LA	501	GTP	PB-O3A-PA-O2A
56	ME	501	GTP	PB-O3A-PA-O1A
56	QG	501	GTP	PB-O3A-PA-O2A
56	RB	501	GTP	PB-O3A-PA-O2A
56	RI	501	GTP	PB-O3A-PA-O2A
56	SA	501	GTP	PB-O3A-PA-O2A
56	SG	501	GTP	PB-O3A-PA-O1A
56	TA	501	GTP	PB-O3A-PA-O2A
56	TB	501	GTP	PB-O3A-PA-O2A
56	UA	501	GTP	PB-O3A-PA-O2A
56	VE	501	GTP	PB-O3A-PA-O2A
58	HL	501	GDP	C3'-C4'-C5'-O5'
56	II	501	GTP	C4'-C5'-O5'-PA
56	CM	501	GTP	C4'-C5'-O5'-PA
56	NB	501	GTP	PB-O3B-PG-O1G
56	CK	501	GTP	O4'-C4'-C5'-O5'
56	FK	501	GTP	O4'-C4'-C5'-O5'
56	RE	501	GTP	C3'-C4'-C5'-O5'
56	VK	501	GTP	O4'-C4'-C5'-O5'
58	LF	501	GDP	C3'-C4'-C5'-O5'
58	VL	501	GDP	O4'-C4'-C5'-O5'
56	AE	501	GTP	PB-O3A-PA-O2A
56	BI	501	GTP	PB-O3A-PA-O1A
56	BM	501	GTP	PB-O3A-PA-O1A
56	GA	501	GTP	PB-O3A-PA-O2A
56	IM	501	GTP	PA-O3A-PB-O2B
56	ME	501	GTP	PB-O3A-PA-O2A
56	PG	501	GTP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
56	RB	501	GTP	PB-O3A-PA-O1A
56	WI	501	GTP	PB-O3A-PA-O2A
56	AK	501	GTP	C4'-C5'-O5'-PA
56	LK	501	GTP	C4'-C5'-O5'-PA
56	DG	501	GTP	O4'-C4'-C5'-O5'
56	FE	501	GTP	O4'-C4'-C5'-O5'
56	BM	501	GTP	PB-O3B-PG-O1G
58	UD	501	GDP	PA-O3A-PB-O1B
56	AA	501	GTP	PB-O3B-PG-O2G
56	HK	501	GTP	PB-O3B-PG-O2G
56	HK	501	GTP	PB-O3B-PG-O3G
56	IK	501	GTP	PB-O3B-PG-O2G
56	MA	501	GTP	PB-O3B-PG-O2G
56	NB	501	GTP	PB-O3B-PG-O2G
56	NB	501	GTP	PB-O3B-PG-O3G
56	RL	501	GTP	PB-O3B-PG-O2G
56	RL	501	GTP	PB-O3B-PG-O3G
56	UK	501	GTP	PB-O3B-PG-O2G
58	QH	501	GDP	PA-O3A-PB-O3B
56	AK	501	GTP	C3'-C4'-C5'-O5'
58	JJ	501	GDP	C3'-C4'-C5'-O5'
58	SF	501	GDP	C3'-C4'-C5'-O5'
56	HA	501	GTP	C3'-C4'-C5'-O5'
58	VM	501	GDP	C3'-C4'-C5'-O5'
56	AE	501	GTP	PB-O3A-PA-O1A
56	AM	501	GTP	PB-O3A-PA-O1A
56	AM	501	GTP	PB-O3A-PA-O2A
56	BG	501	GTP	PA-O3A-PB-O1B
56	FE	501	GTP	PB-O3A-PA-O2A
56	GA	501	GTP	PB-O3A-PA-O1A
56	HI	501	GTP	PB-O3A-PA-O2A
56	IG	501	GTP	PB-O3A-PA-O1A
56	II	501	GTP	PB-O3A-PA-O2A
56	LK	501	GTP	PB-O3A-PA-O2A
56	NB	501	GTP	PA-O3A-PB-O2B
56	QA	501	GTP	PB-O3A-PA-O2A
56	QG	501	GTP	PB-O3A-PA-O1A
56	TA	501	GTP	PB-O3A-PA-O1A
56	TB	501	GTP	PB-O3A-PA-O1A
56	TI	501	GTP	PA-O3A-PB-O2B
56	UK	501	GTP	PB-O3A-PA-O2A
56	WI	501	GTP	PB-O3A-PA-O1A

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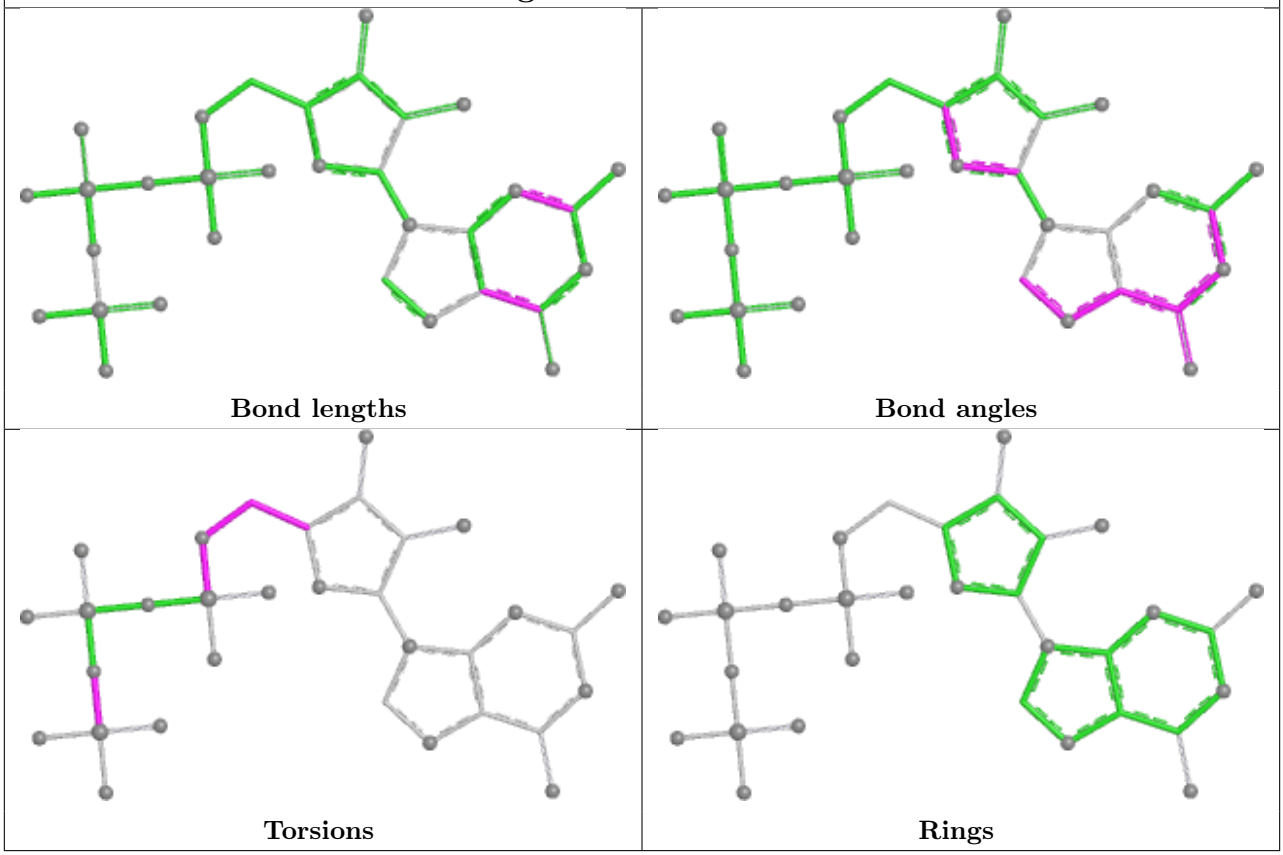
Mol	Chain	Res	Type	Atoms
56	WK	501	GTP	PB-O3A-PA-O2A
56	LA	501	GTP	C3'-C4'-C5'-O5'
56	LK	501	GTP	O4'-C4'-C5'-O5'
56	RG	501	GTP	C3'-C4'-C5'-O5'
56	RL	501	GTP	O4'-C4'-C5'-O5'
56	VG	501	GTP	C3'-C4'-C5'-O5'
58	UM	501	GDP	C3'-C4'-C5'-O5'
56	DK	501	GTP	PA-O3A-PB-O1B
56	JK	501	GTP	PA-O3A-PB-O1B
56	LA	501	GTP	PB-O3A-PA-O1A
56	LK	501	GTP	PB-O3A-PA-O1A
56	NG	501	GTP	PA-O3A-PB-O2B
56	QL	501	GTP	PB-O3A-PA-O2A
56	RI	501	GTP	PB-O3A-PA-O1A
56	UA	501	GTP	PB-O3A-PA-O1A
58	SD	501	GDP	PB-O3A-PA-O2A
56	IB	501	GTP	C3'-C4'-C5'-O5'
56	QB	501	GTP	C3'-C4'-C5'-O5'
58	MJ	501	GDP	C3'-C4'-C5'-O5'
58	QF	501	GDP	C3'-C4'-C5'-O5'

There are no ring outliers.

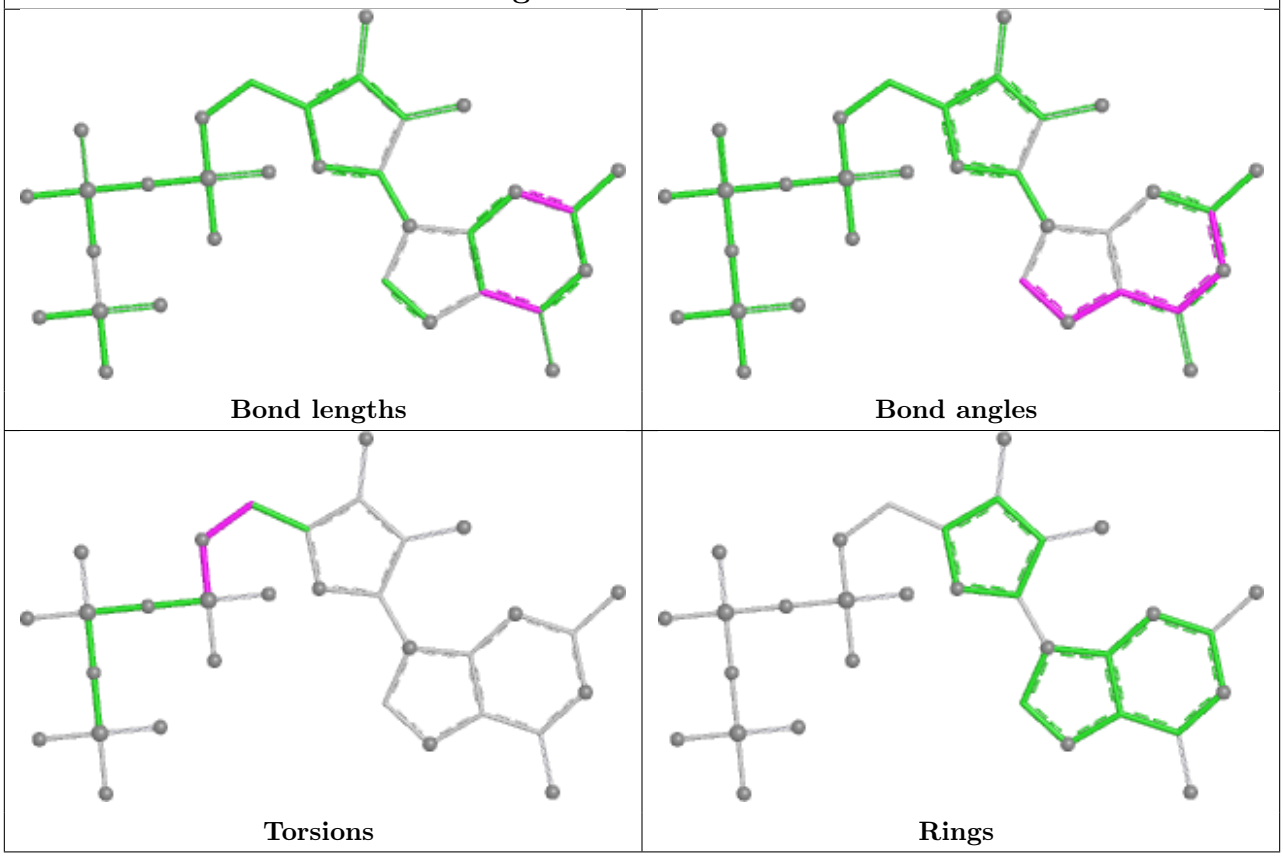
No monomer is involved in short contacts.

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 IB 501



Ligand GTP PE 501



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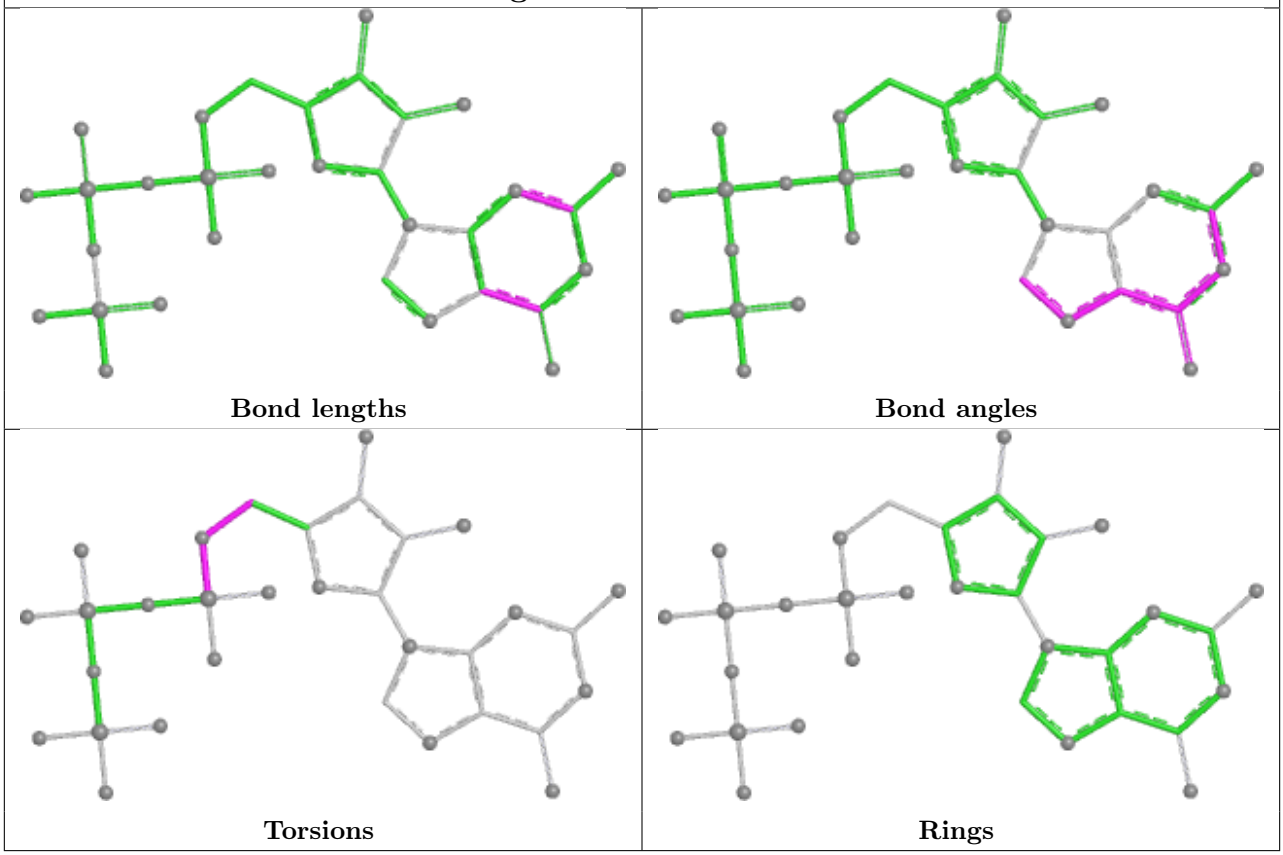
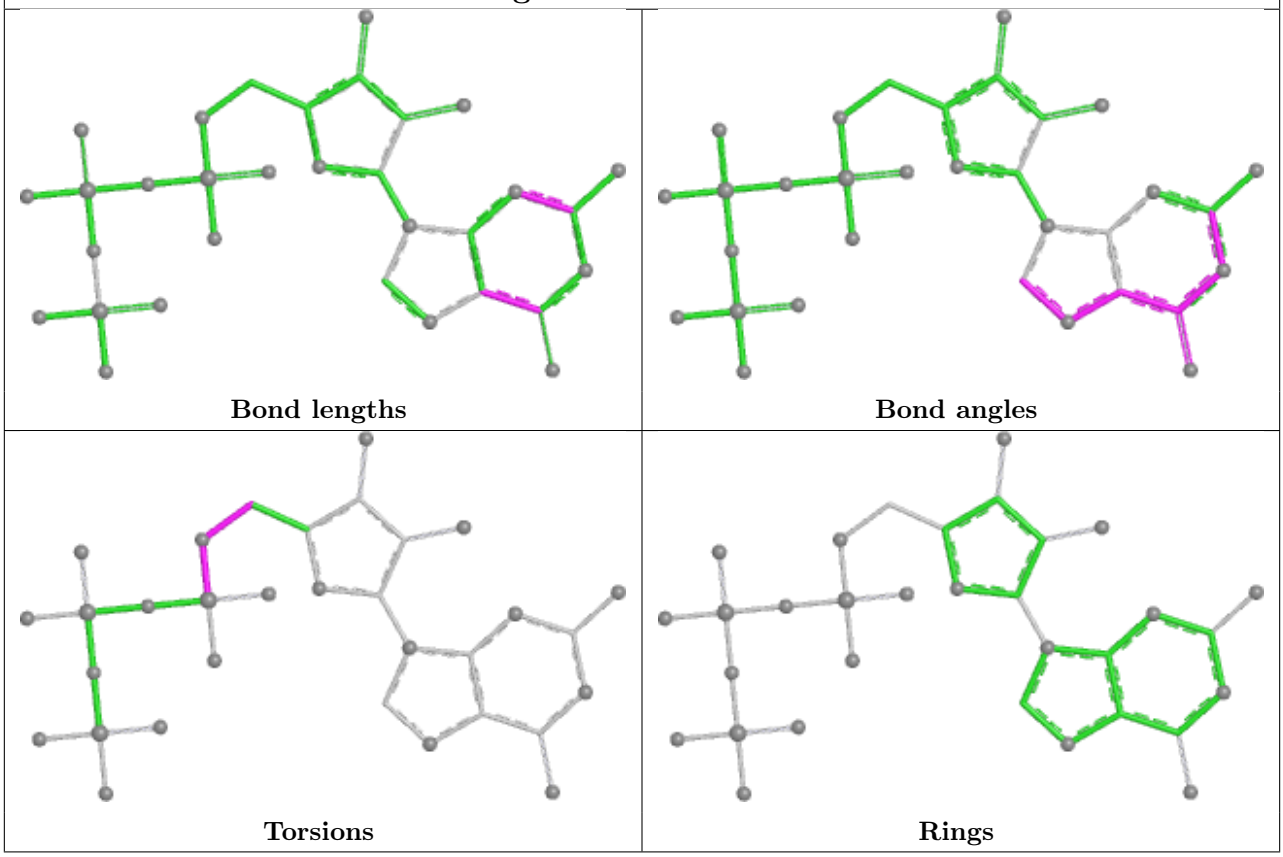


Ligand GTP LB 501



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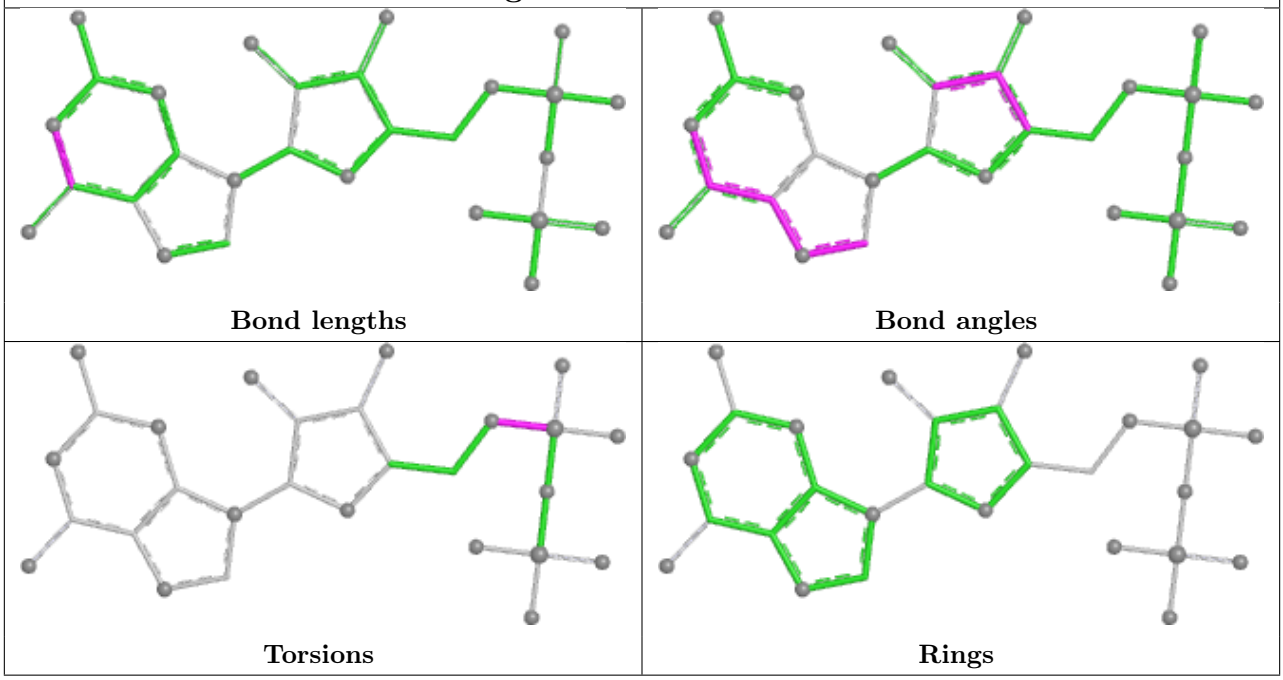

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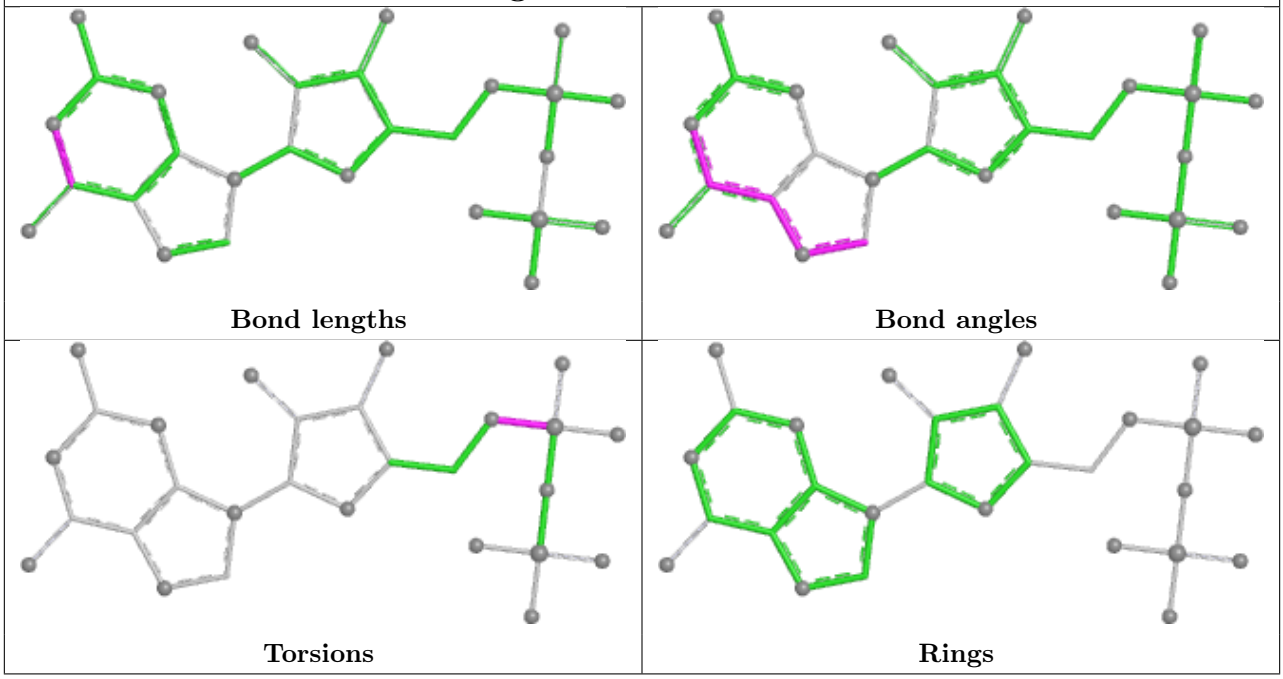

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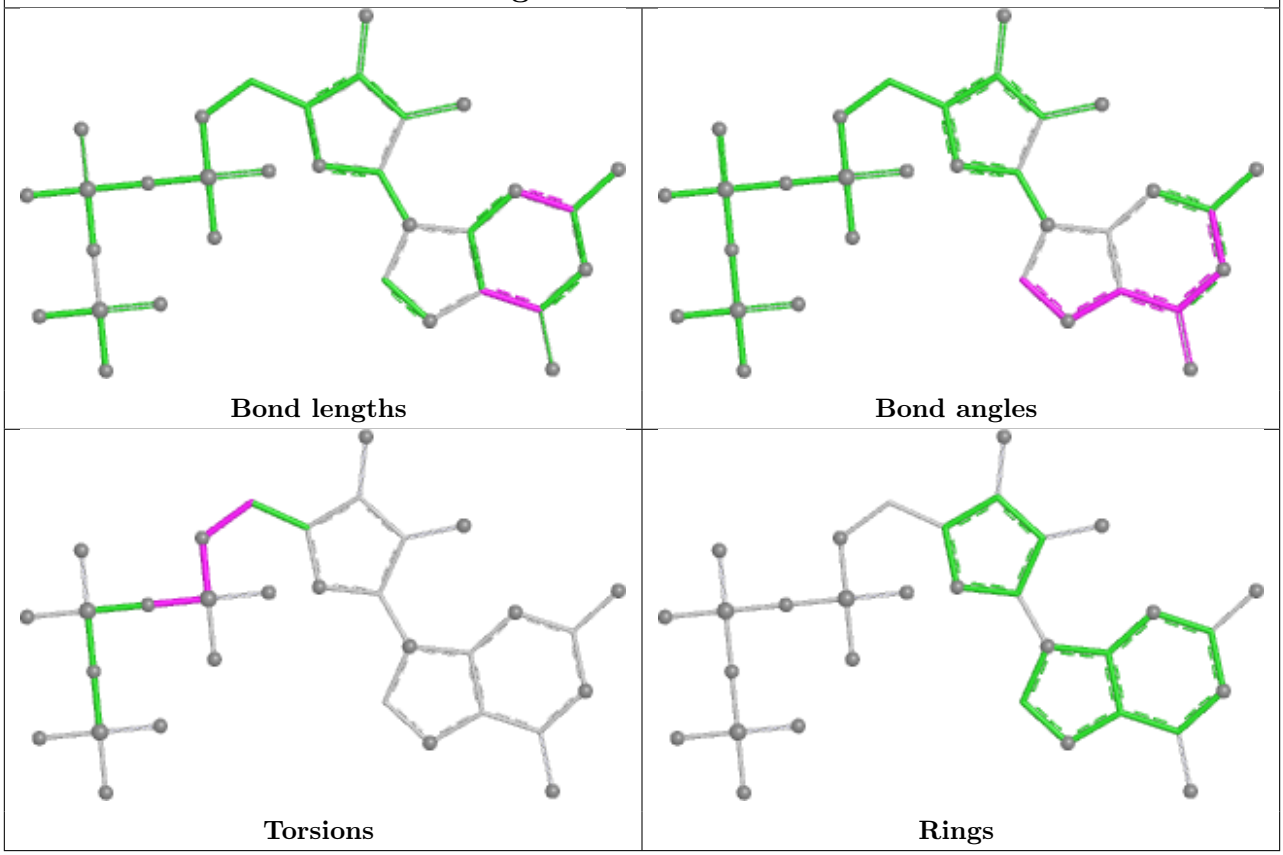

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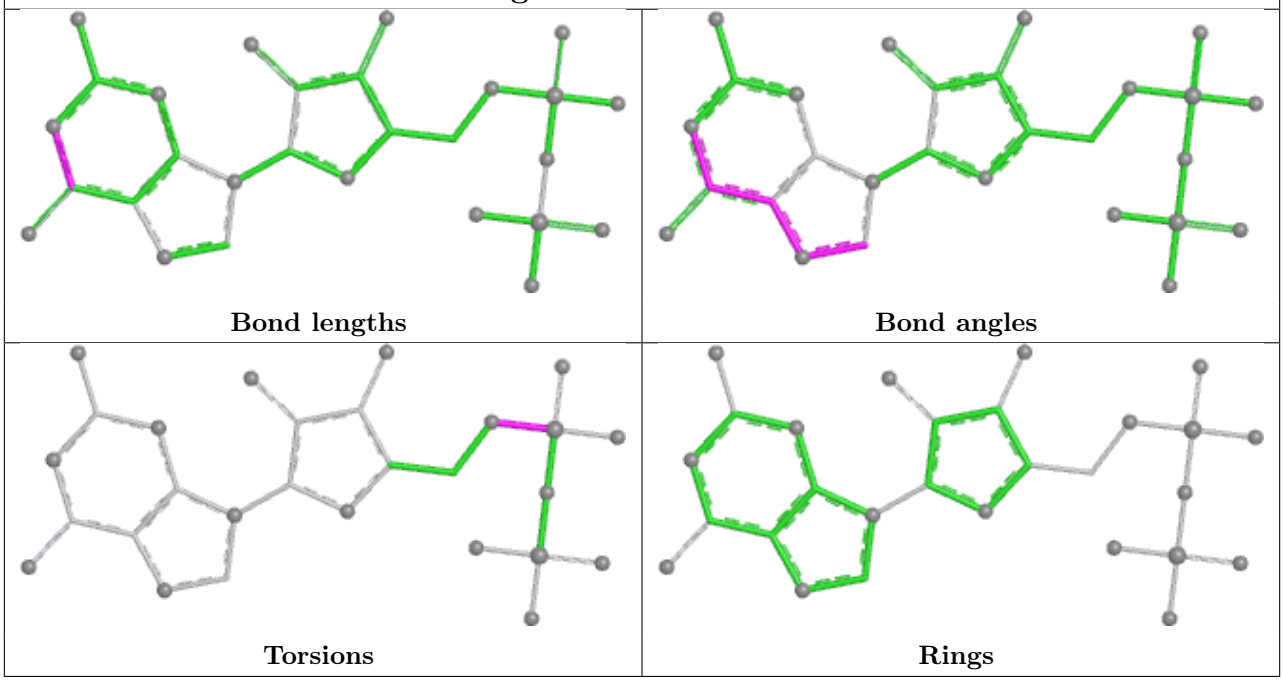

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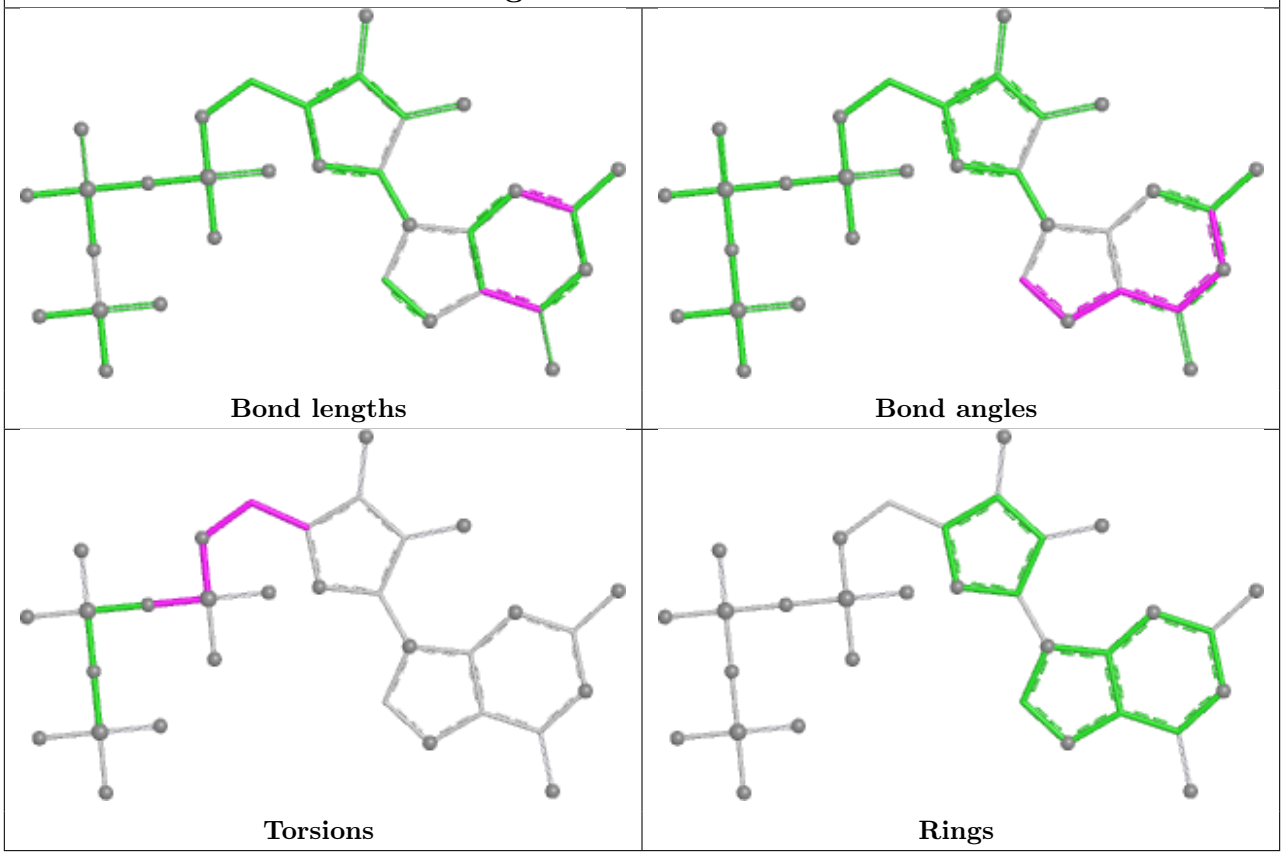

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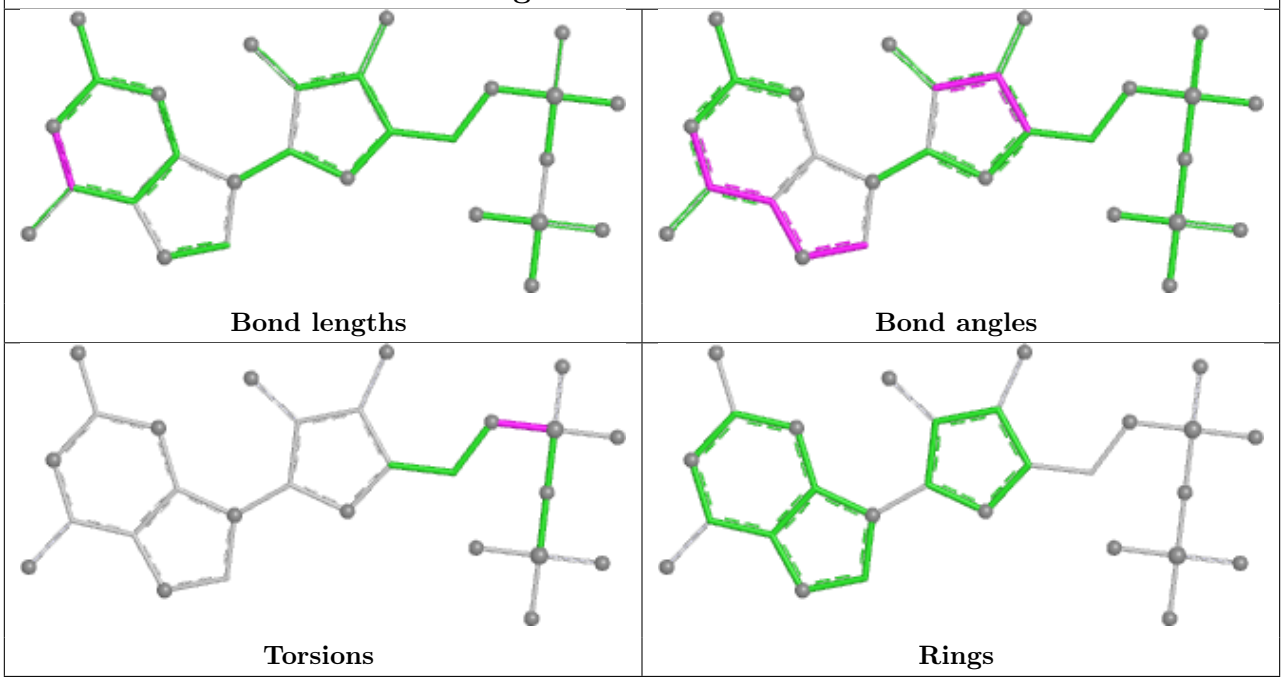

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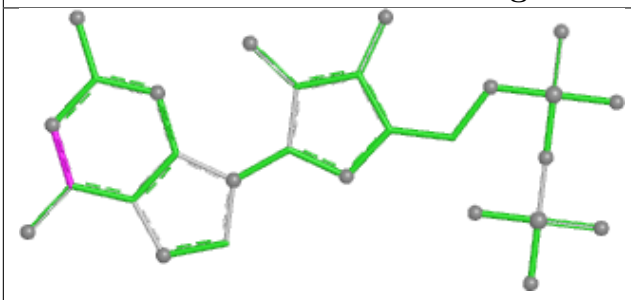
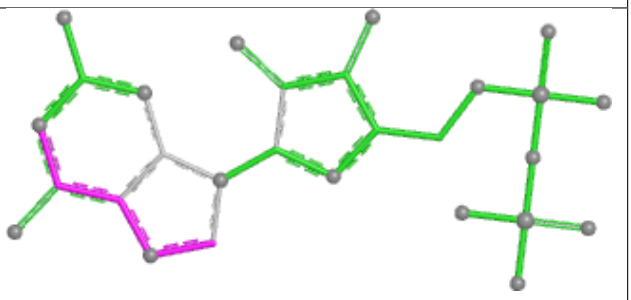
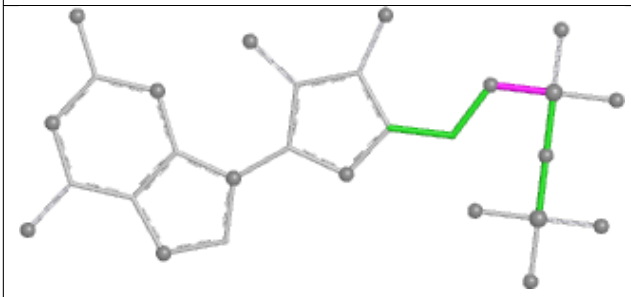
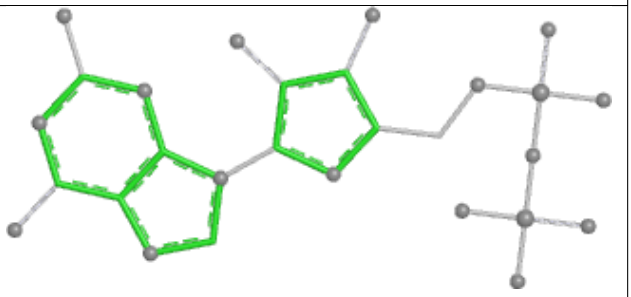
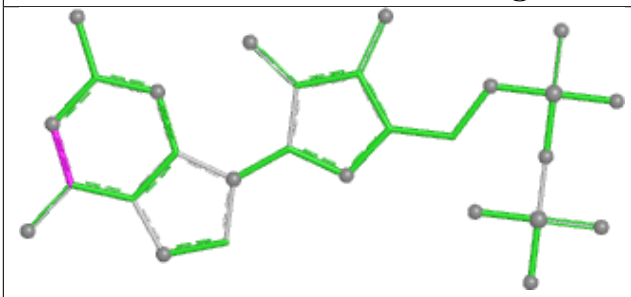
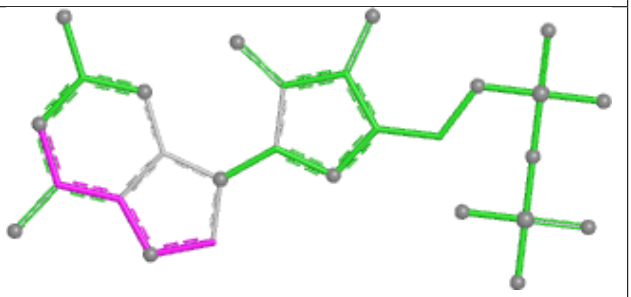
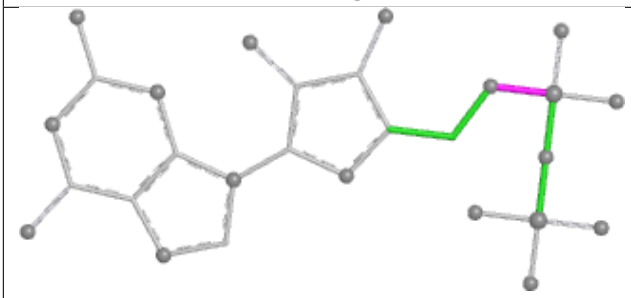
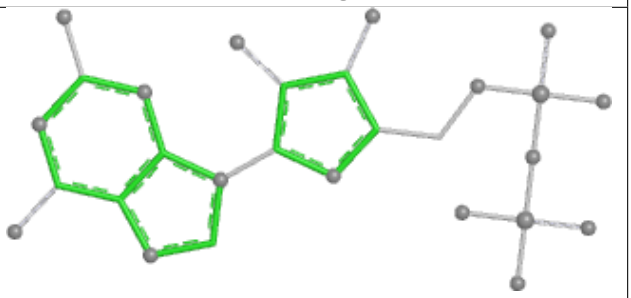
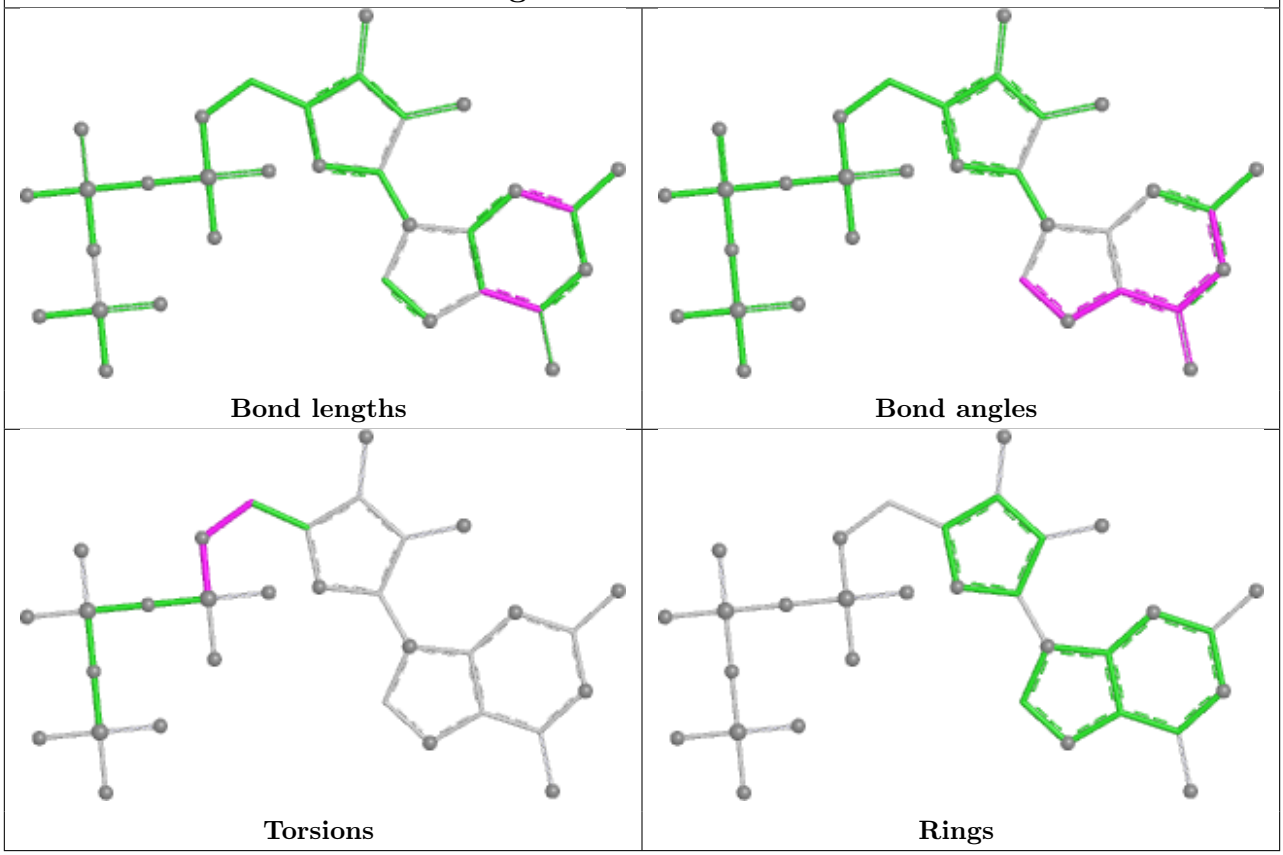
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP GJ 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP NA 501



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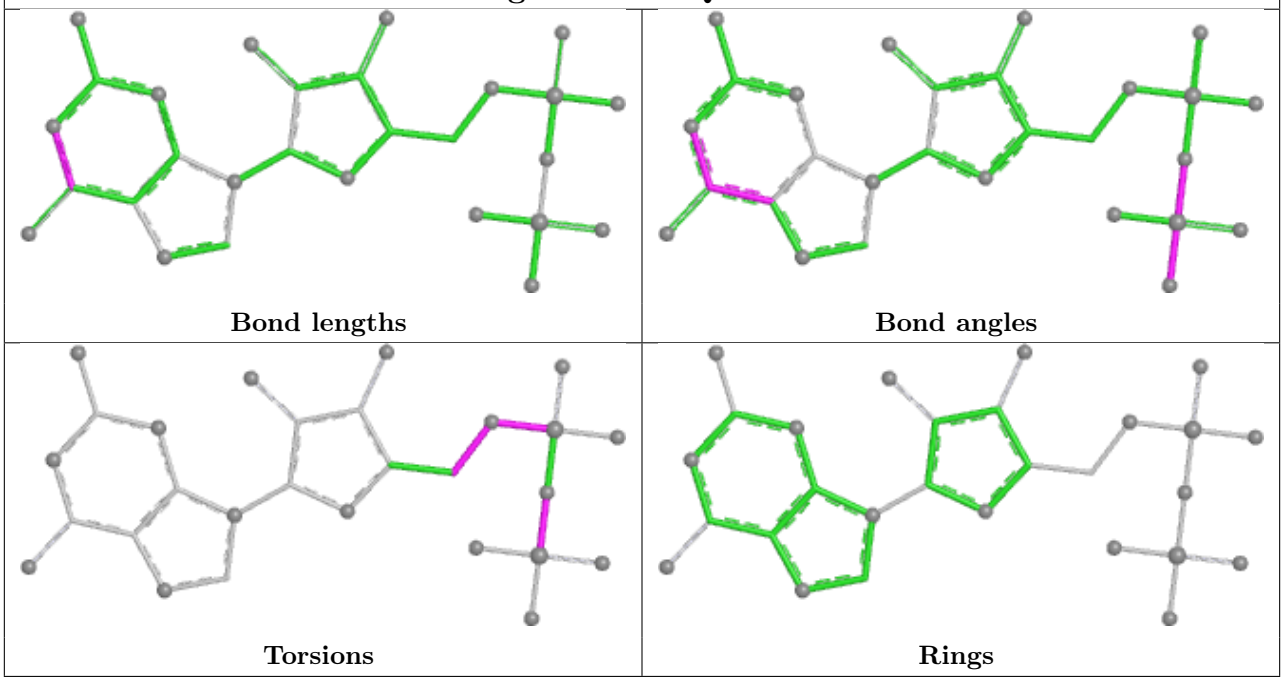

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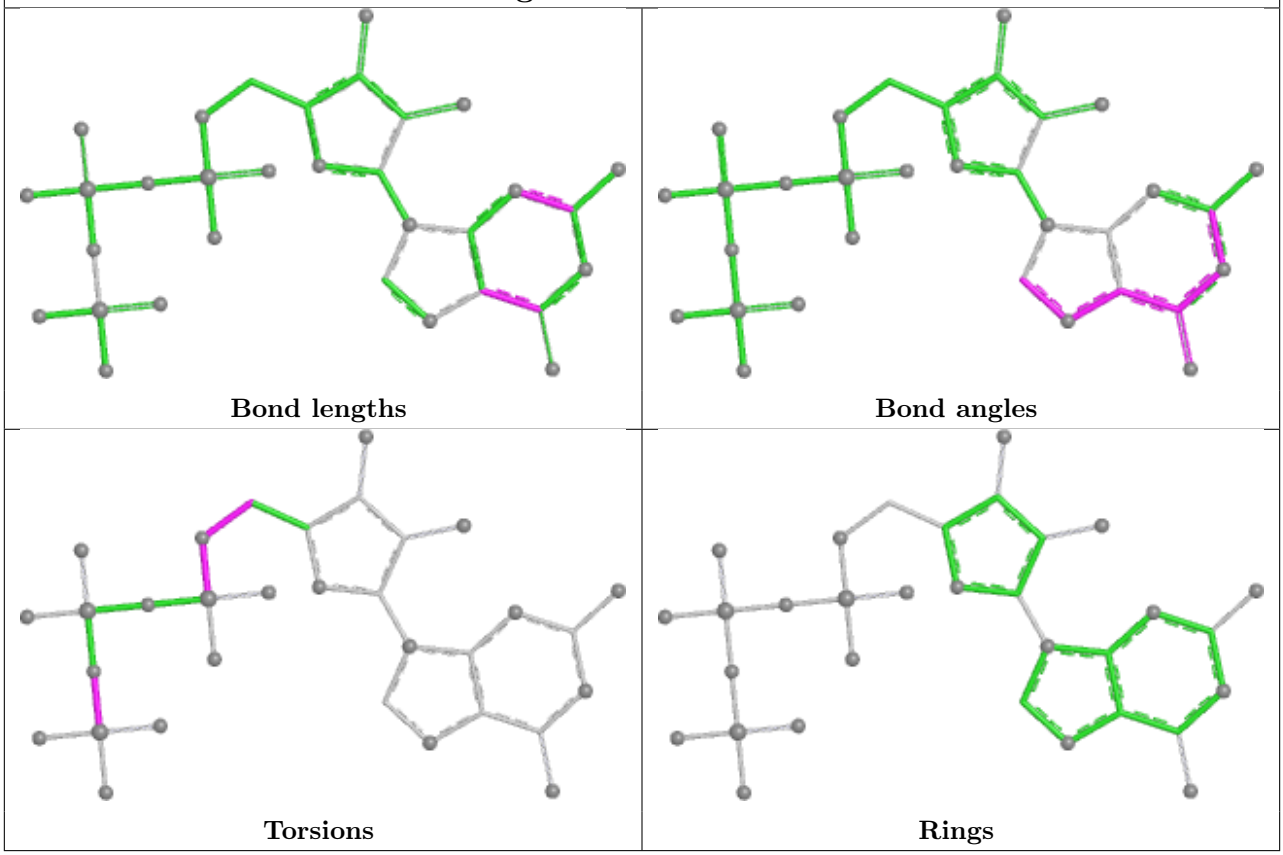

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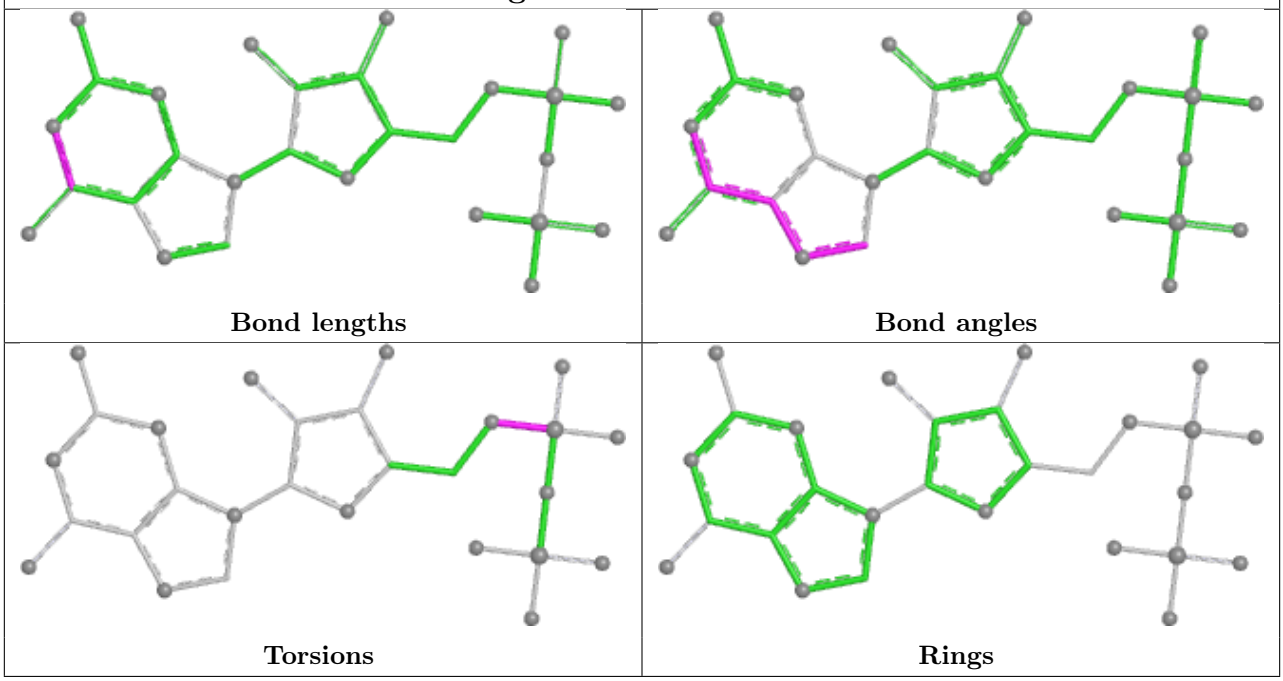

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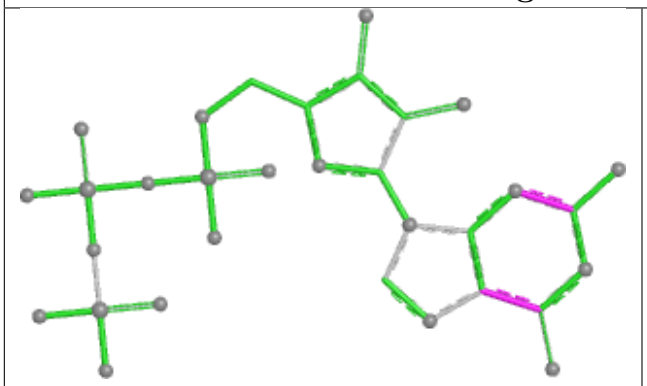
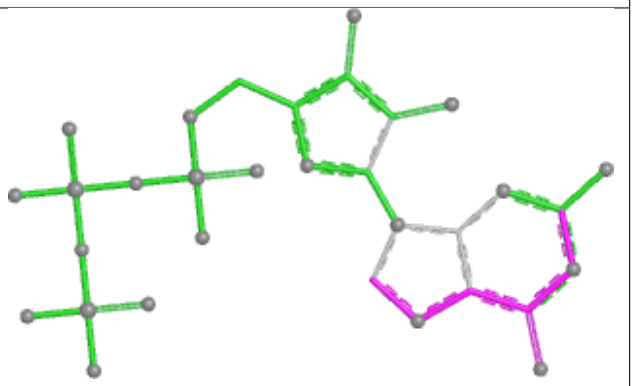
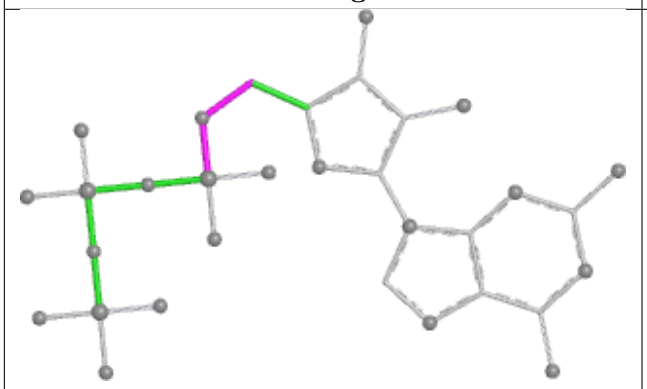


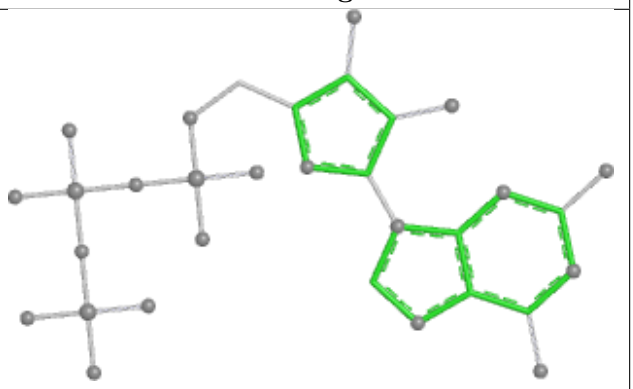
Bond lengths



Bond angles

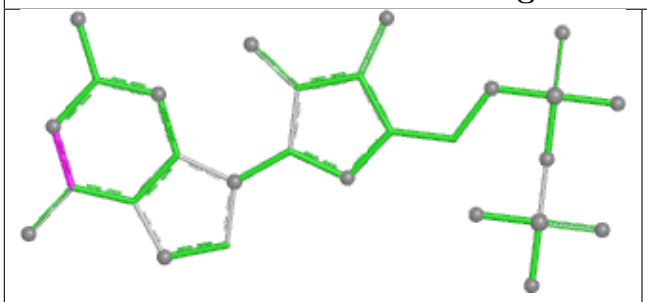


Torsions



Rings

Ligand GDP IF 501



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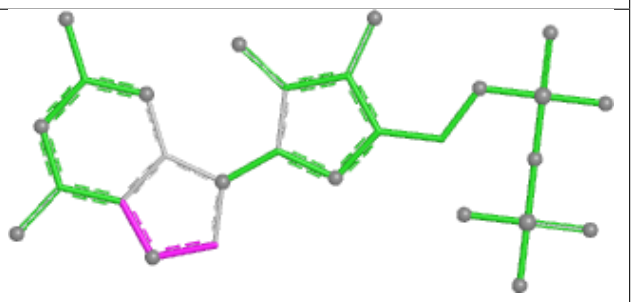
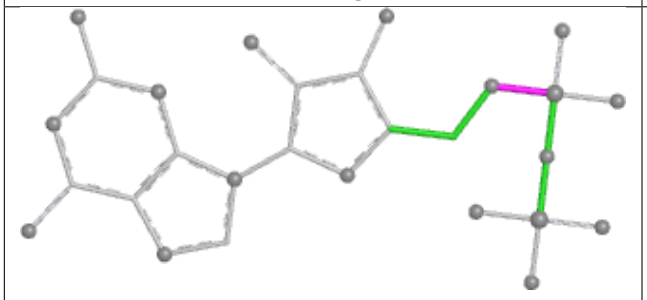
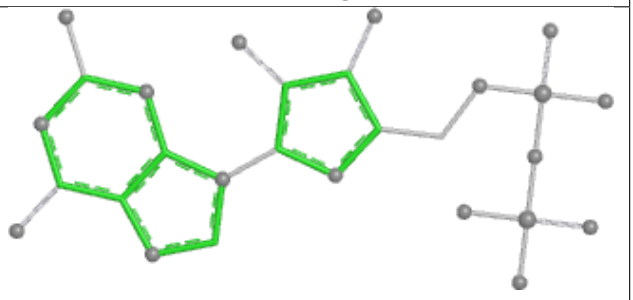


Bond angles

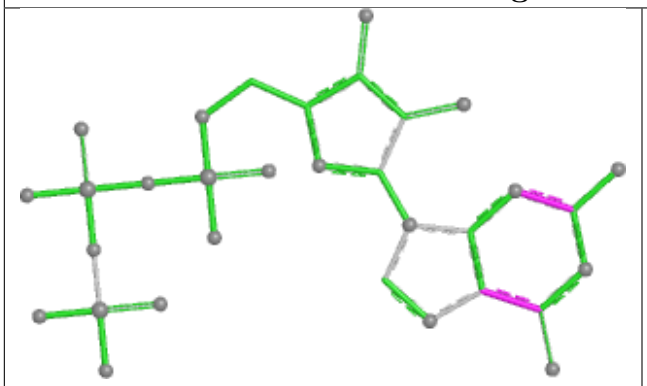


Torsions



Rings

Ligand GTP BB 501



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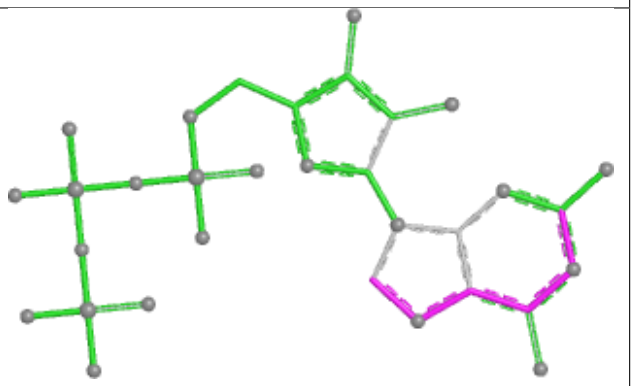
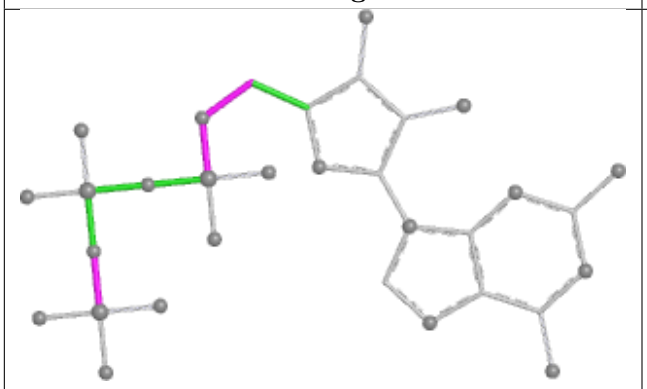


Bond angles



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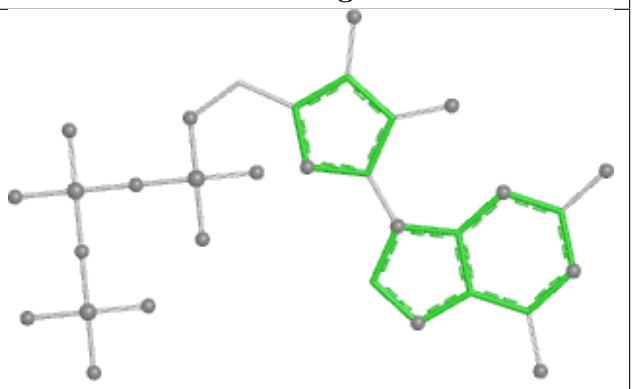
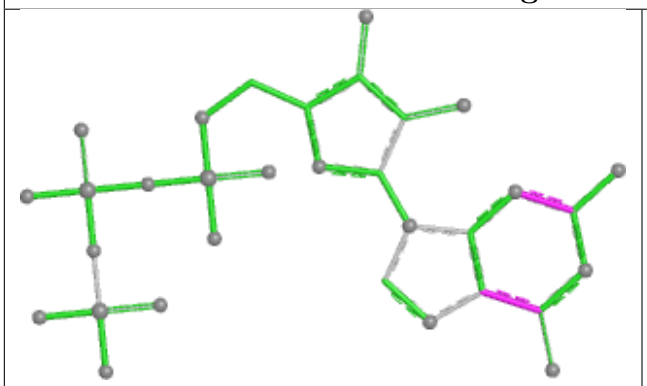


Rings

Ligand GTP JI 501



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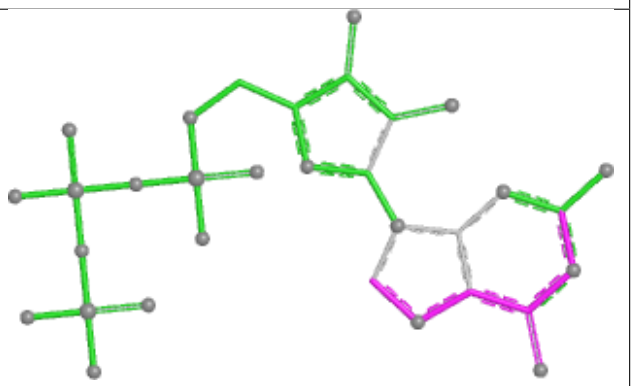
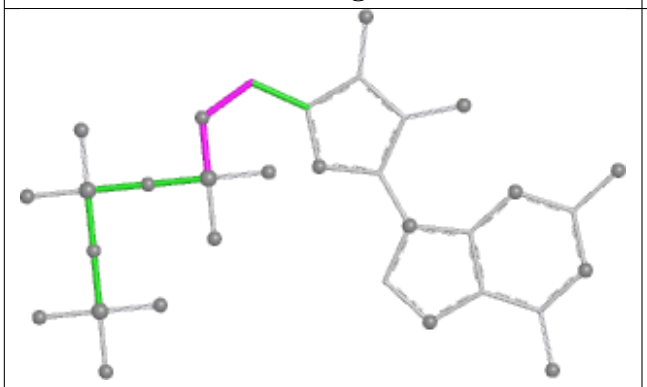


Bond angles



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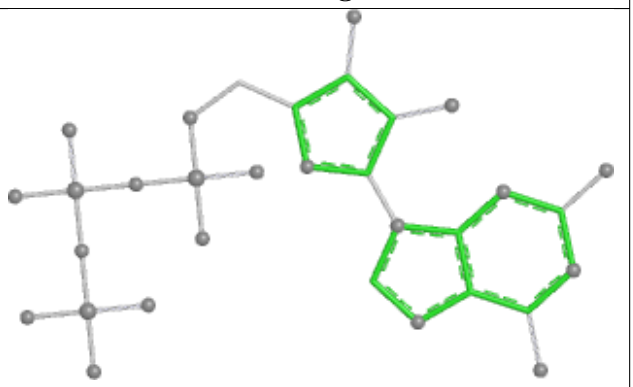
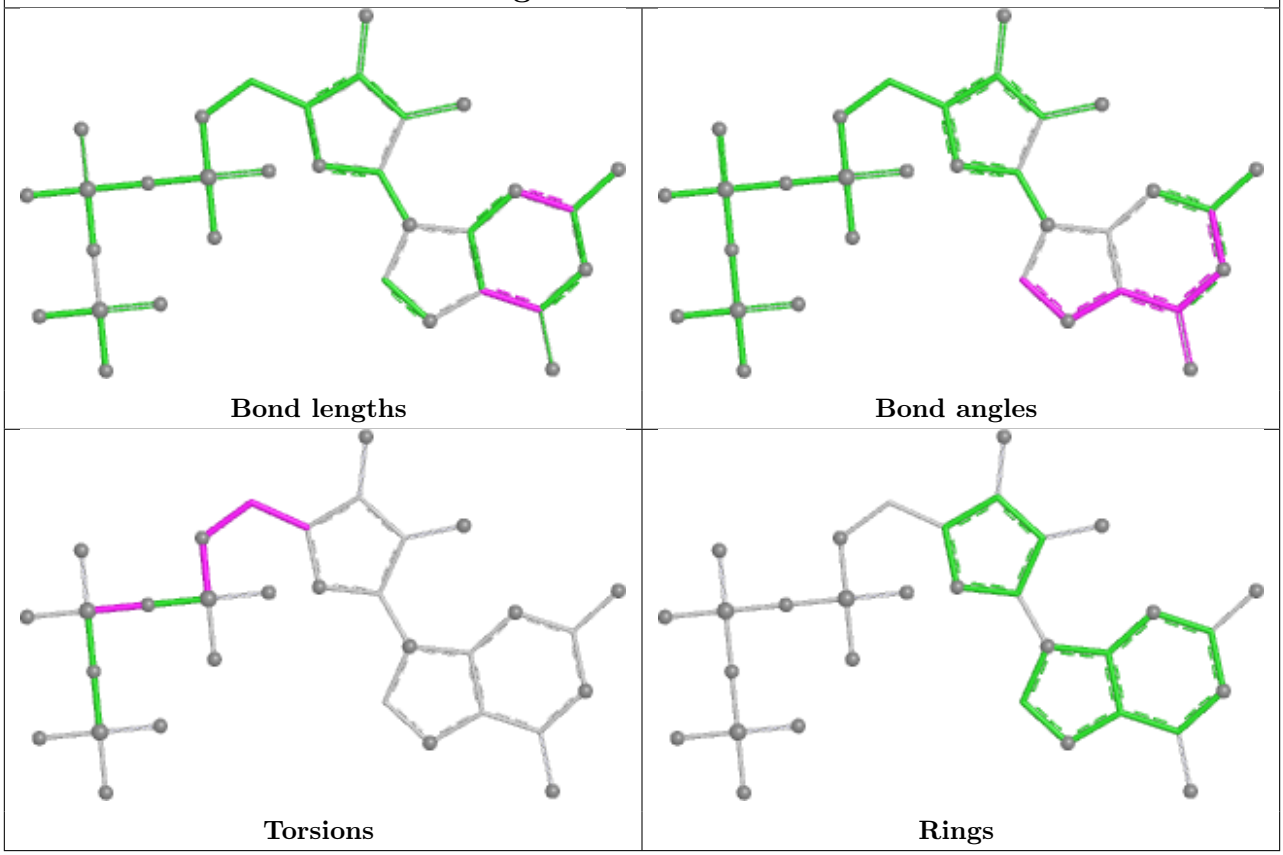


Rings

Ligand GTP JK 501



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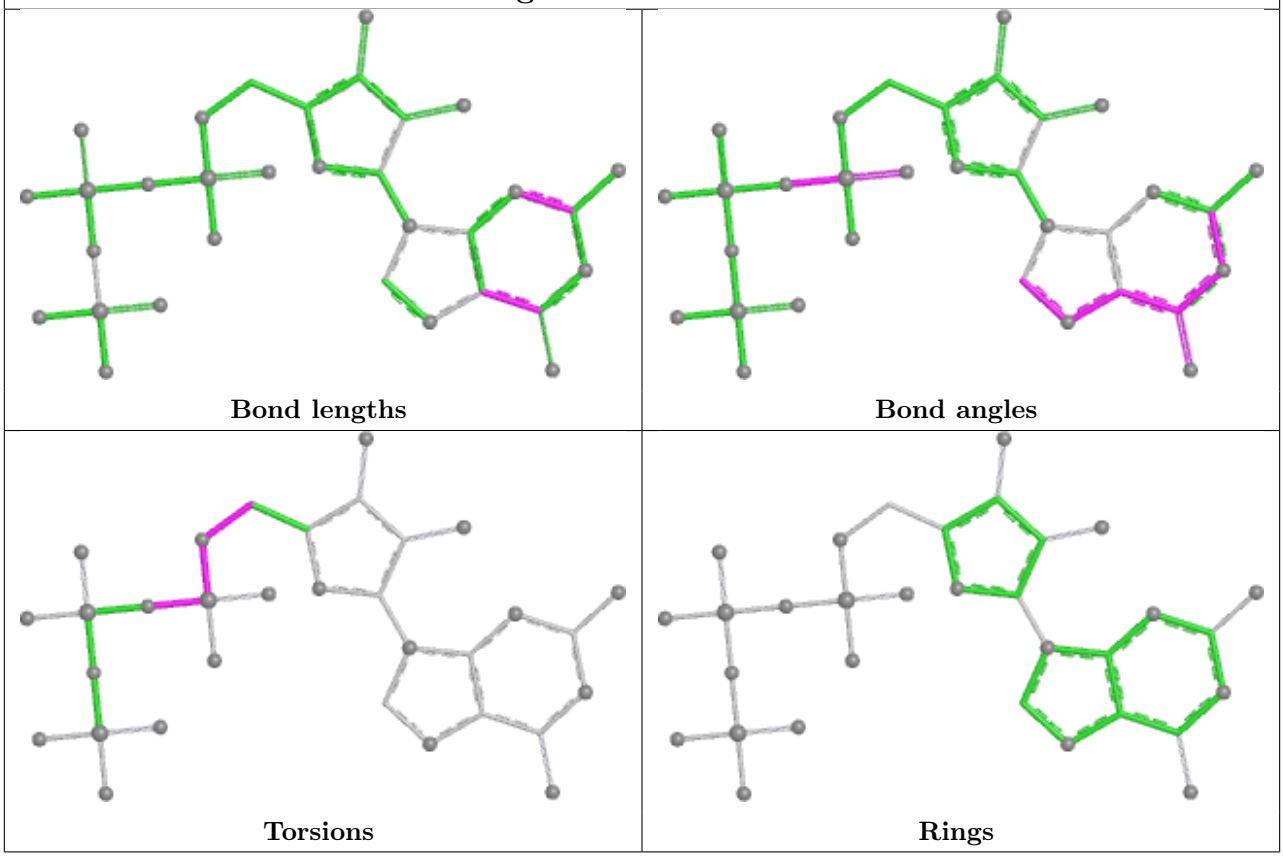

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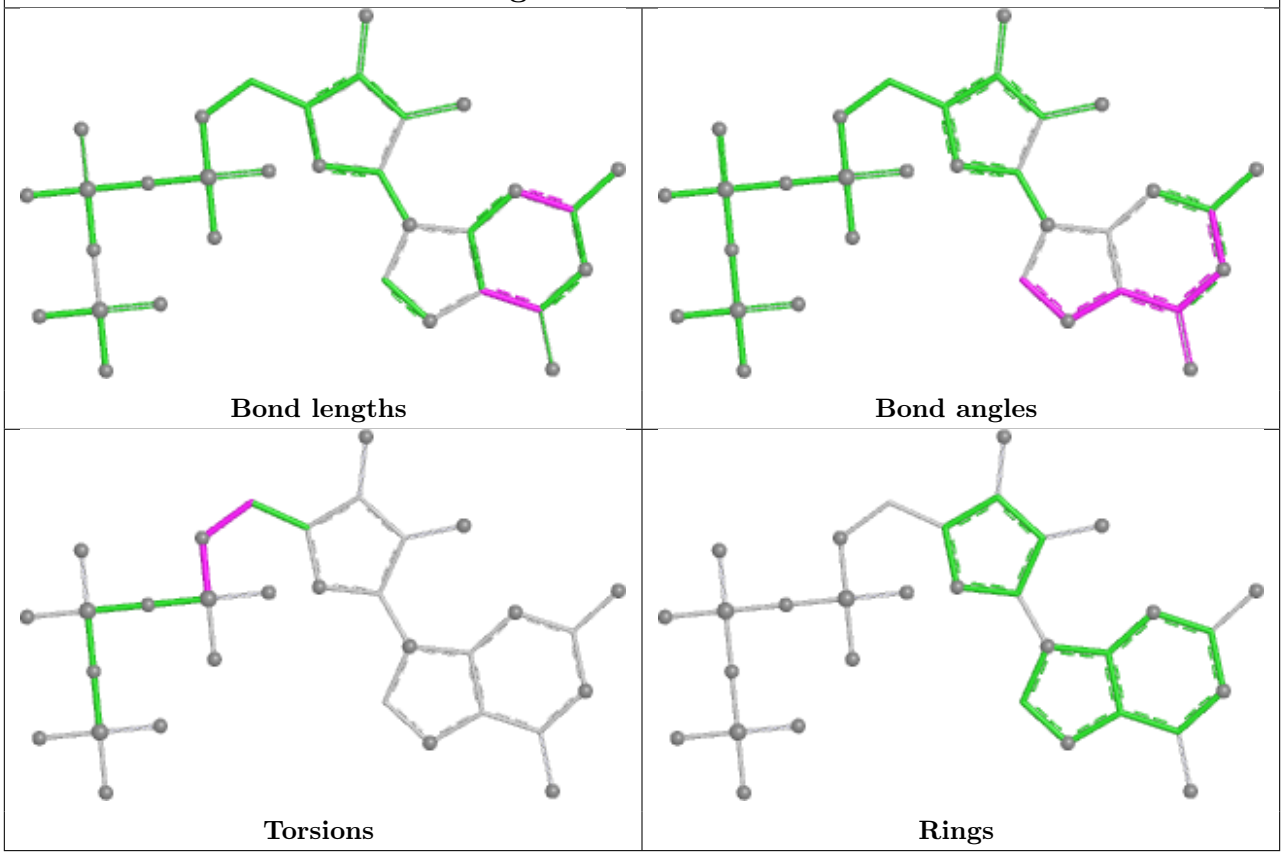

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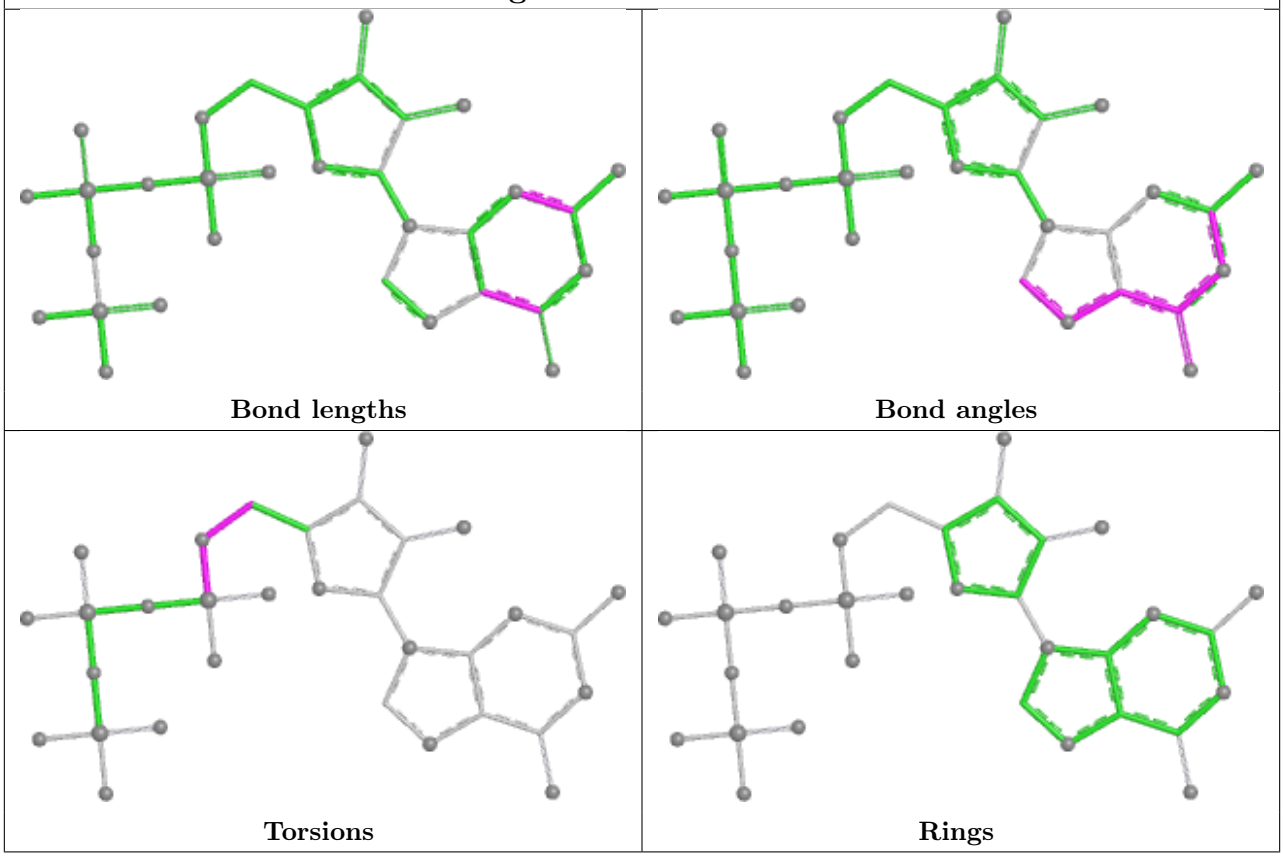

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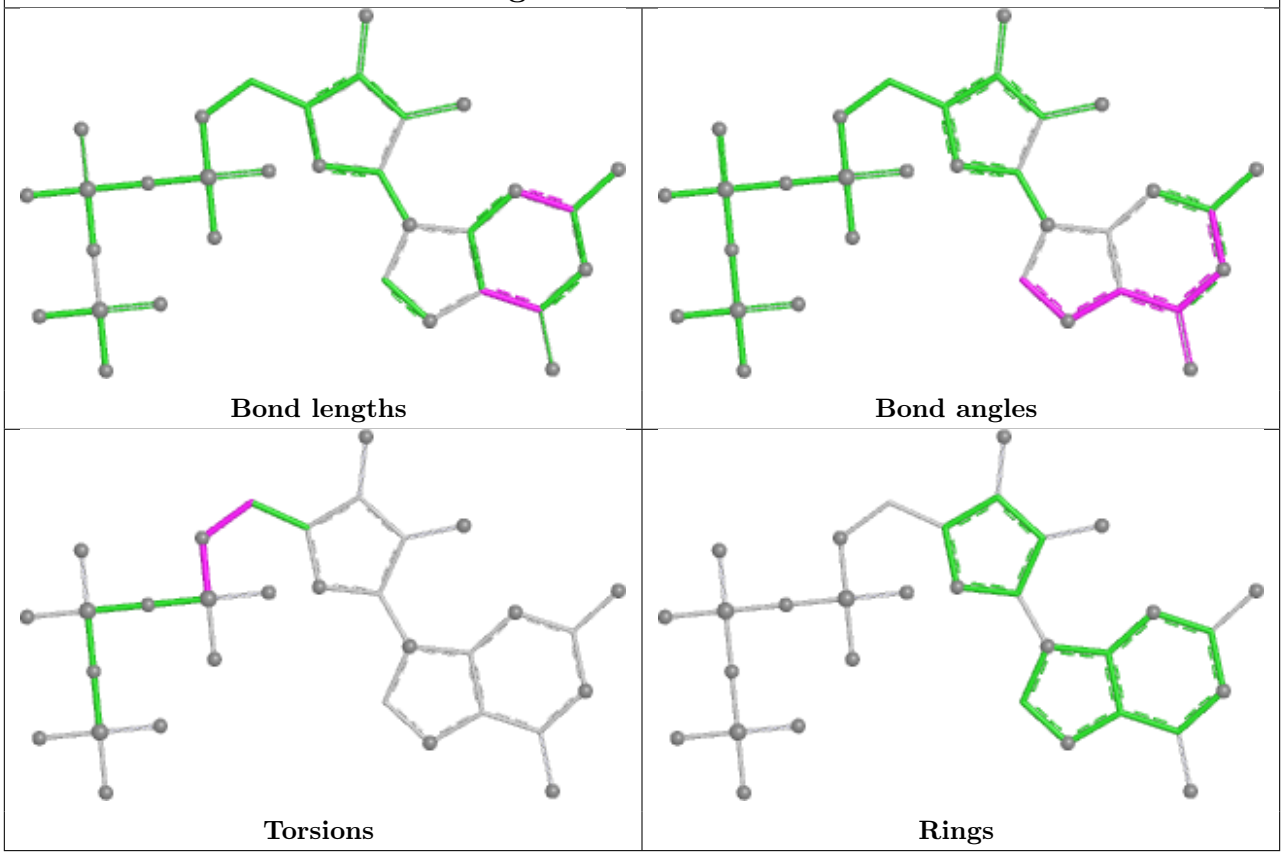

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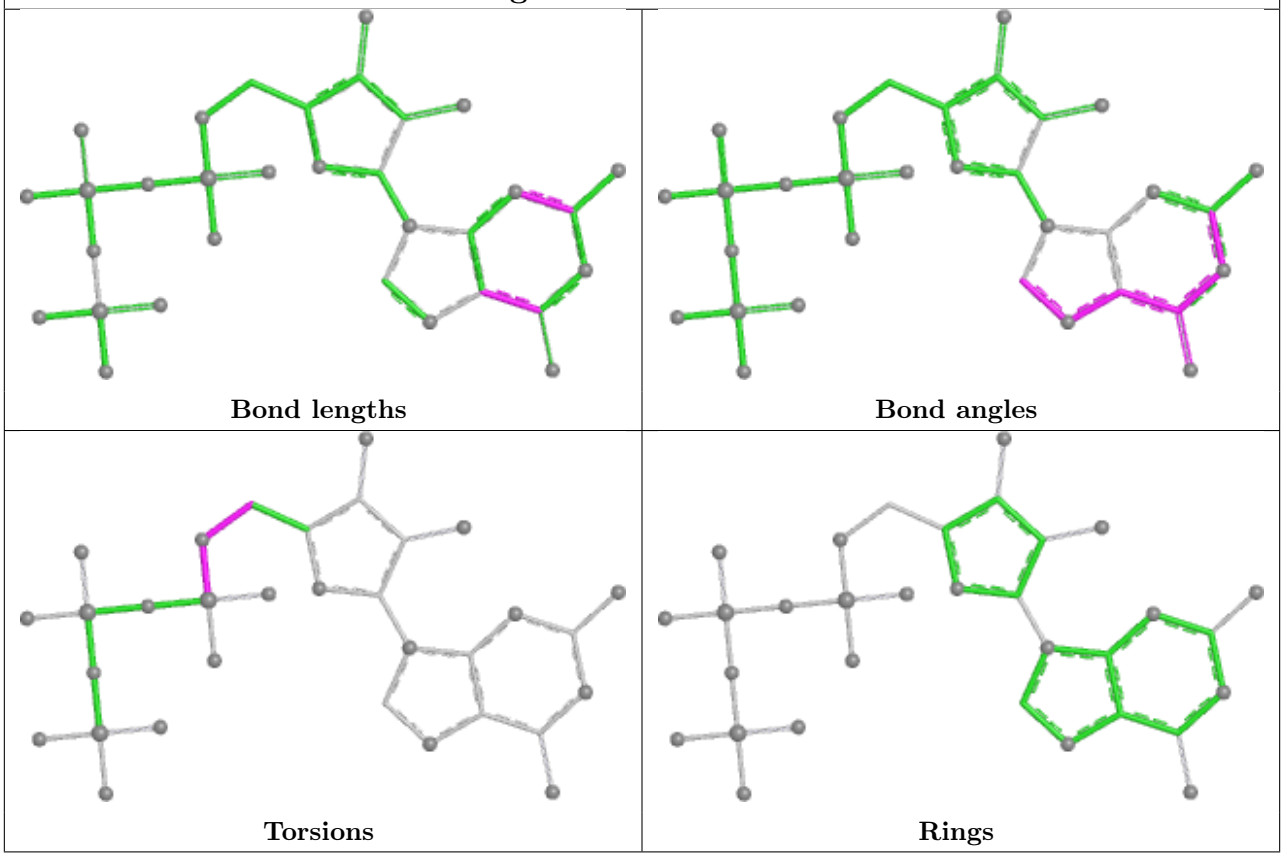
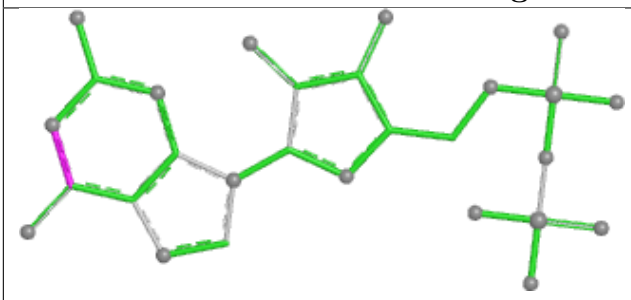
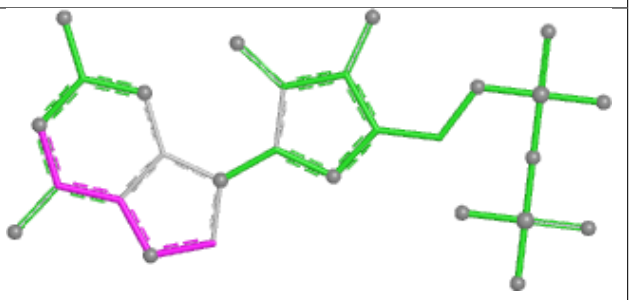


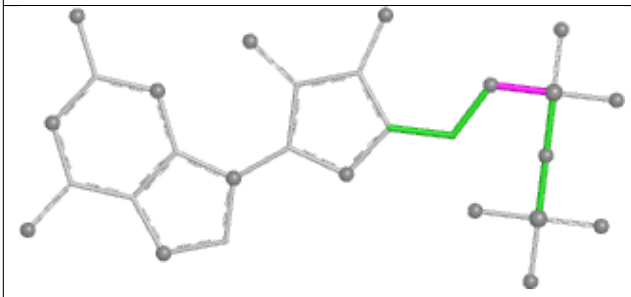
Ligand GDP TF 501



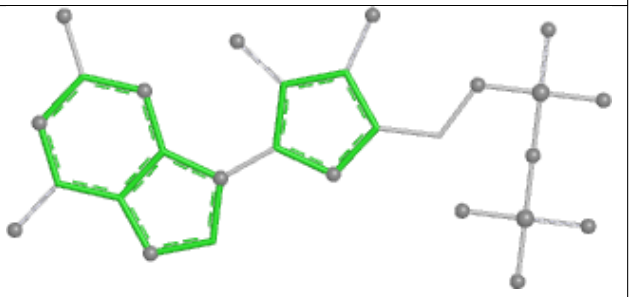
Bond lengths



Bond angles

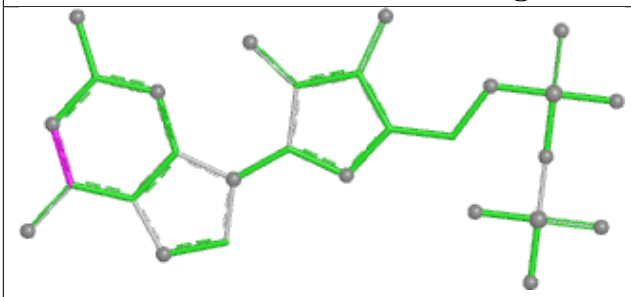


Torsions



Rings

Ligand GDP LF 501



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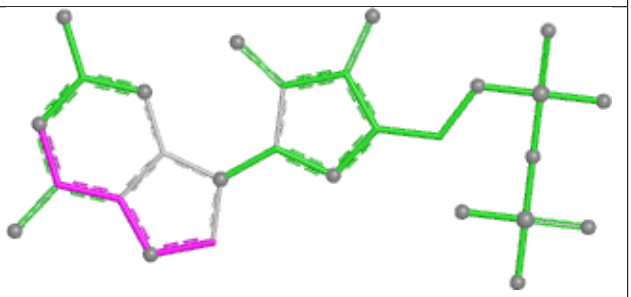

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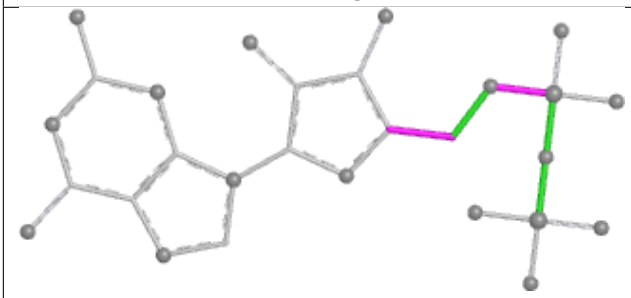

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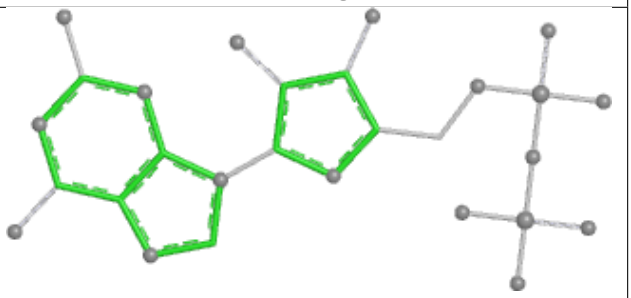
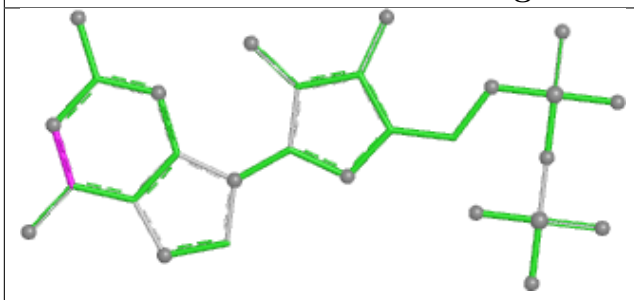


Rings

Ligand GDP LL 501



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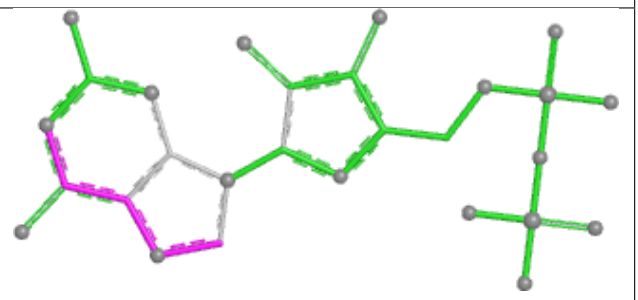

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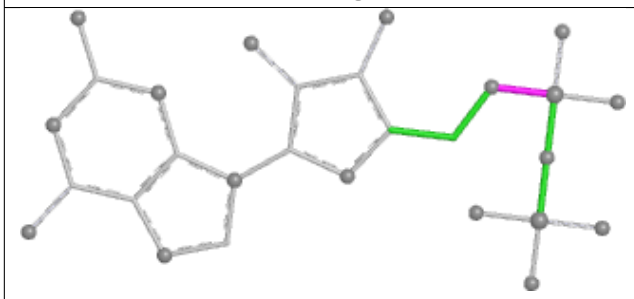

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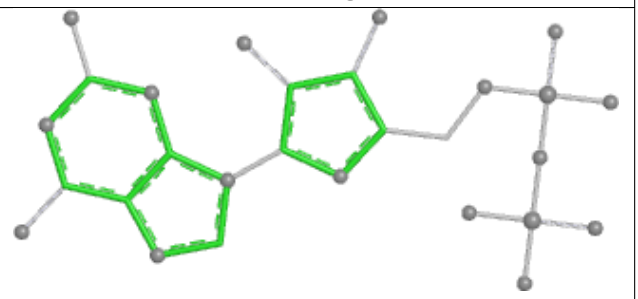
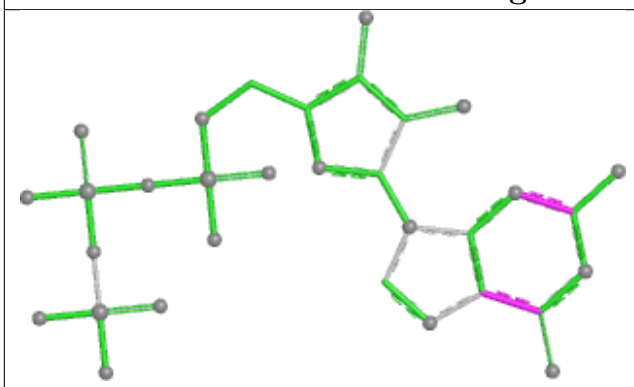


Rings

Ligand GTP UA 501



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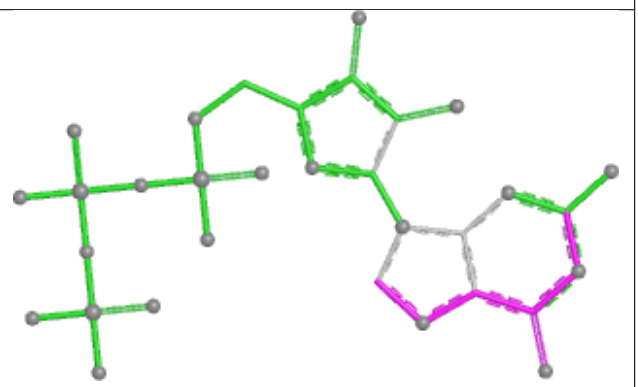

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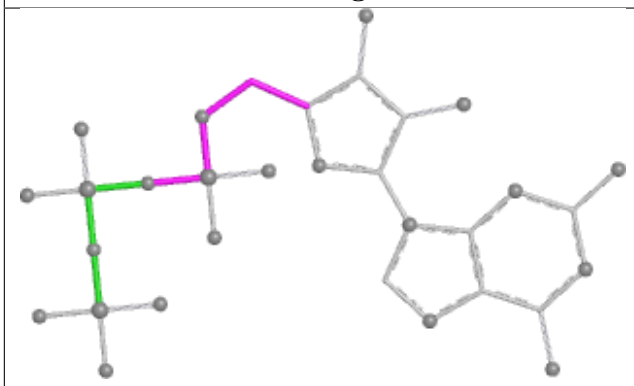

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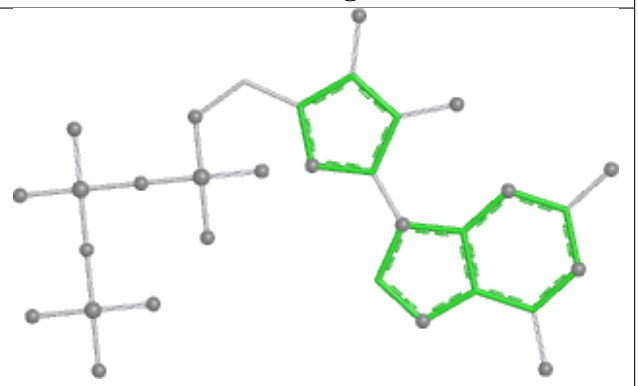
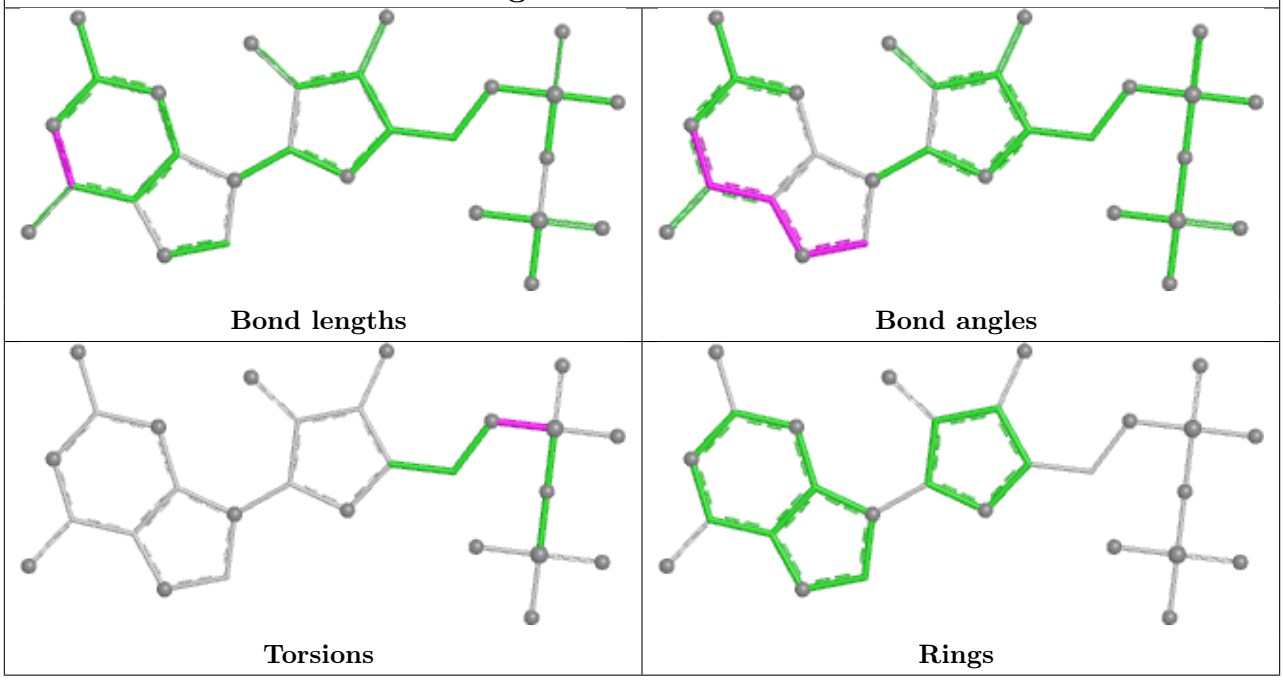
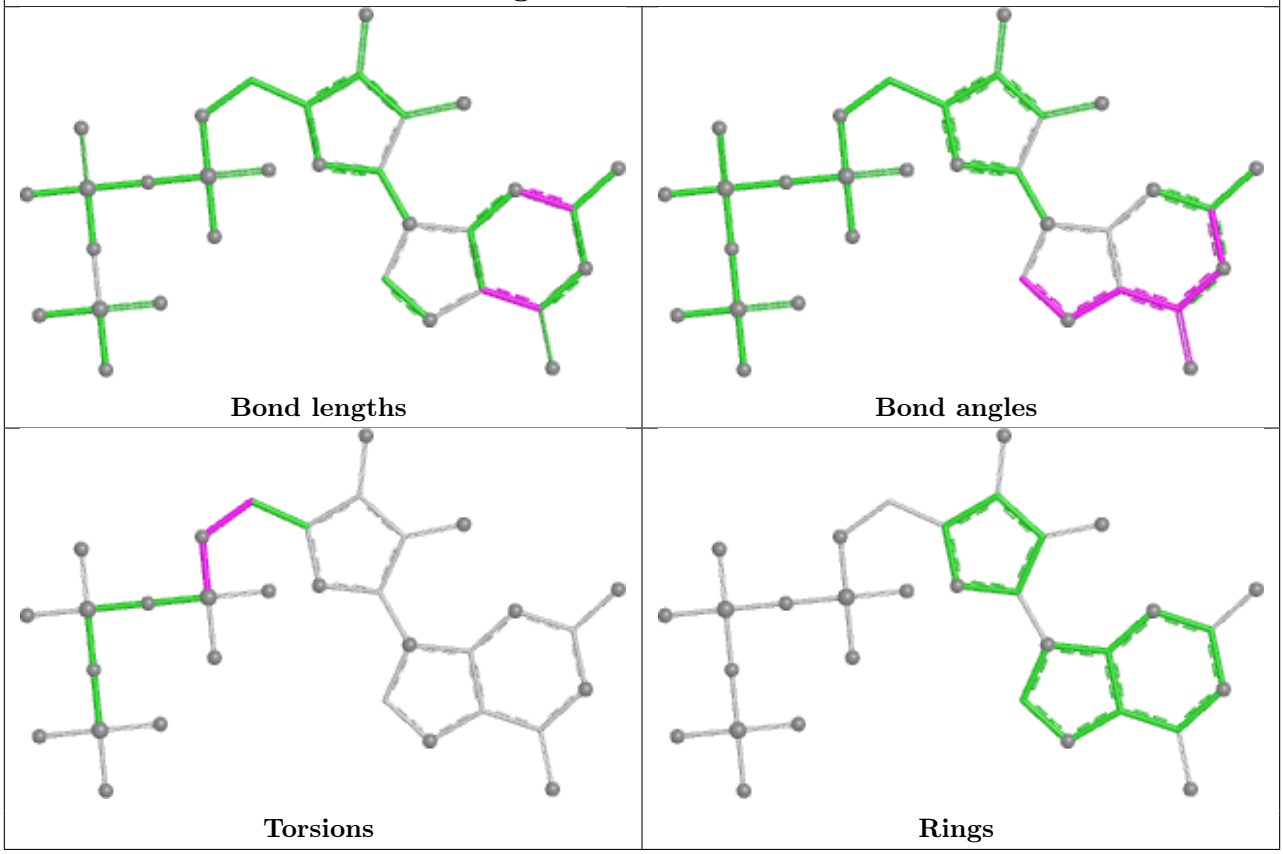


Rings

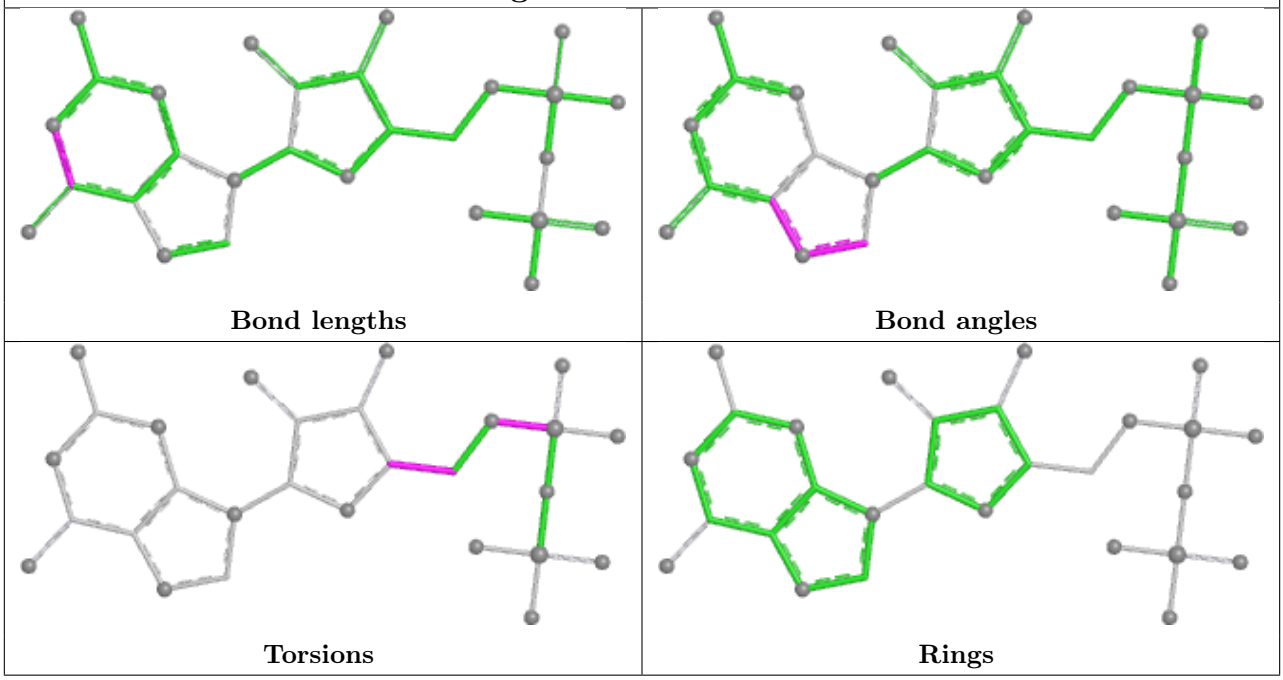
Ligand GDP GC 501



Ligand GTP TE 501



Ligand GDP HL 501



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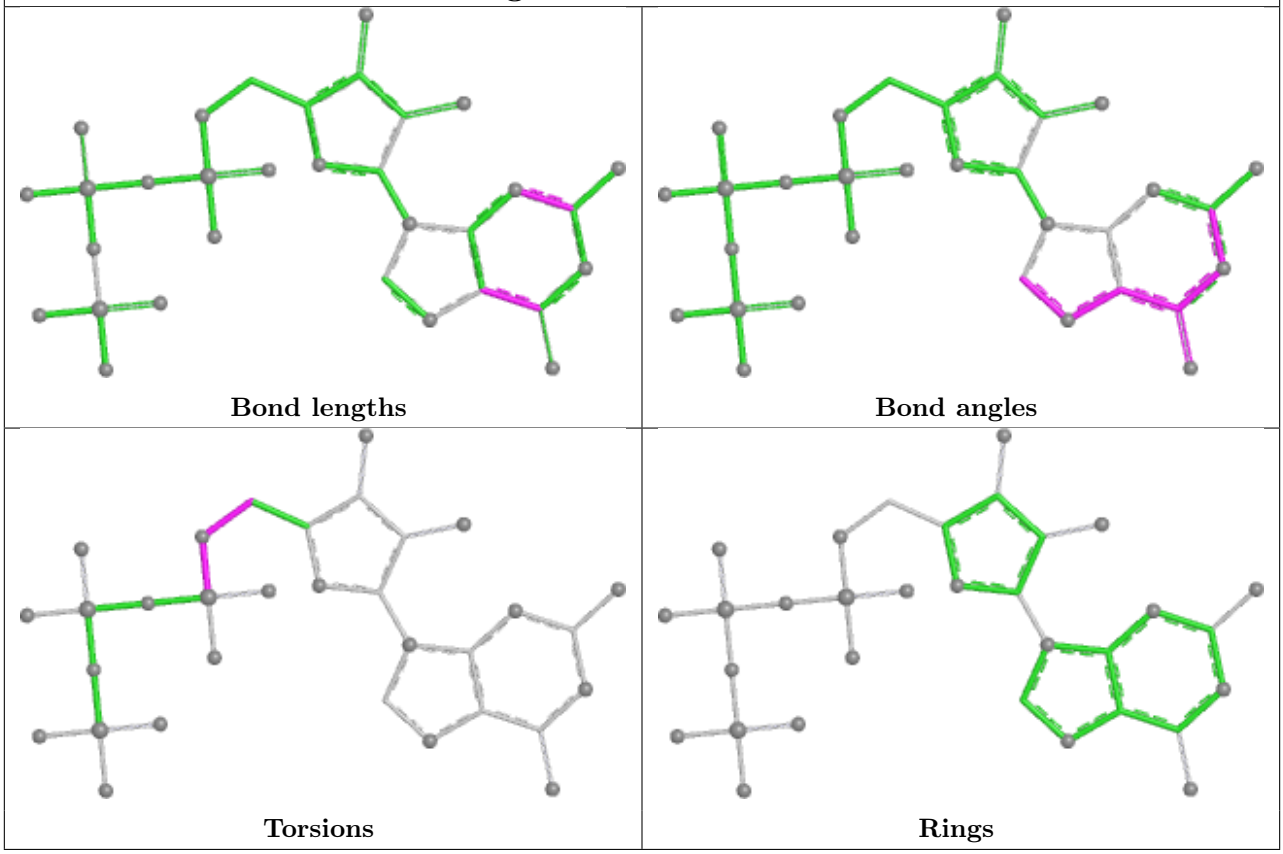

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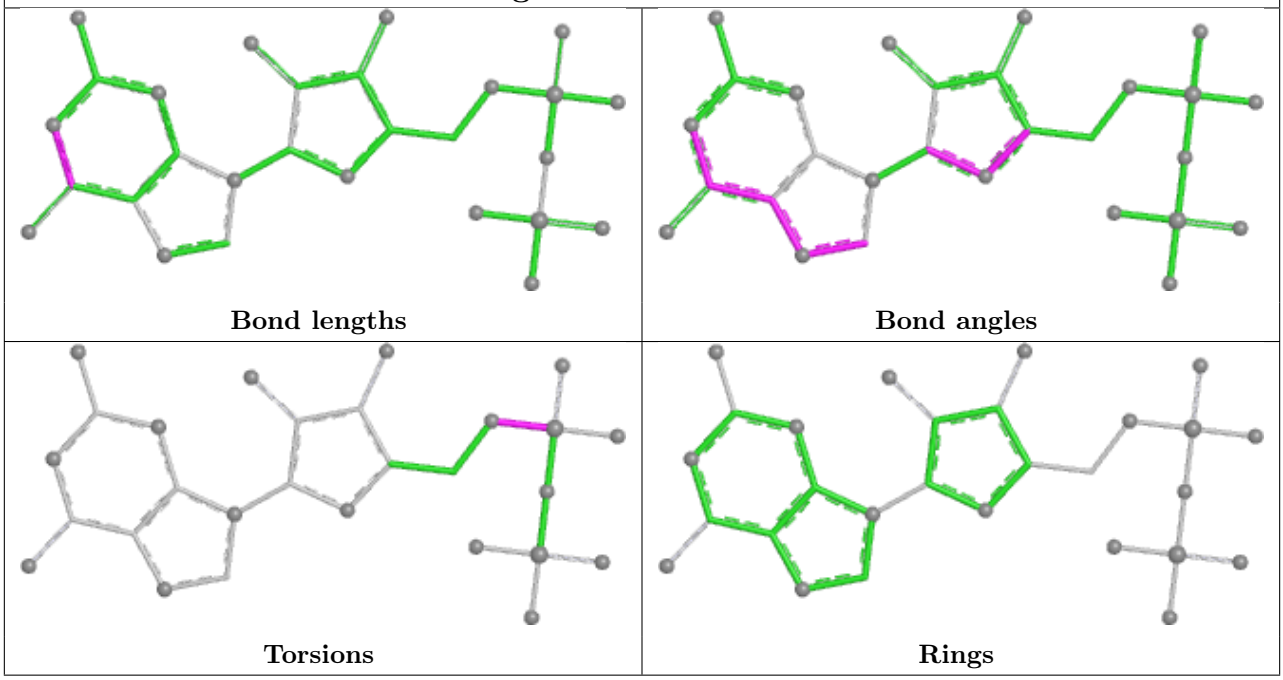

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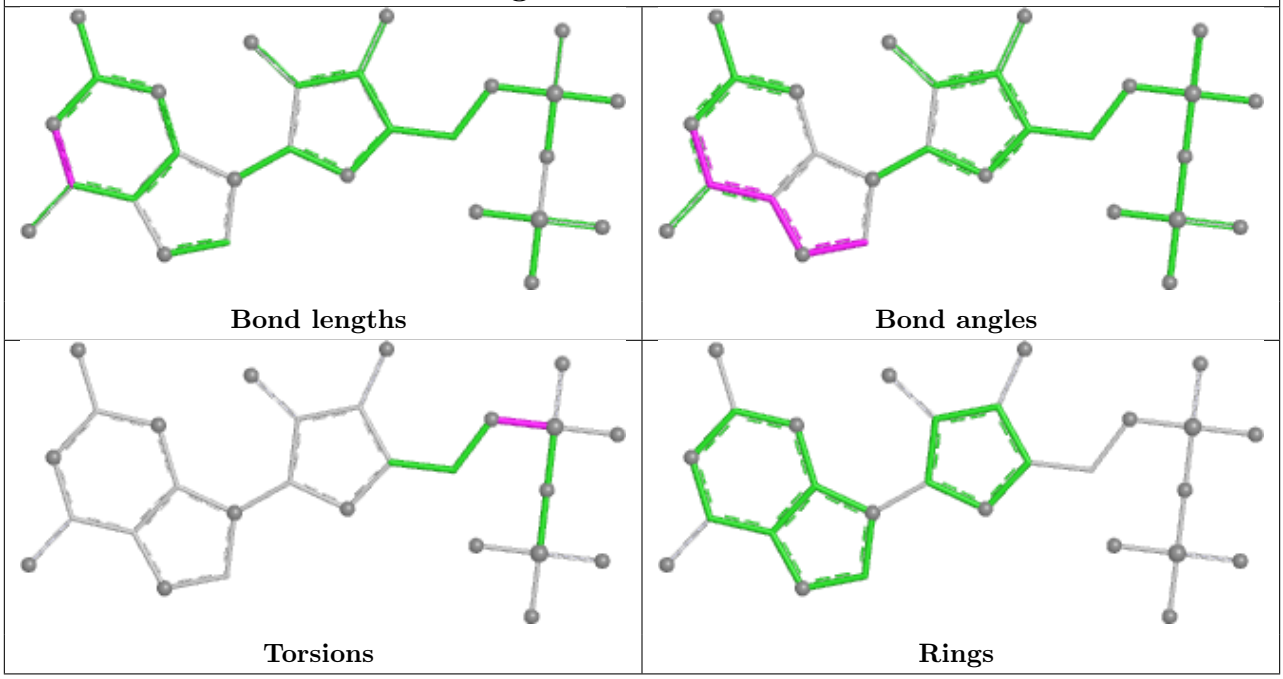

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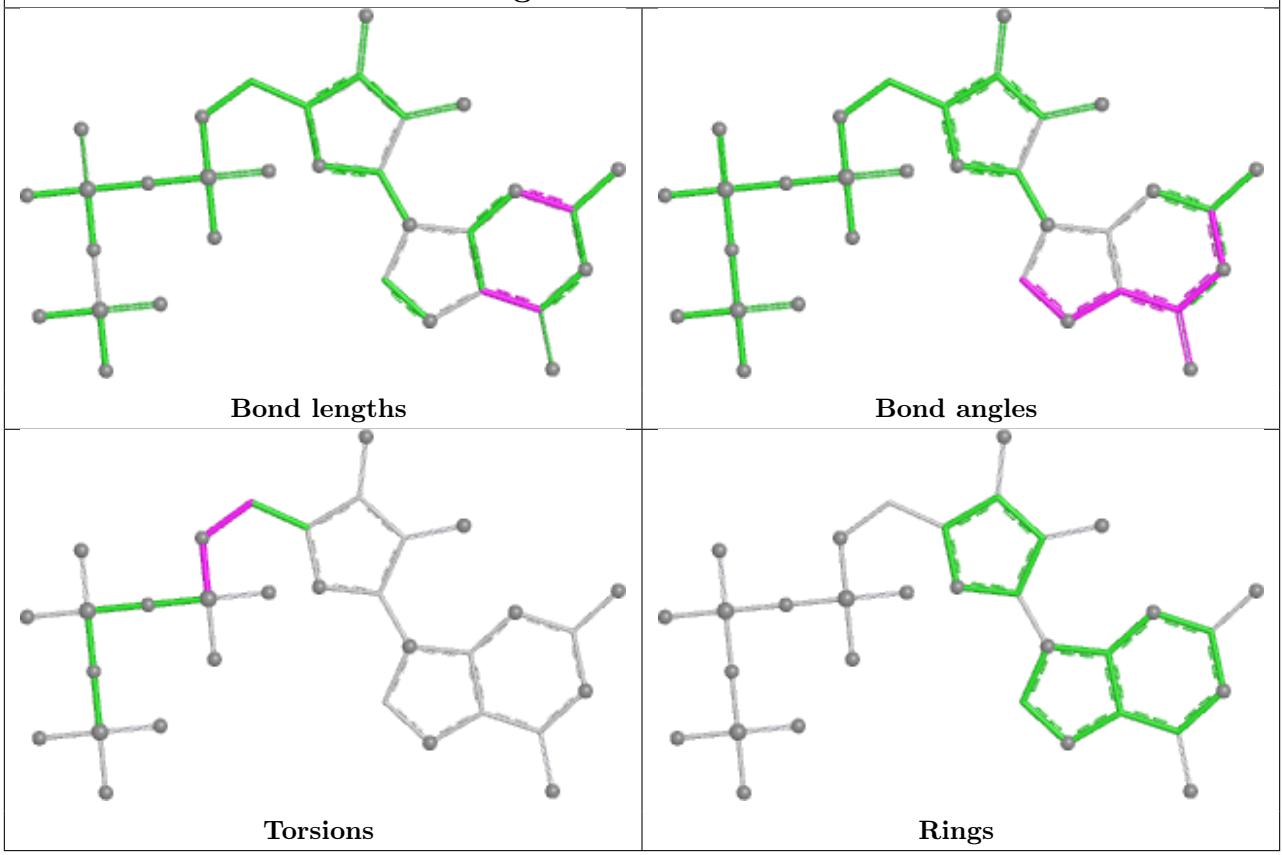

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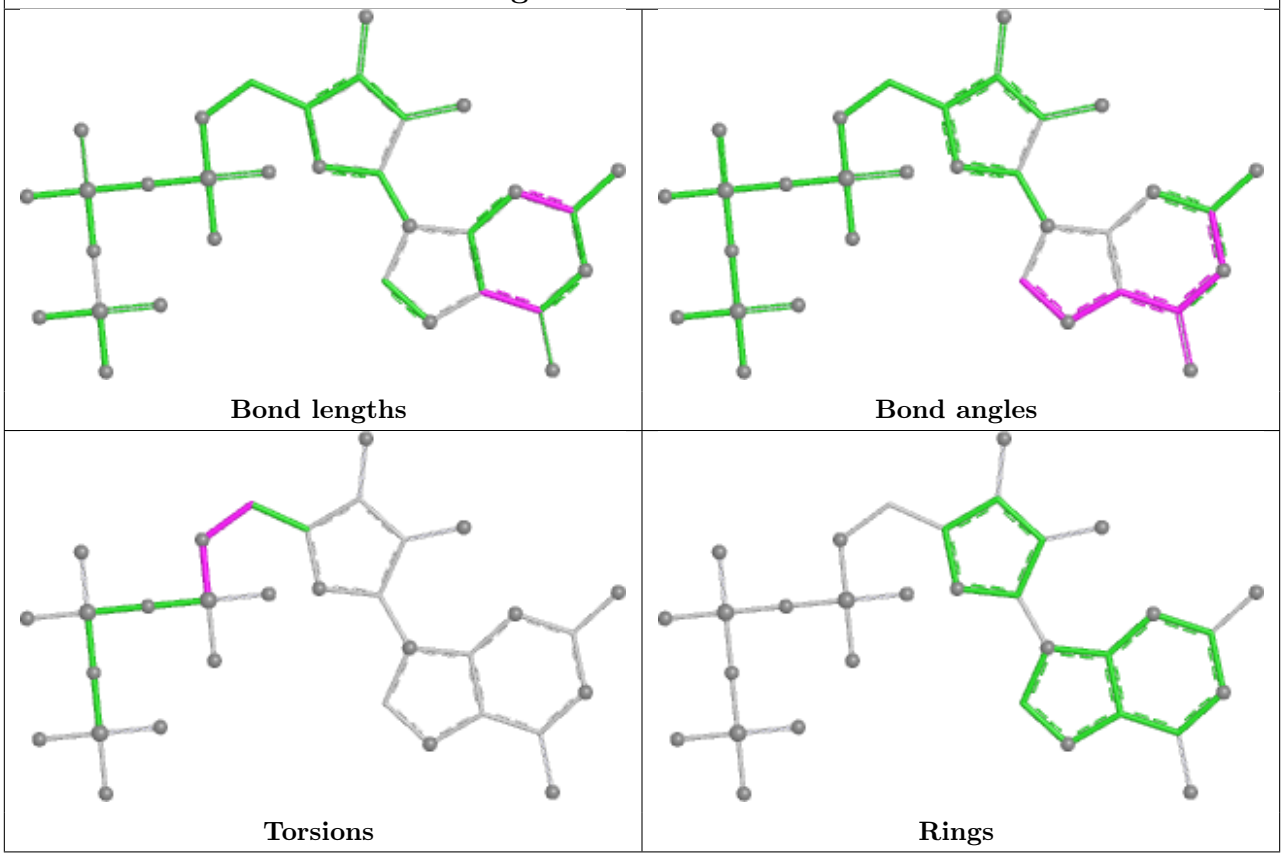

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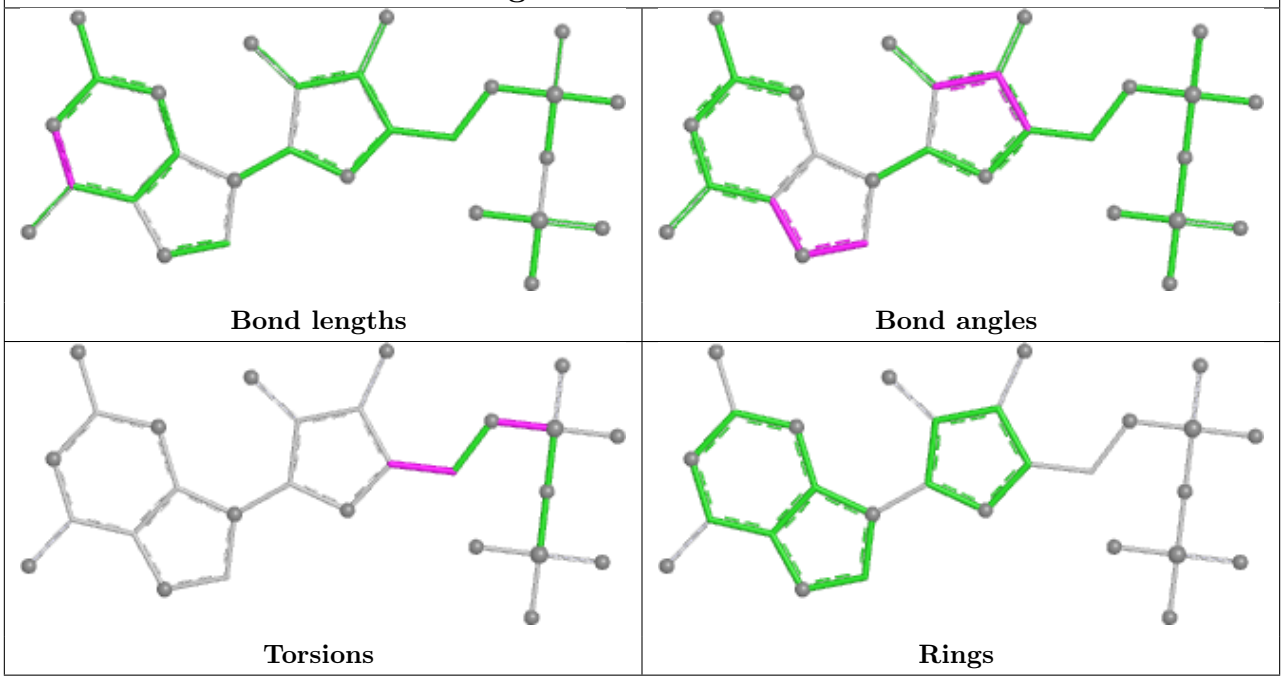

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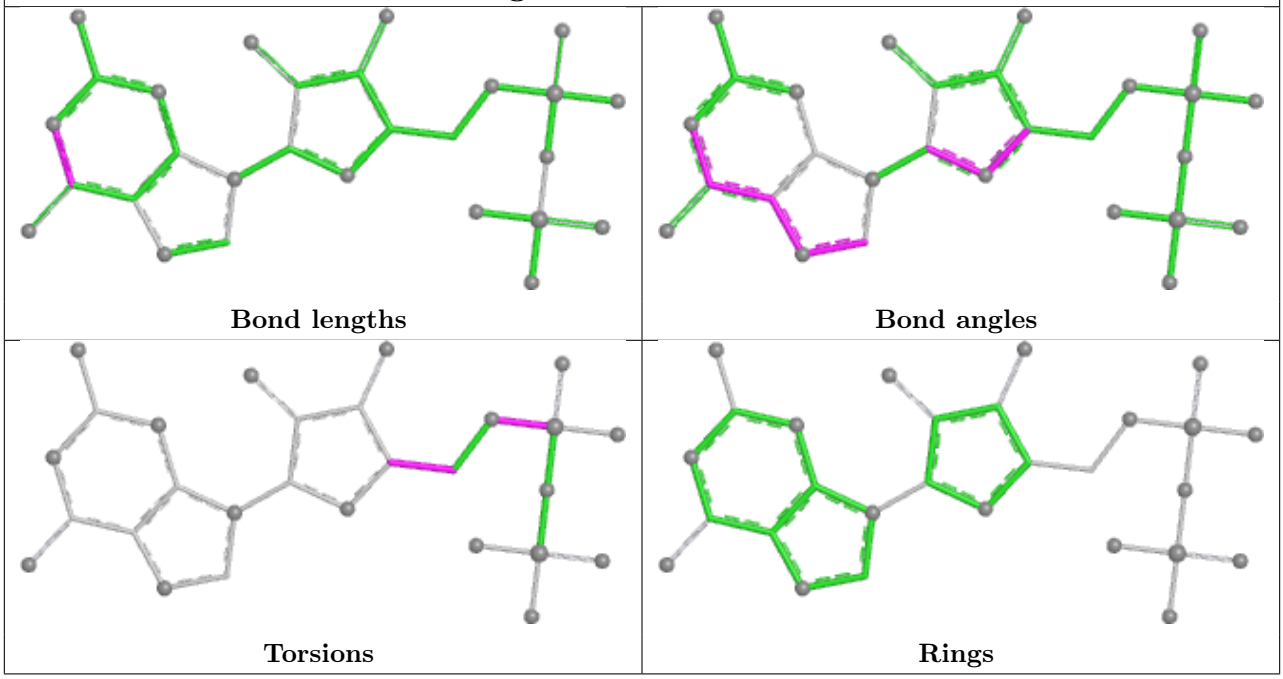

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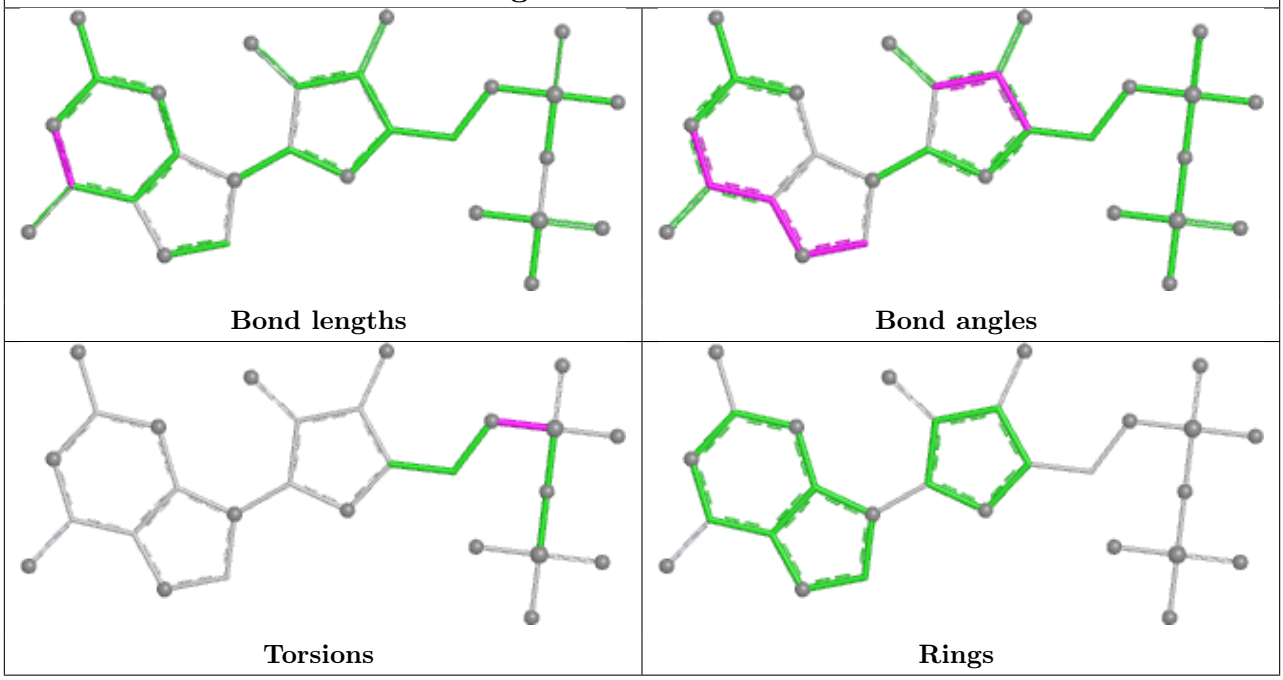

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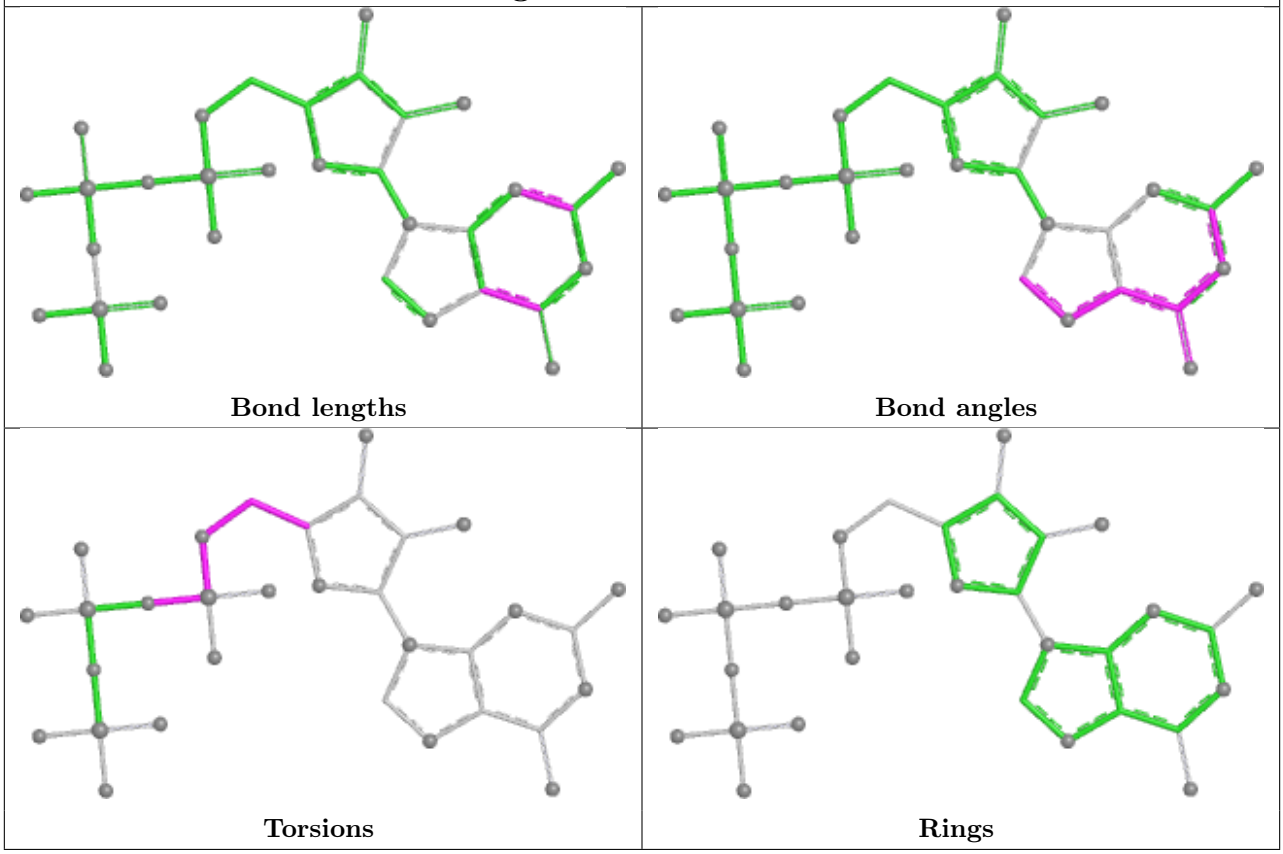

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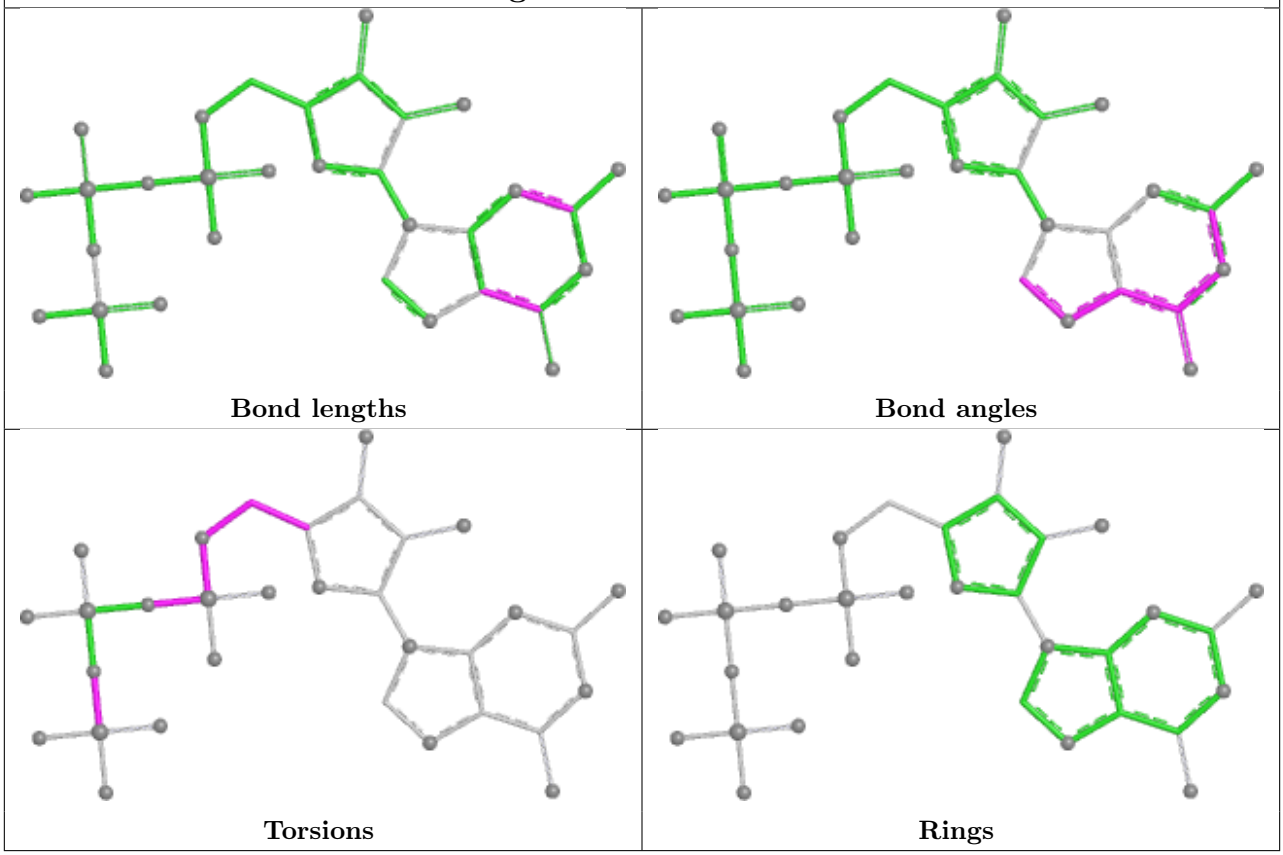

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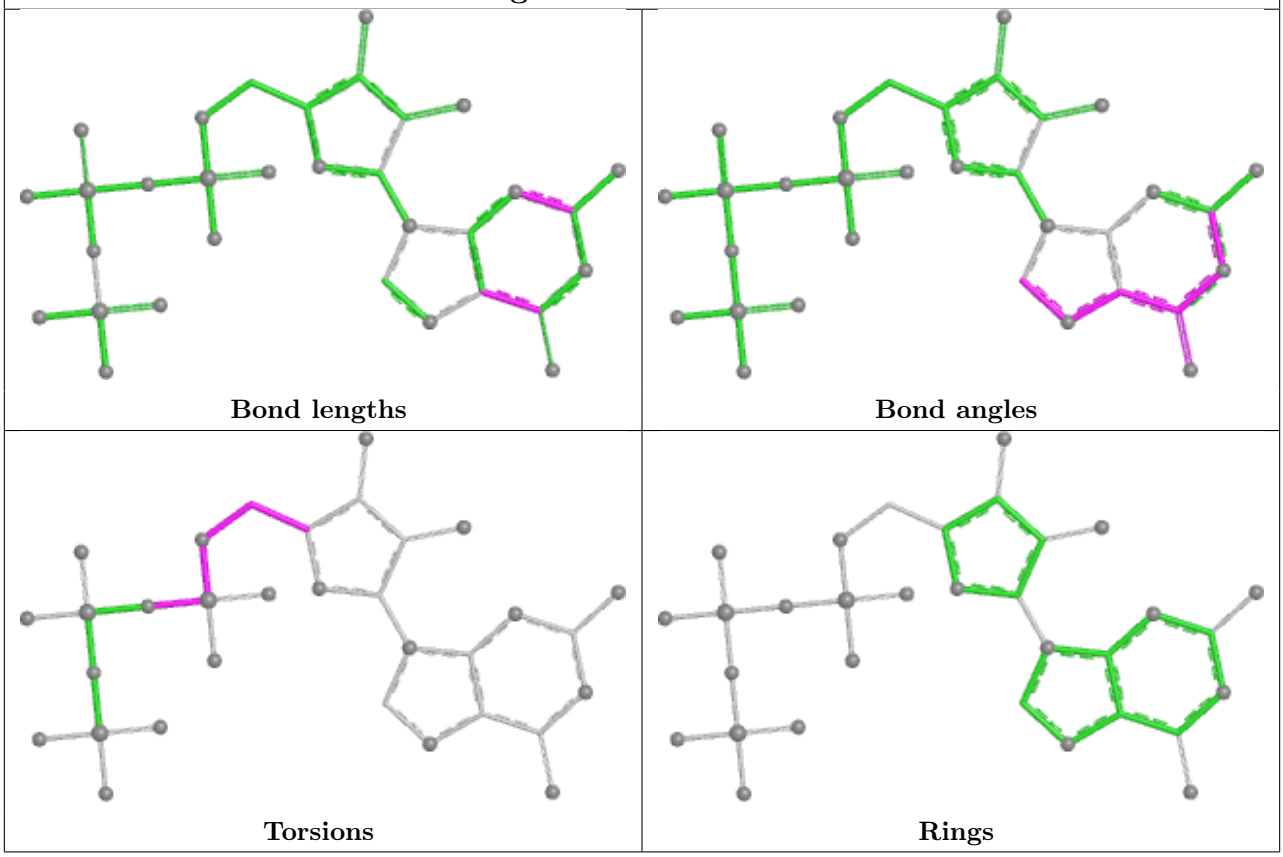

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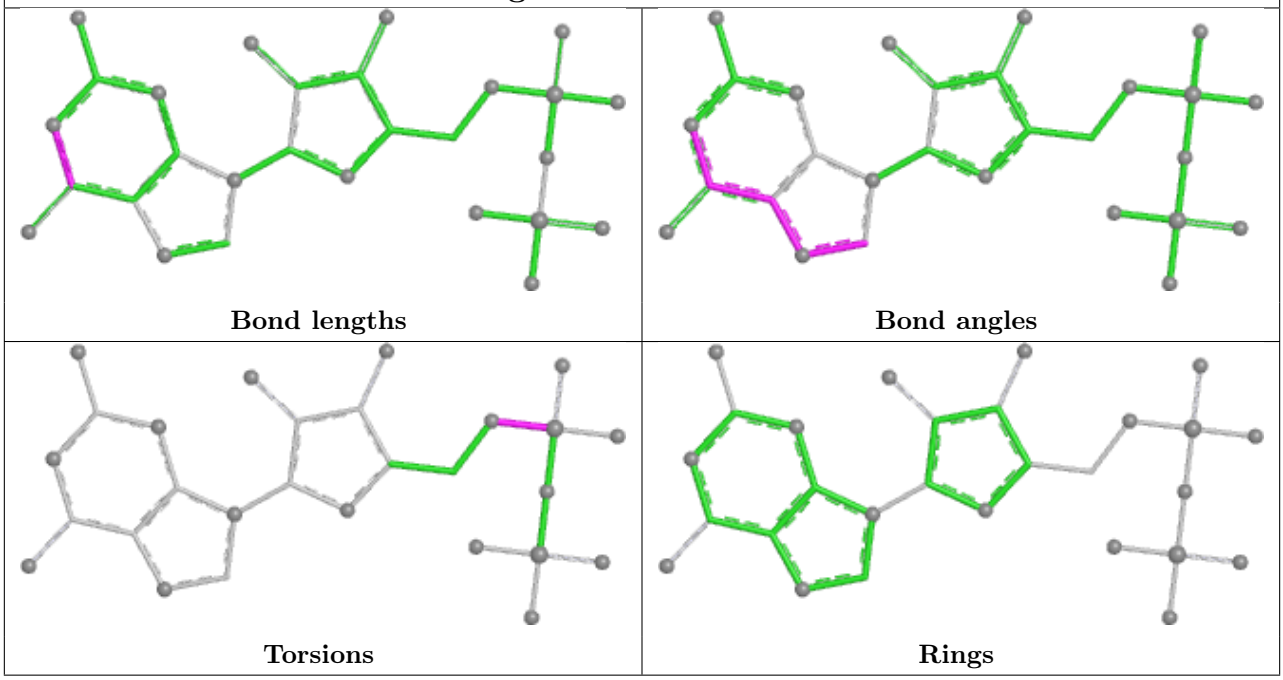

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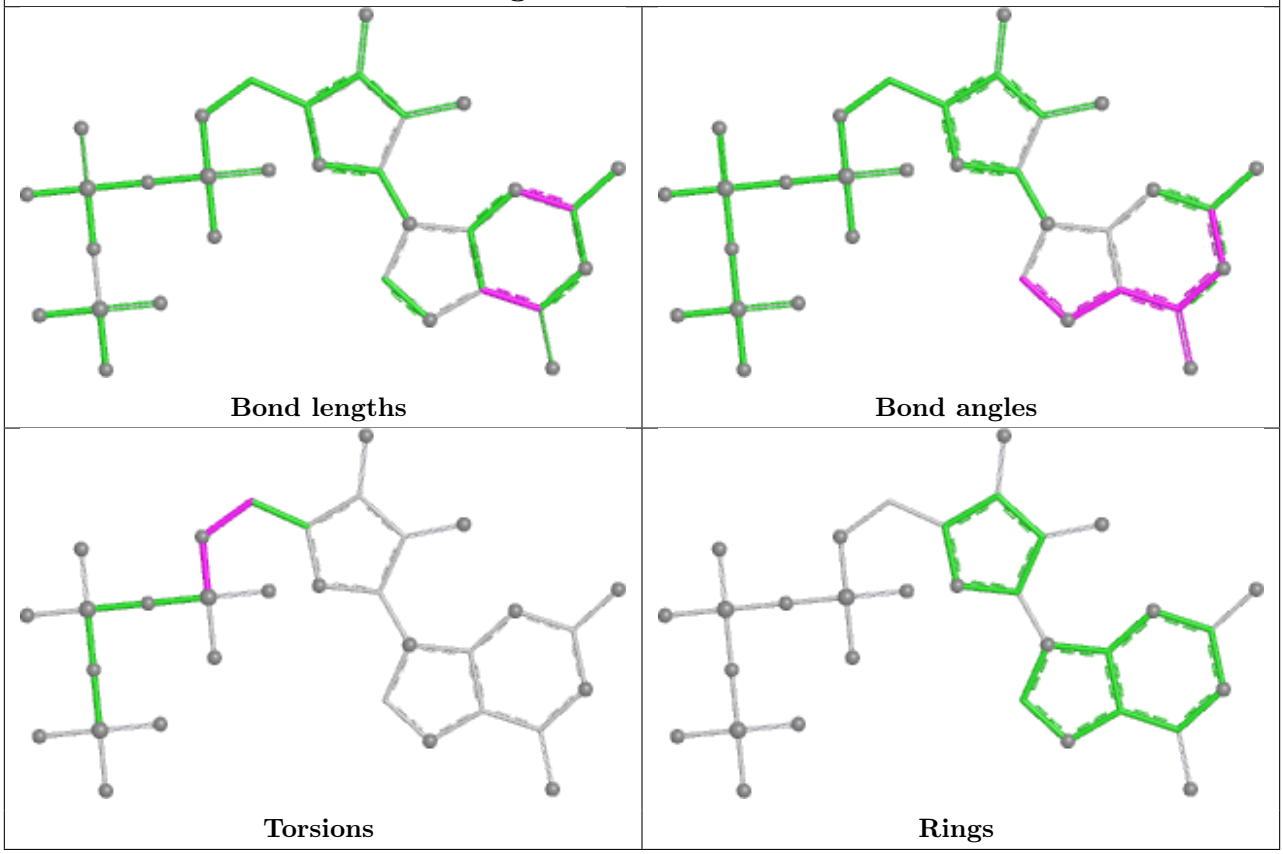
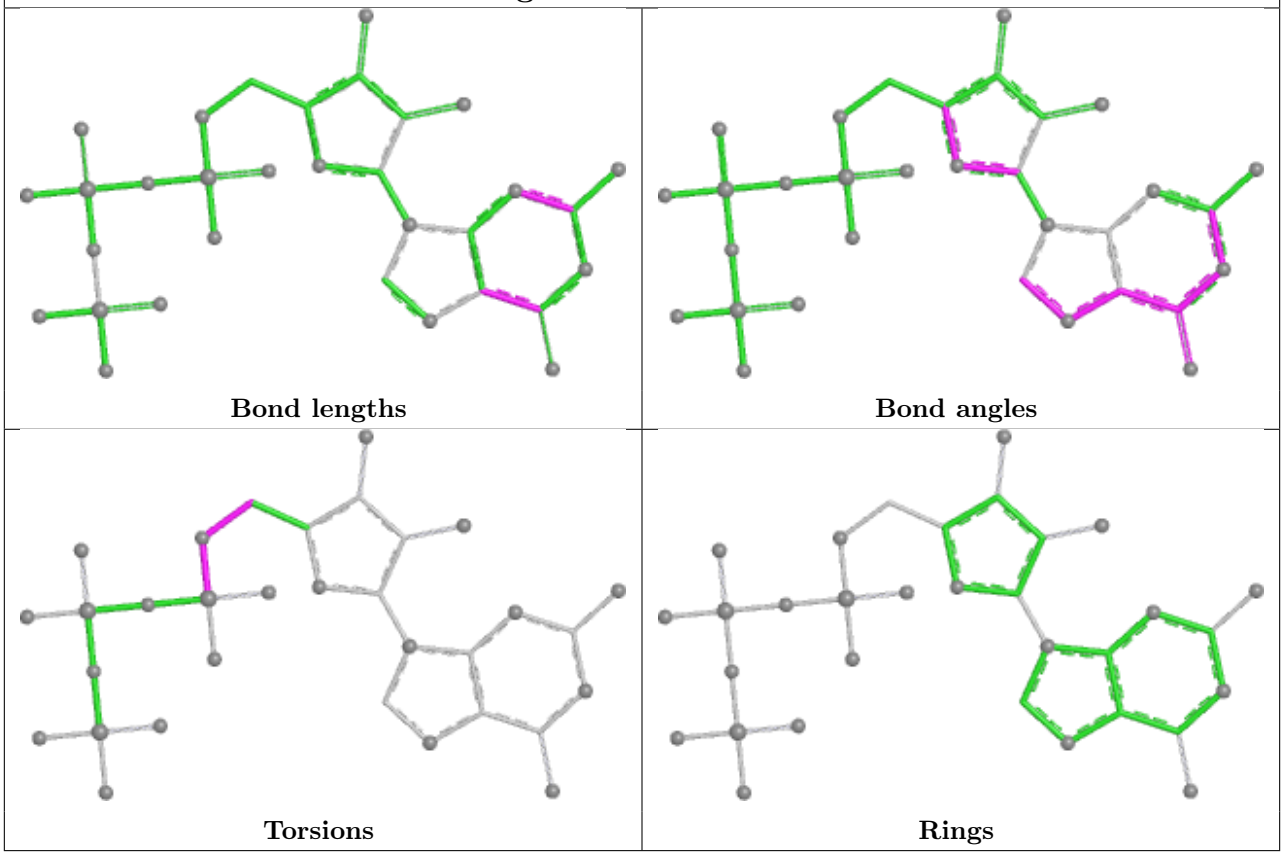
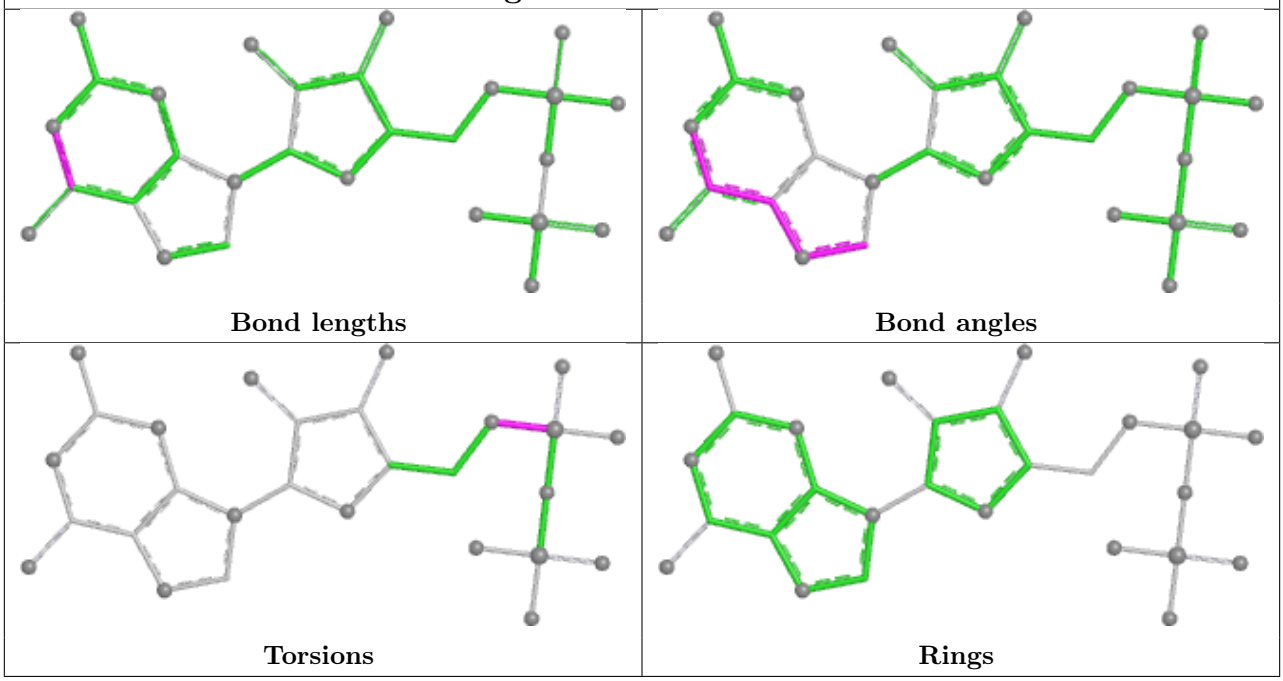


Ligand GTP UI 501



Ligand GDP HM 501



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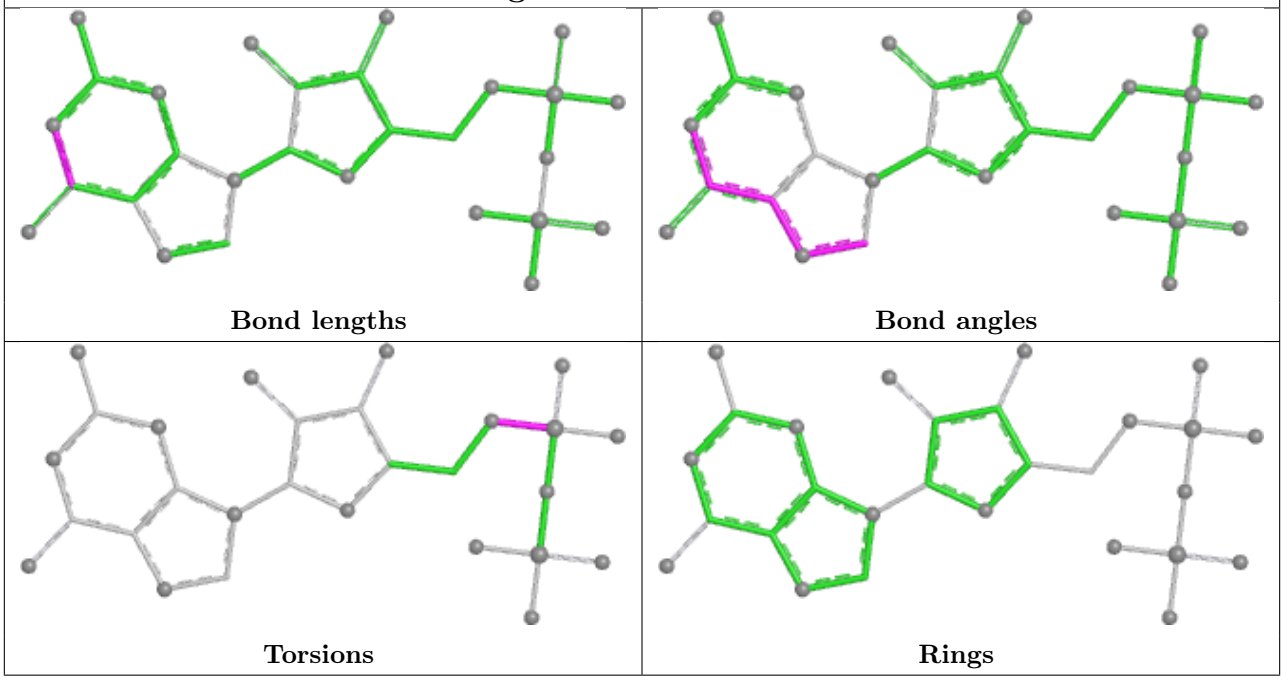
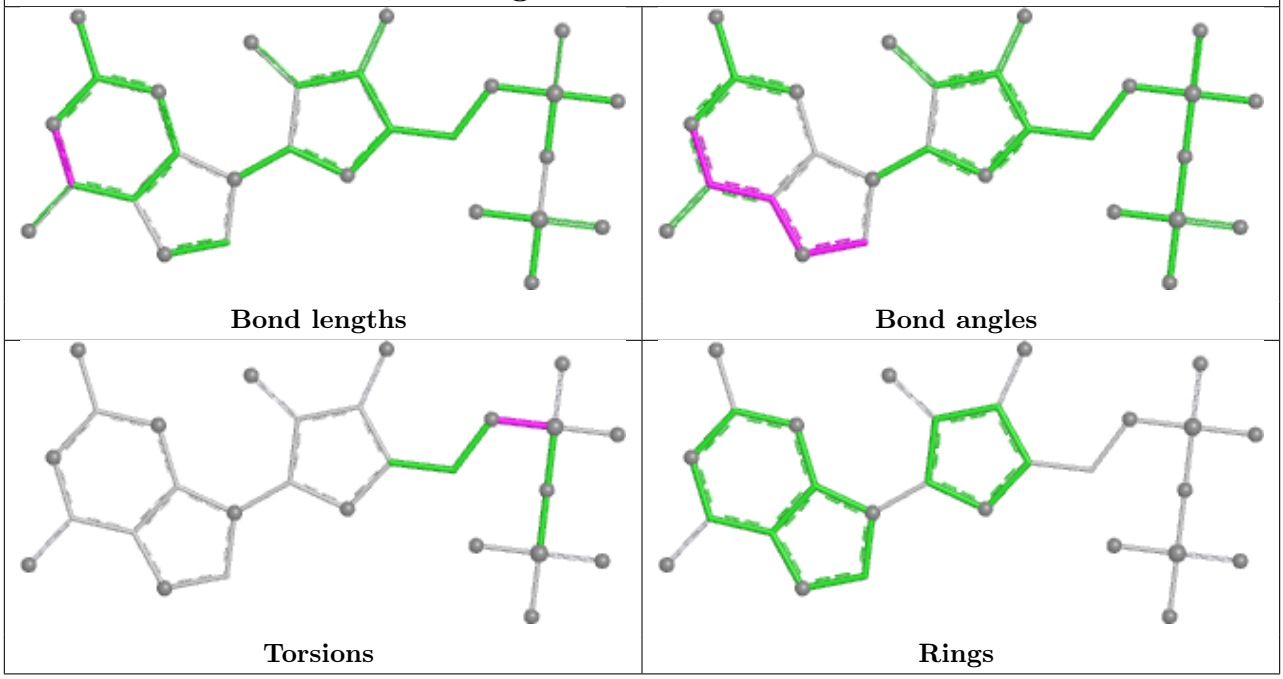


Ligand GDP SH 501



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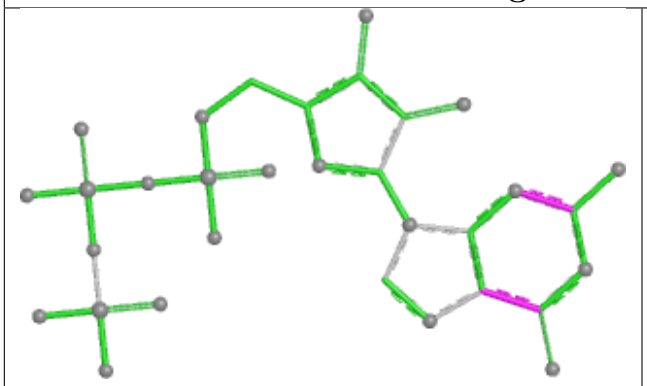
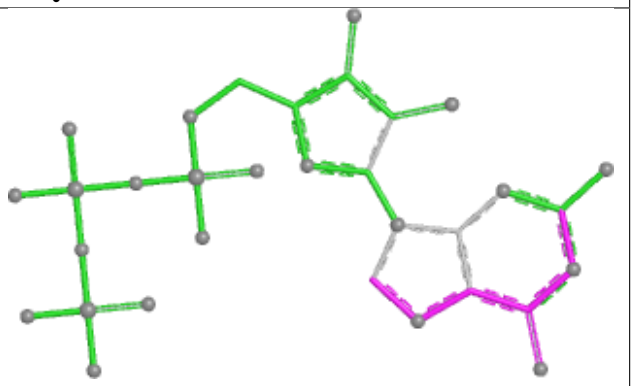
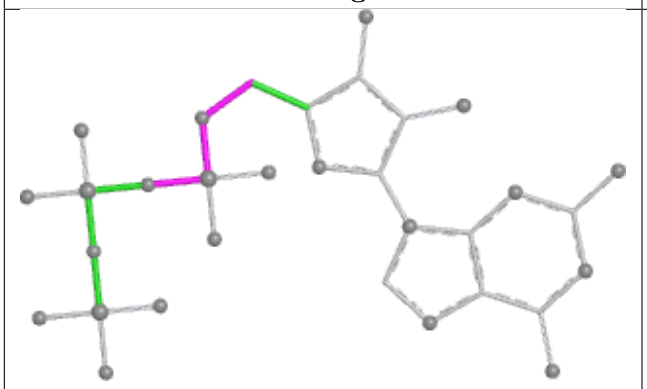


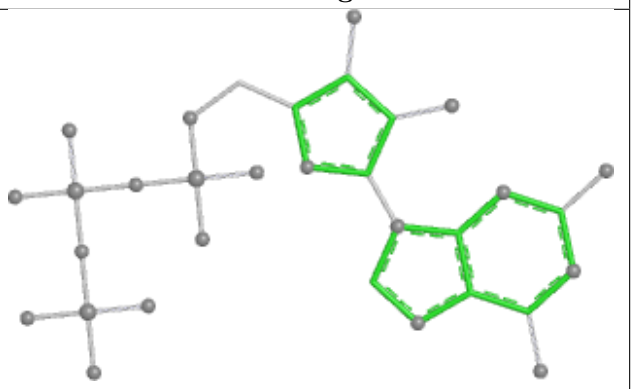
Bond lengths



Bond angles

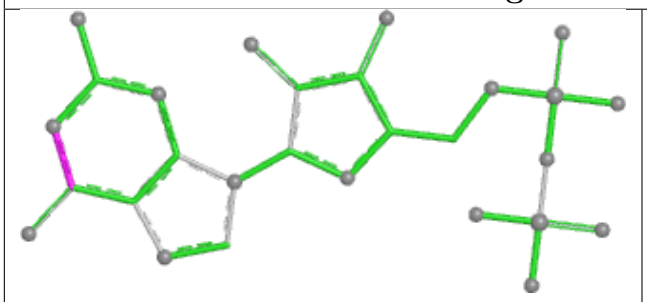


Torsions



Rings

Ligand GDP WL 501



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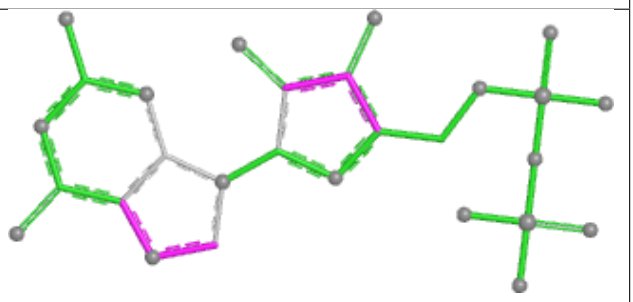

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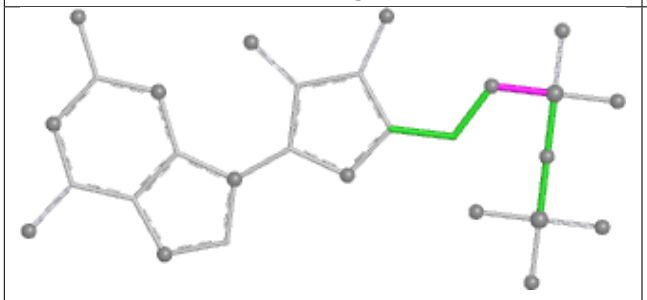

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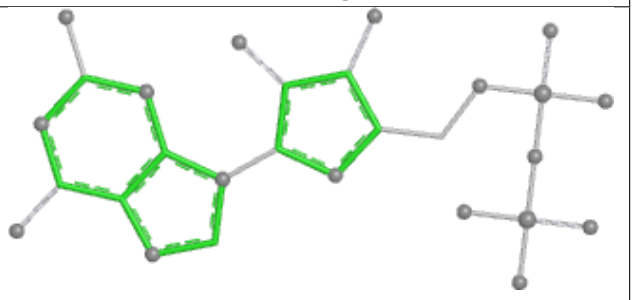
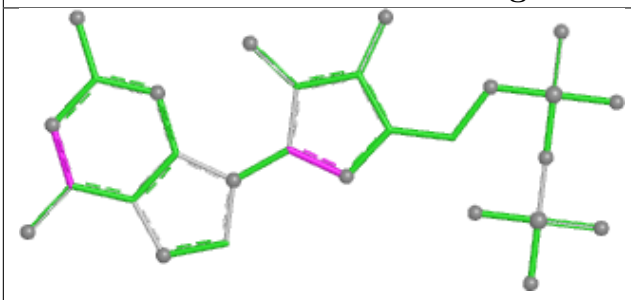


Rings

Ligand GDP DF 501



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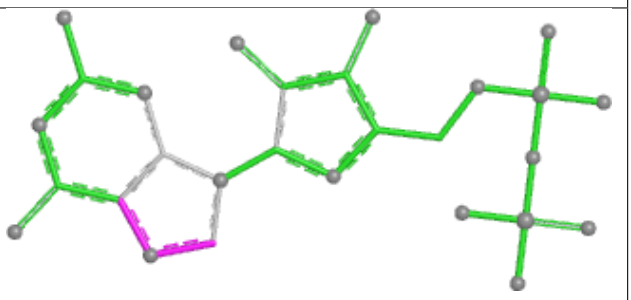

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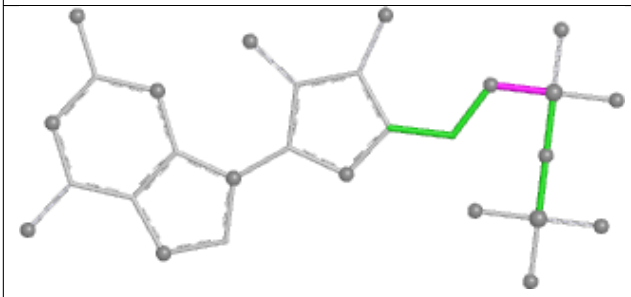

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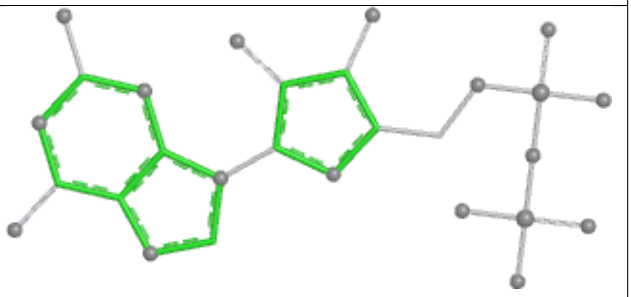

Rings

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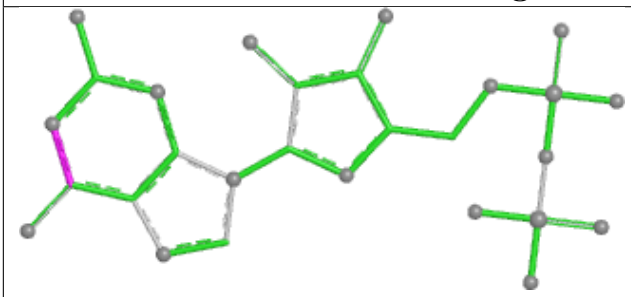

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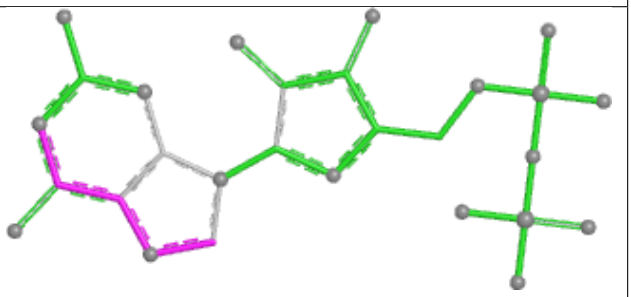

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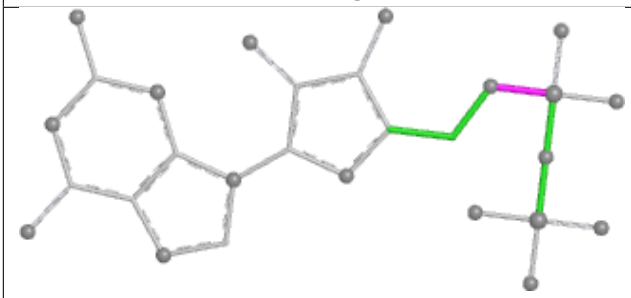

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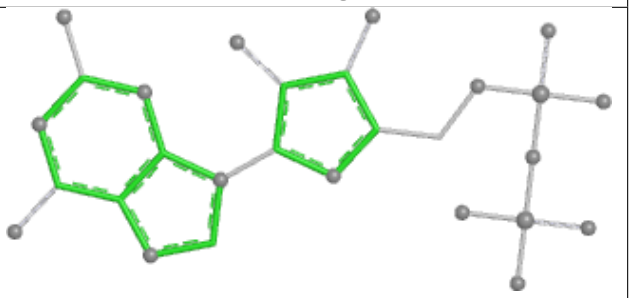
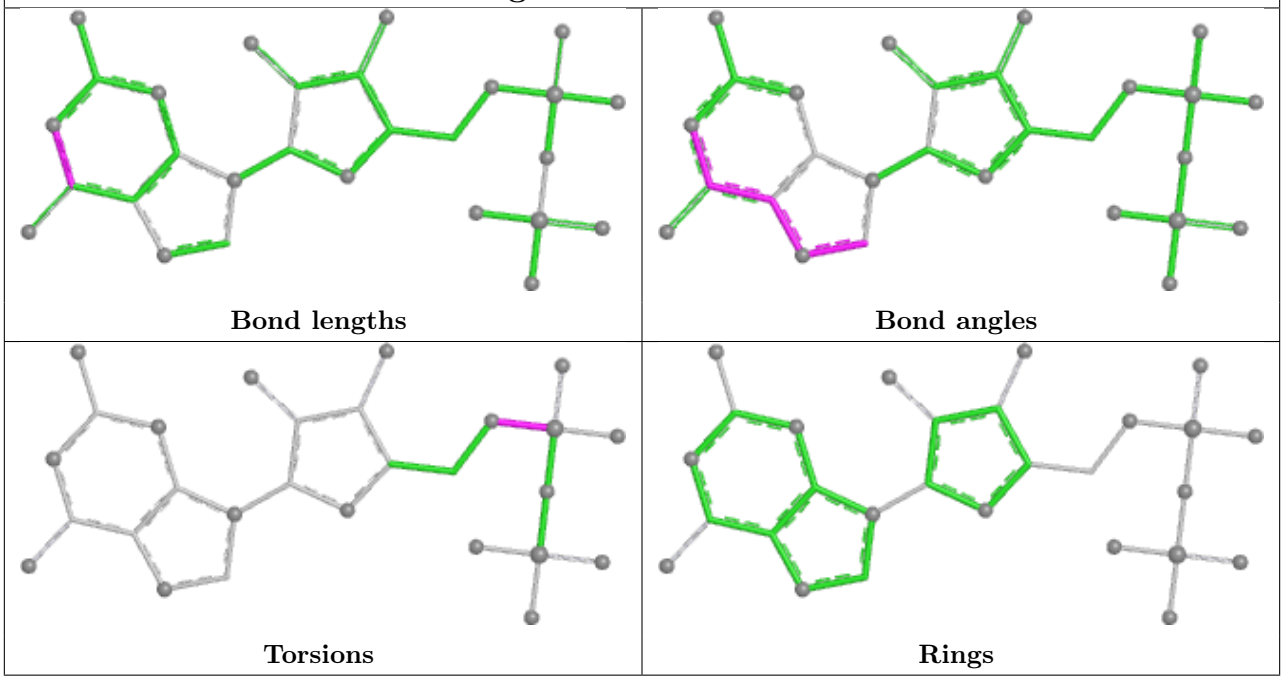
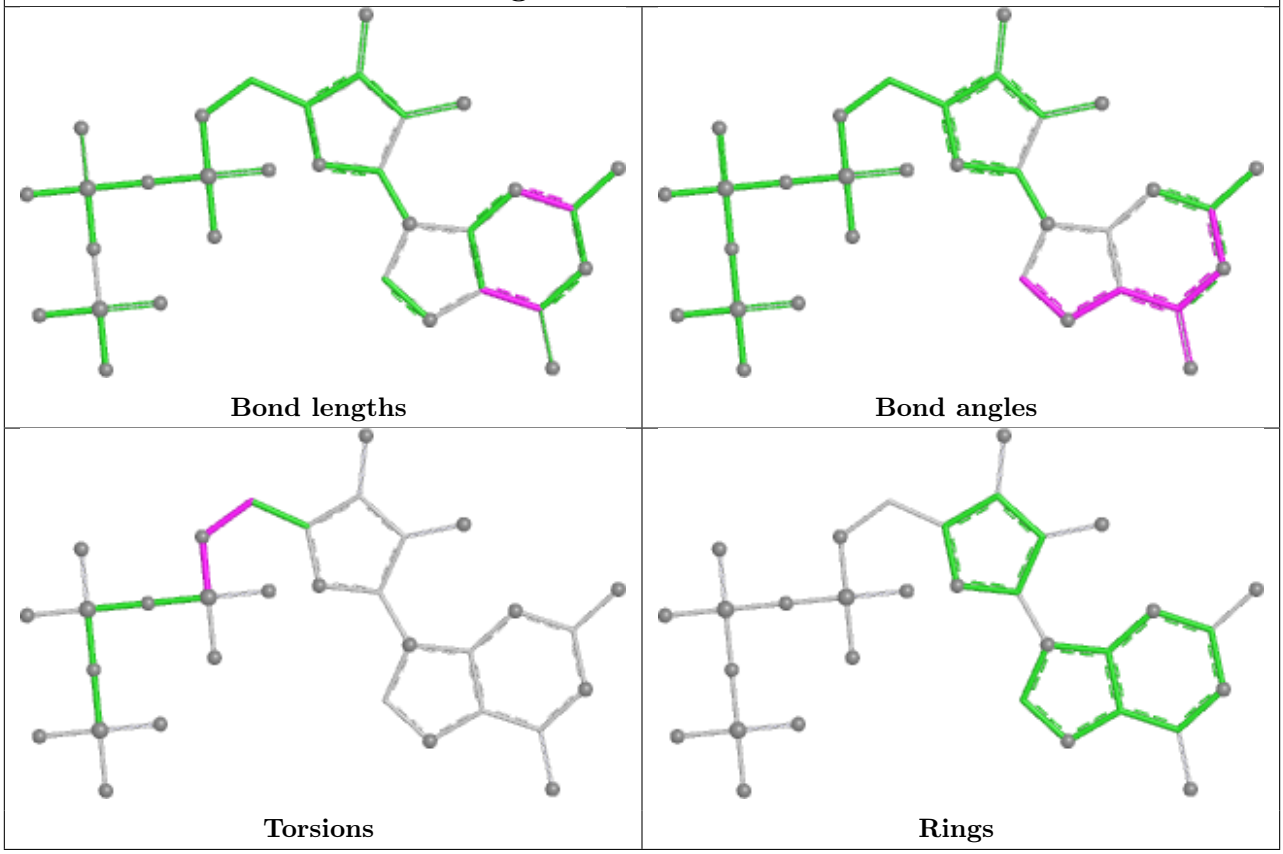


Rings

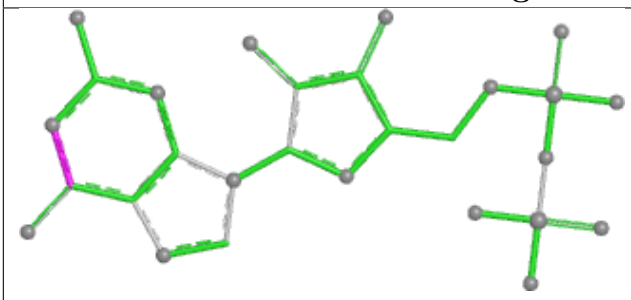
Ligand GDP BH 501



Ligand GTP TK 501



Ligand GDP CJ 501



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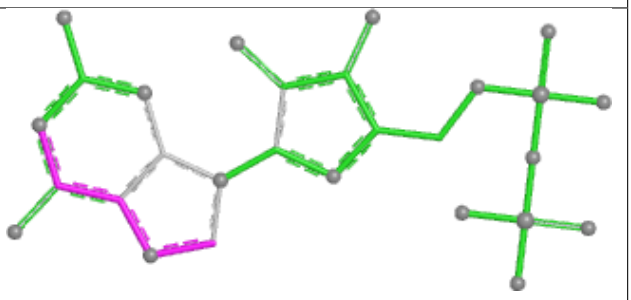
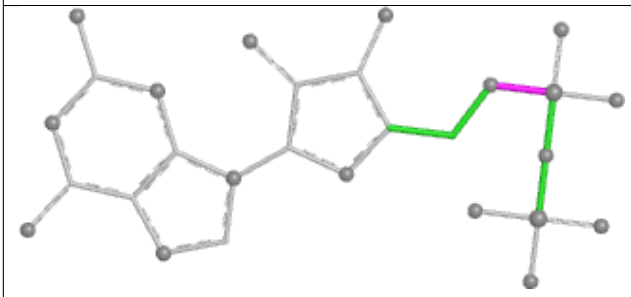


Bond angles



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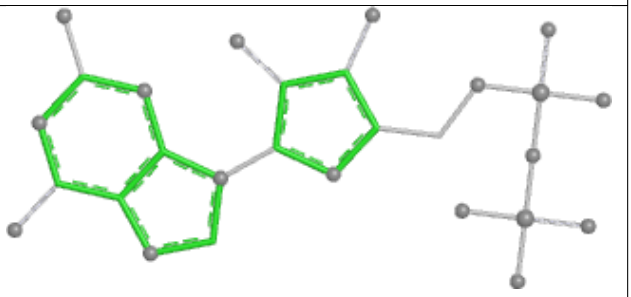

Rings

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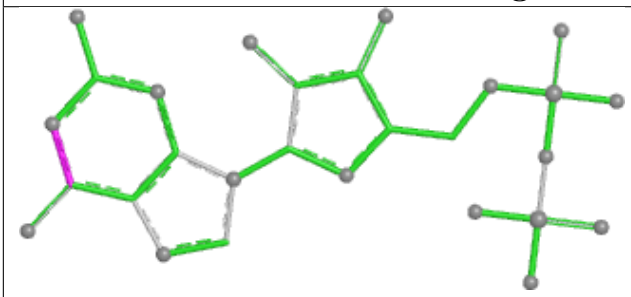

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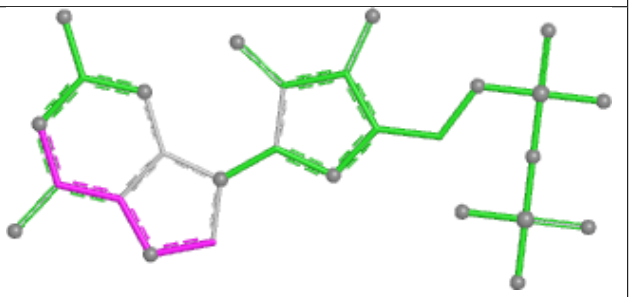
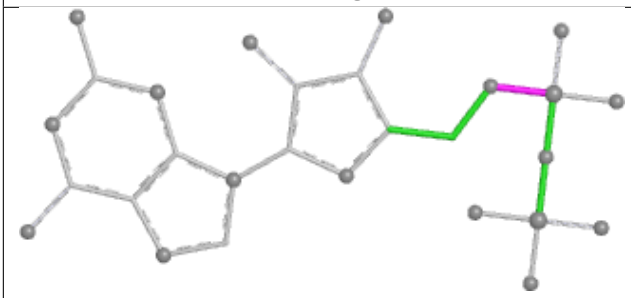
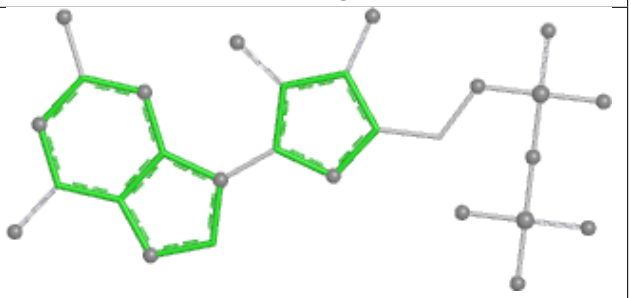


Bond angles

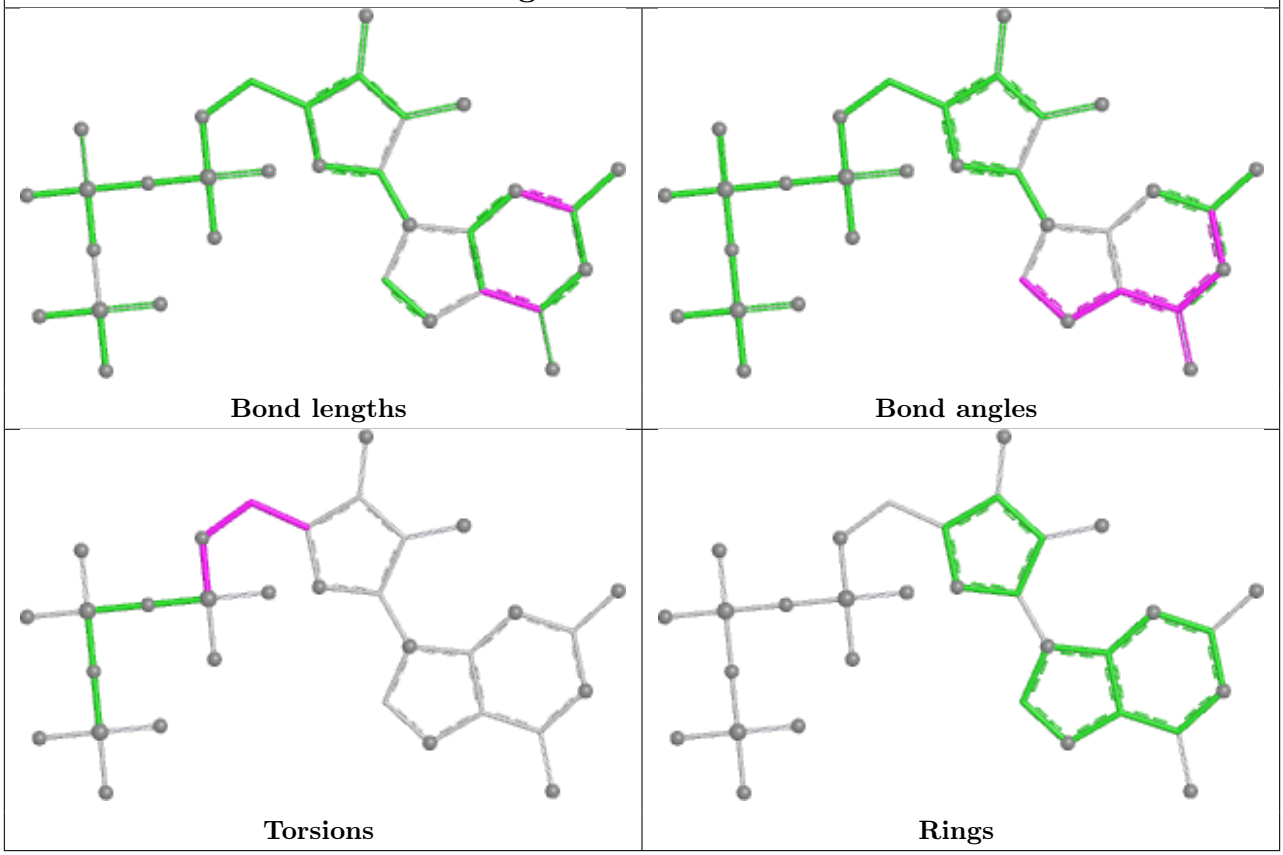


Torsions



Rings

Ligand GTP IE 501



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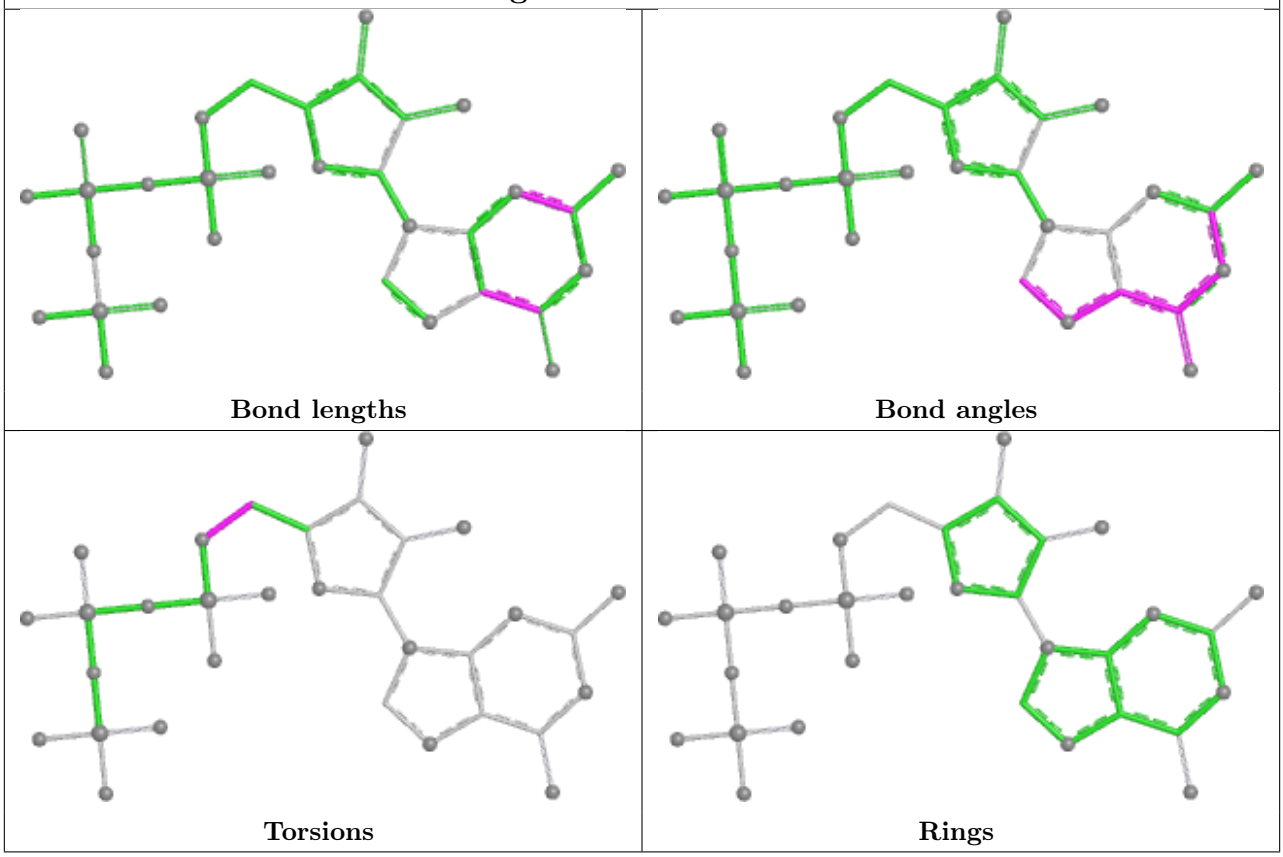

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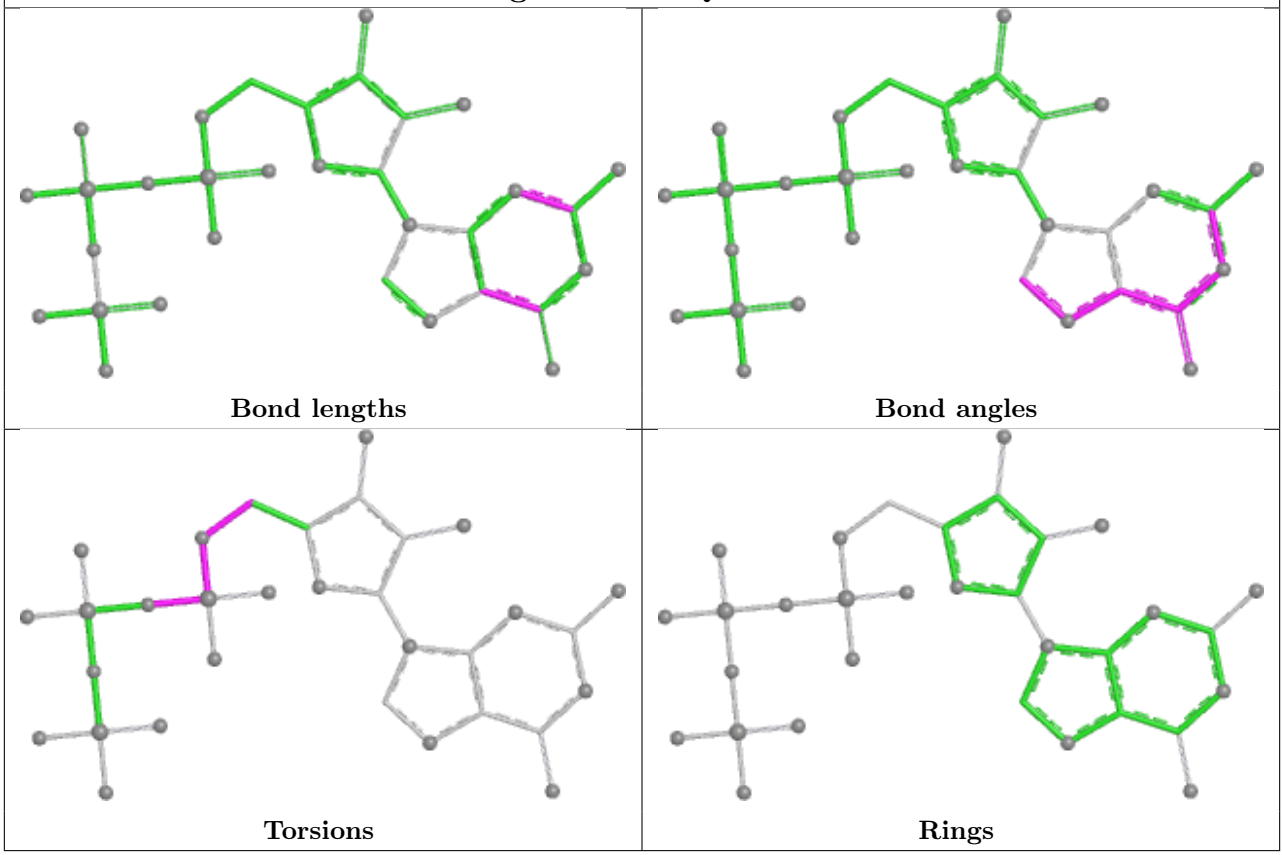

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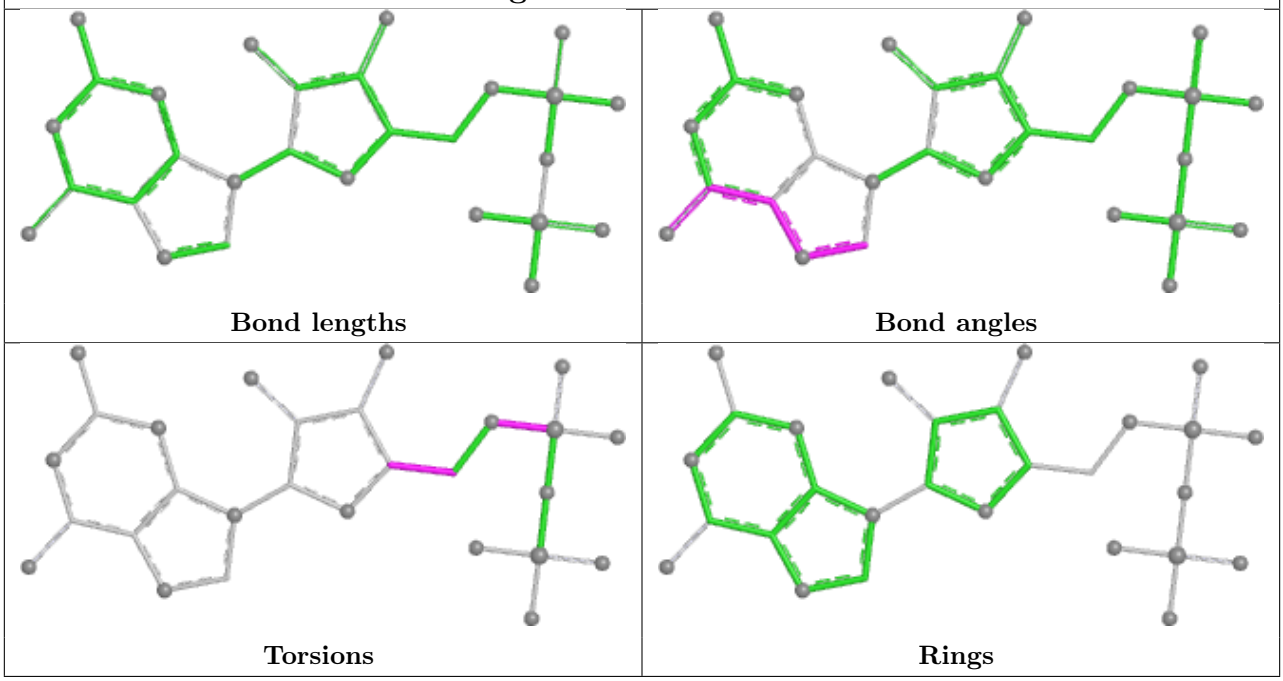

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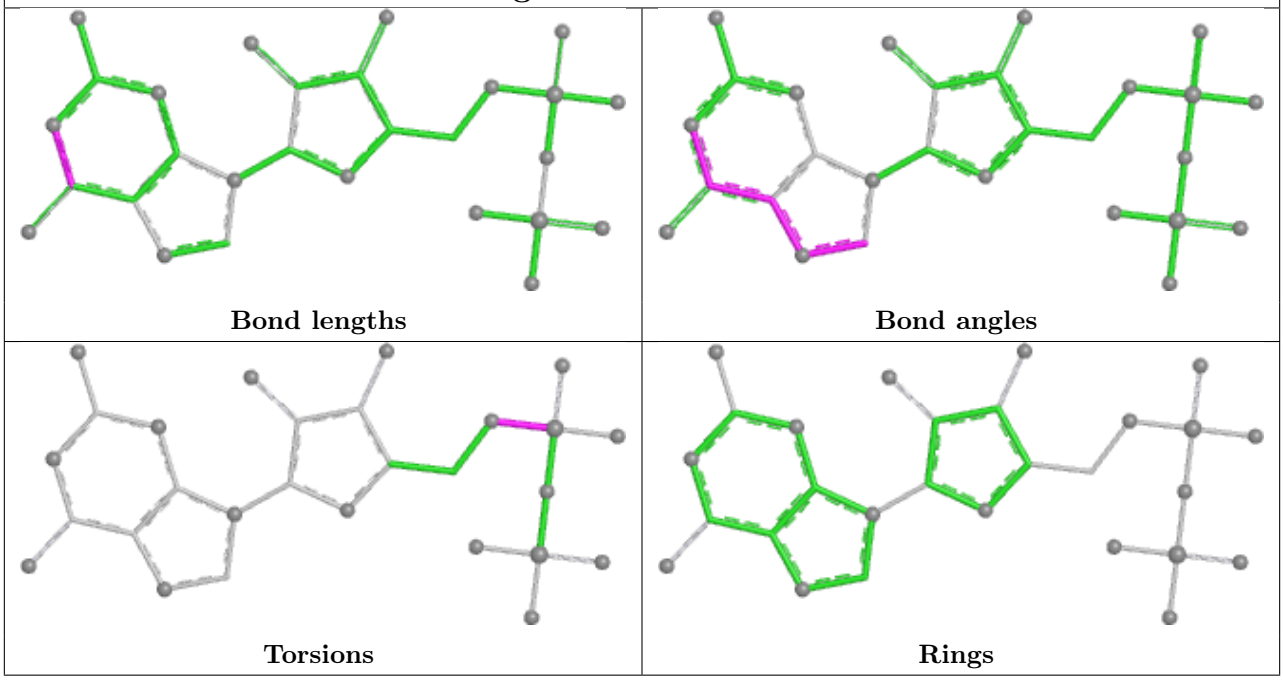

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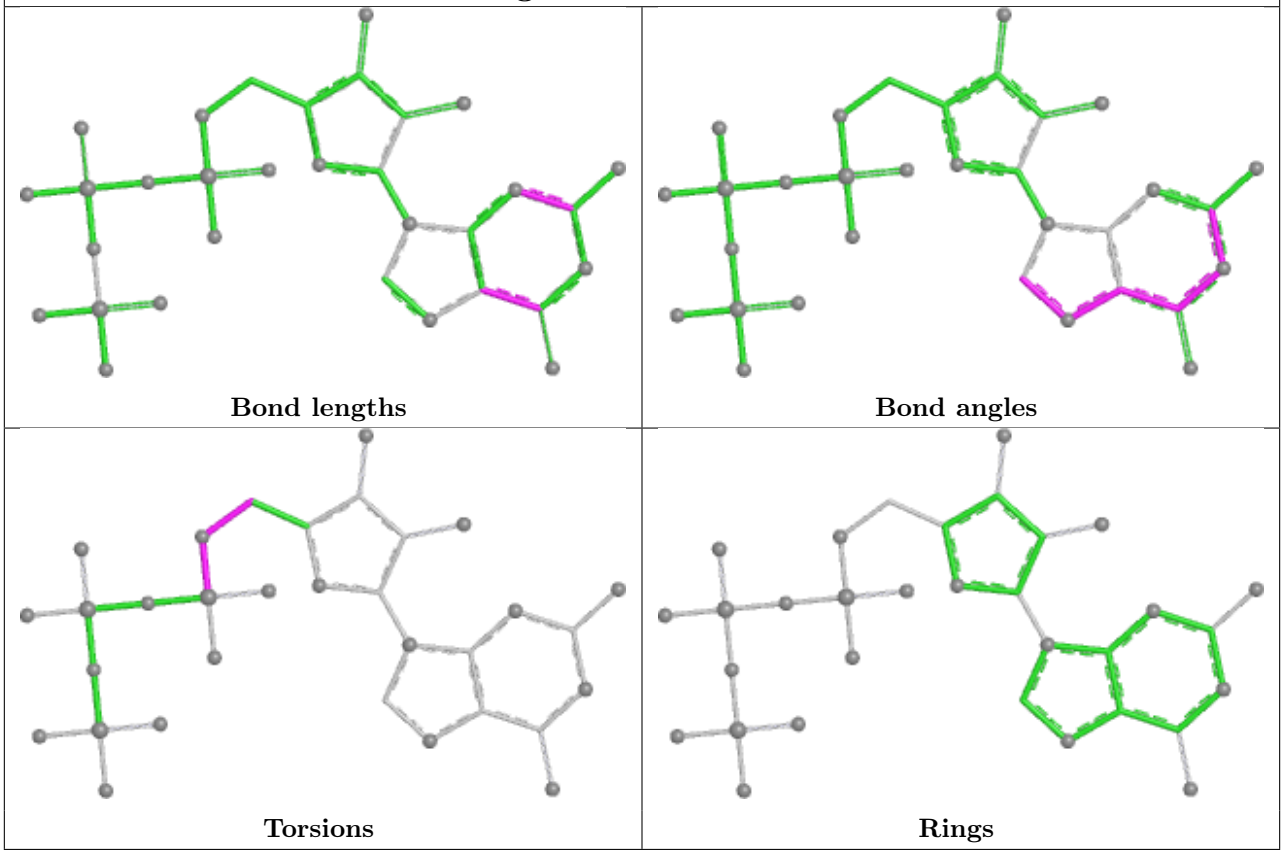

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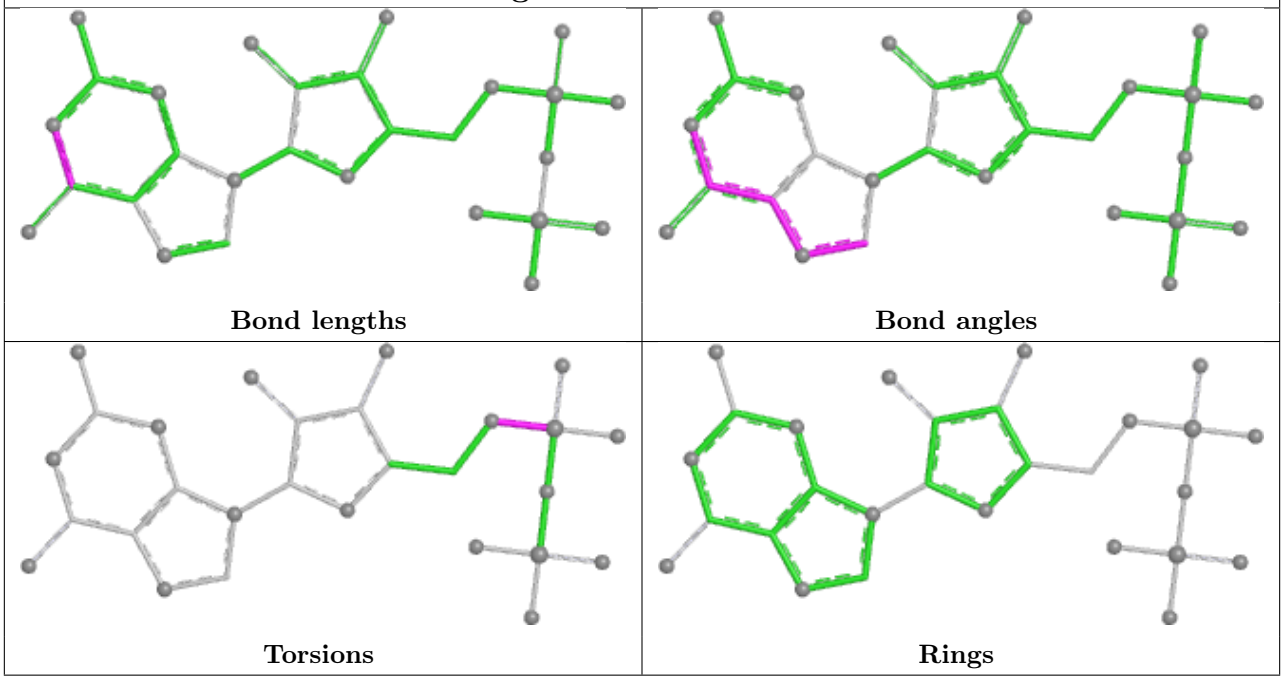
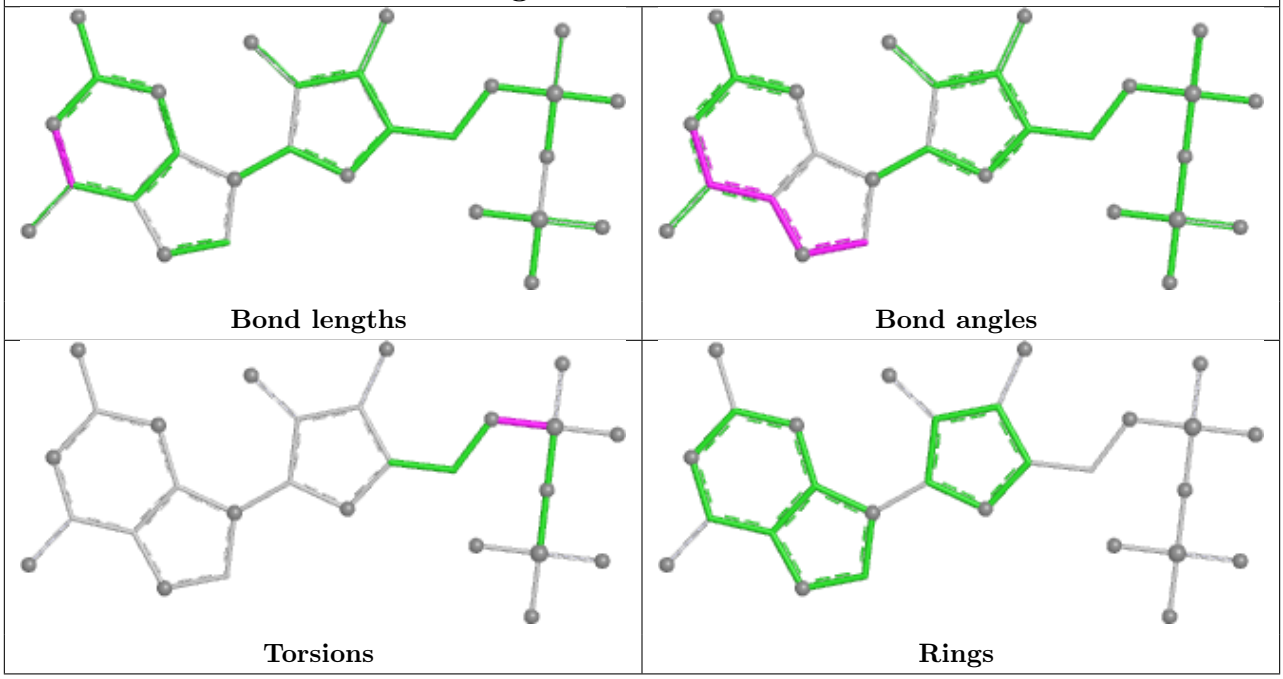
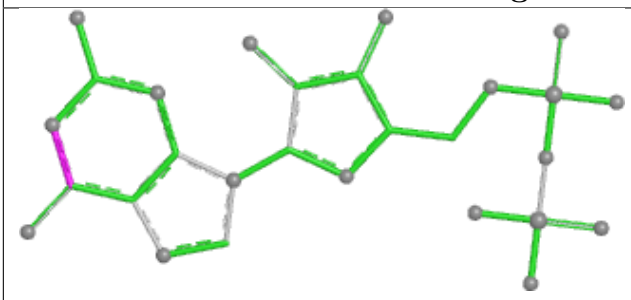


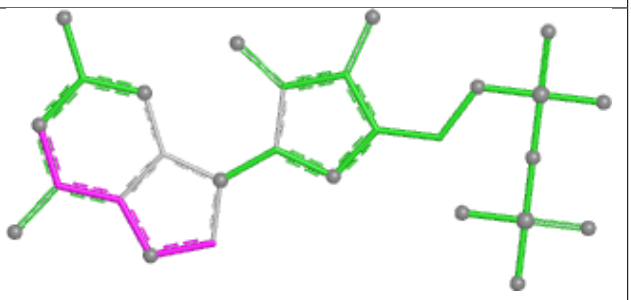
Ligand GDP VF 501



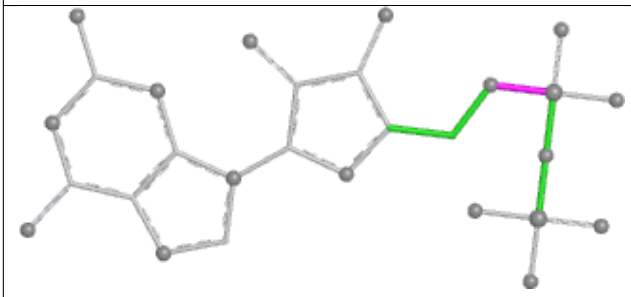
Ligand GDP LC 501



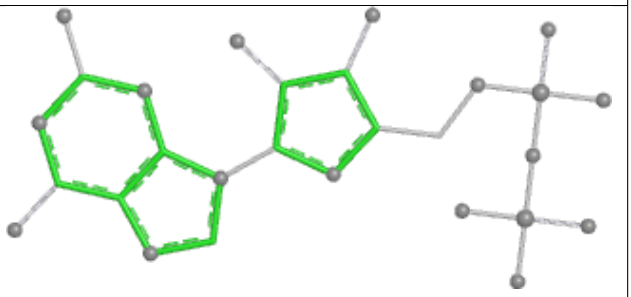
Bond lengths



Bond angles

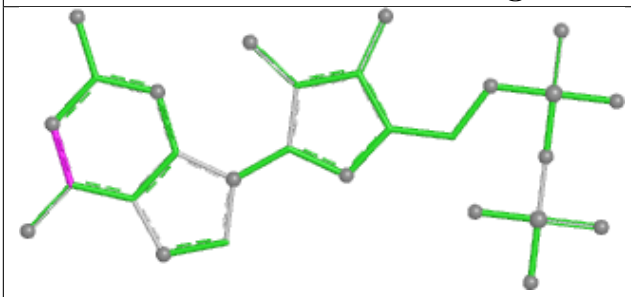


Torsions



Rings

Ligand GDP DH 501



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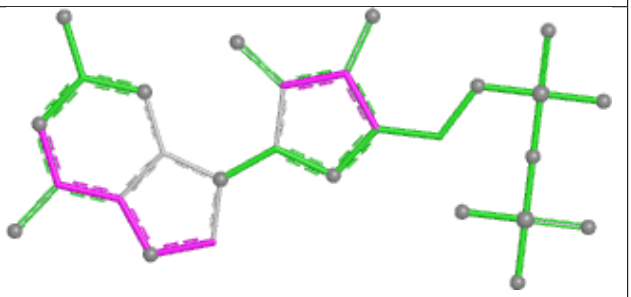
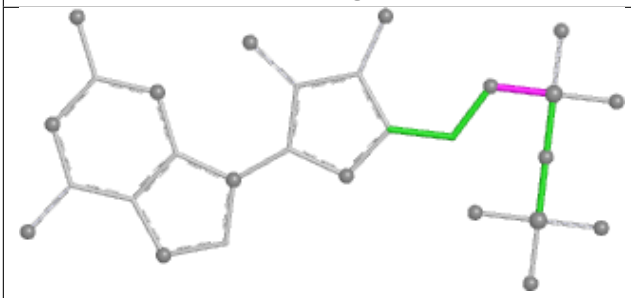


Bond angles



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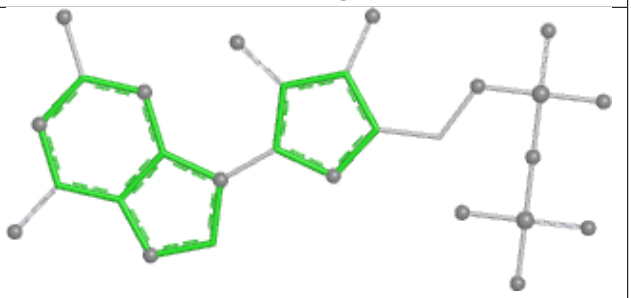
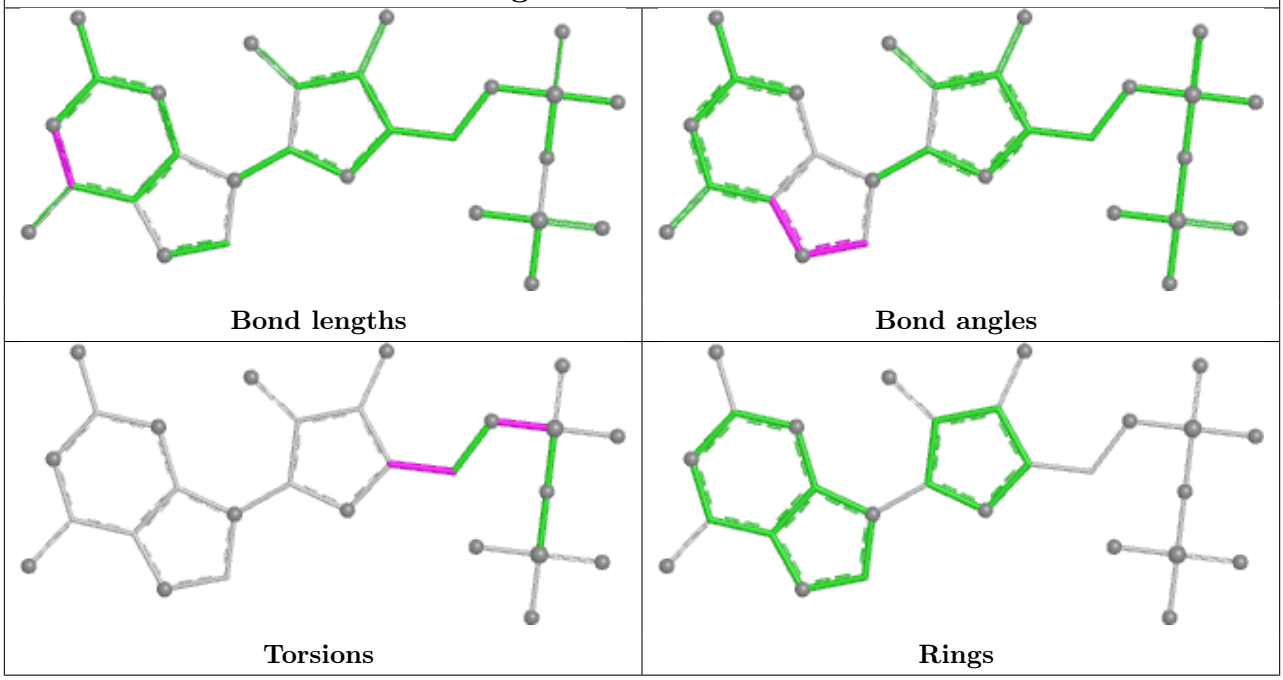
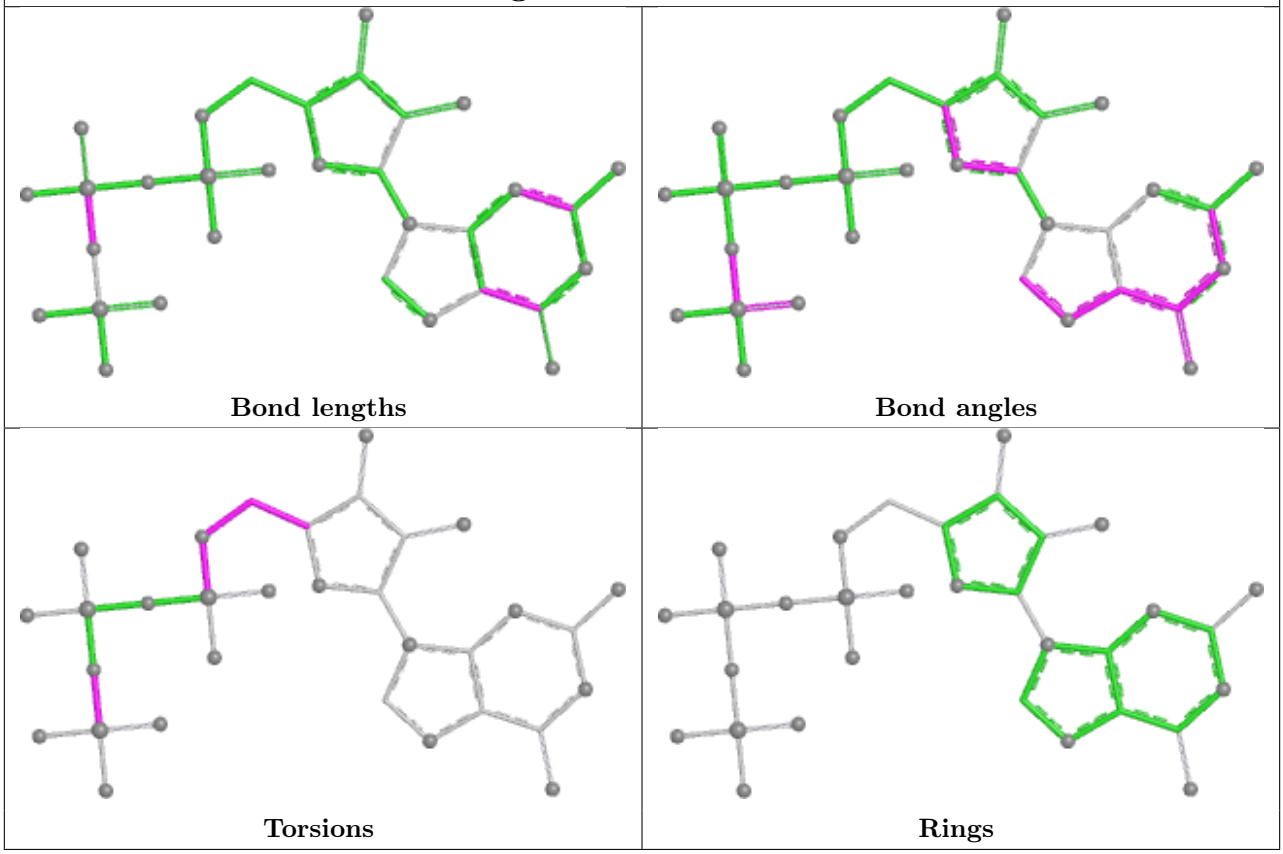


Rings

Ligand GDP VL 501



Ligand GTP BK 501



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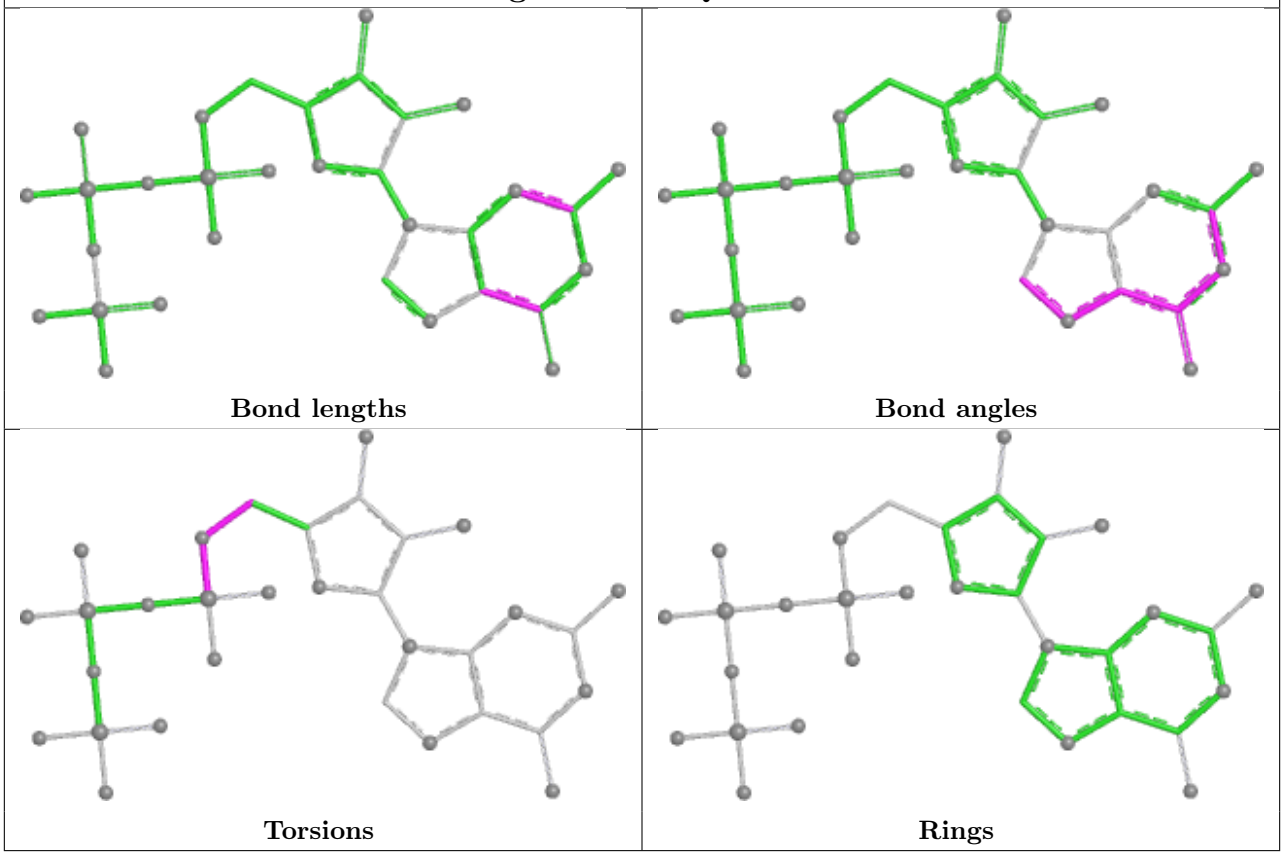

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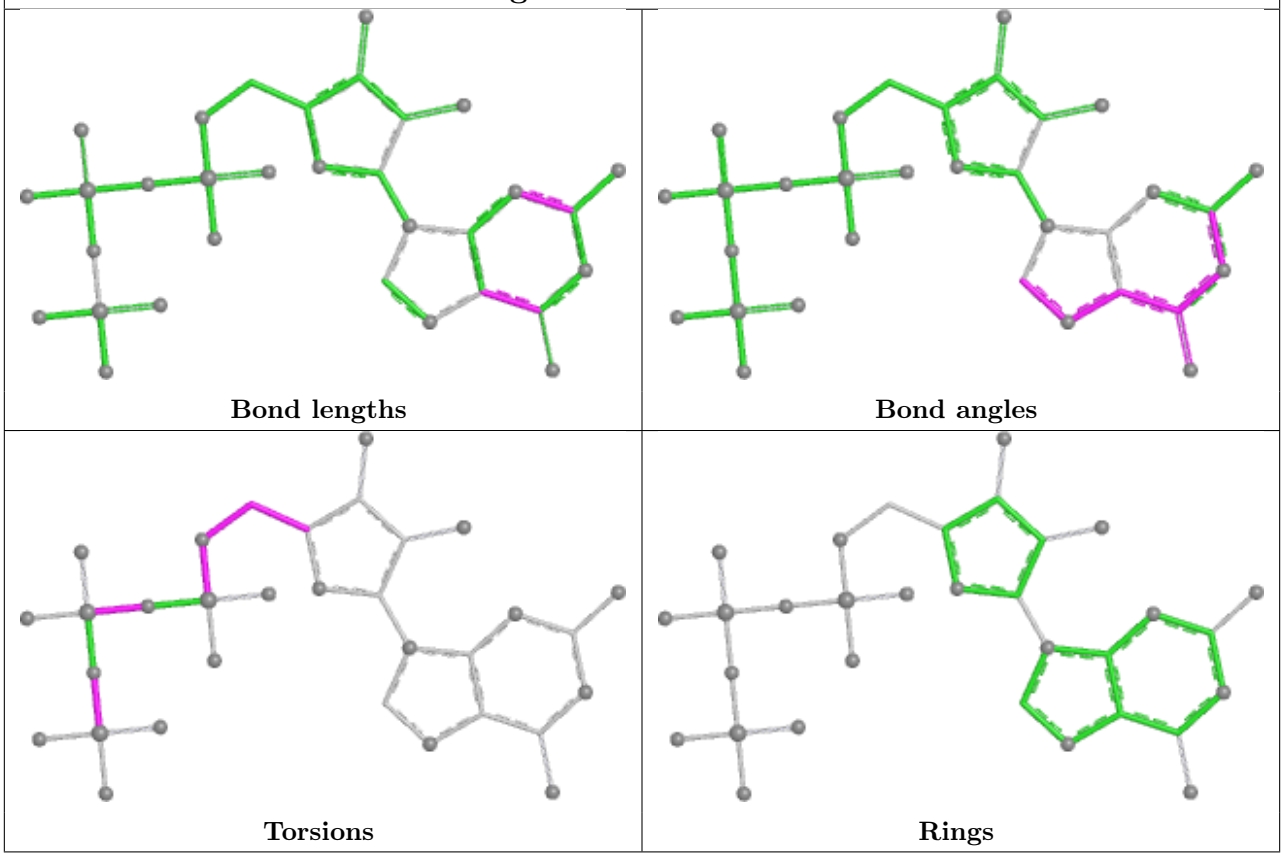
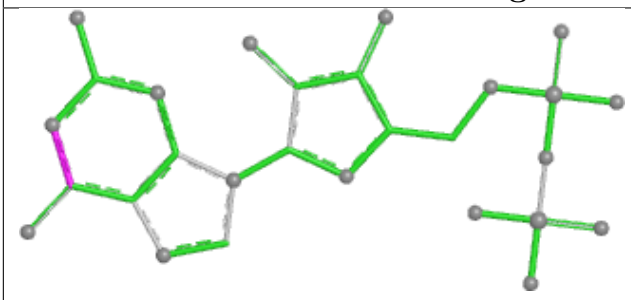
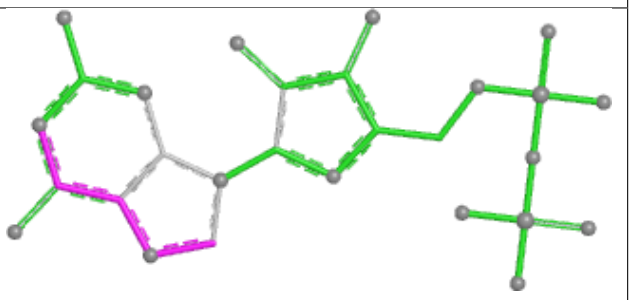


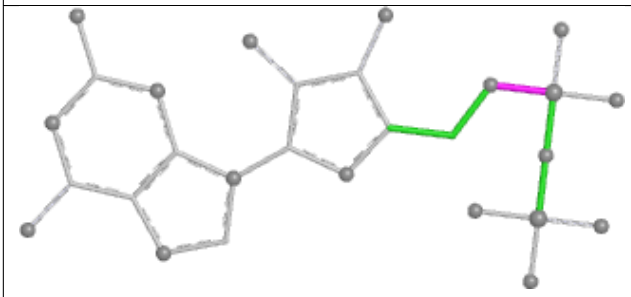
Ligand GDP PC 501



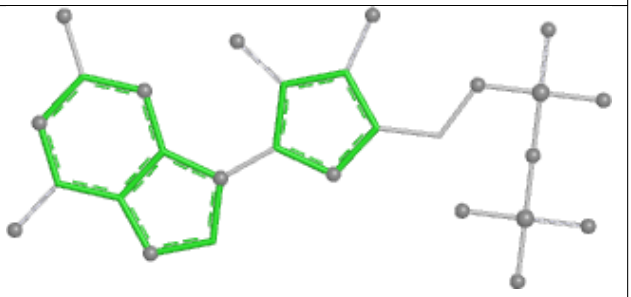
Bond lengths



Bond angles

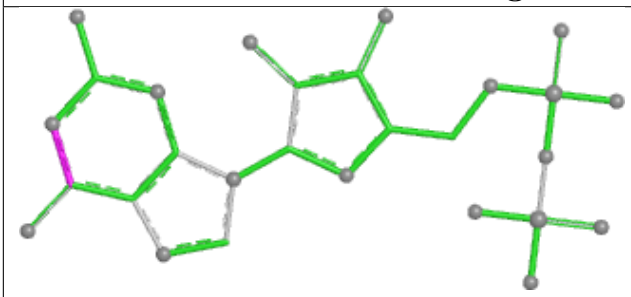


Torsions



Rings

Ligand GDP GH 501



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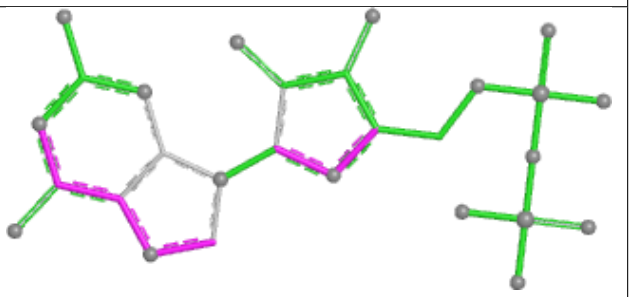
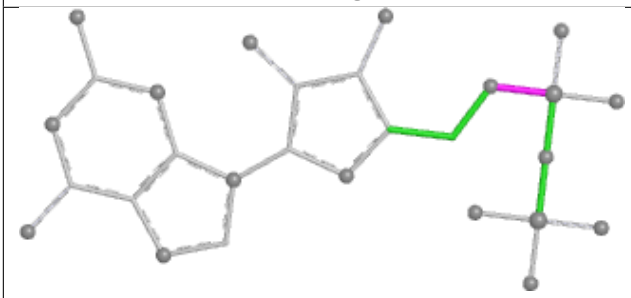


Bond angles



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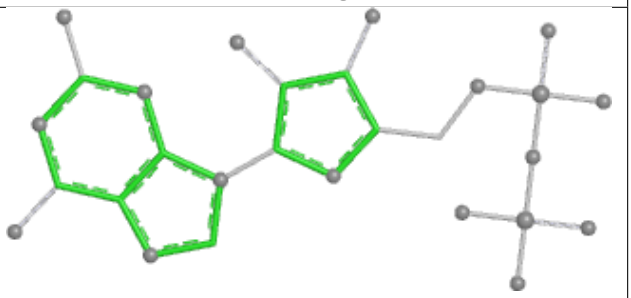
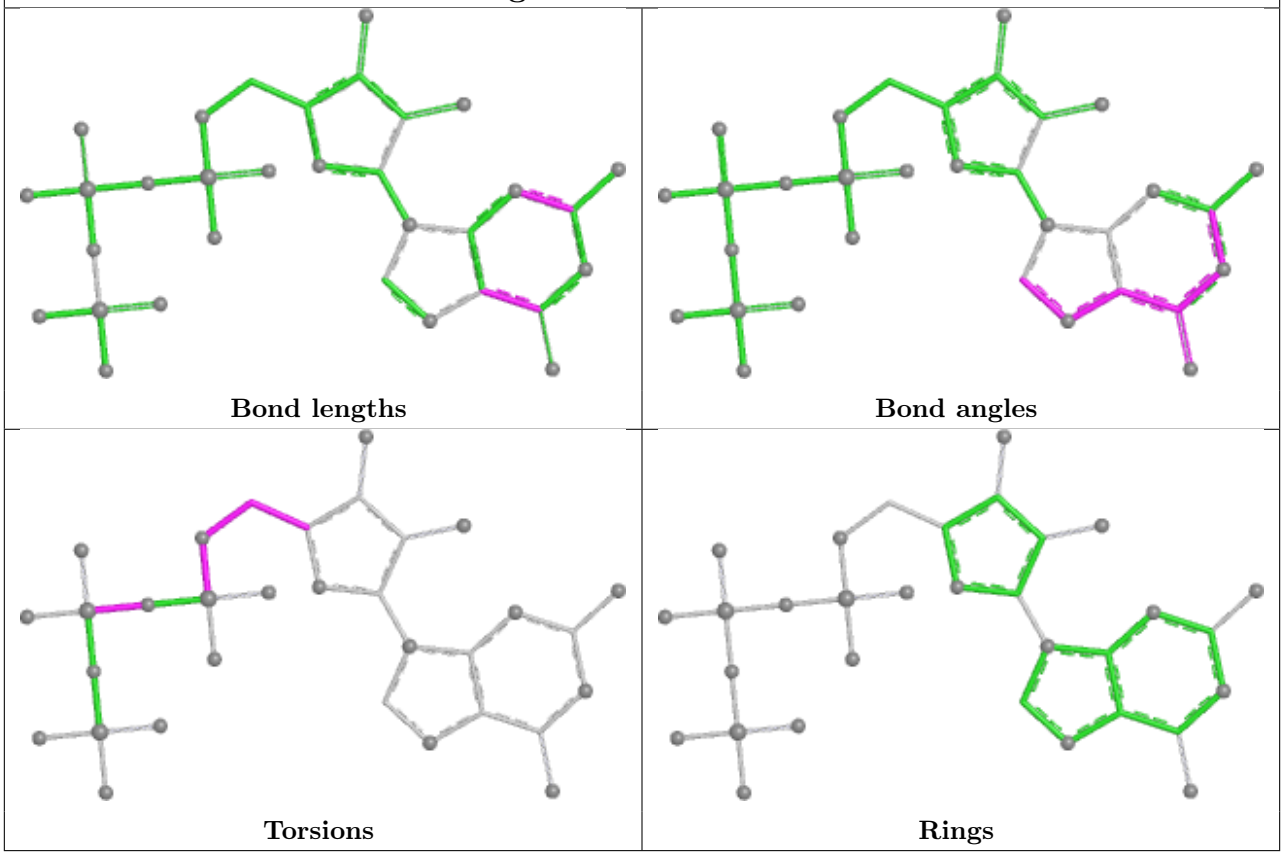
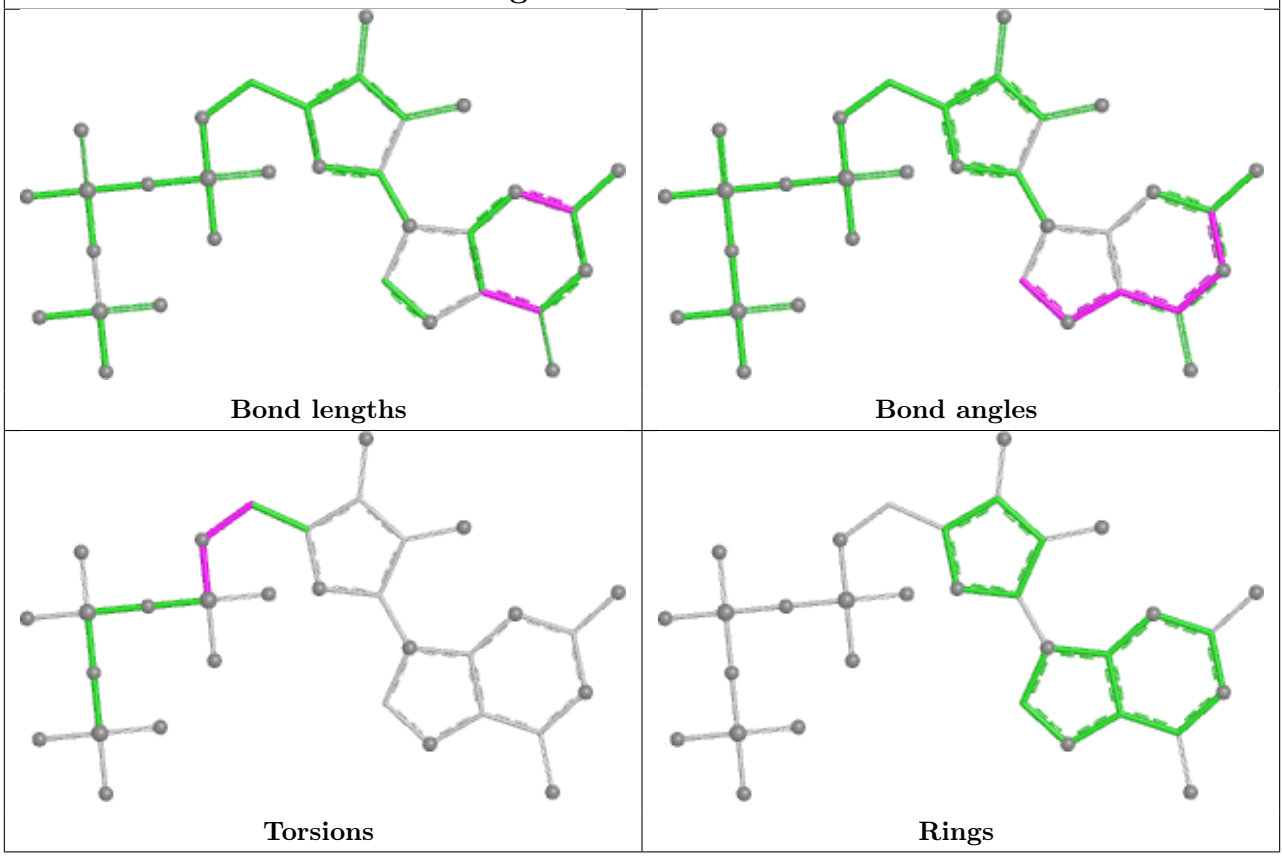


Rings

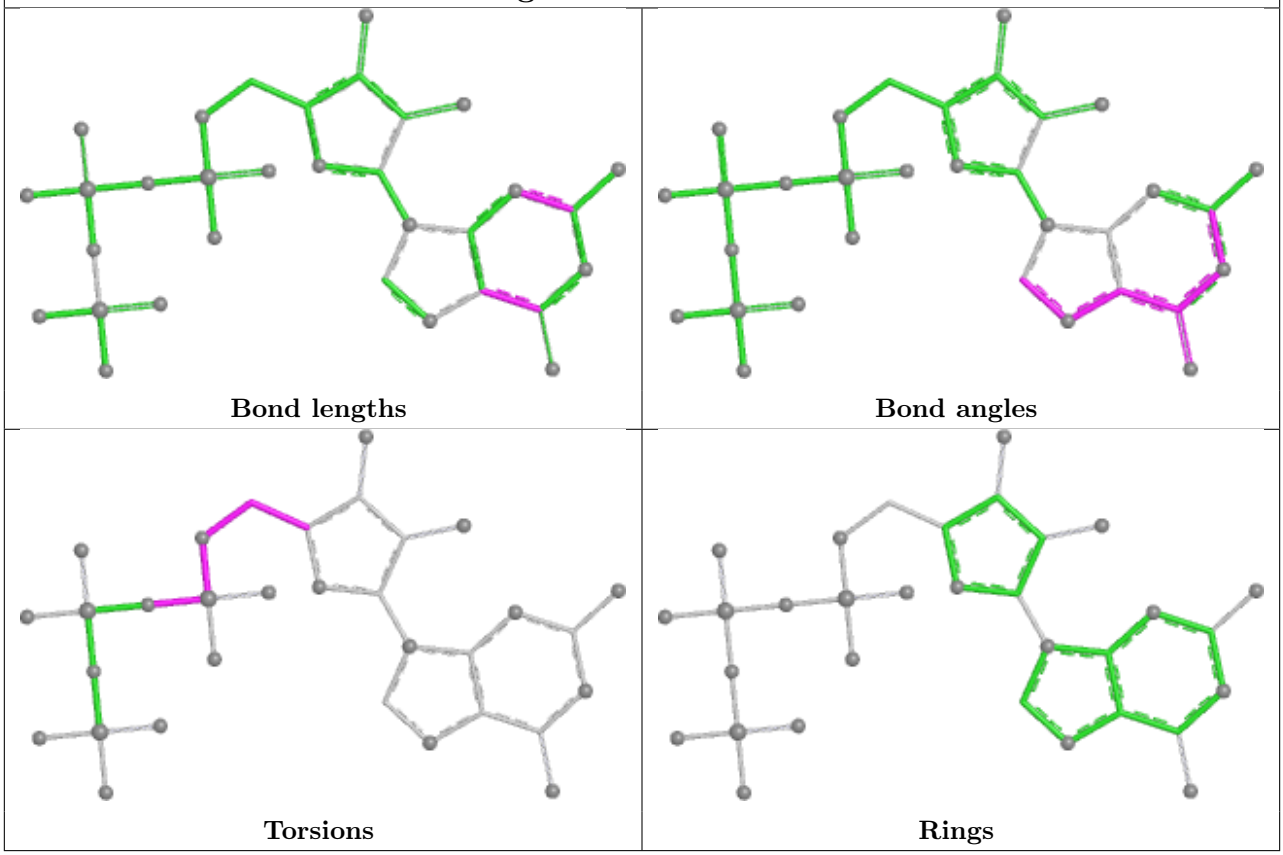
Ligand GTP NG 501



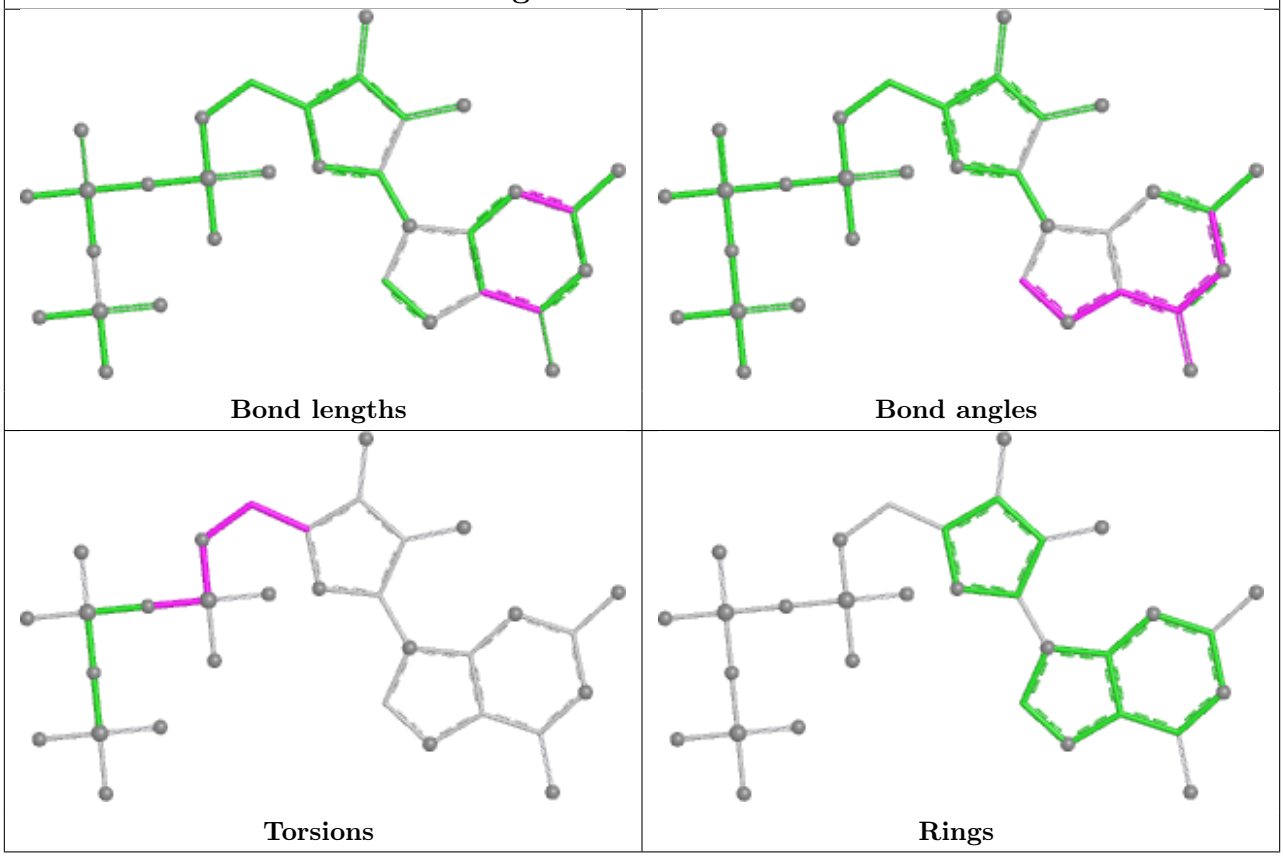
Ligand GTP CA 501



Ligand GTP BI 501



Ligand GTP LA 501



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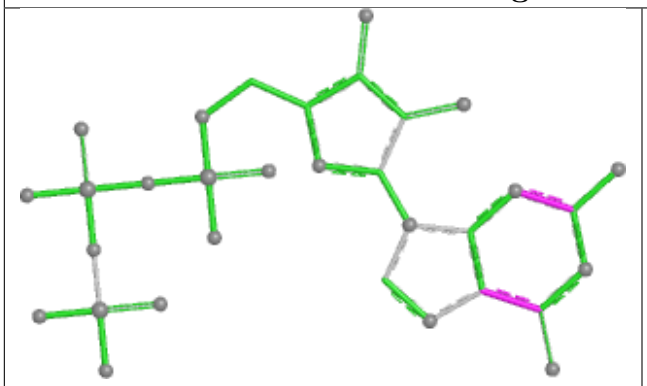
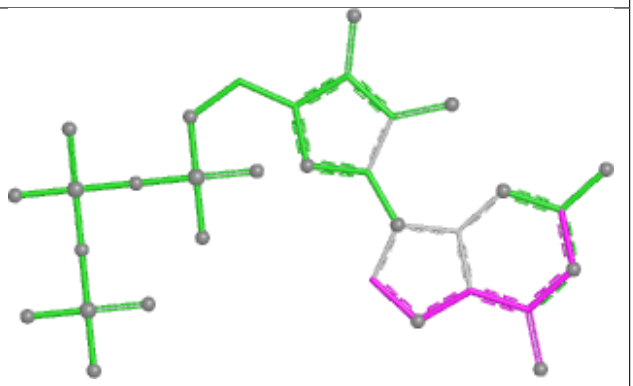
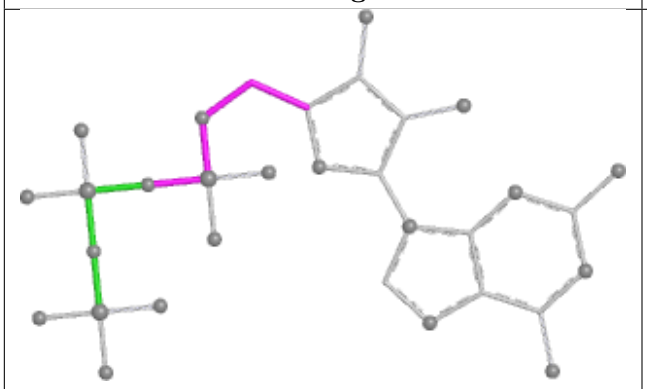


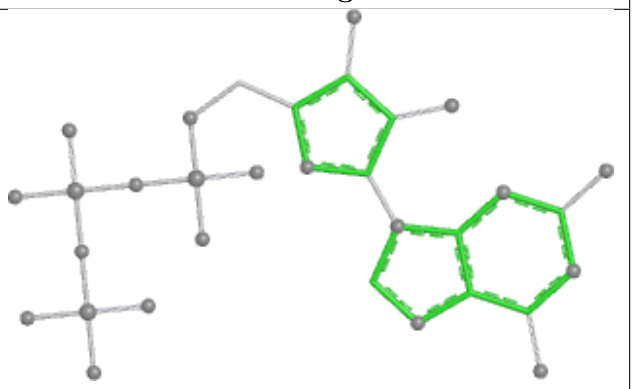
Bond lengths



Bond angles

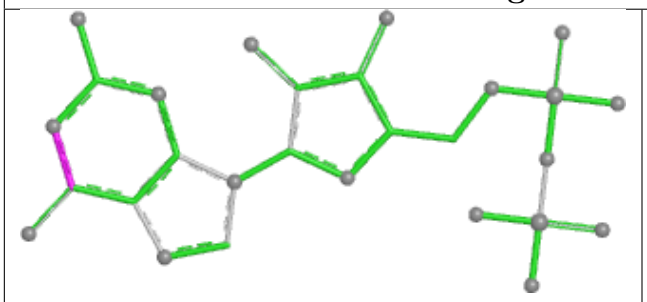


Torsions



Rings

Ligand GDP GD 501



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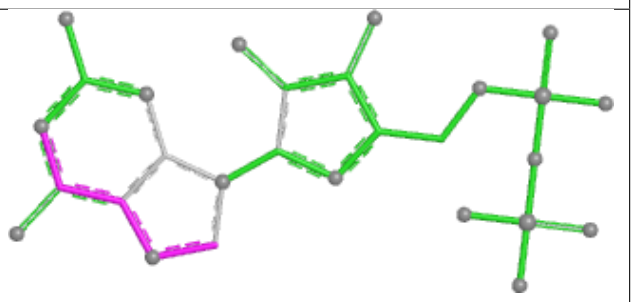

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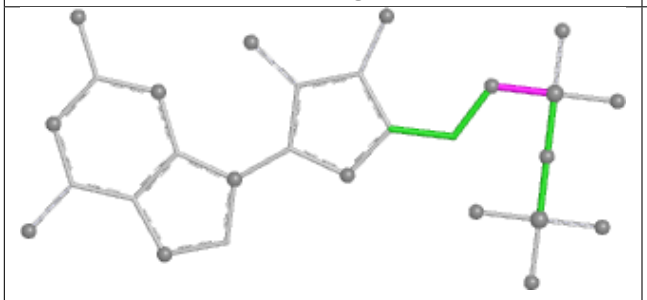

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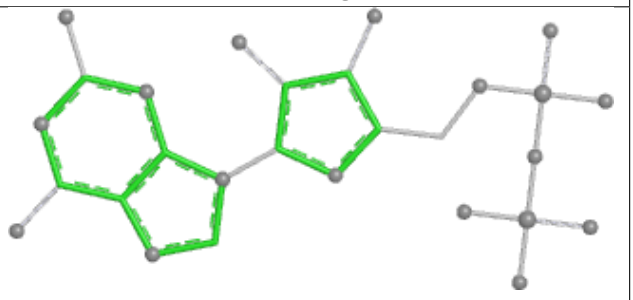

Rings

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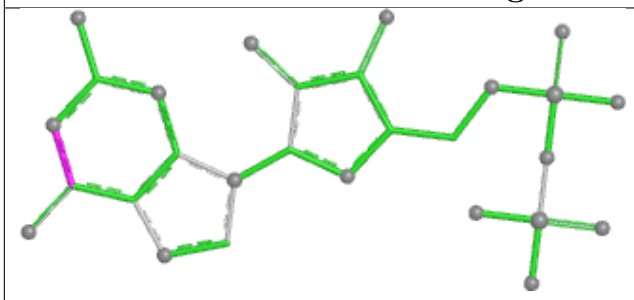

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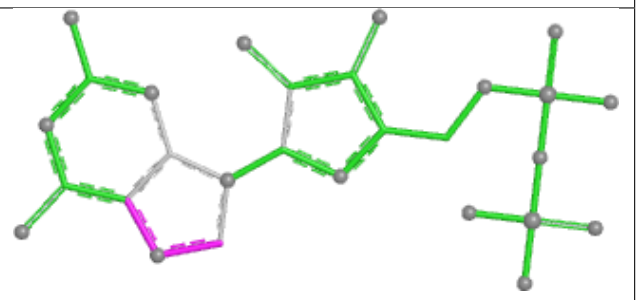

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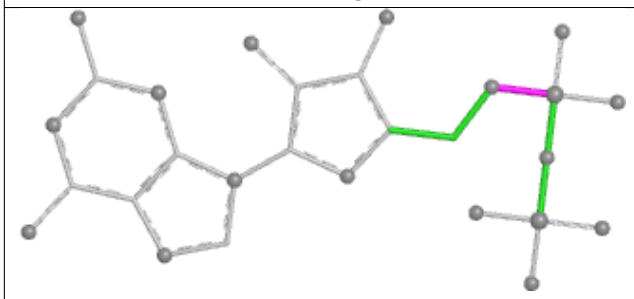

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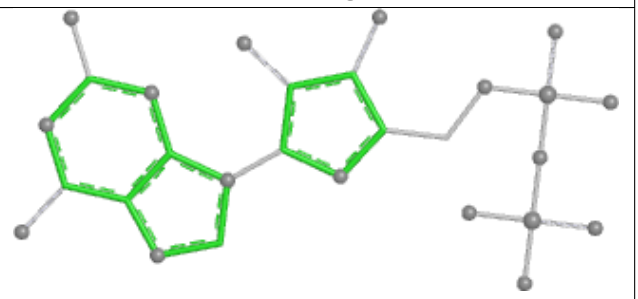

Rings

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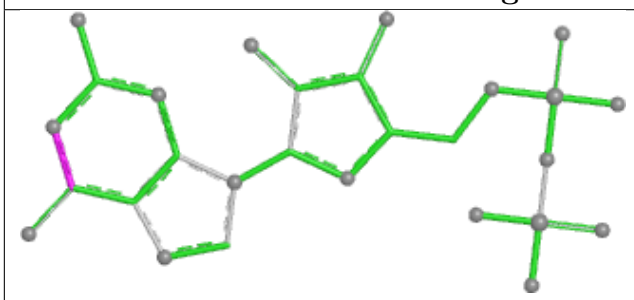

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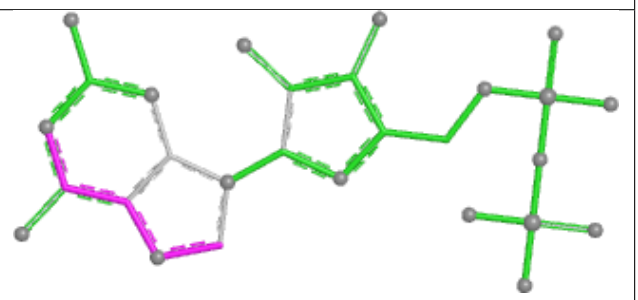

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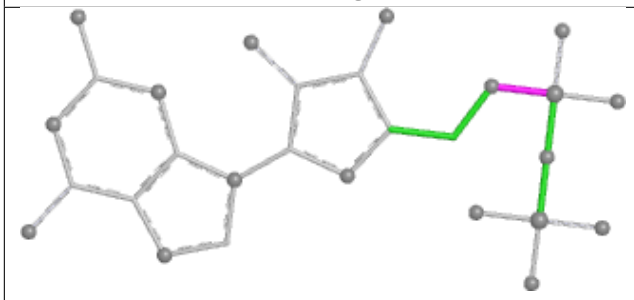

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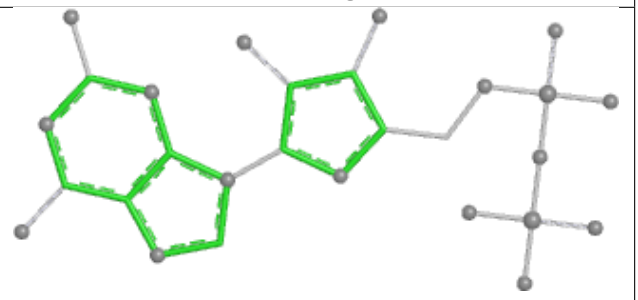

Rings

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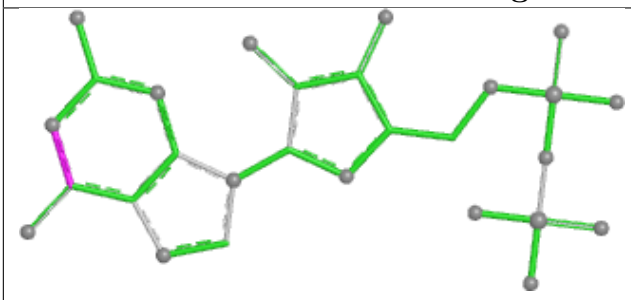
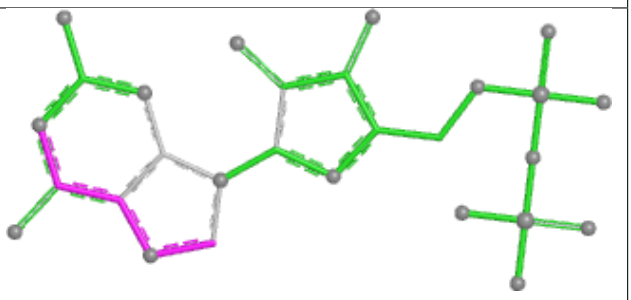
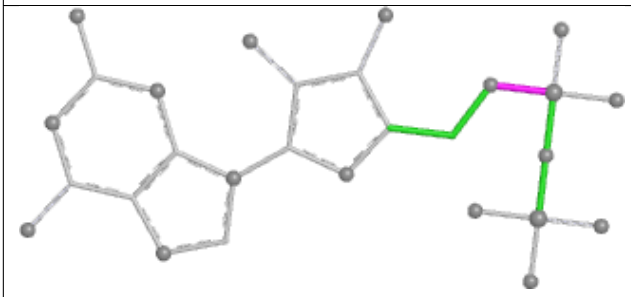
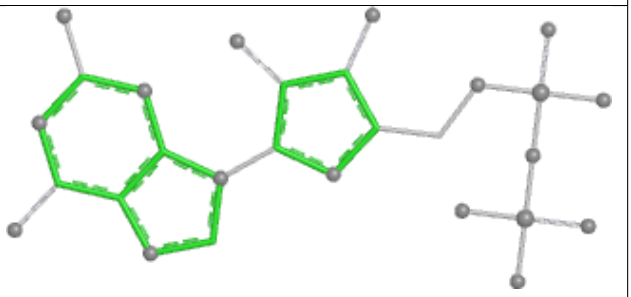
 Bond lengths	 Bond angles
 Torsions	 Rings

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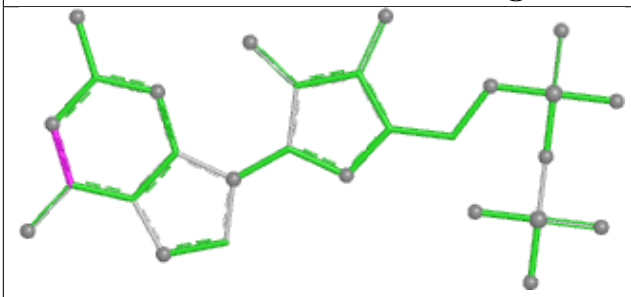
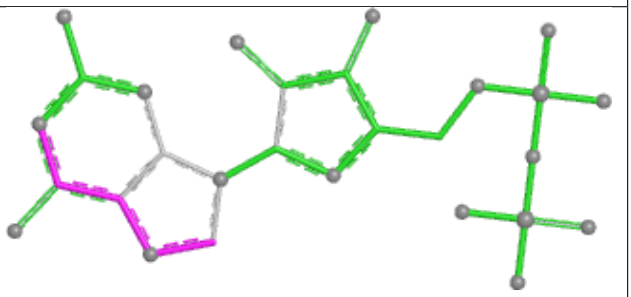
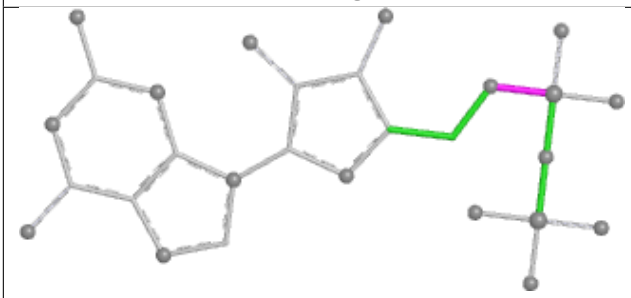
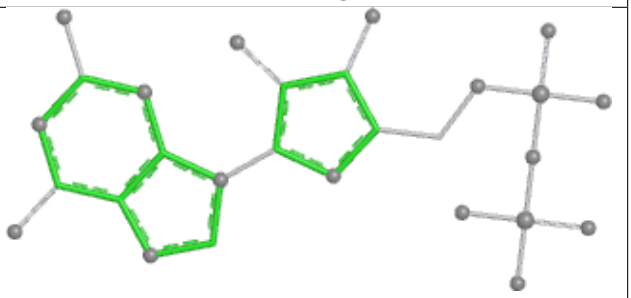
 Bond lengths	 Bond angles
 Torsions	 Rings

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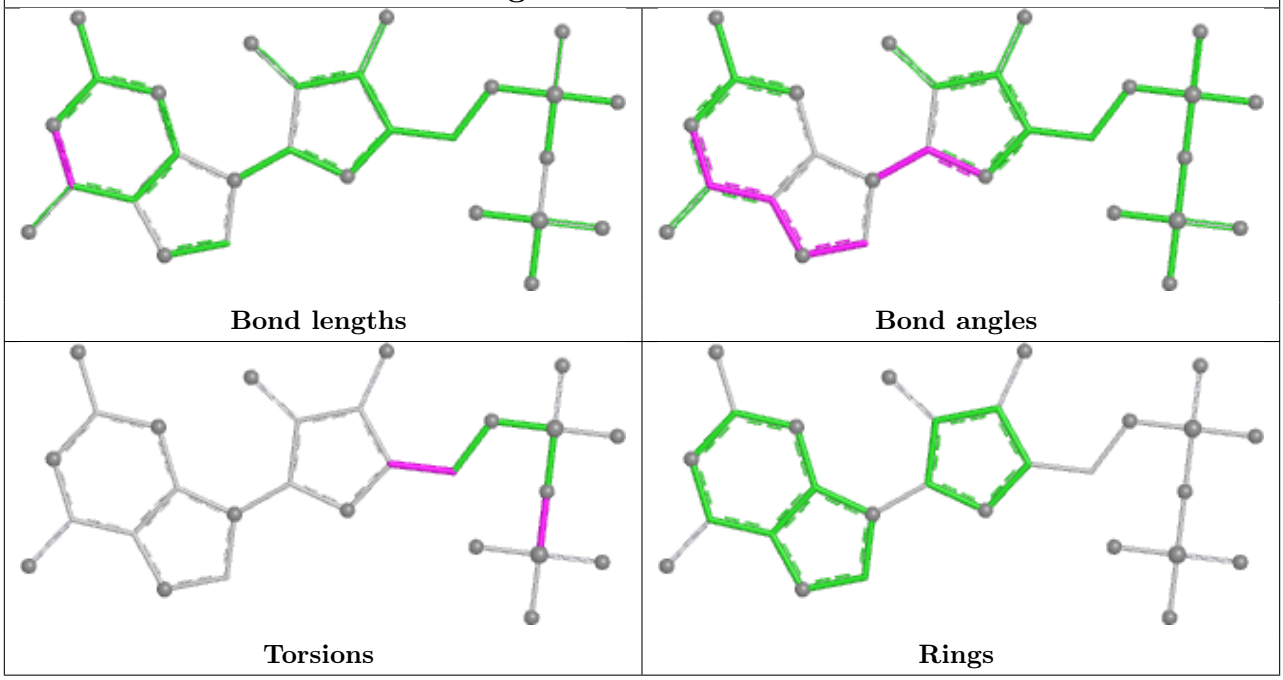
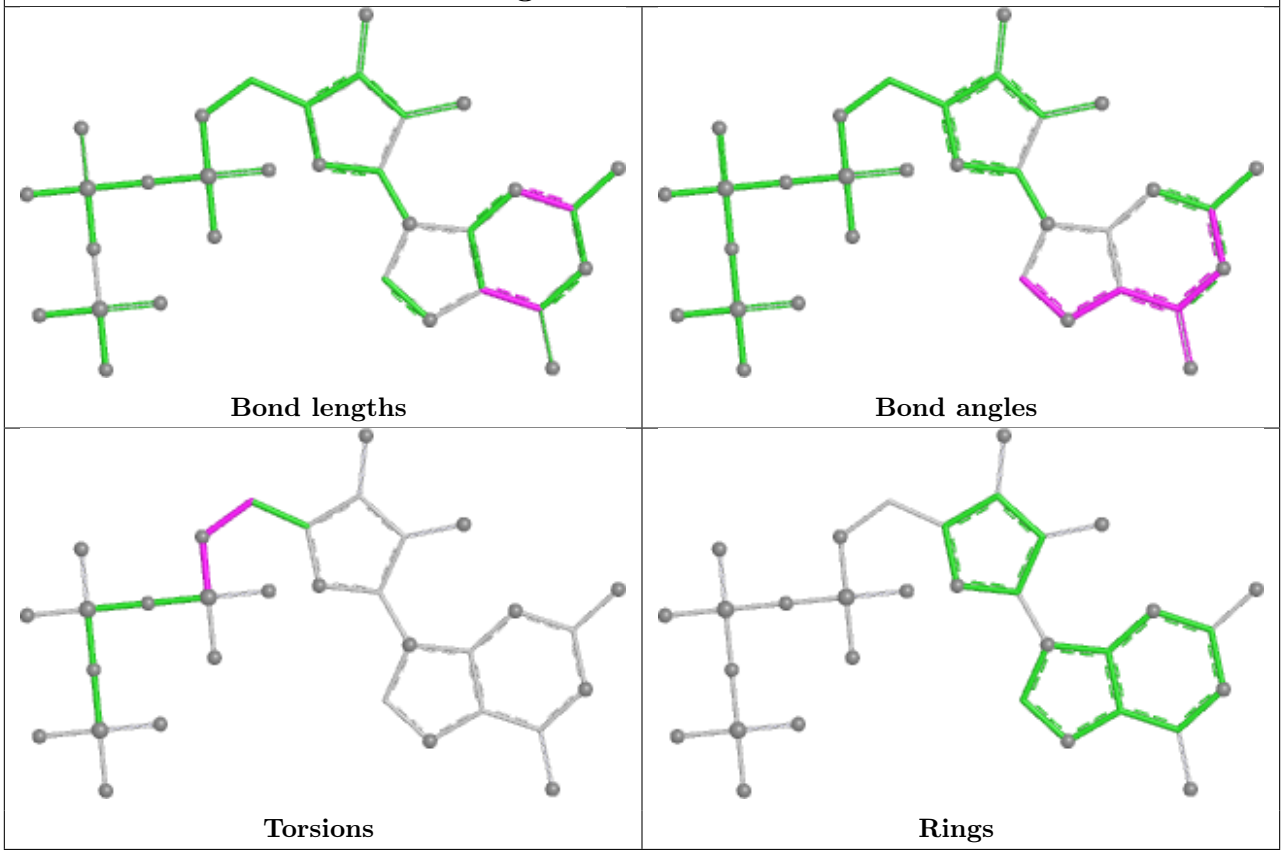


Ligand GTP IA 501



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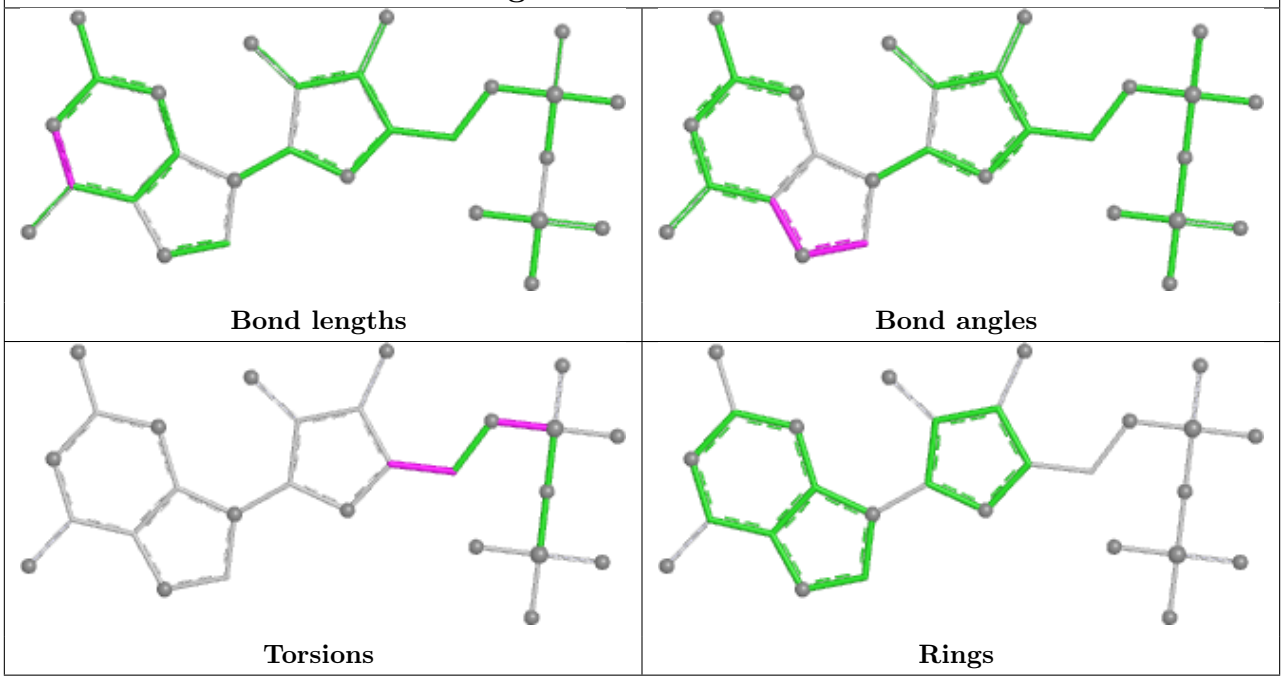

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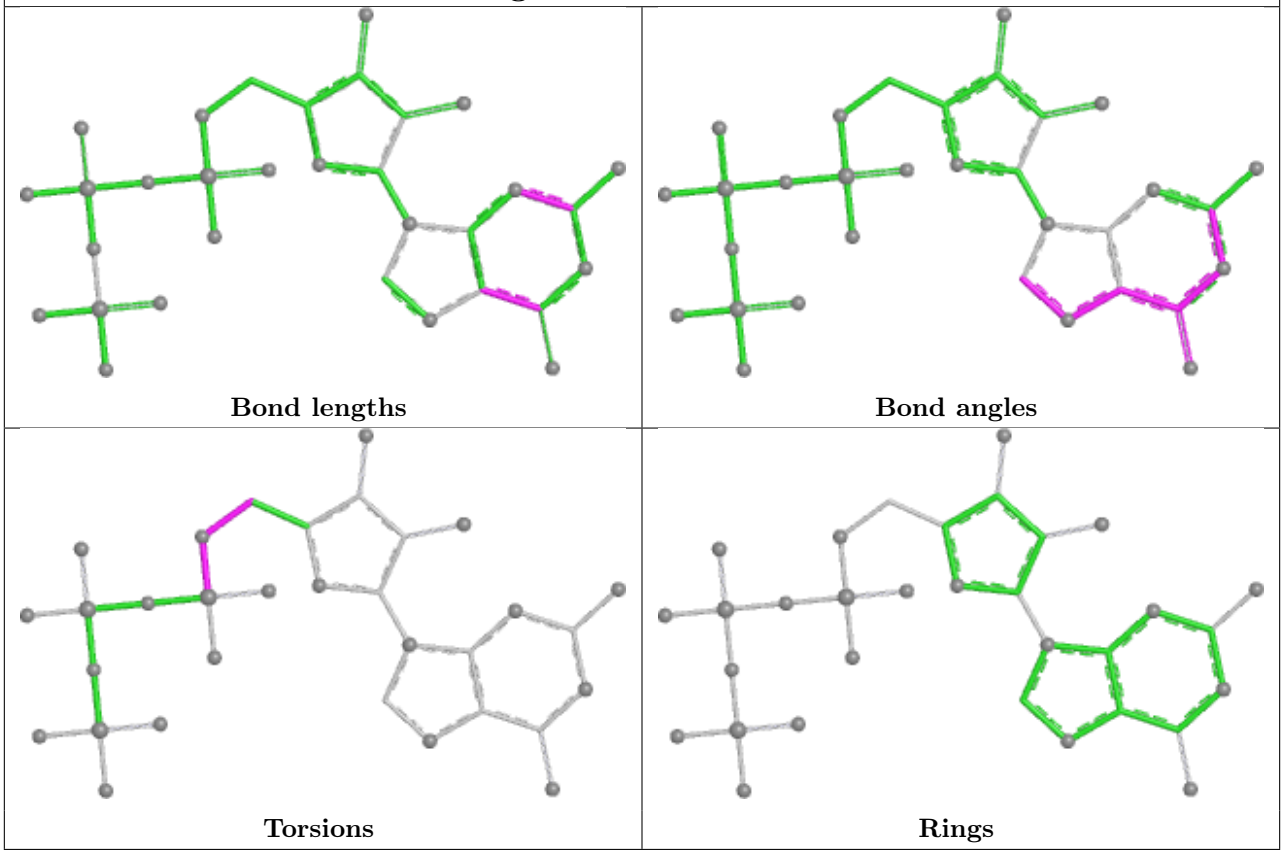

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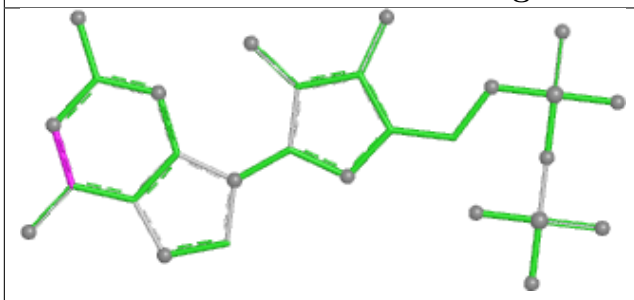

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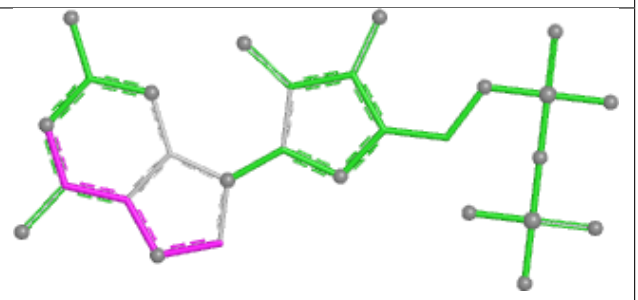
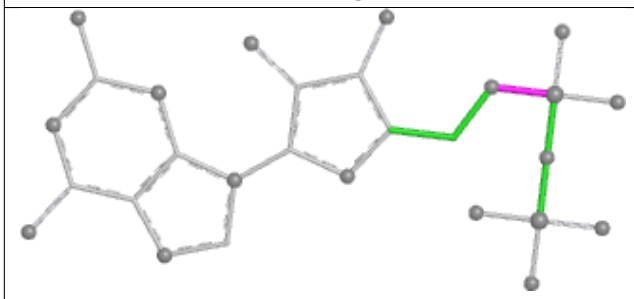
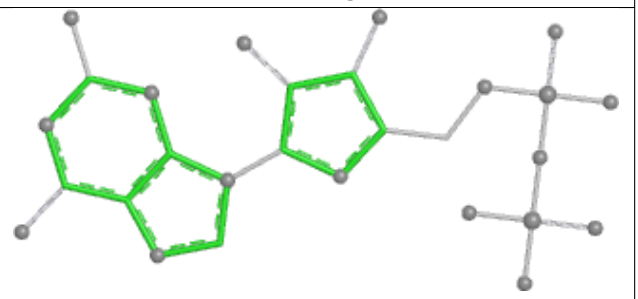


Bond angles

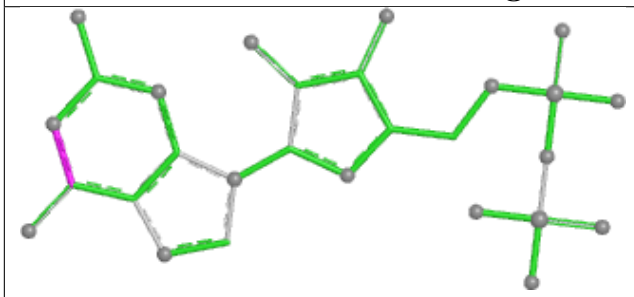


Torsions



Rings

Ligand GDP QM 501



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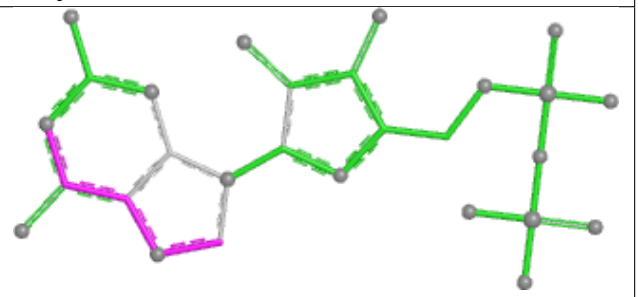

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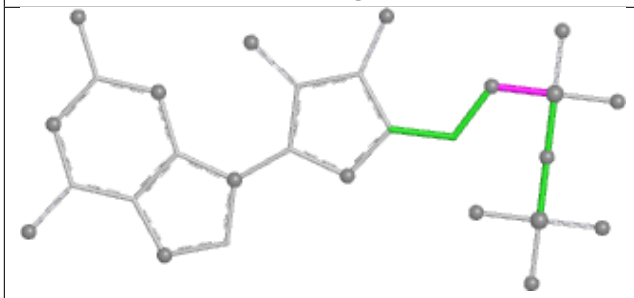

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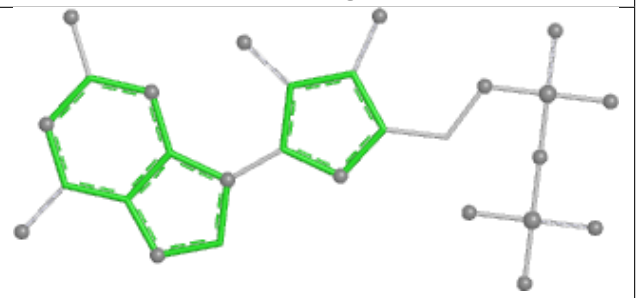

Rings

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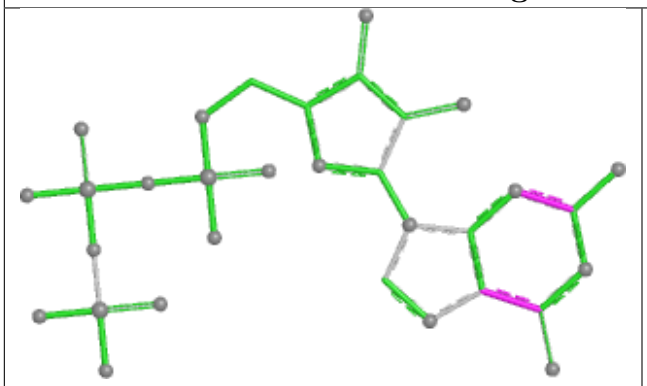

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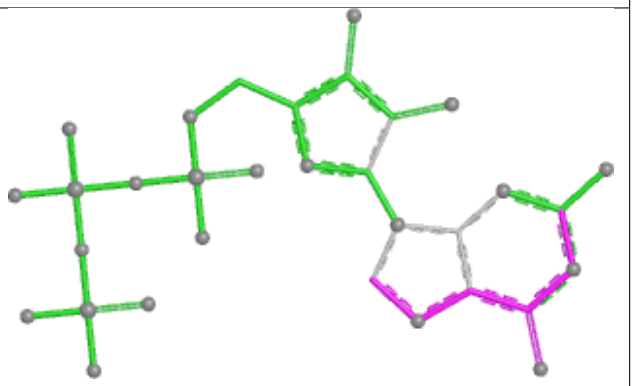

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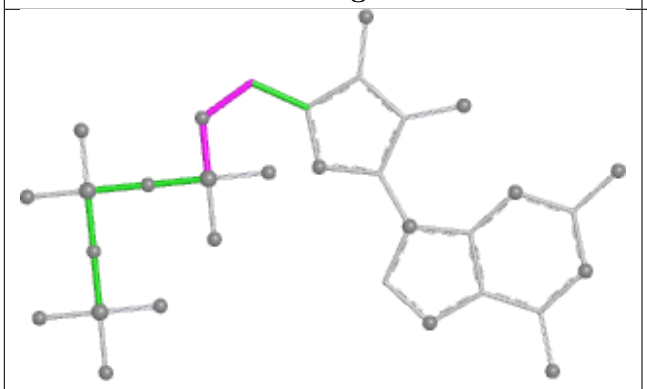

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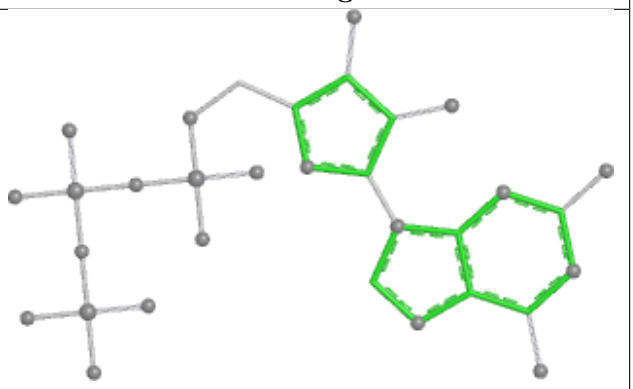

Rings

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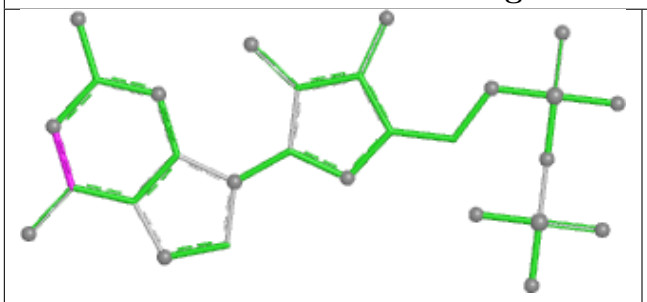

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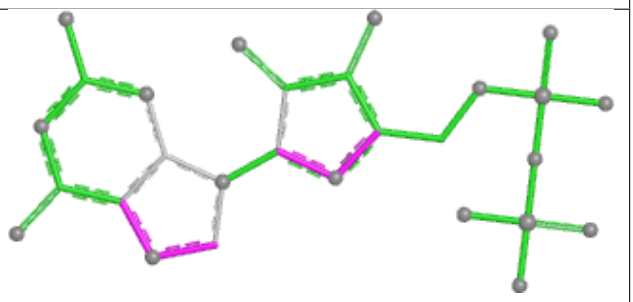

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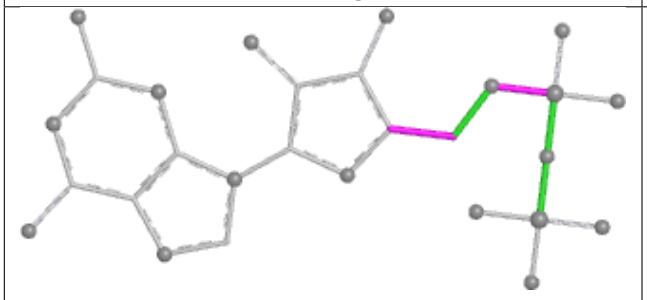

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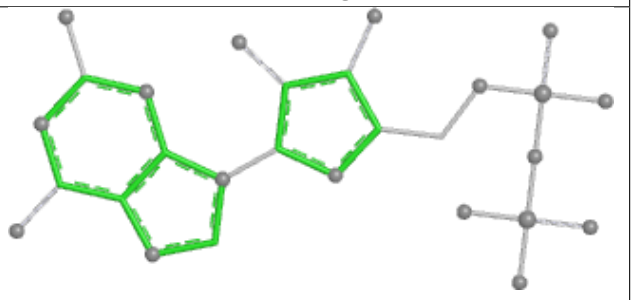

Rings

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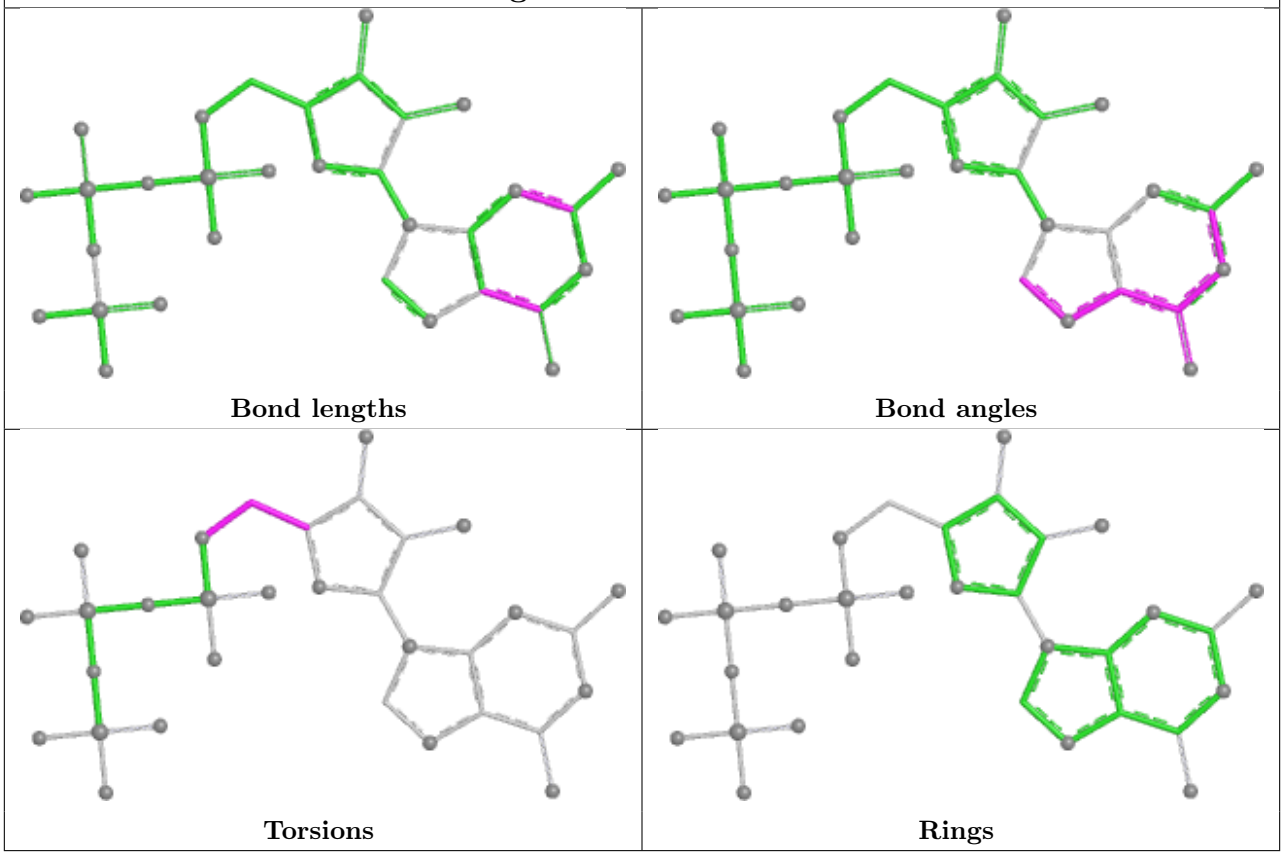

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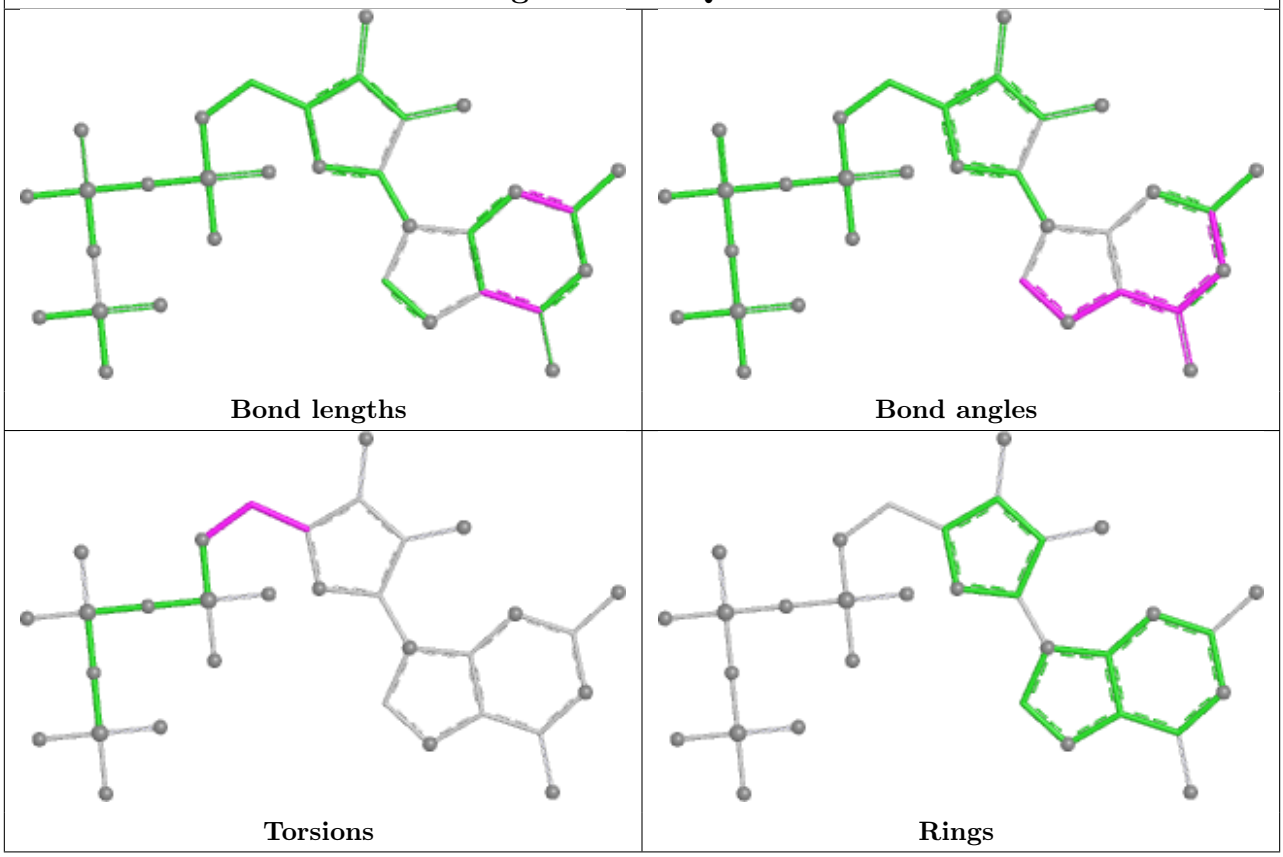
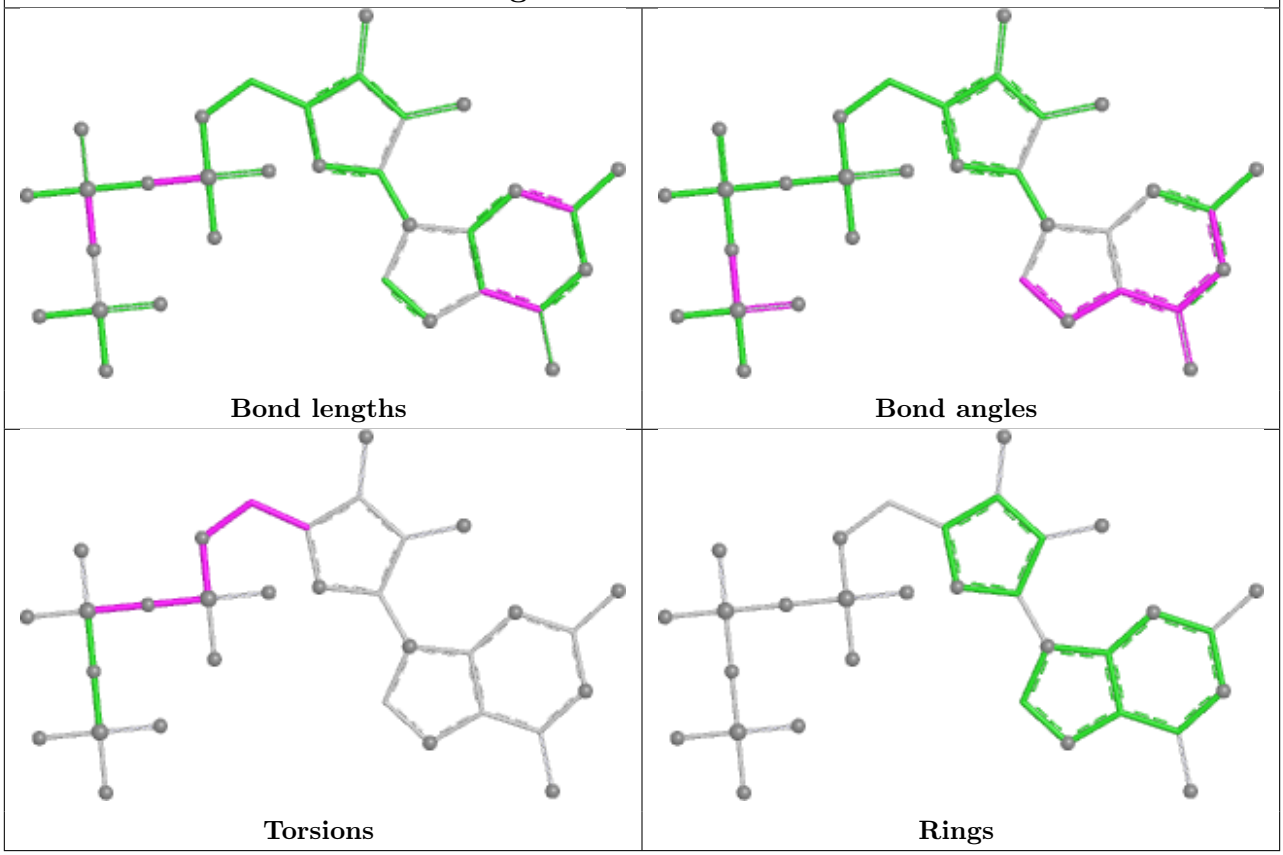


Ligand GTP CK 501



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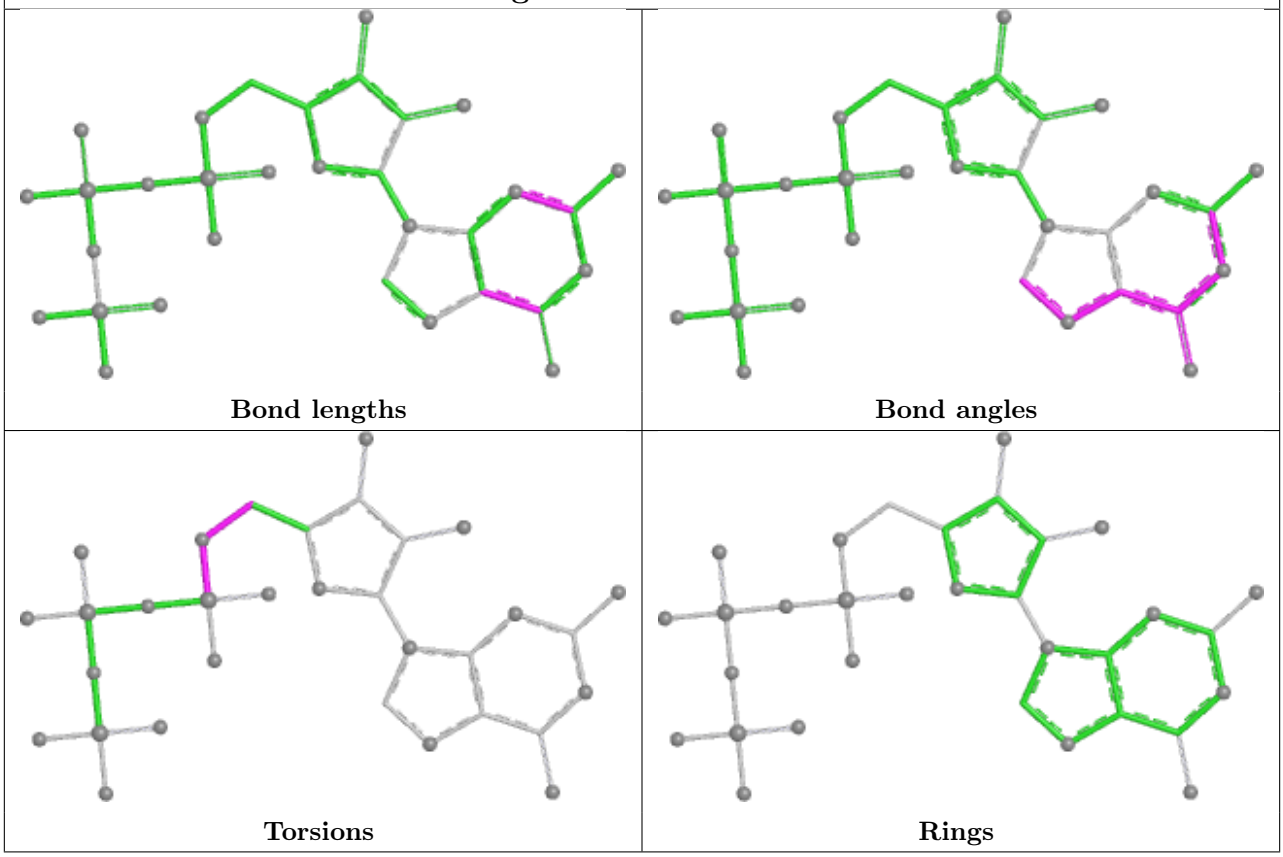

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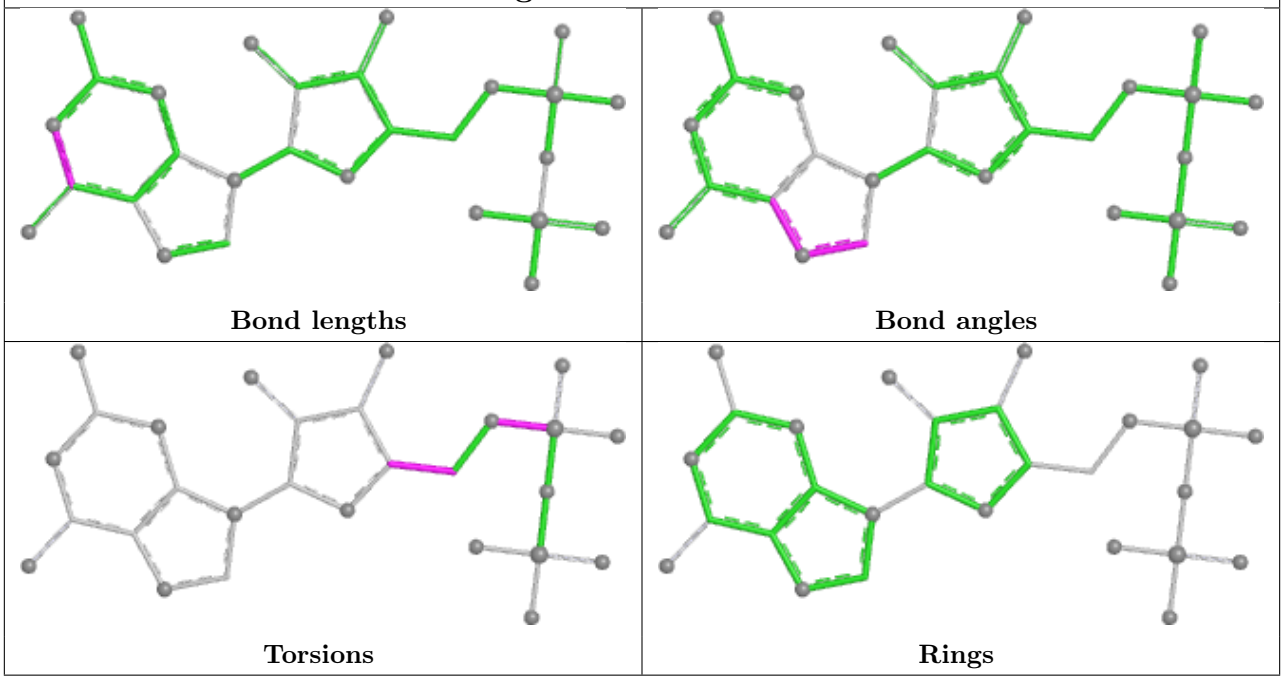

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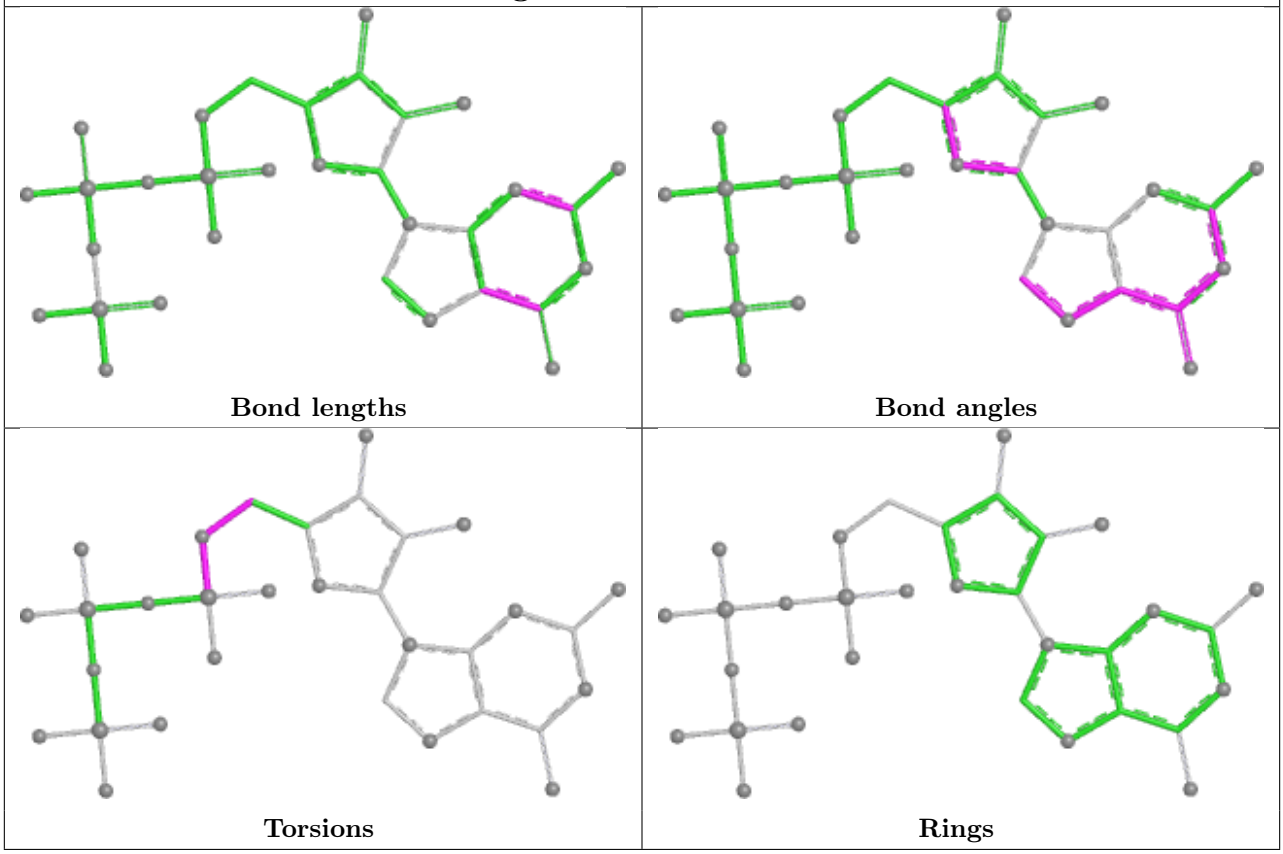

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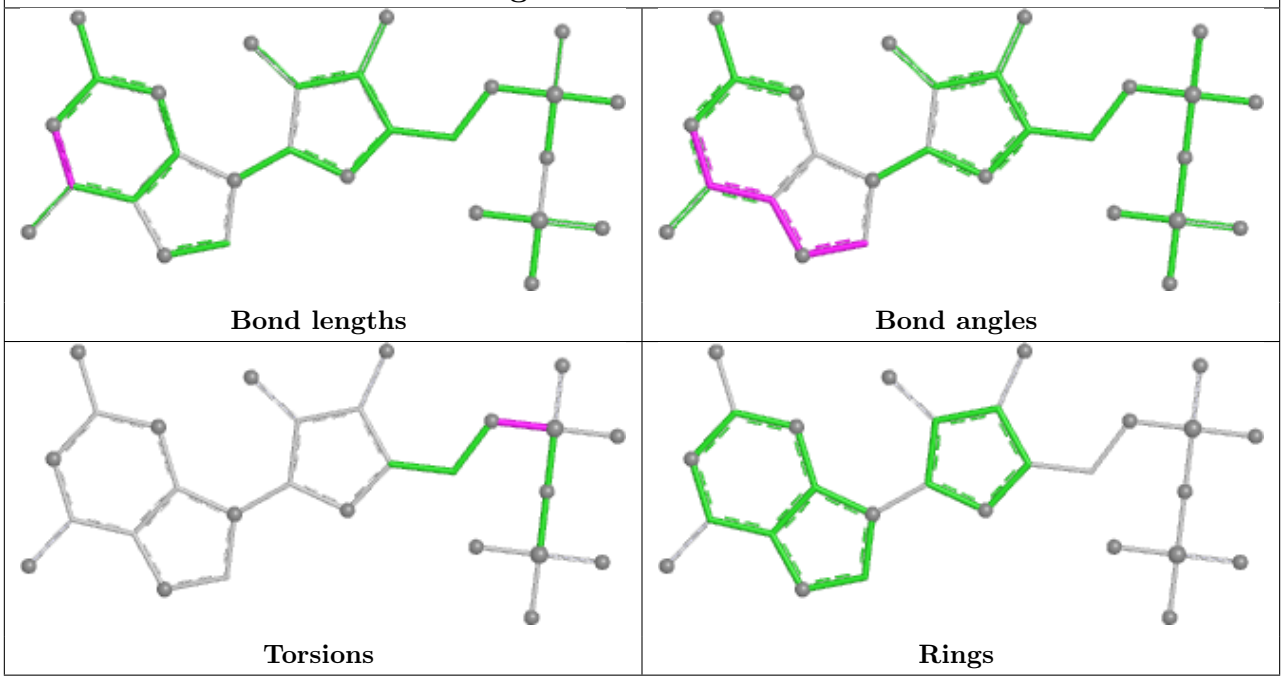

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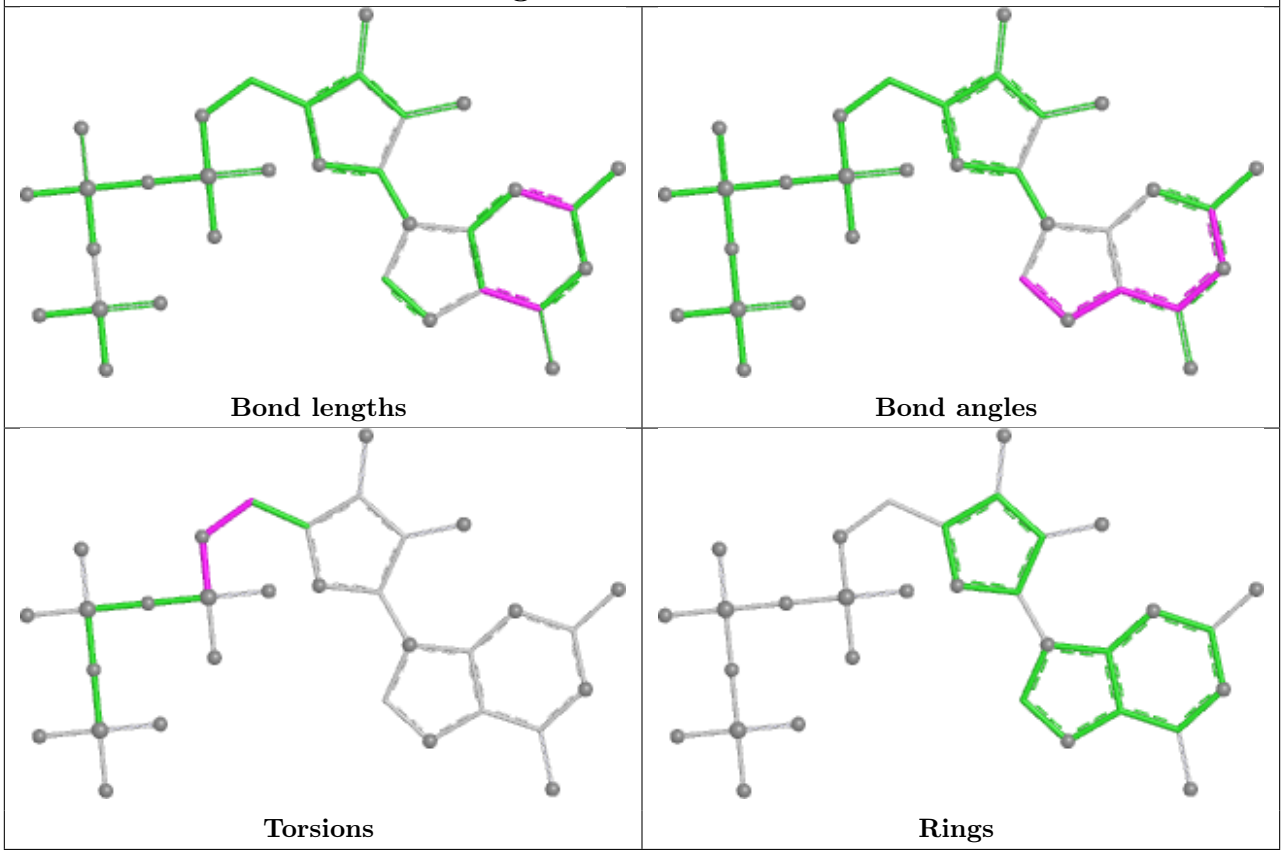

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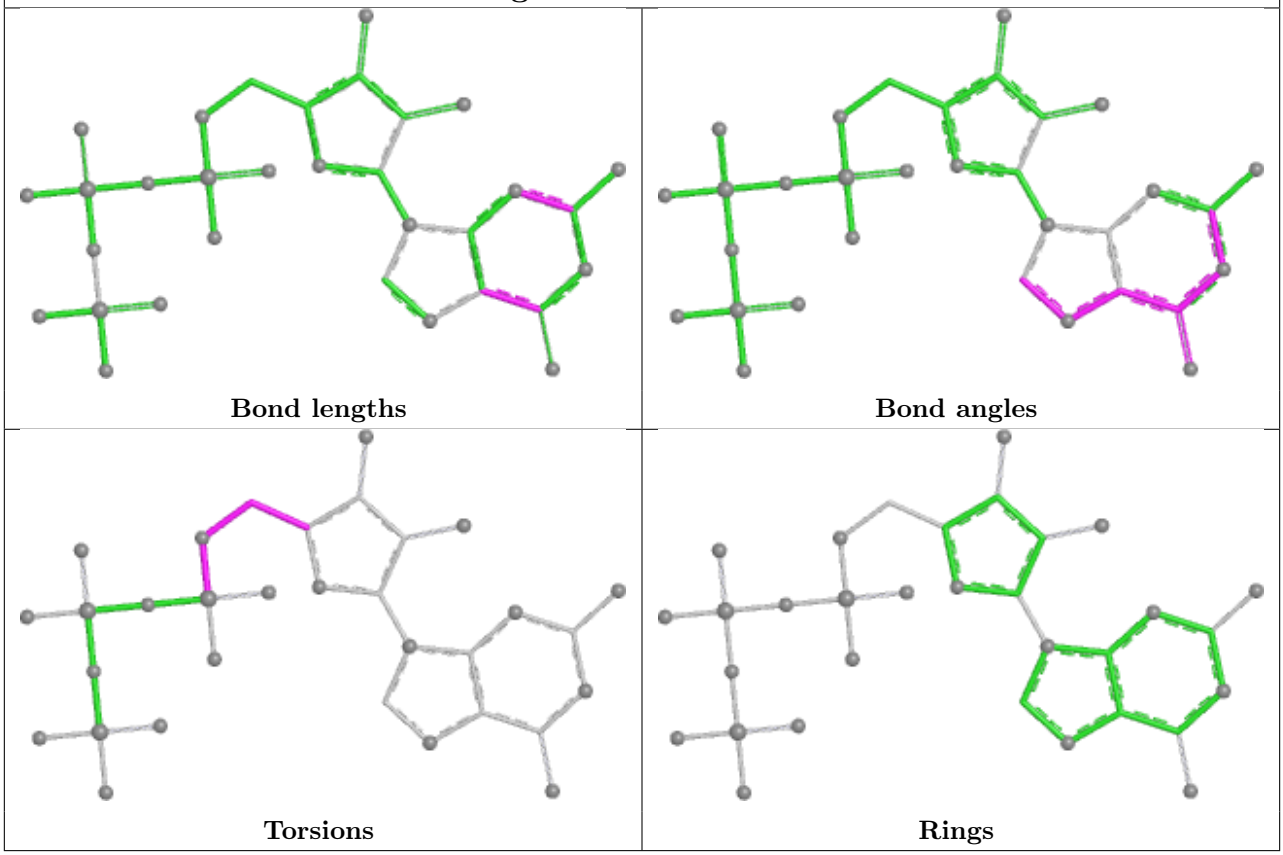
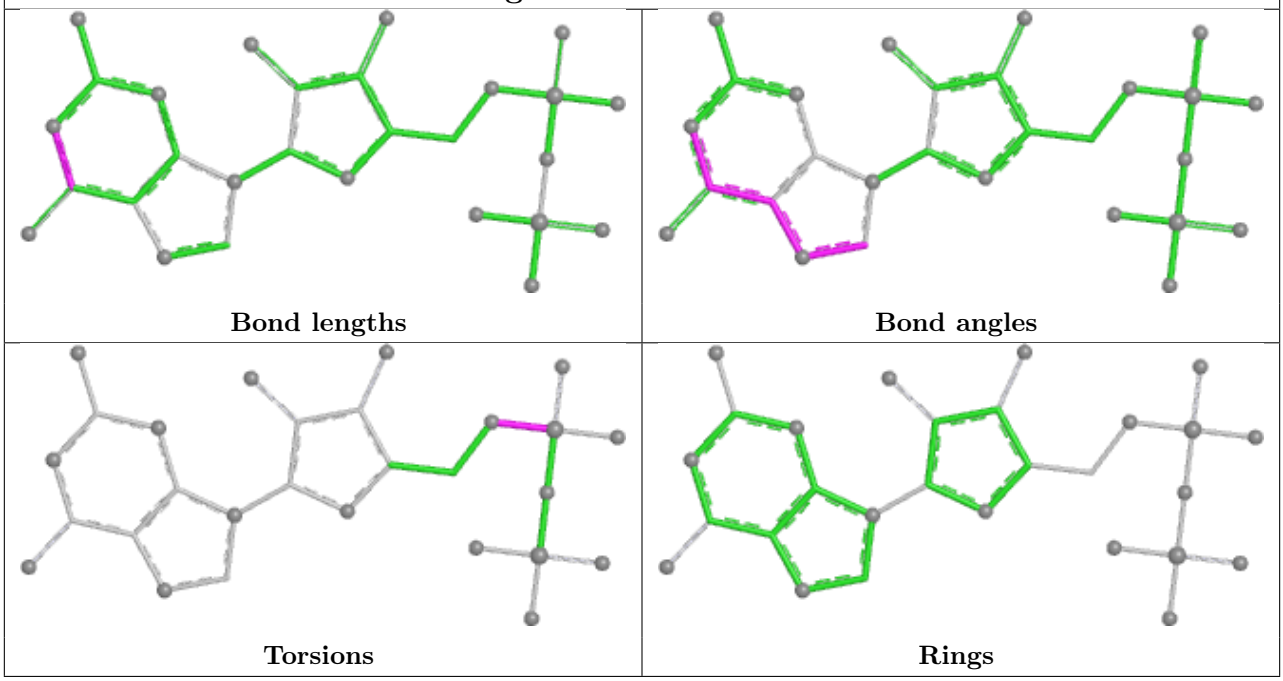
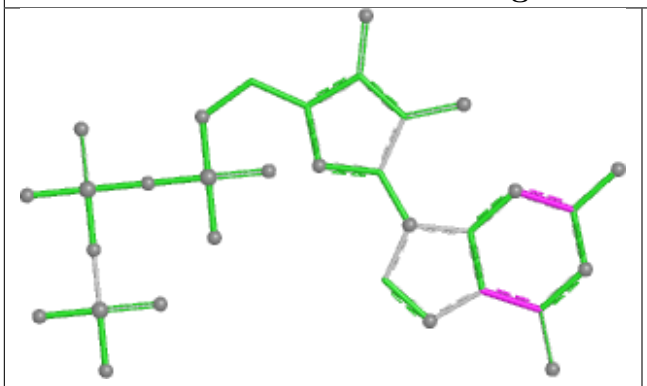


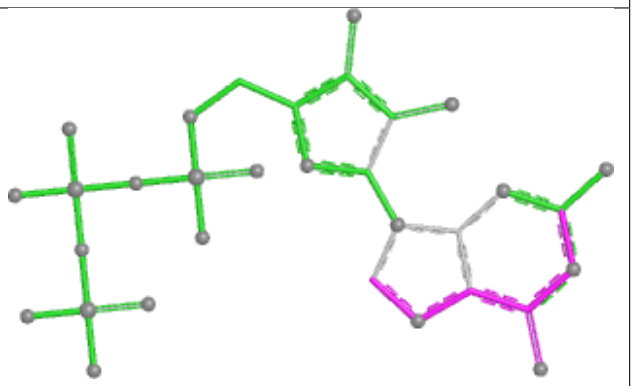
Ligand GDP MC 501



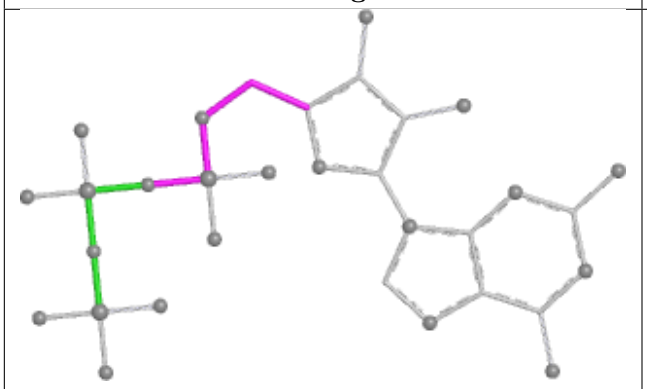
Ligand GTP OE 501



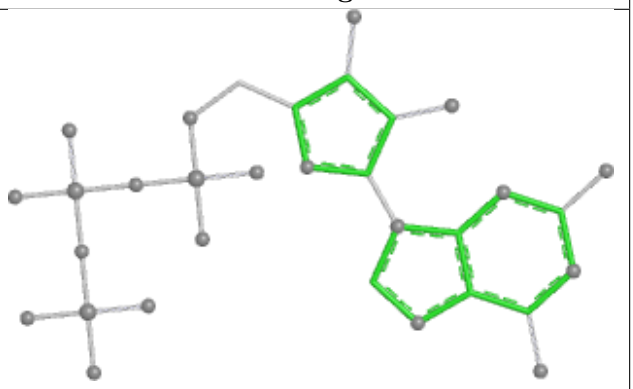
Bond lengths



Bond angles

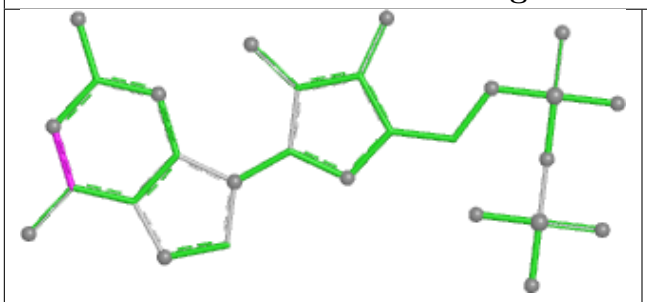


Torsions



Rings

Ligand GDP ED 501



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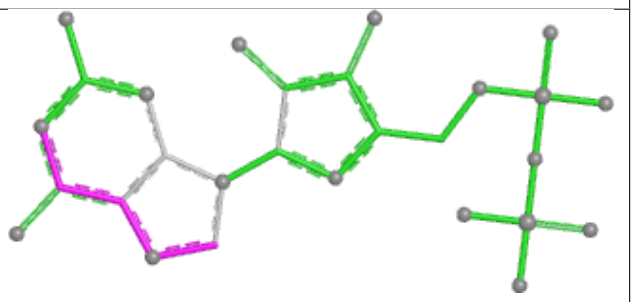
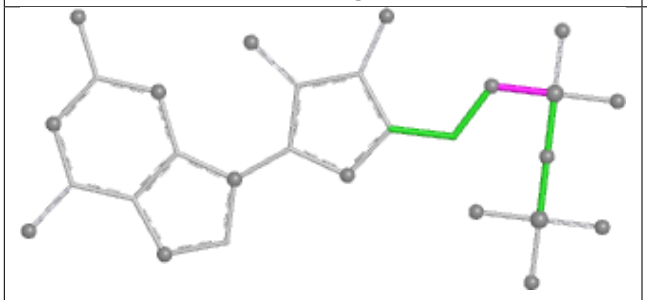


Bond angles



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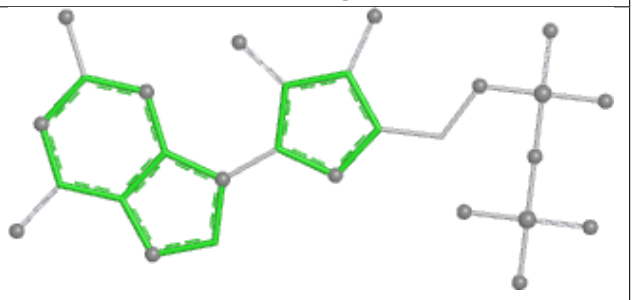
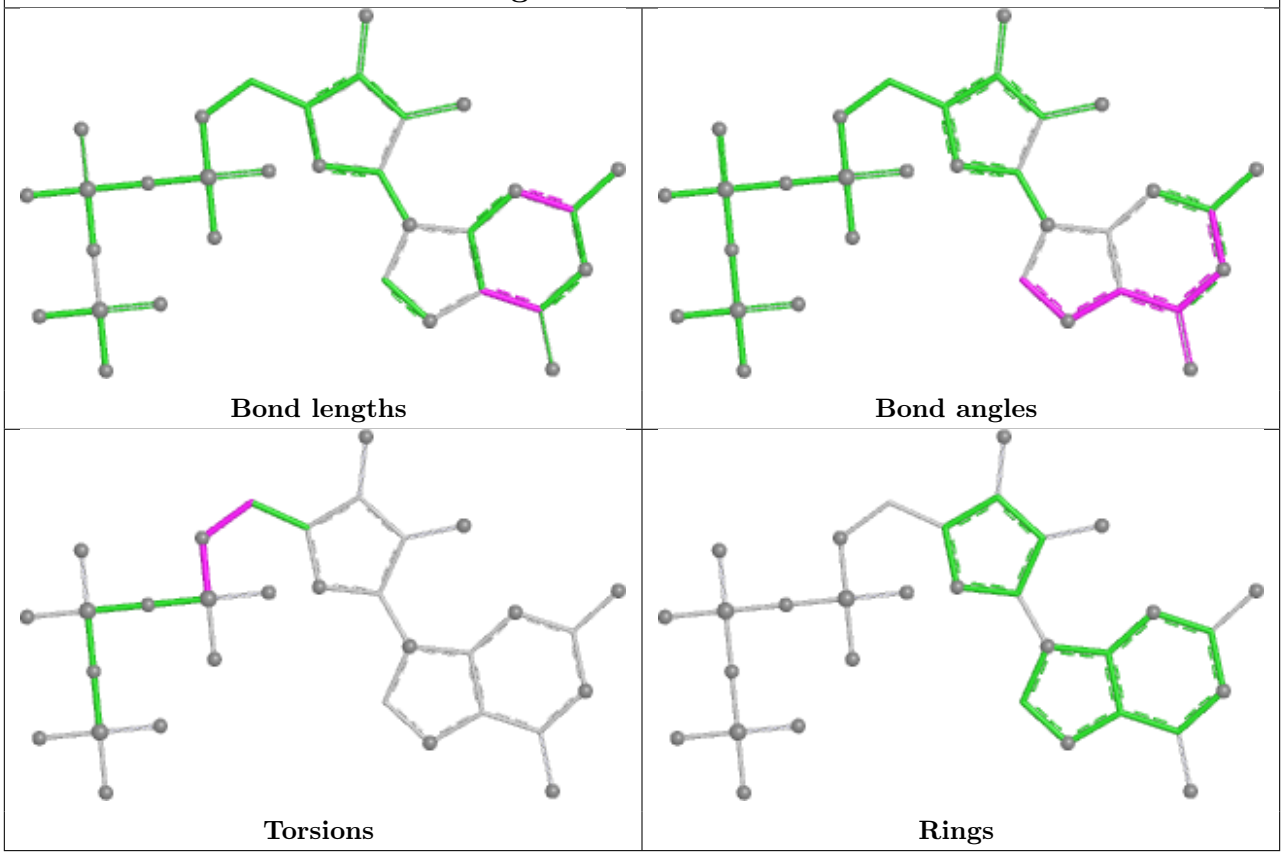
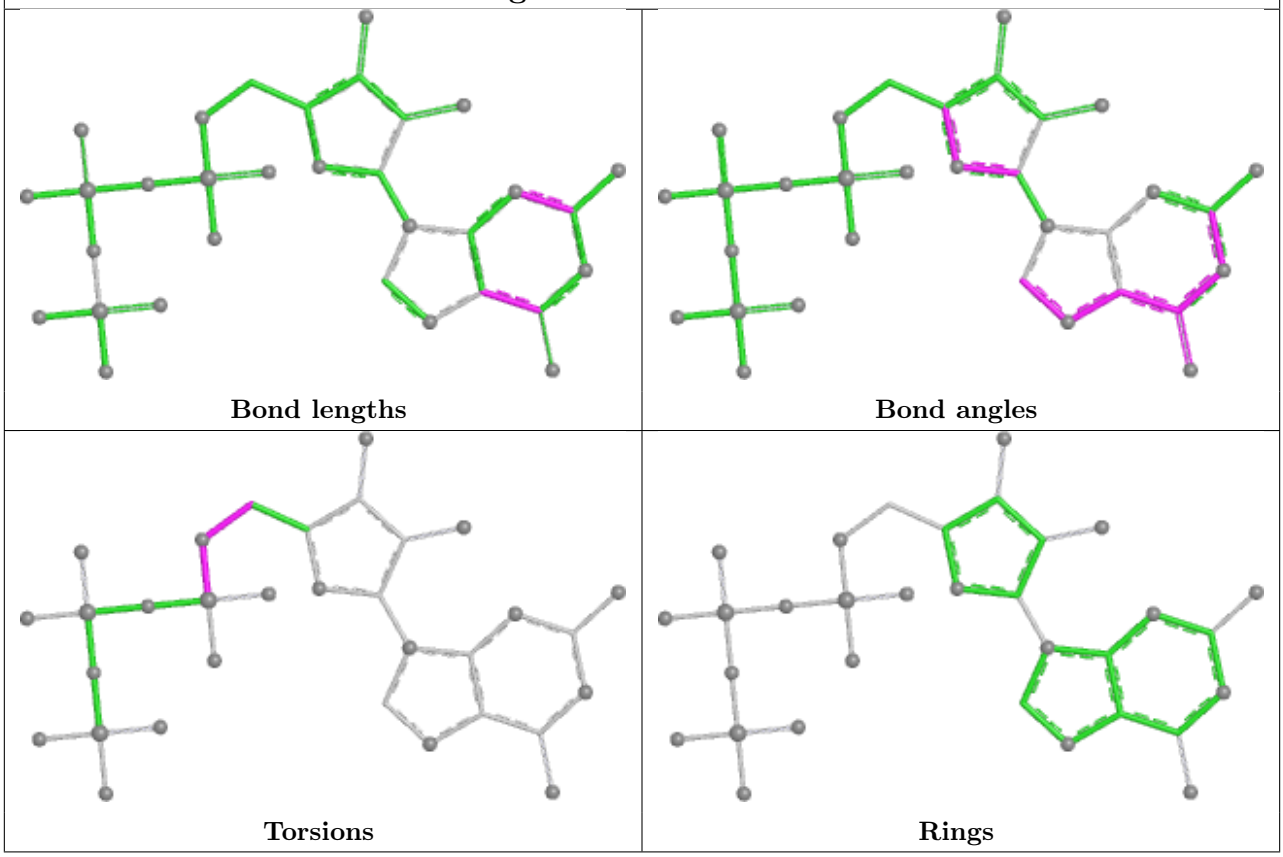


Rings

Ligand GTP EK 501



Ligand GTP ML 501



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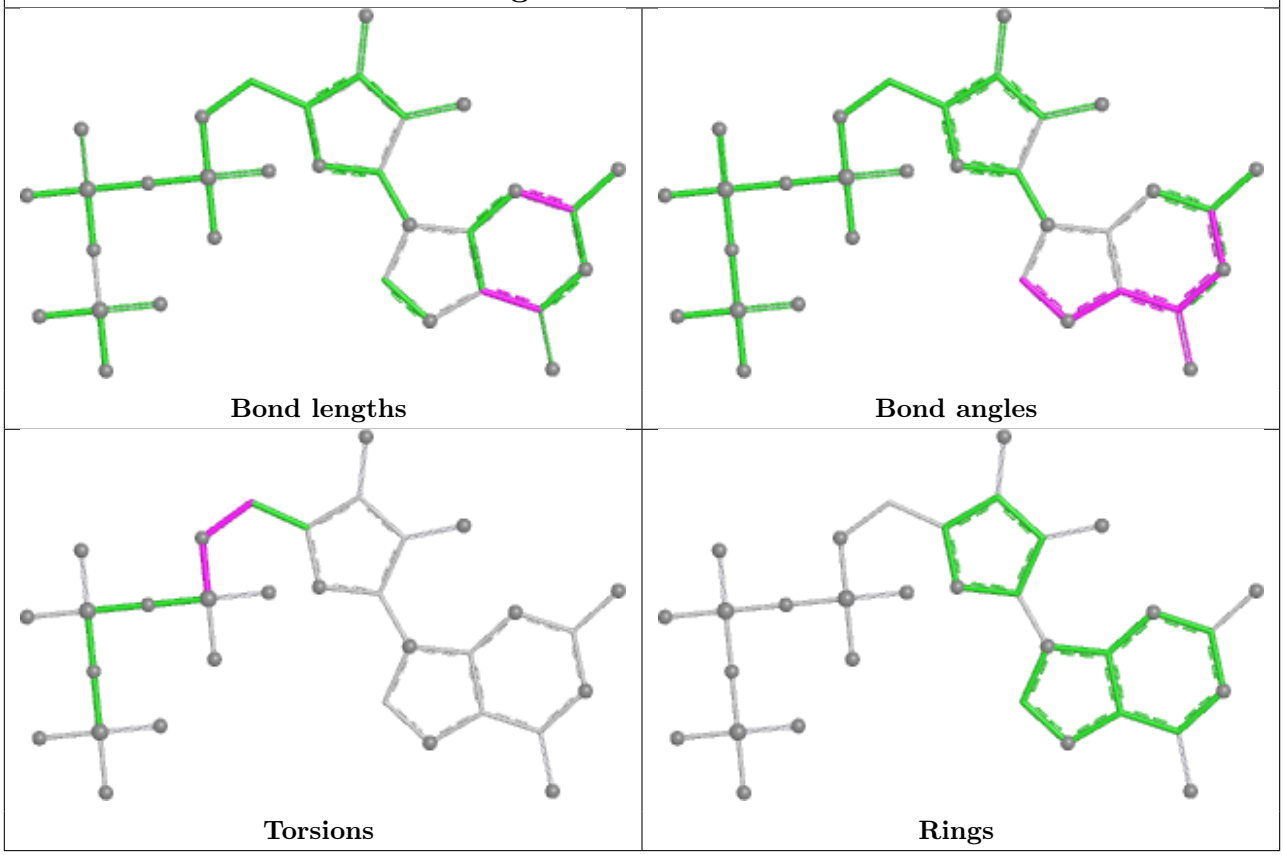
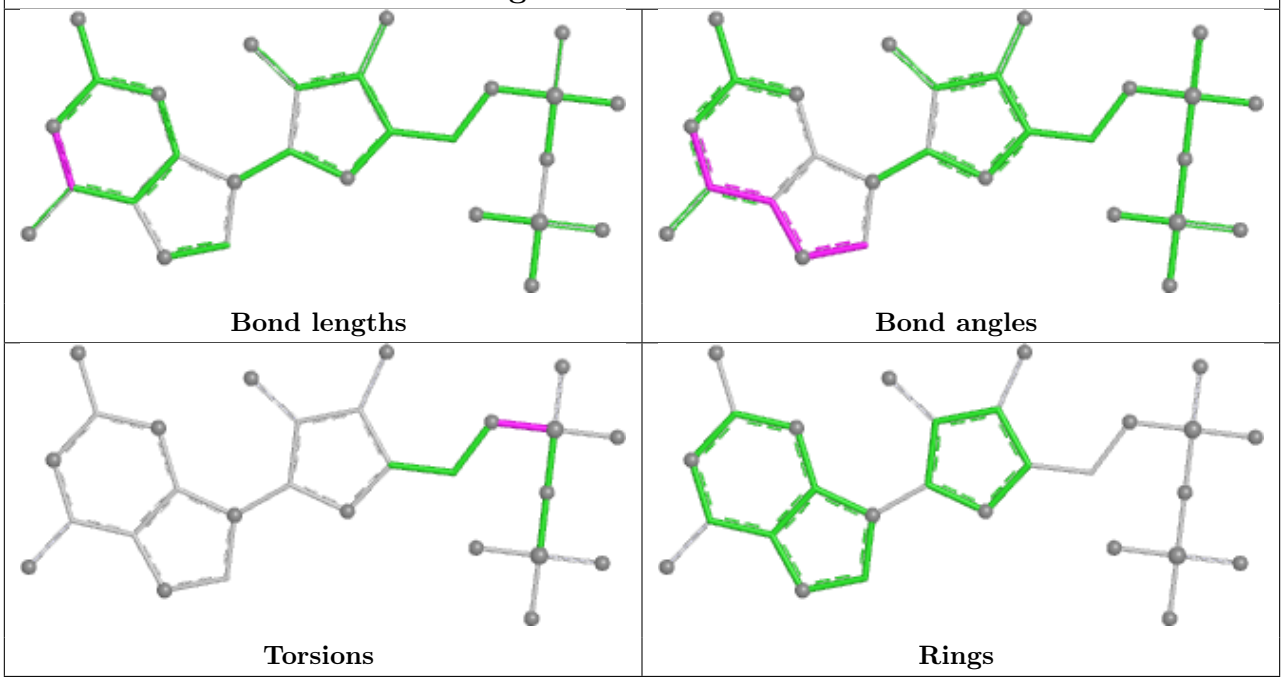


Ligand GDP JM 501



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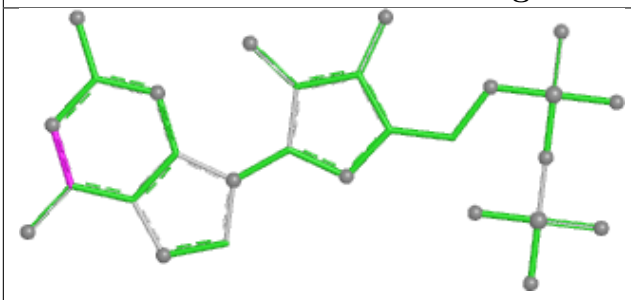
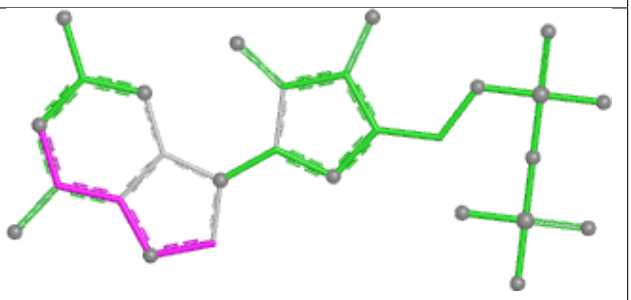
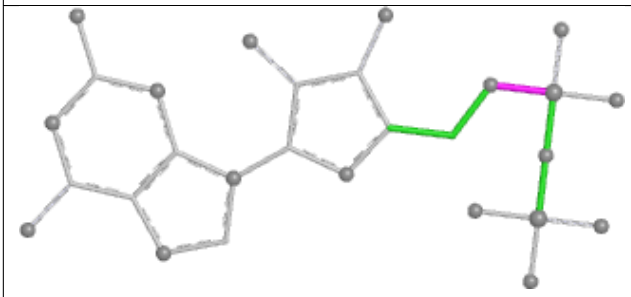


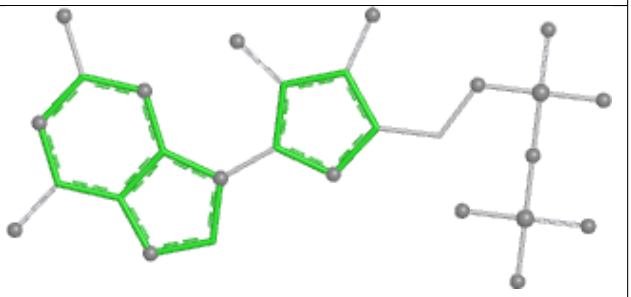
Bond lengths



Bond angles

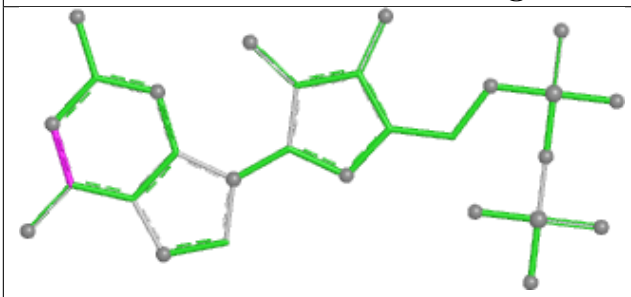


Torsions



Rings

Ligand GDP CD 501



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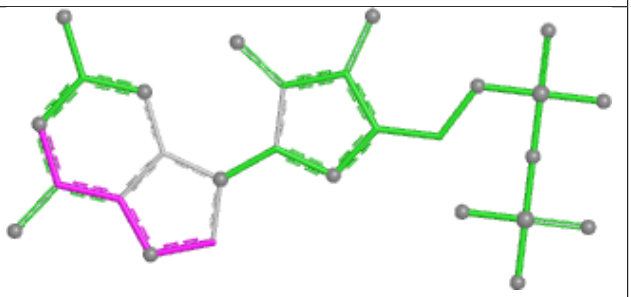

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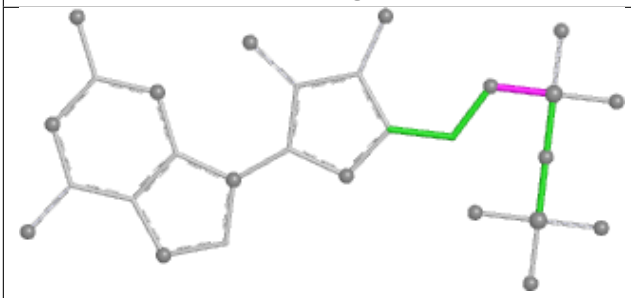

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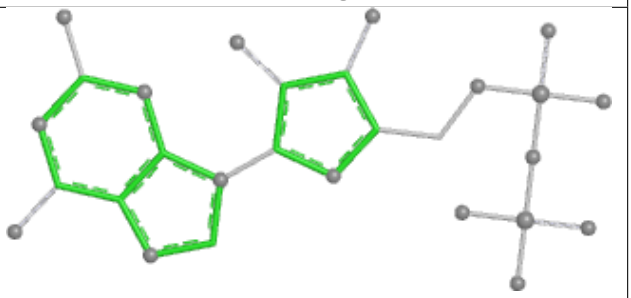
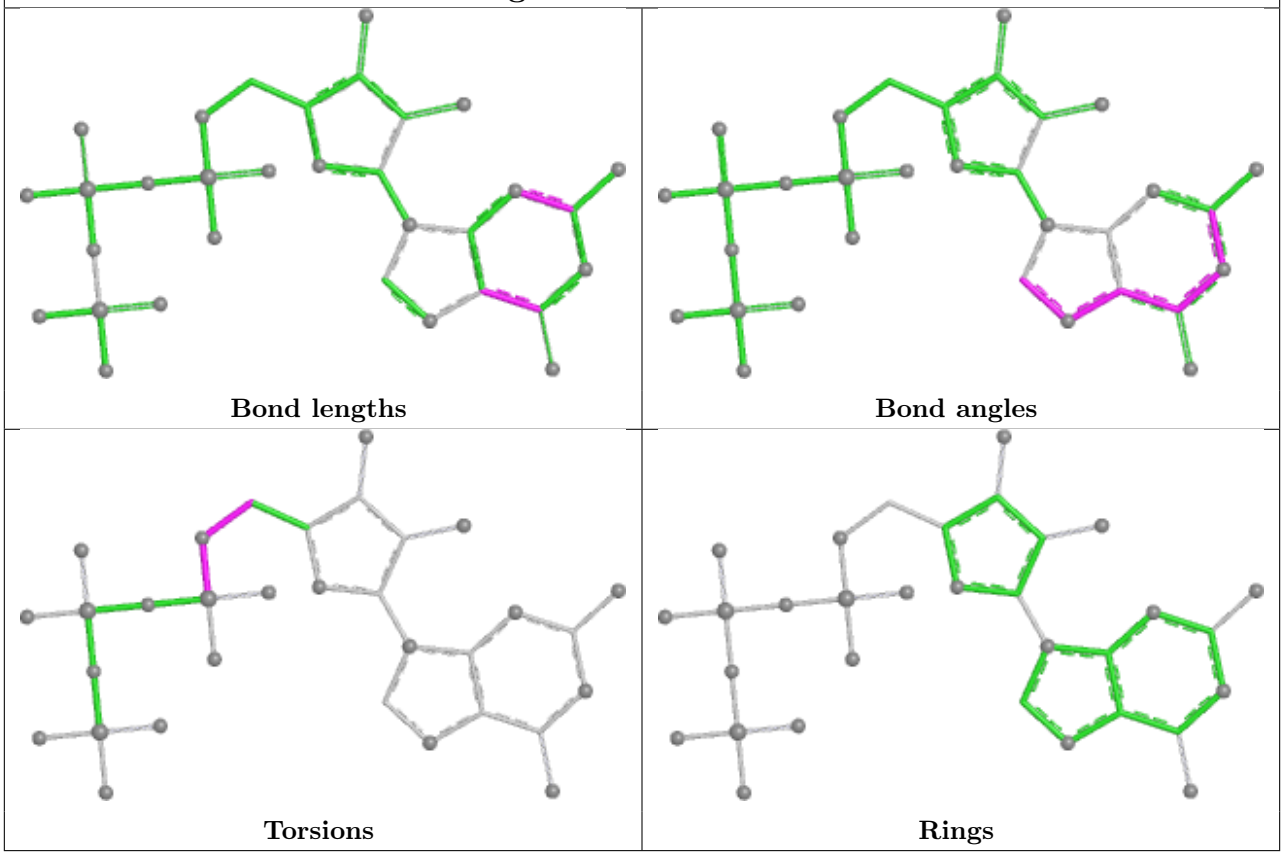
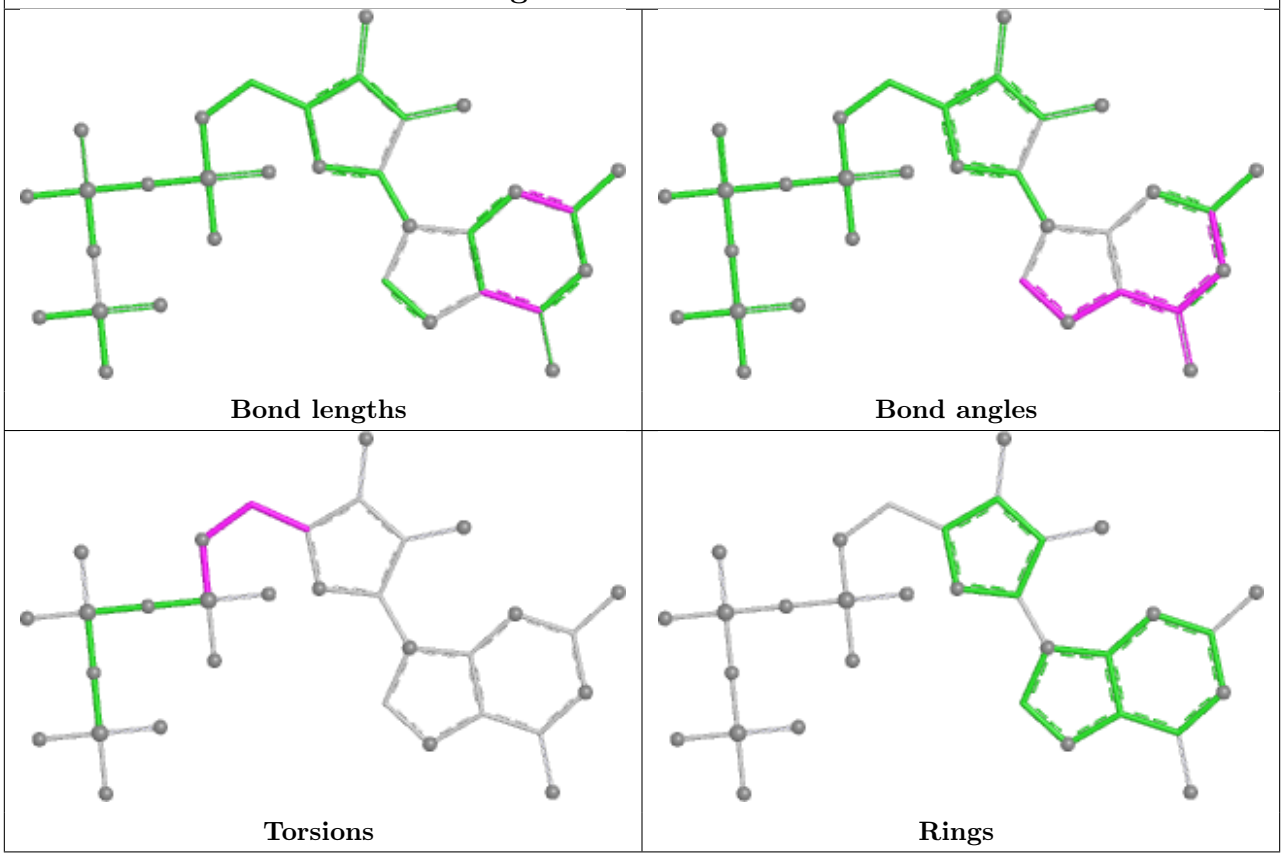


Rings

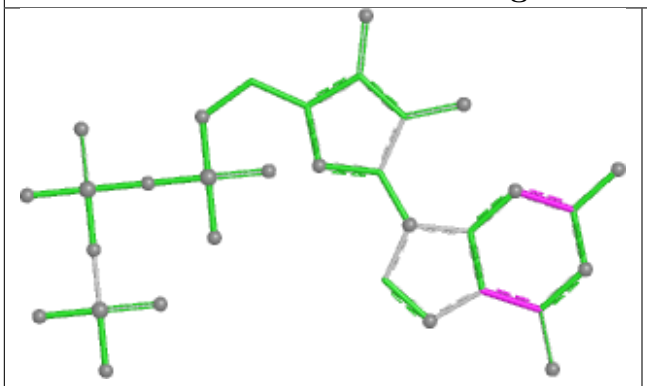
Ligand GTP GG 501



Ligand GTP VB 501



Ligand GTP QB 501



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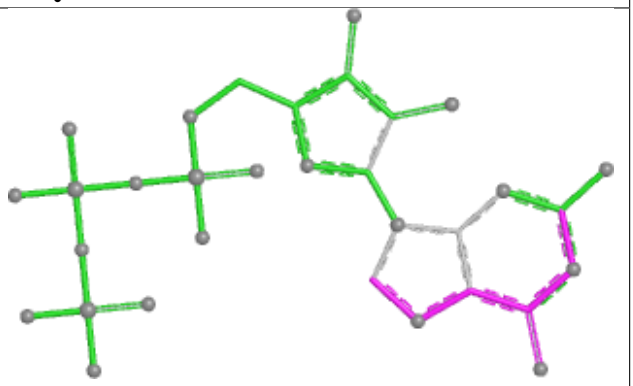
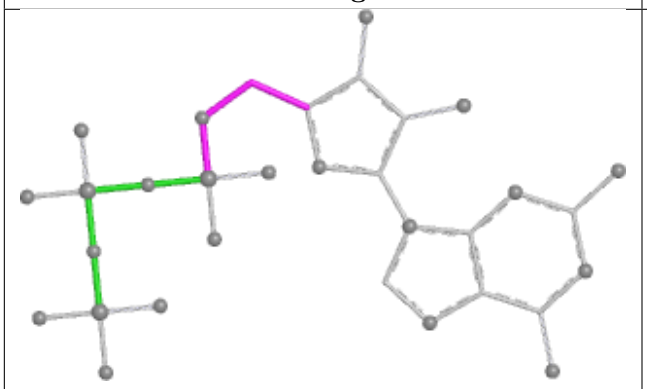


Bond angles



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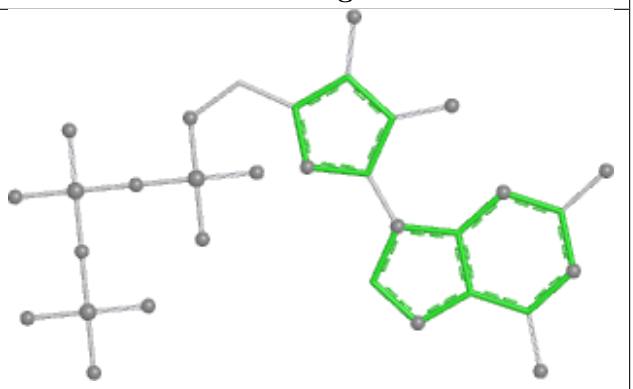

Rings

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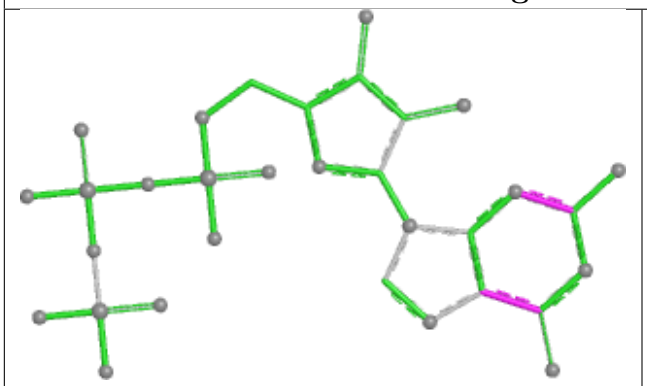

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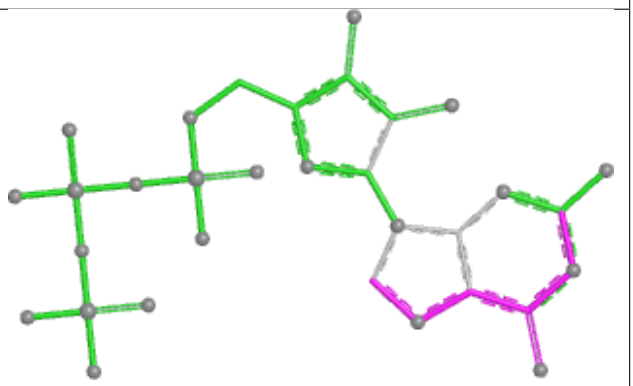
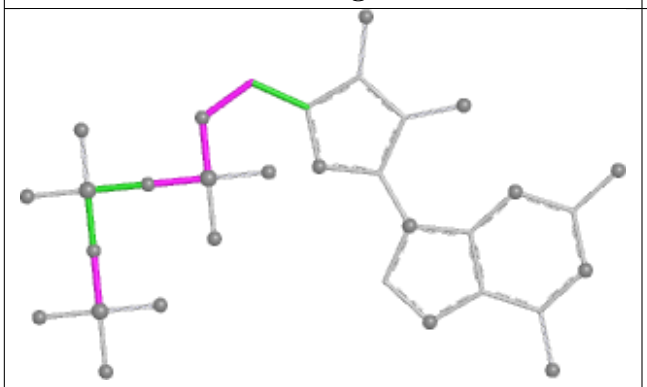


Bond angles



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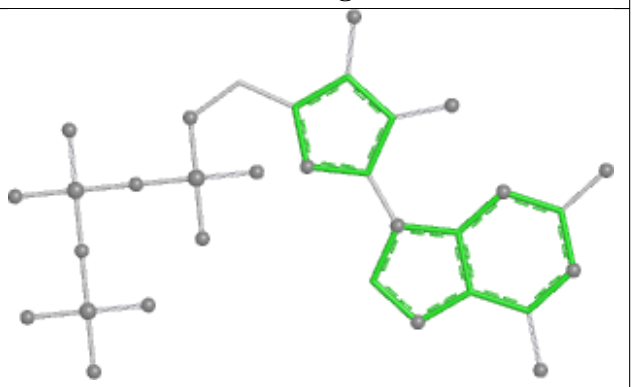
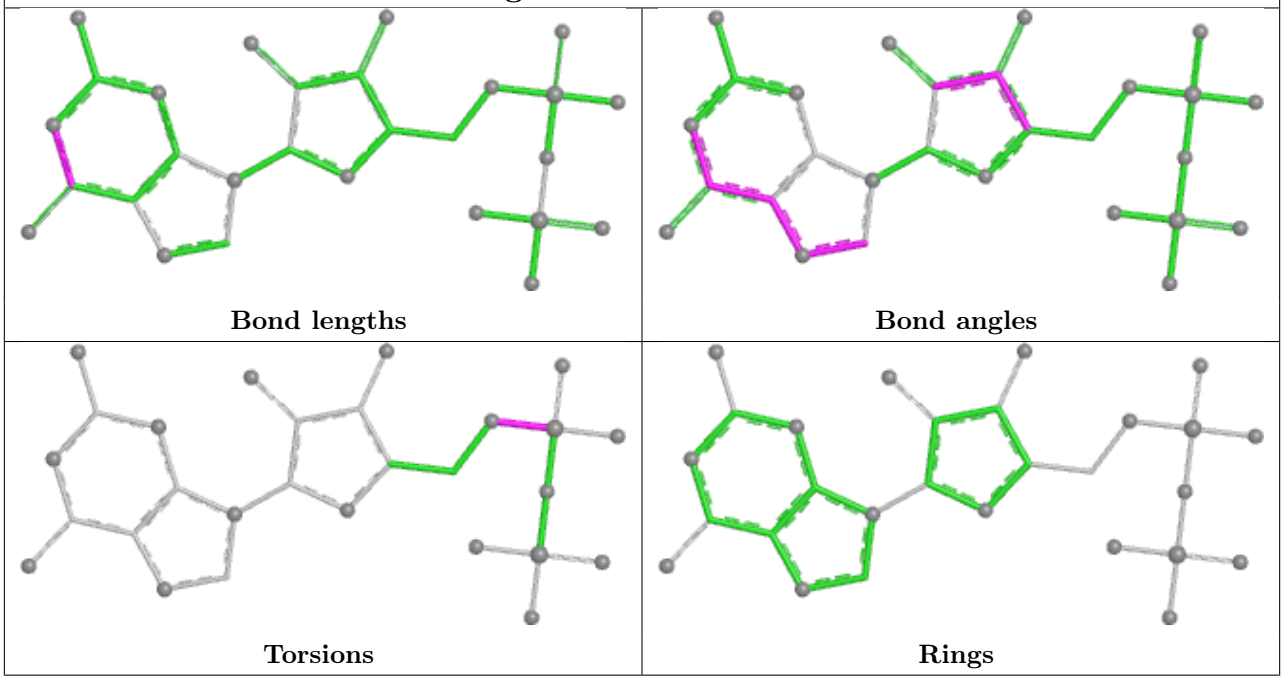
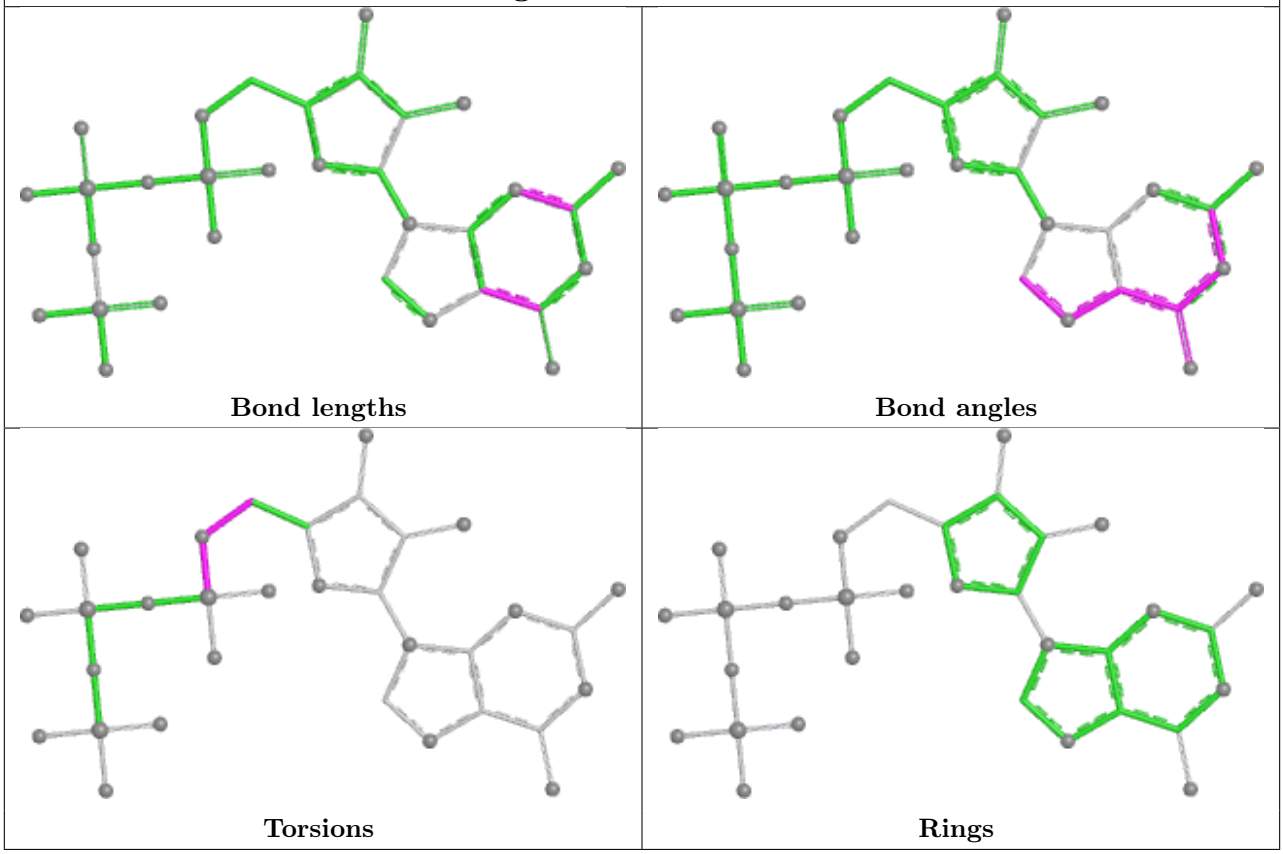


Rings

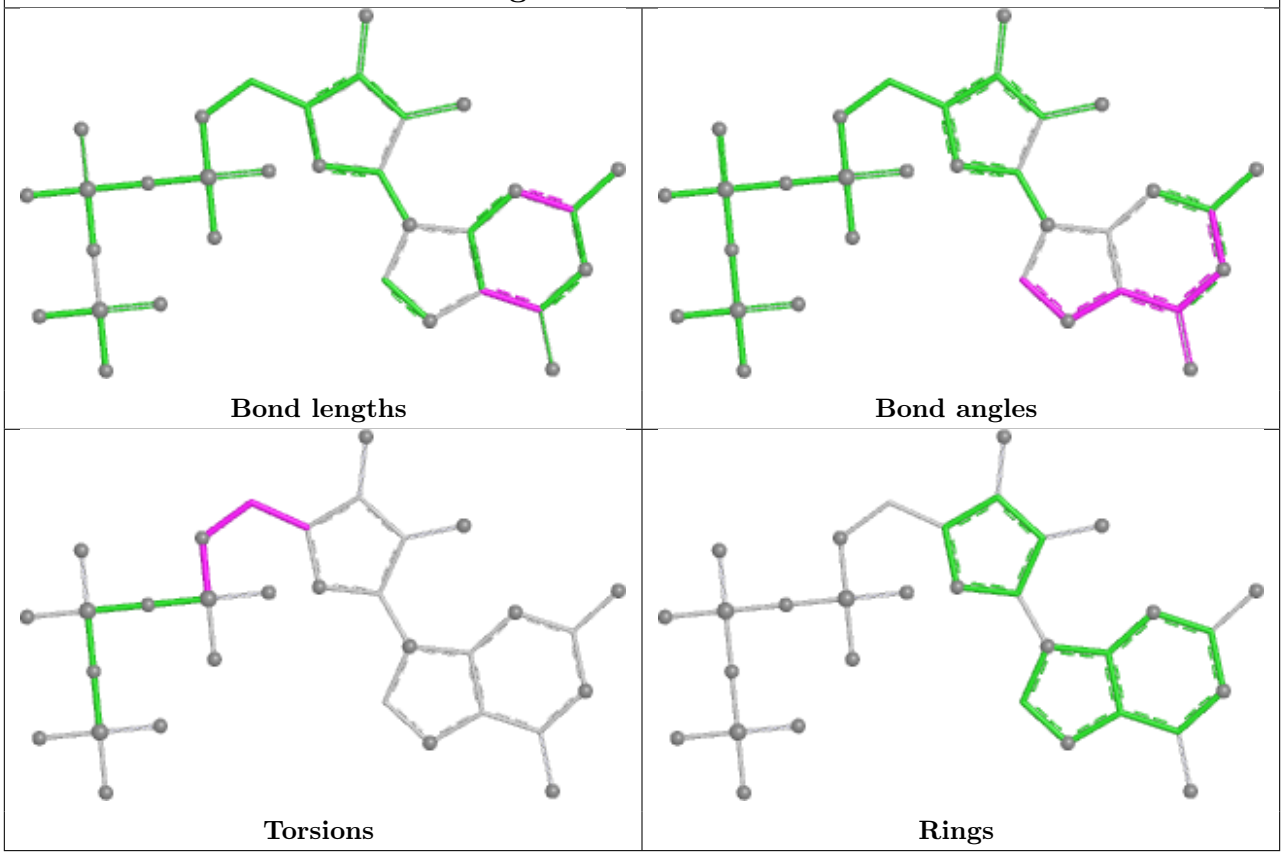
Ligand GDP RM 501



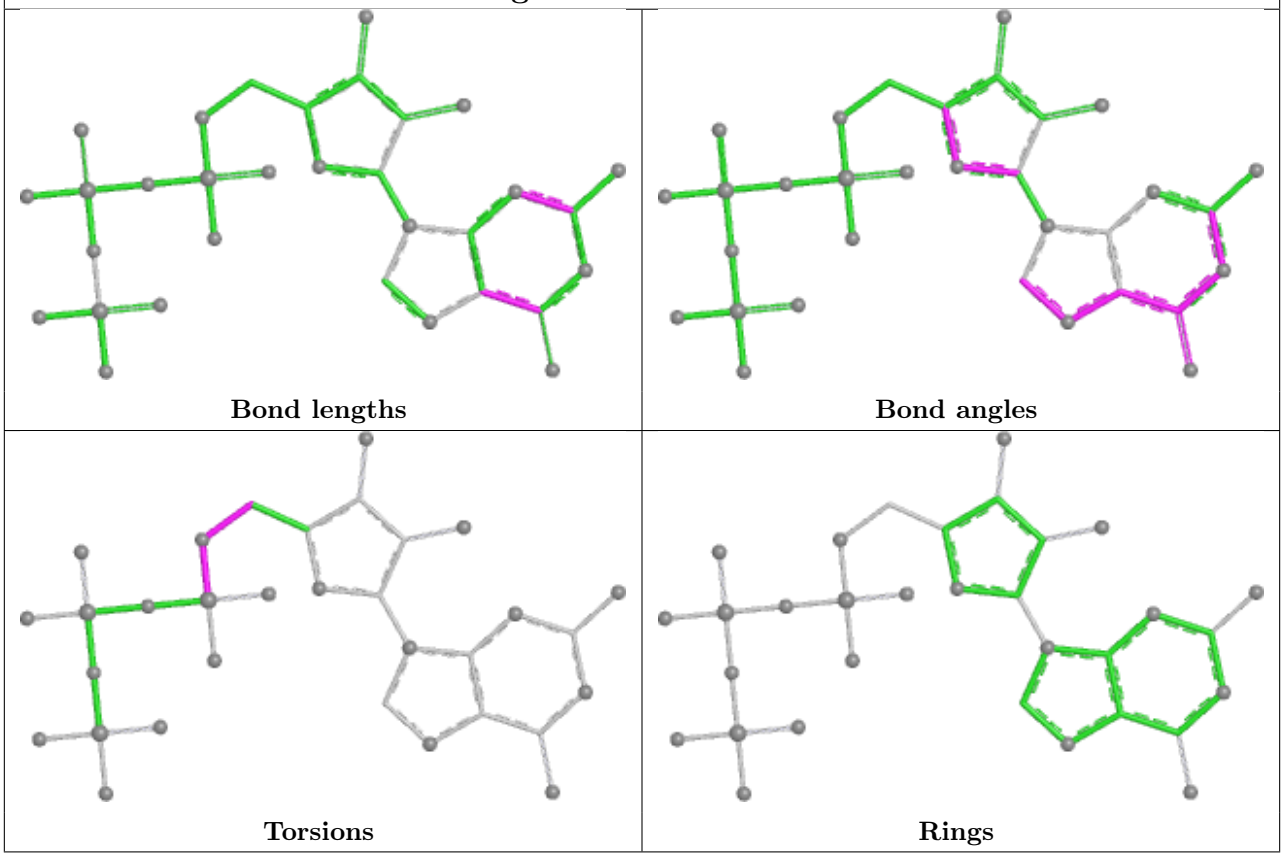
Ligand GTP FB 501



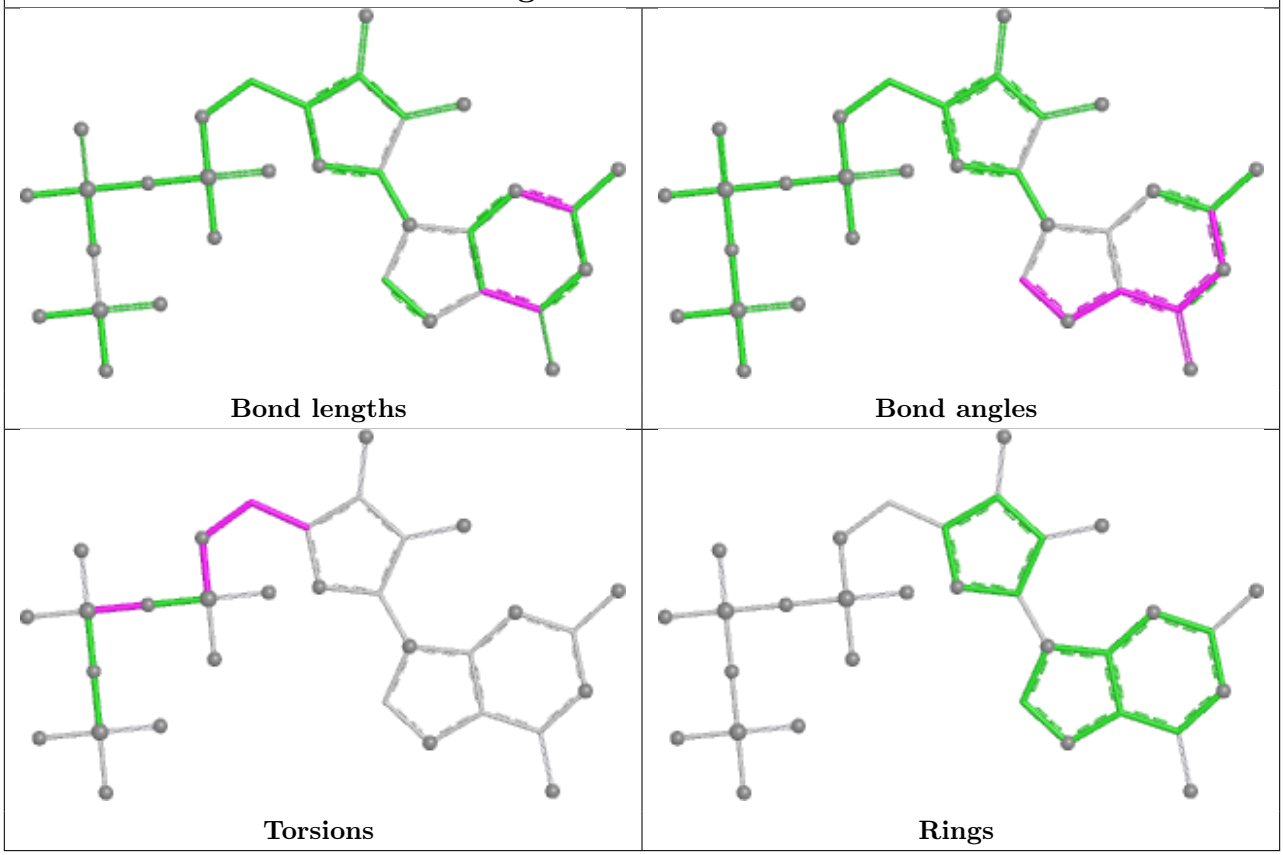
Ligand GTP RK 501



Ligand GTP EA 501



Ligand GTP TI 501



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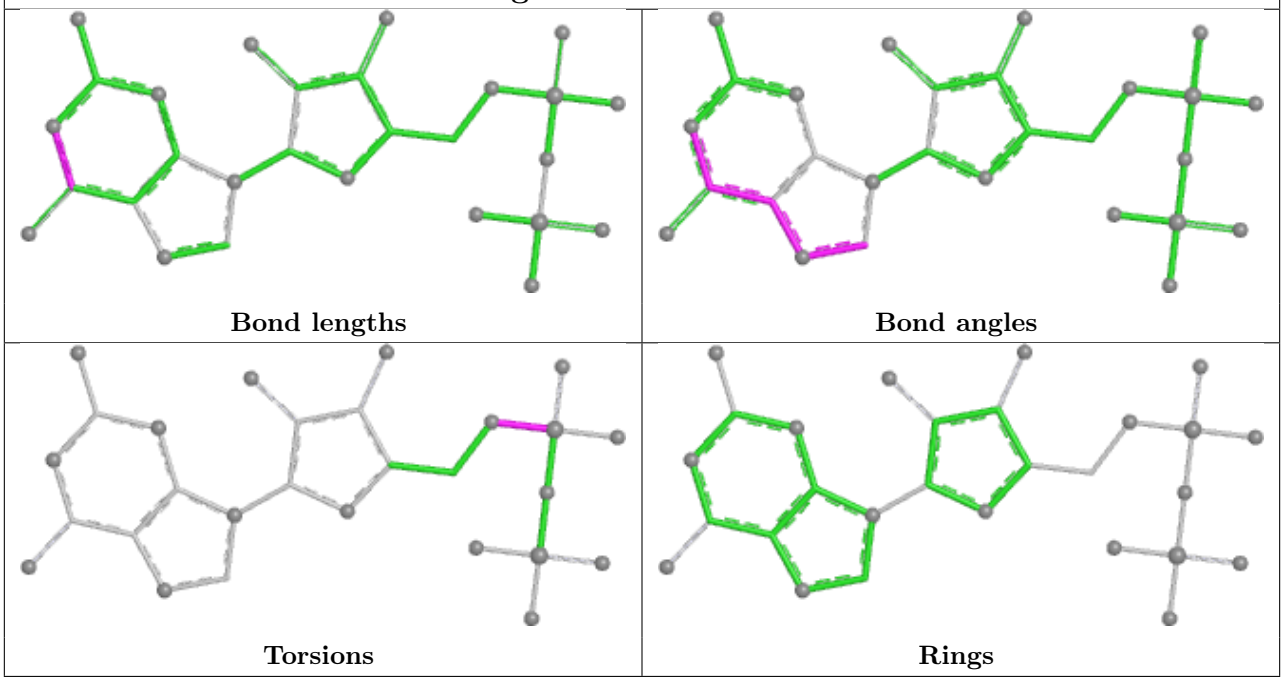
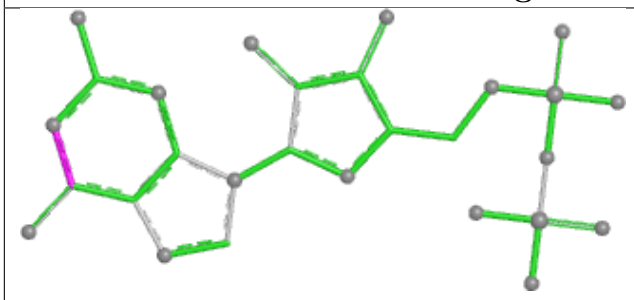
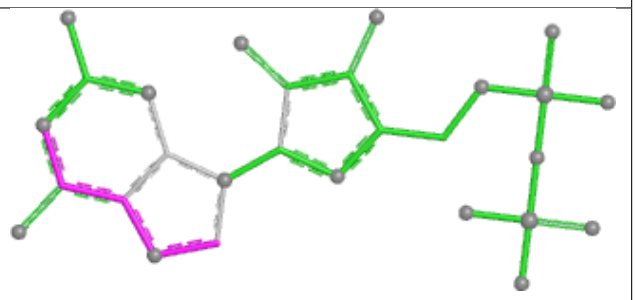


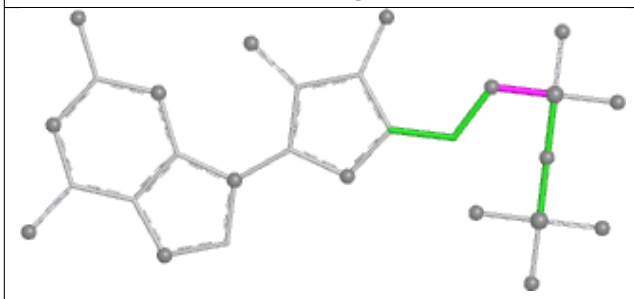
Ligand GDP IH 501



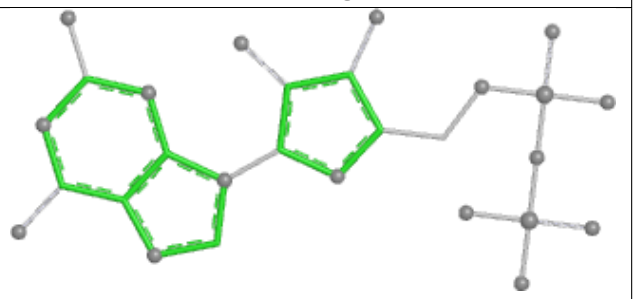
Bond lengths



Bond angles

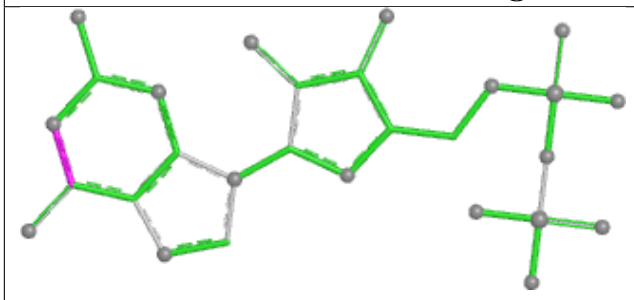


Torsions



Rings

Ligand GDP AD 501



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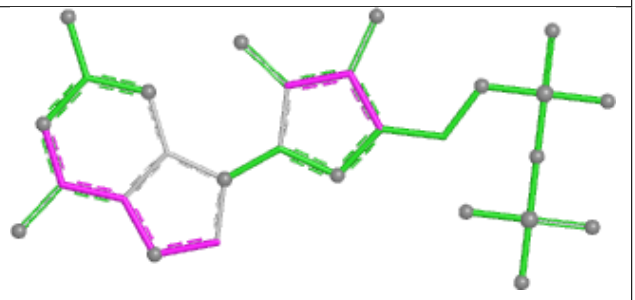

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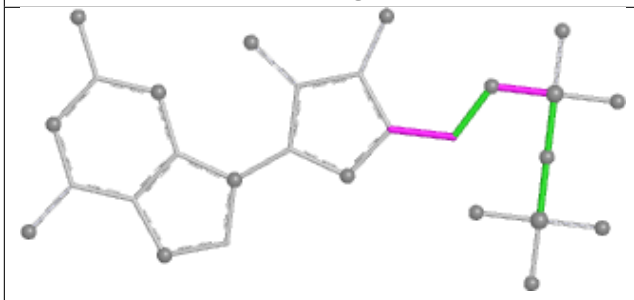

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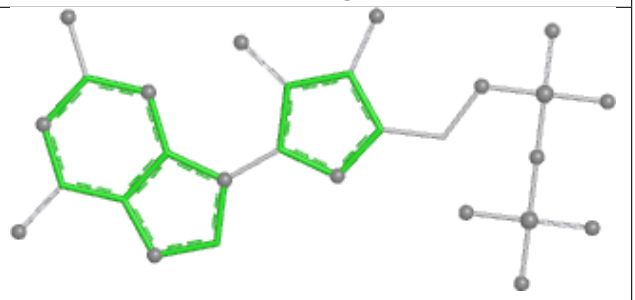

Rings

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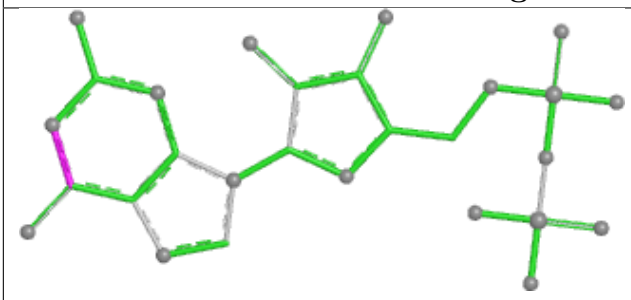

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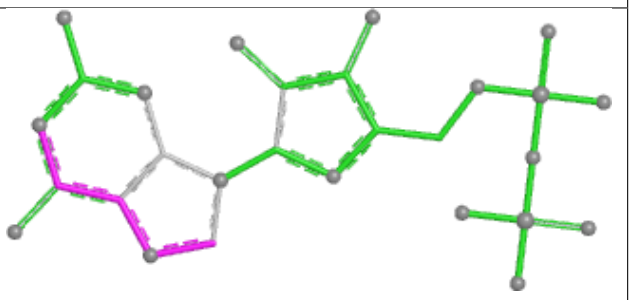
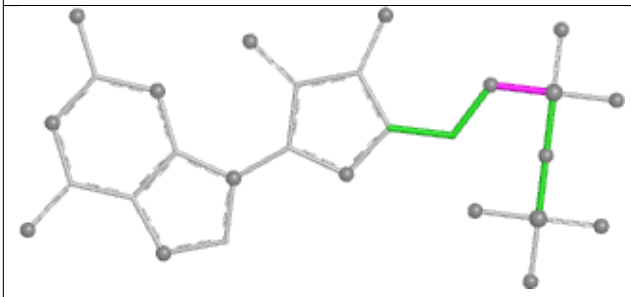
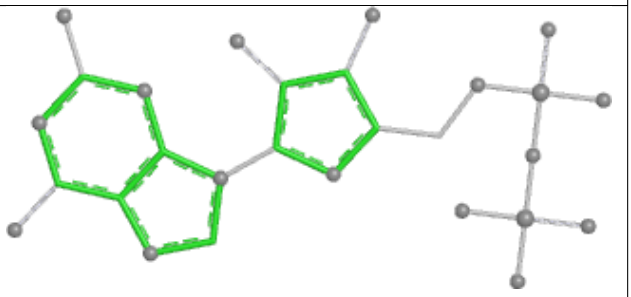


Bond angles

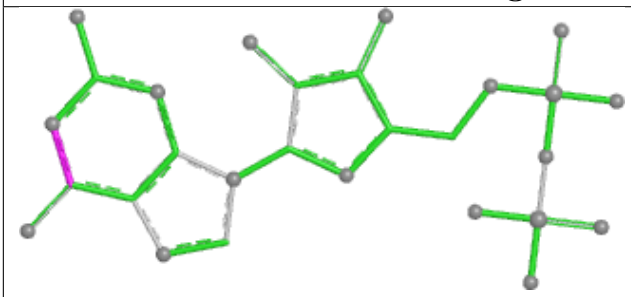


Torsions



Rings

Ligand GDP ND 501



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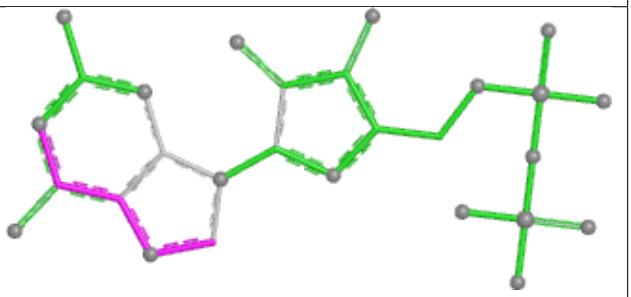
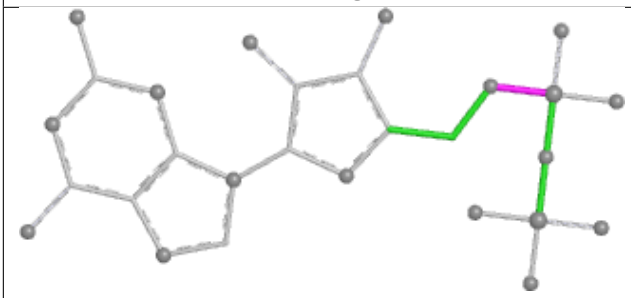


Bond angles



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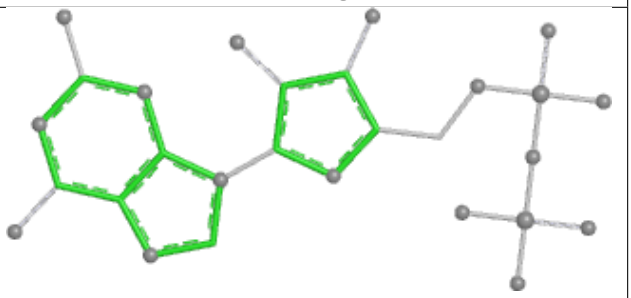
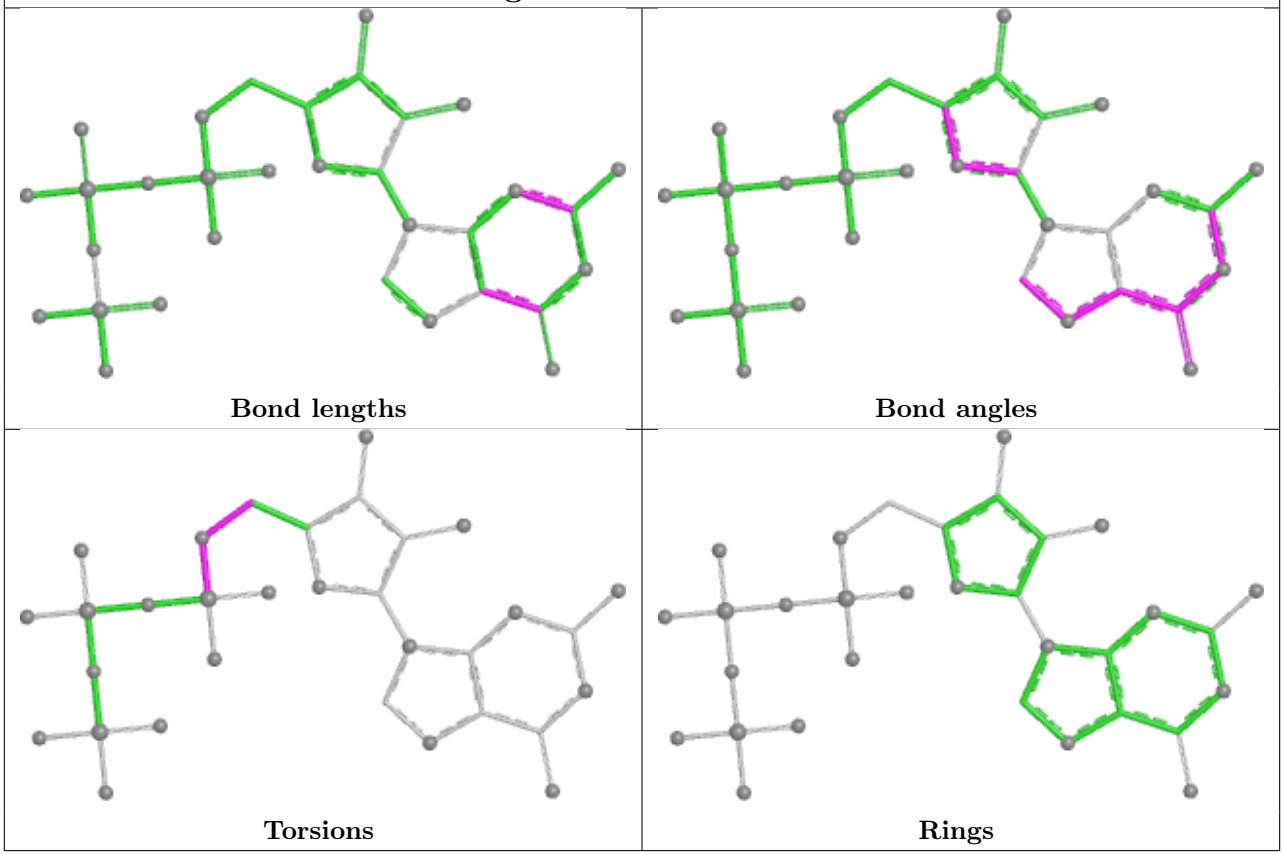
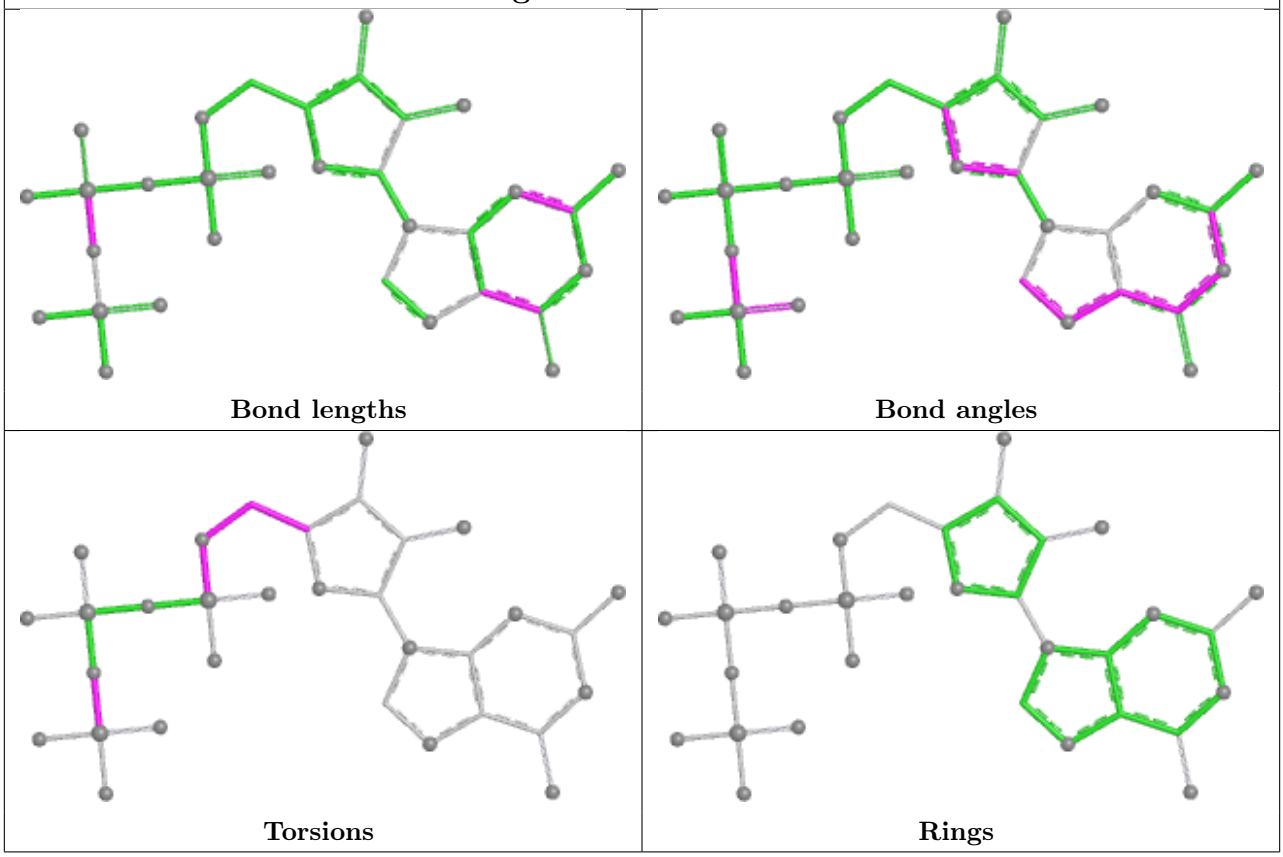


Rings

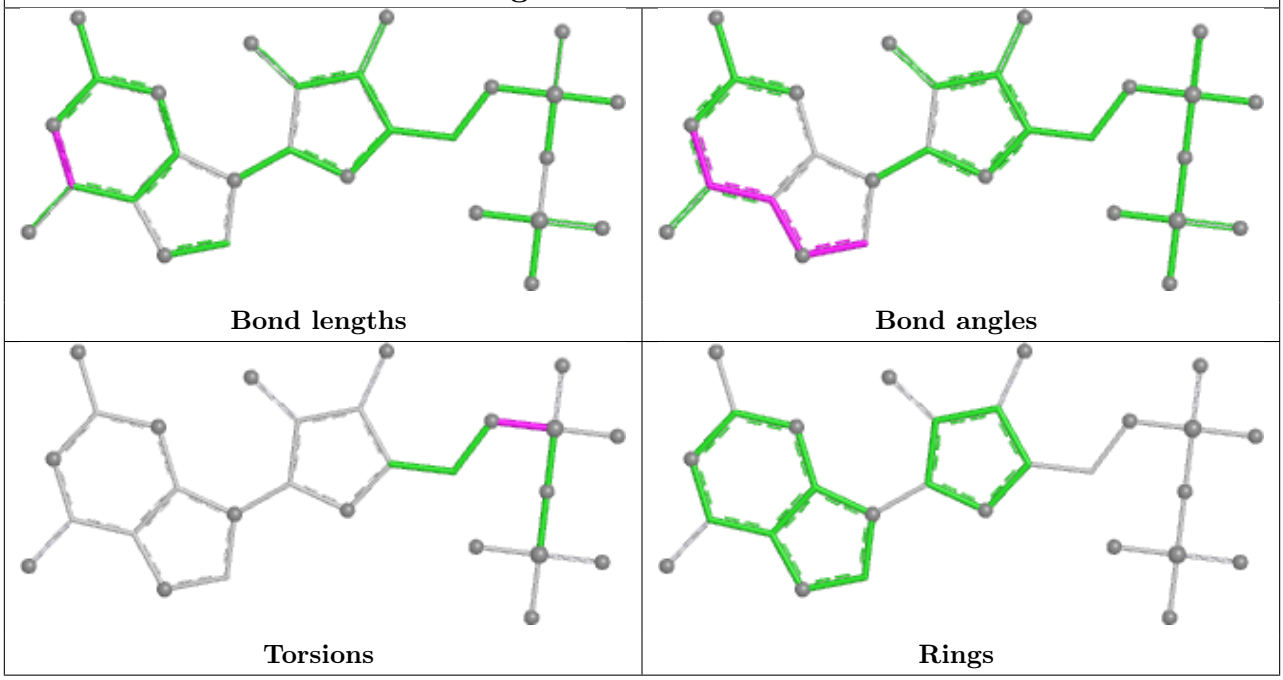
Ligand GTP WG 501



Ligand GTP RL 501



Ligand GDP AF 501



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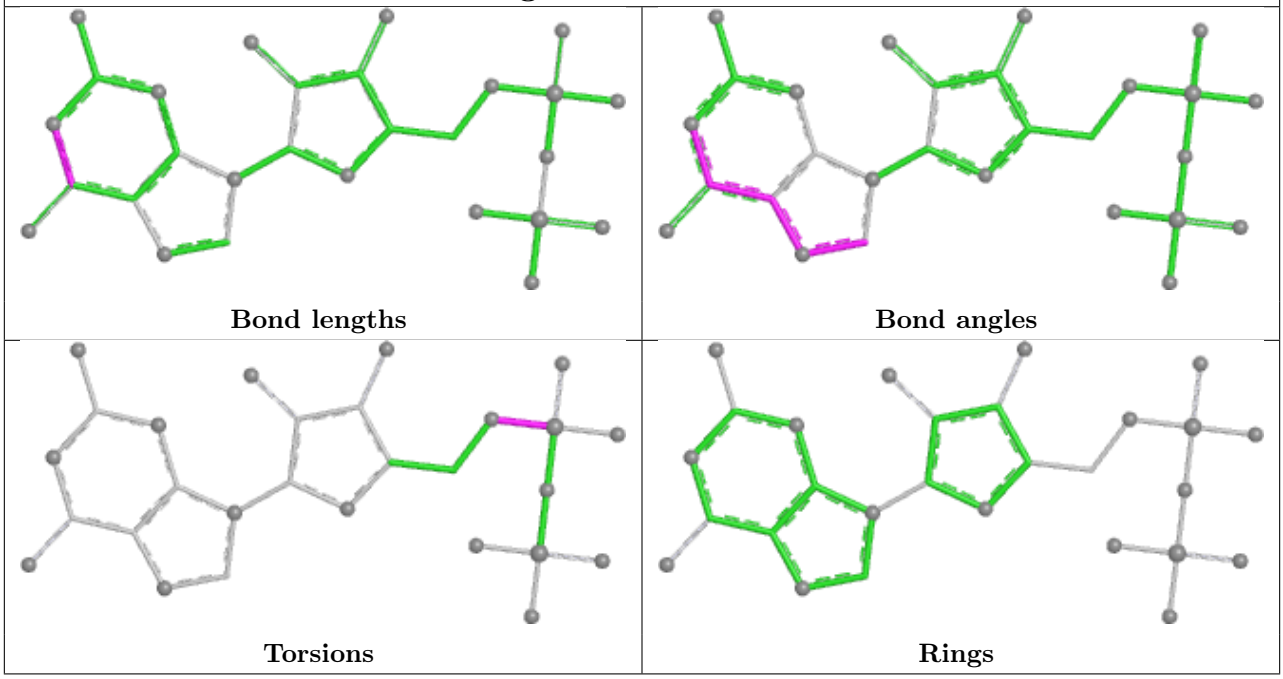

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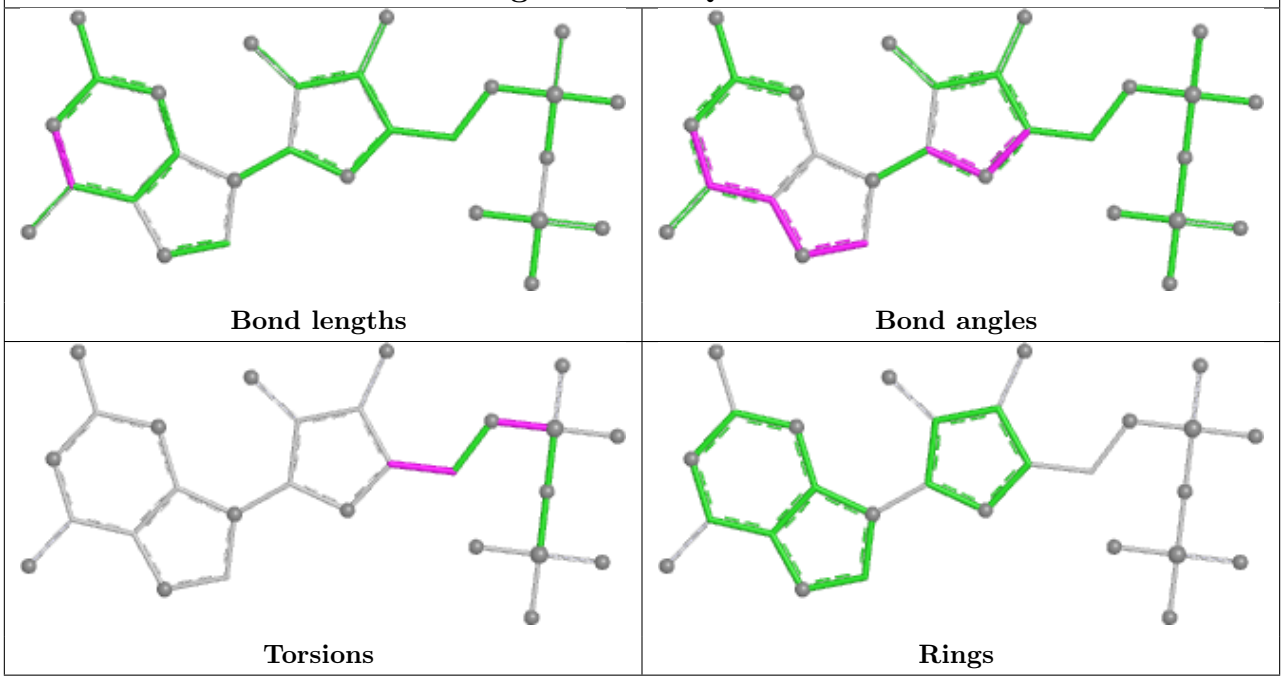

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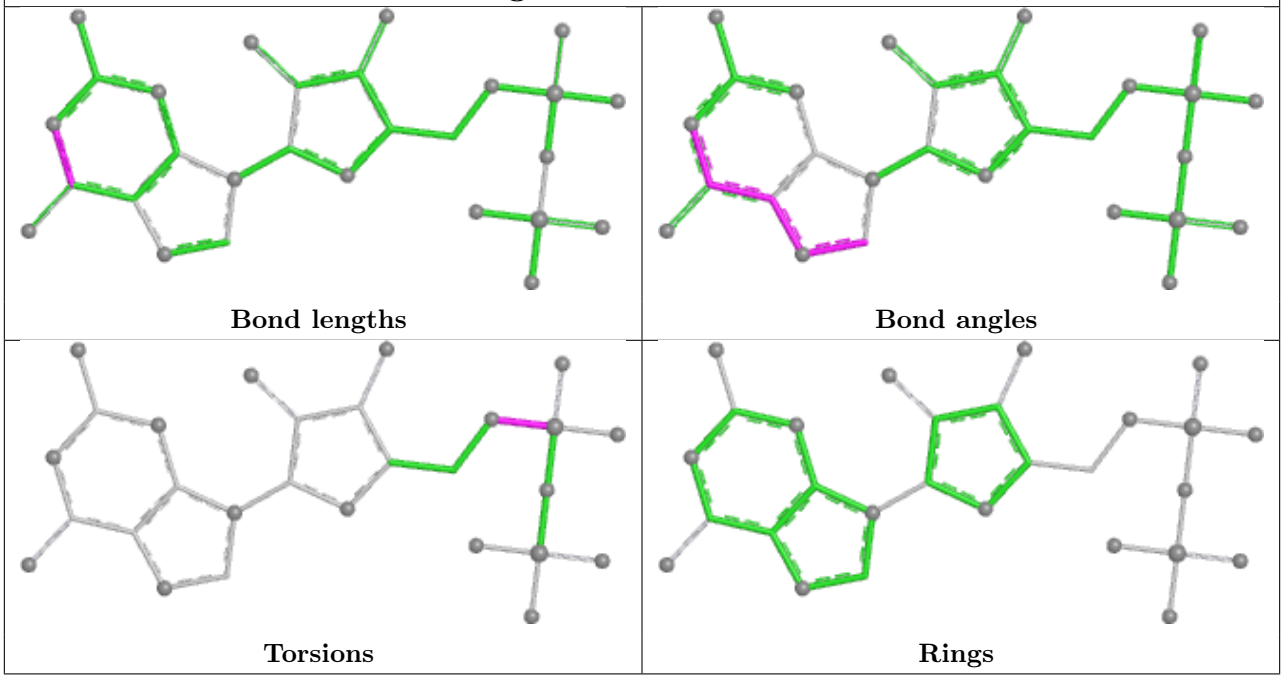

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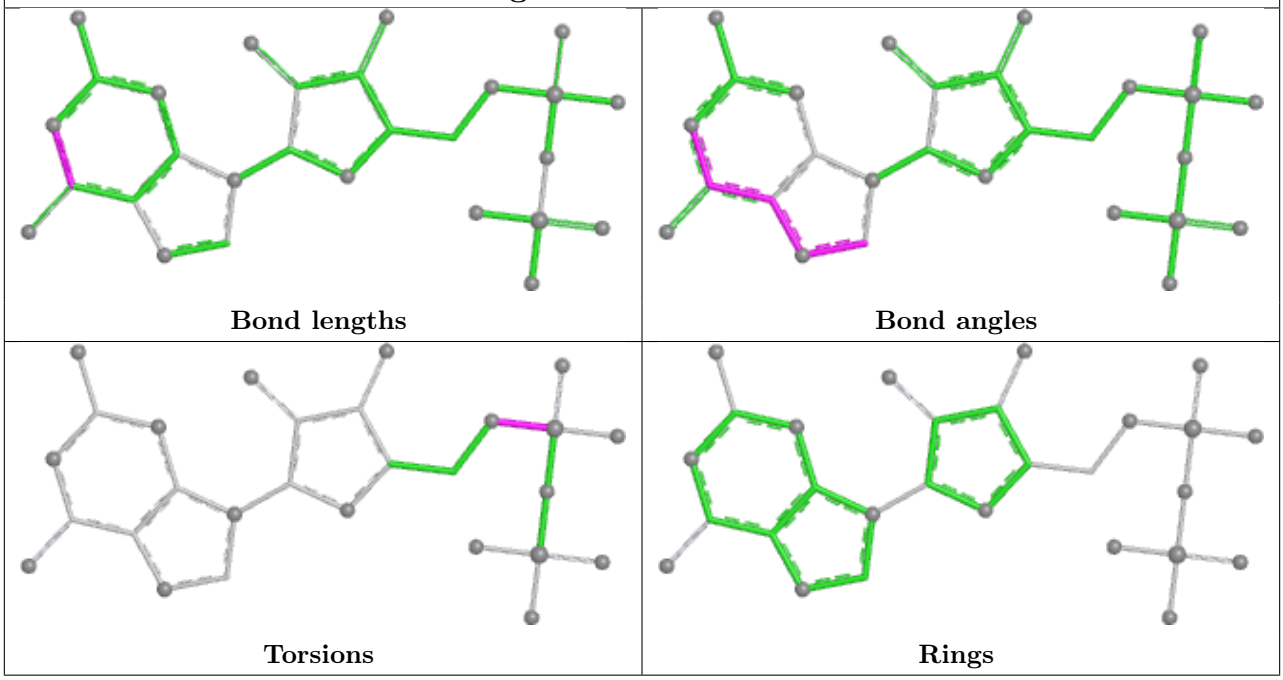

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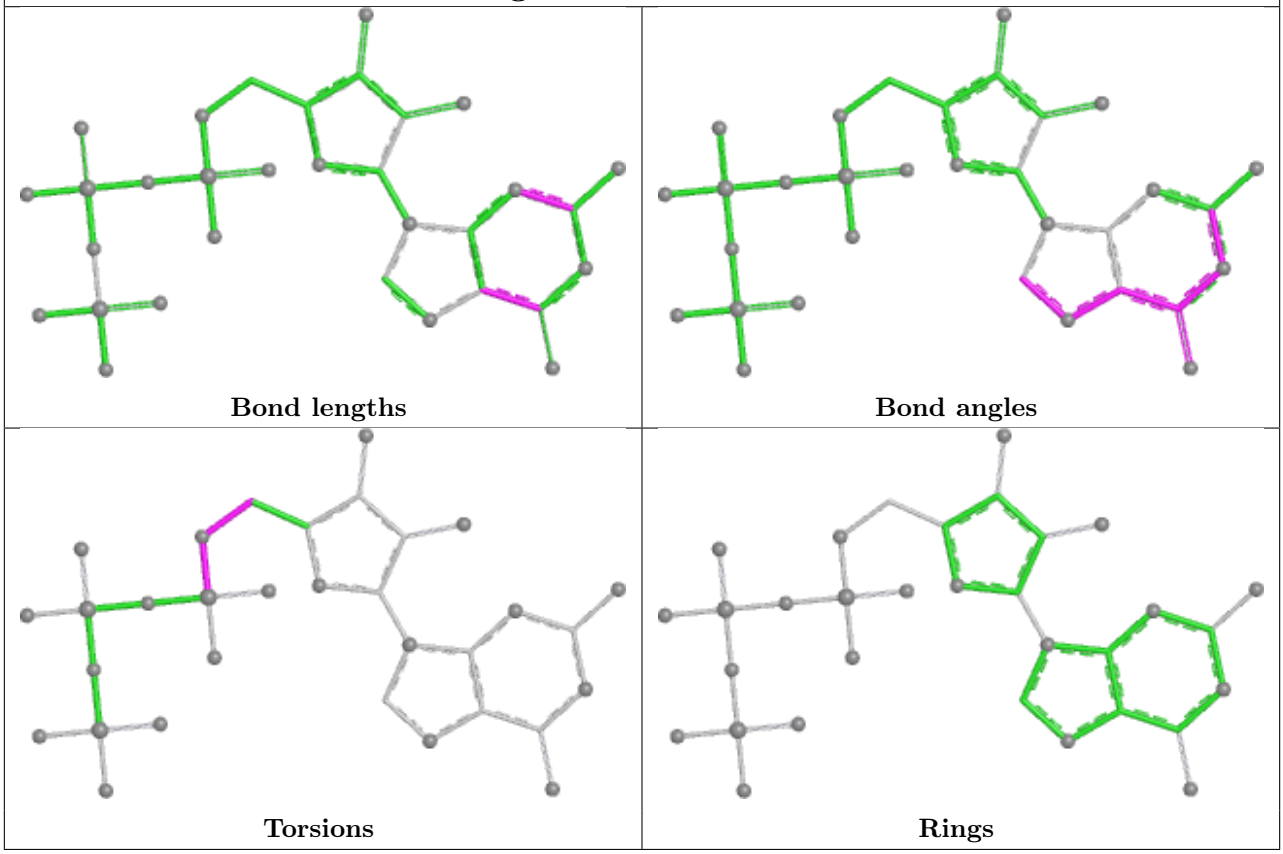

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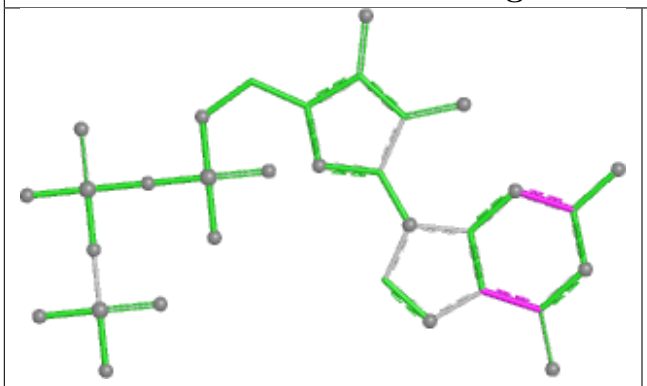
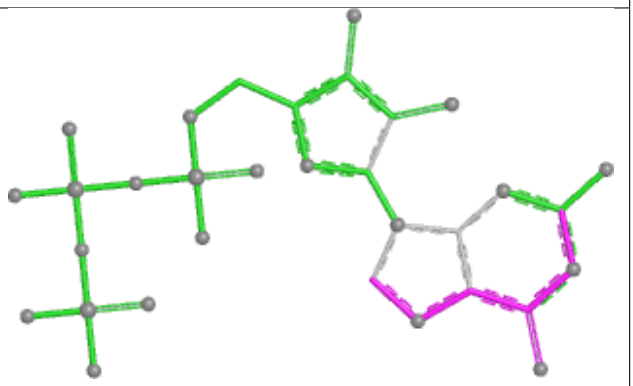
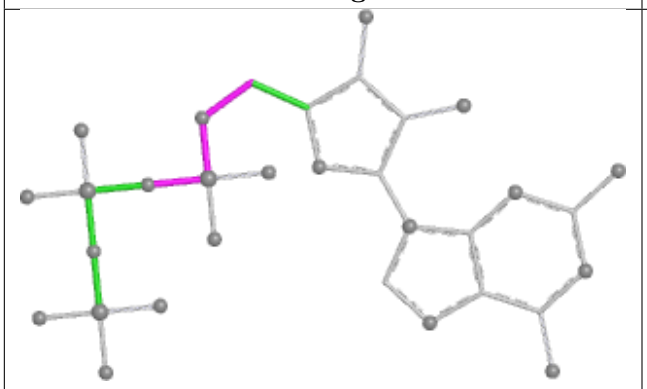


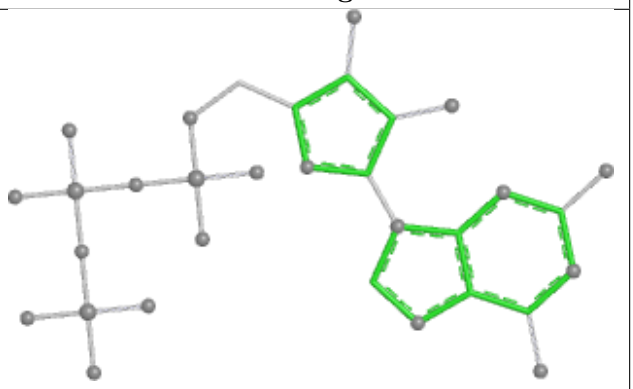
Bond lengths



Bond angles

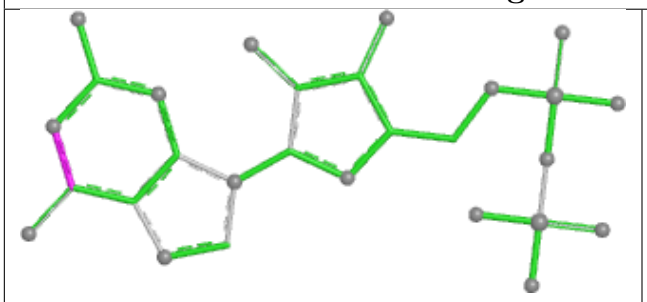


Torsions



Rings

Ligand GDP KH 501



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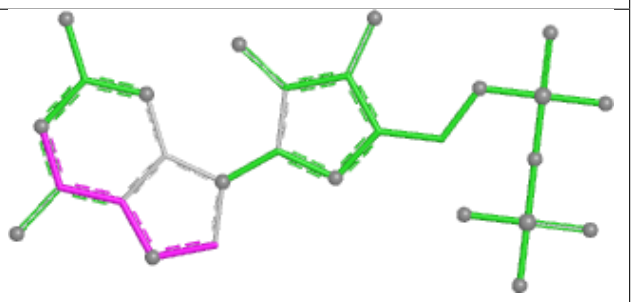
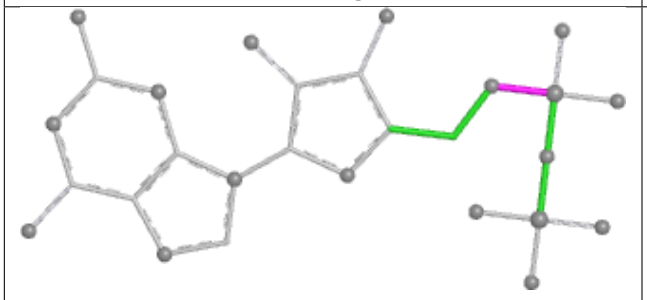
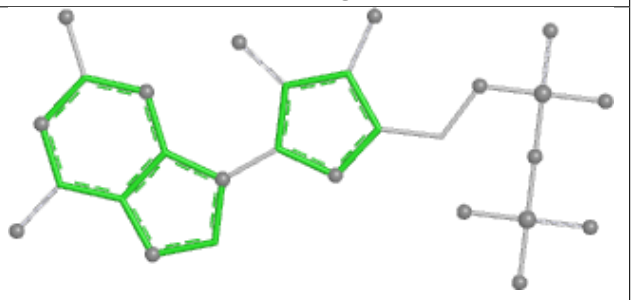


Bond angles

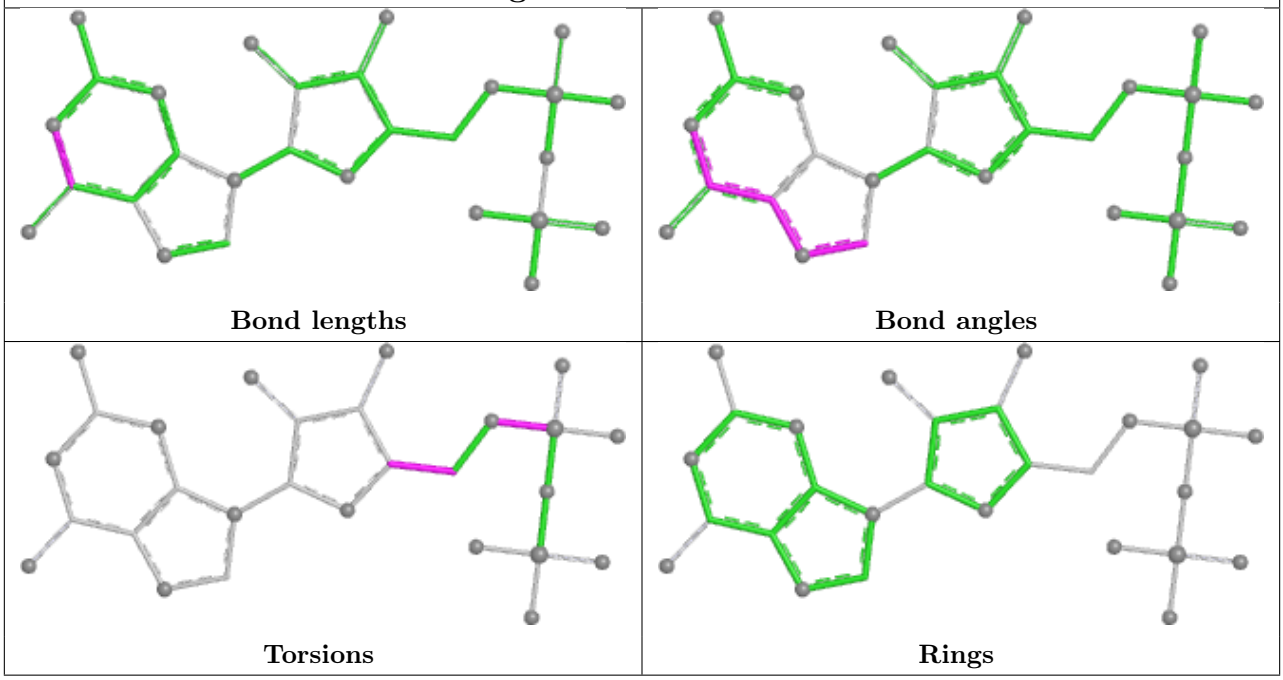


Torsions

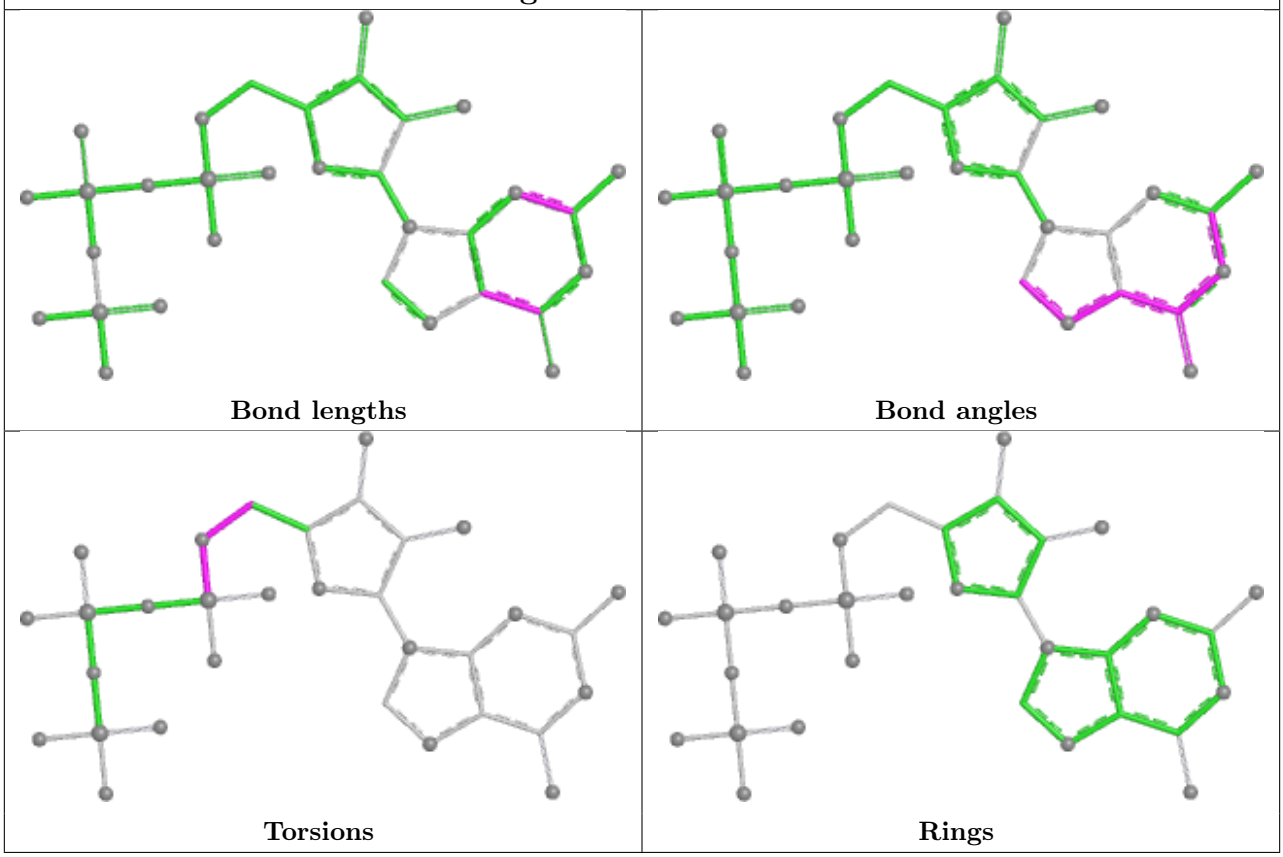


Rings

Ligand GDP MJ 501



Ligand GTP SI 501



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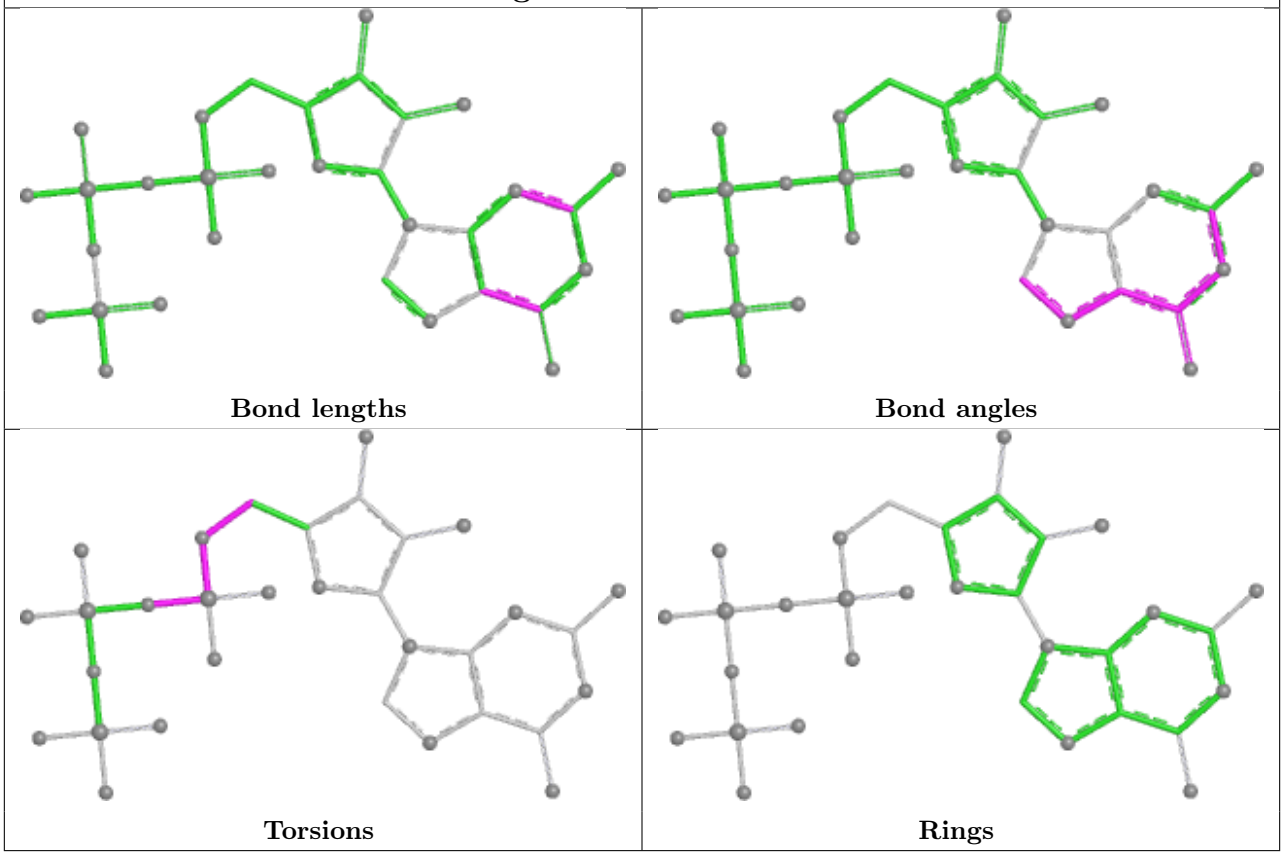

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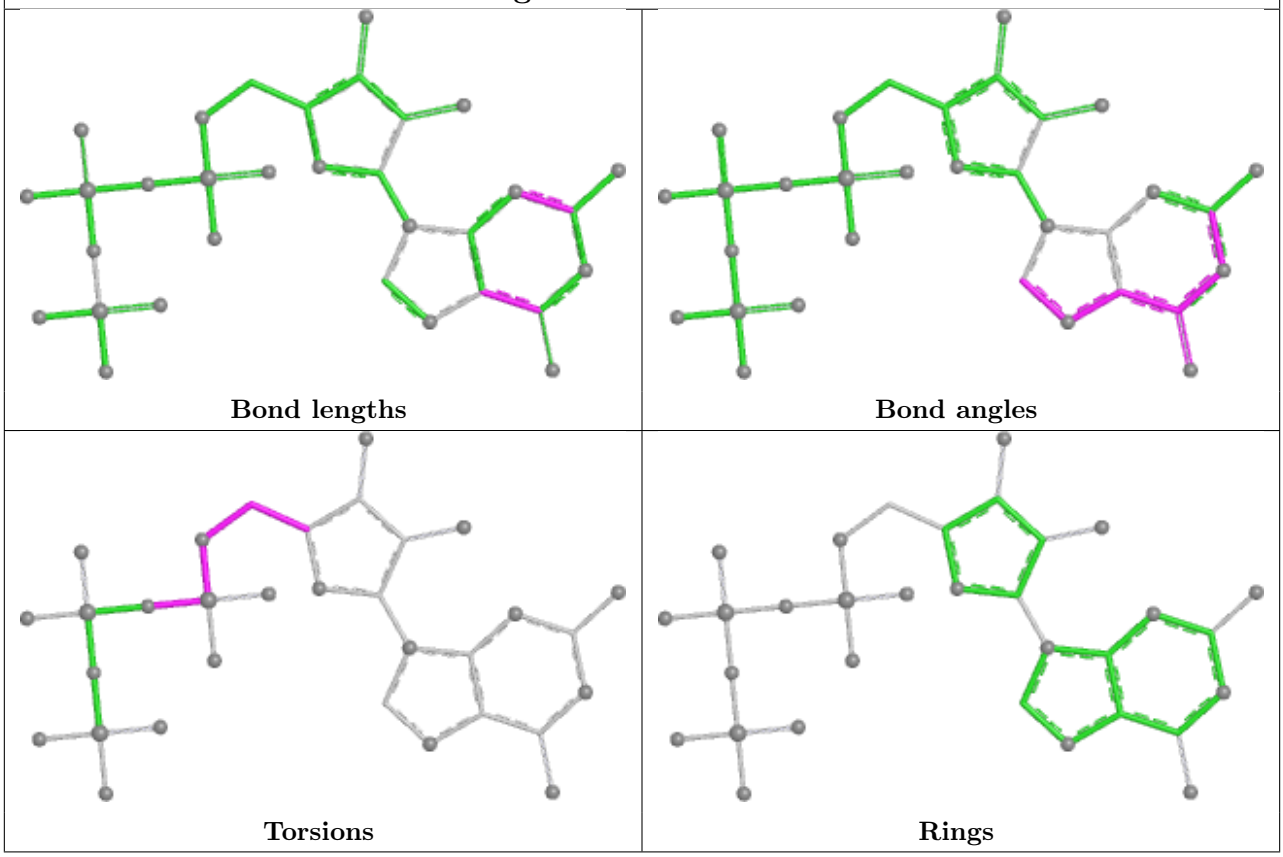

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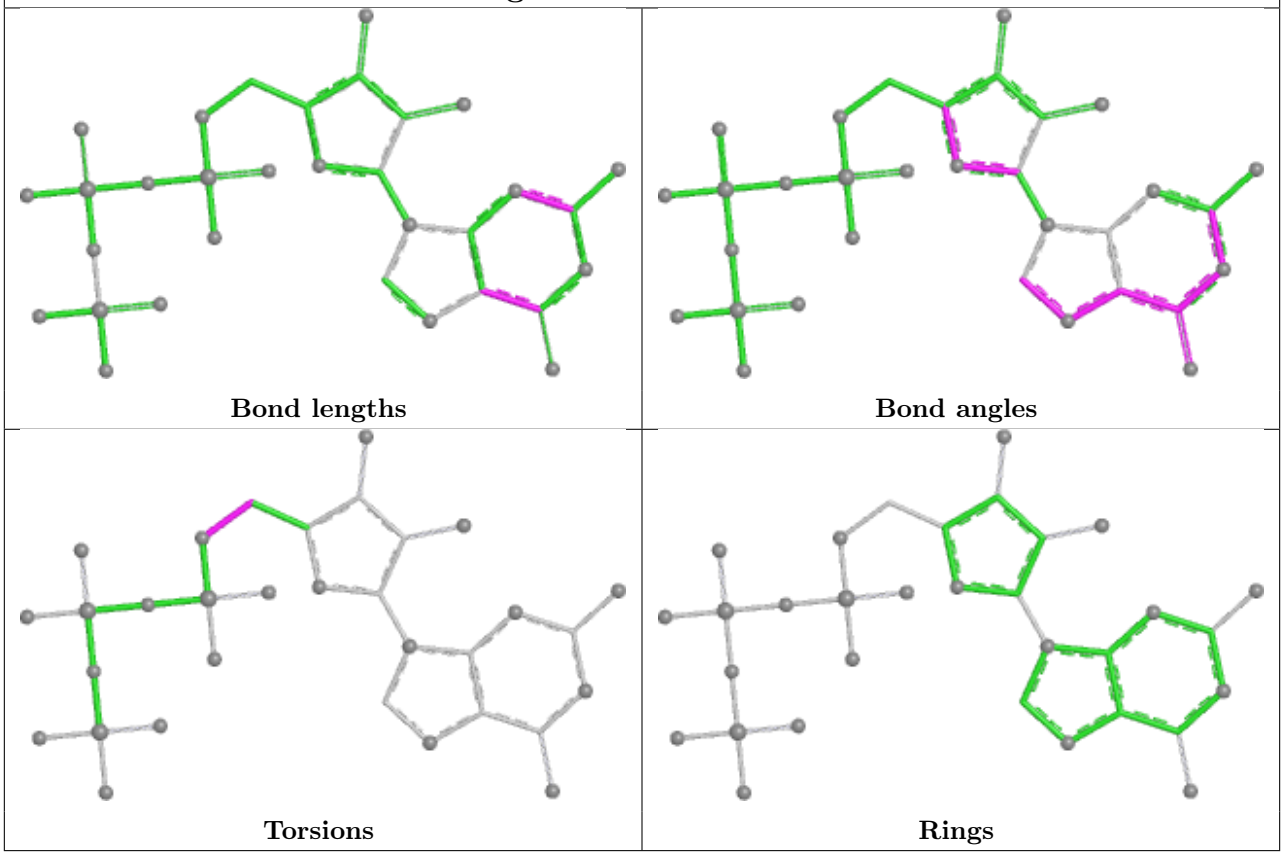

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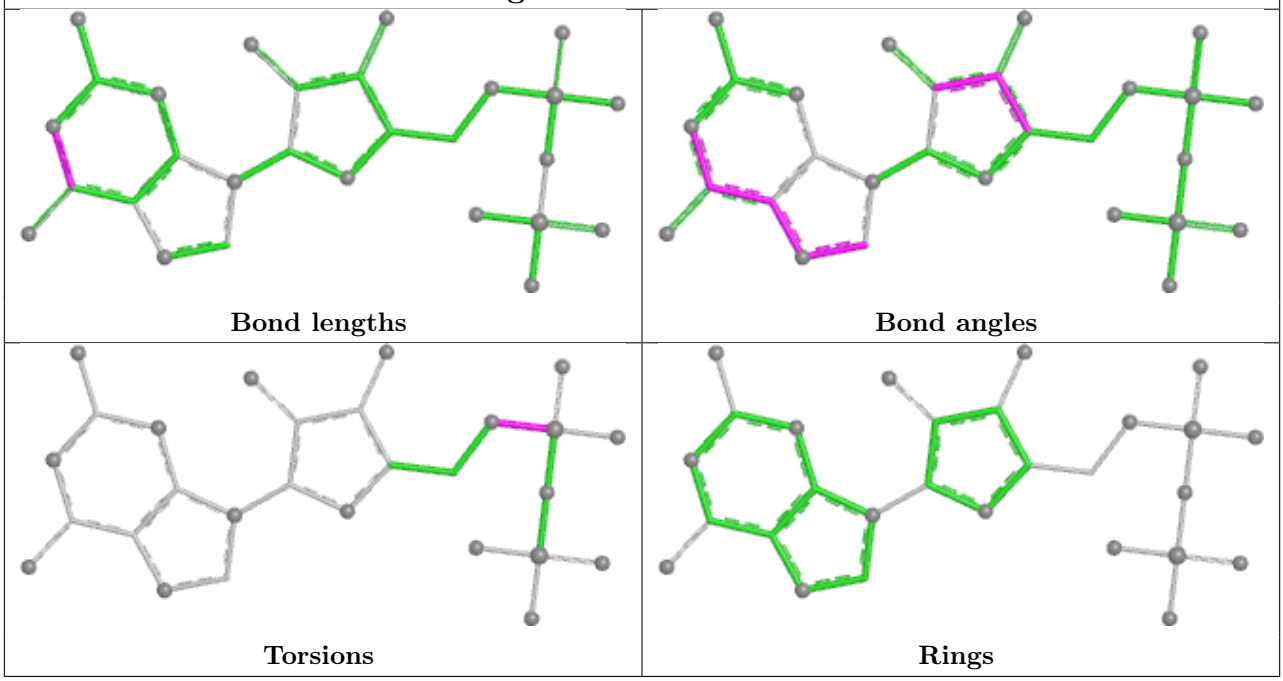

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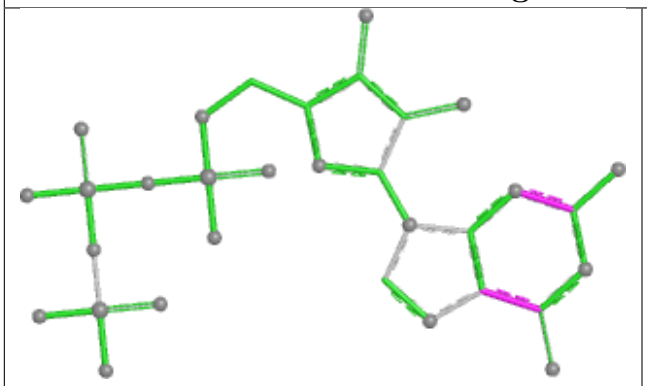
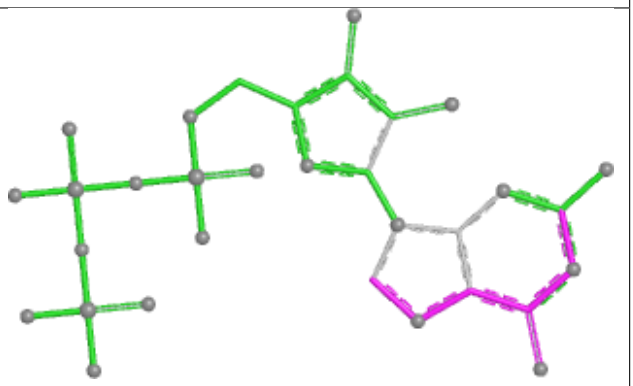
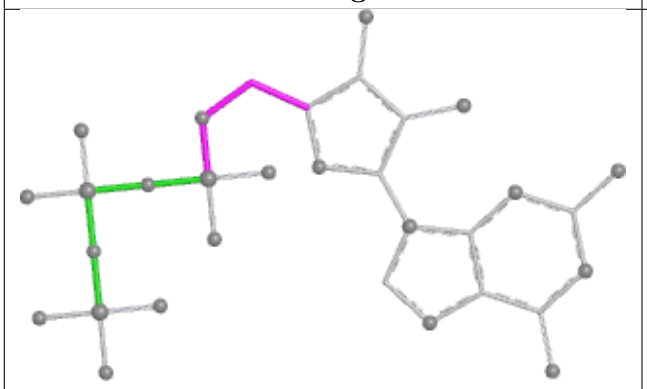


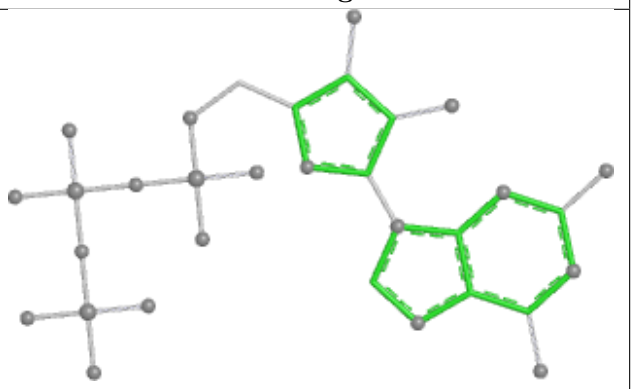
Bond lengths



Bond angles

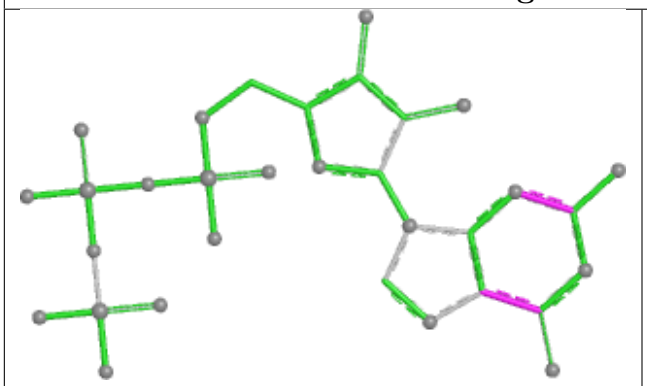


Torsions



Rings

Ligand GTP CI 501



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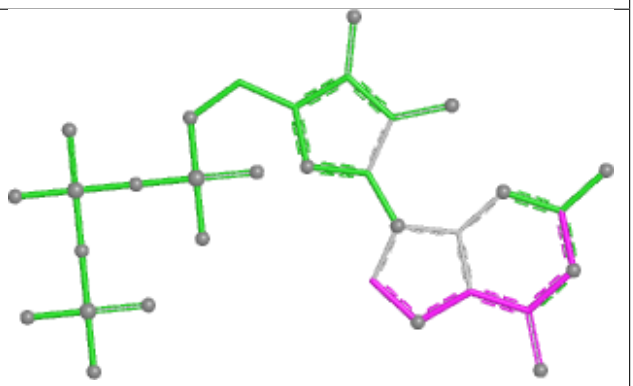

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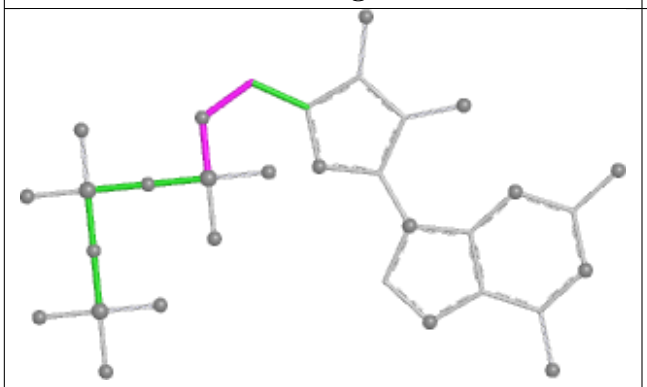

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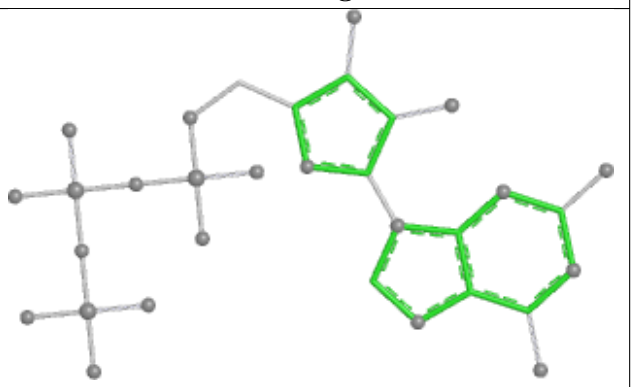
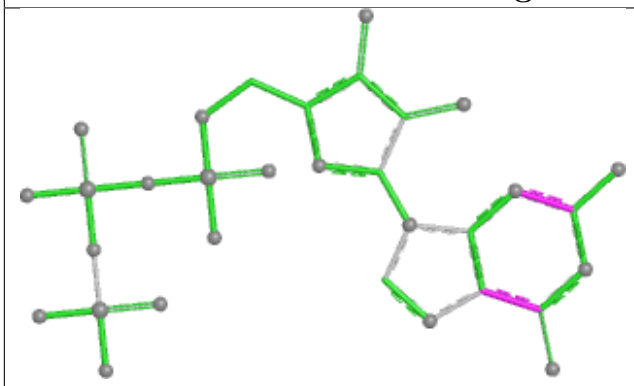


Rings

Ligand GTP JB 501



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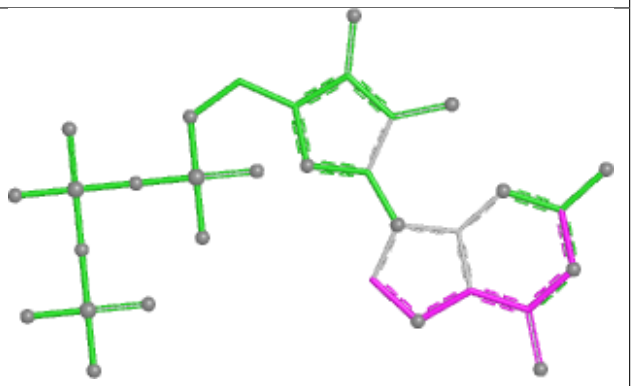
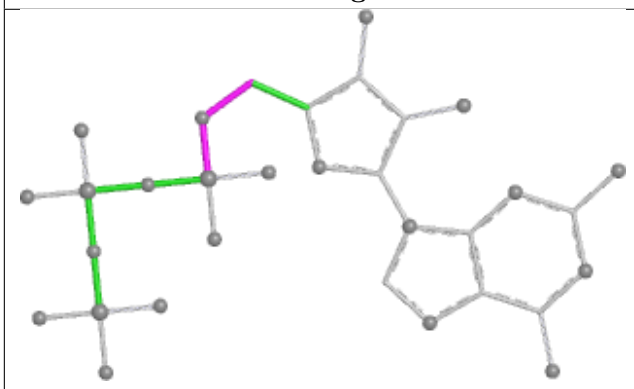


Bond angles



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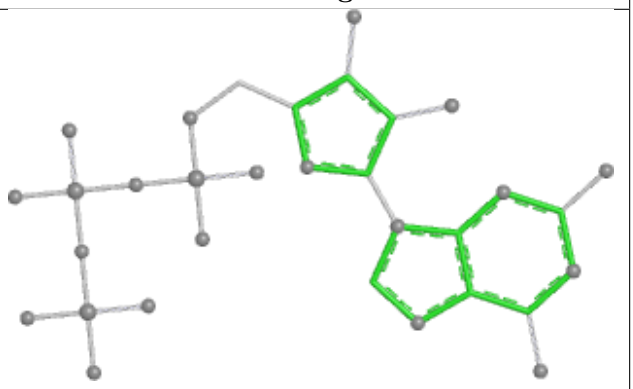

Rings

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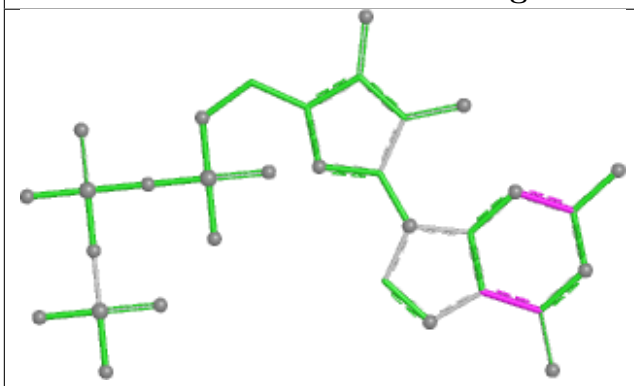

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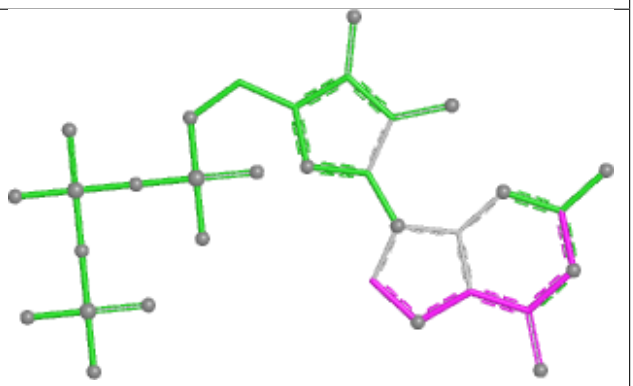

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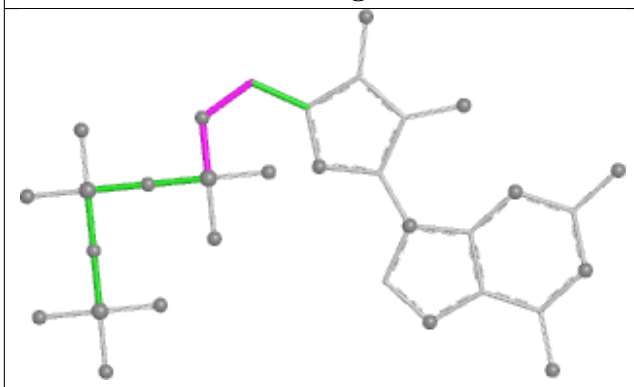

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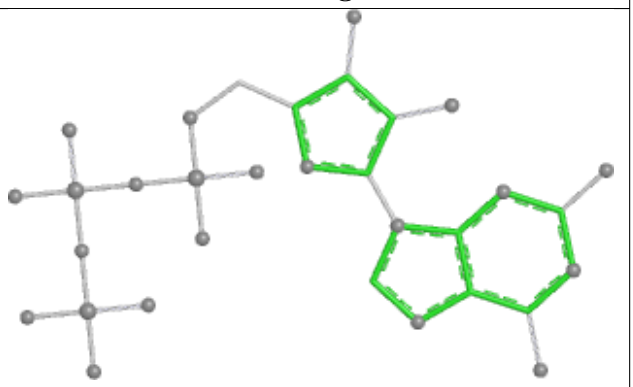
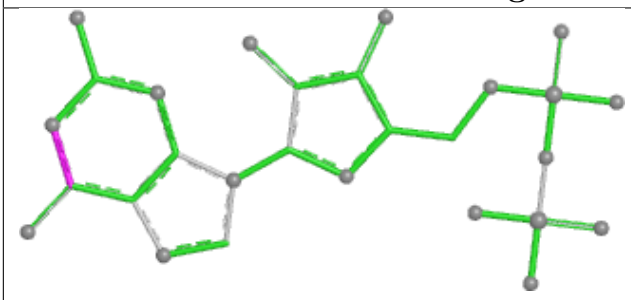
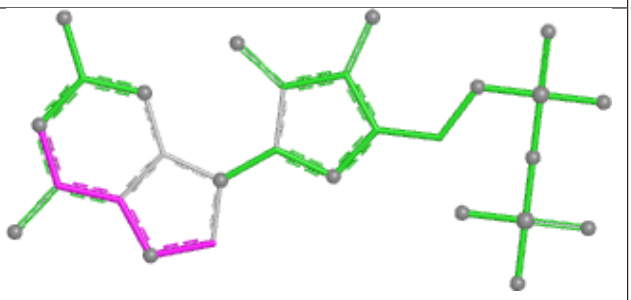
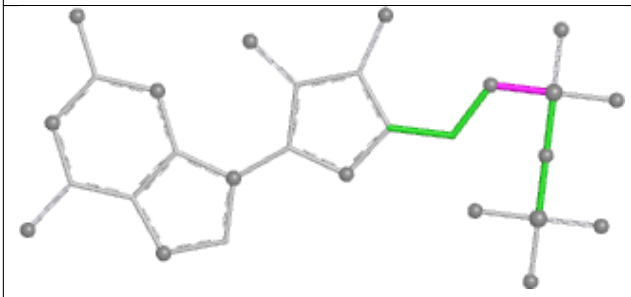
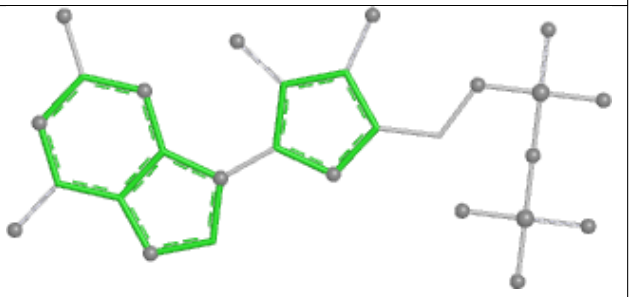
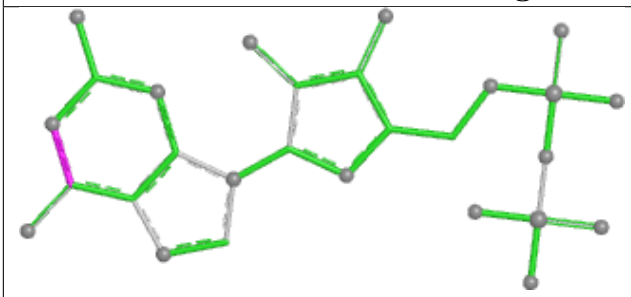
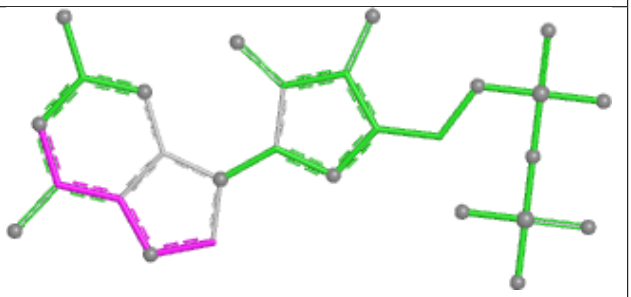
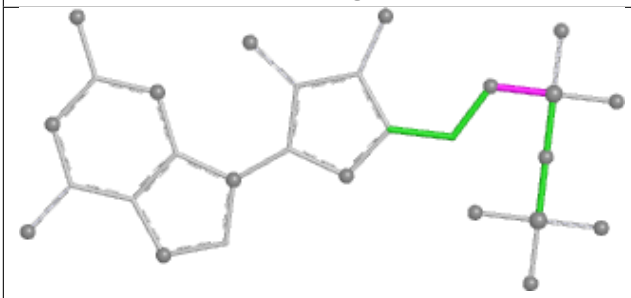
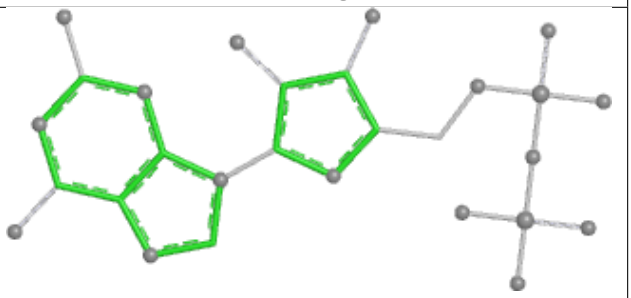
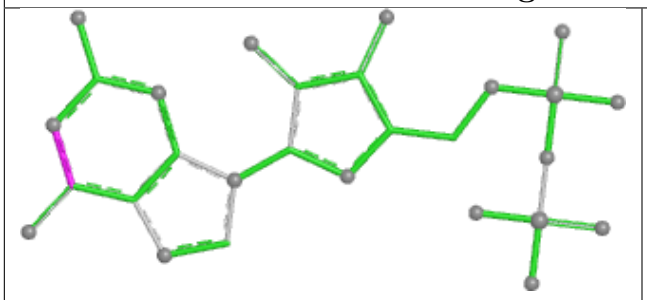


Rings

Ligand GDP AC 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP FJ 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP IL 501



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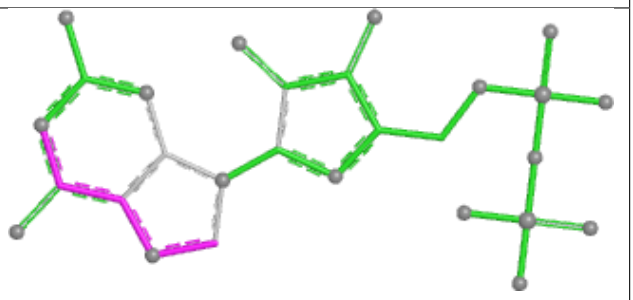
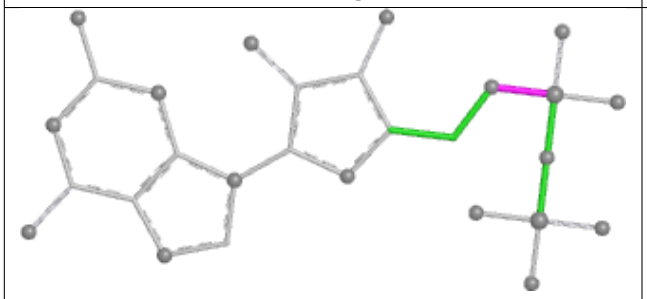


Bond angles



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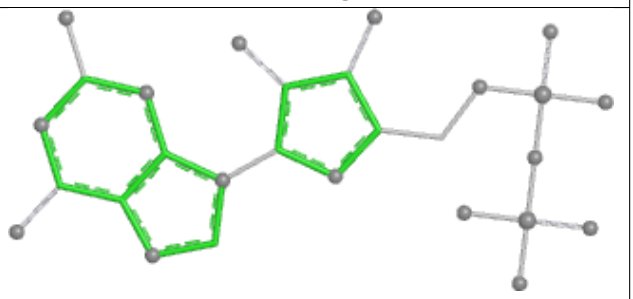
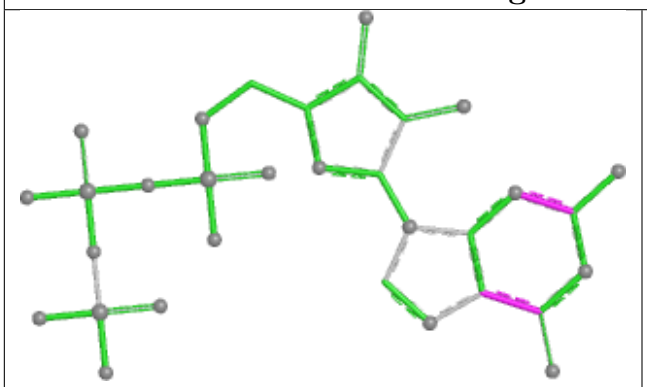


Rings

Ligand GTP DG 501



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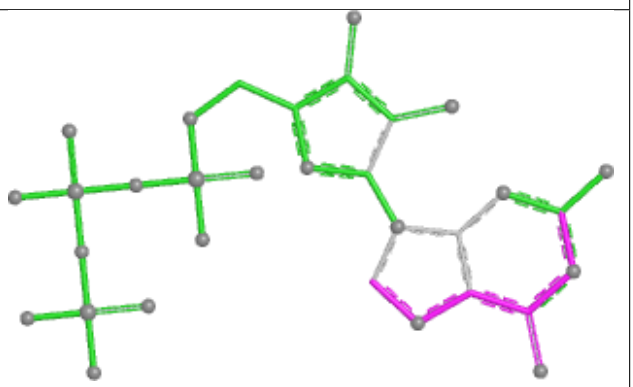
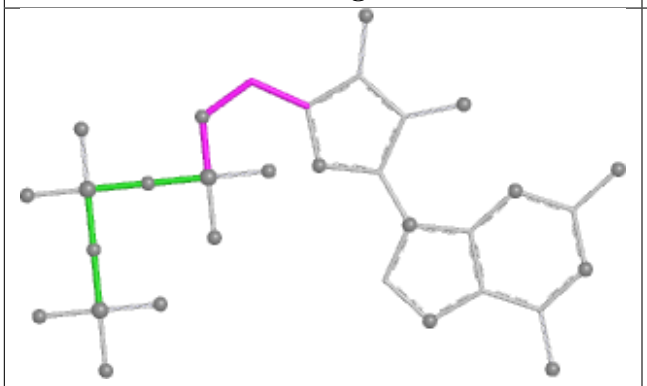


Bond angles



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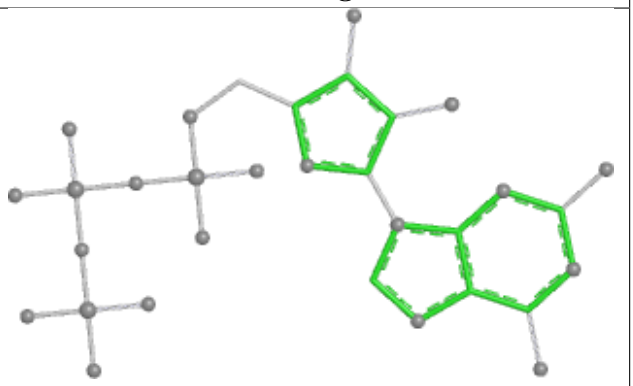
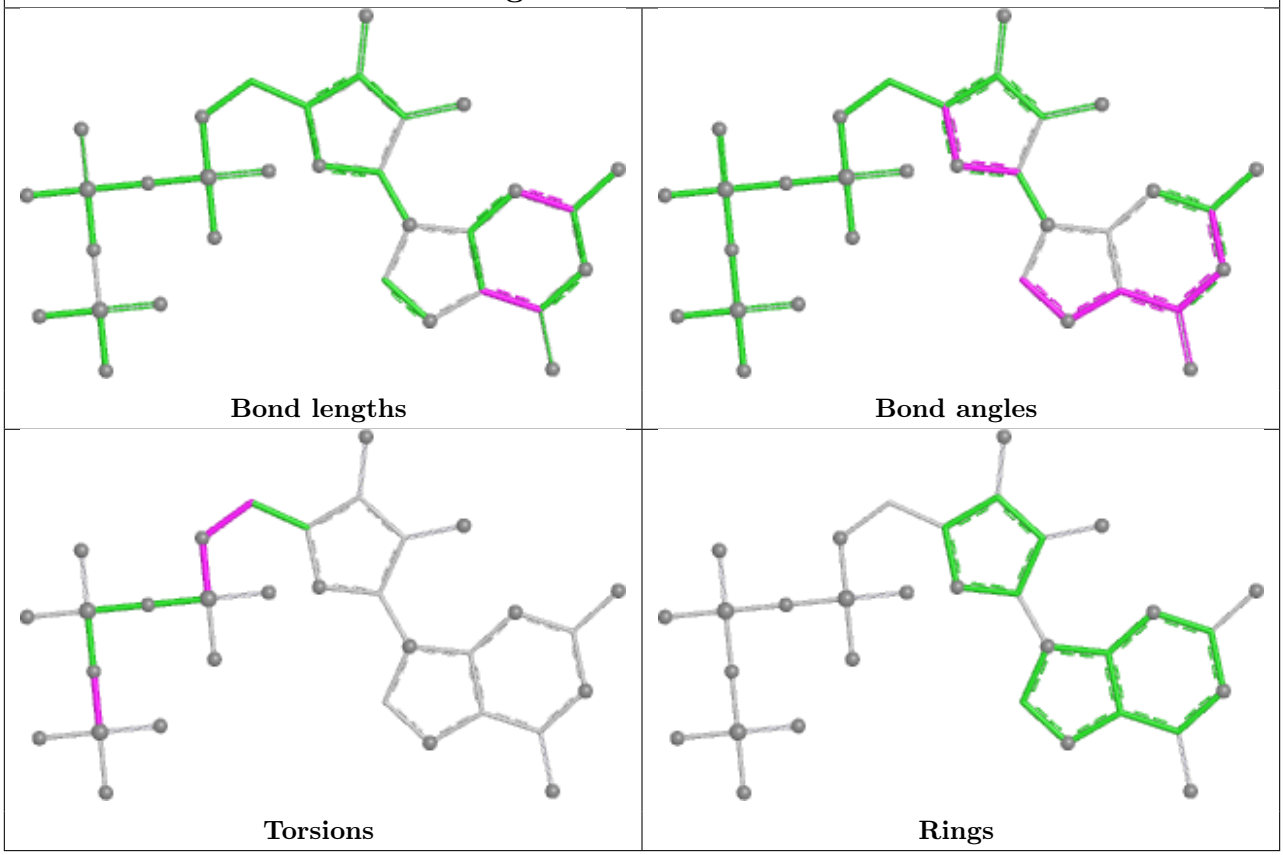
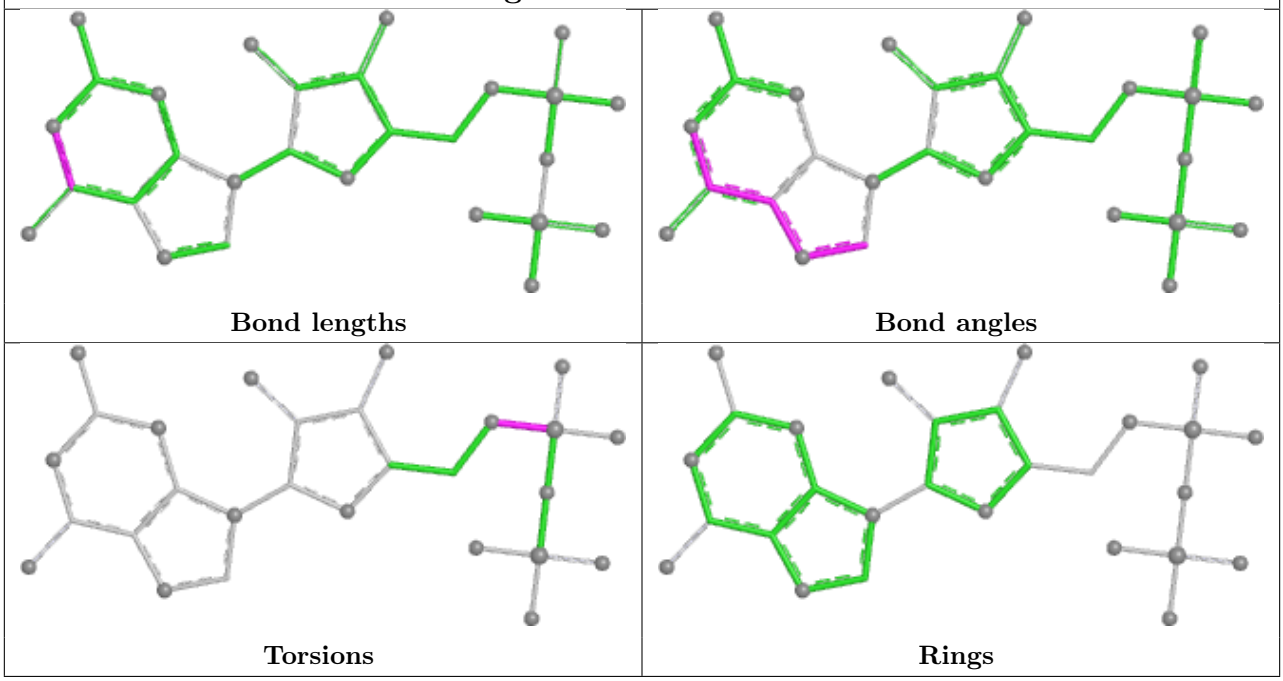


Rings

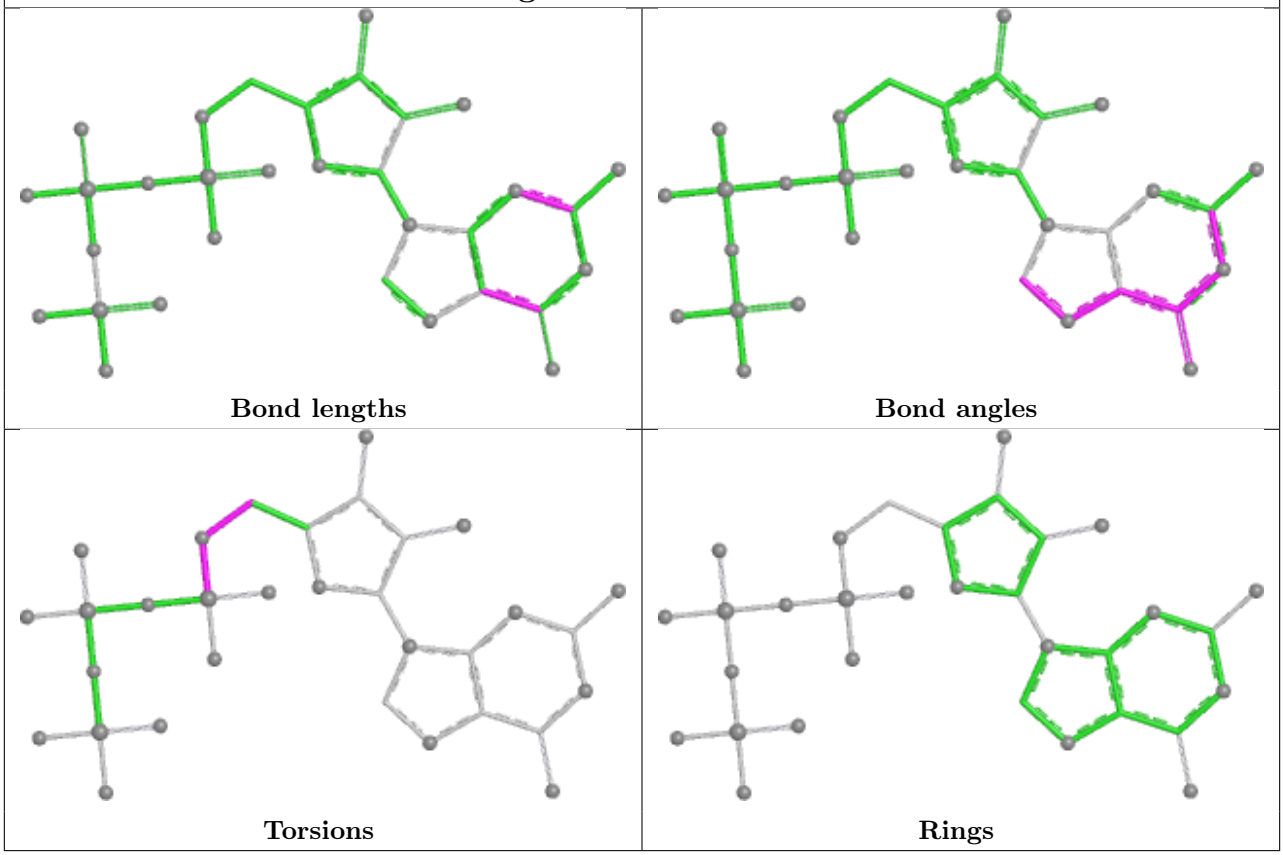
Ligand GTP MA 501



Ligand GDP MH 501



Ligand GTP EI 501



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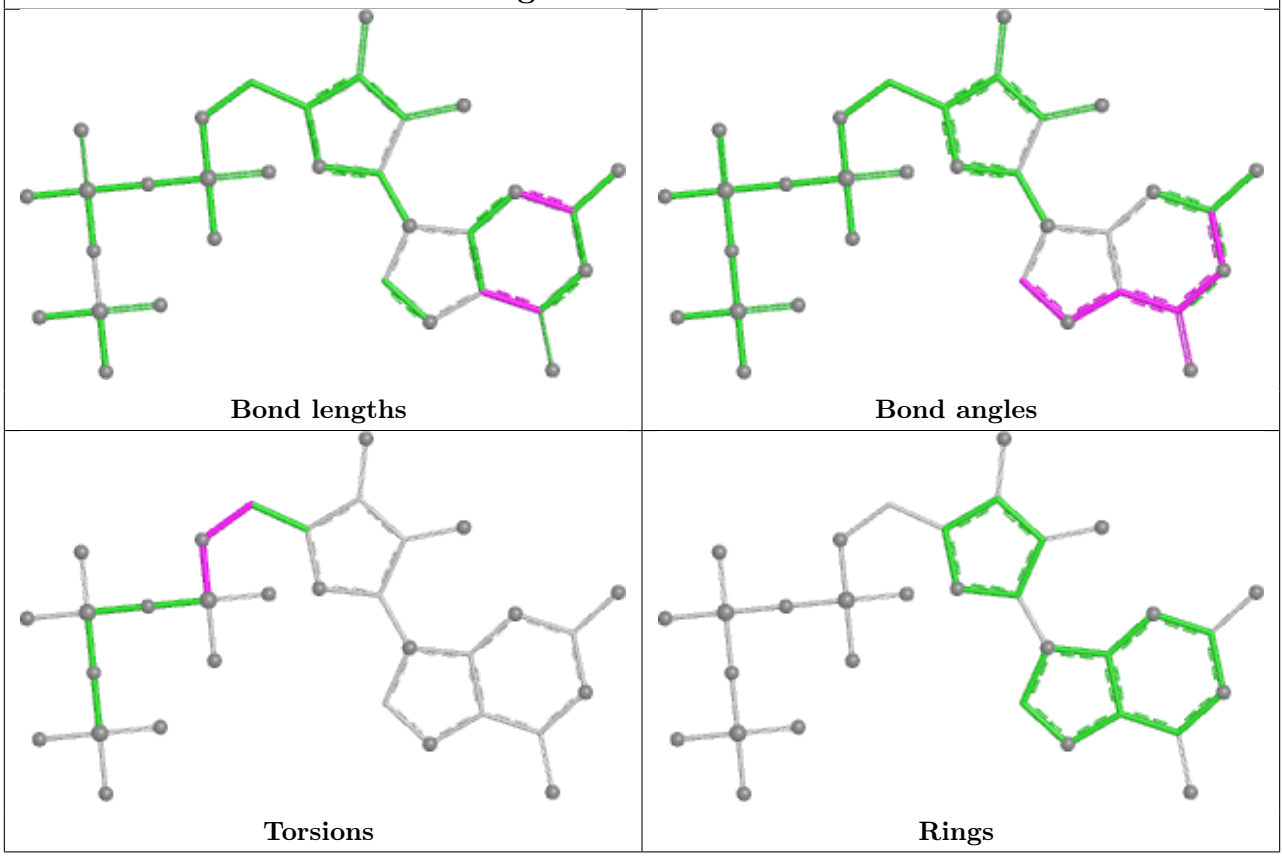

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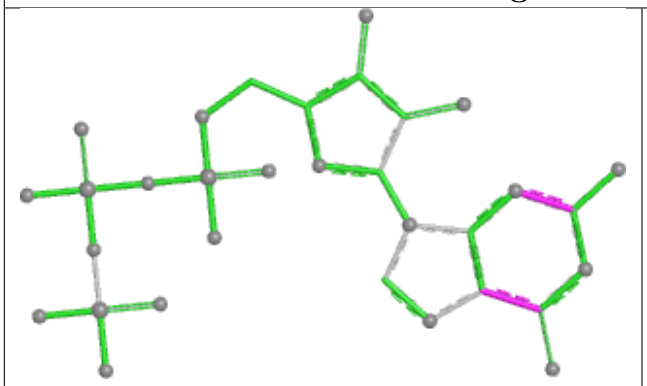
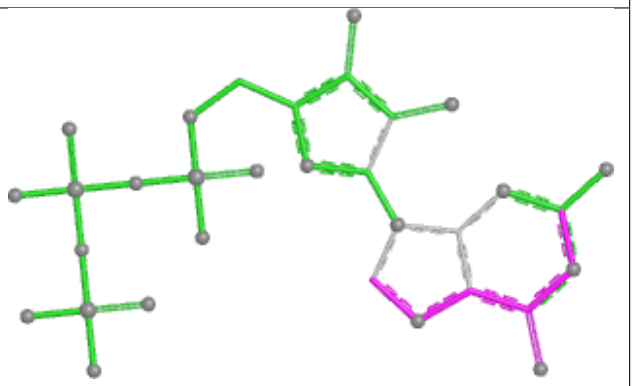
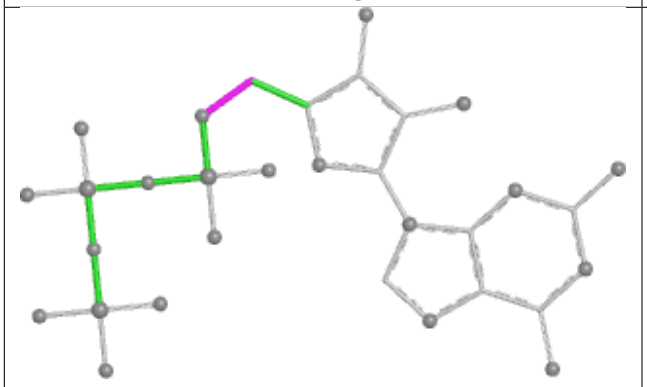


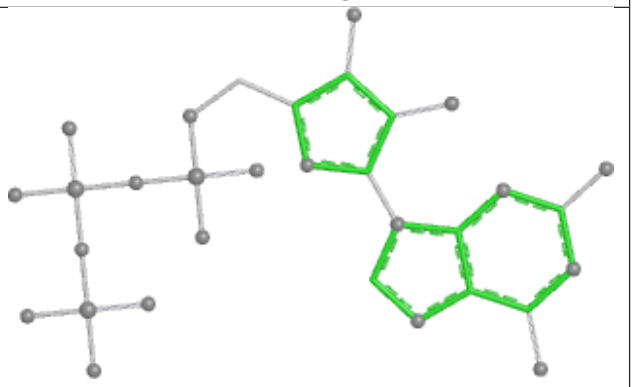
Bond lengths



Bond angles

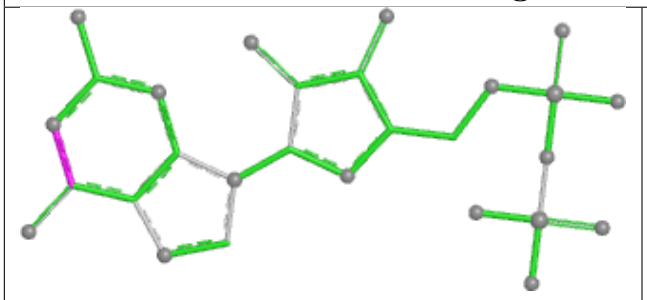


Torsions



Rings

Ligand GDP FC 501



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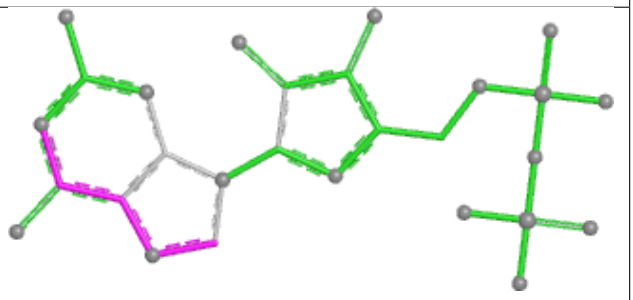

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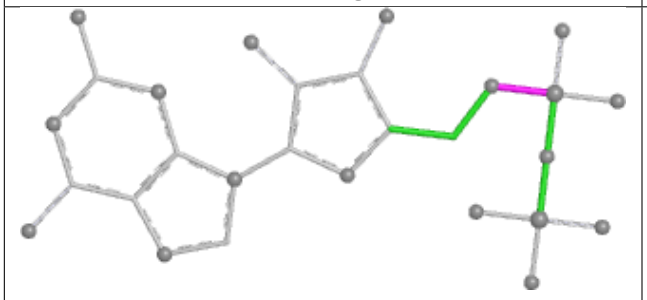

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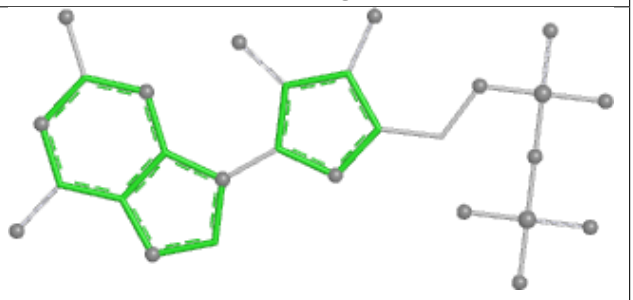

Rings

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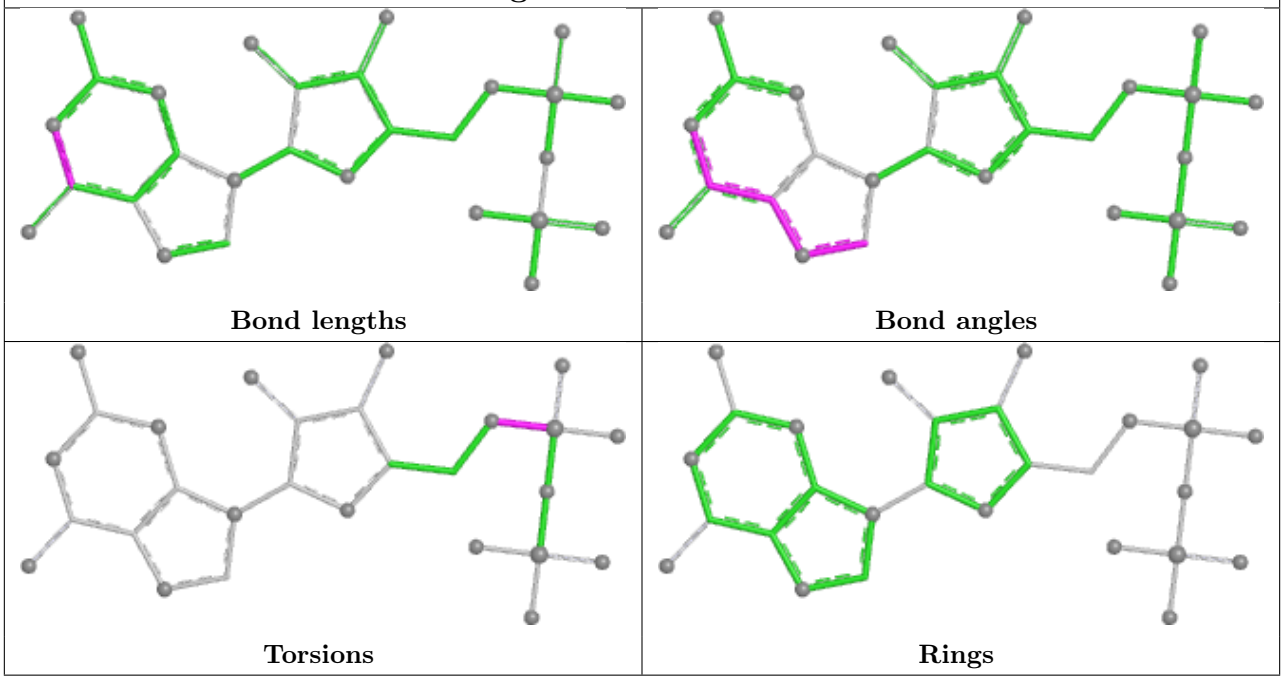

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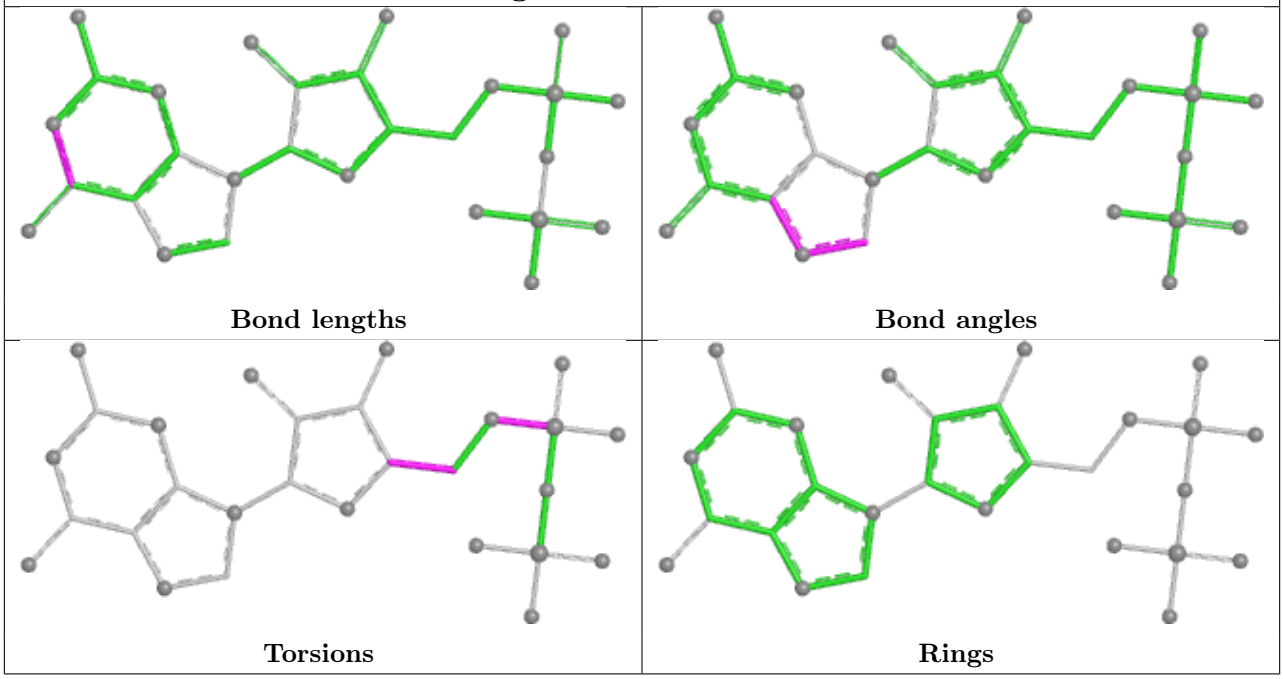

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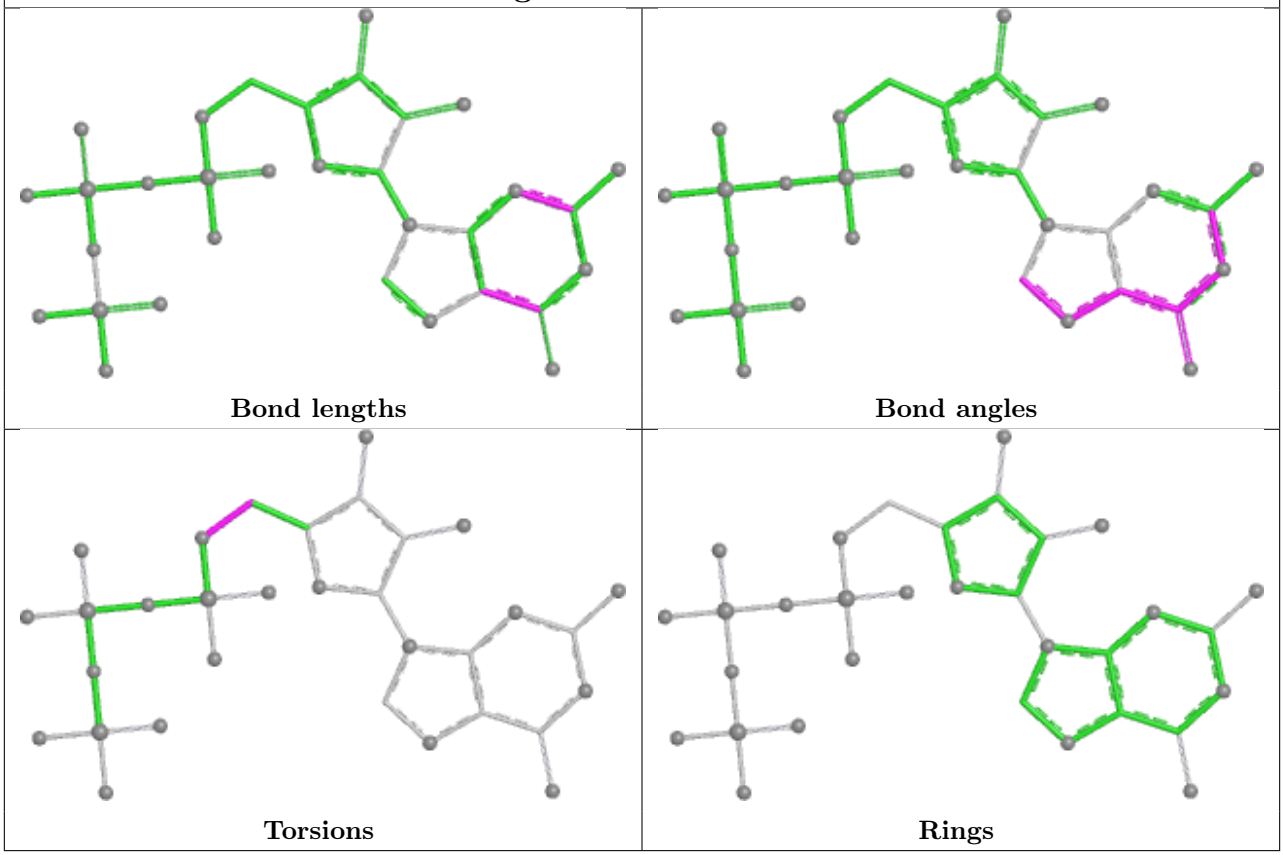

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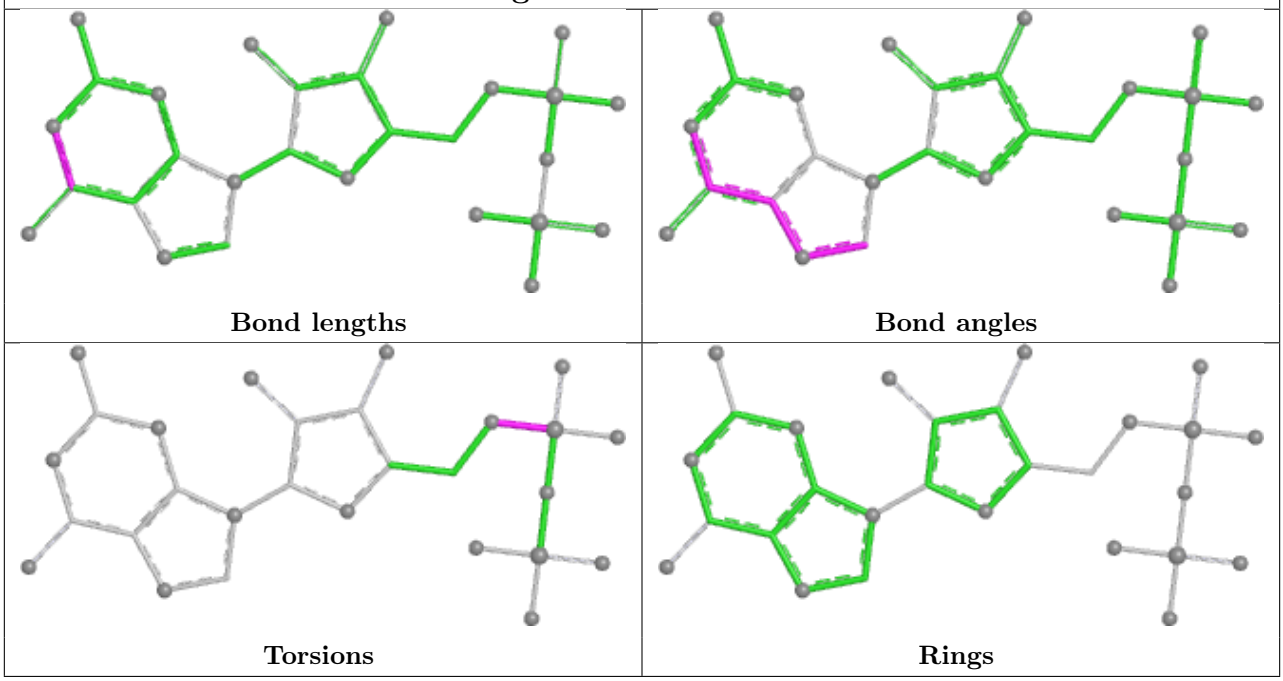

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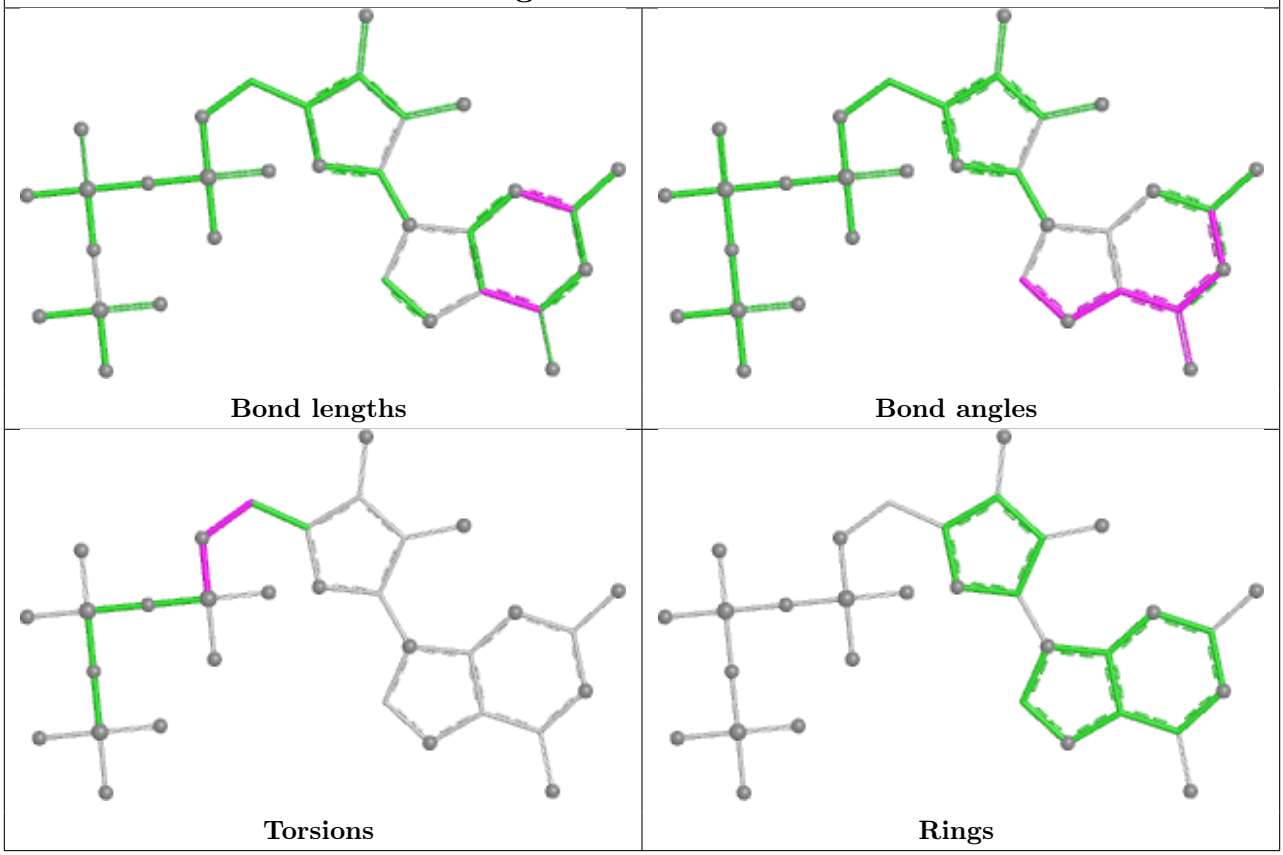

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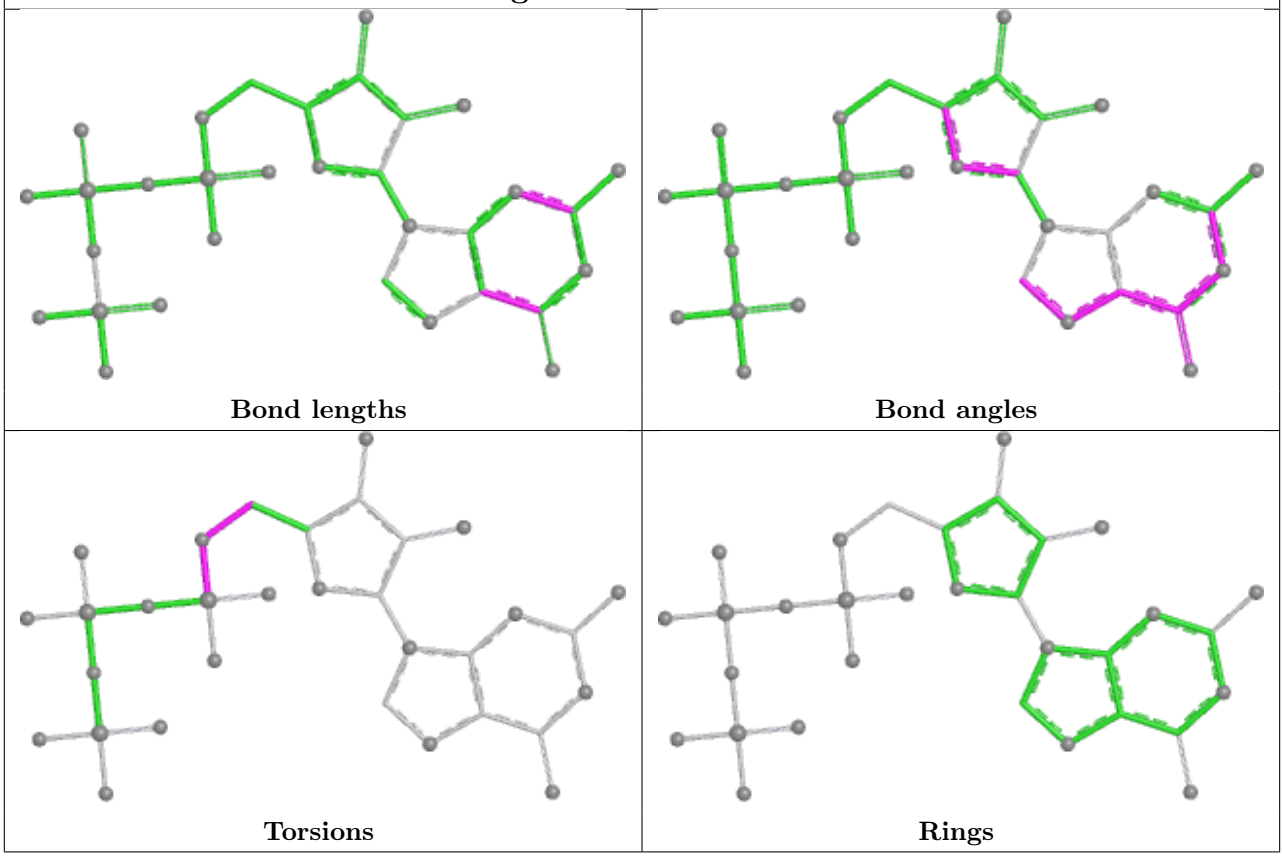

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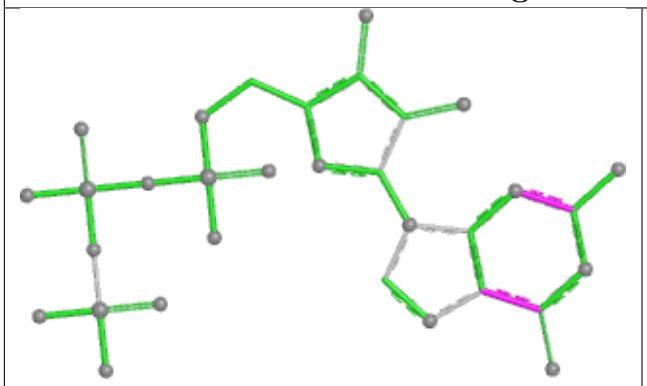

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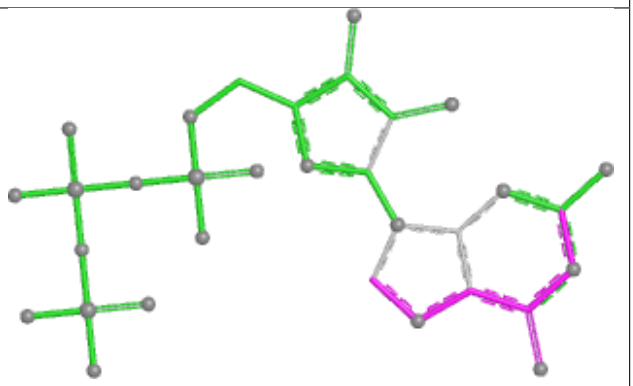
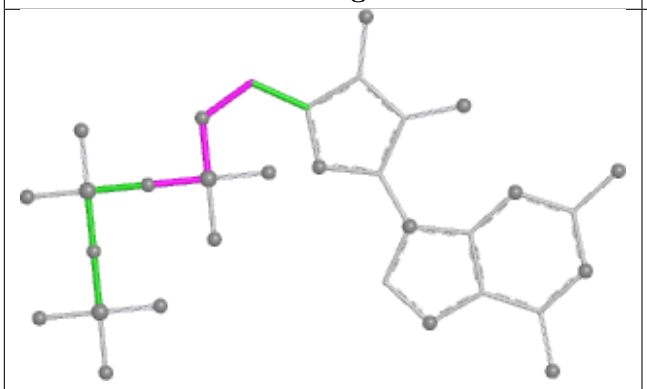
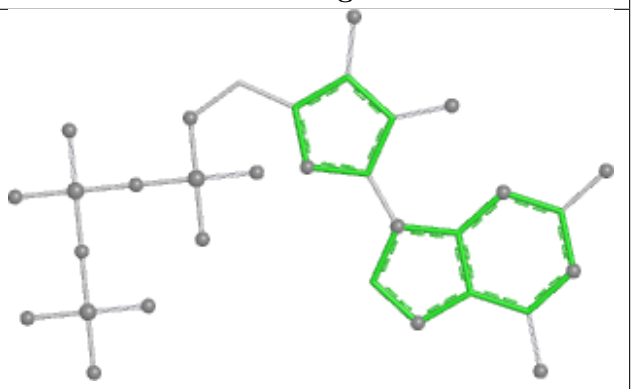


Bond angles

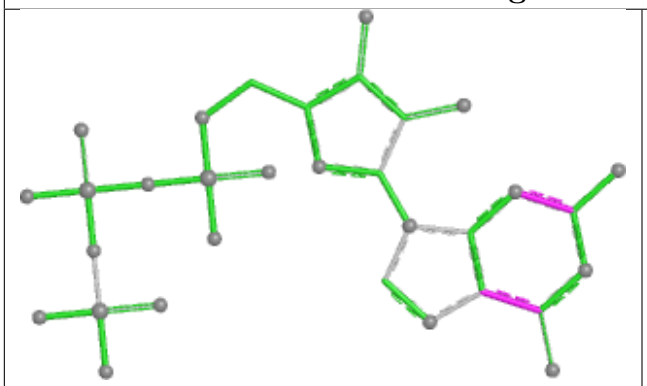


Torsions



Rings

Ligand GTP HG 501



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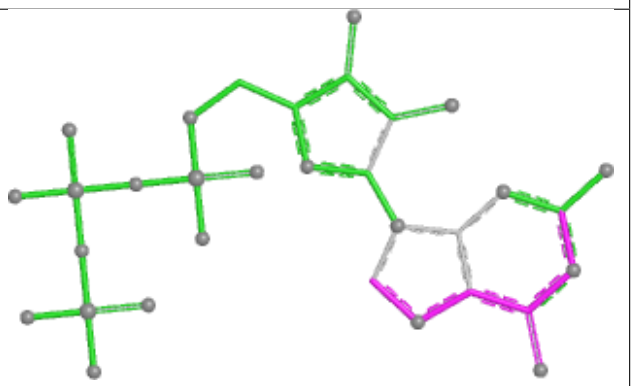

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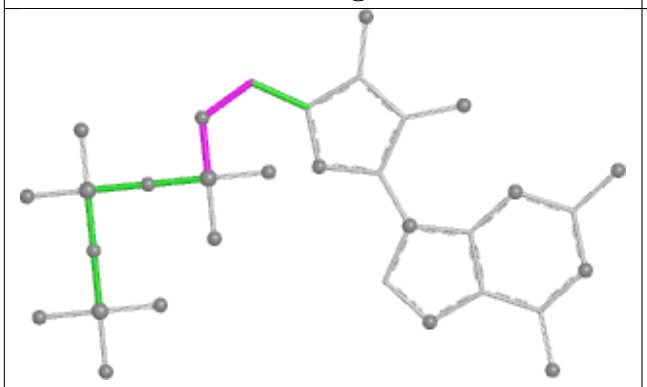

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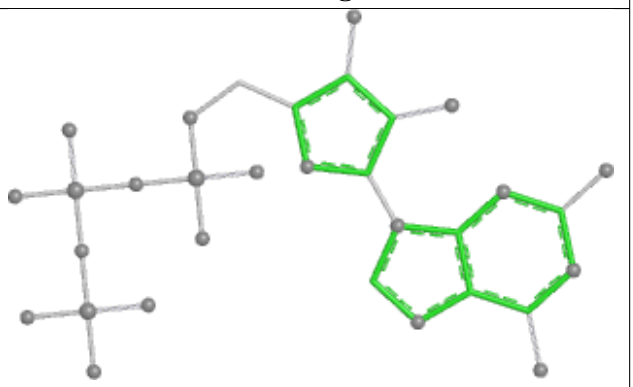
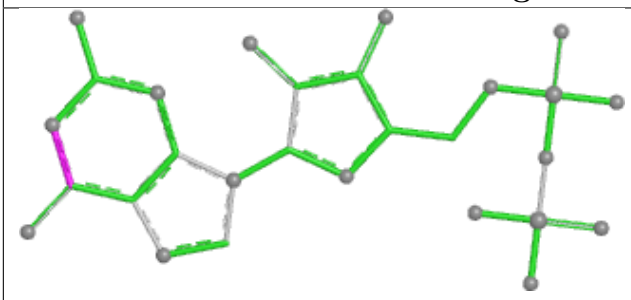


Rings

Ligand GDP PJ 501



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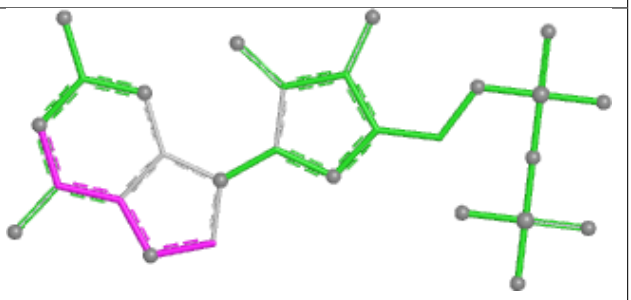

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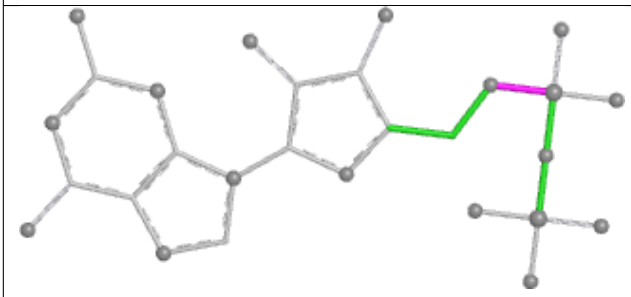

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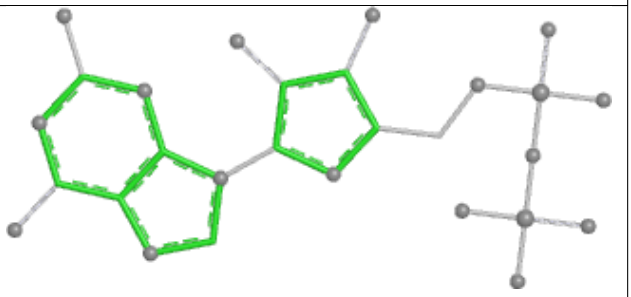

Rings

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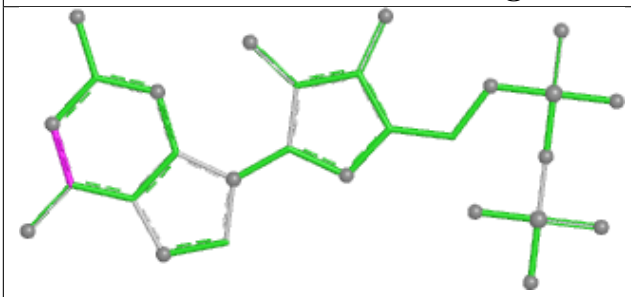

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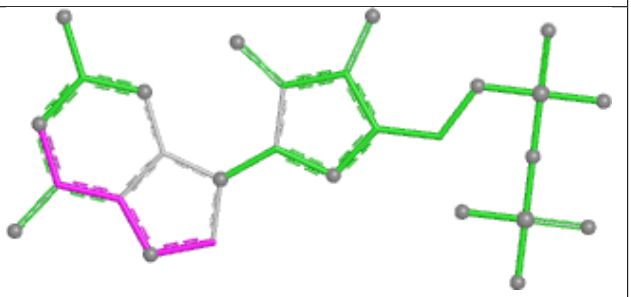

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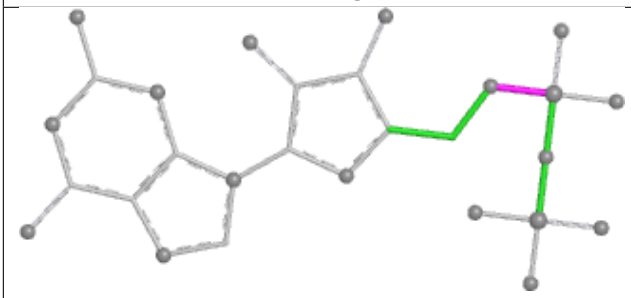

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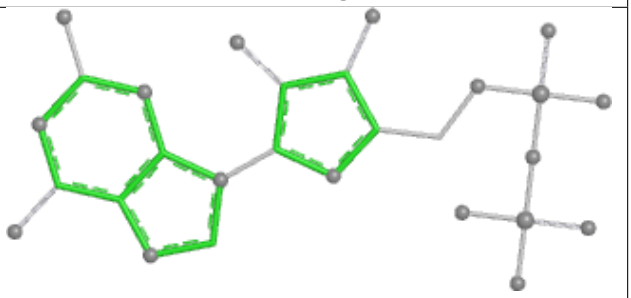
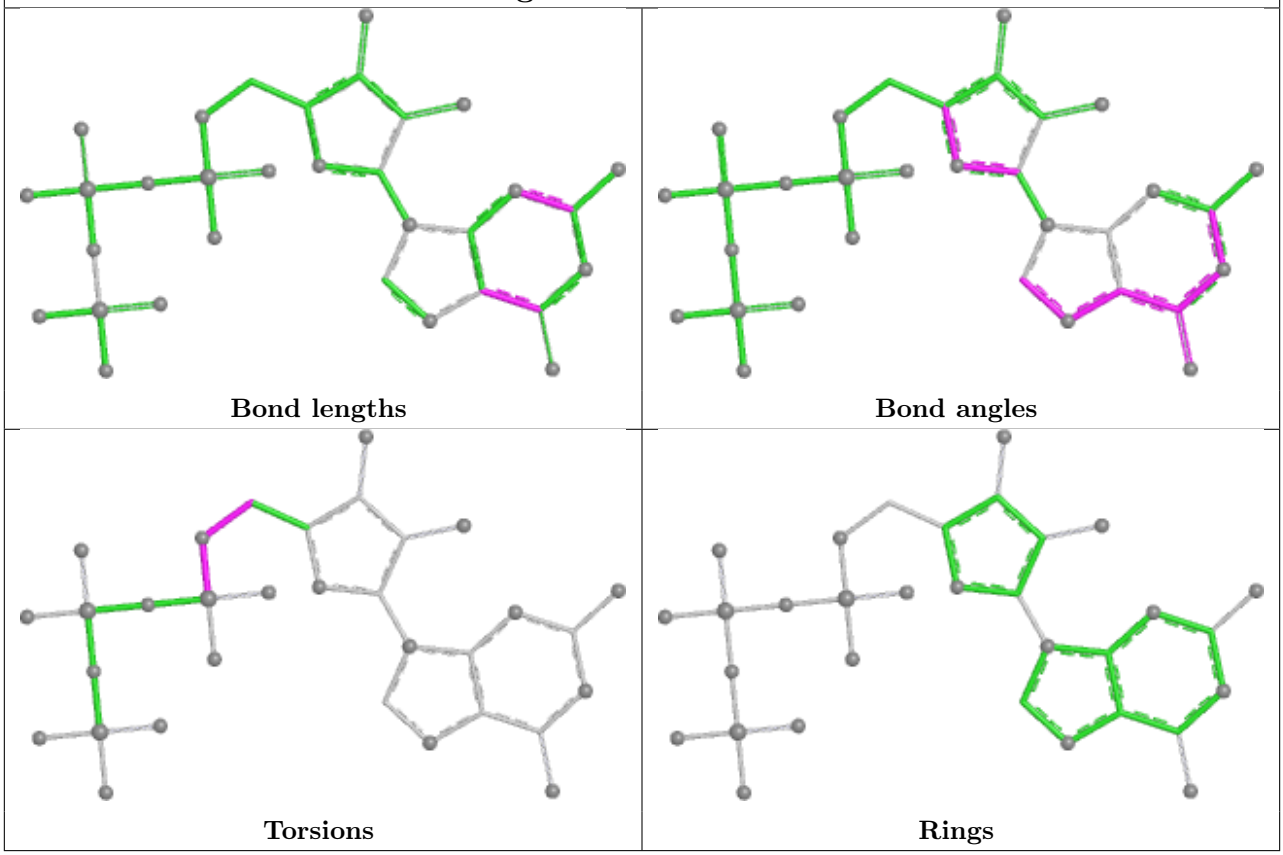
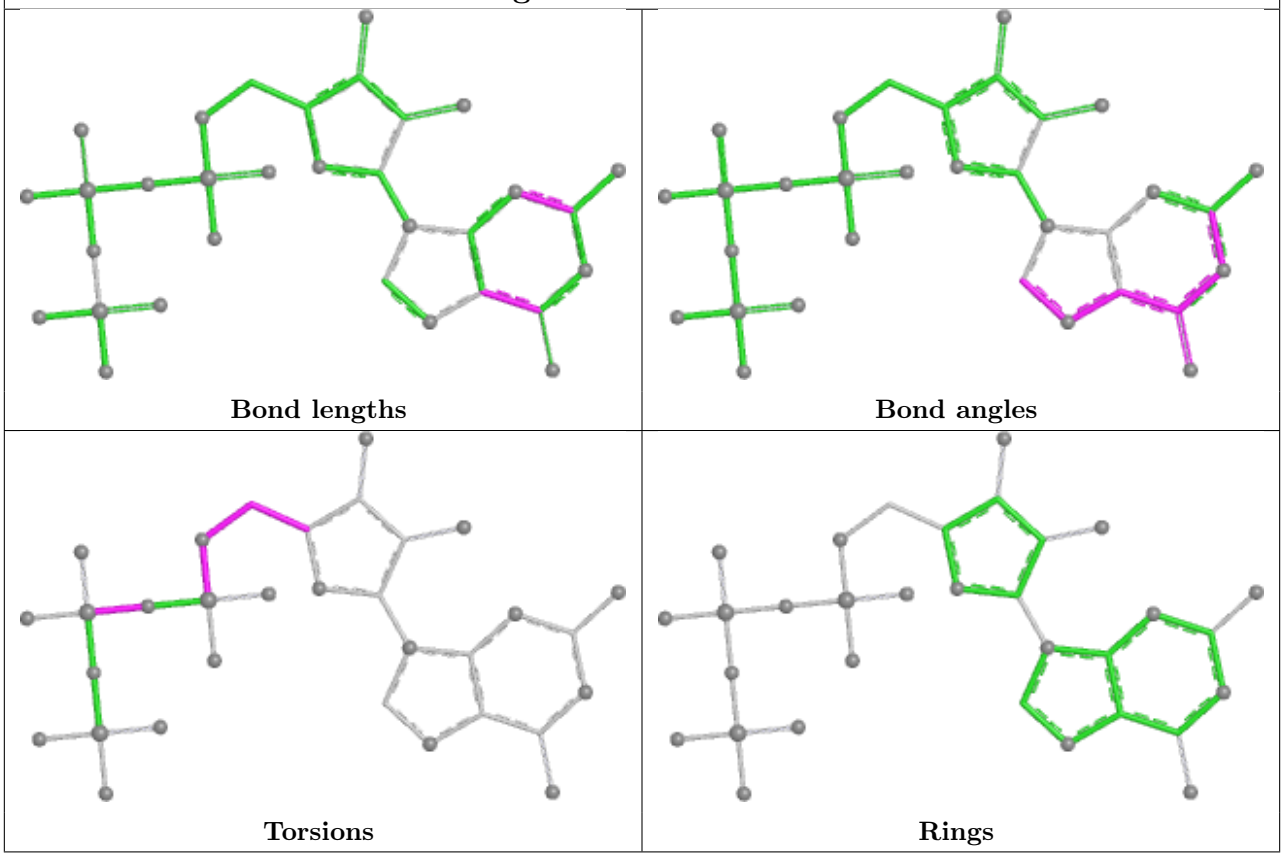


Rings

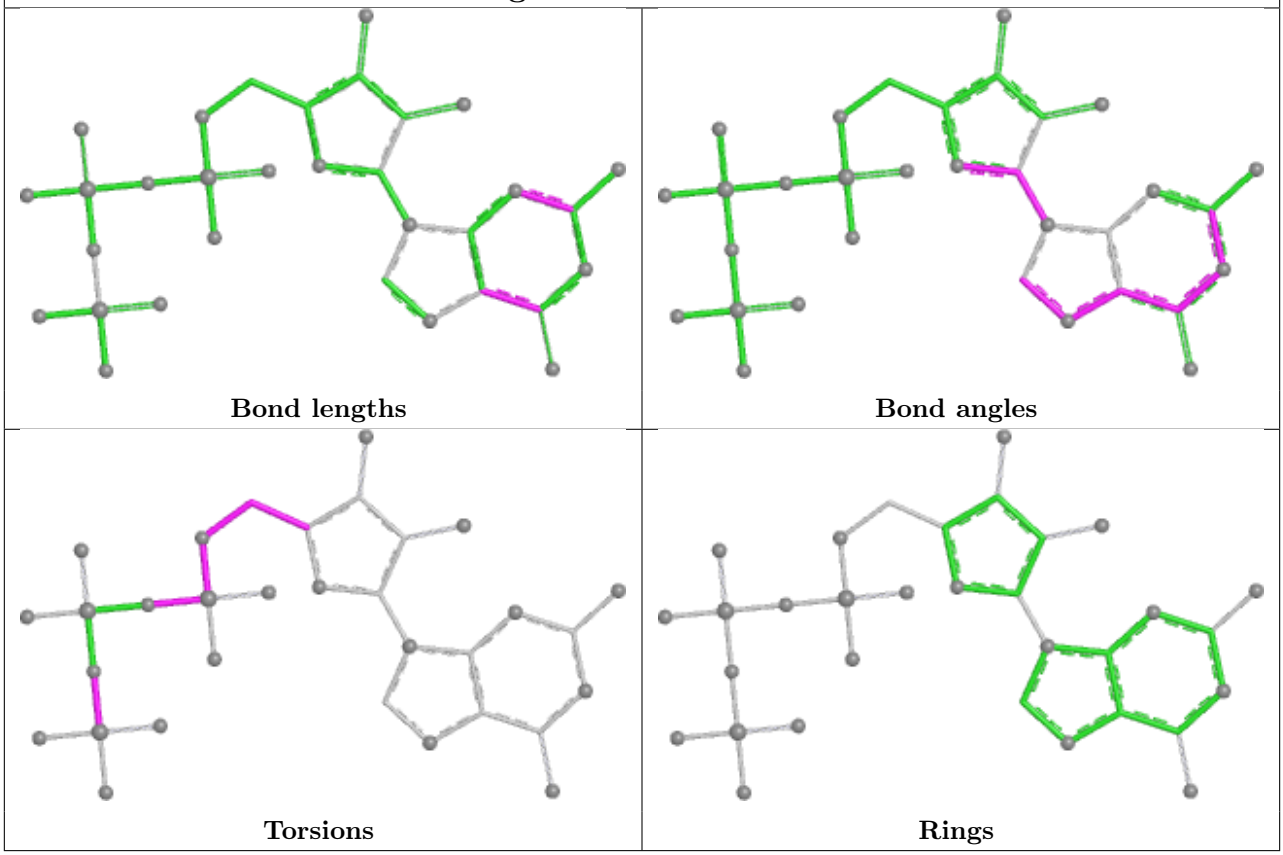
Ligand GTP AI 501



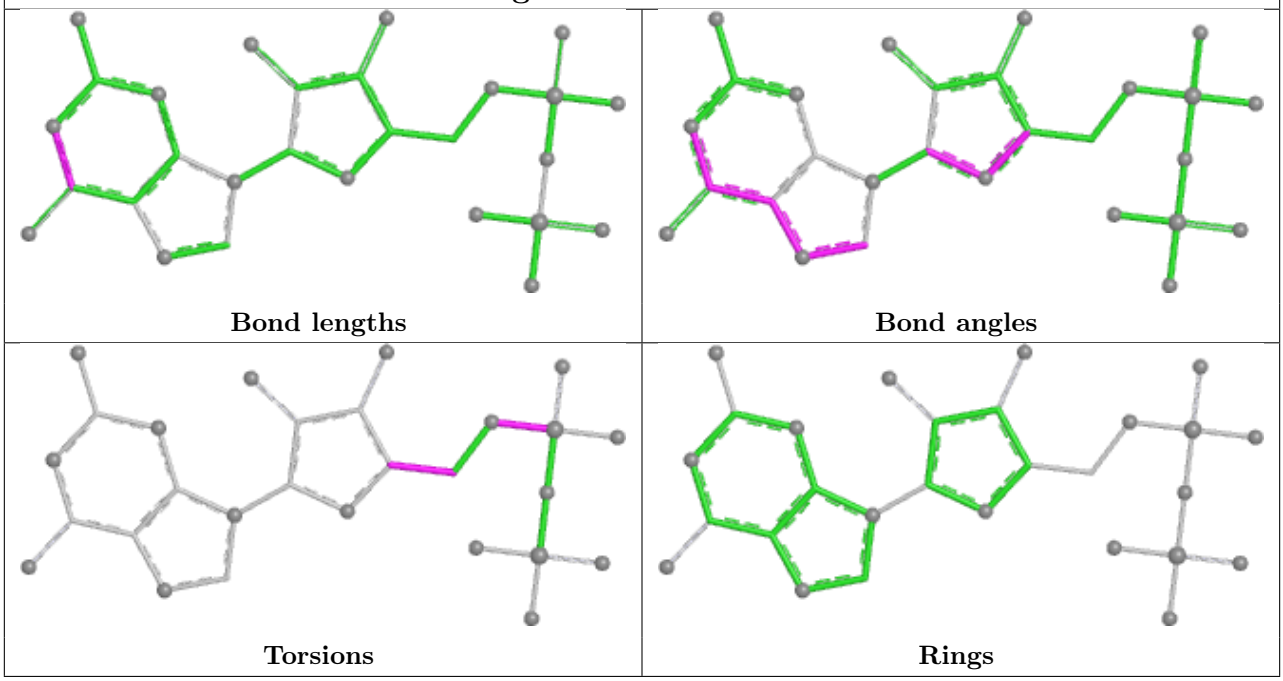
Ligand GTP IM 501



Ligand GTP HK 501



Ligand GDP DJ 501



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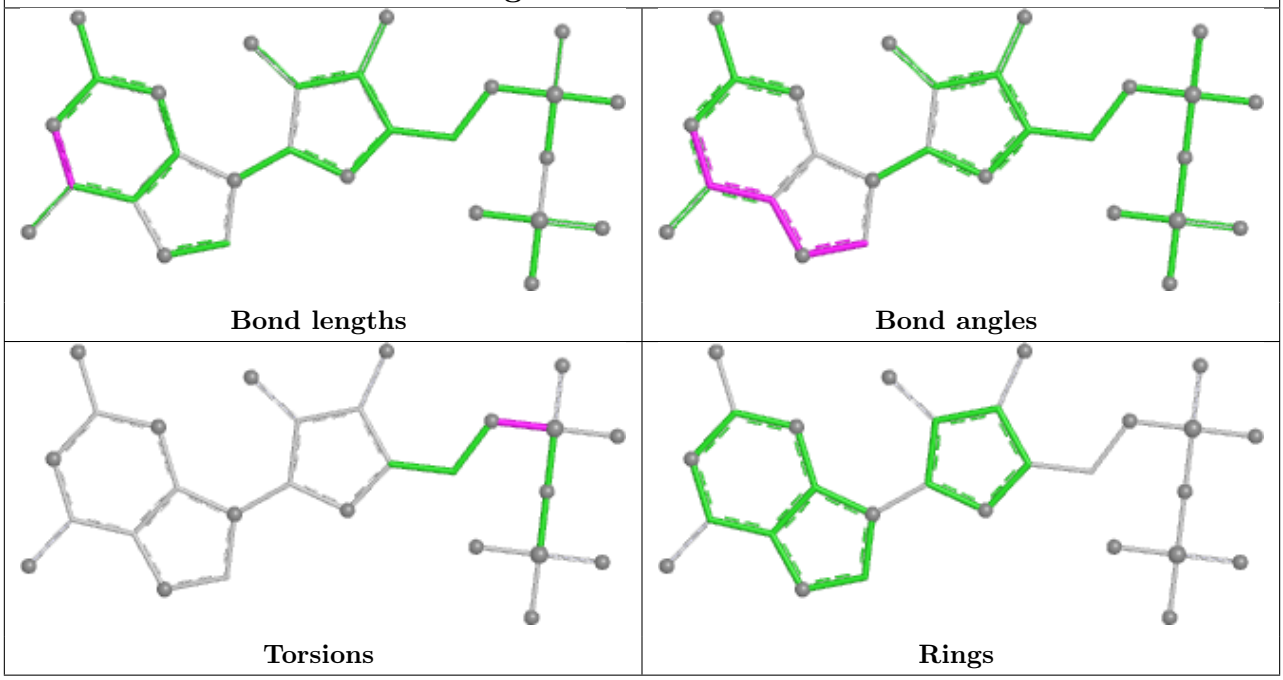

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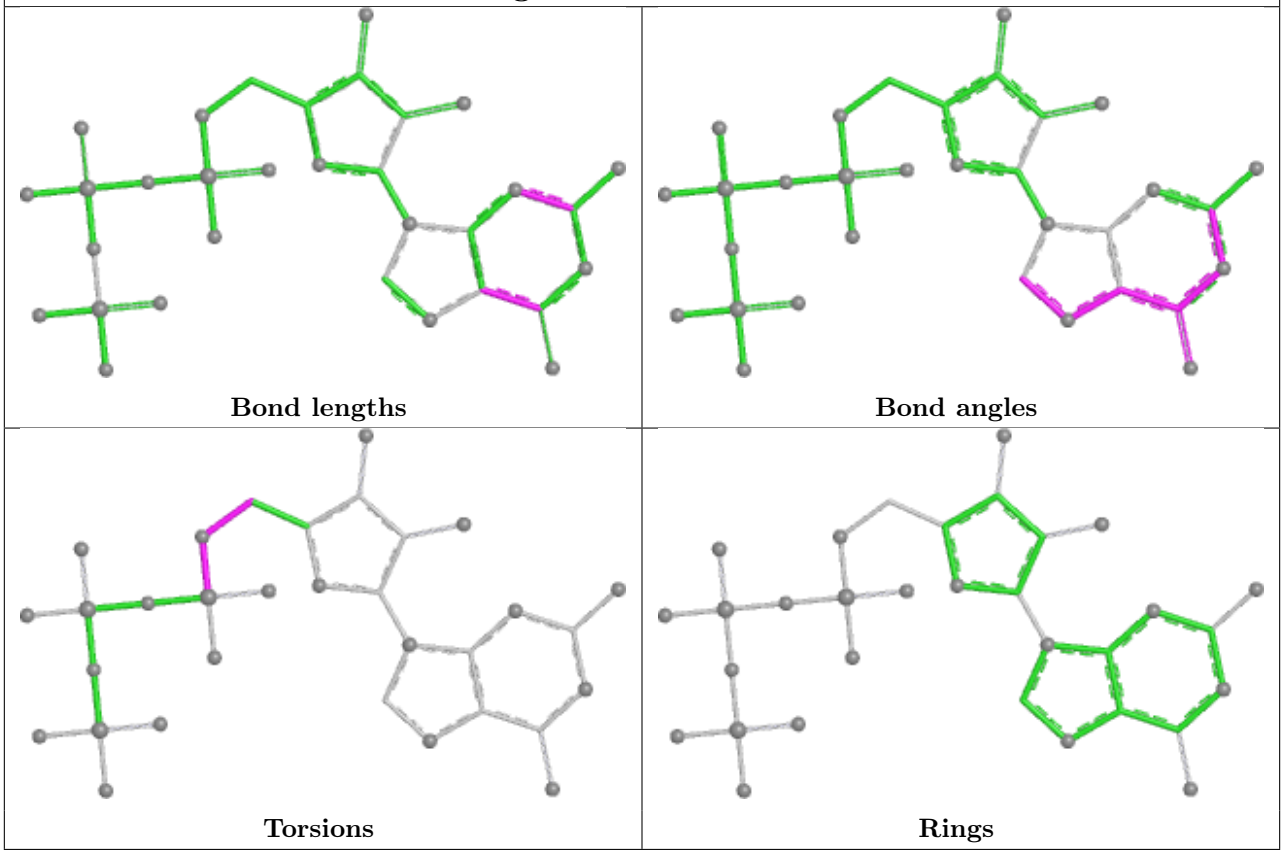
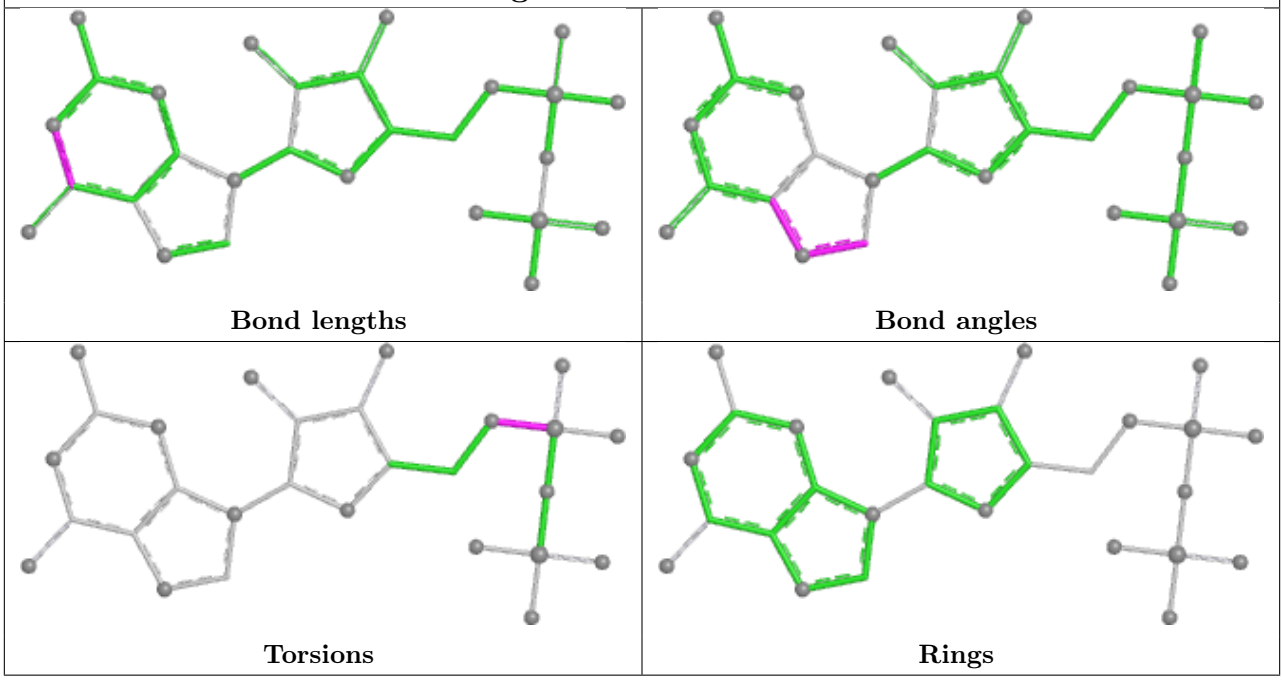


Ligand GDP DL 501



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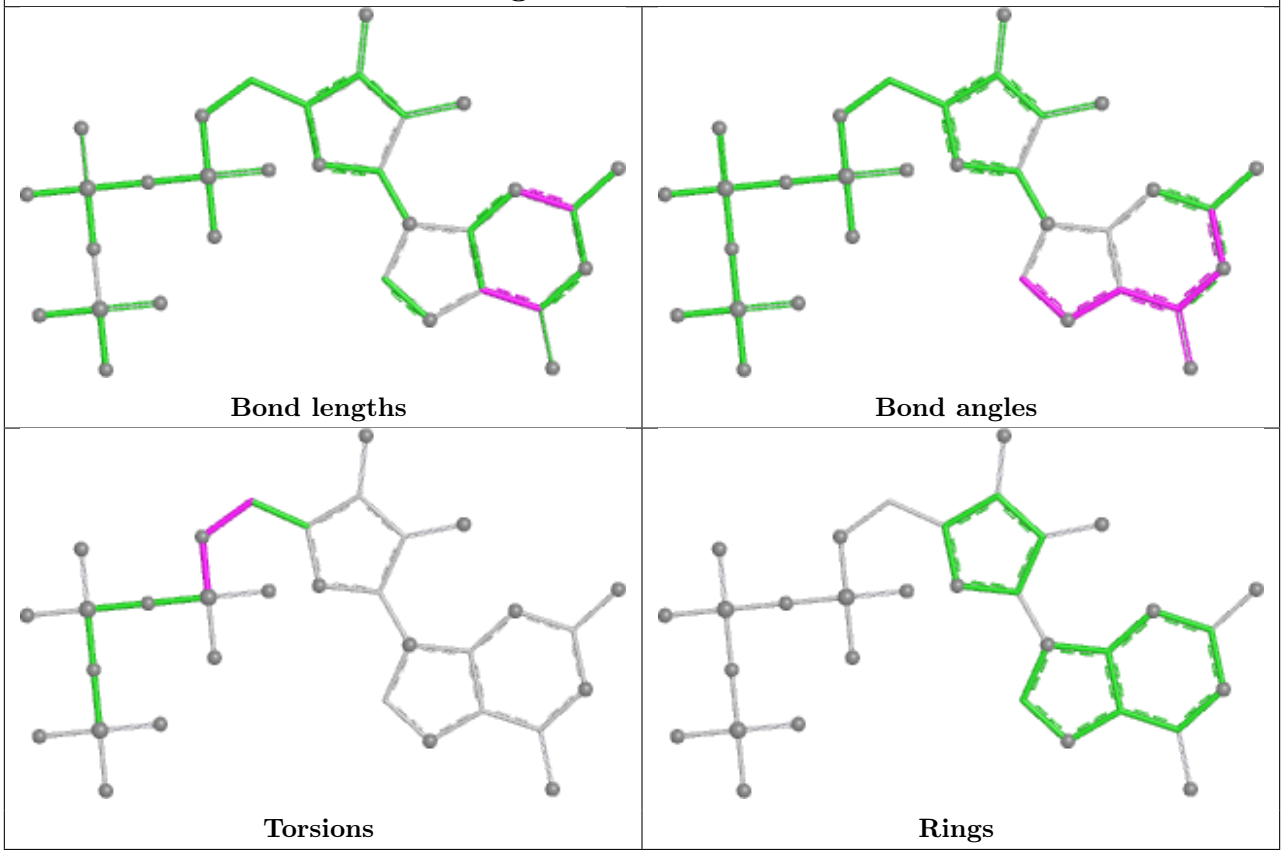

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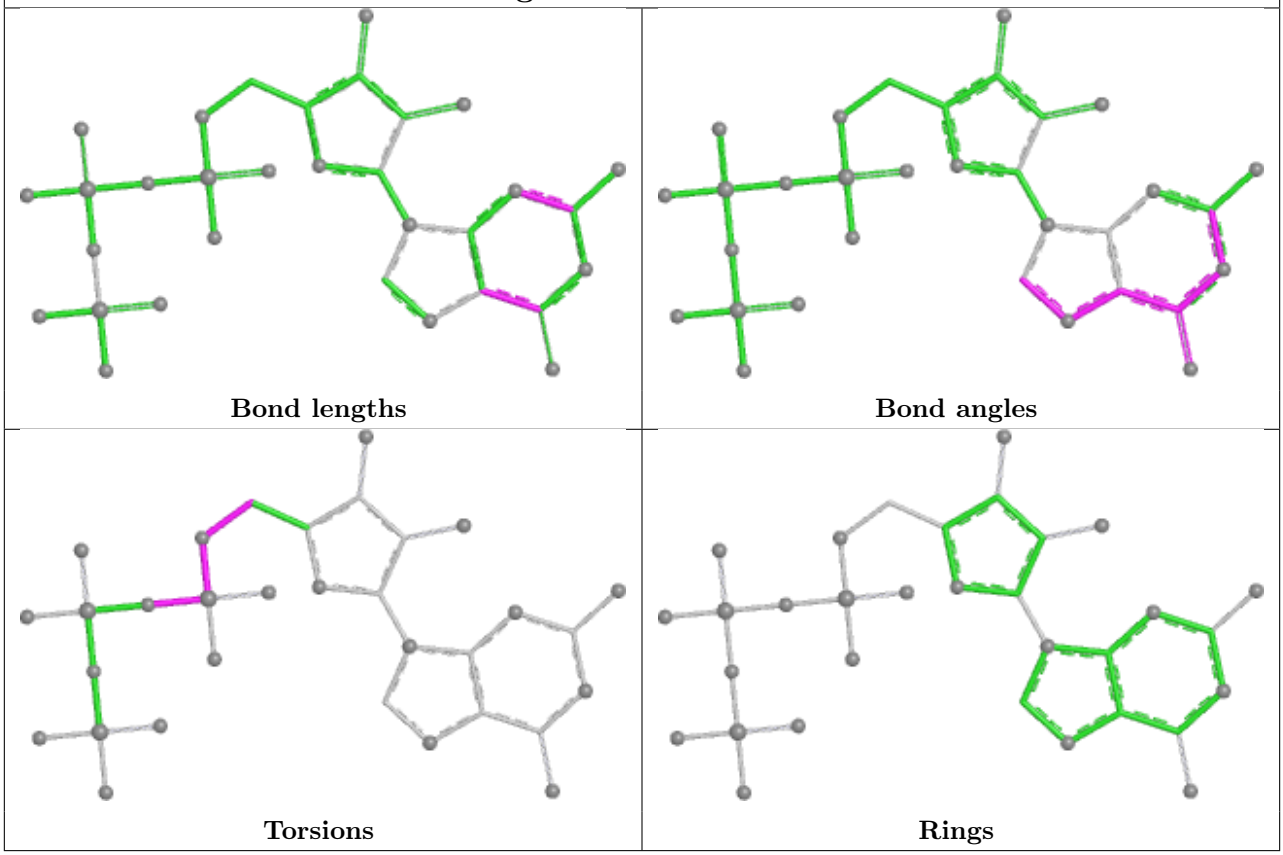

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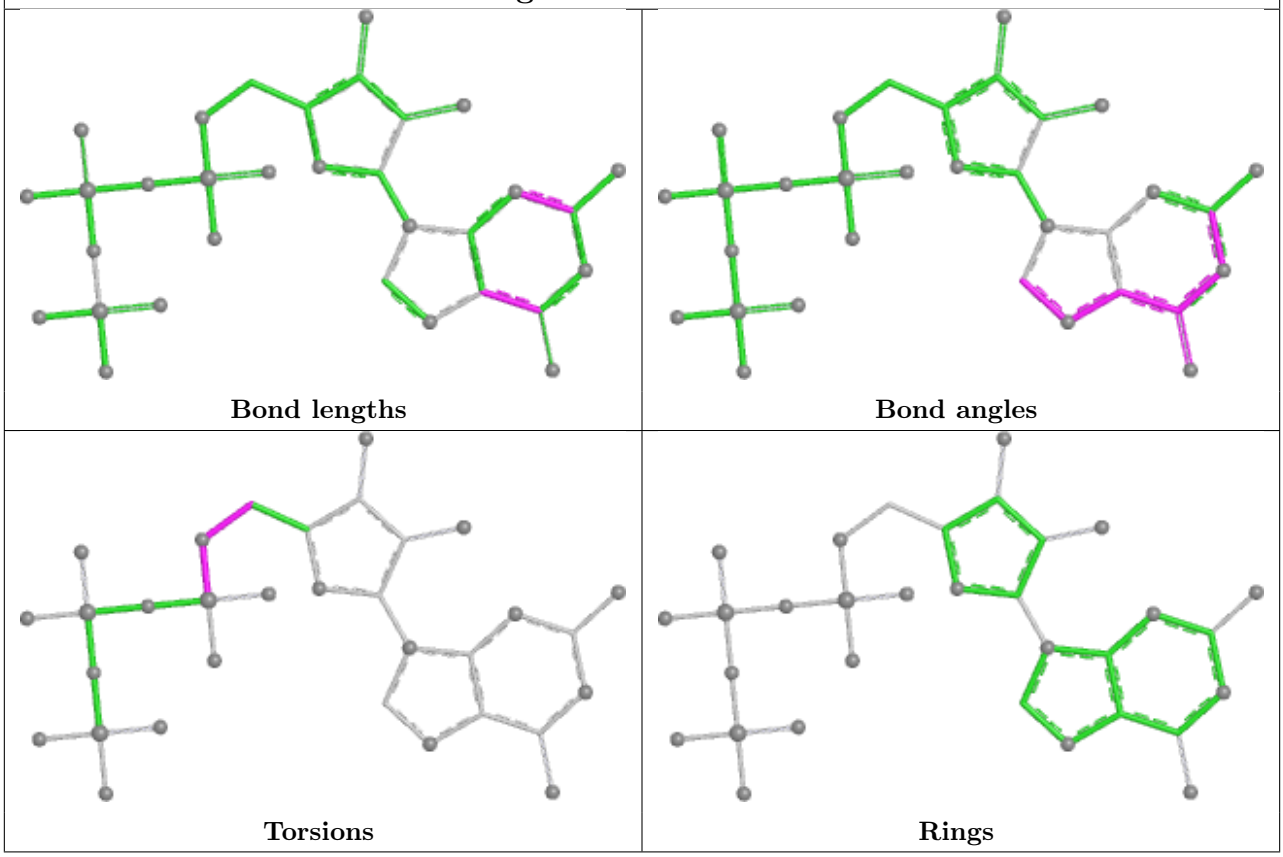

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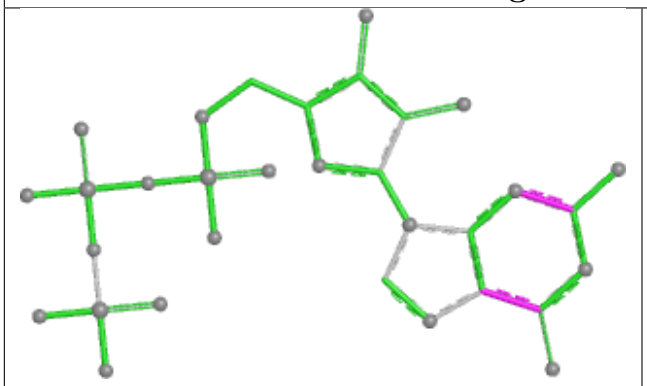
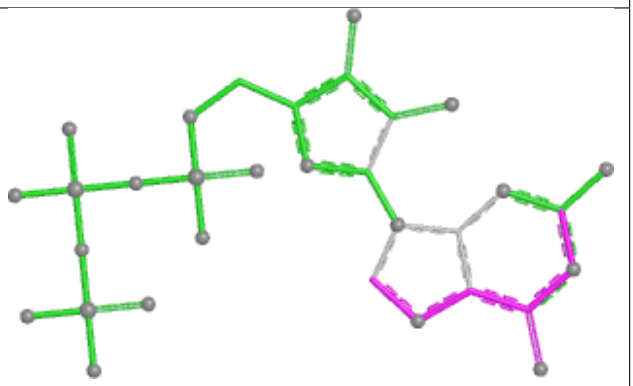
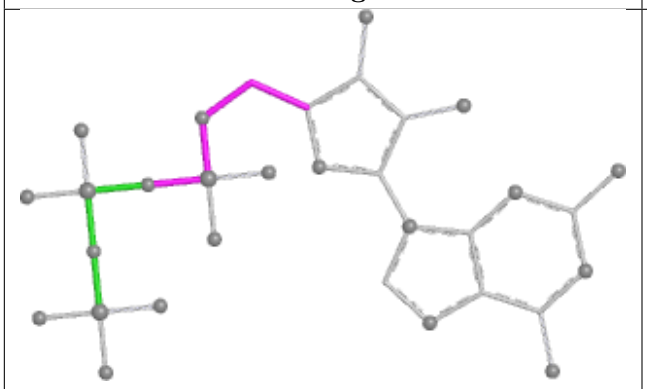


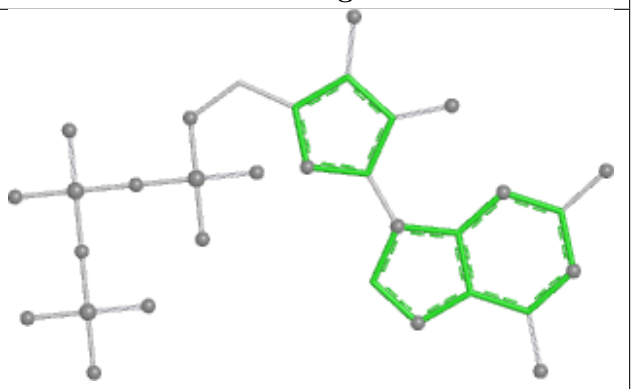
Bond lengths



Bond angles

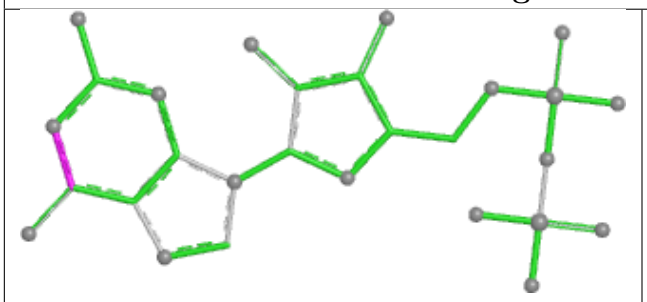


Torsions



Rings

Ligand GDP VJ 501



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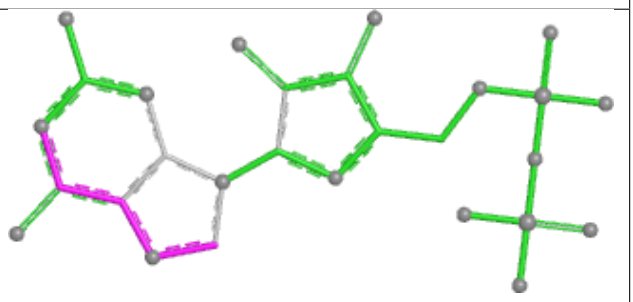
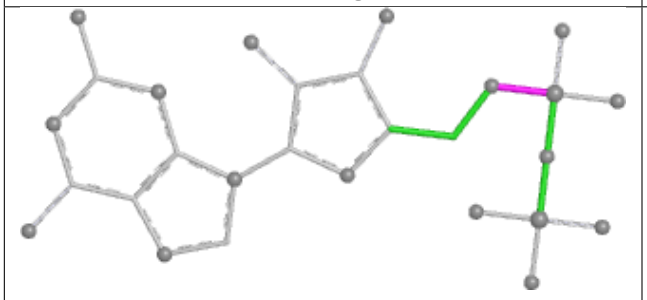


Bond angles



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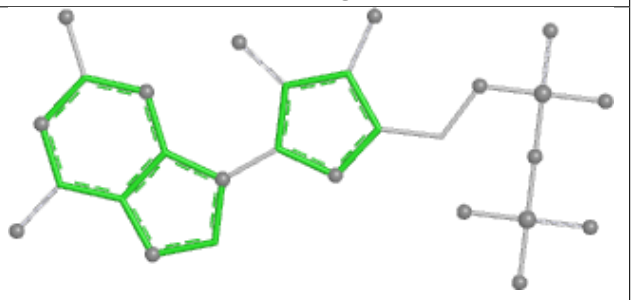

Rings

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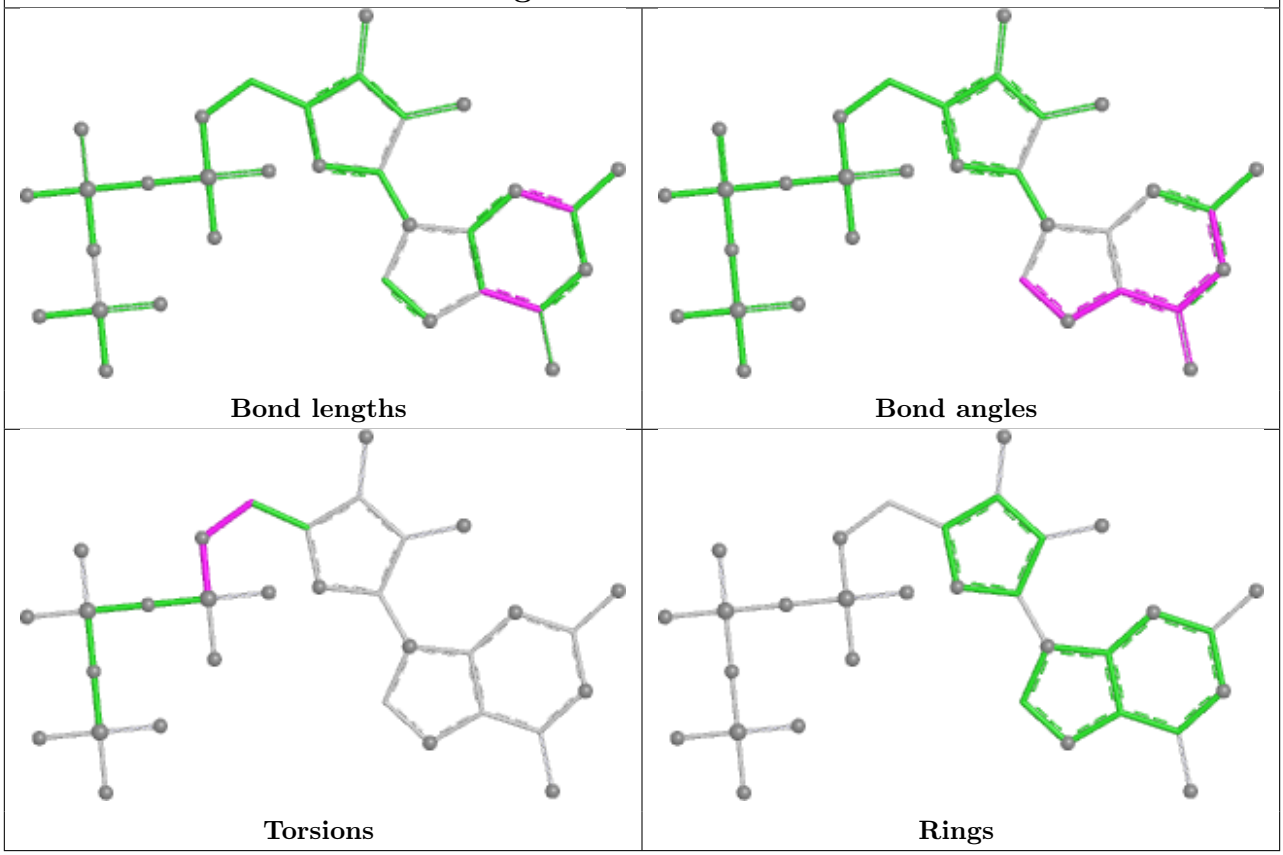

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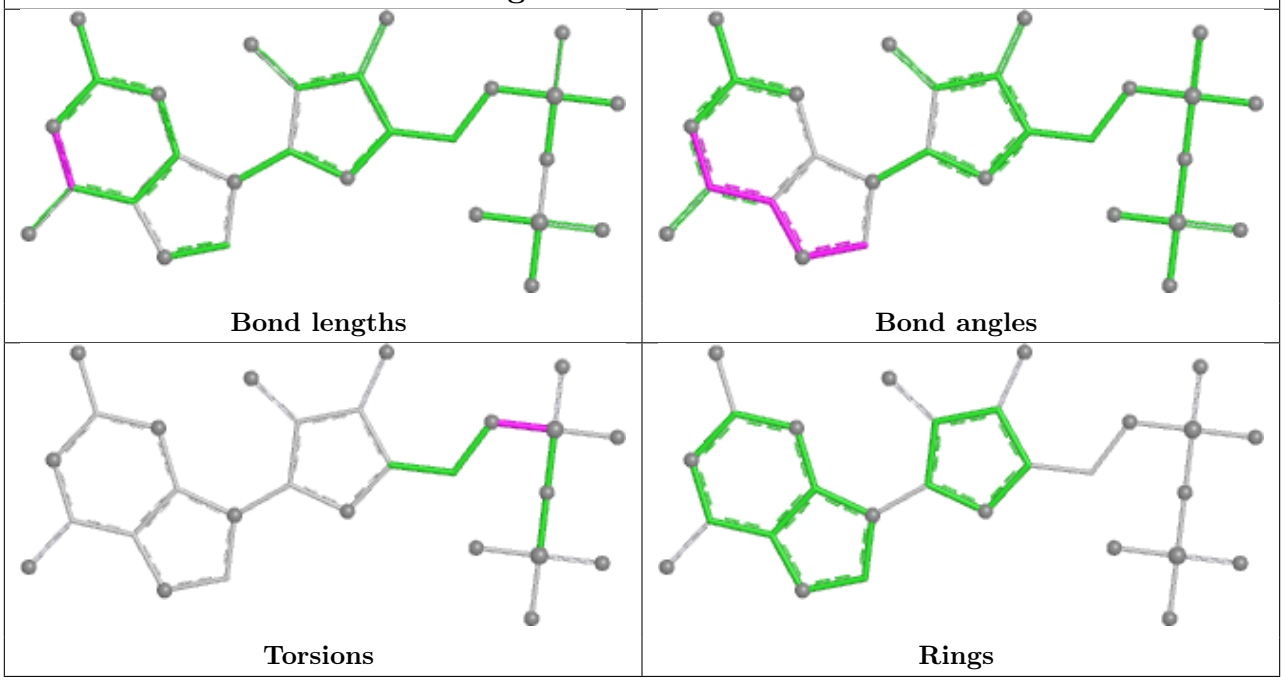

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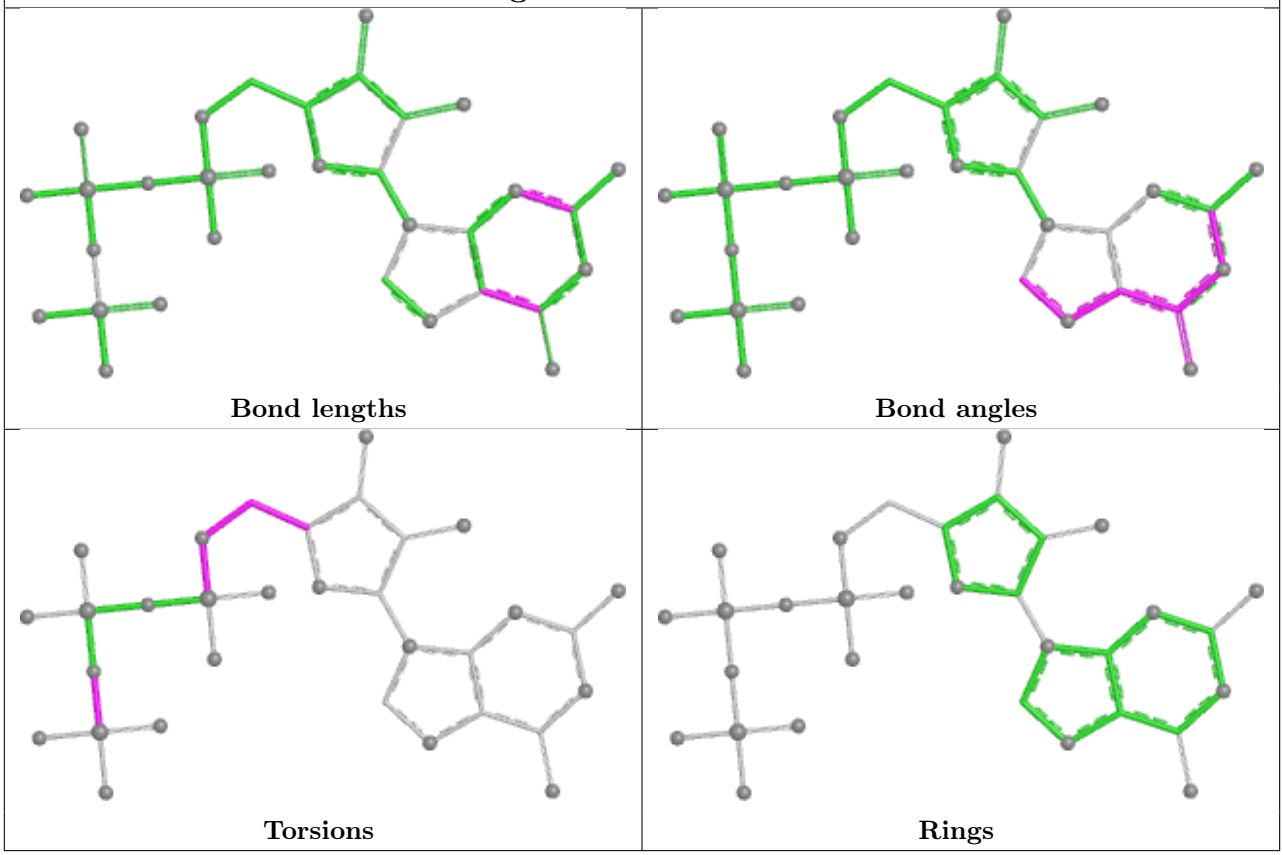
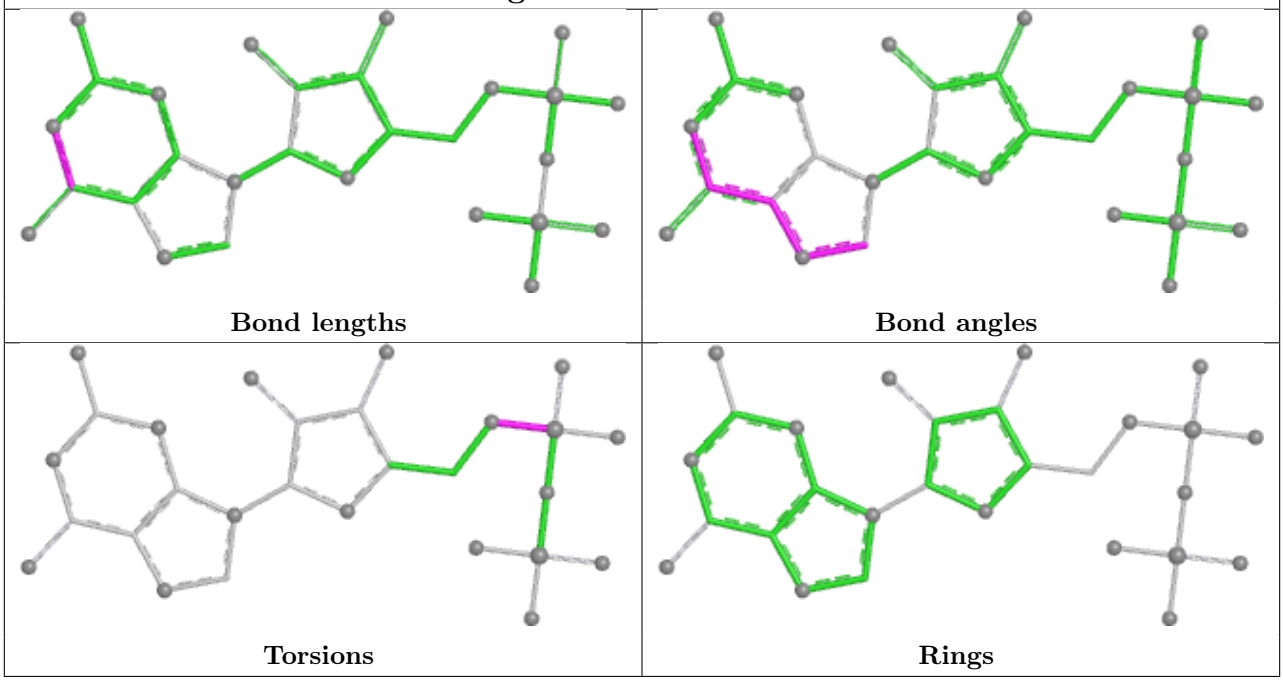


Ligand GDP UH 501



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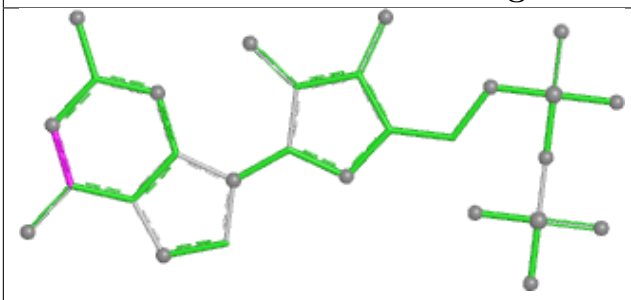

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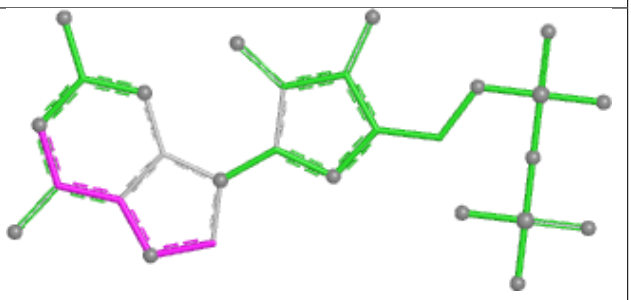

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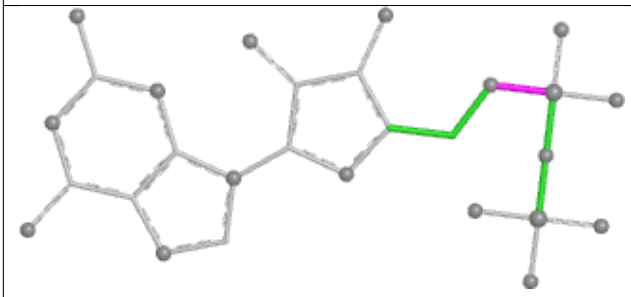
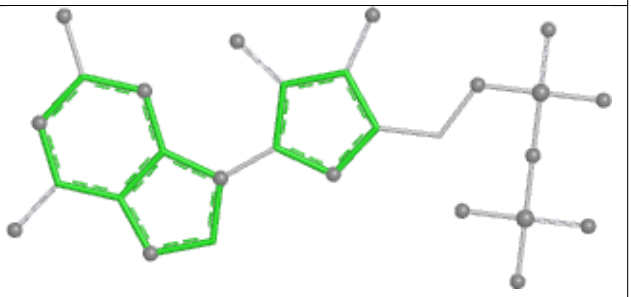
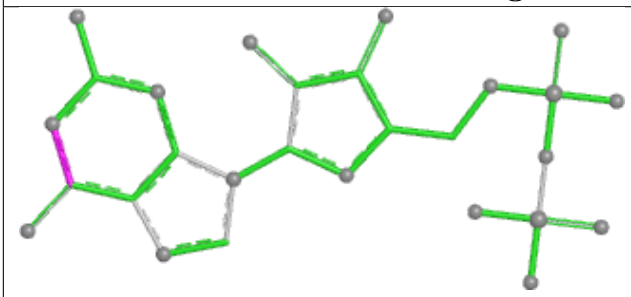


Torsions



Rings

Ligand GDP VH 501



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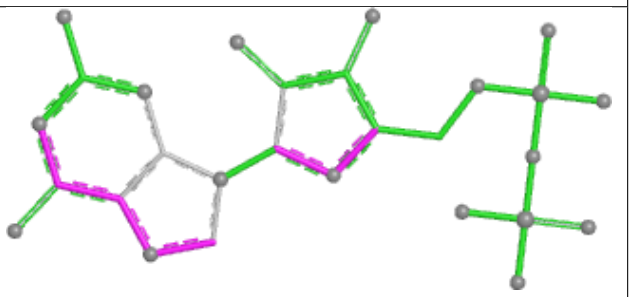

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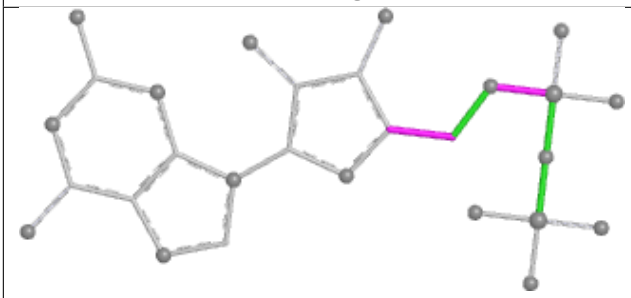

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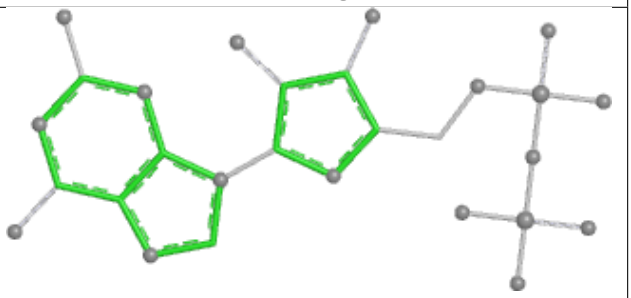

Rings

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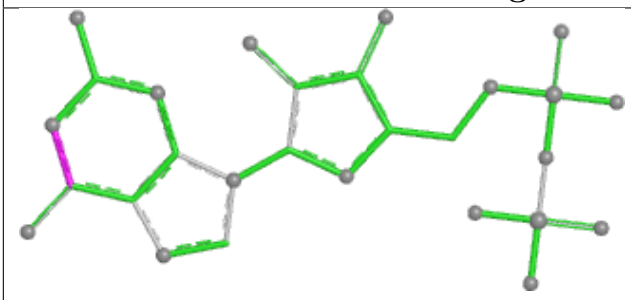

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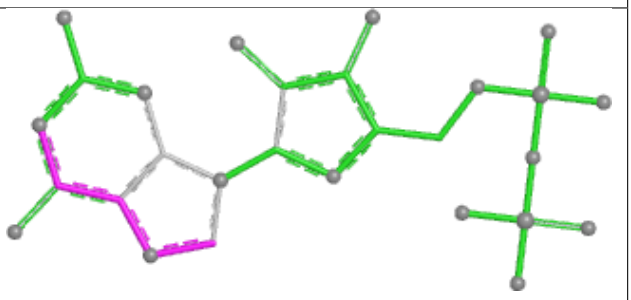

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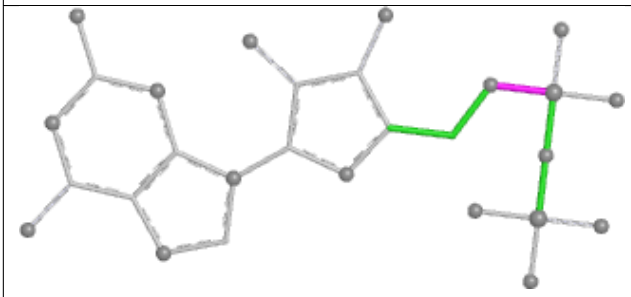

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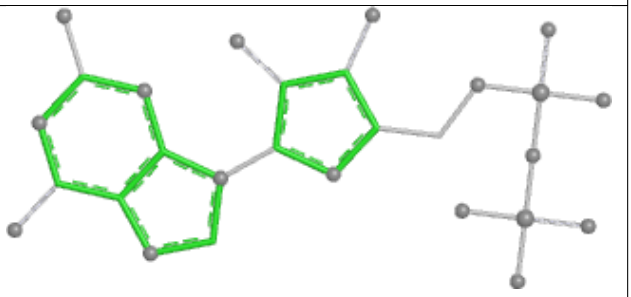

Rings

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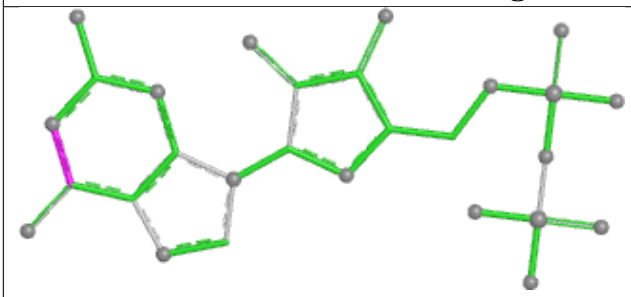

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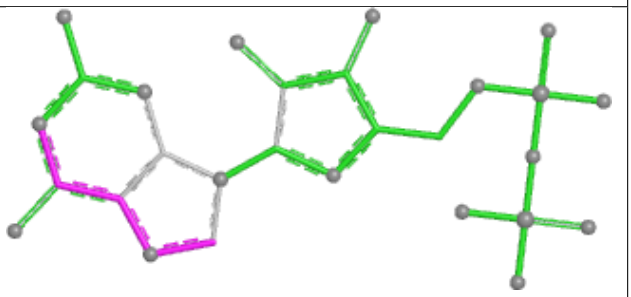

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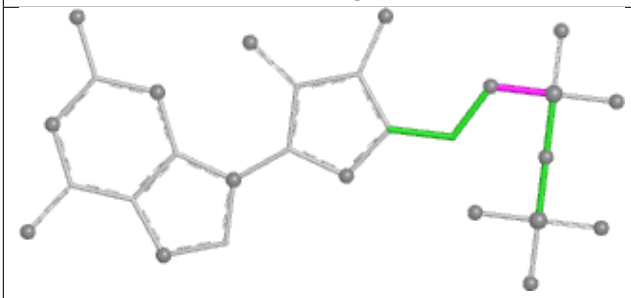

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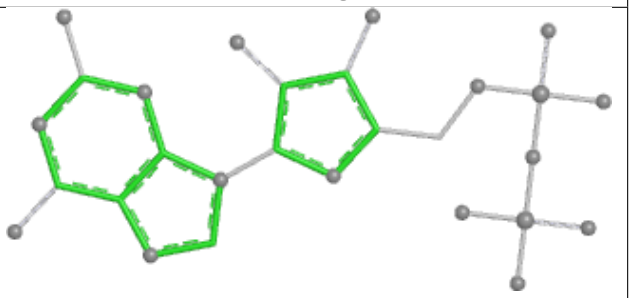

Rings

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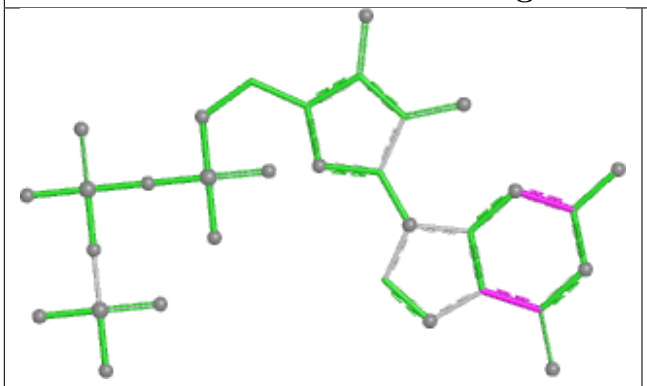

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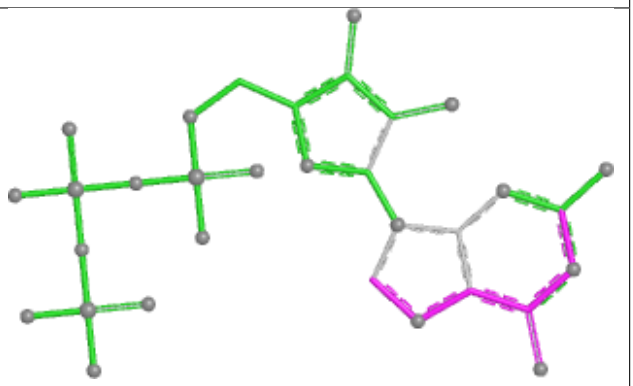

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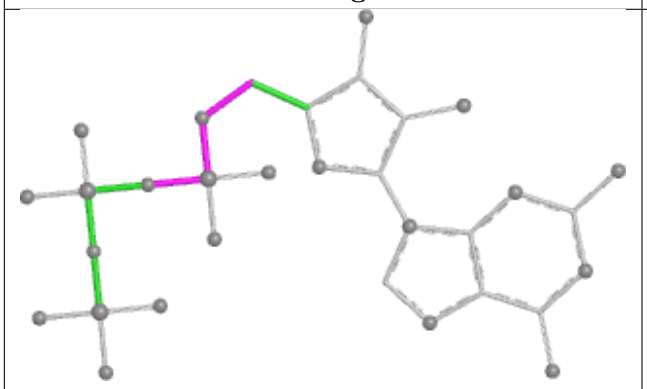

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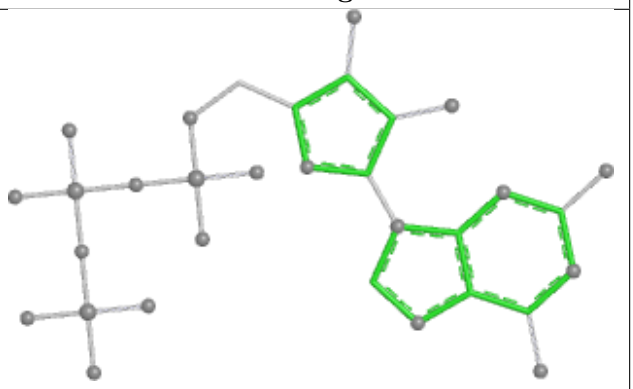

Rings

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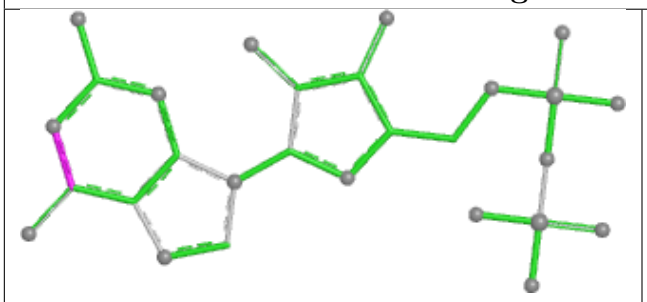

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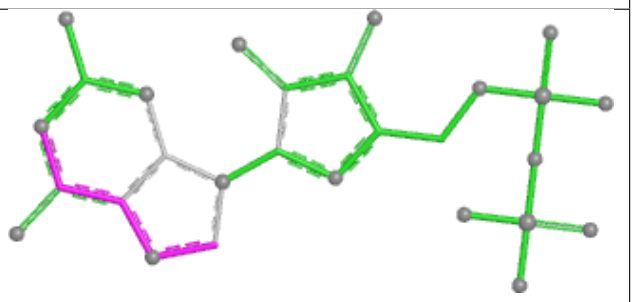

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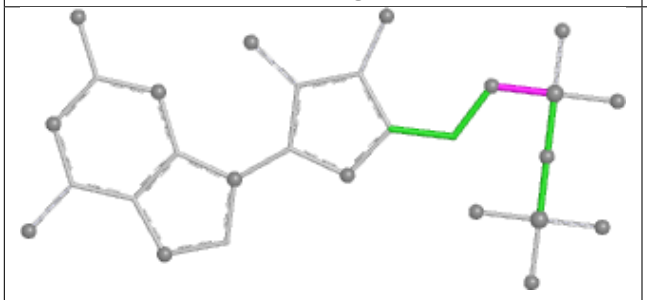

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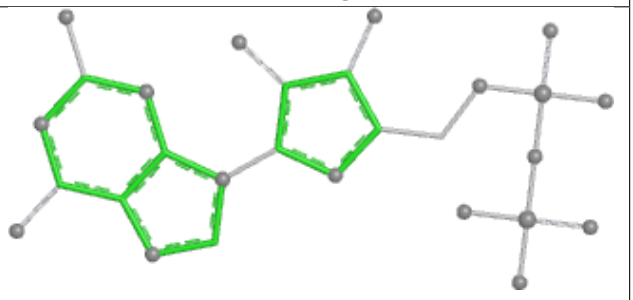

Rings

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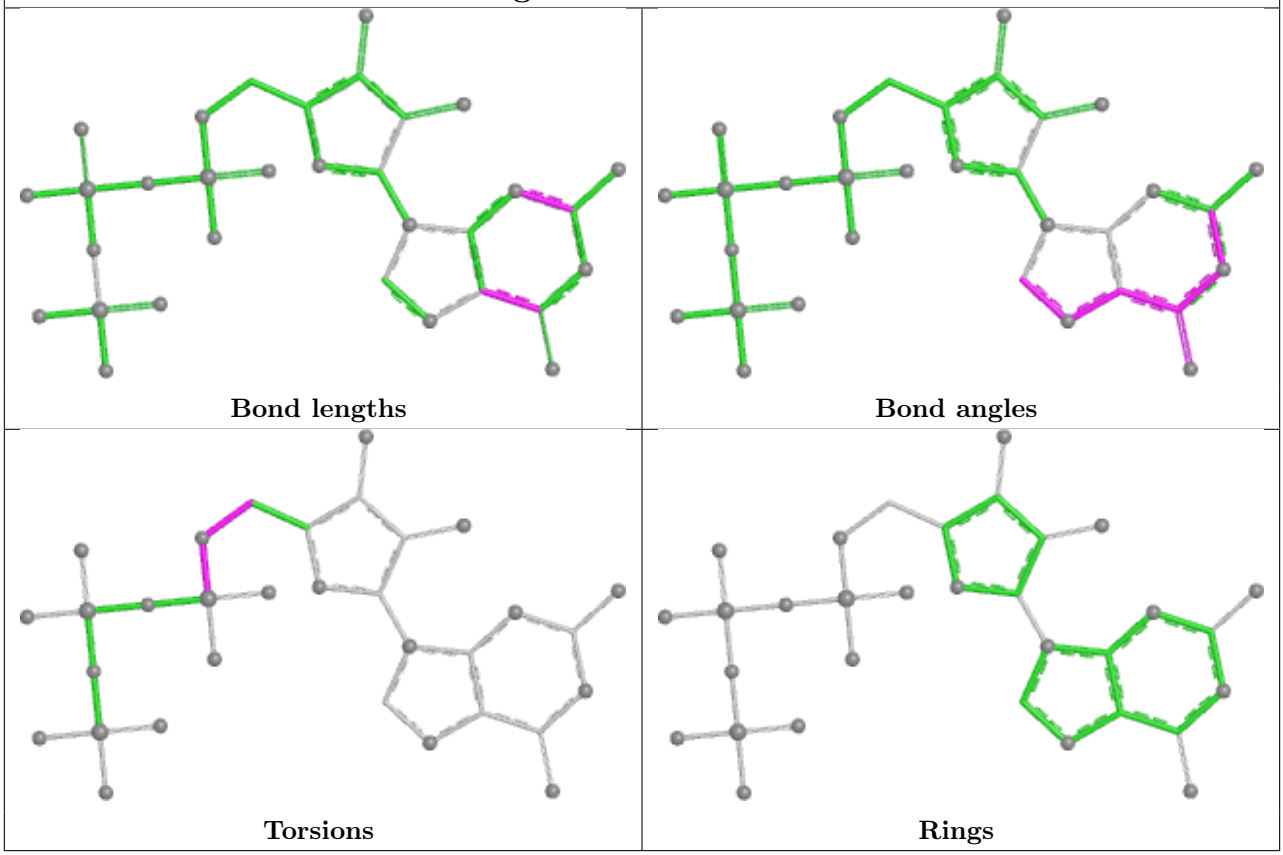

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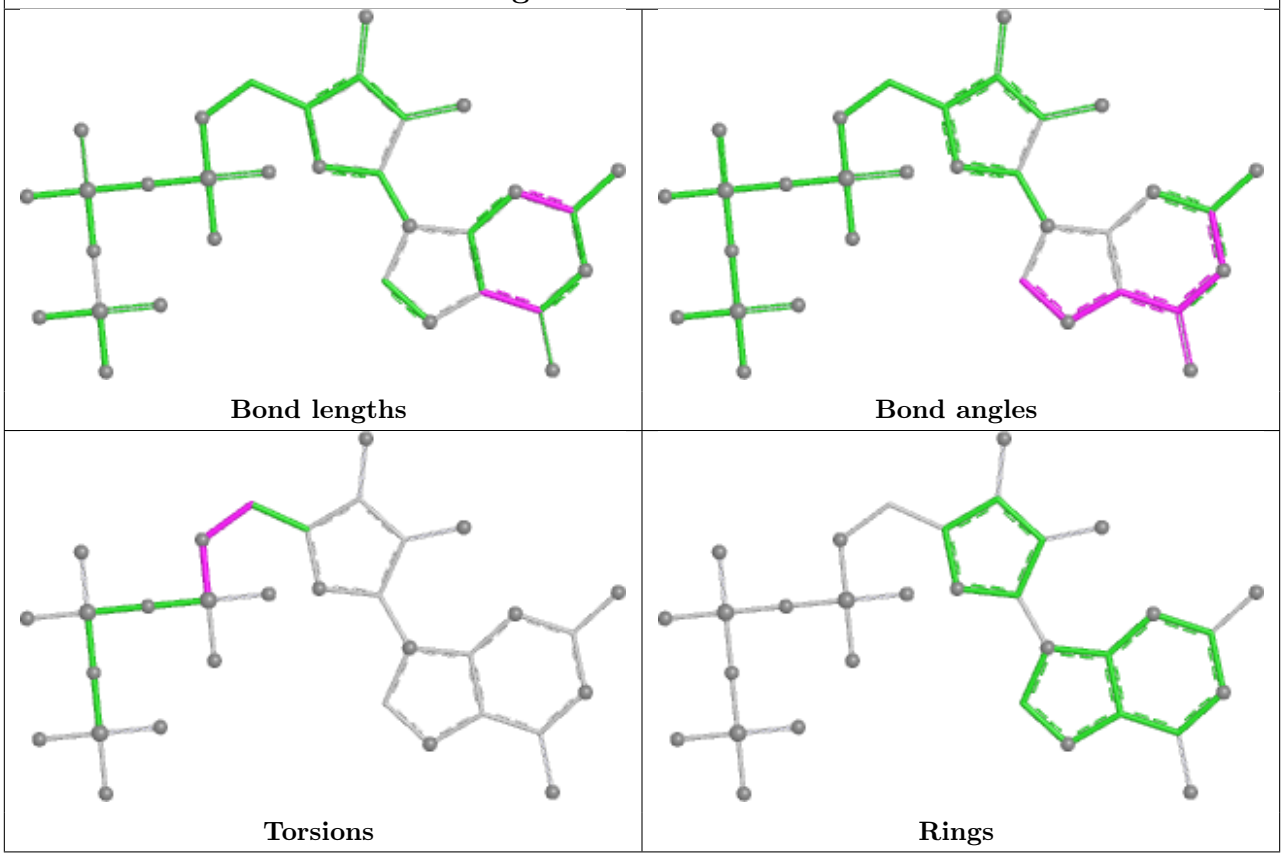

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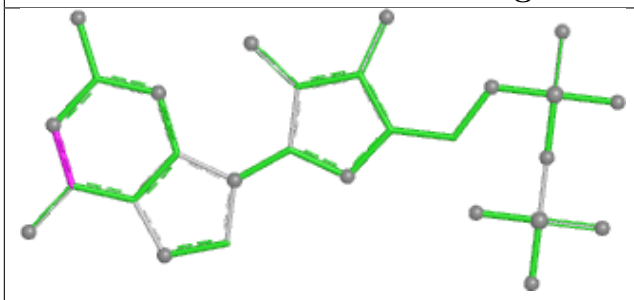

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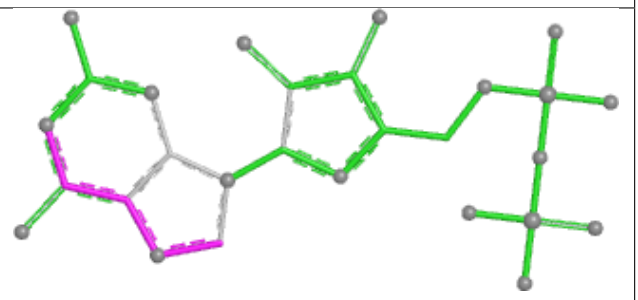

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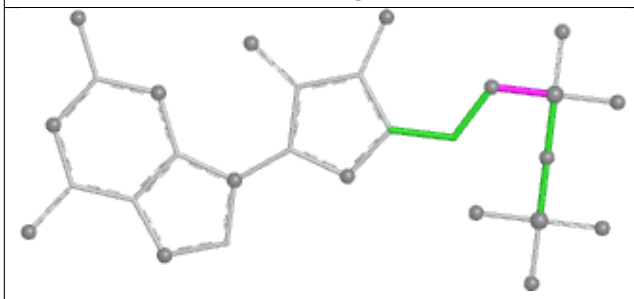

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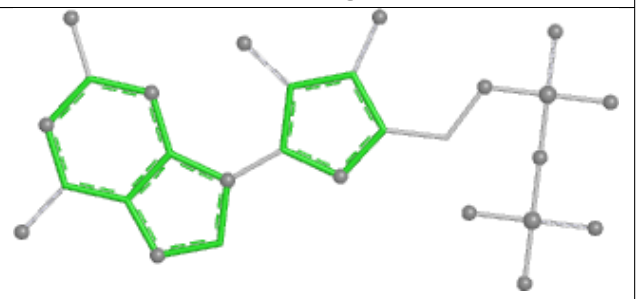

Rings

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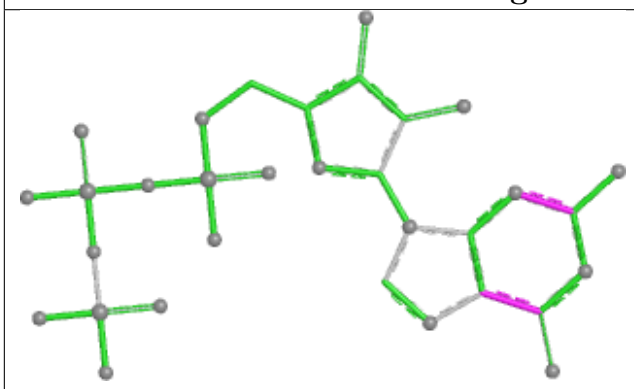

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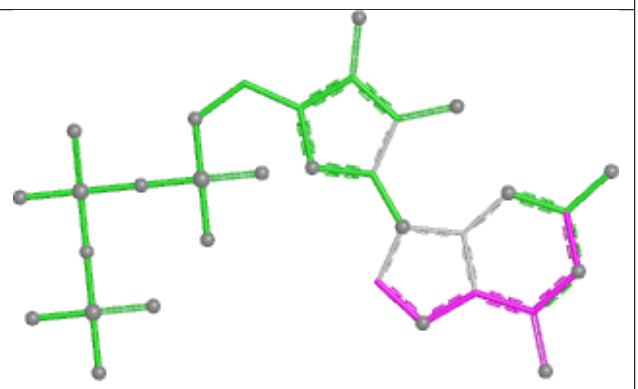

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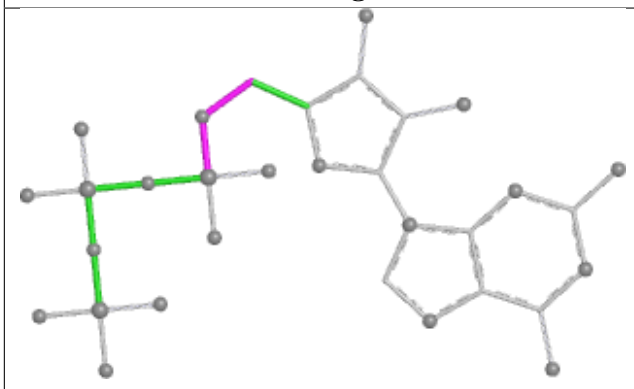

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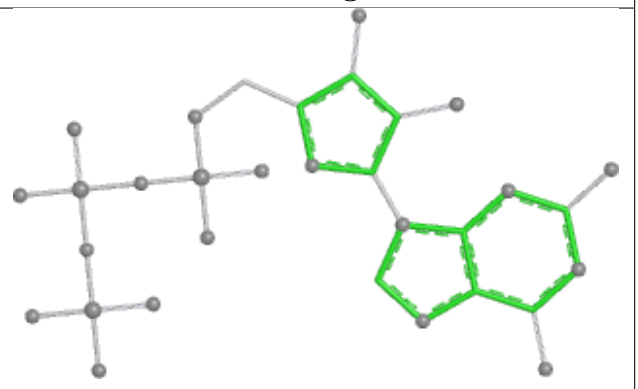

Rings

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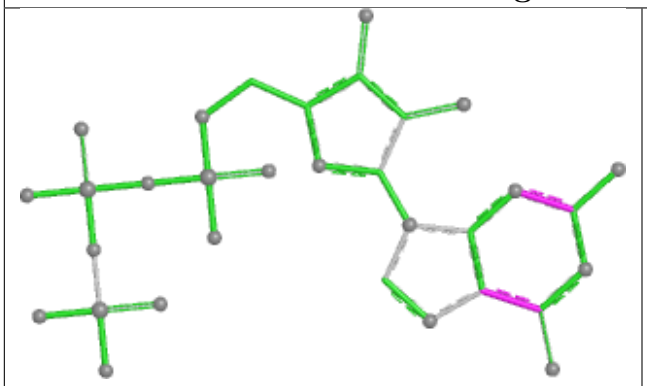

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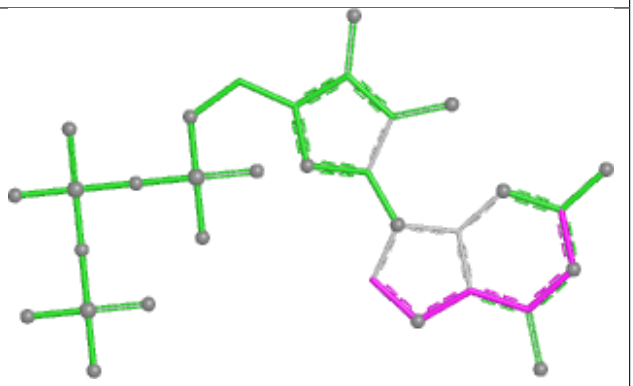

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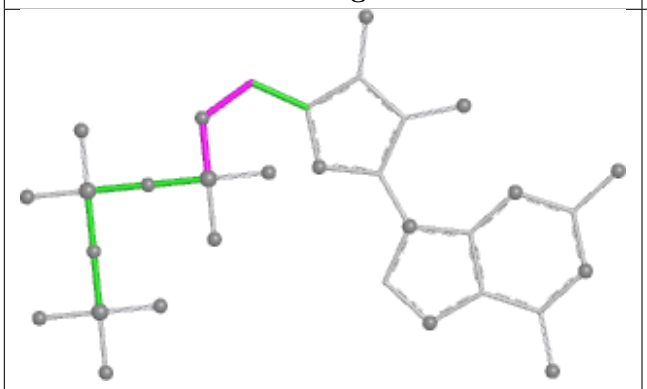

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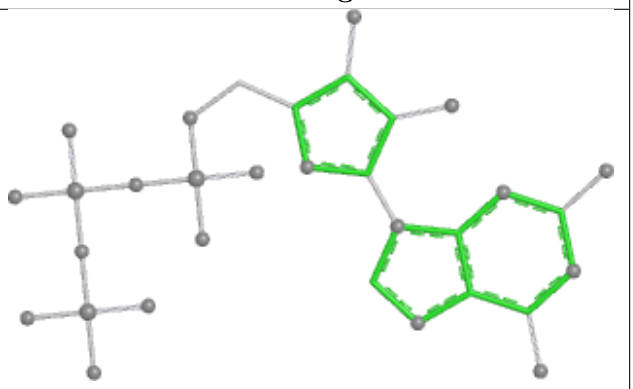

Rings

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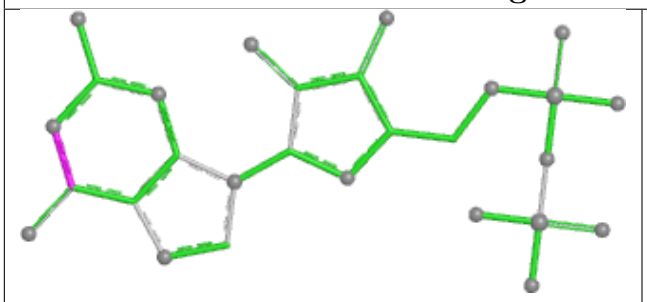

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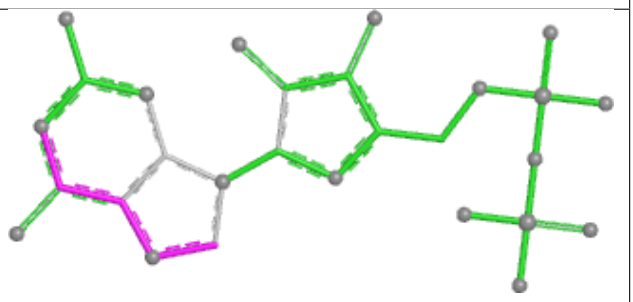

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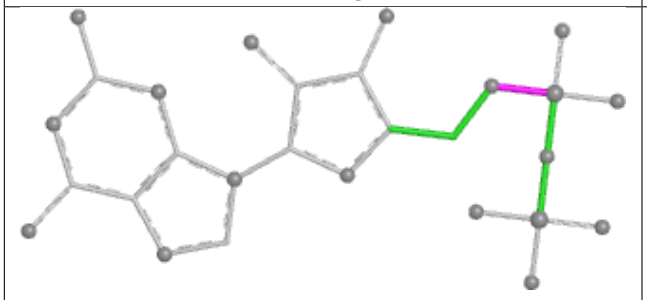

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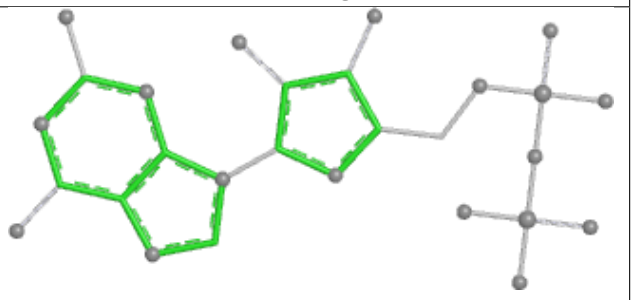

Rings

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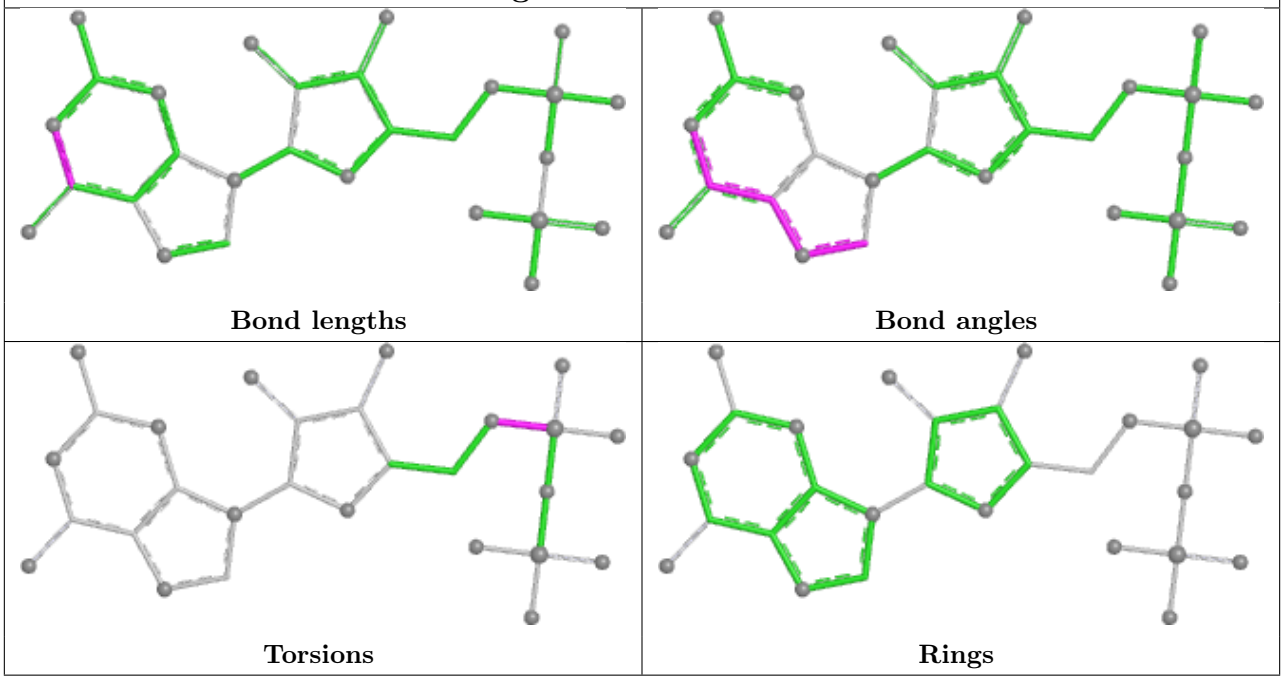

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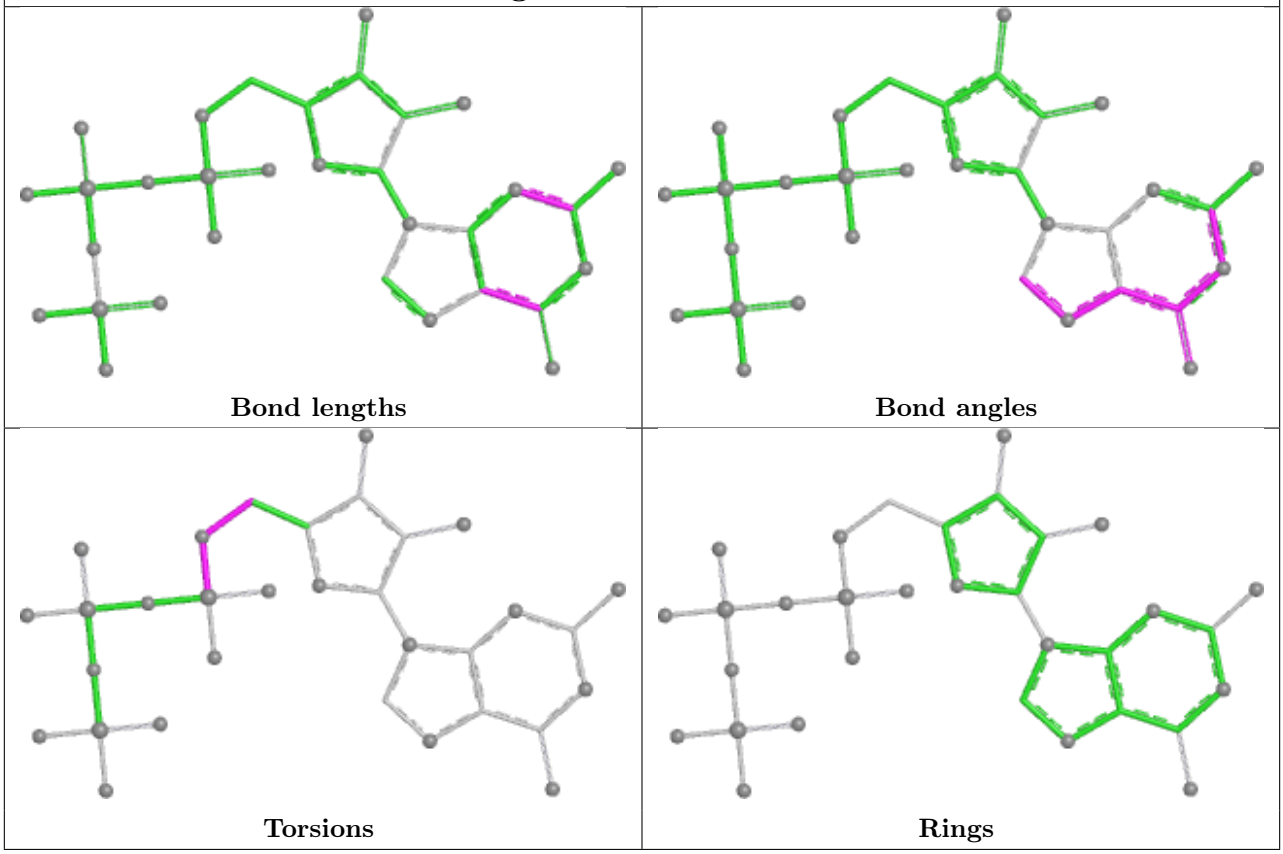

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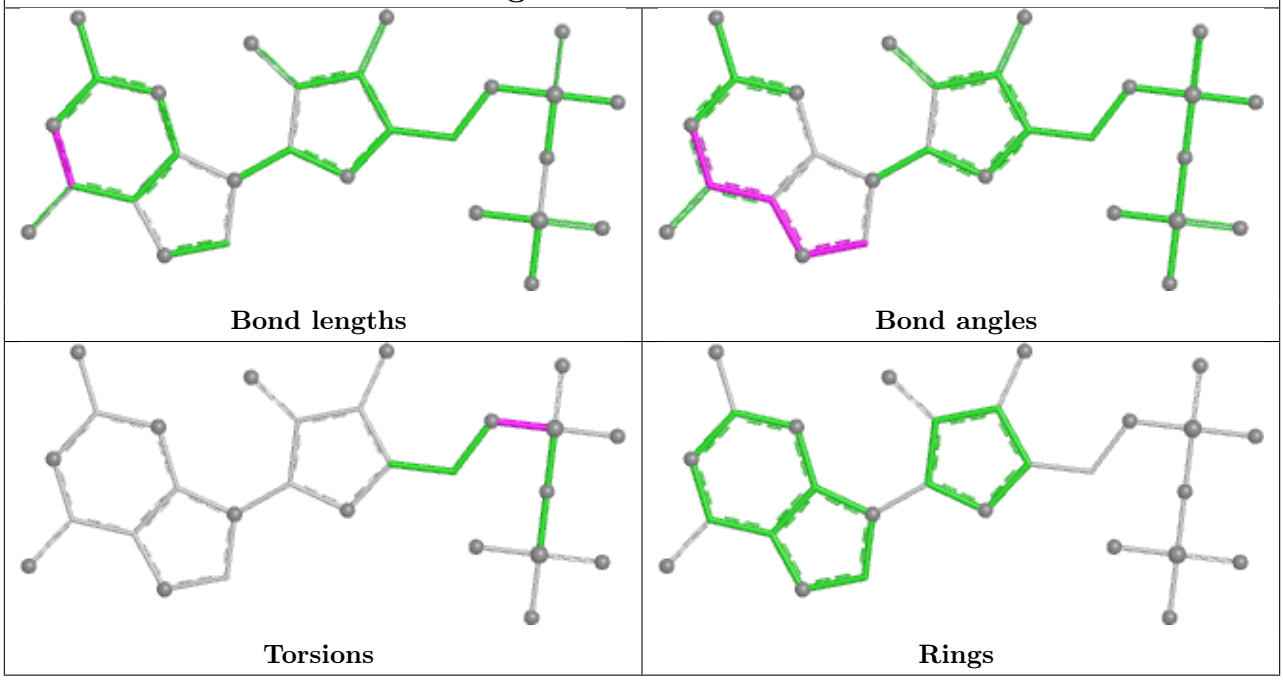

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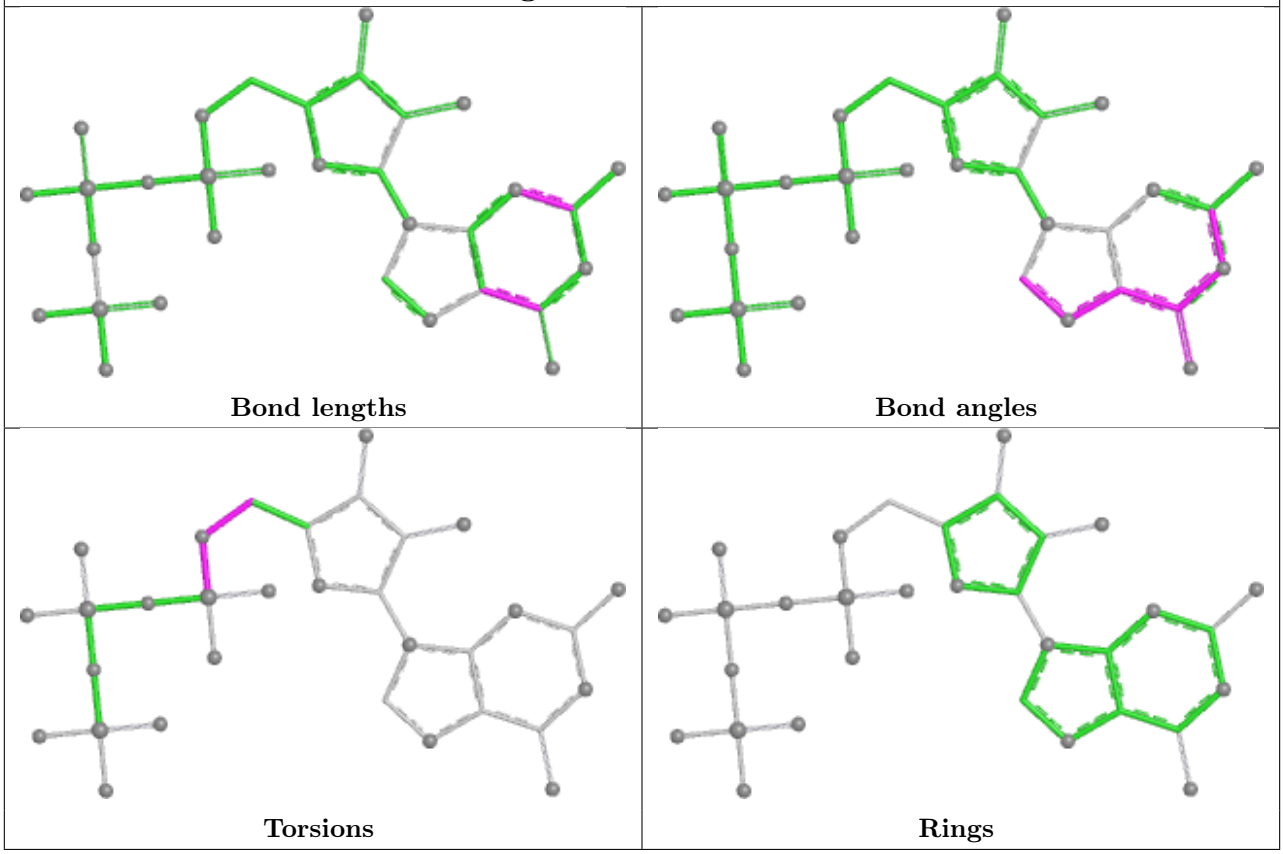

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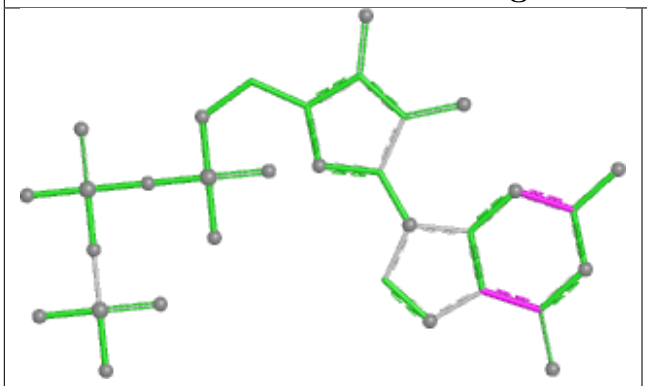

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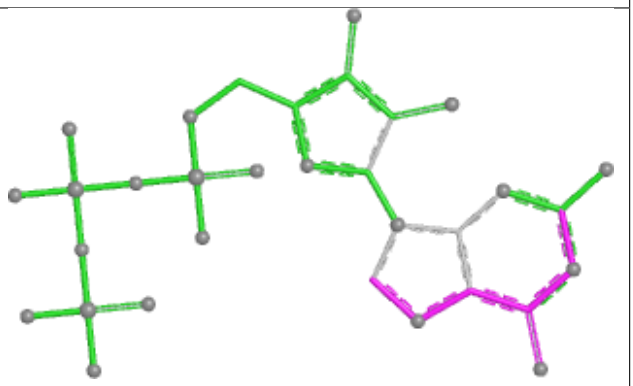
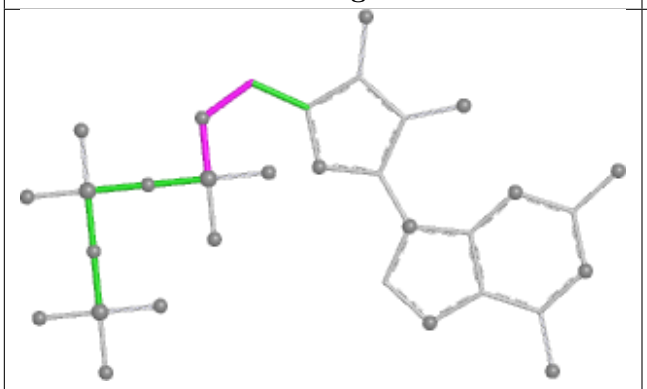
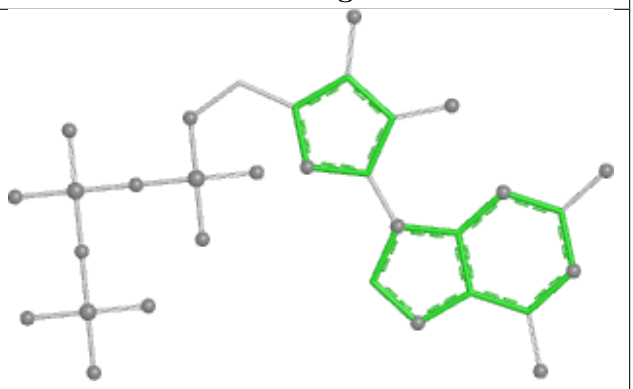


Bond angles

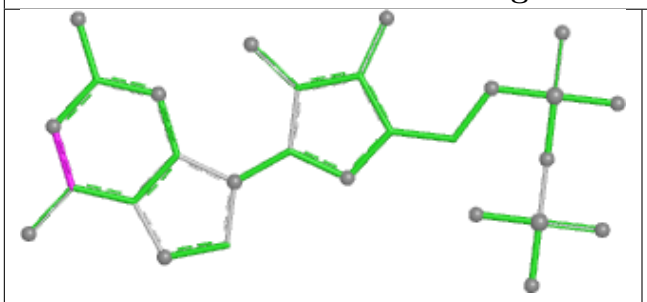


Torsions



Rings

Ligand GDP LD 501



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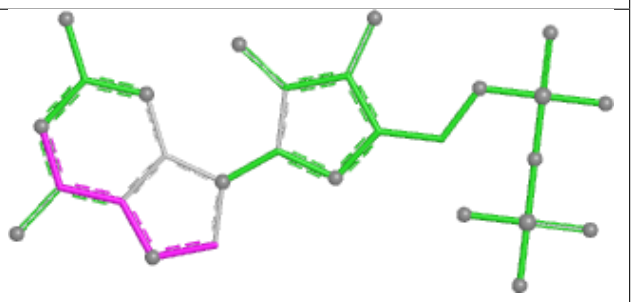

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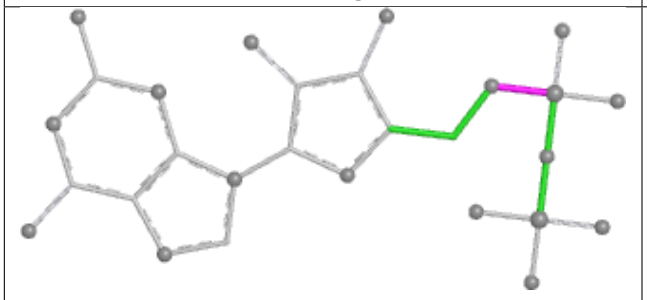
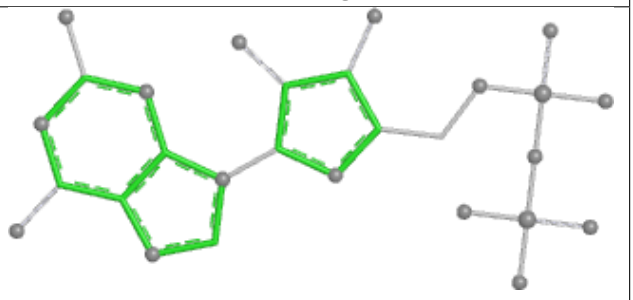
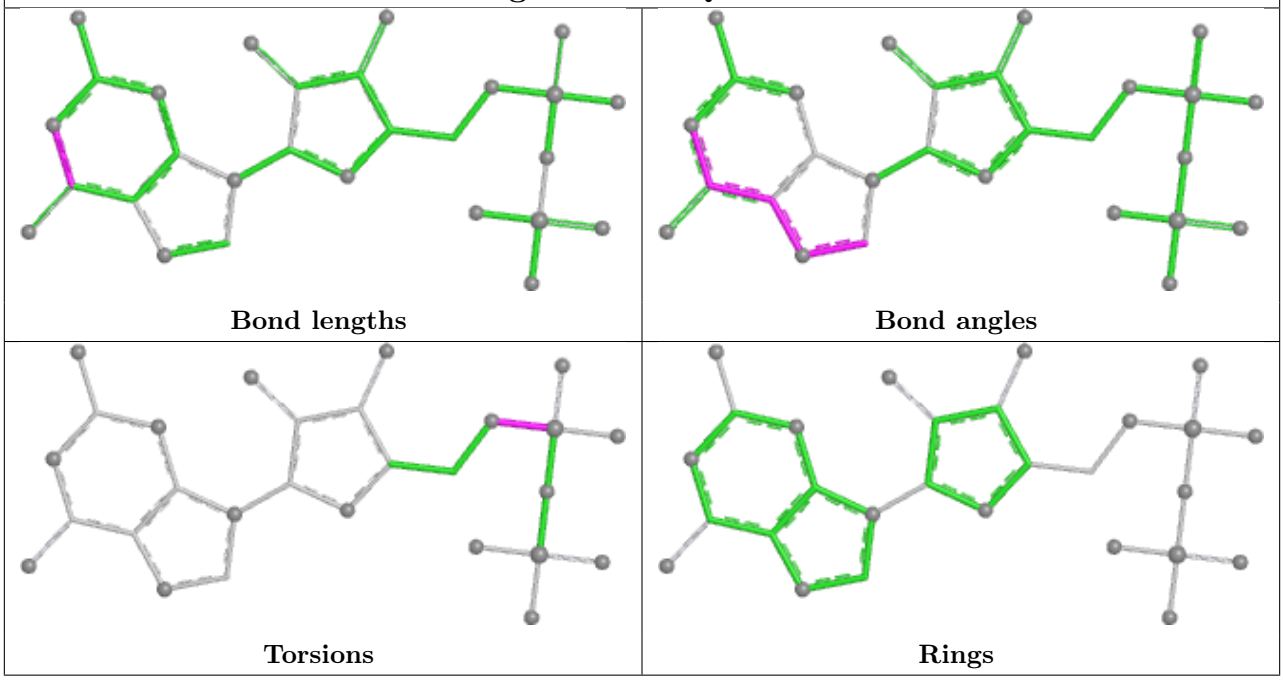


Torsions



Rings

Ligand GDP QC 501



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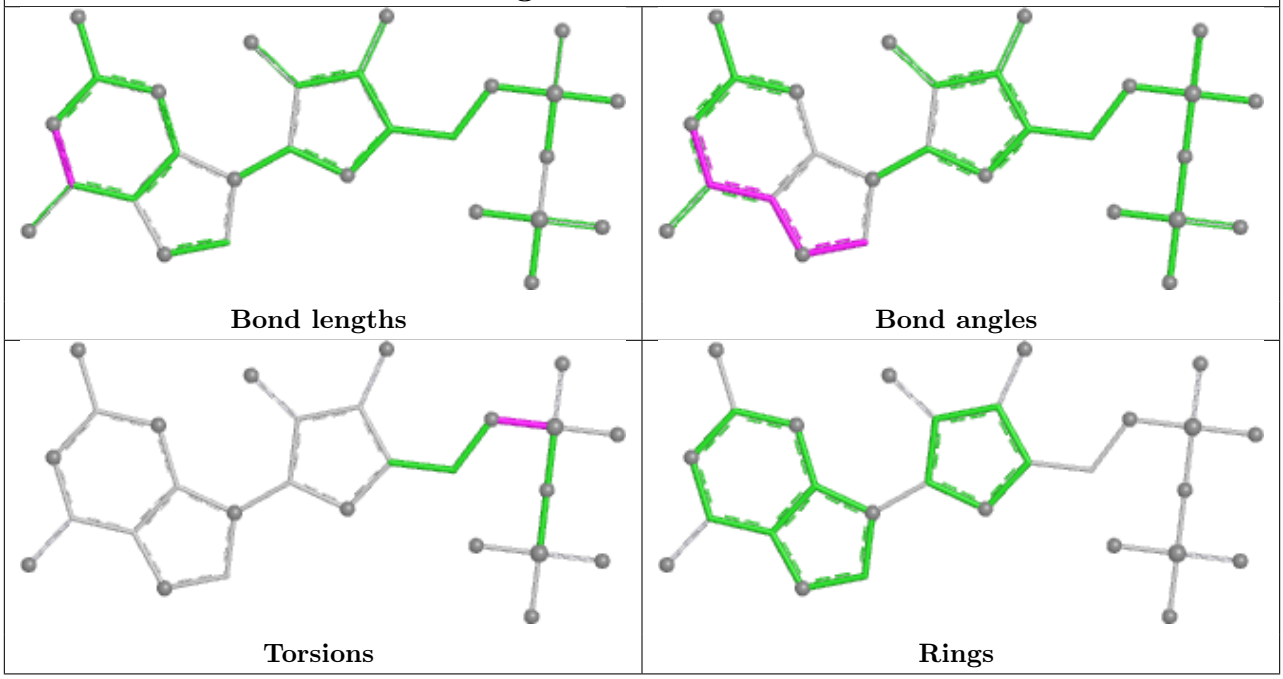

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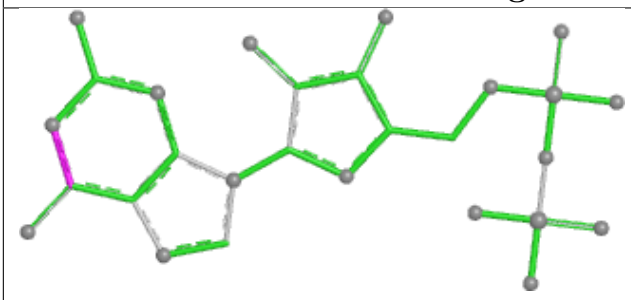
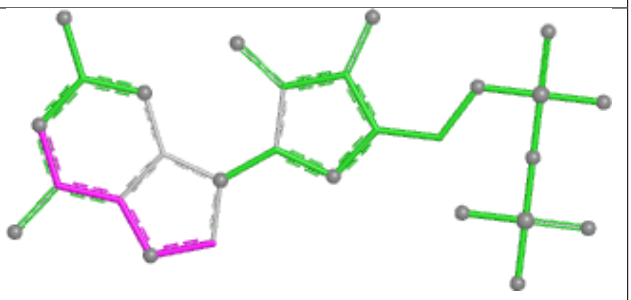


Bond lengths



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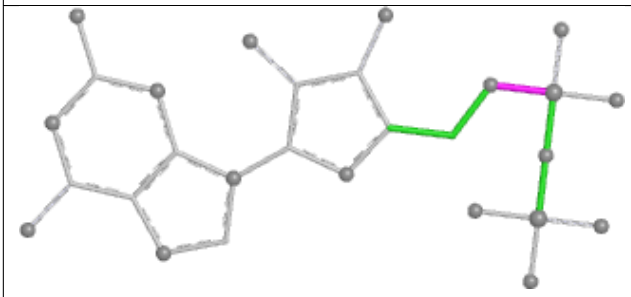

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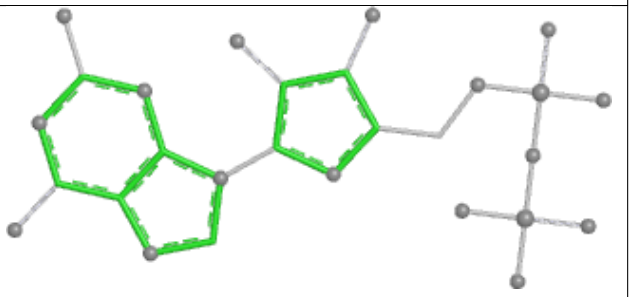

Rings

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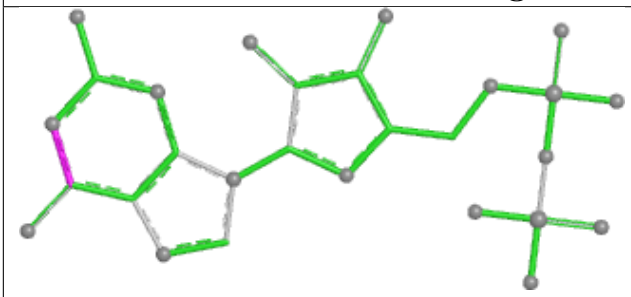

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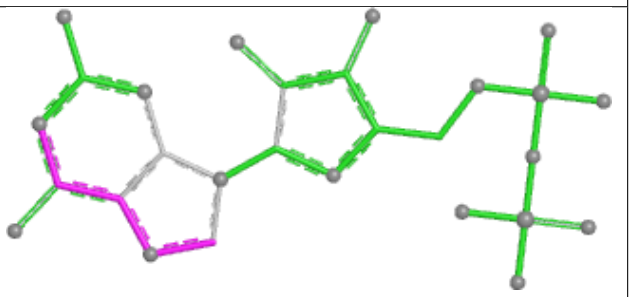

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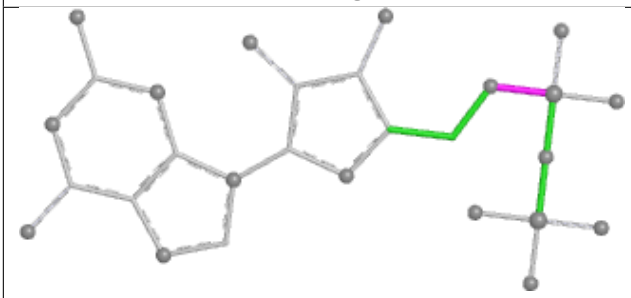

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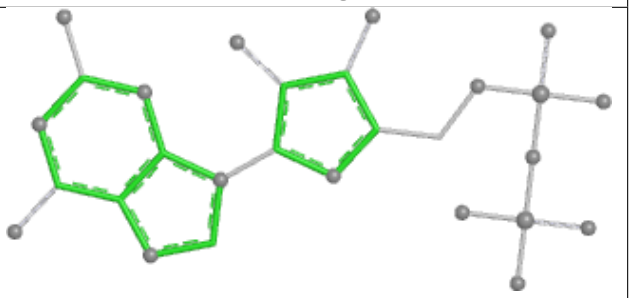

Rings

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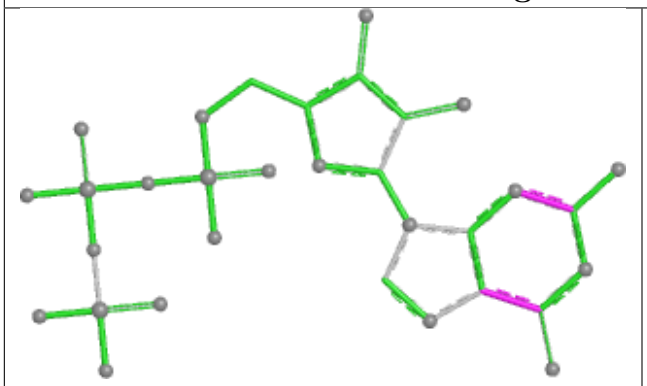

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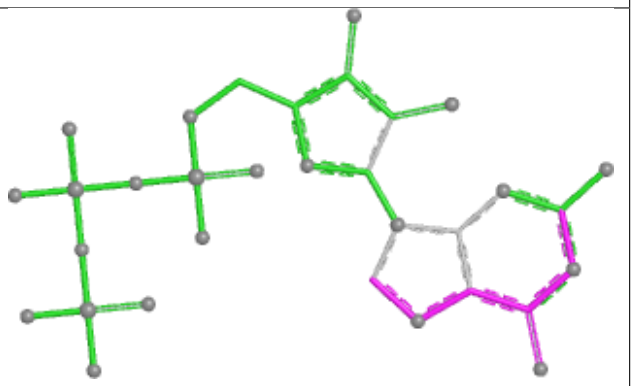

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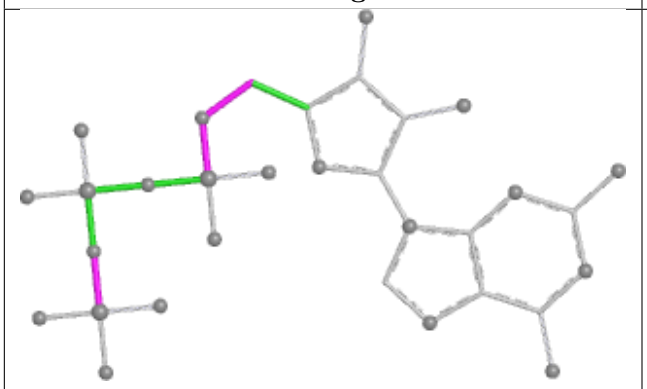

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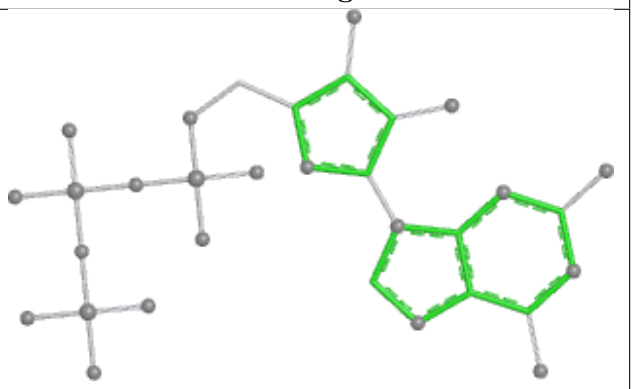

Rings

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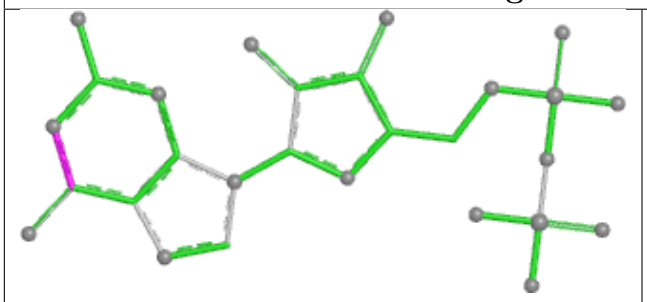

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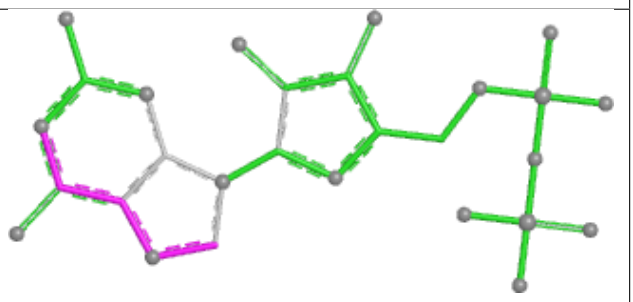

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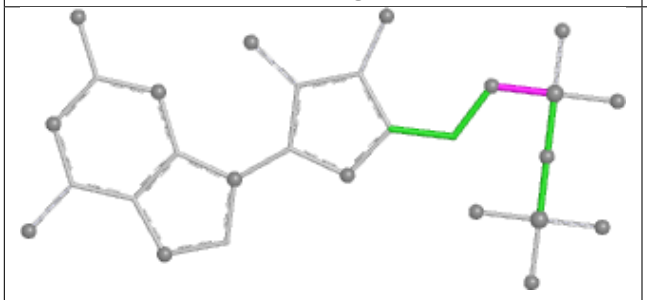

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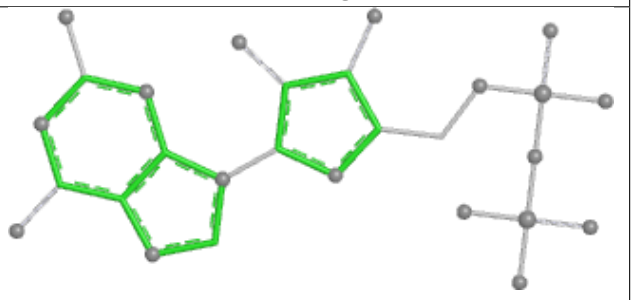

Rings

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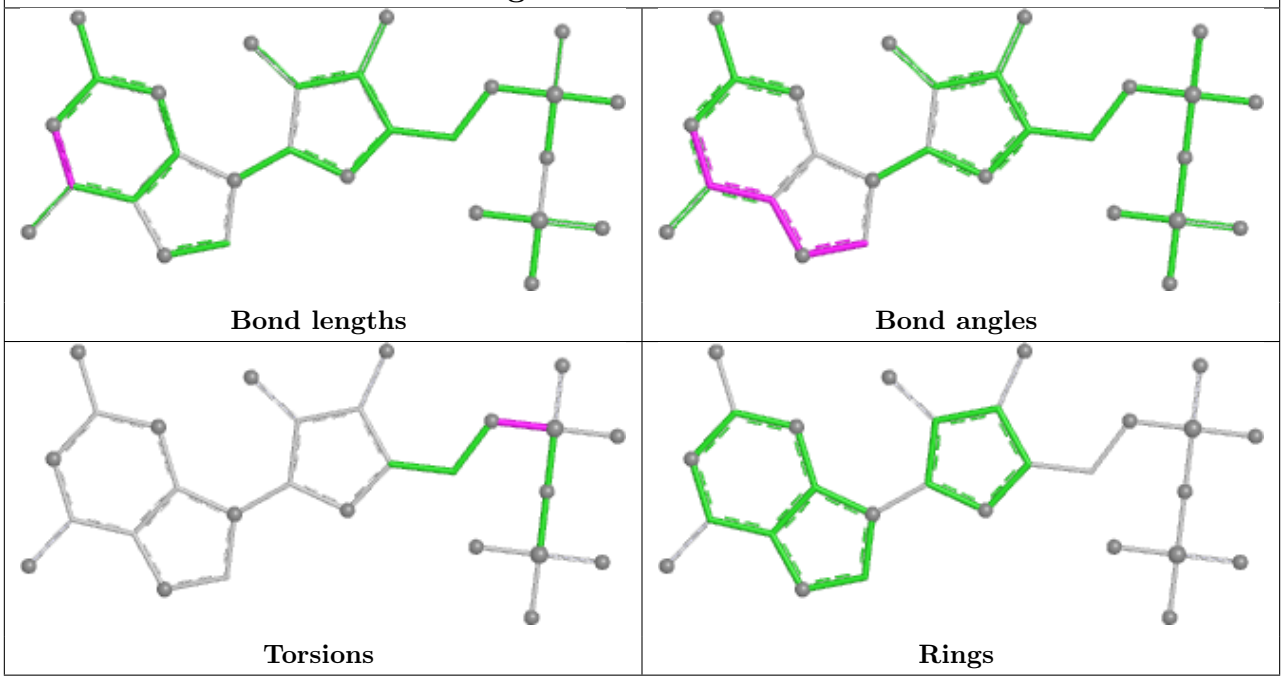

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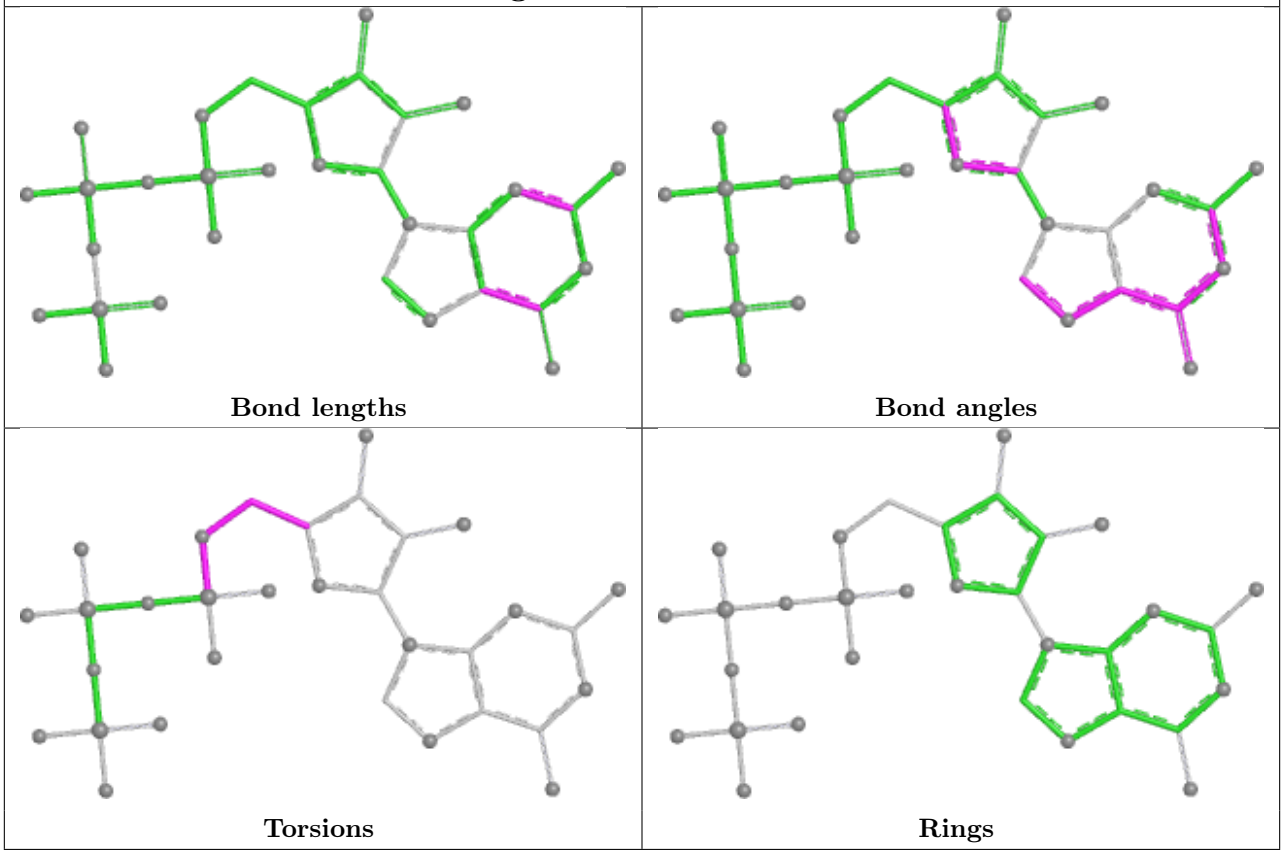

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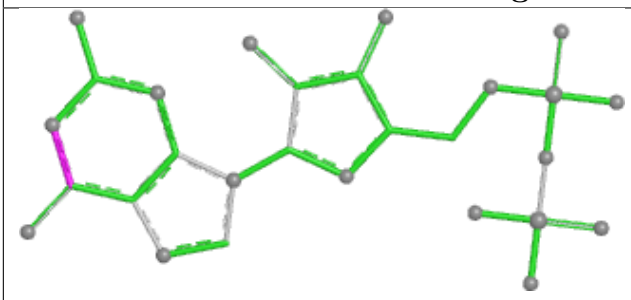

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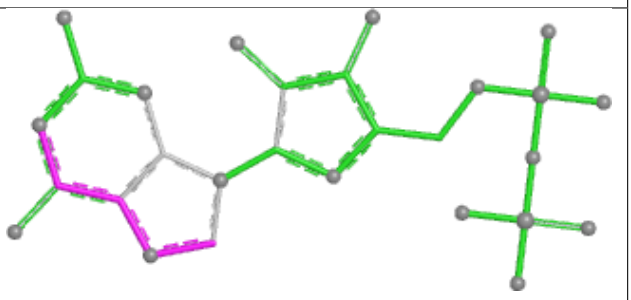

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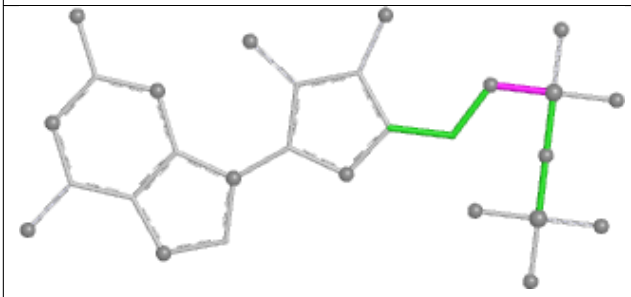

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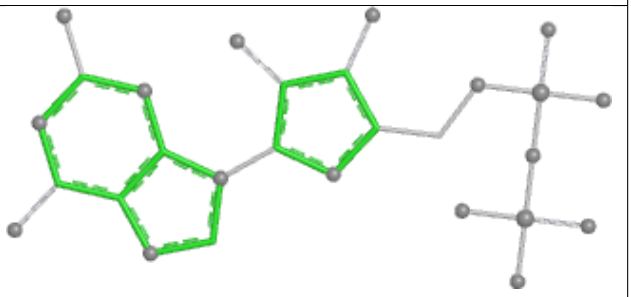

Rings

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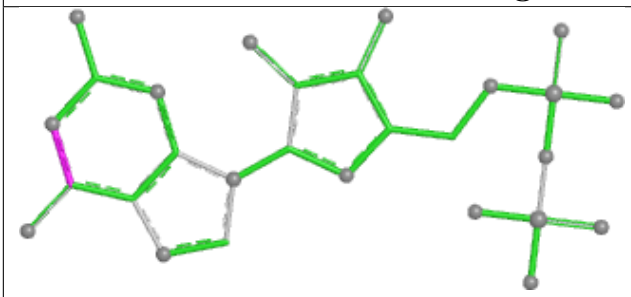

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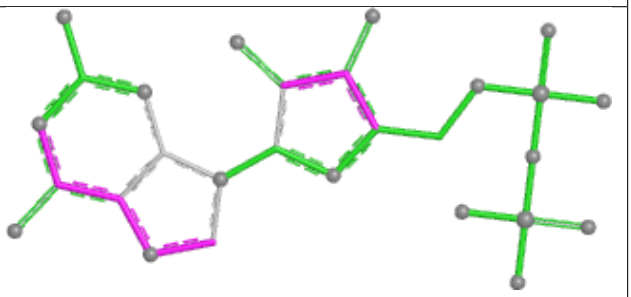

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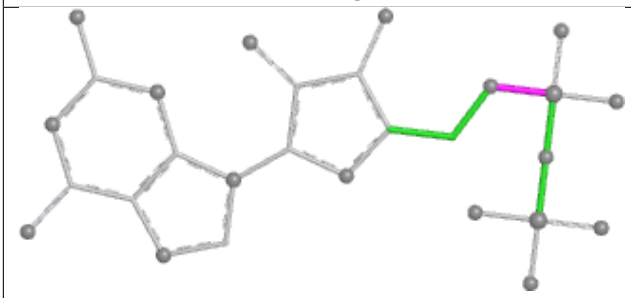

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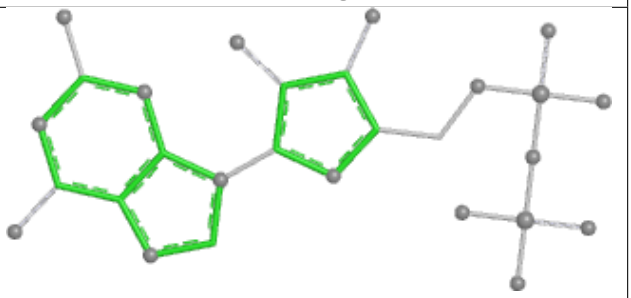

Rings

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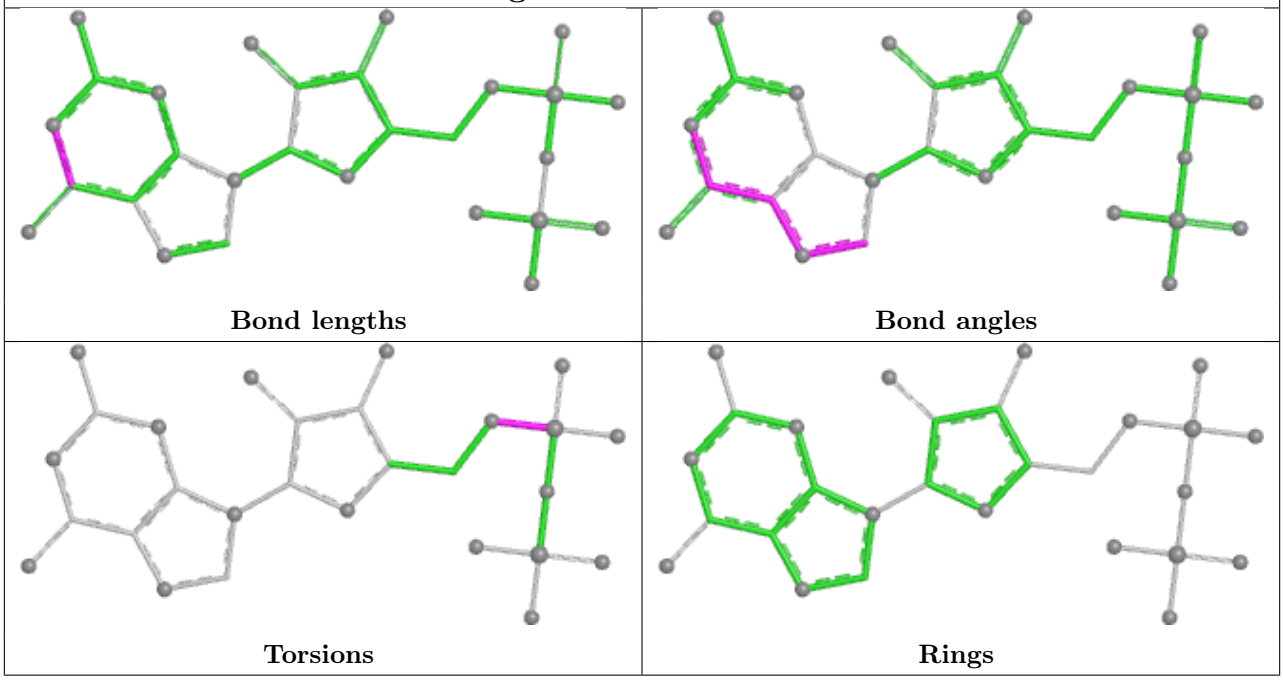

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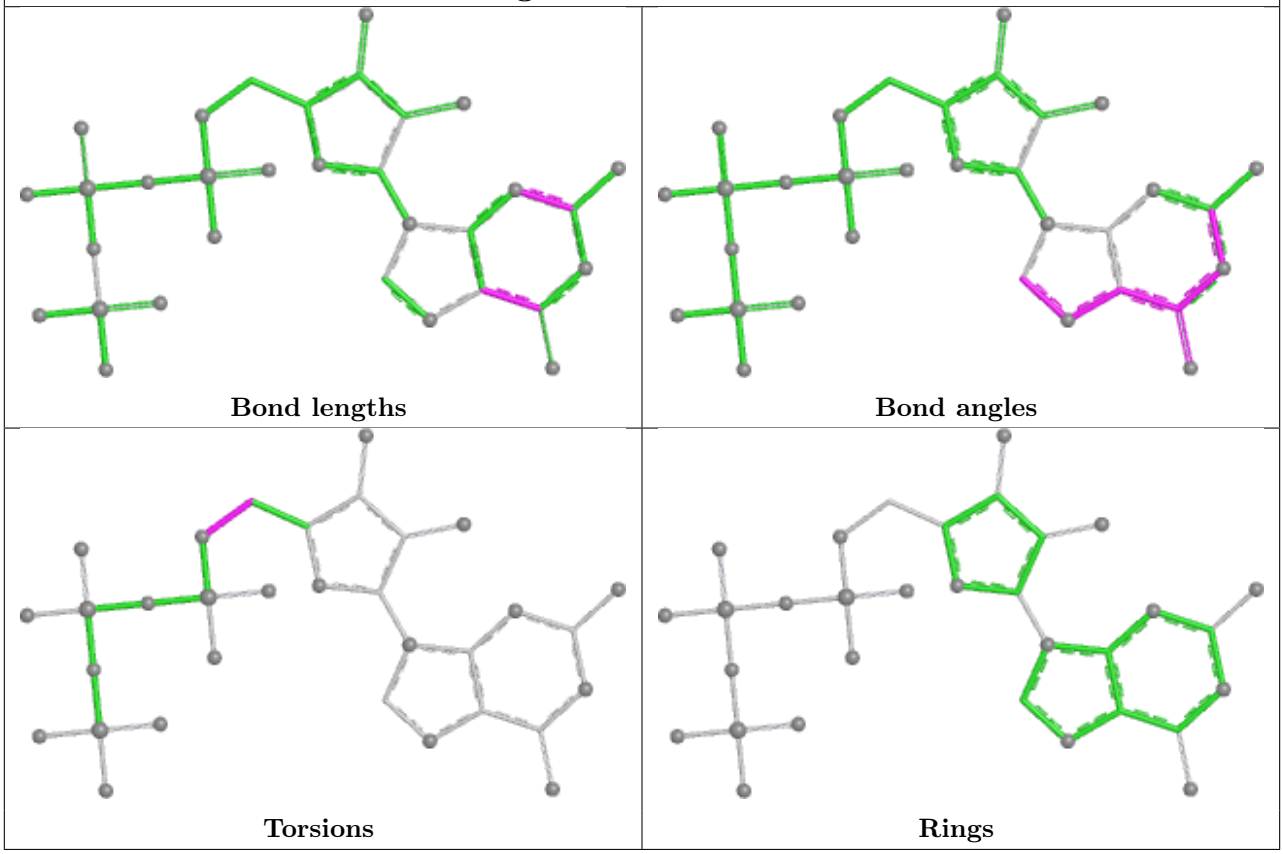

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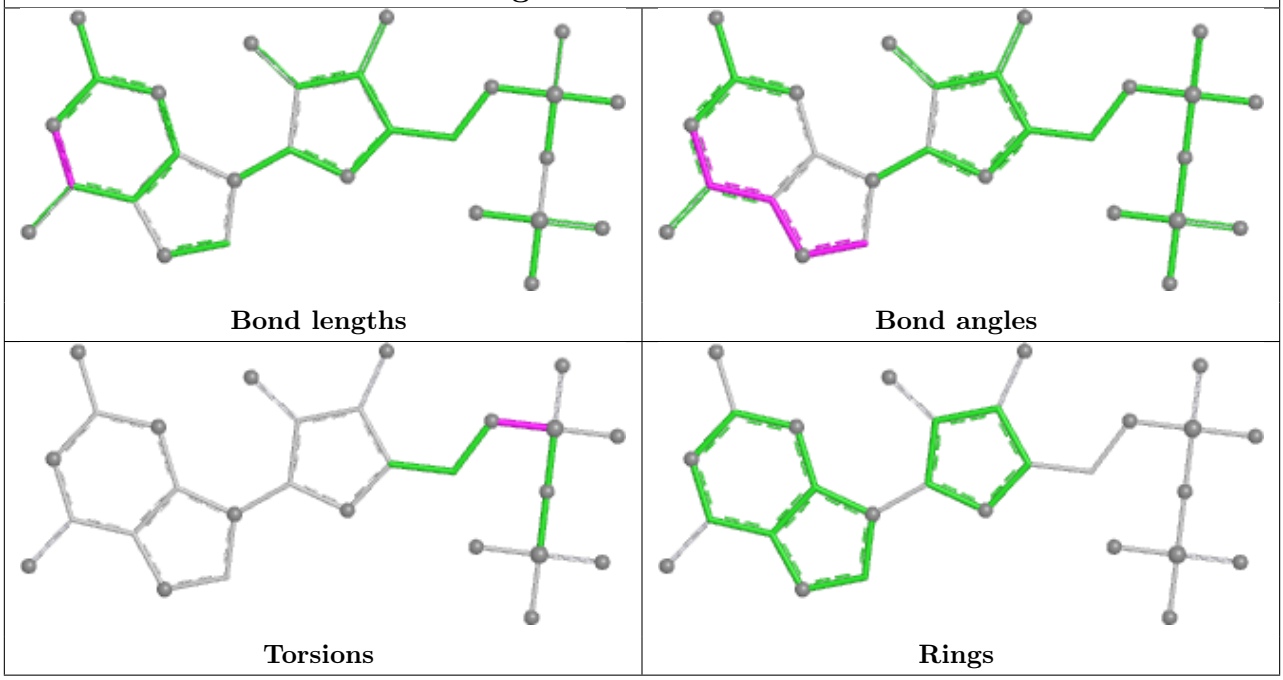

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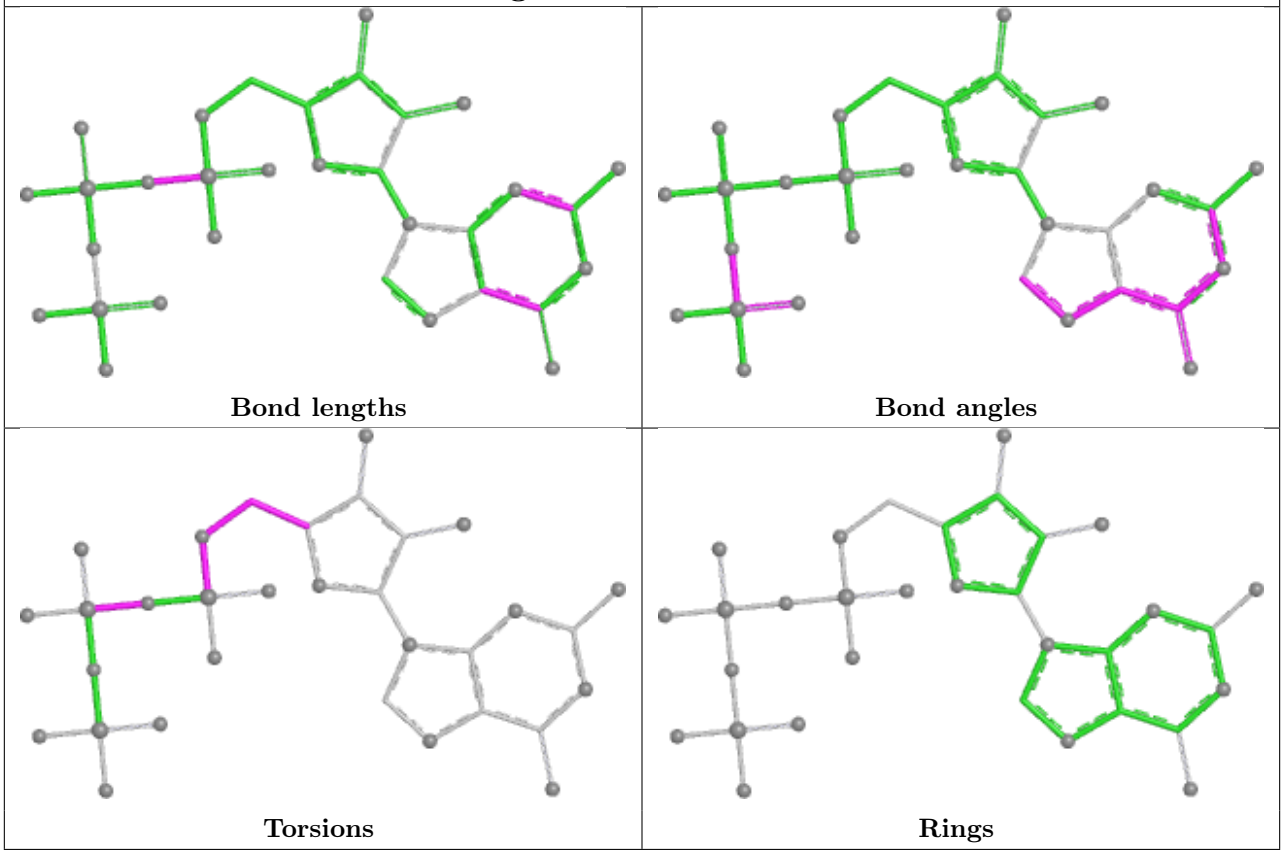

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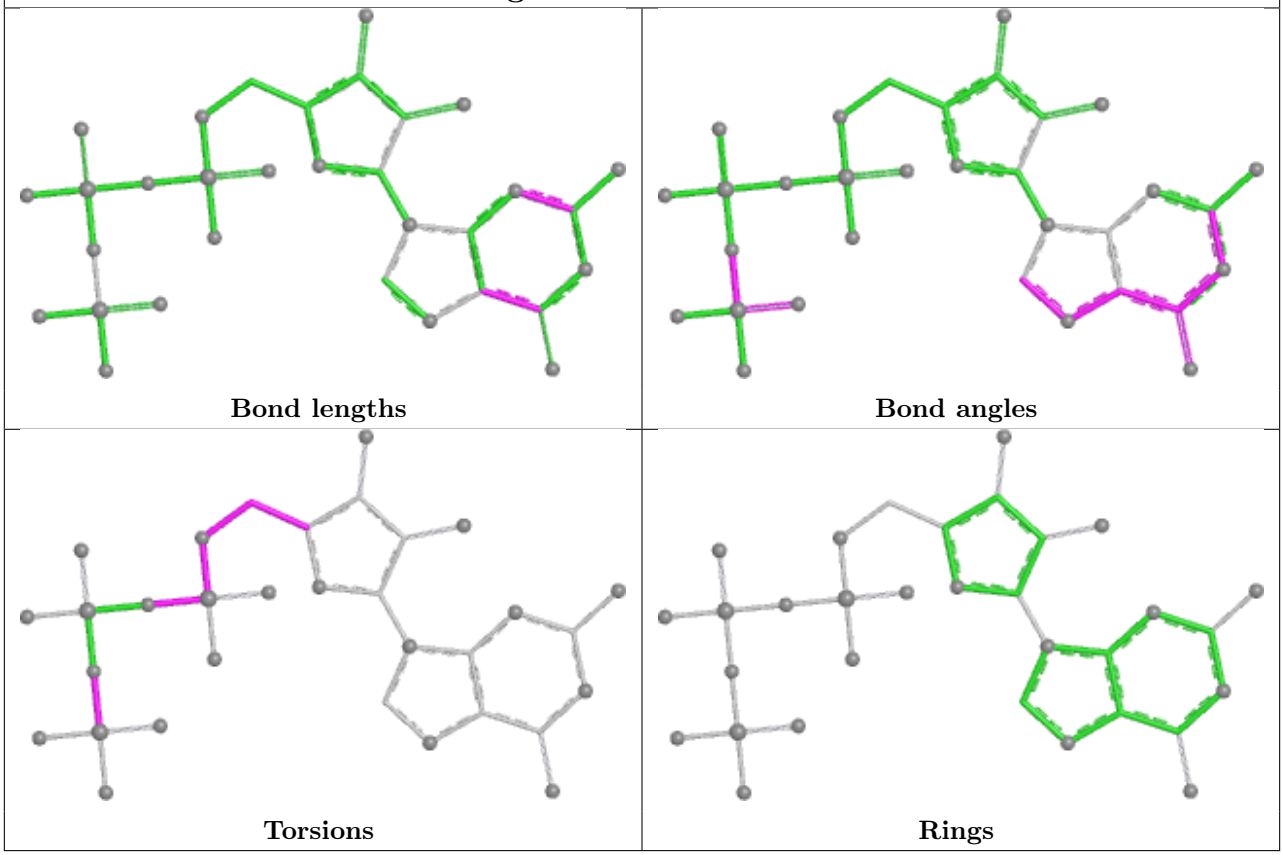

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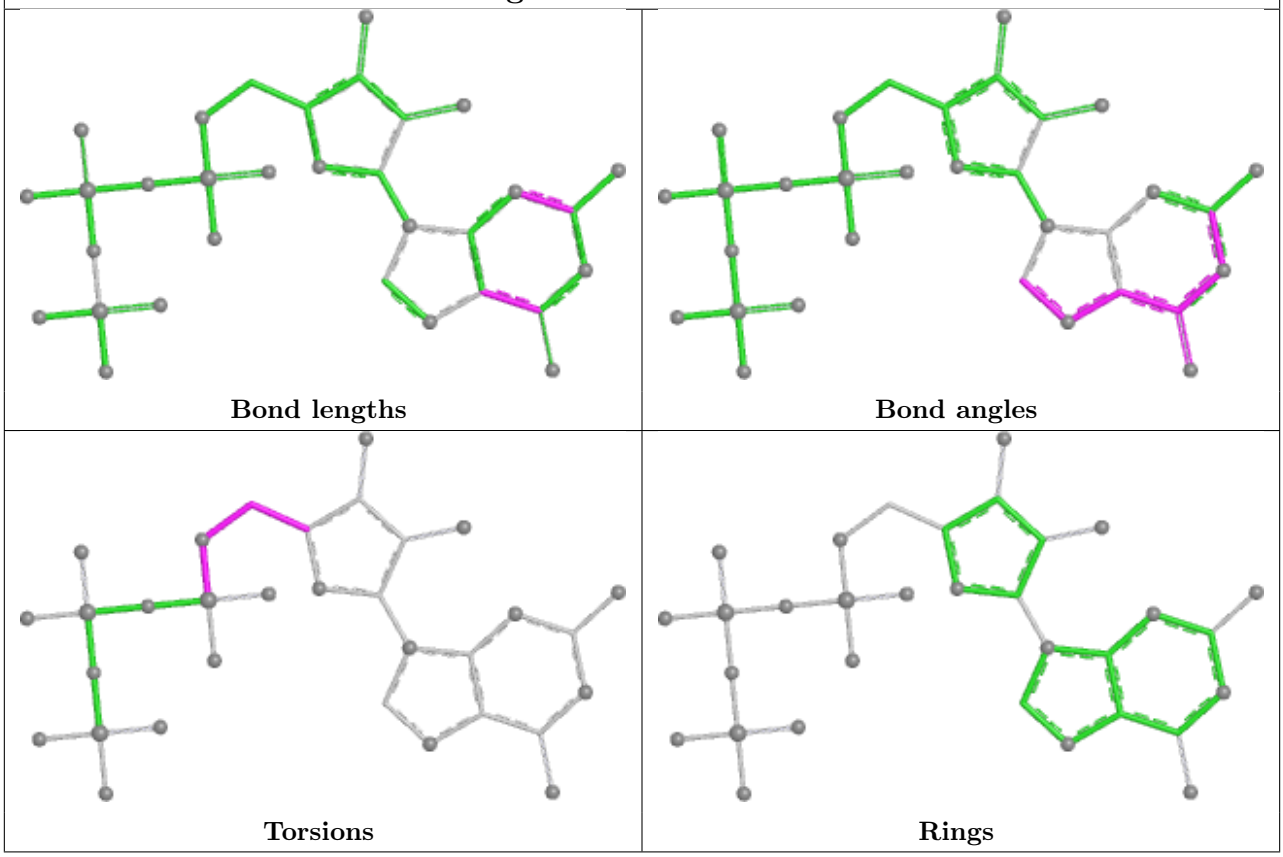

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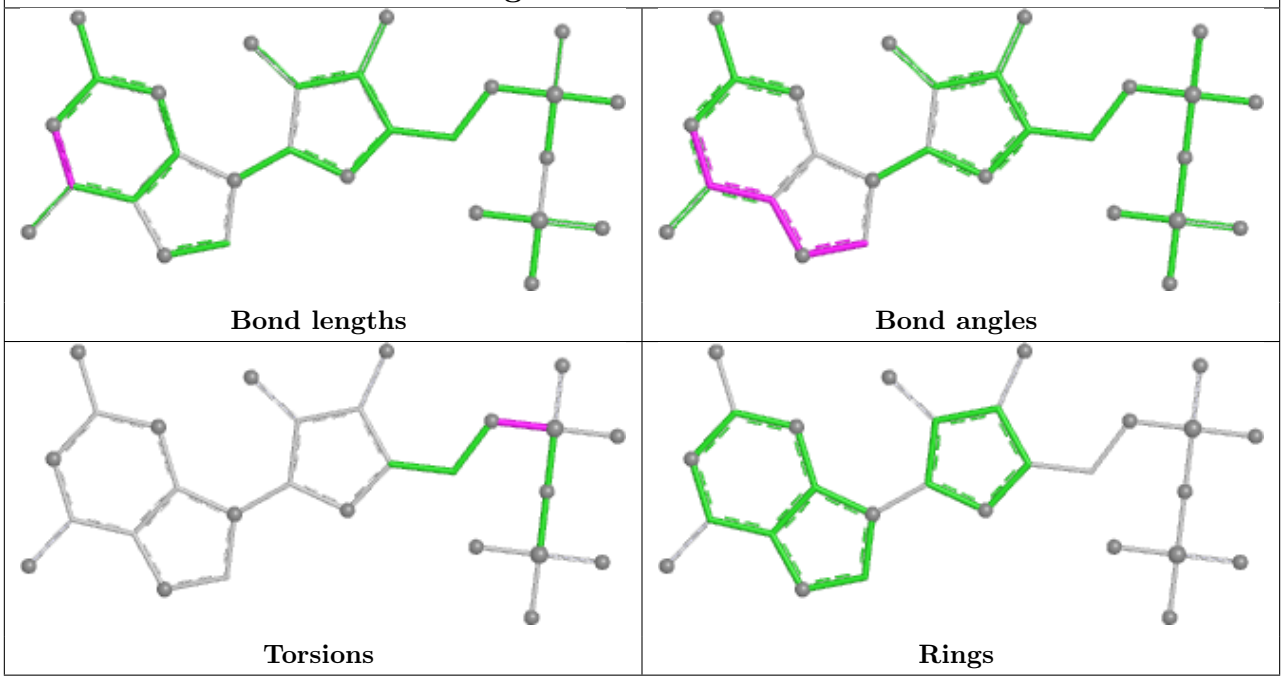

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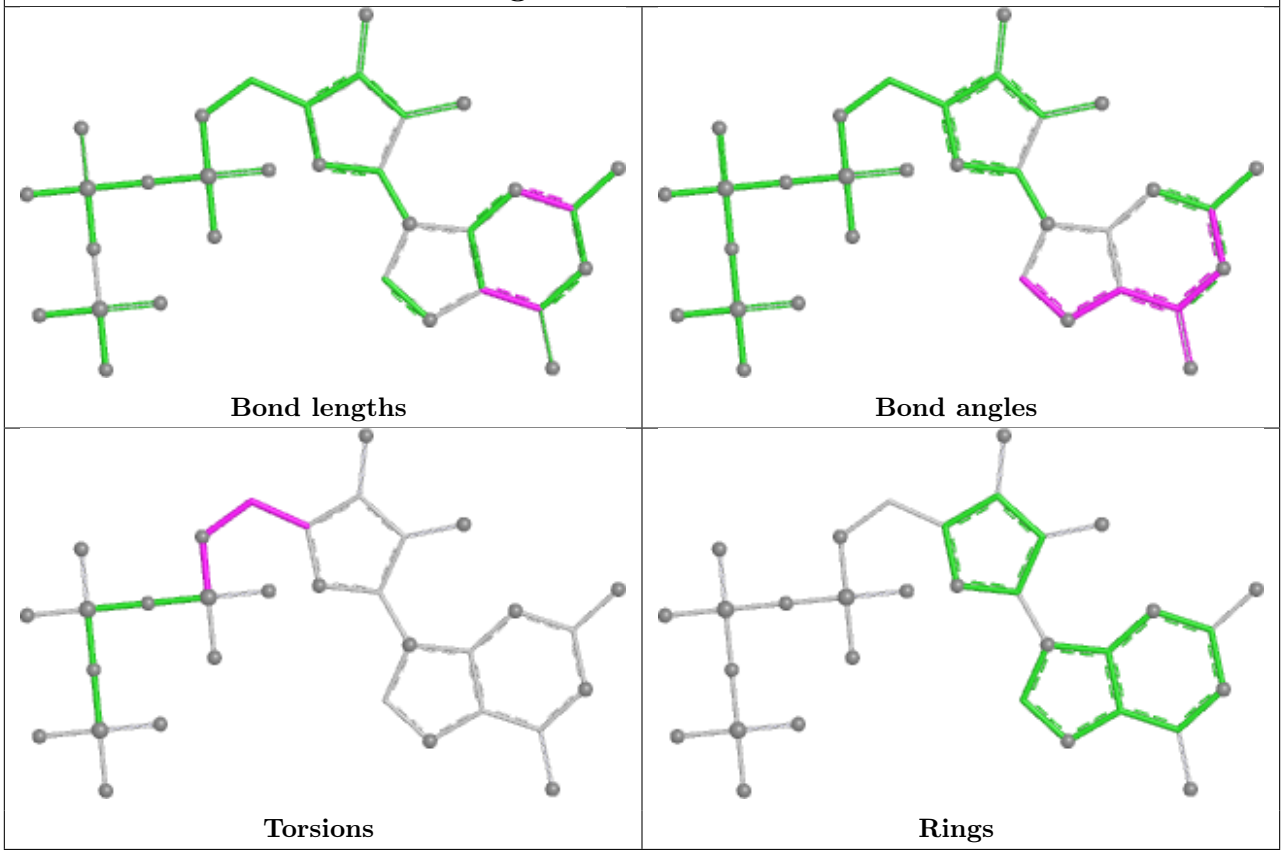

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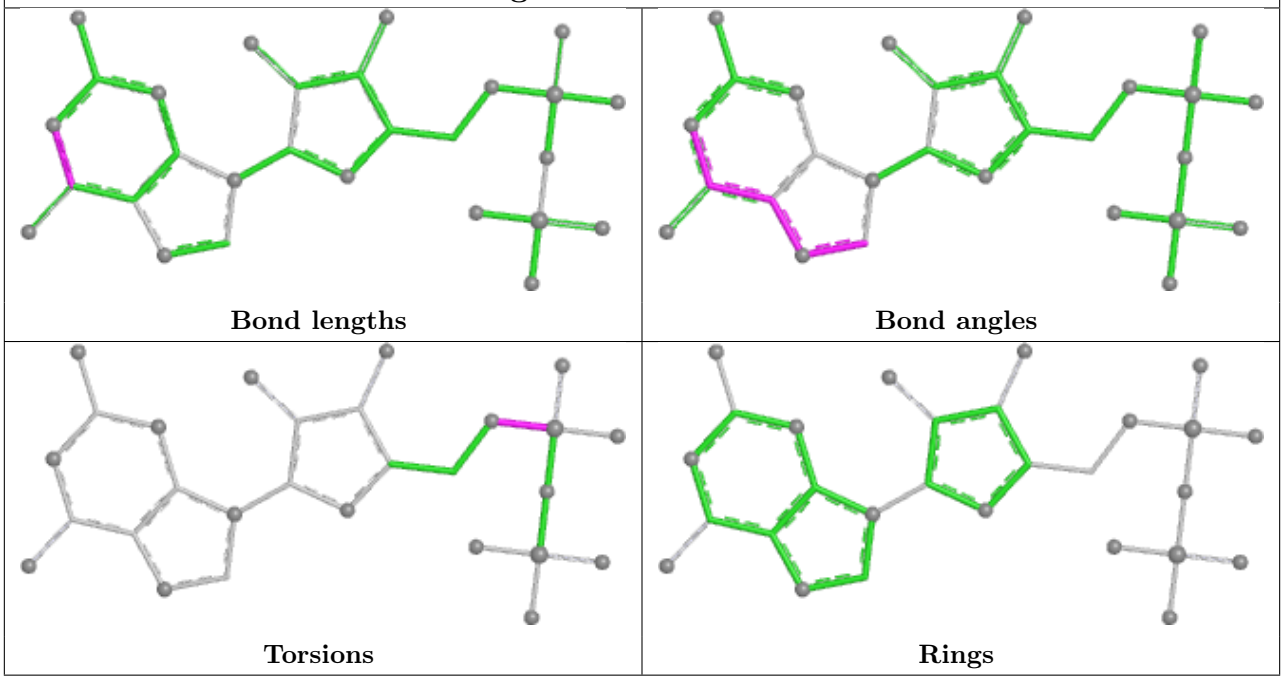

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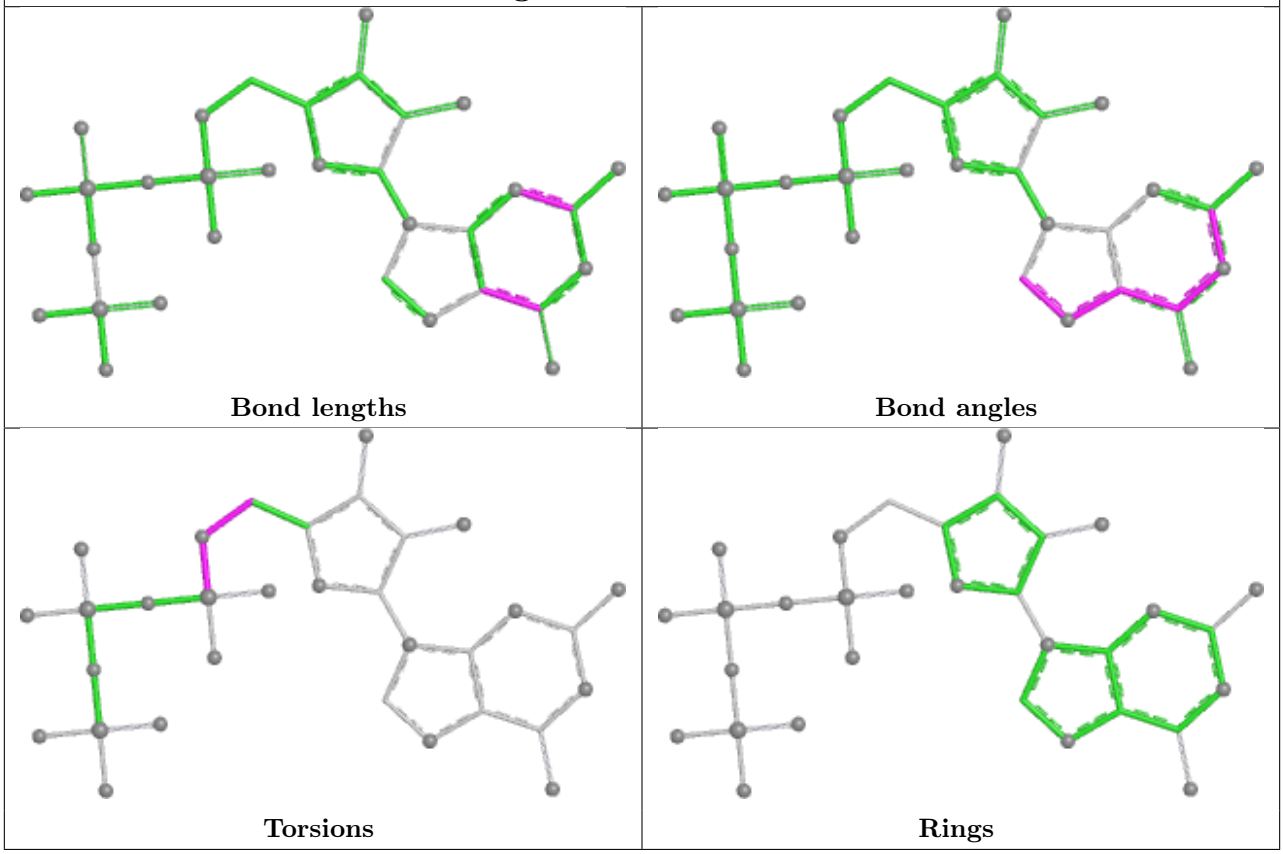

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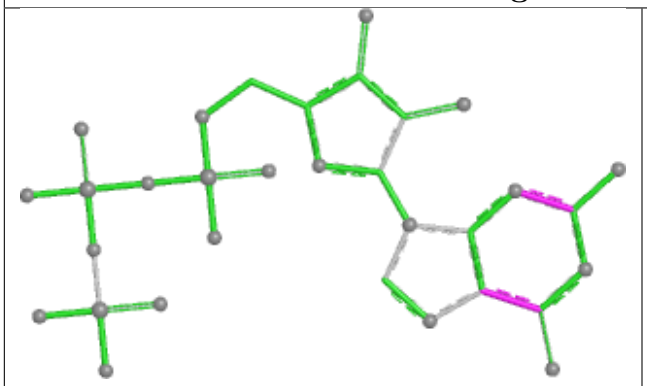
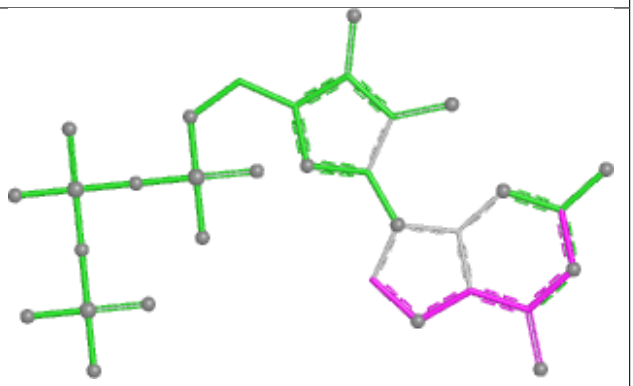
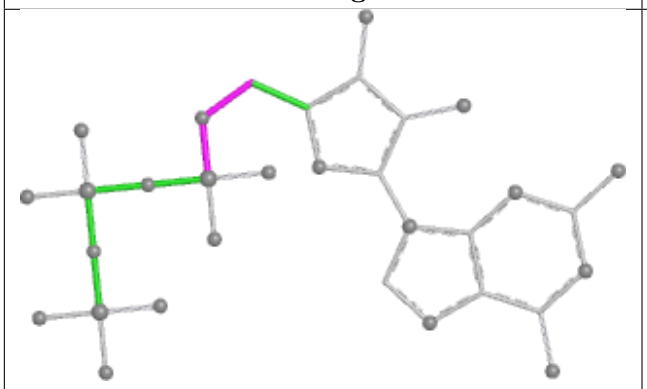


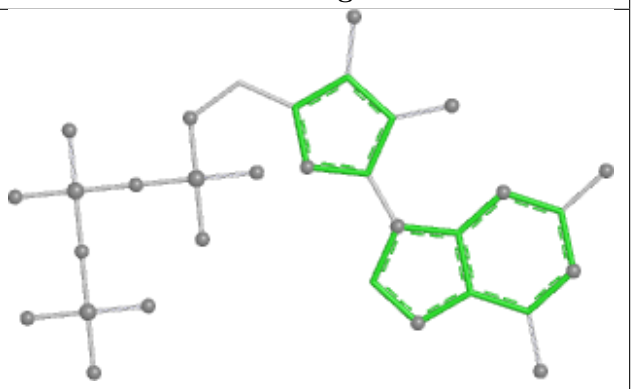
Bond lengths



Bond angles

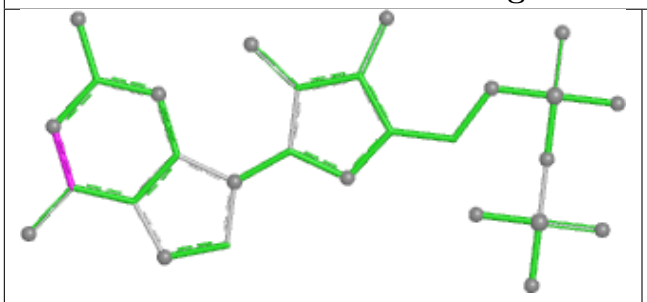


Torsions



Rings

Ligand GDP AH 501



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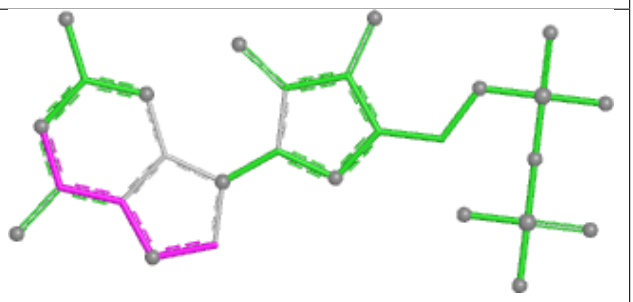
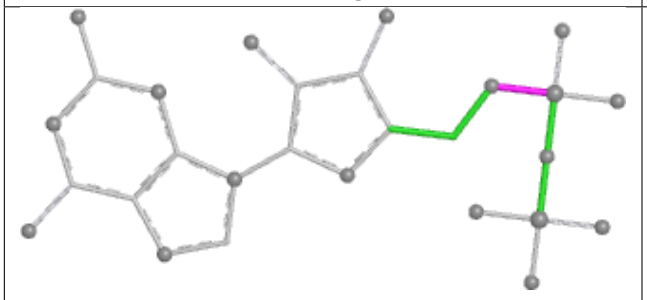
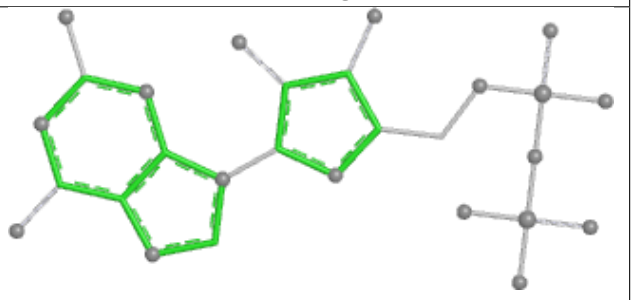


Bond angles

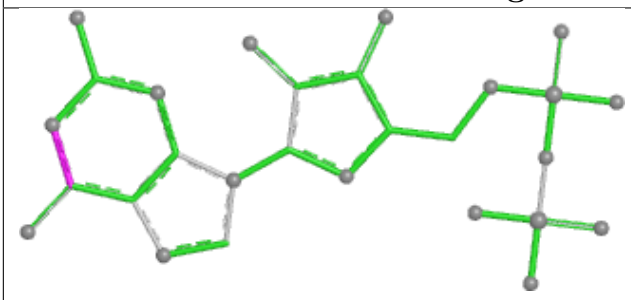


Torsions



Rings

Ligand GDP QD 501



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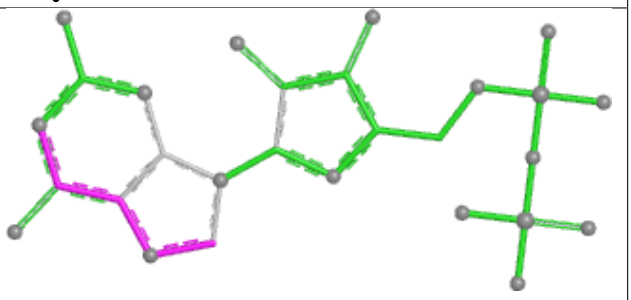
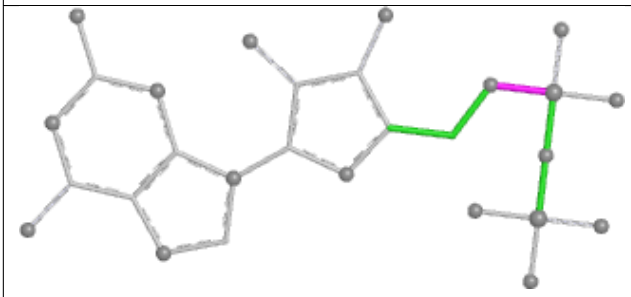


Bond angles



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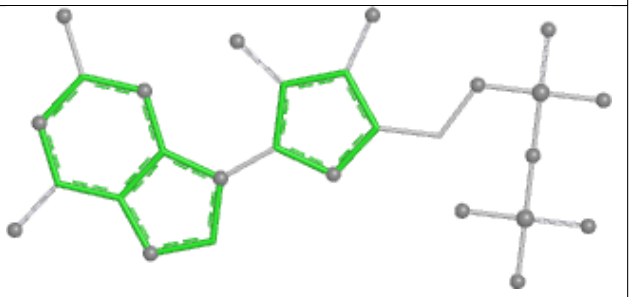
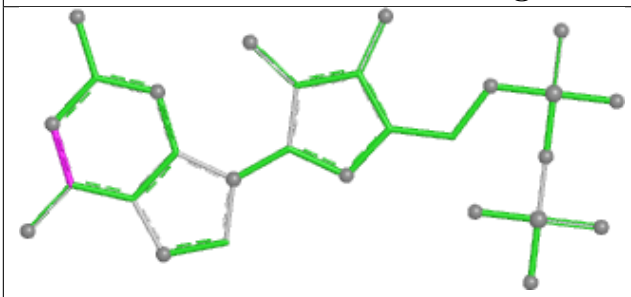


Rings

Ligand GDP SF 501



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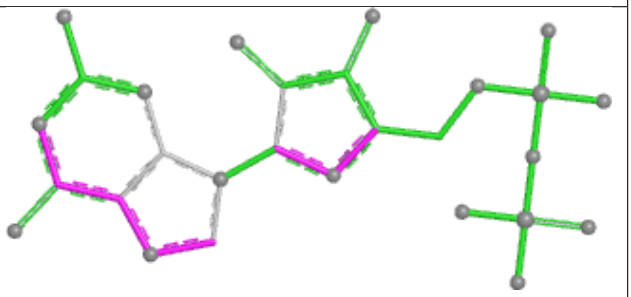

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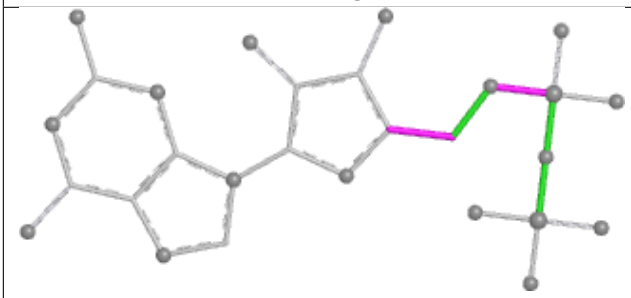
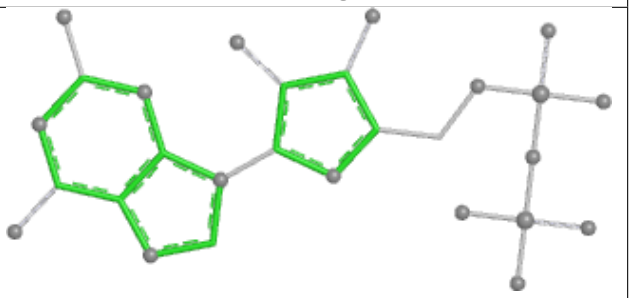
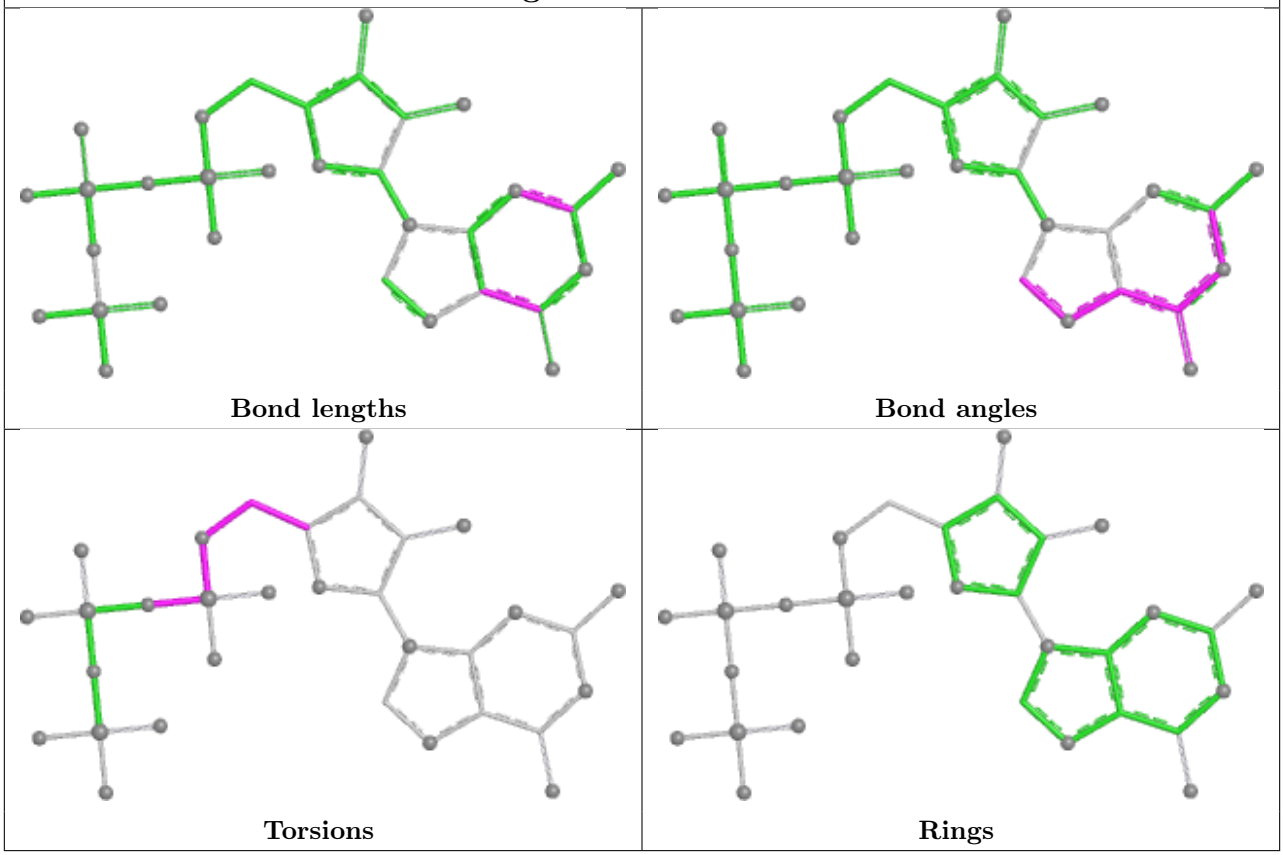


Torsions

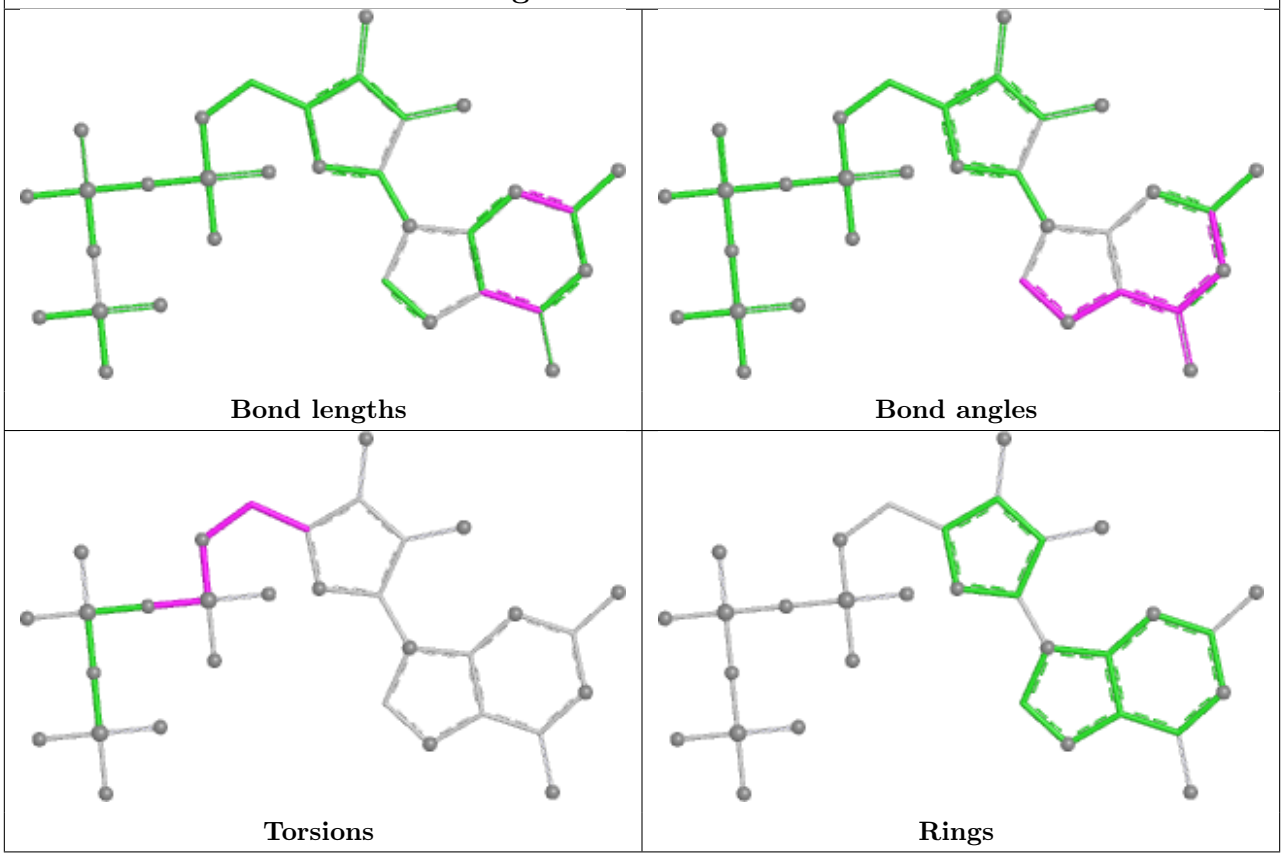


Rings

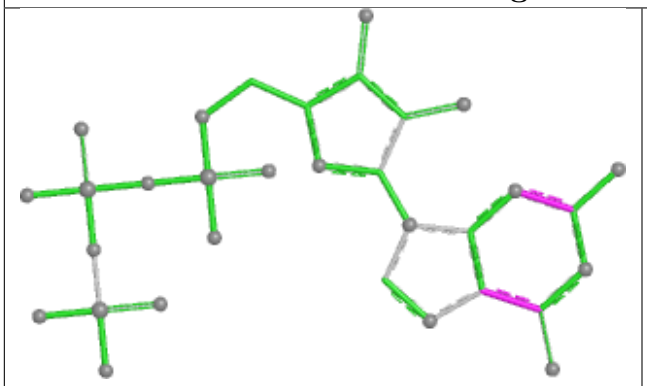
Ligand GTP II 501



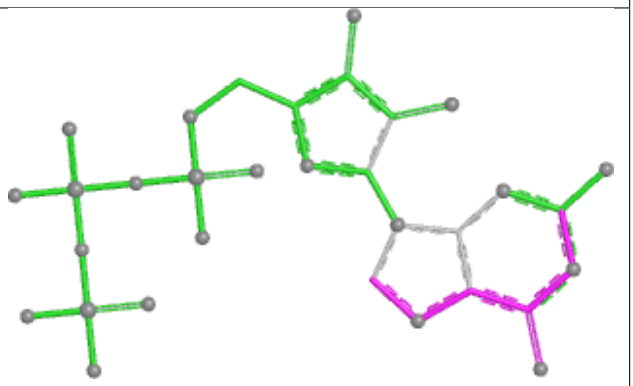
Ligand GTP TA 501



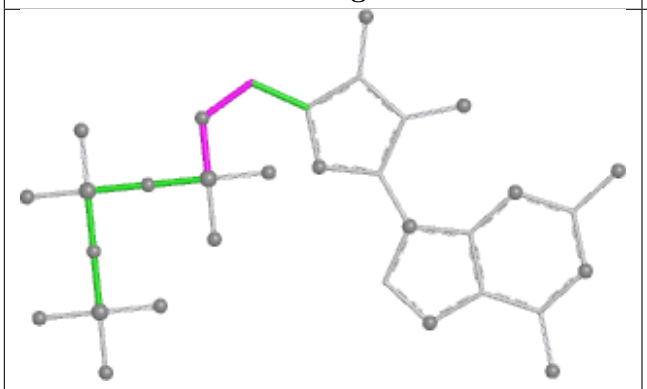
Ligand GTP OB 501



Bond lengths



Bond angles



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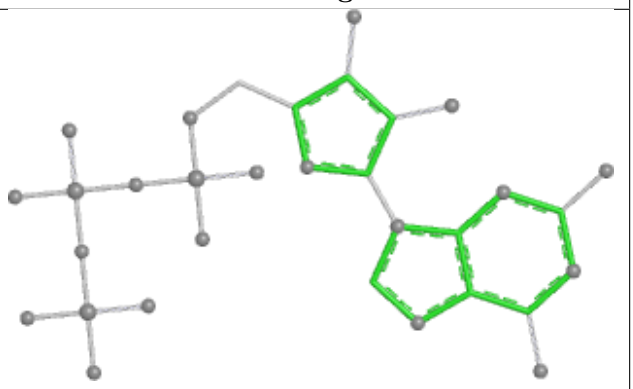
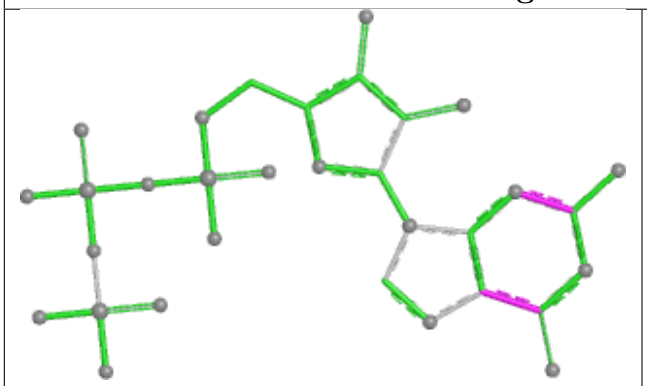


Rings

Ligand GTP QI 501



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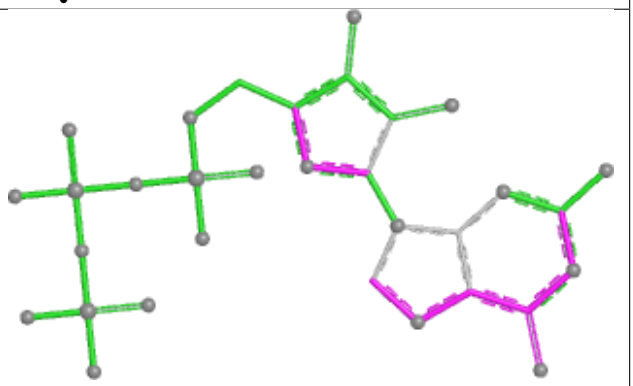
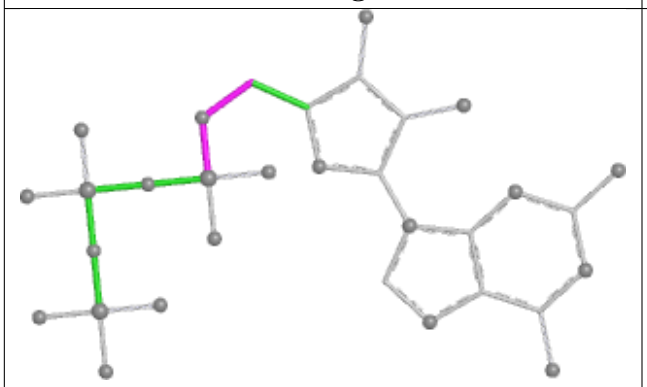


Bond angles



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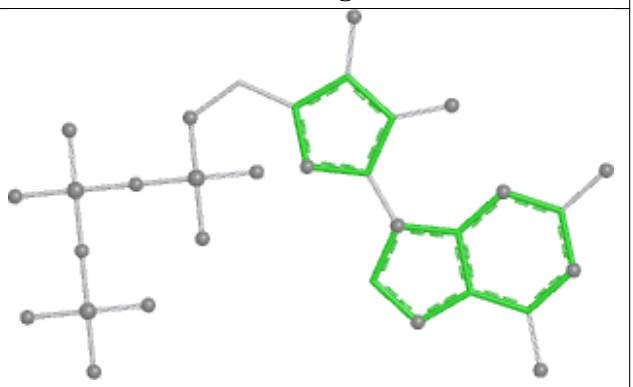
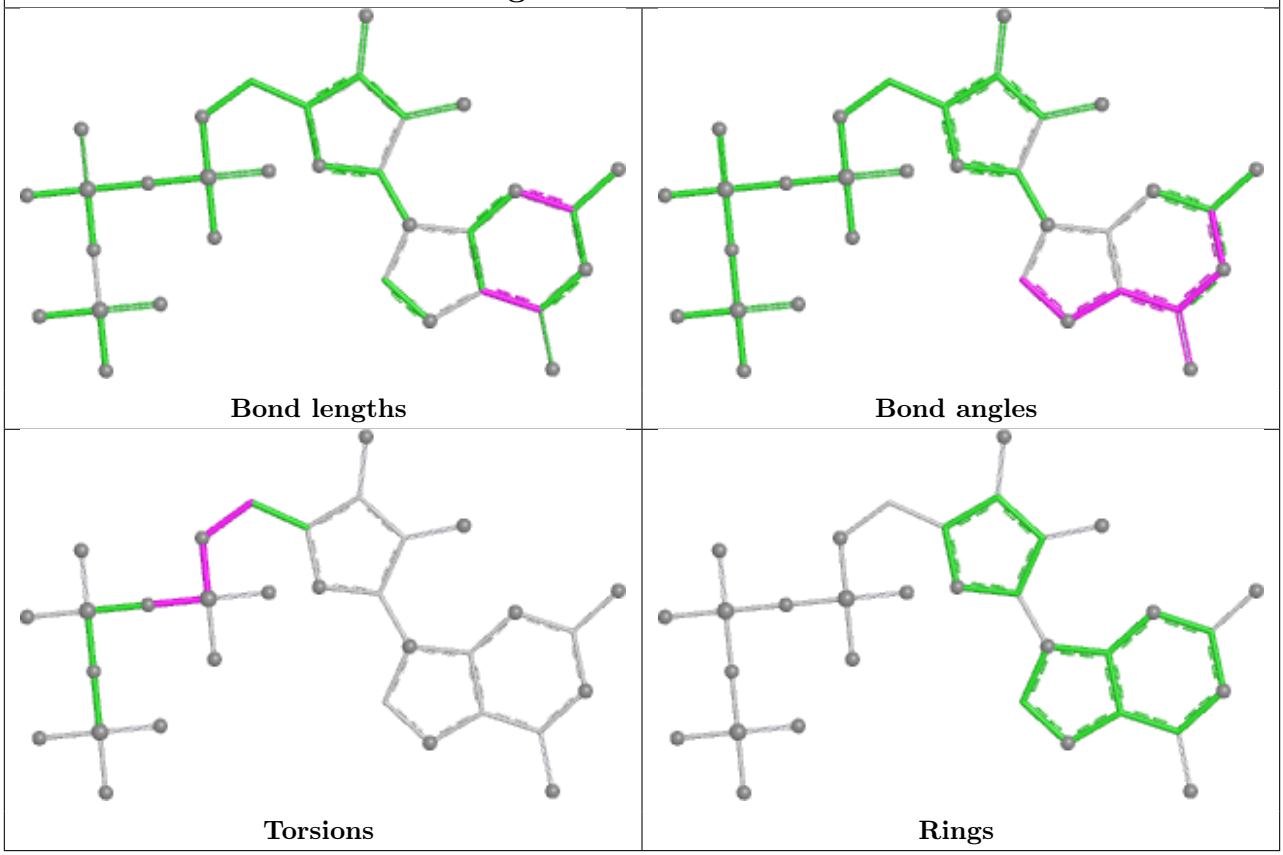
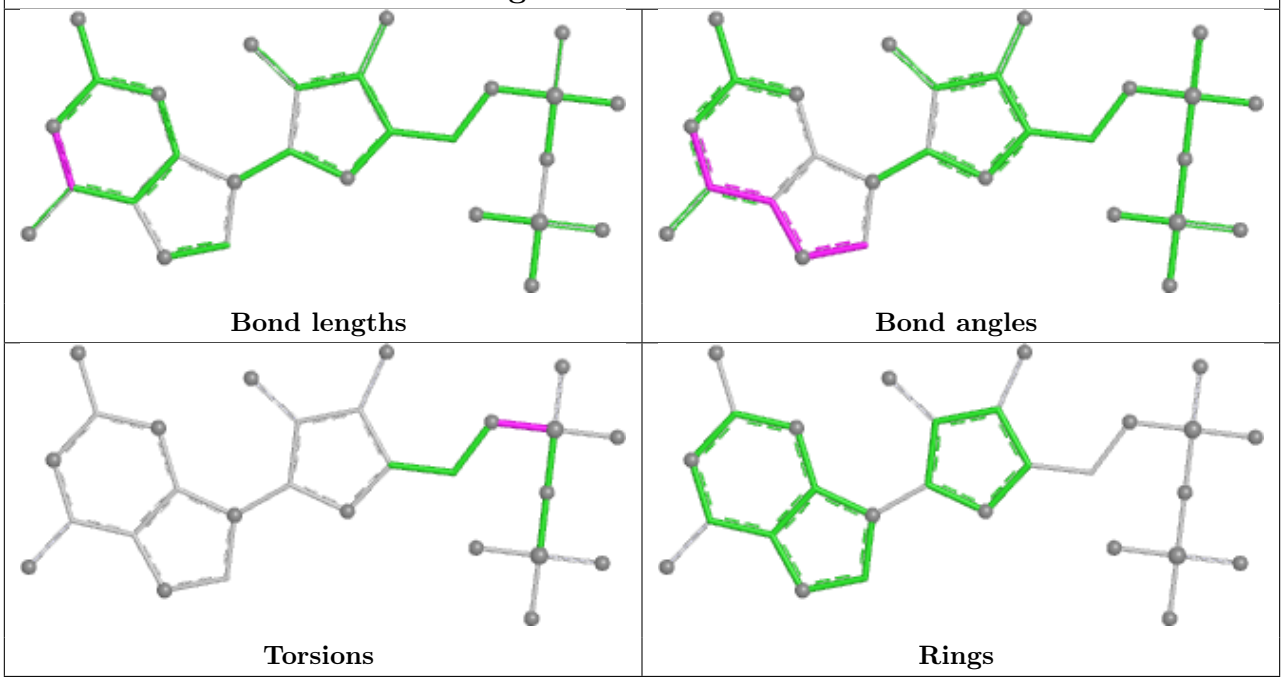


Rings

Ligand GTP ME 501



Ligand GDP UC 501



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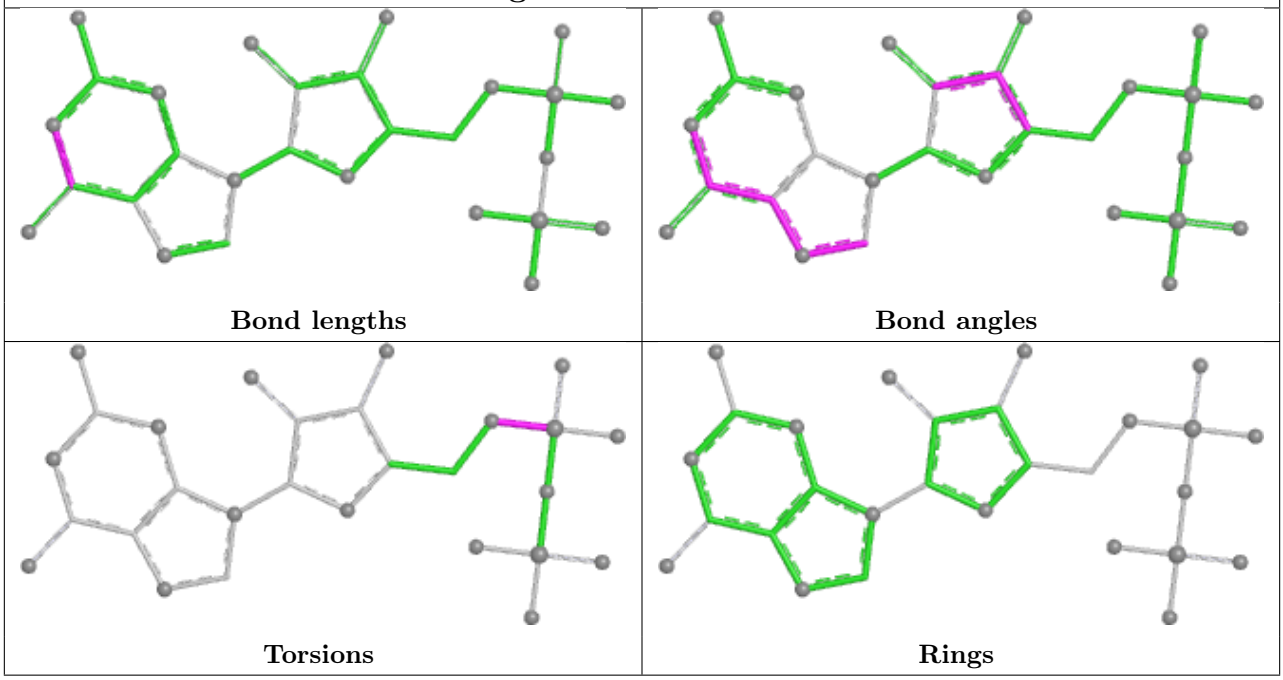

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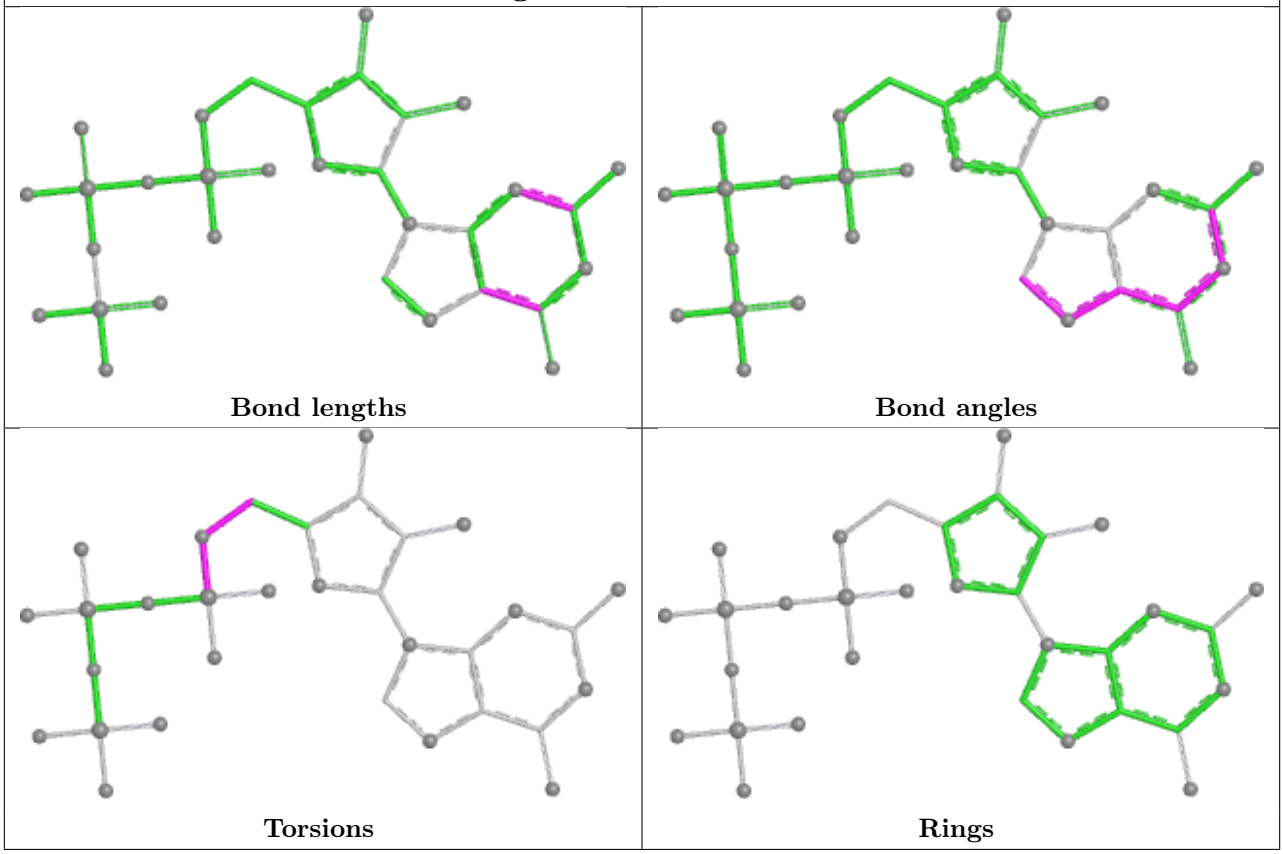

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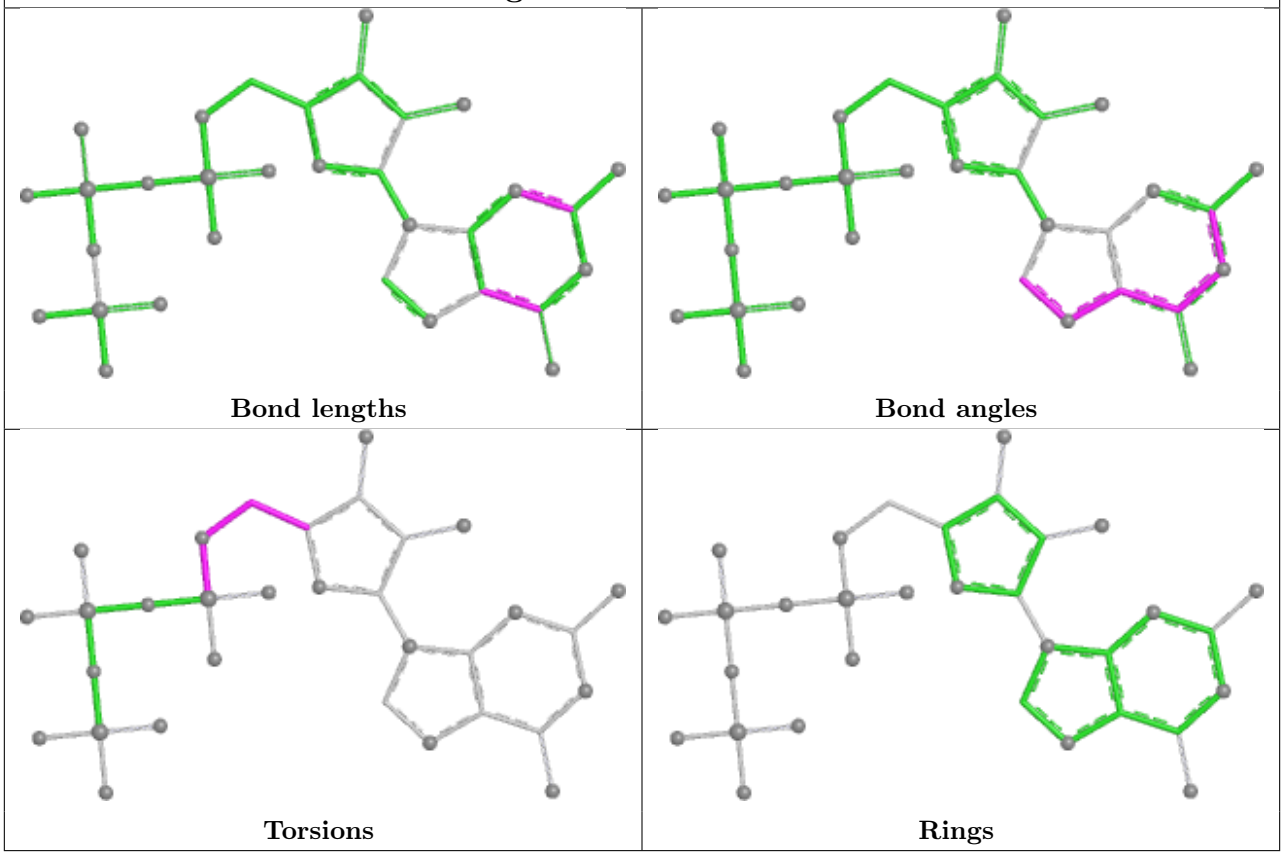

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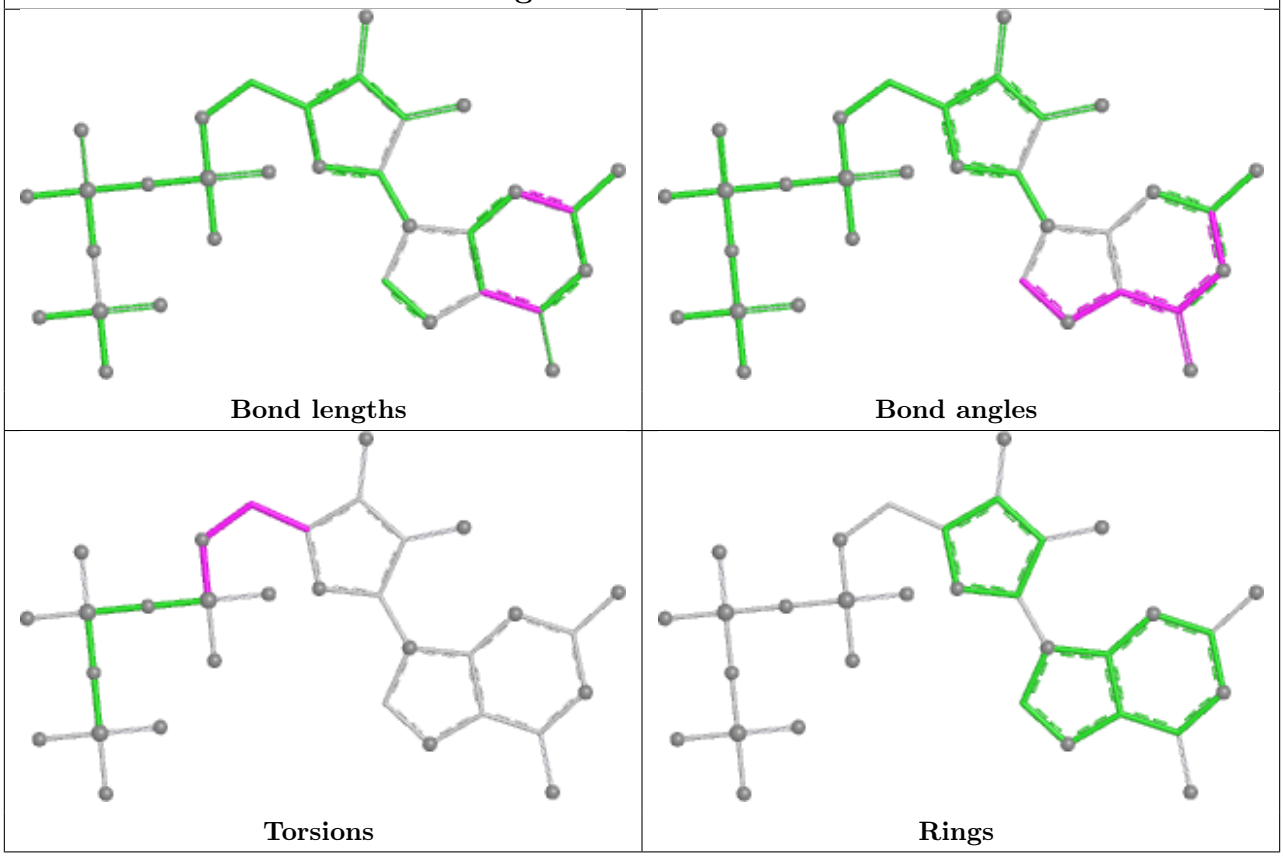

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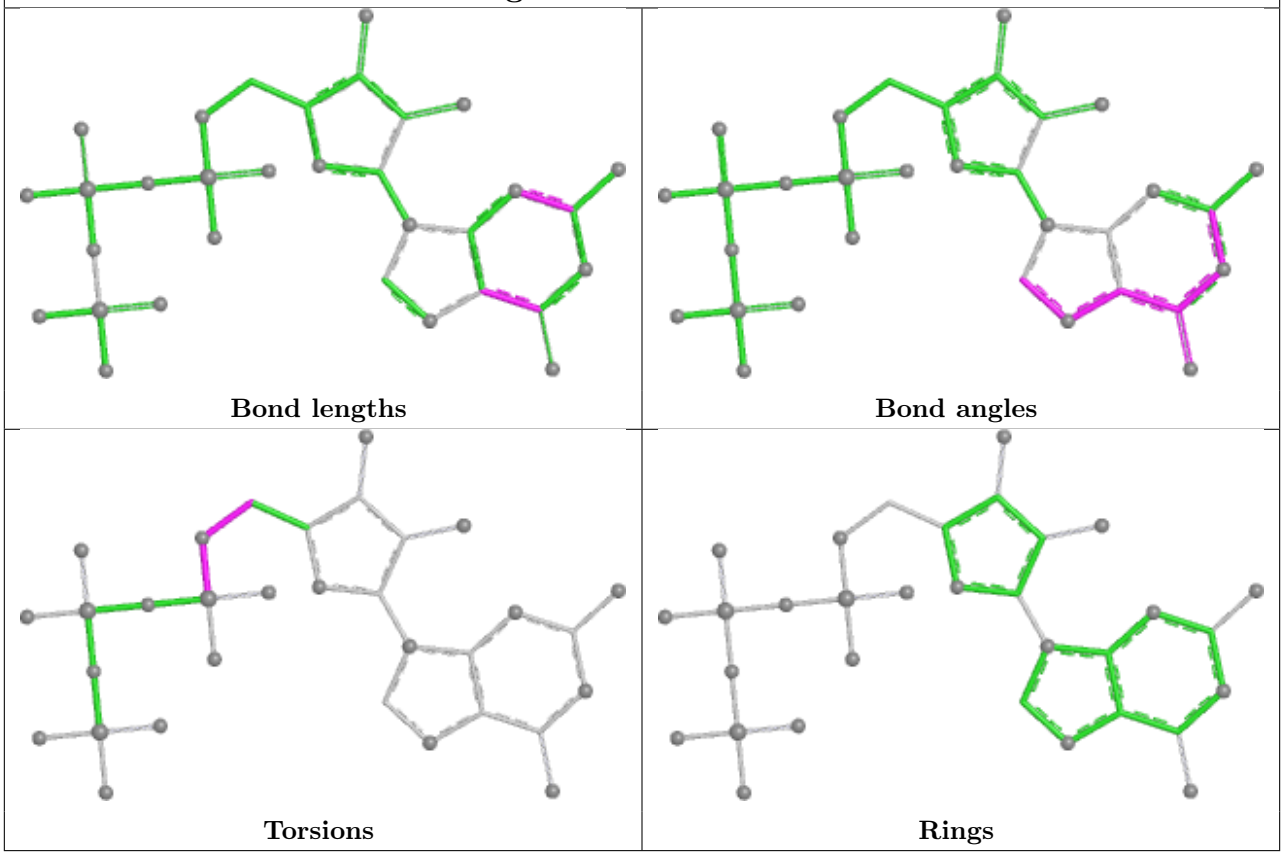

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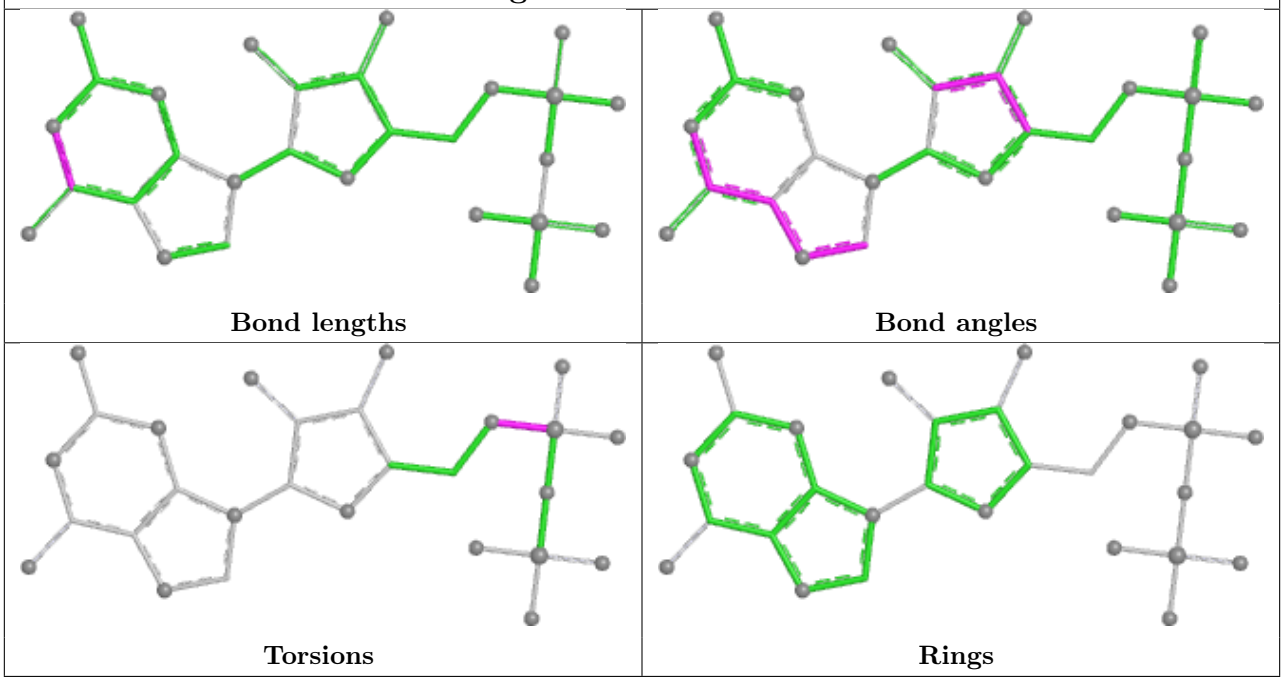
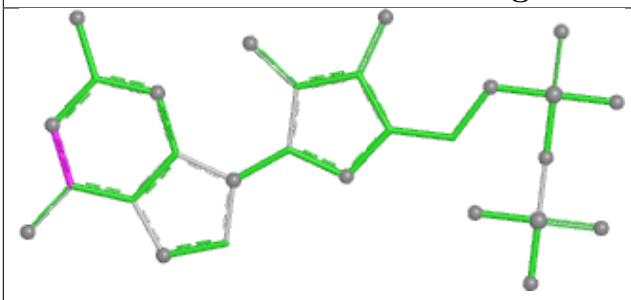
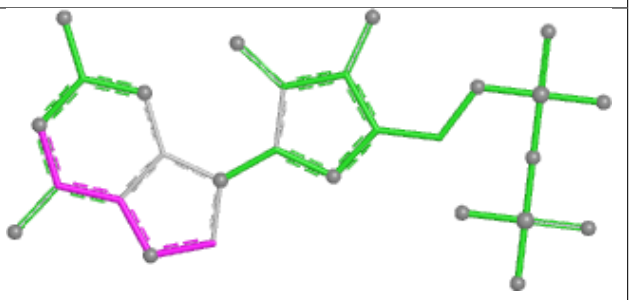


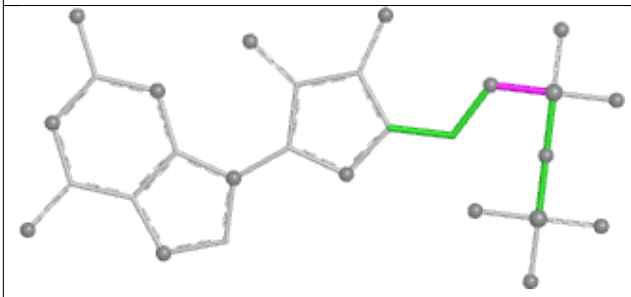
Ligand GDP AJ 501



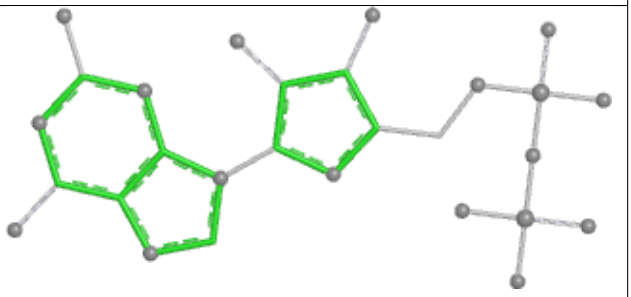
Bond lengths



Bond angles

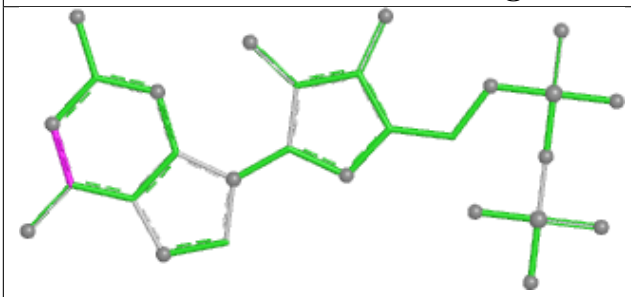


Torsions



Rings

Ligand GDP WF 501



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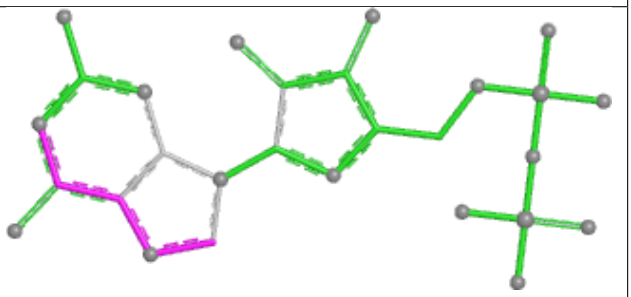

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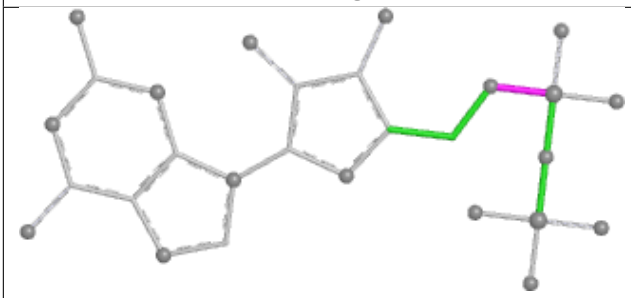

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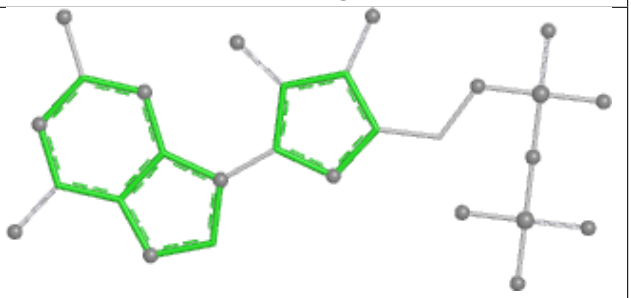
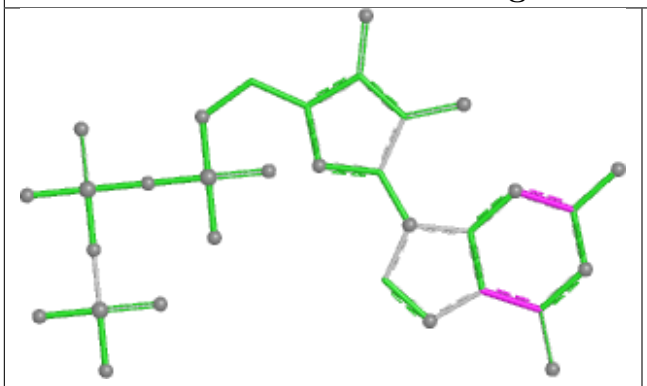


Rings

Ligand GTP KK 501



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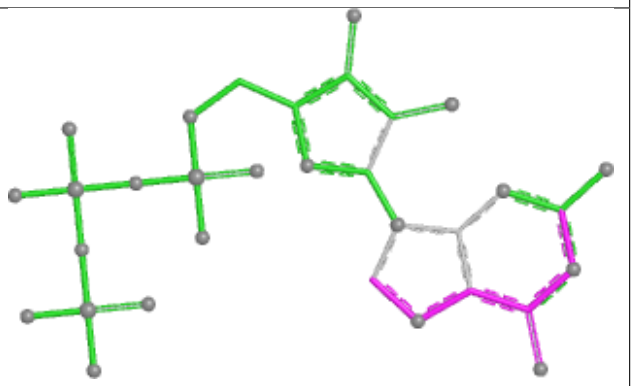
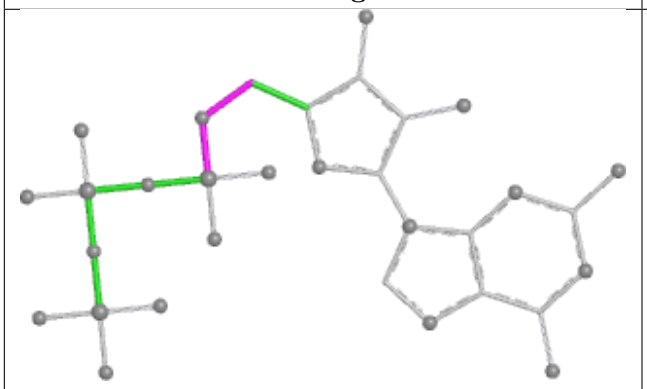


Bond angles



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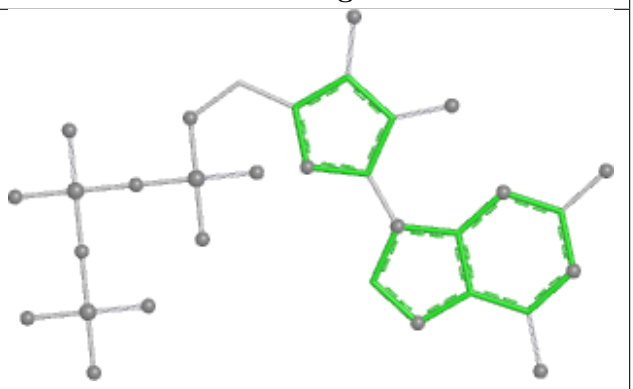
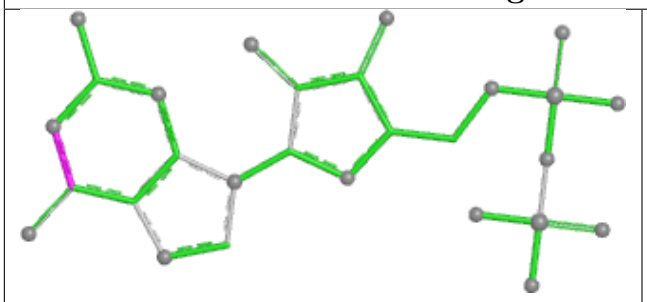


Rings

Ligand GDP FM 501



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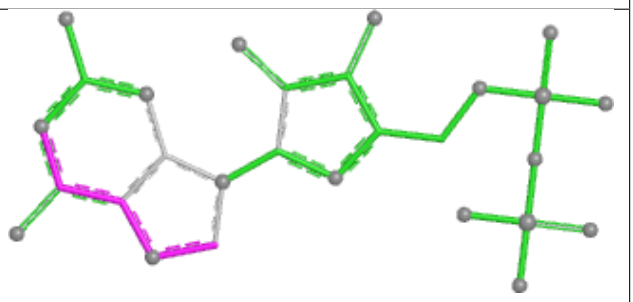
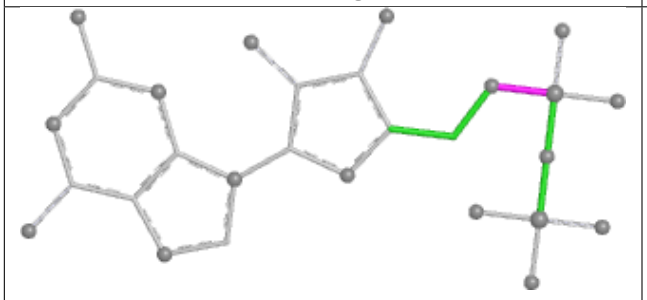


Bond angles



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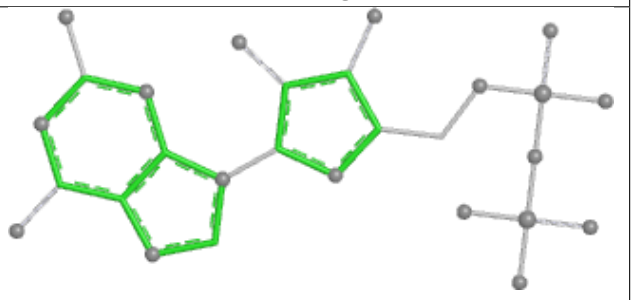
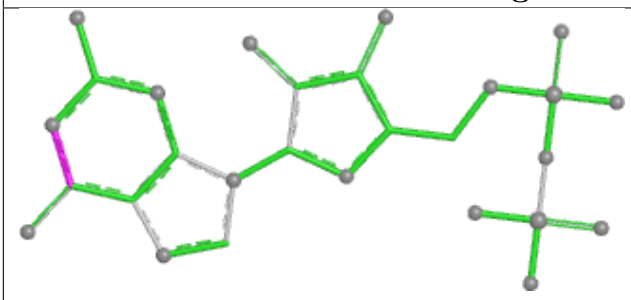


Rings

Ligand GDP RJ 501



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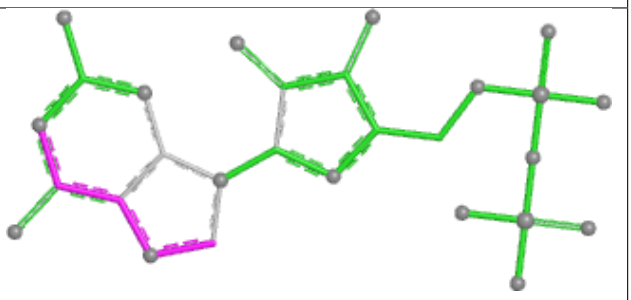

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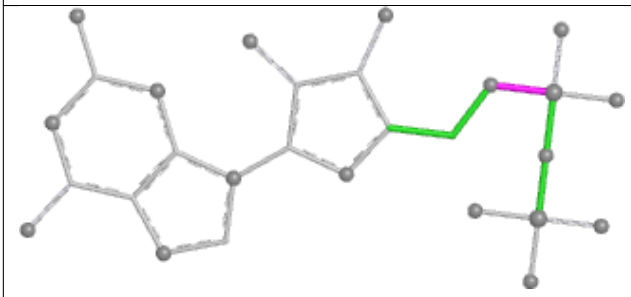

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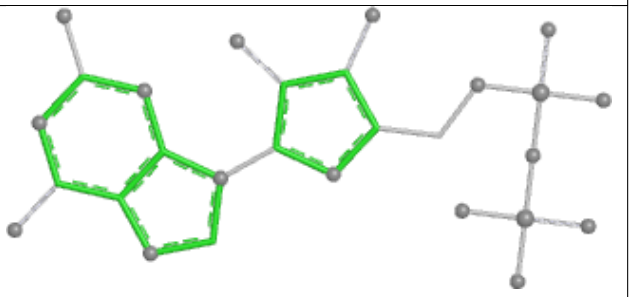
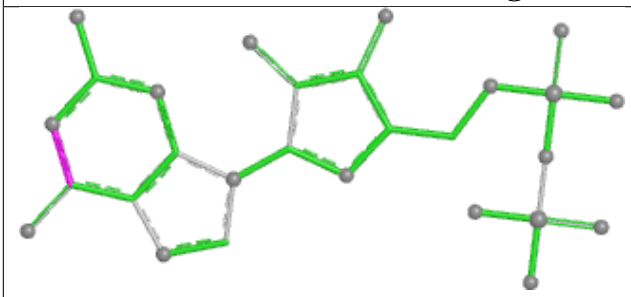


Rings

Ligand GDP EM 501



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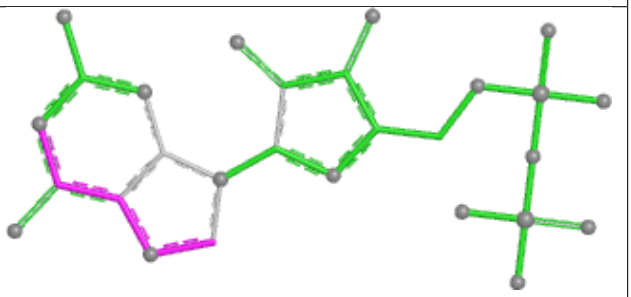

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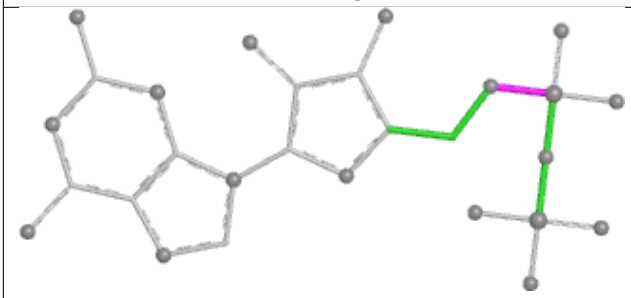

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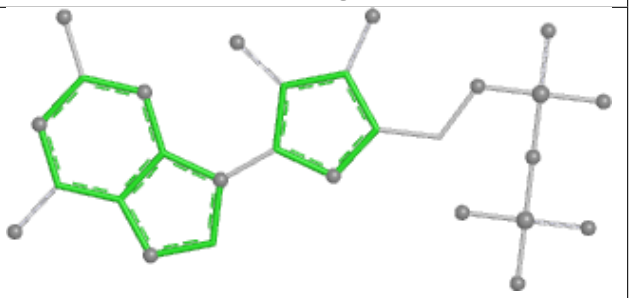
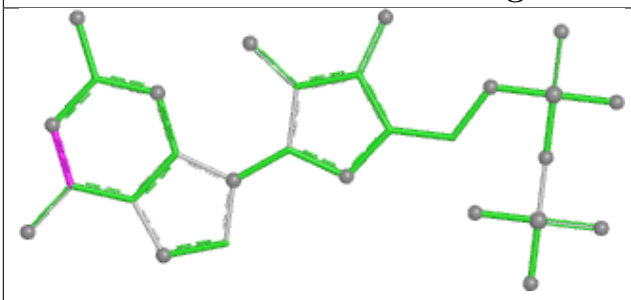


Rings

Ligand GDP KD 501



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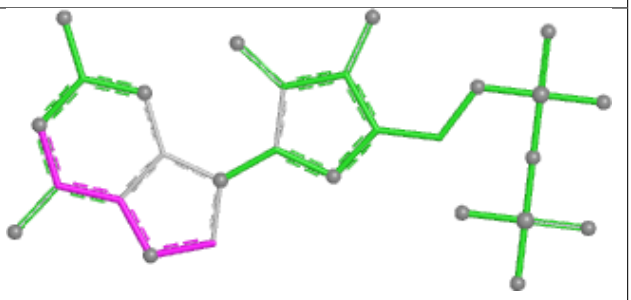
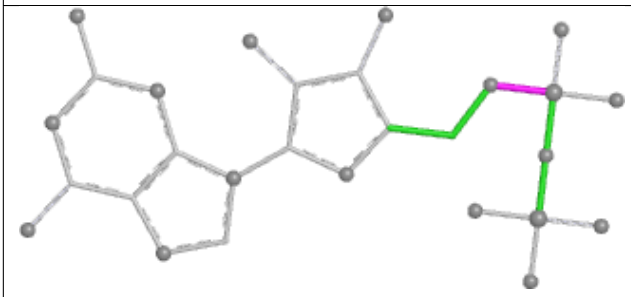


Bond angles



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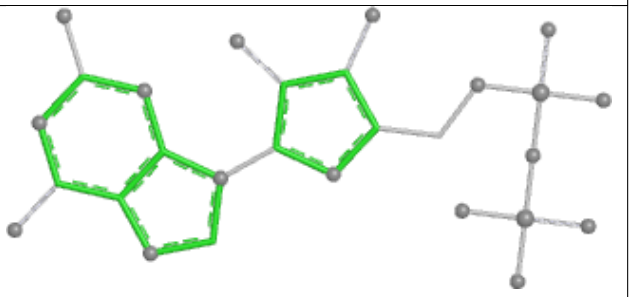
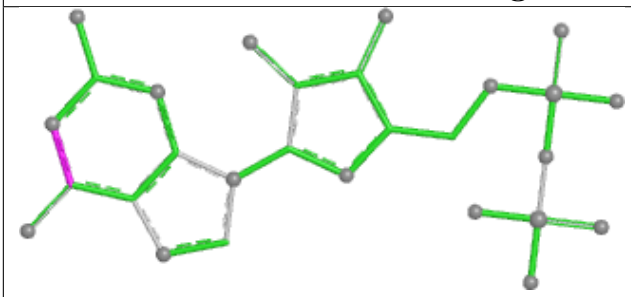


Rings

Ligand GDP UF 501



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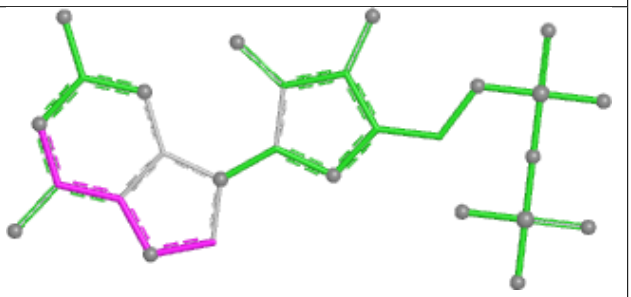

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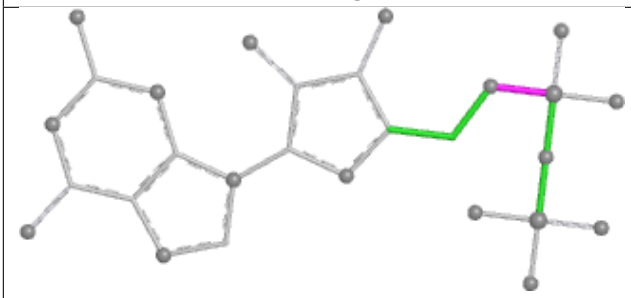

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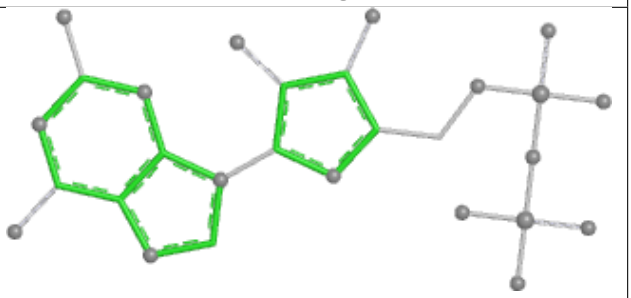
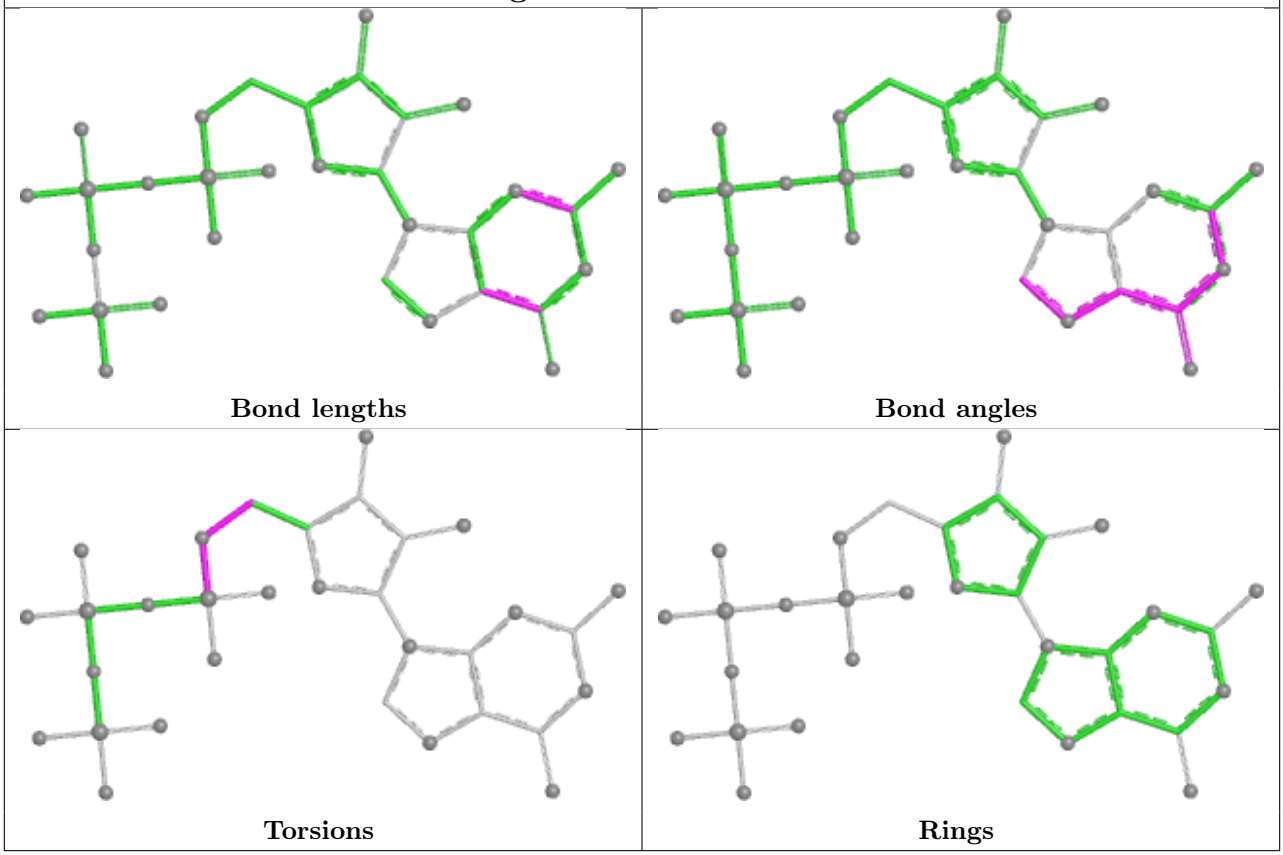
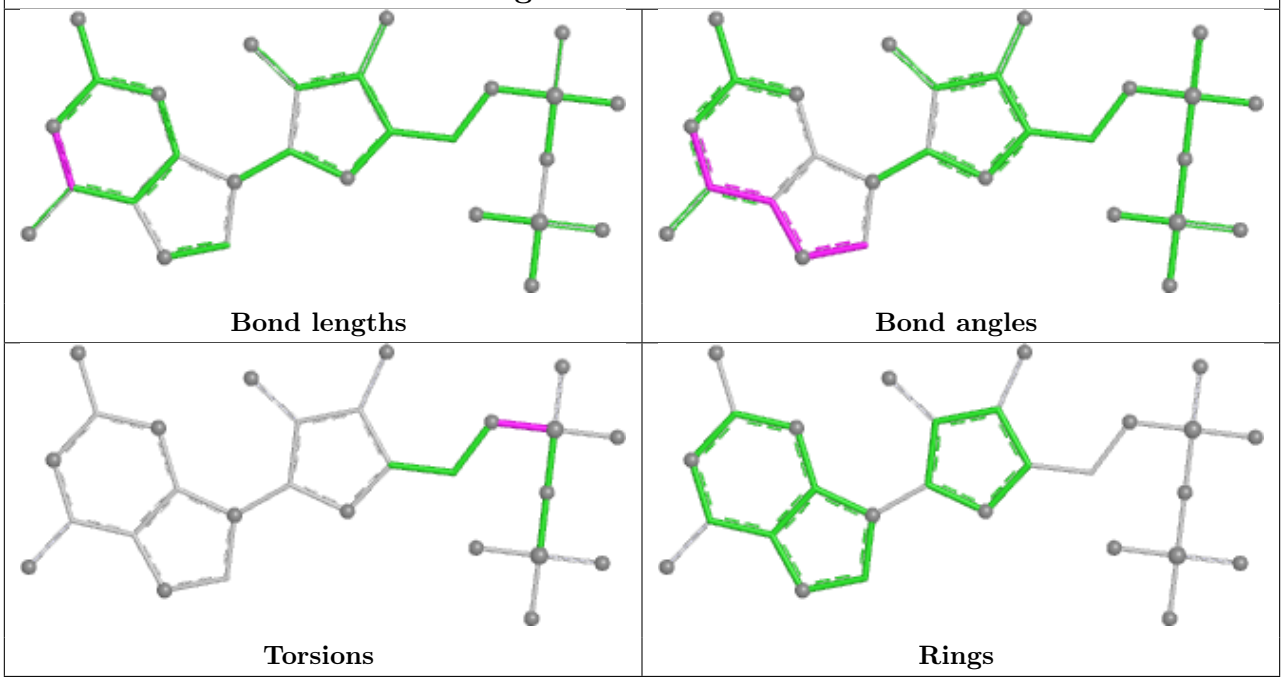


Rings

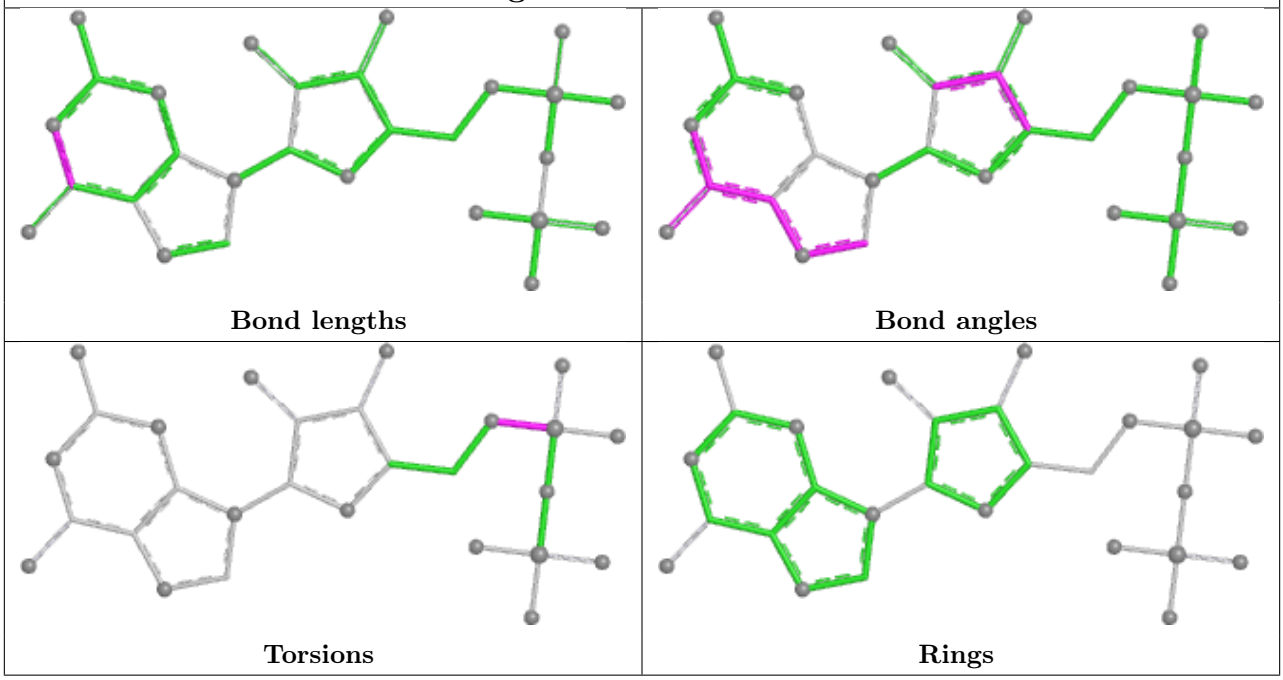
Ligand GTP RA 501



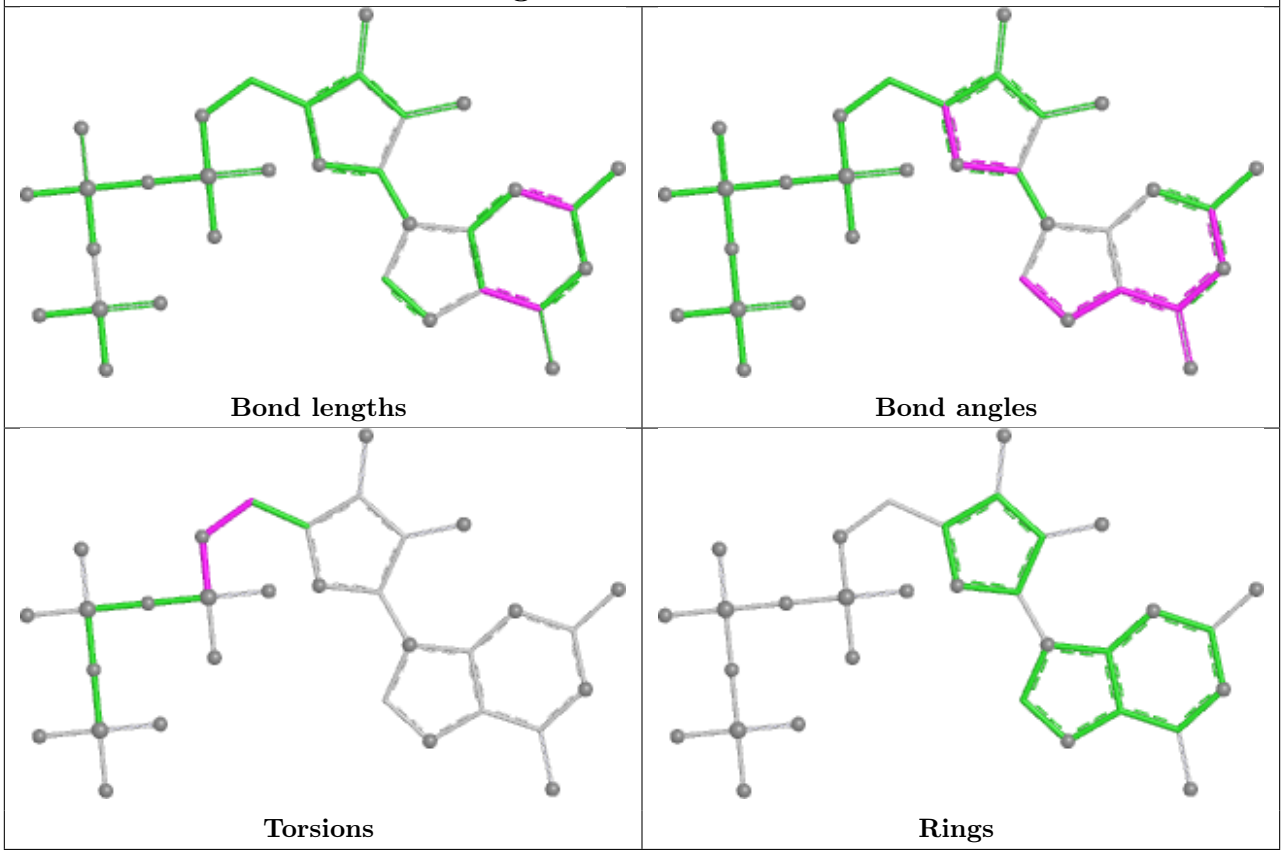
Ligand GDP SL 501



Ligand GDP VD 501



Ligand GTP PA 501



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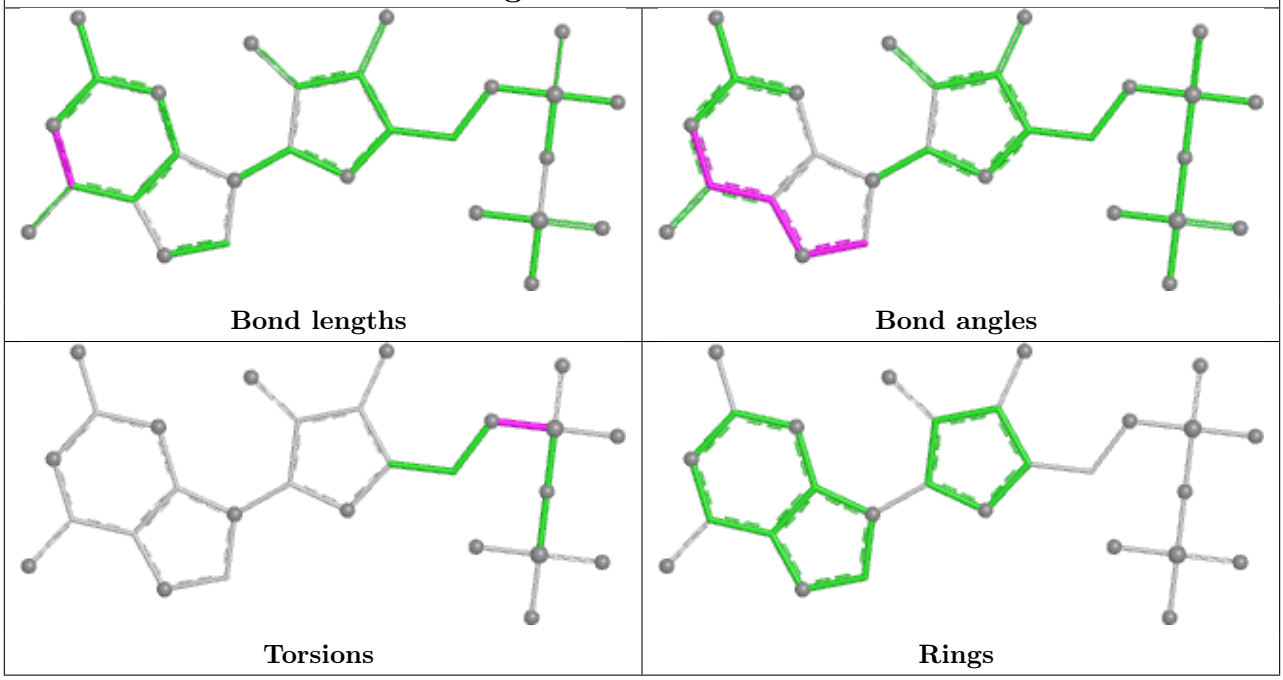

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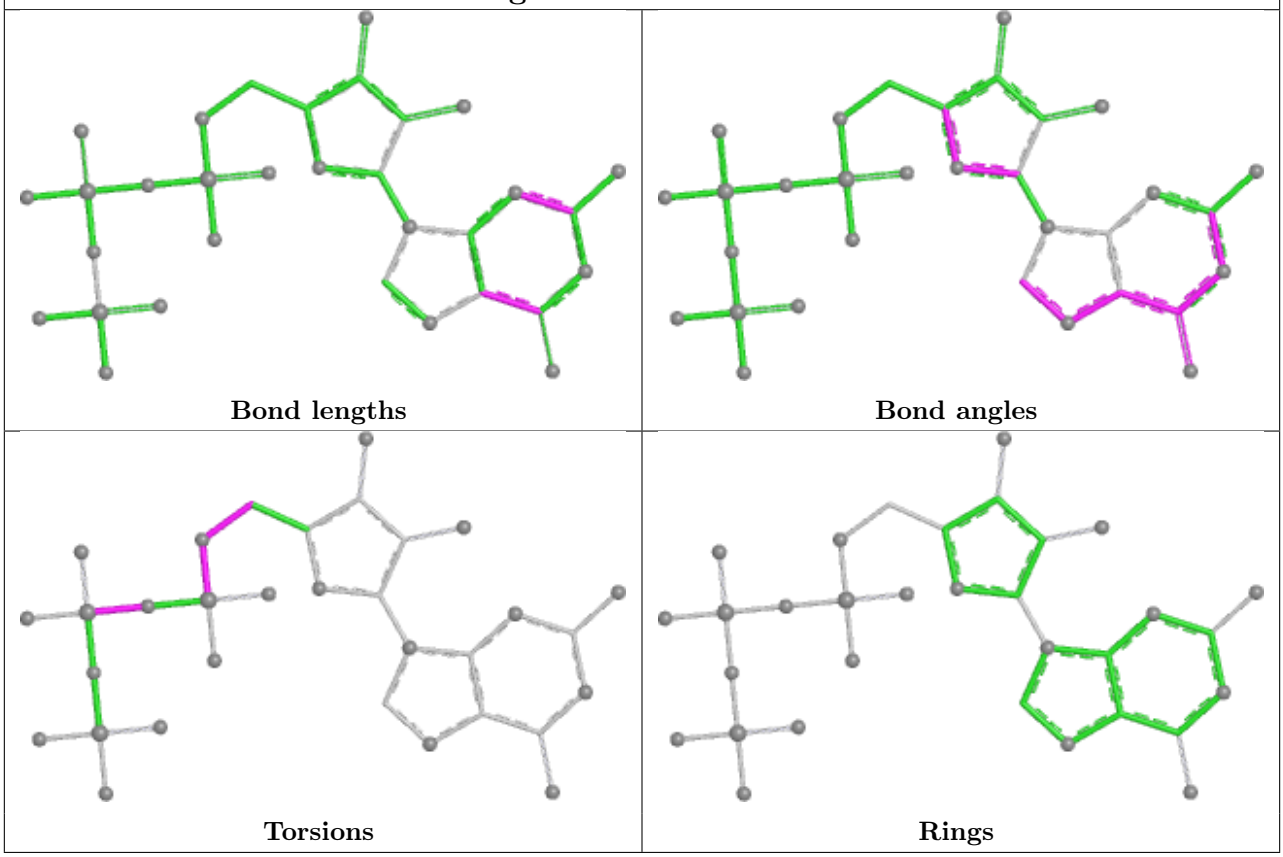

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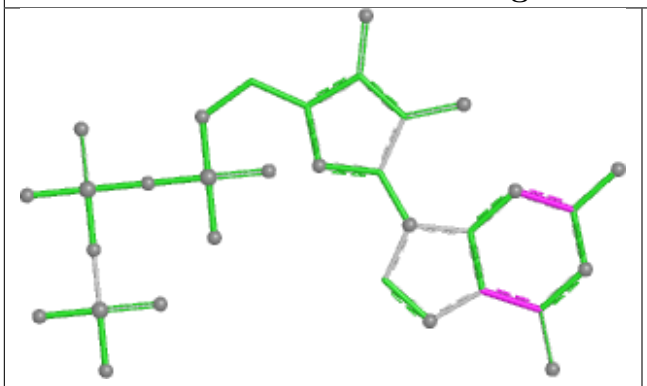
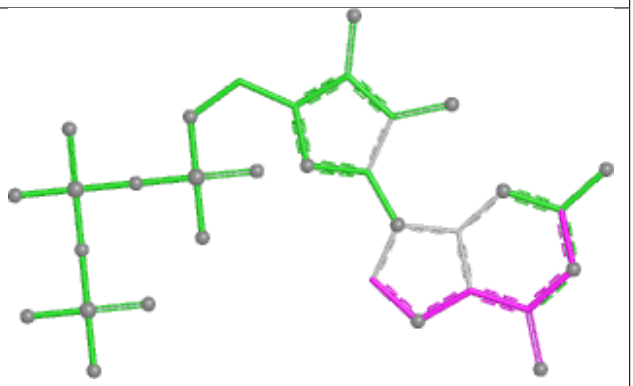


Bond lengths



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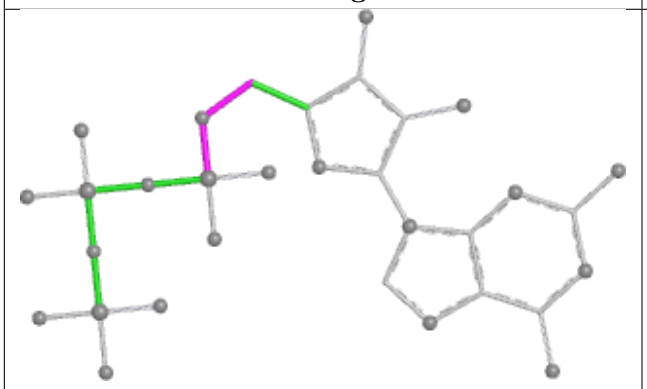
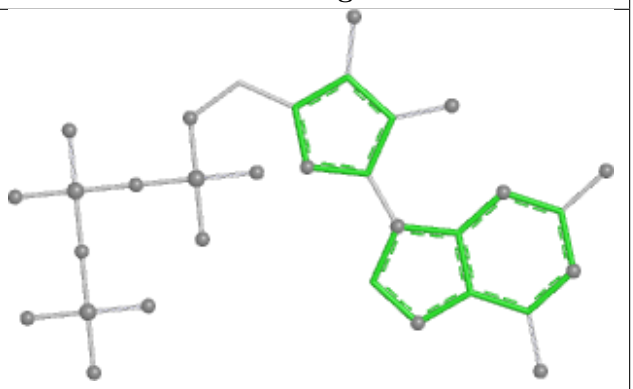
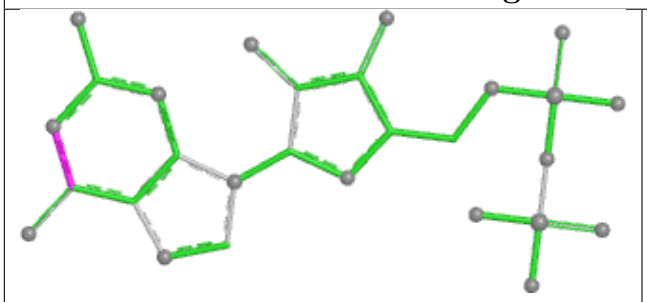


Torsions



Rings

Ligand GDP WD 501



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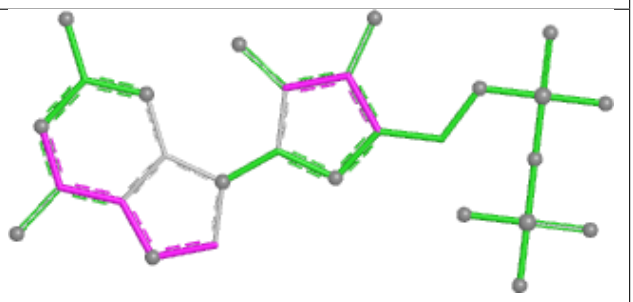

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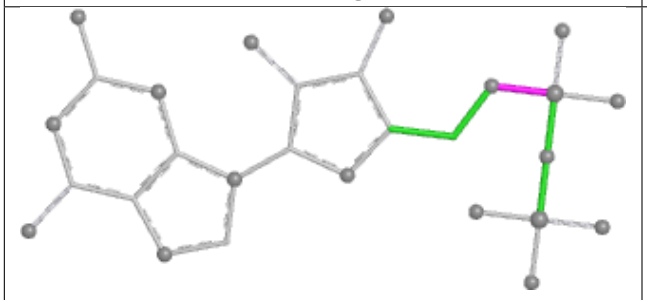

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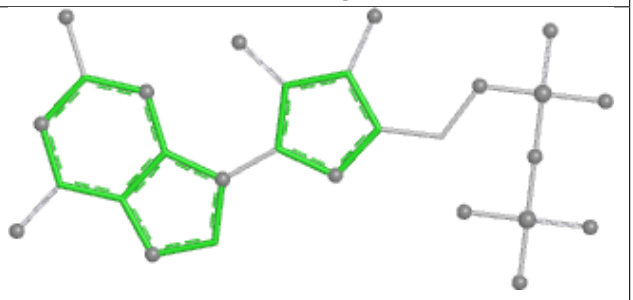

Rings

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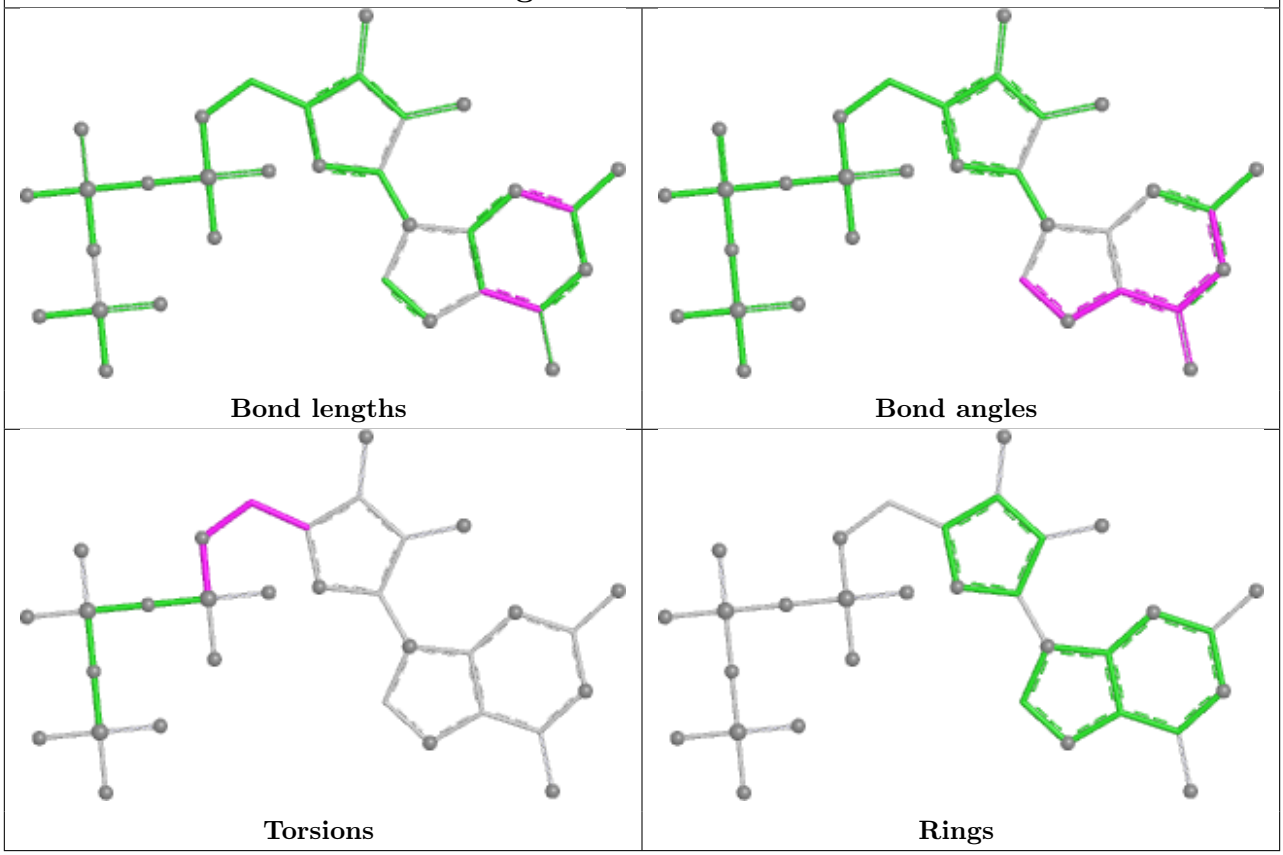

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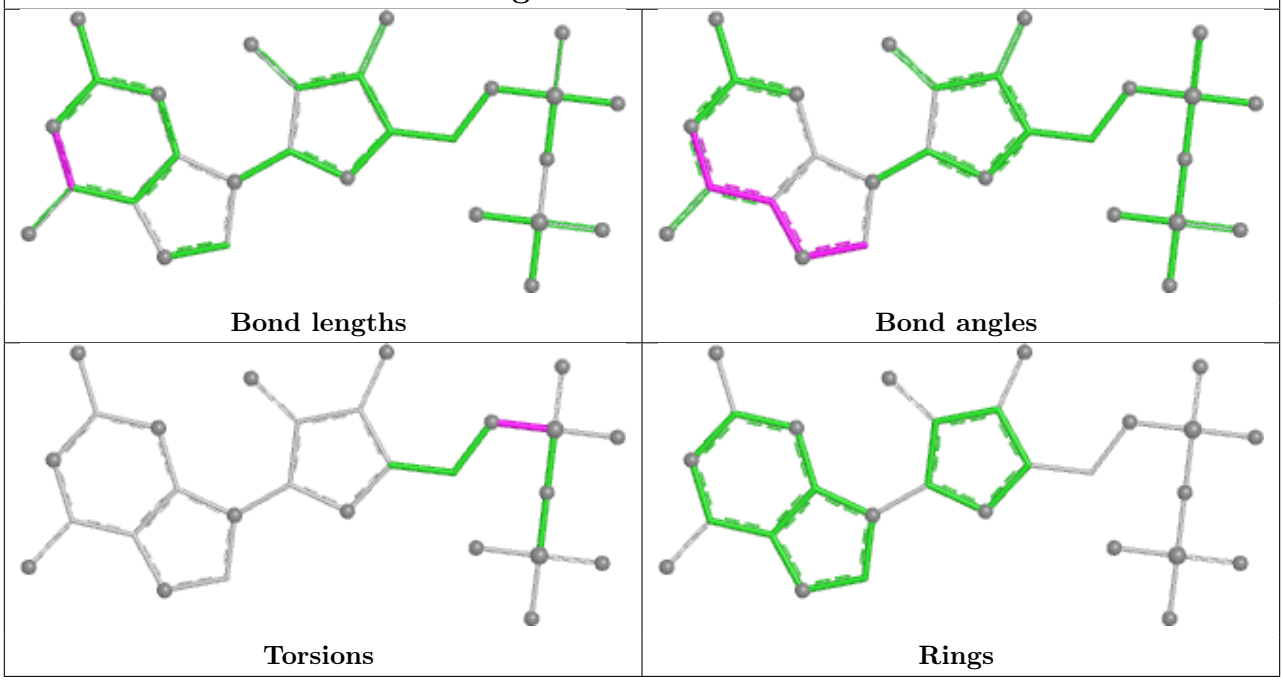

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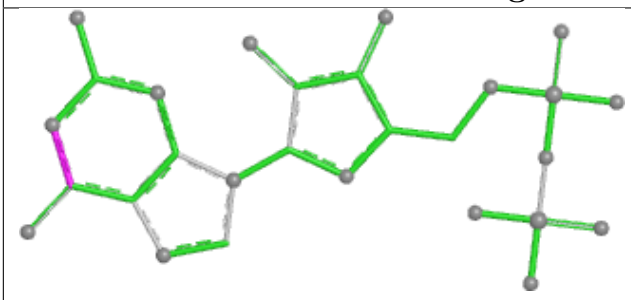

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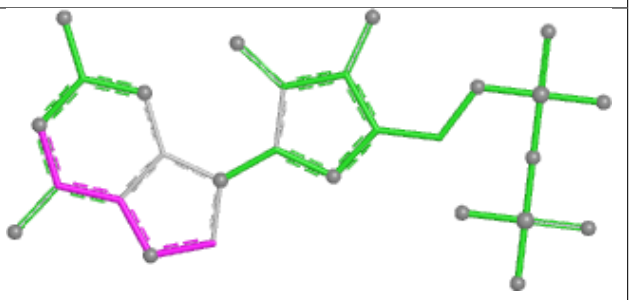

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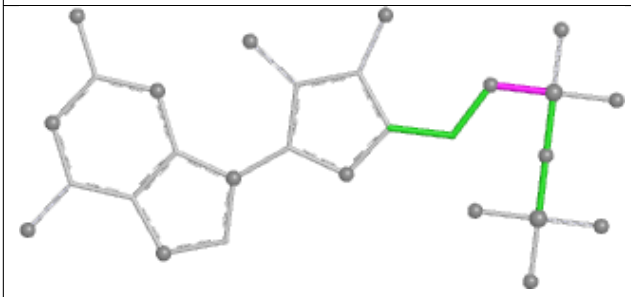

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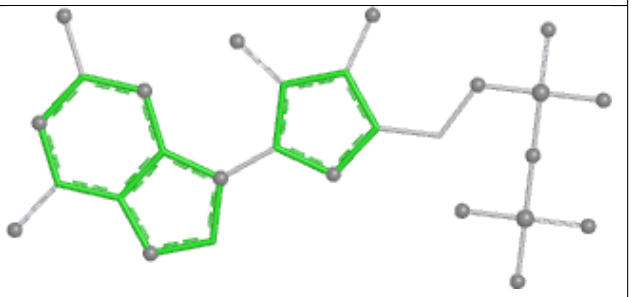

Rings

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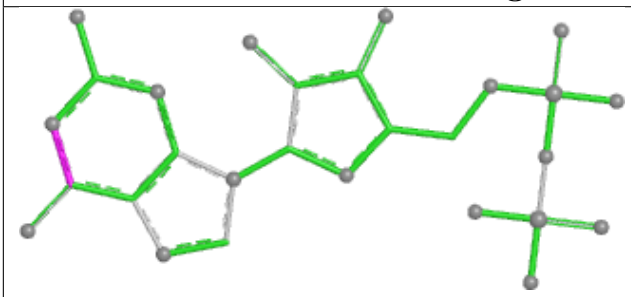

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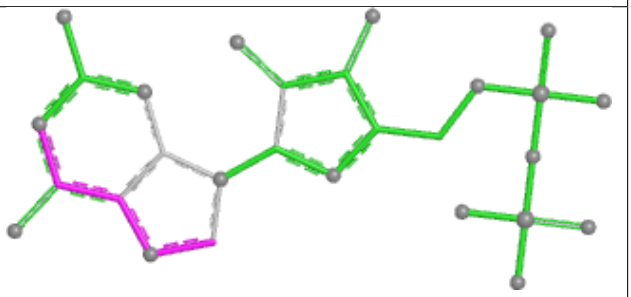

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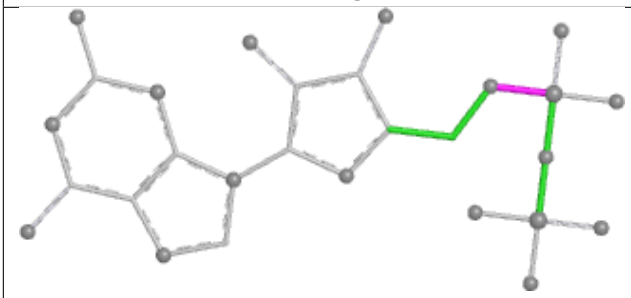

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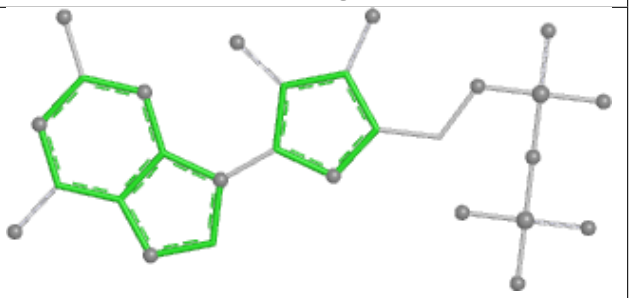

Rings

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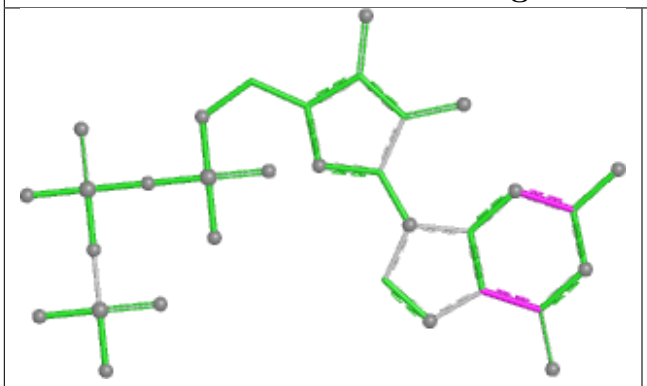

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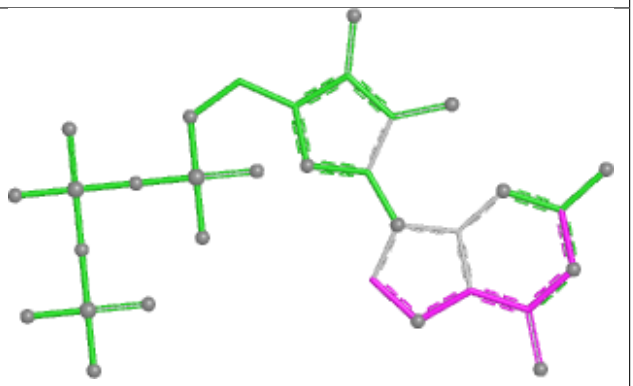

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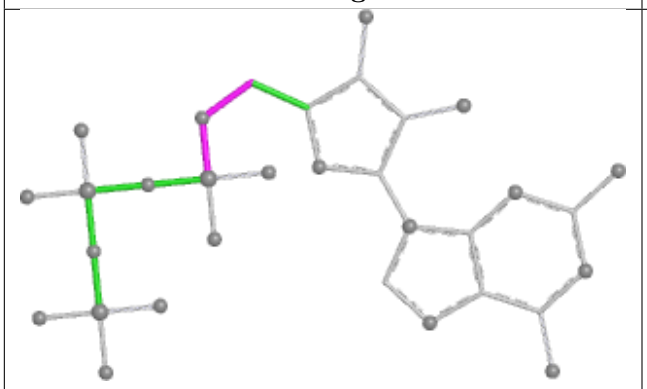

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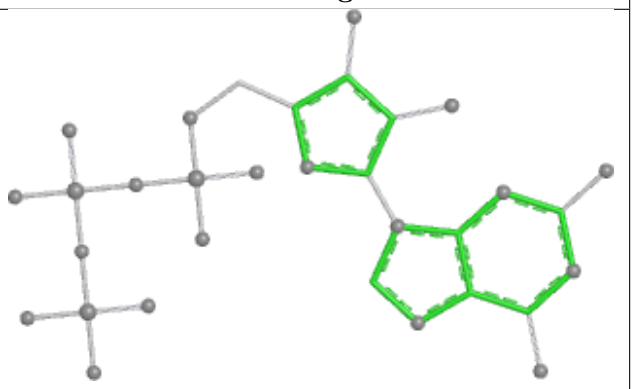

Rings

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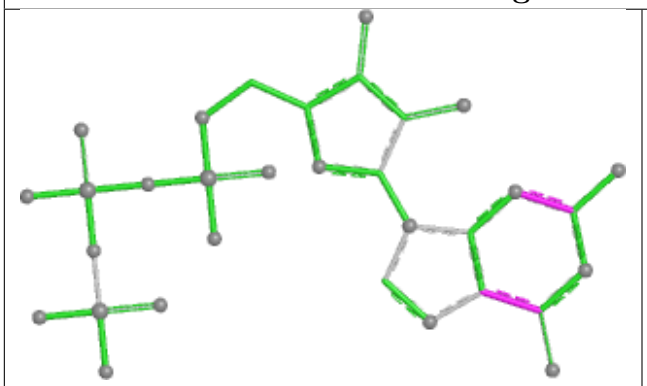

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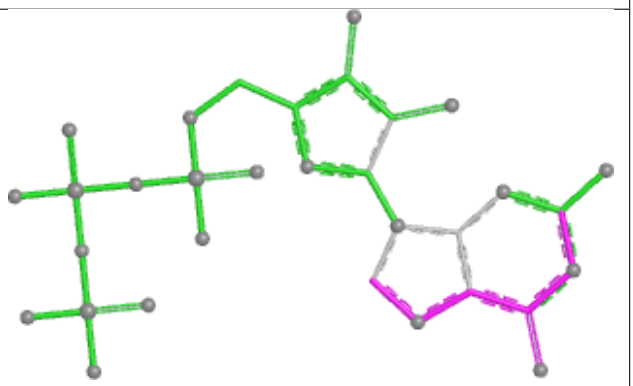

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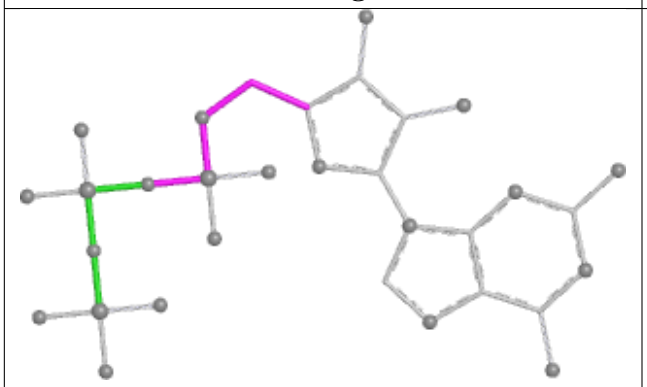

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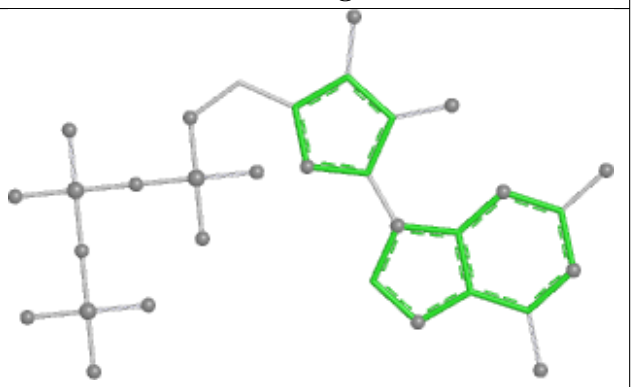

Rings

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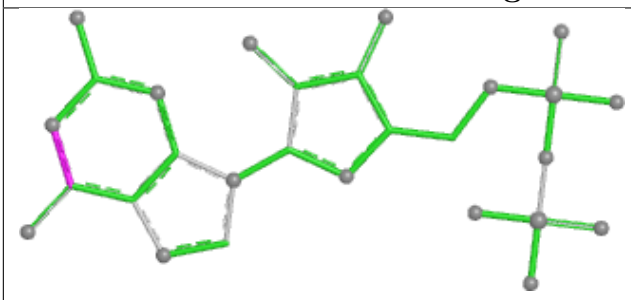
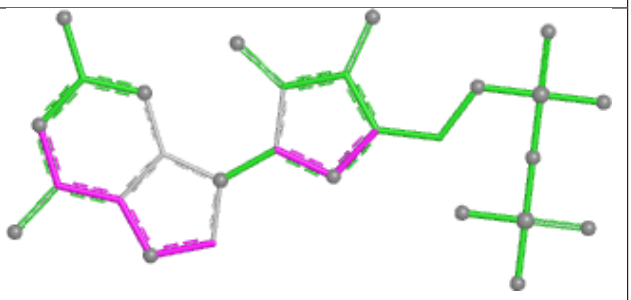
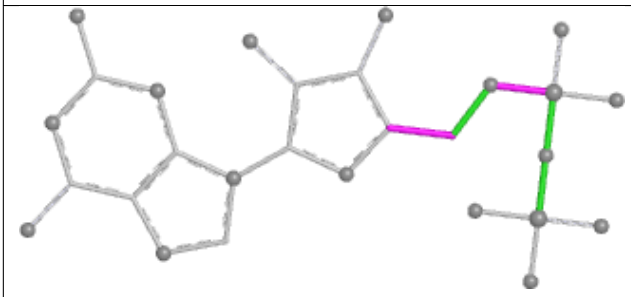
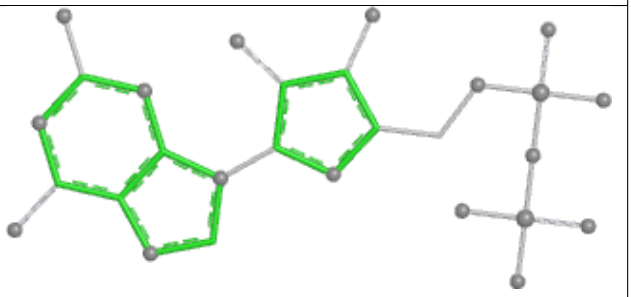
 Bond lengths	 Bond angles
 Torsions	 Rings

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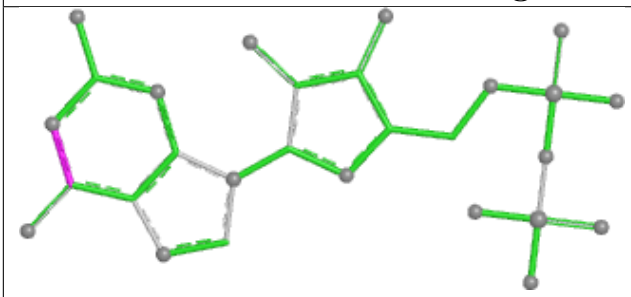
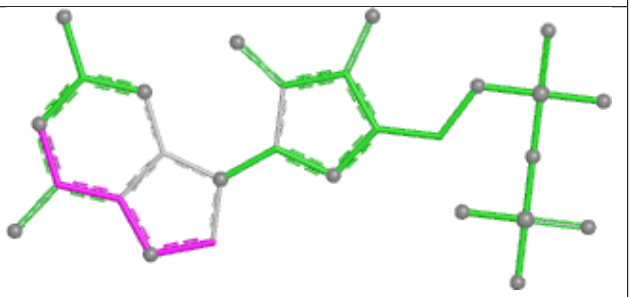
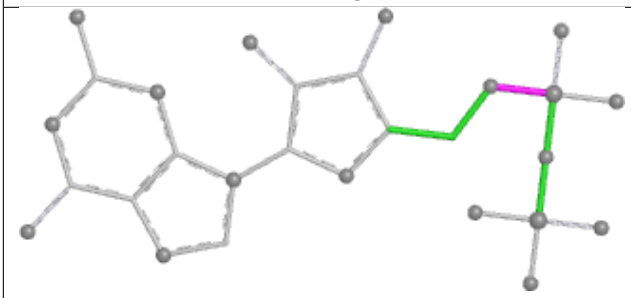
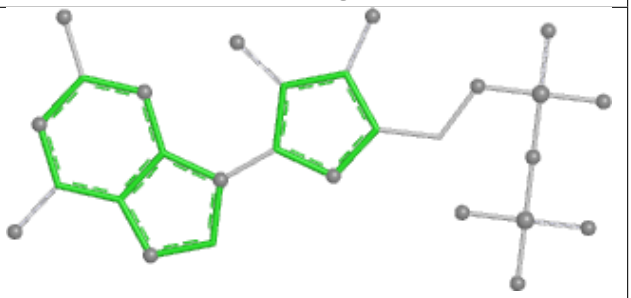
 Bond lengths	 Bond angles
 Torsions	 Rings

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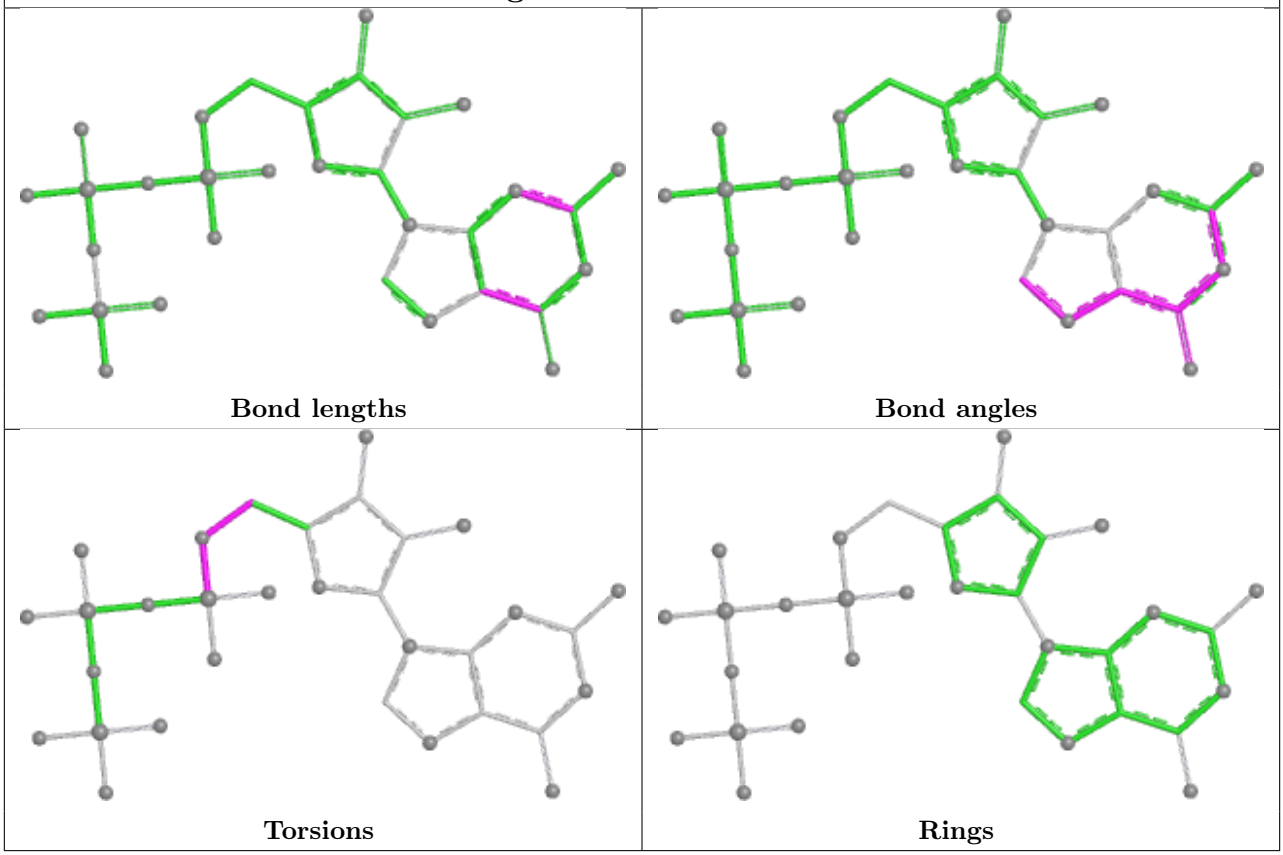

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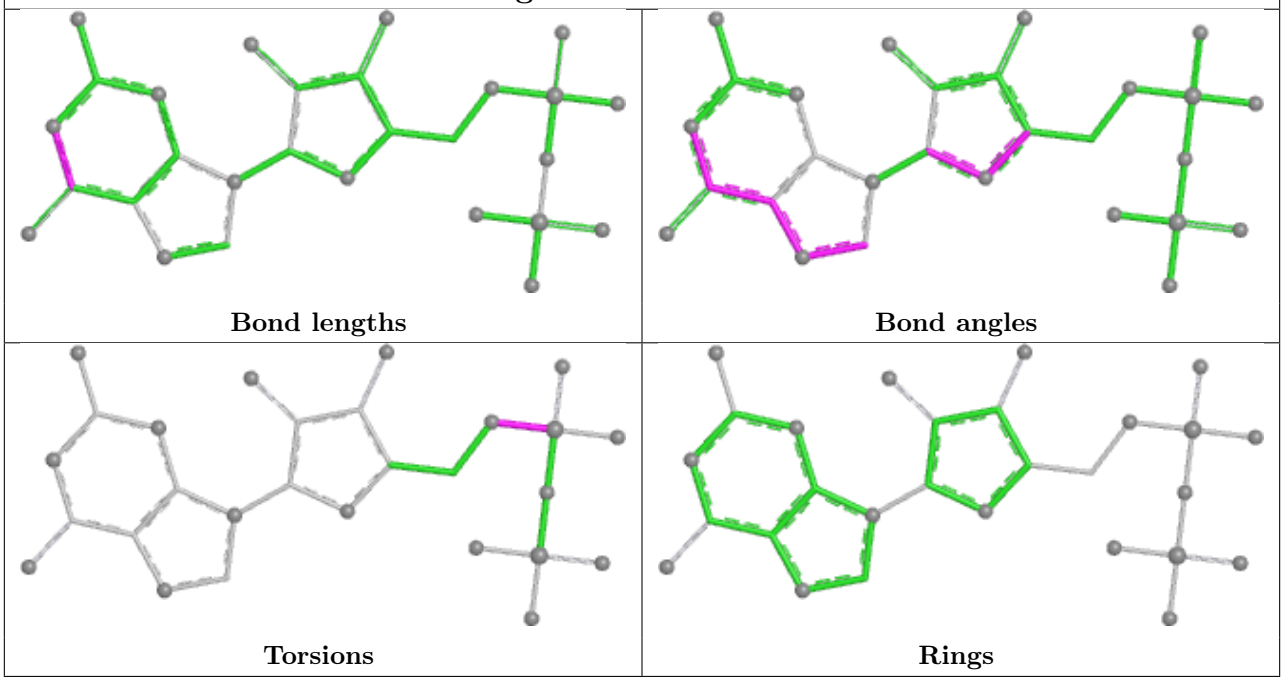

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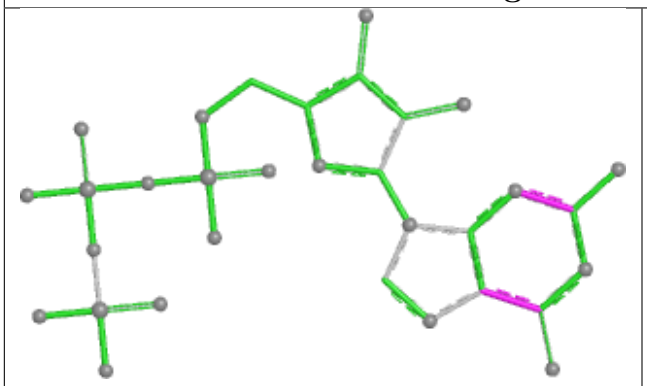
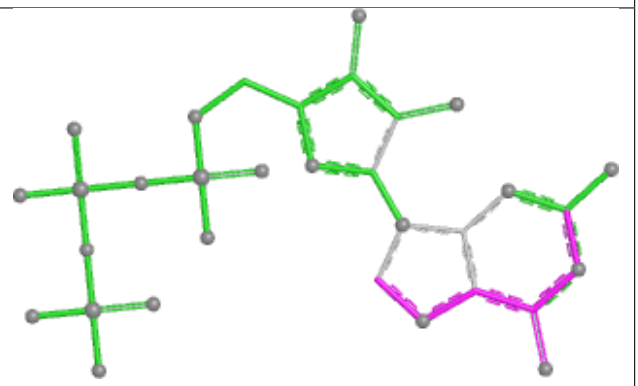
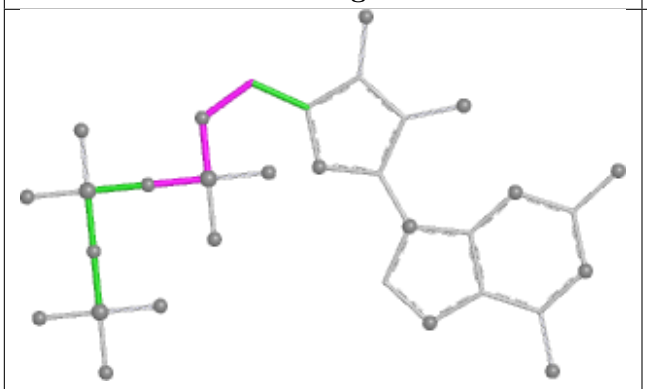


Bond lengths



Bond angles



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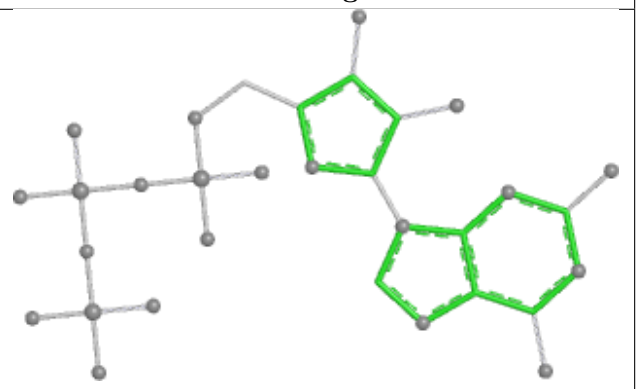

Rings

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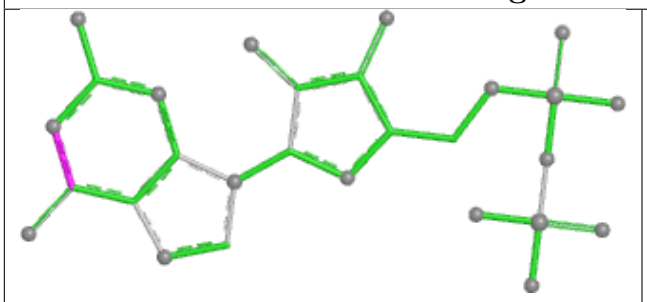

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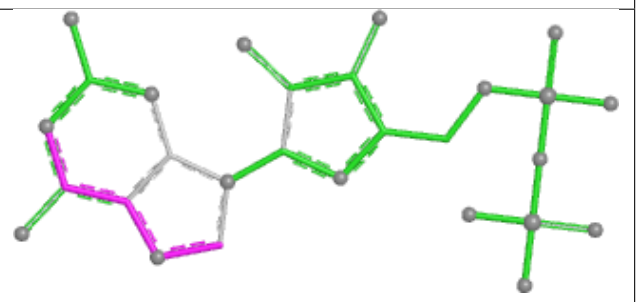

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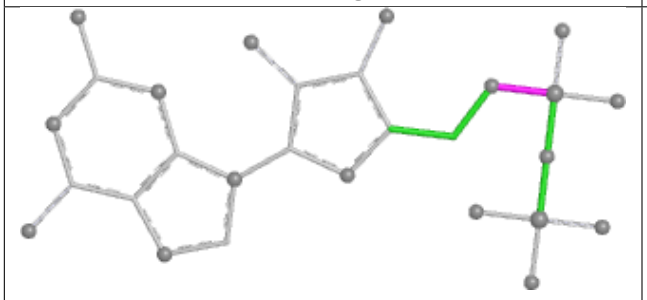

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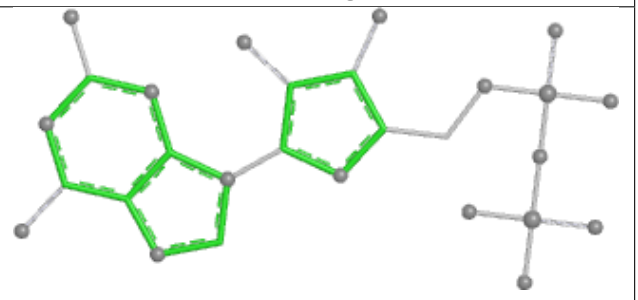

Rings

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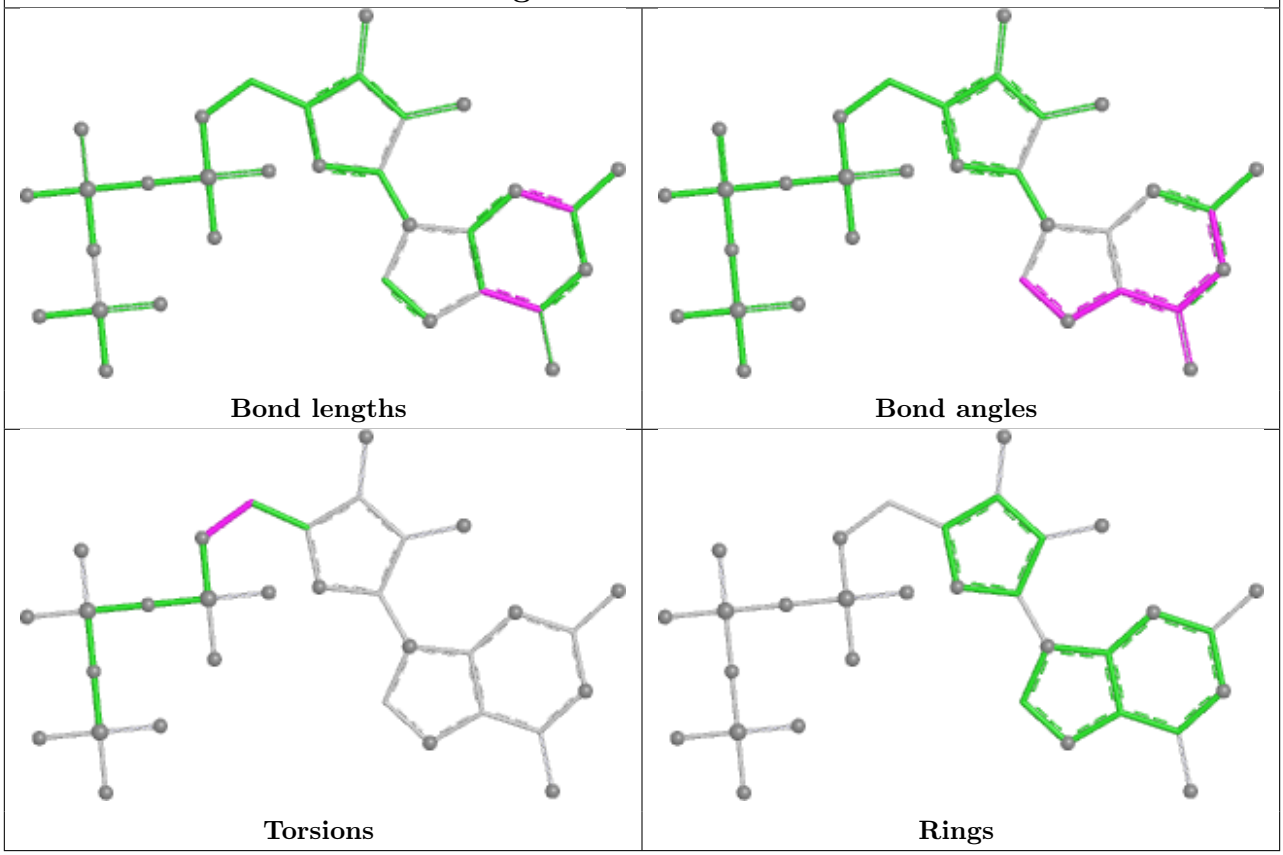

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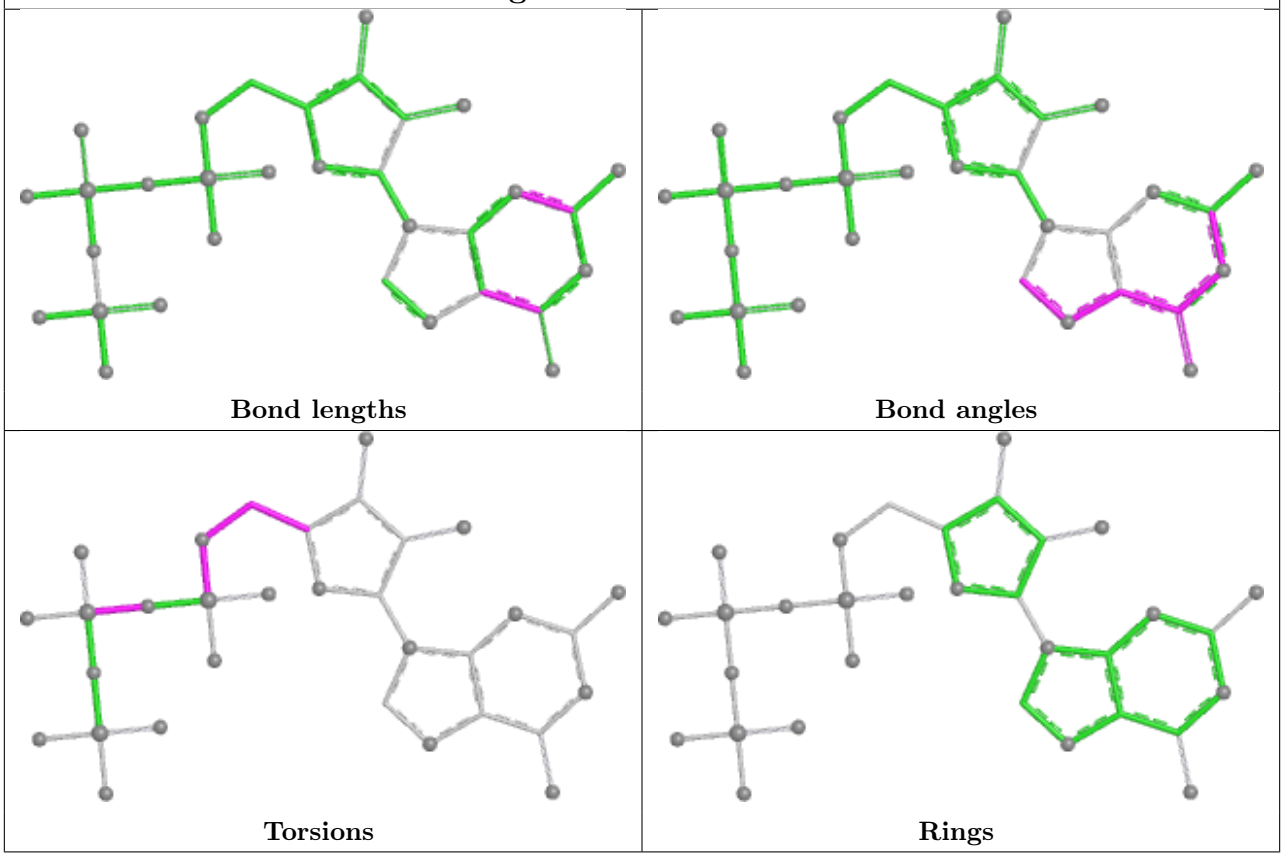

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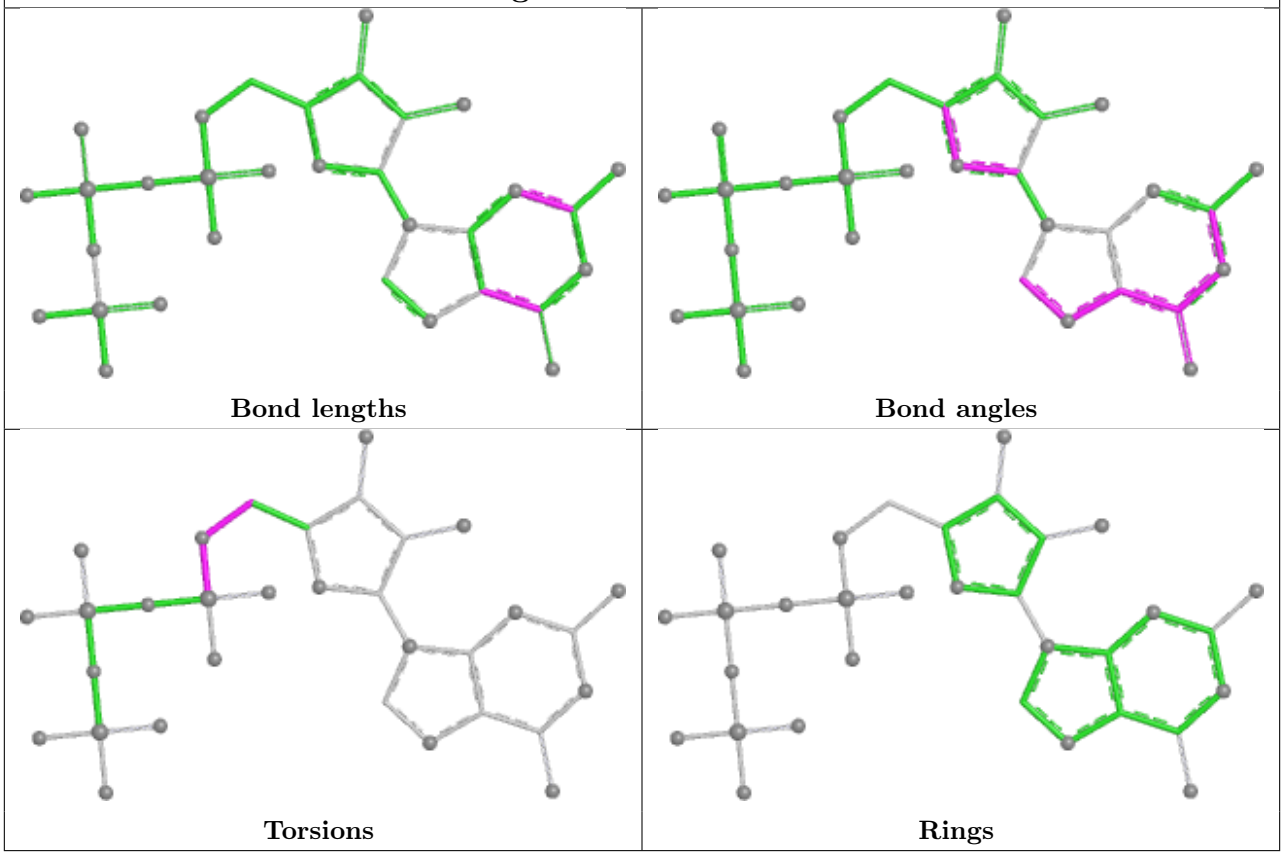

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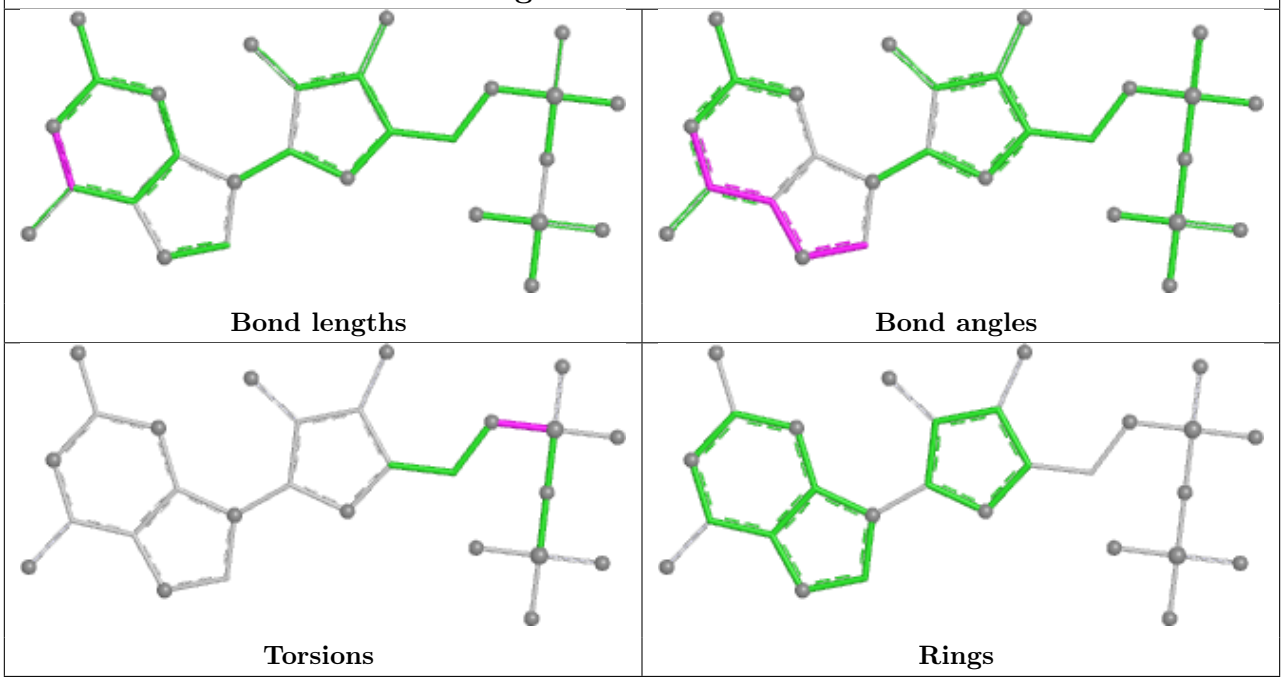

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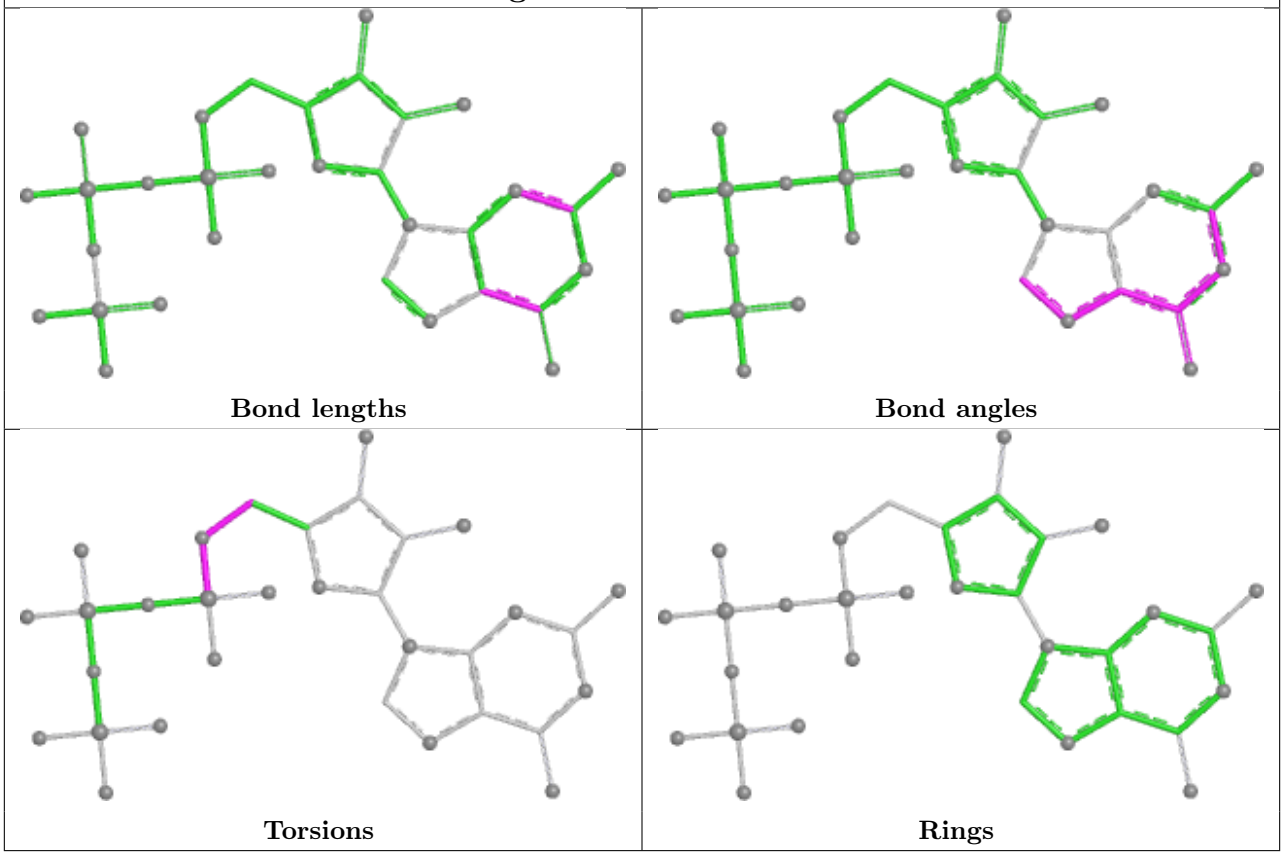

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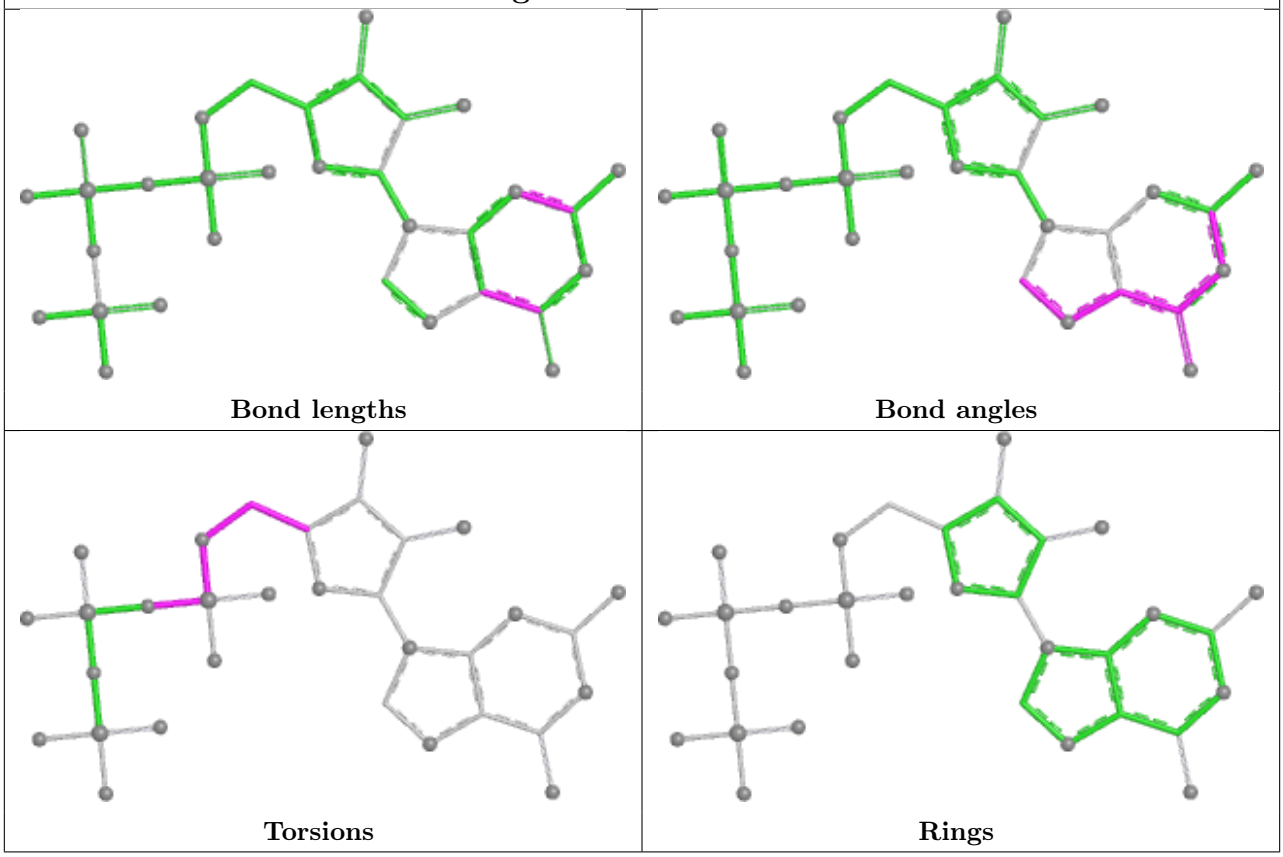

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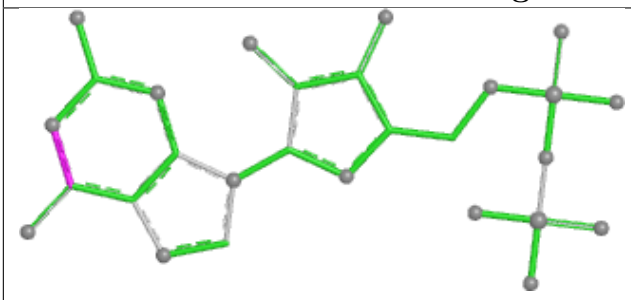
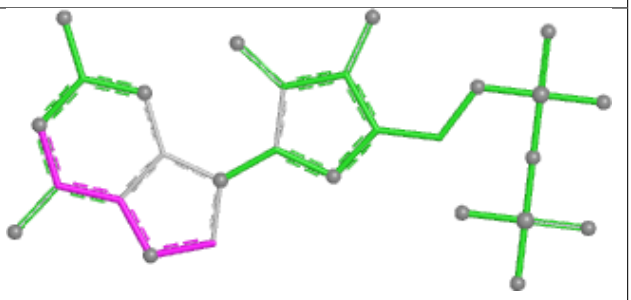


Bond lengths



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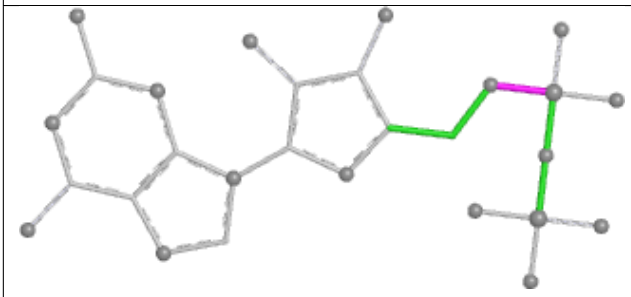
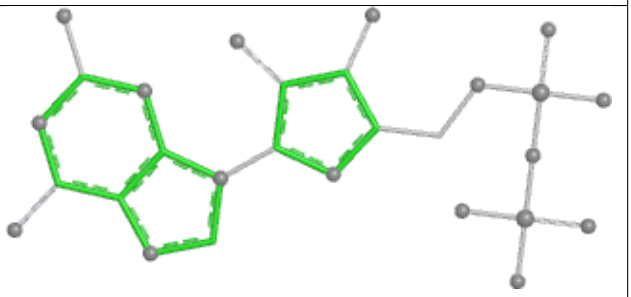
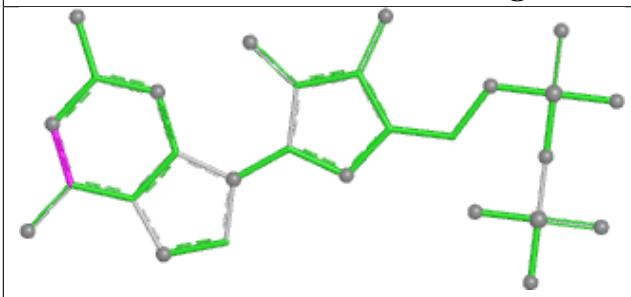


Torsions



Rings

Ligand GDP BC 501



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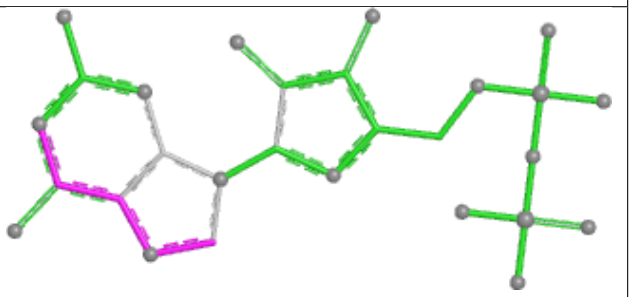

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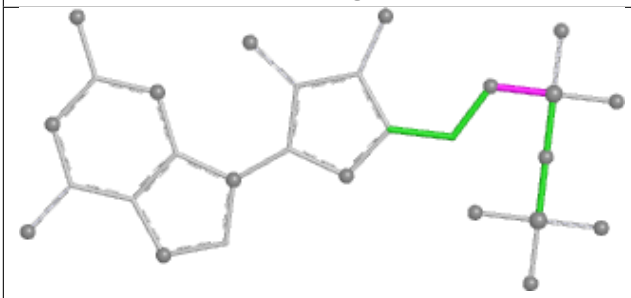

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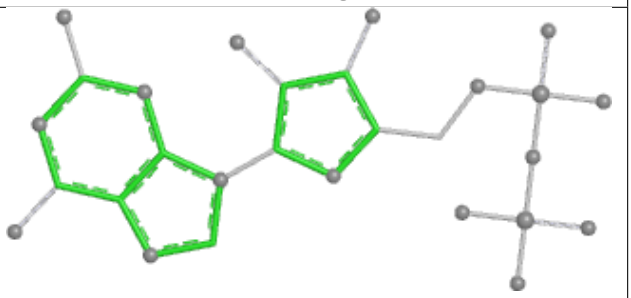

Rings

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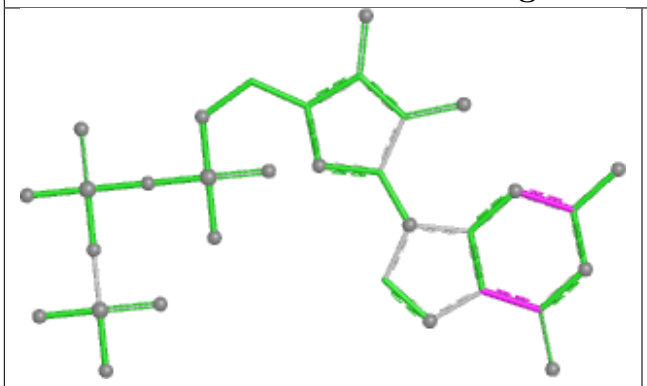

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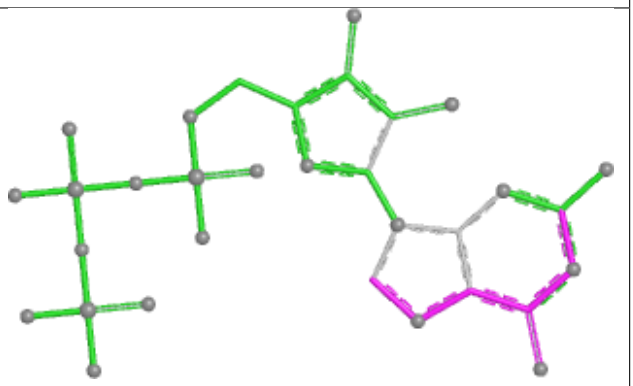

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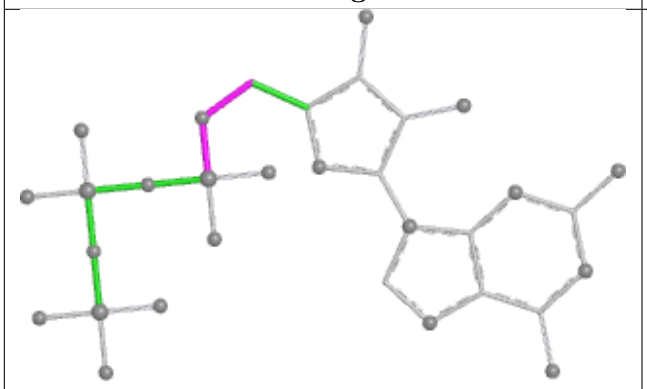

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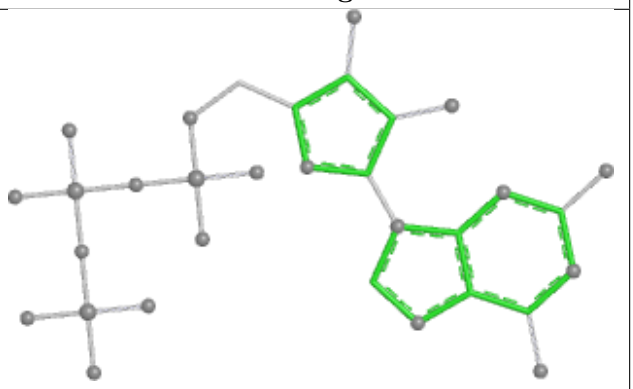

Rings

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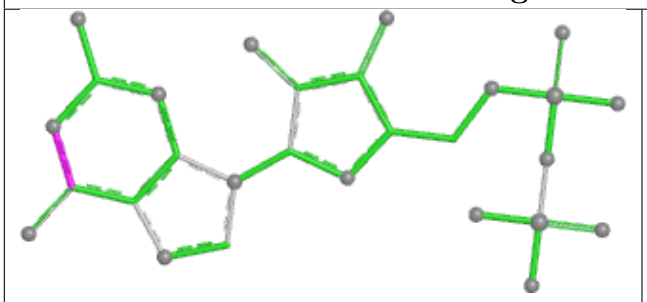

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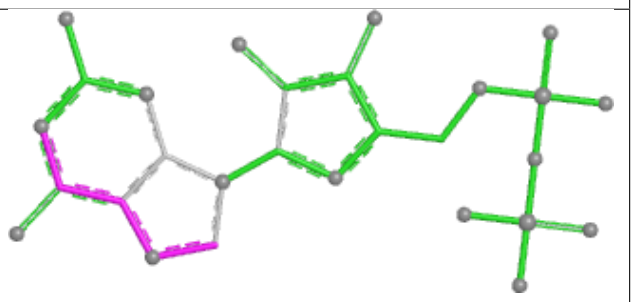

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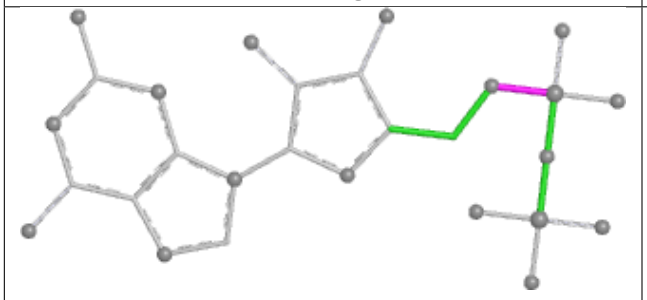

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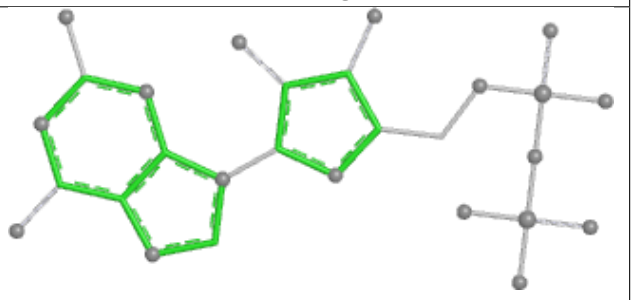

Rings

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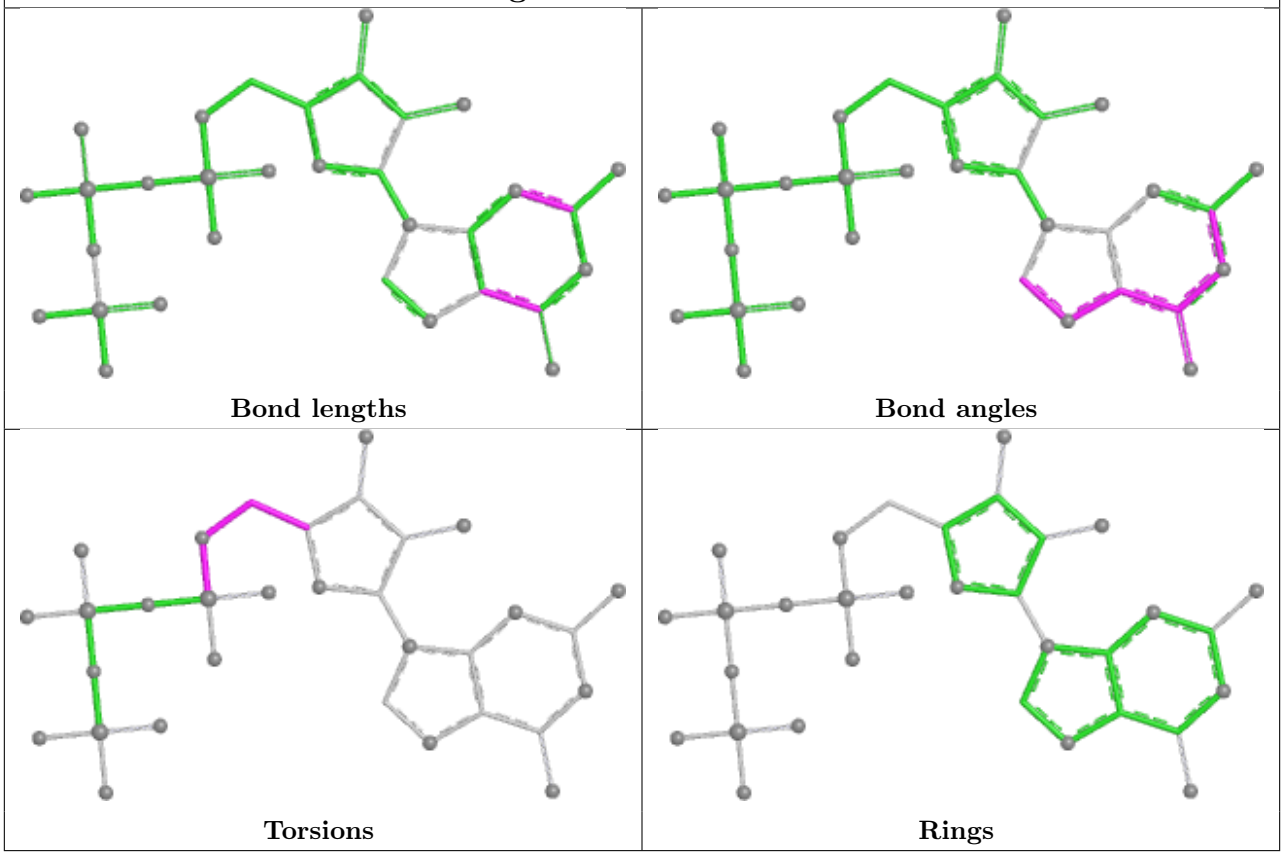

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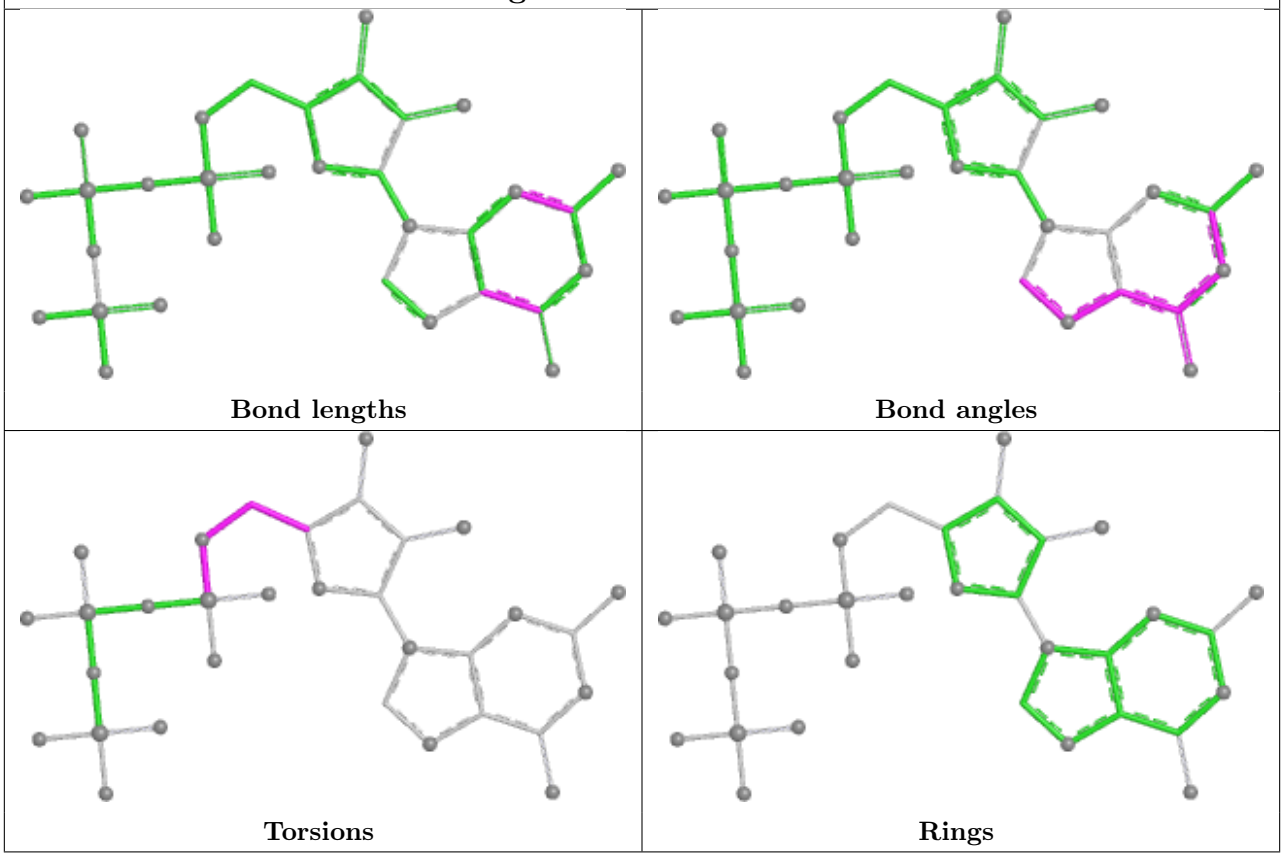

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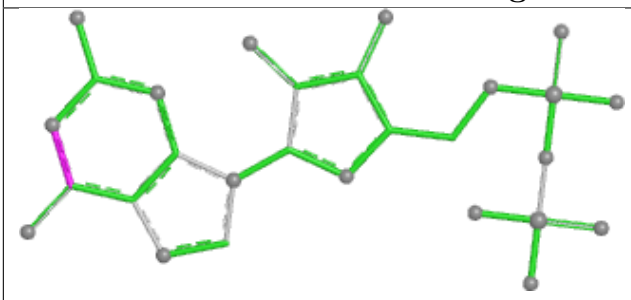

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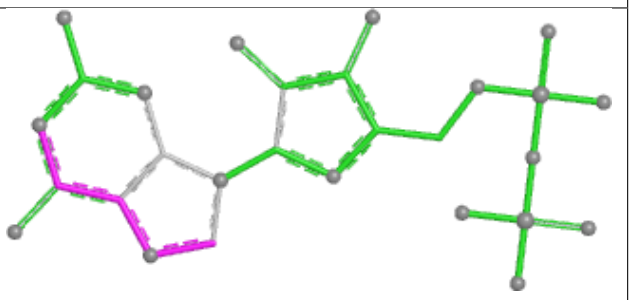

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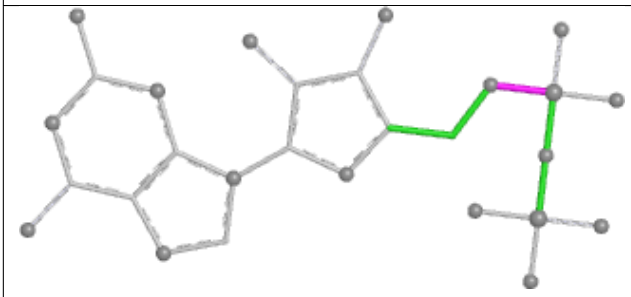

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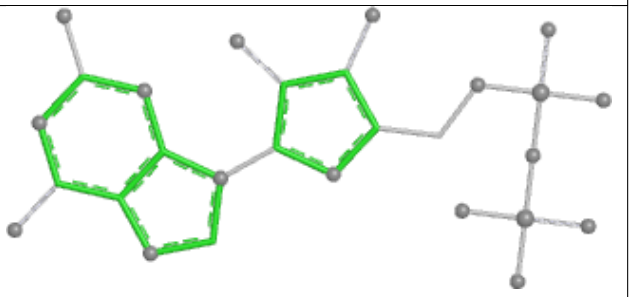

Rings

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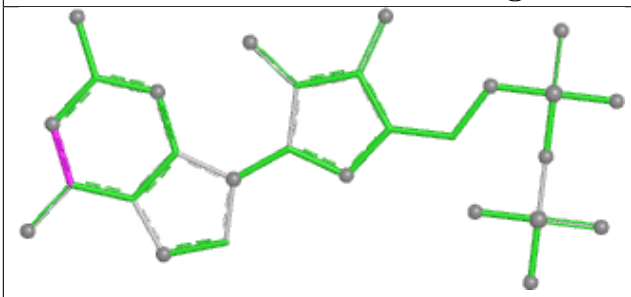

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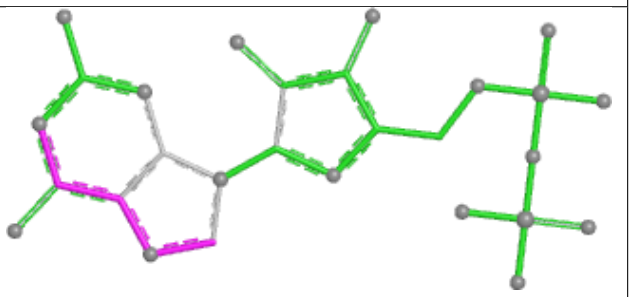

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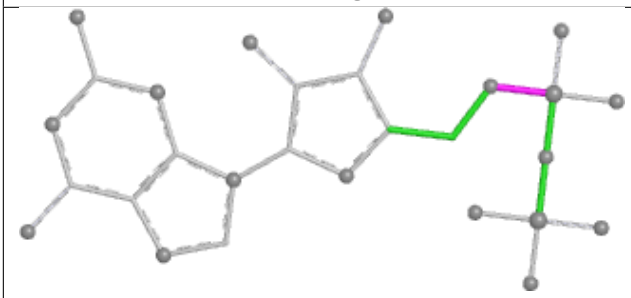

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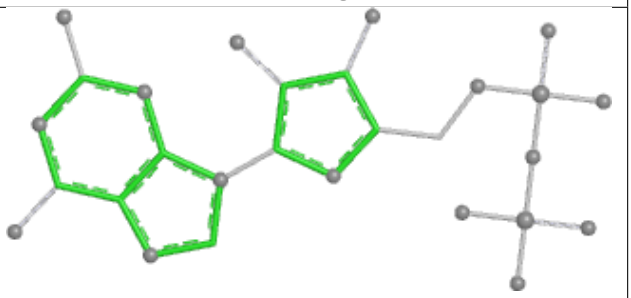
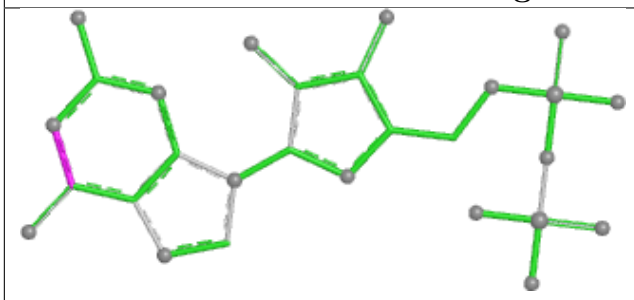


Rings

Ligand GDP TJ 501



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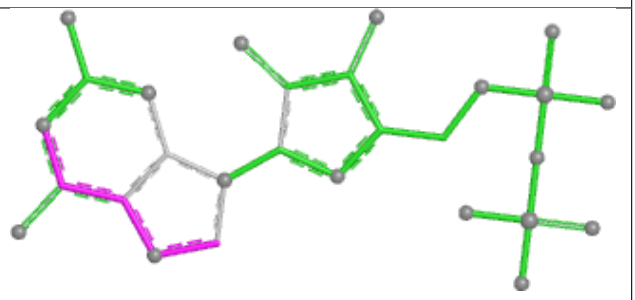

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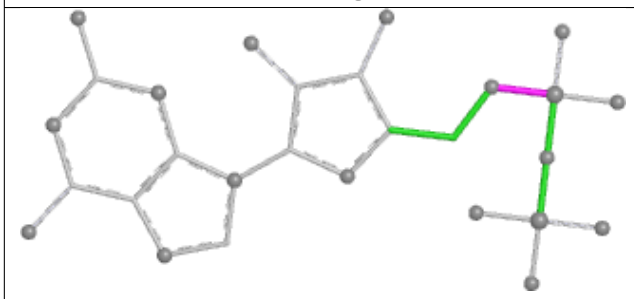

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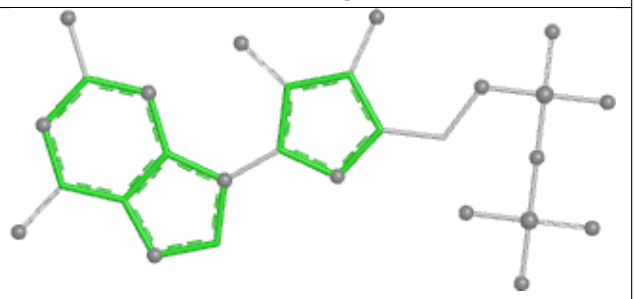

Rings

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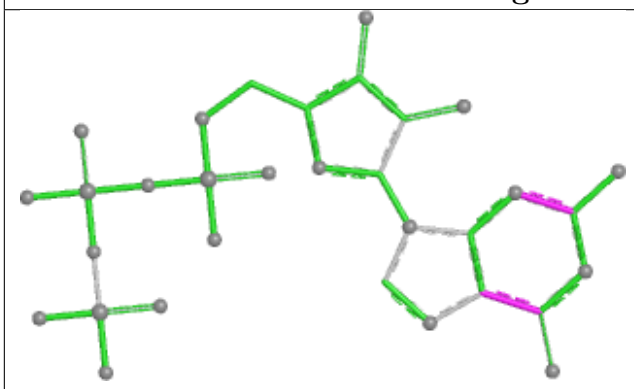

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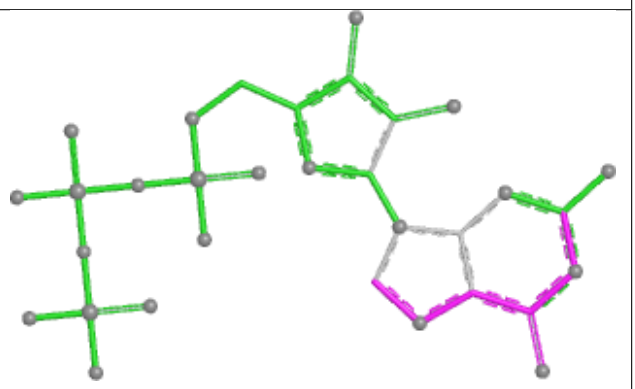

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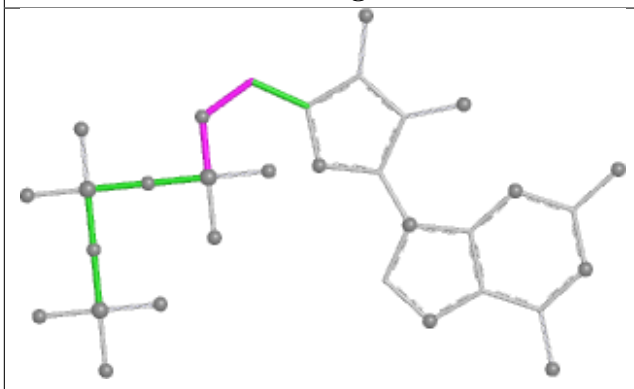

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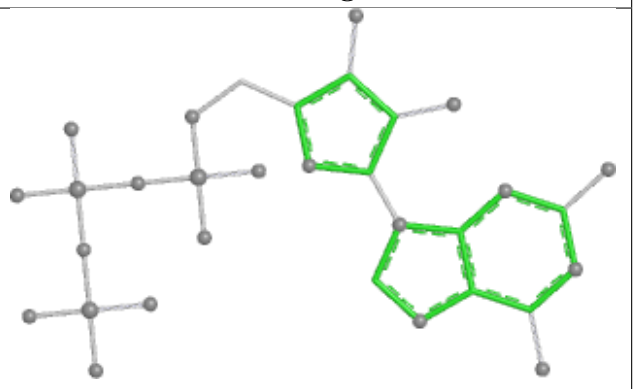

Rings

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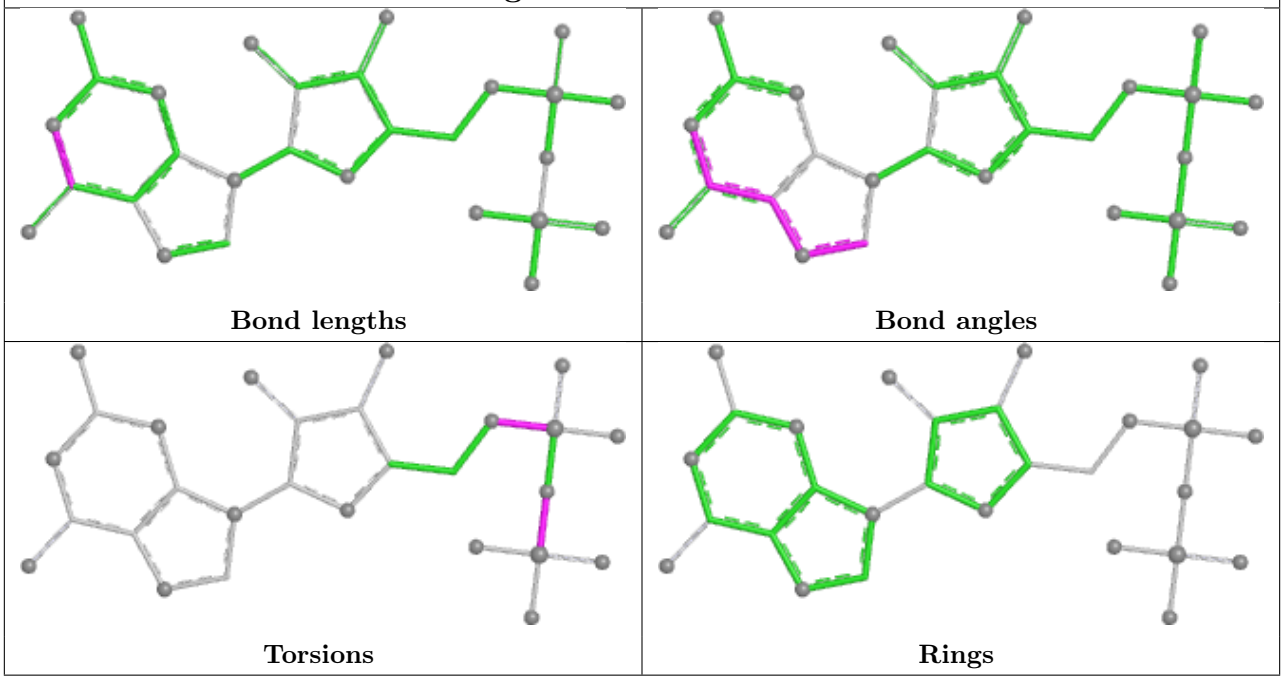

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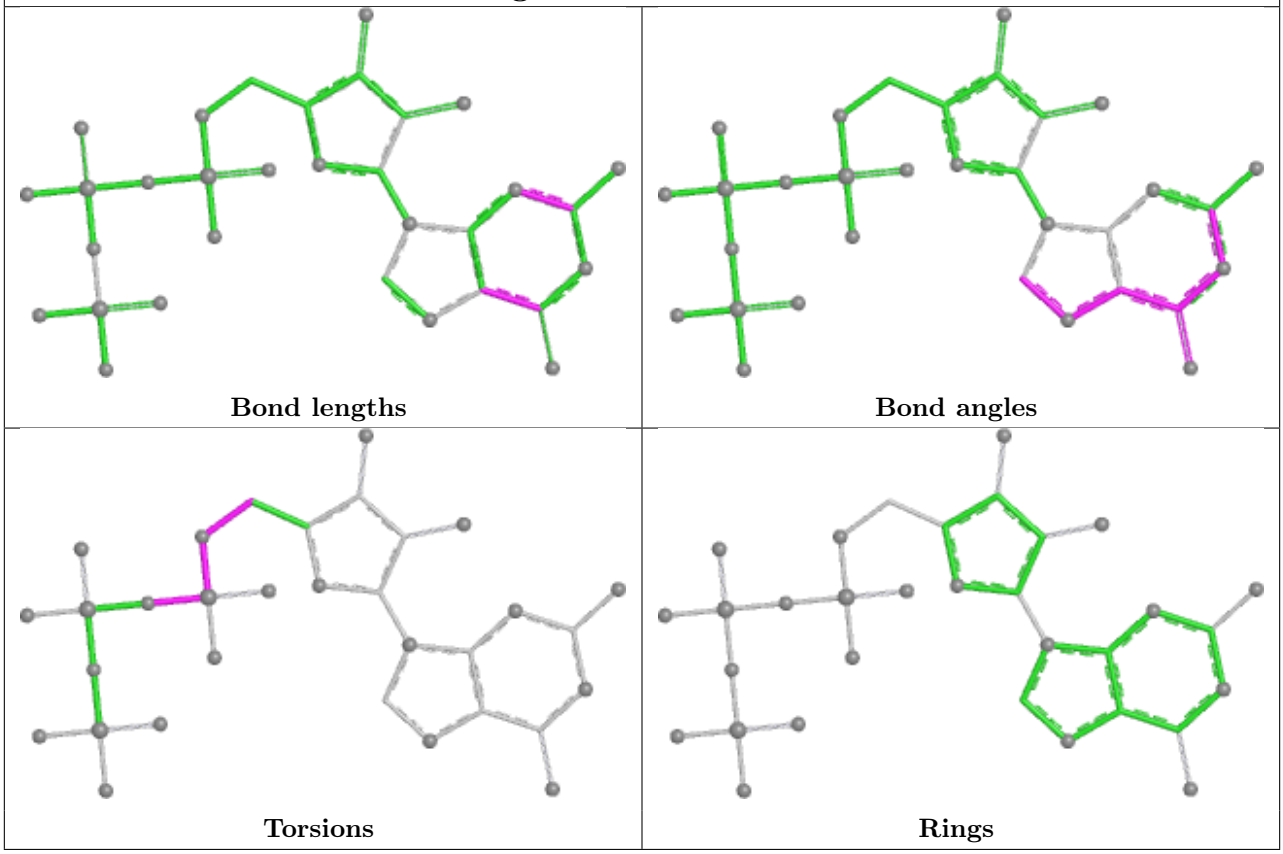

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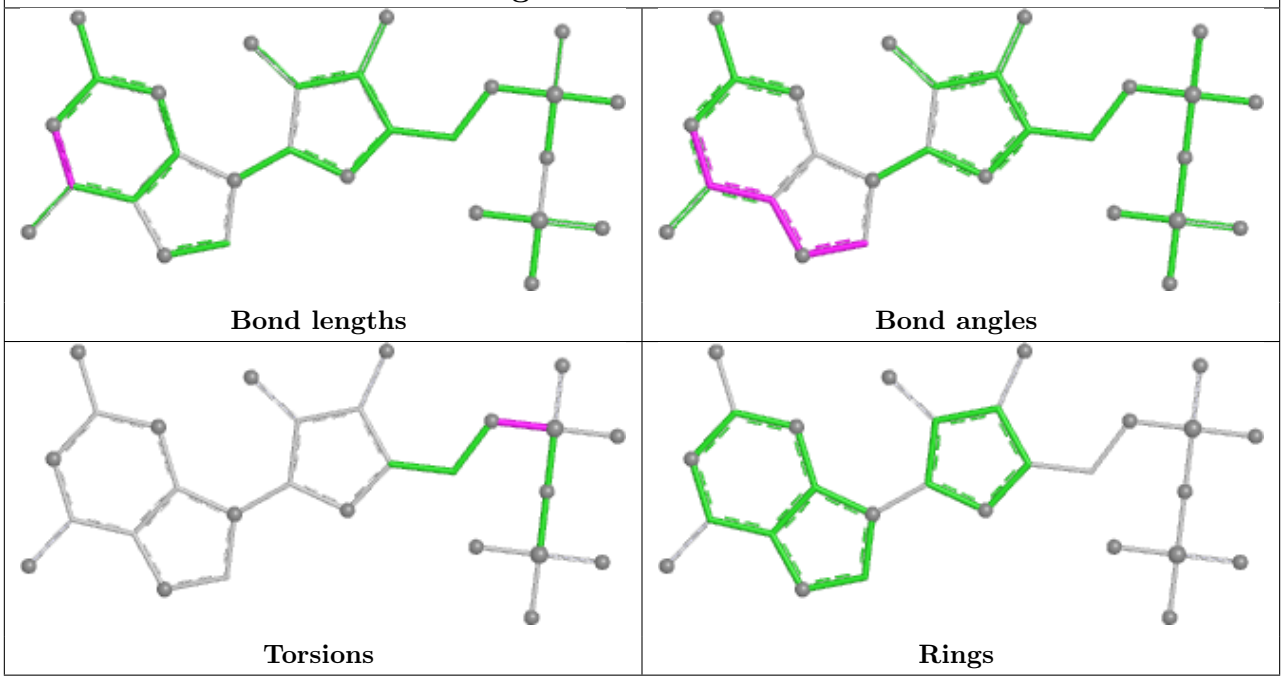

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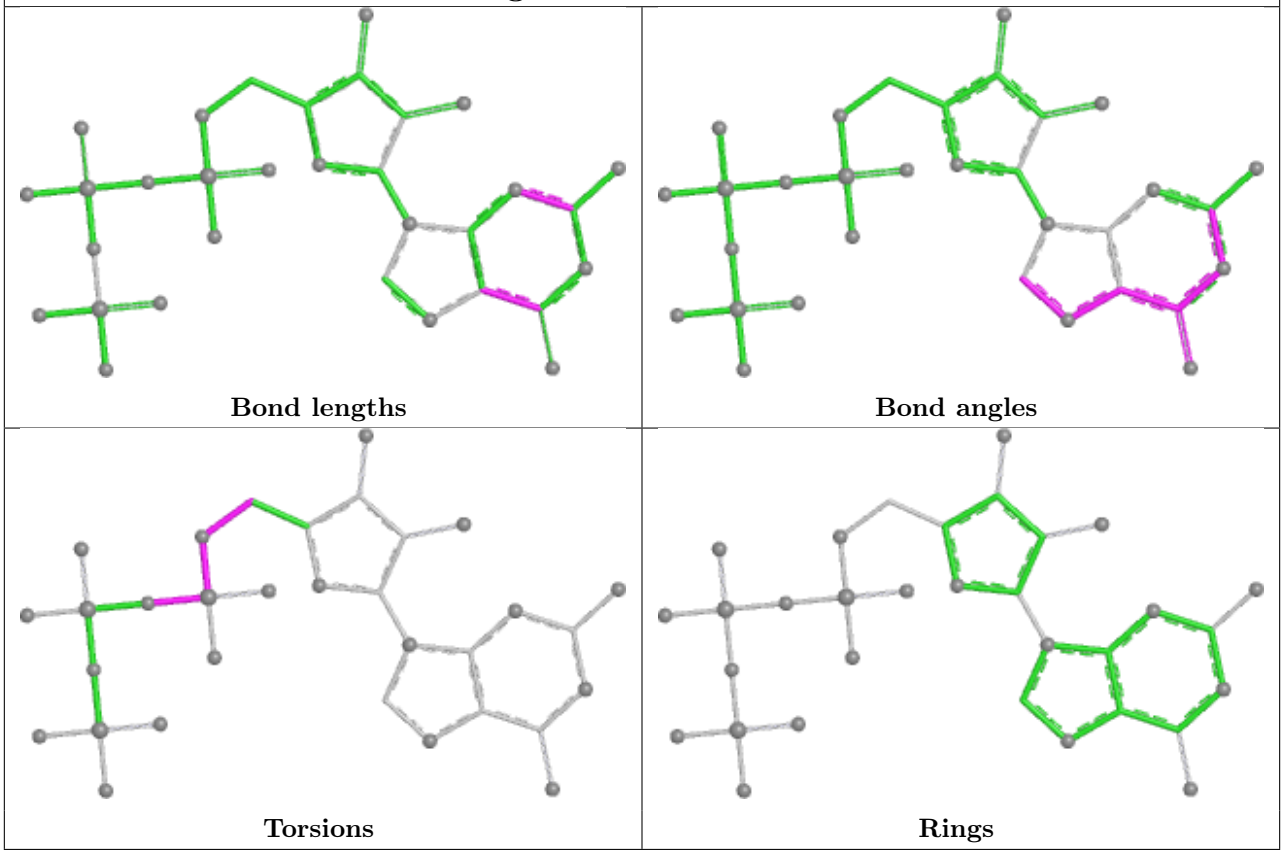

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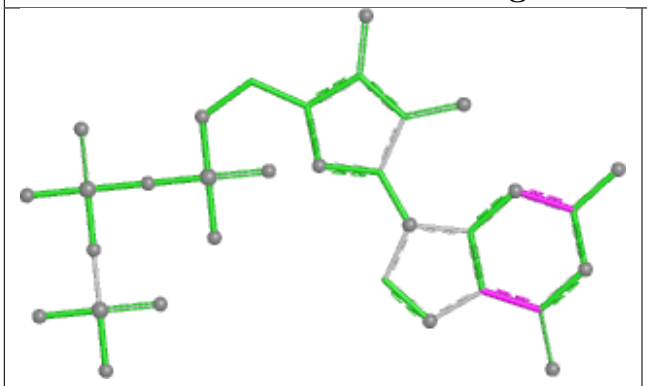

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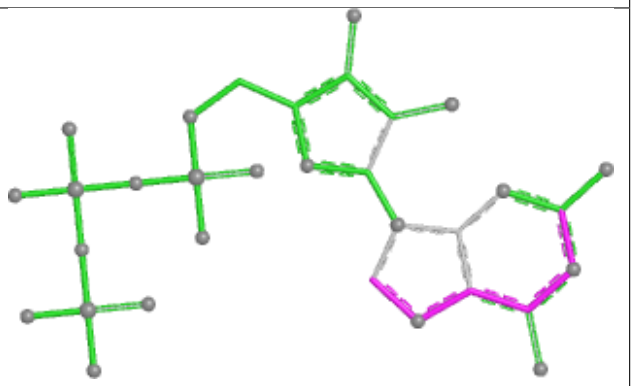

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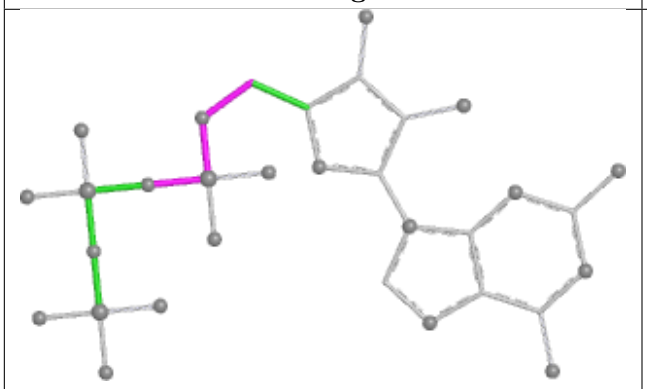

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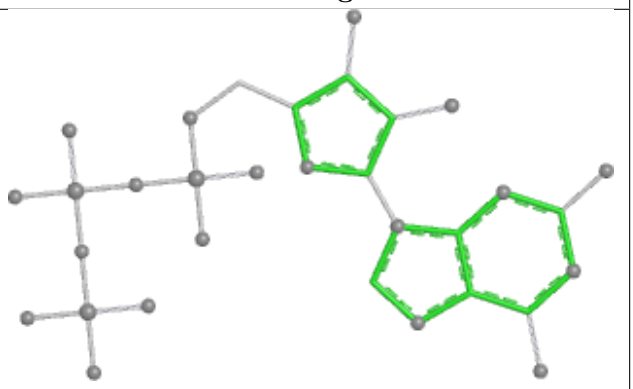
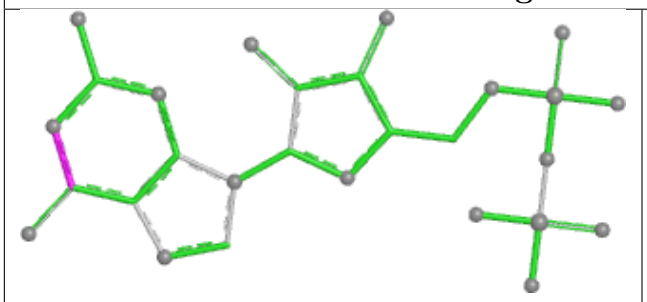


Rings

Ligand GDP LJ 501



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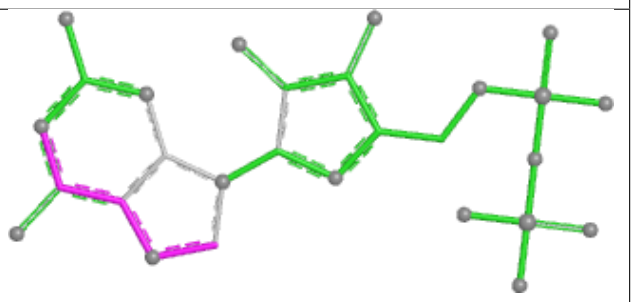

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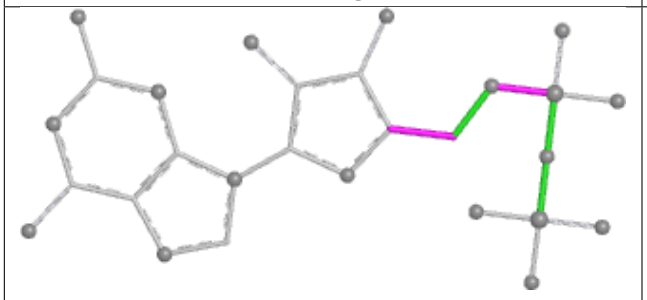

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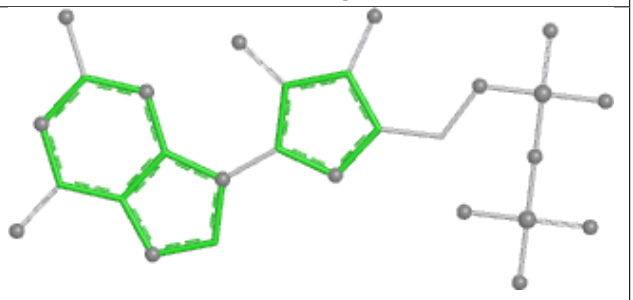

Rings

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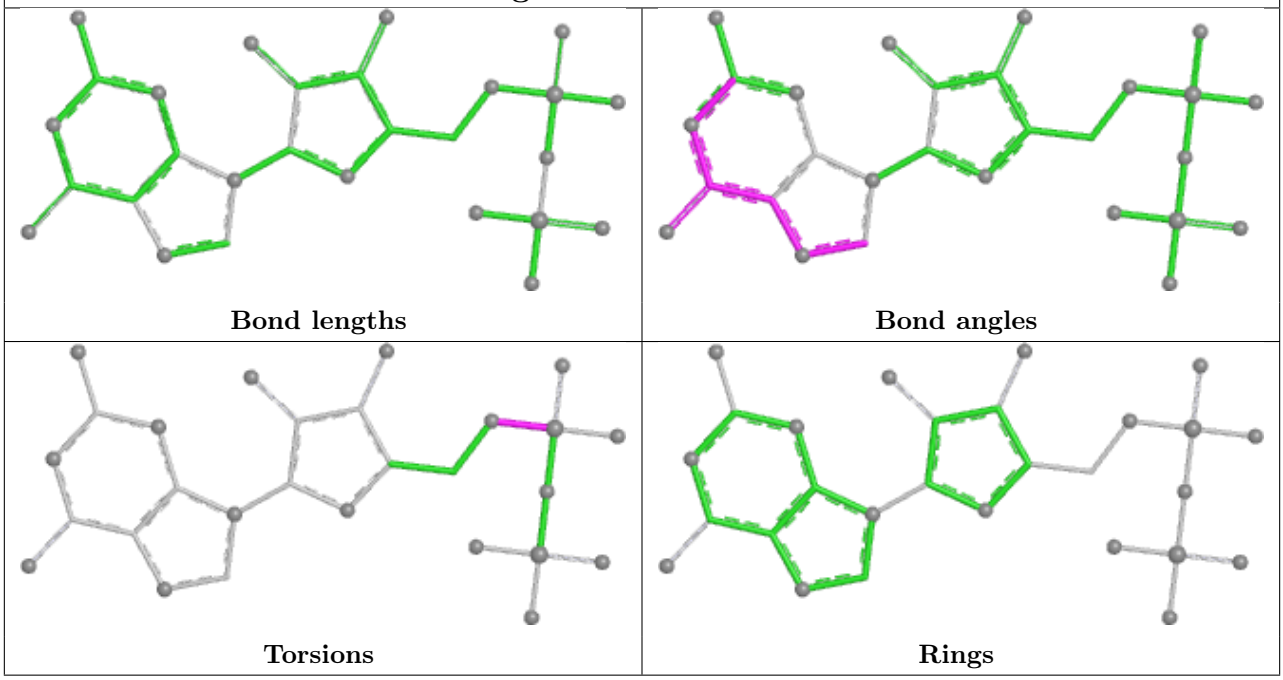

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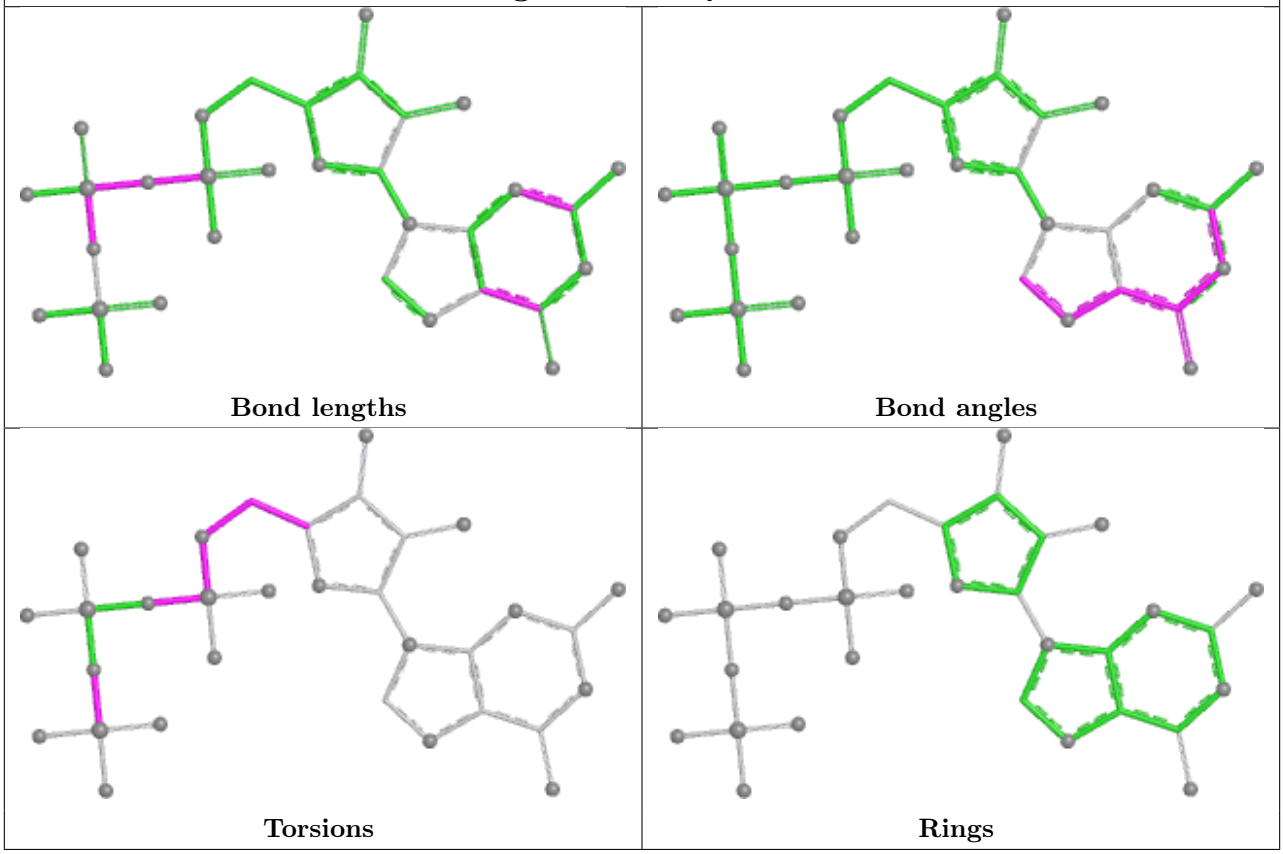

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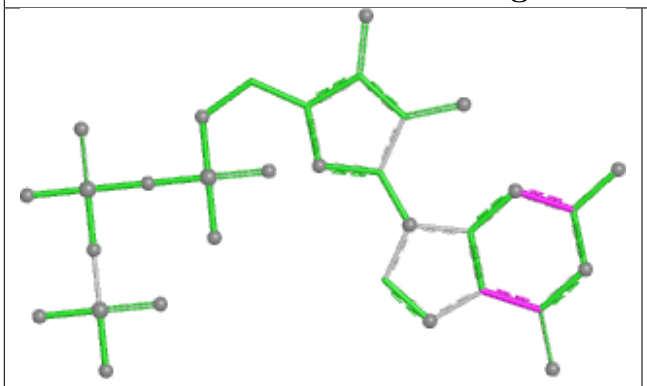

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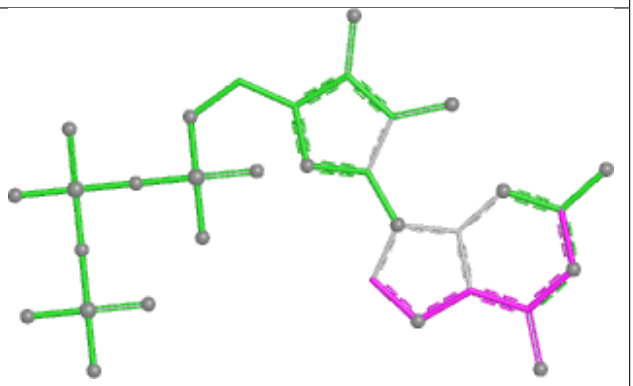

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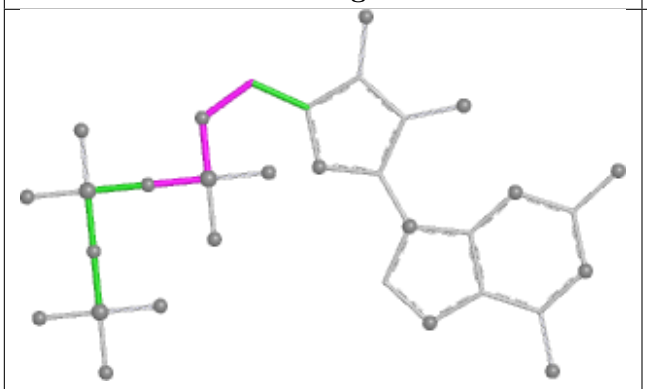

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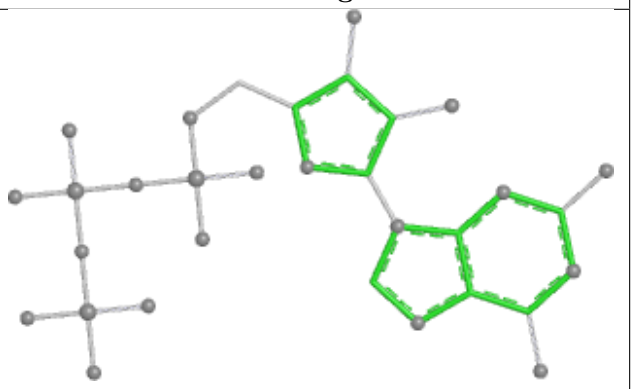

Rings

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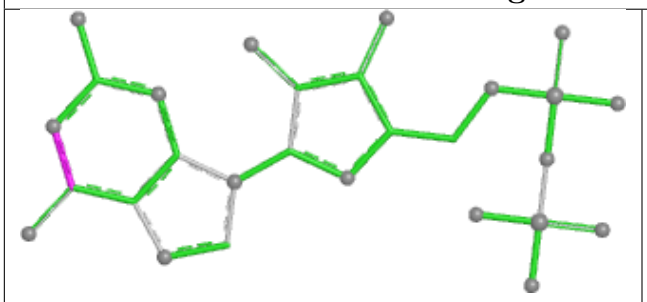

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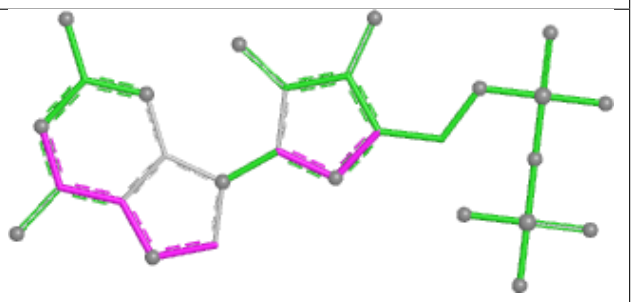

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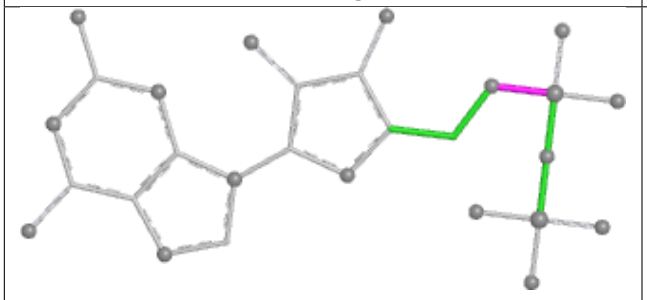
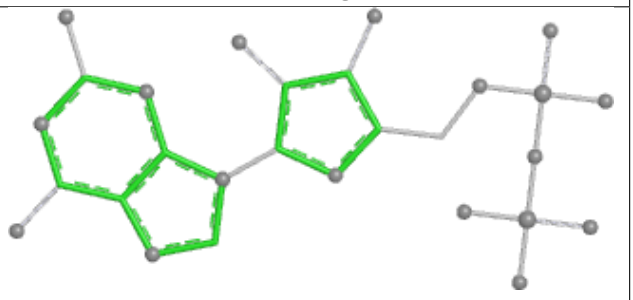
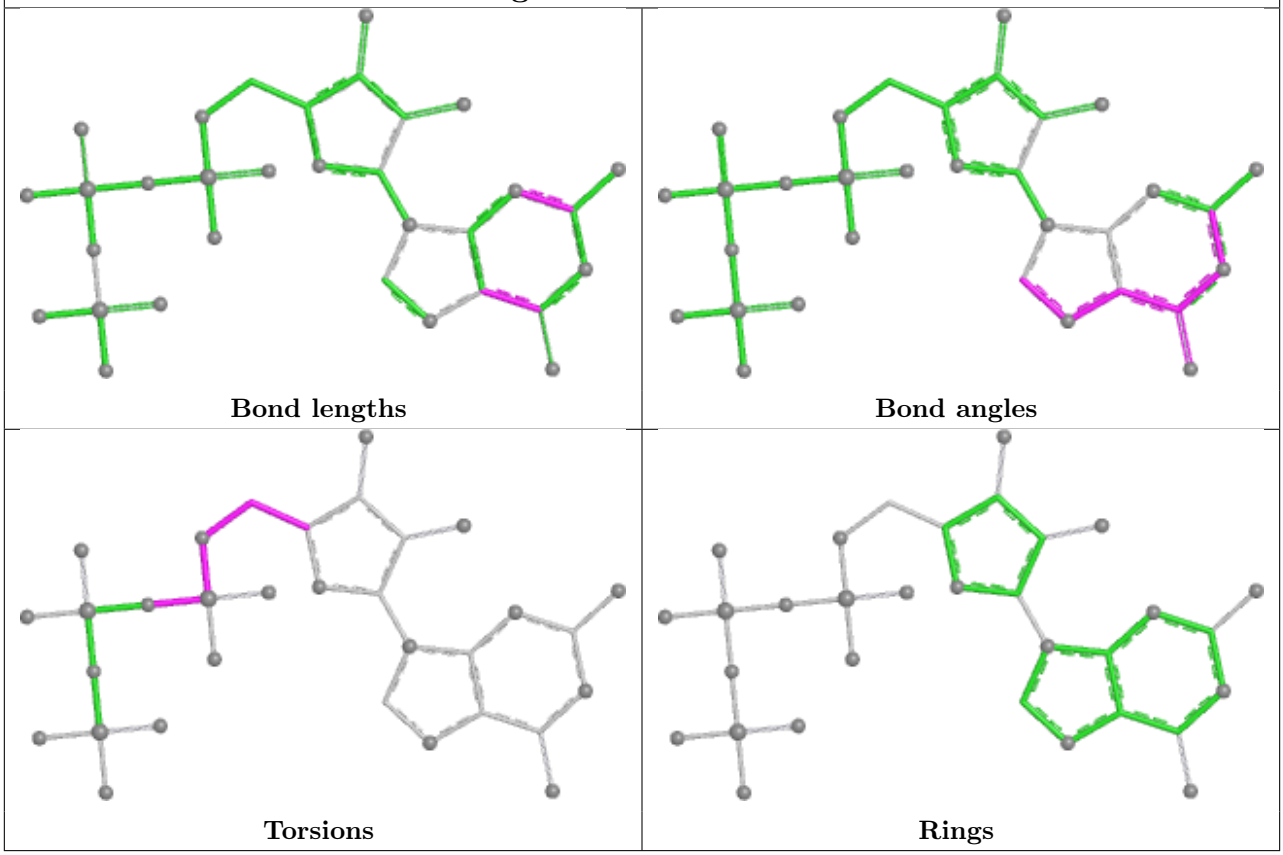


Torsions

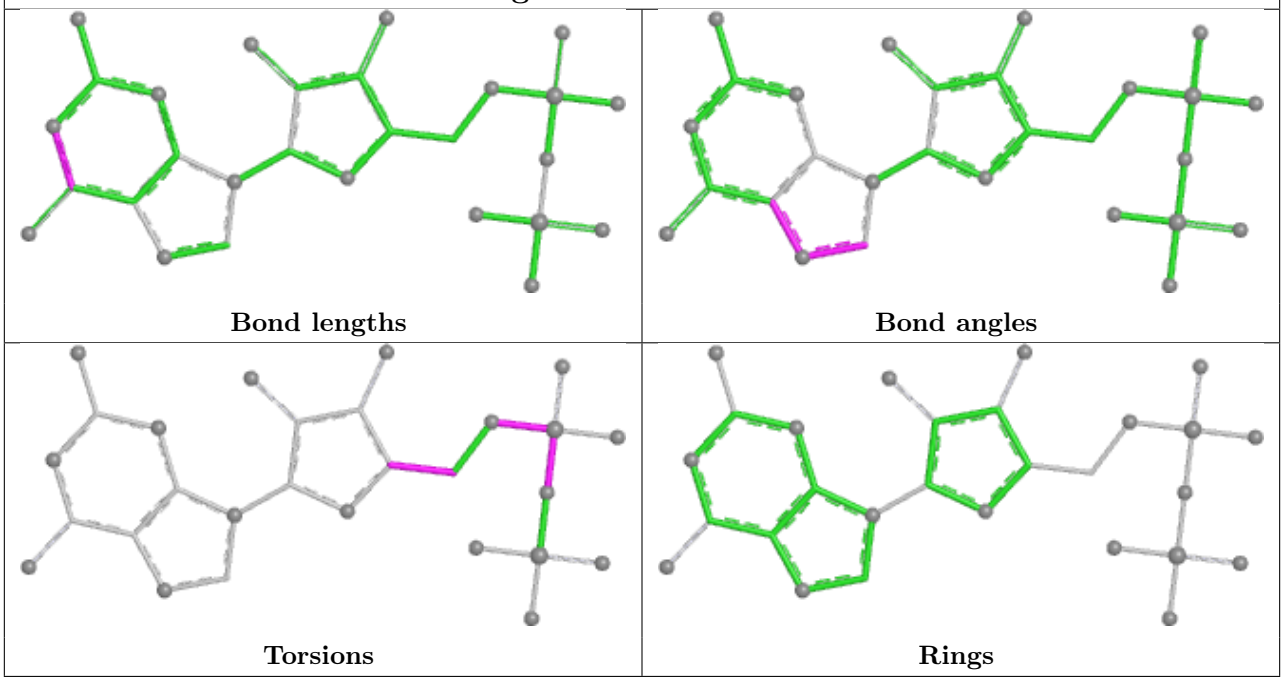


Rings

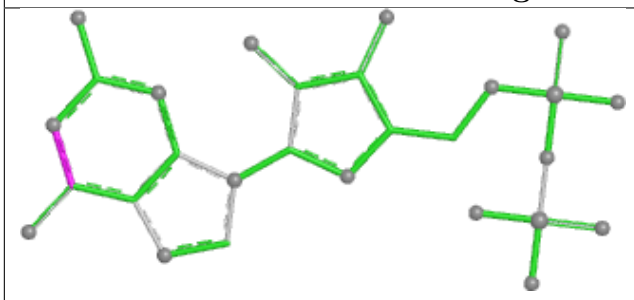
Ligand GTP FK 501



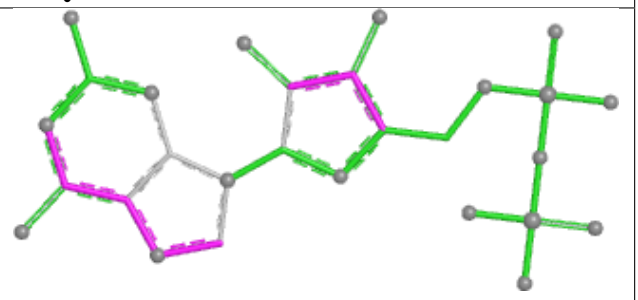
Ligand GDP SD 501



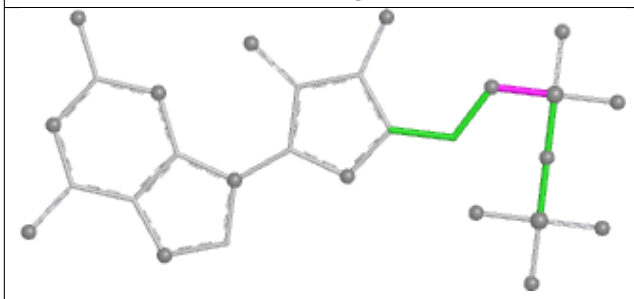
Ligand GDP QJ 501



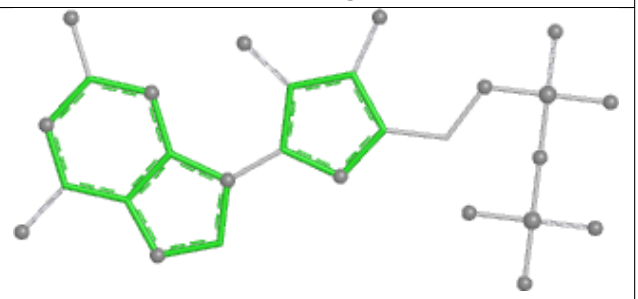
Bond lengths



Bond angles

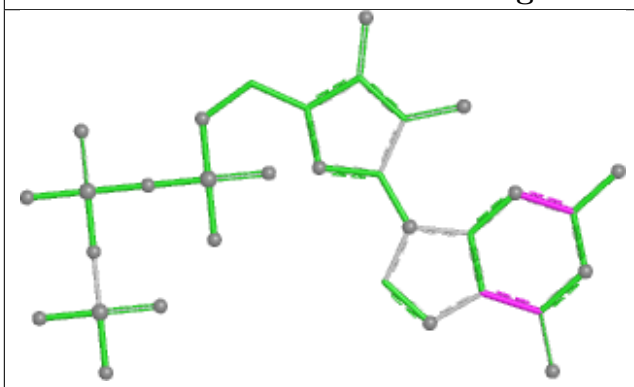


Torsions

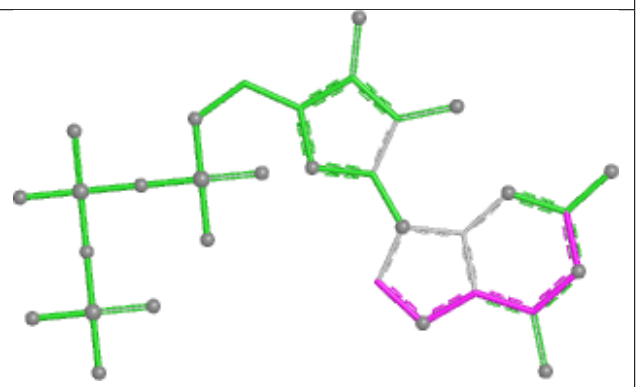


Rings

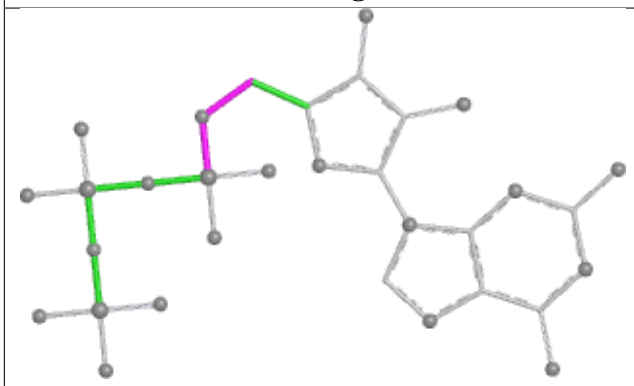
Ligand GTP DI 501



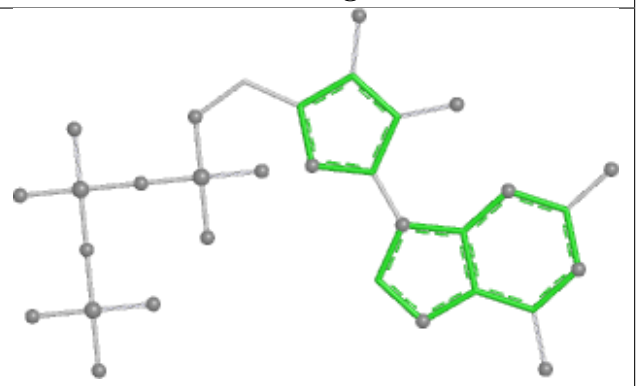
Bond lengths



Bond angles

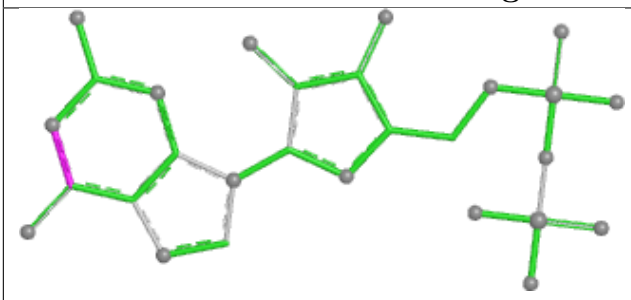


Torsions

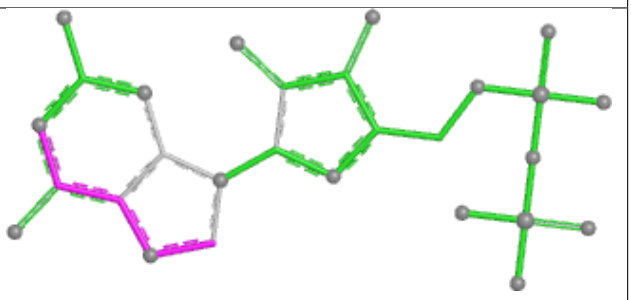


Rings

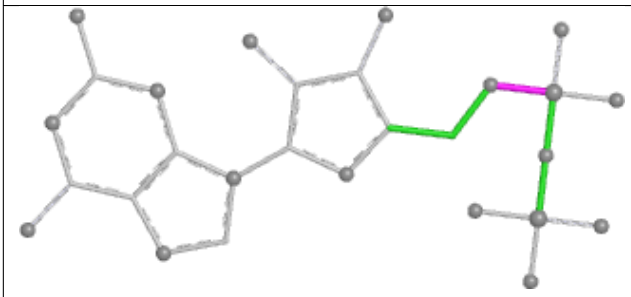
Ligand GDP WH 501



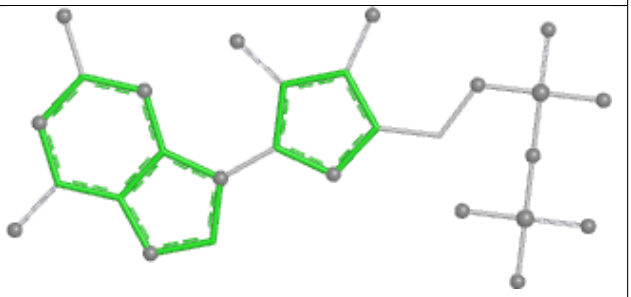
Bond lengths



Bond angles

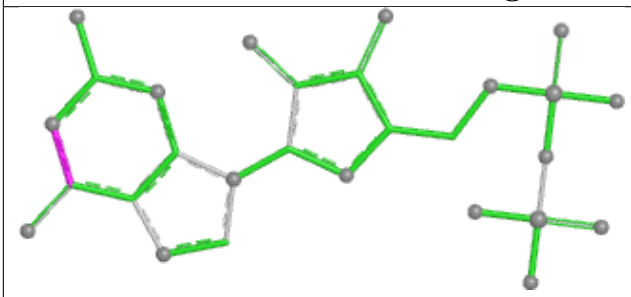


Torsions

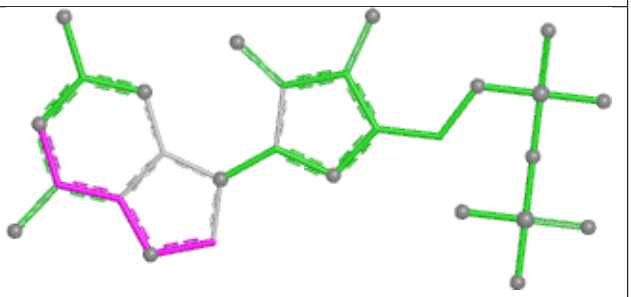


Rings

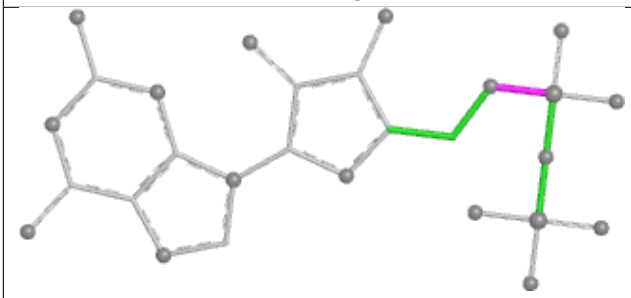
Ligand GDP MD 501



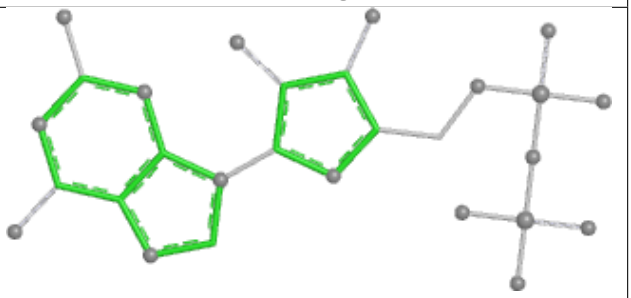
Bond lengths



Bond angles

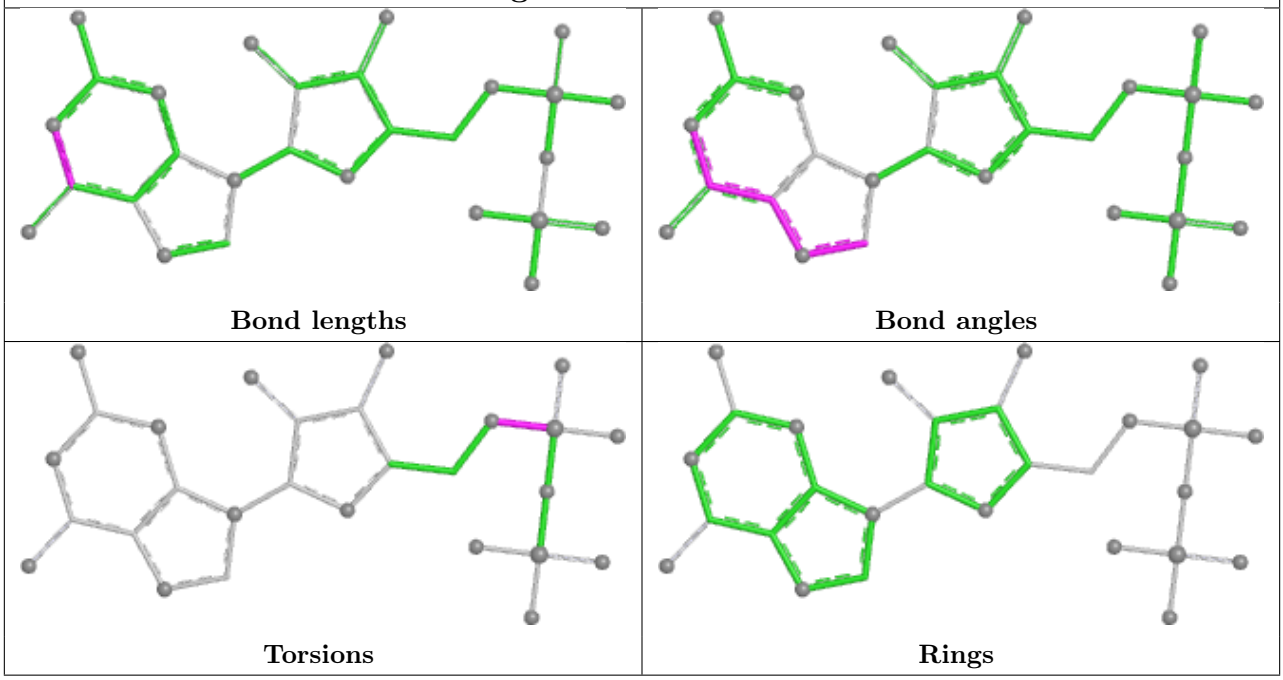


Torsions

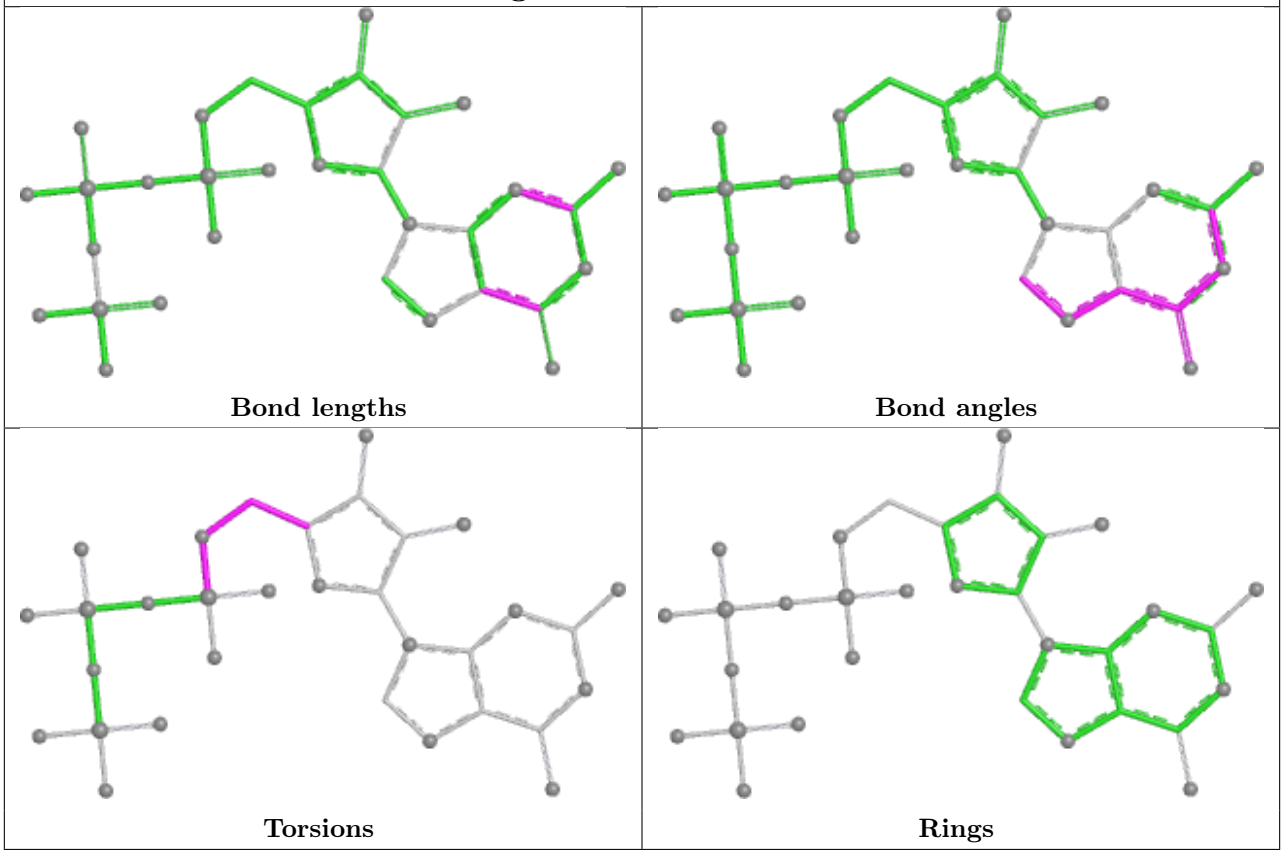


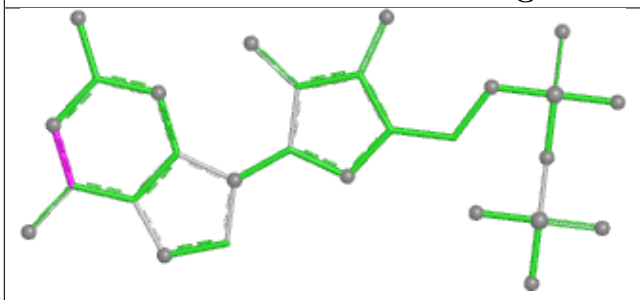
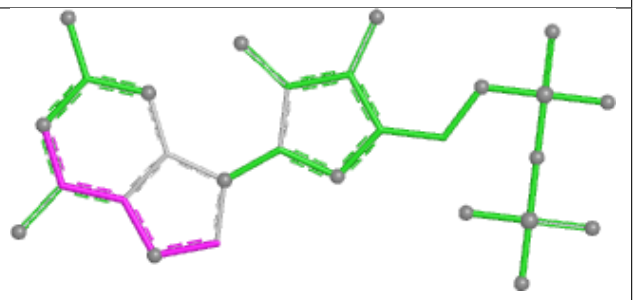
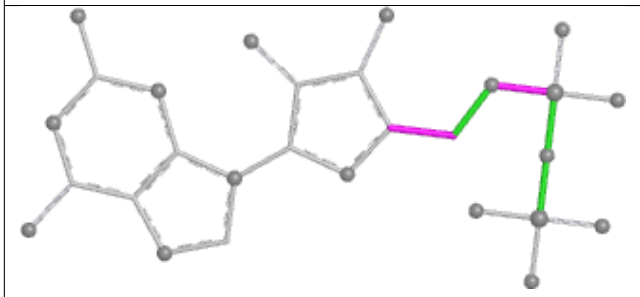
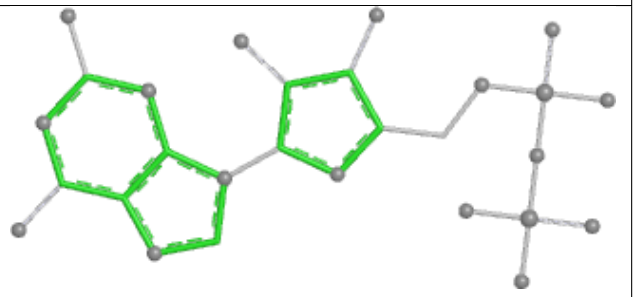
Rings

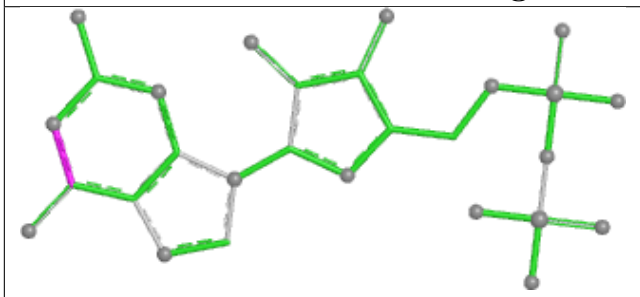
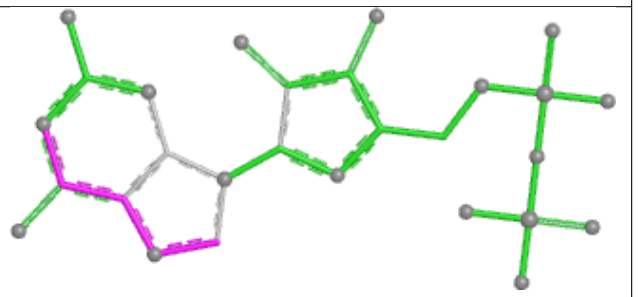
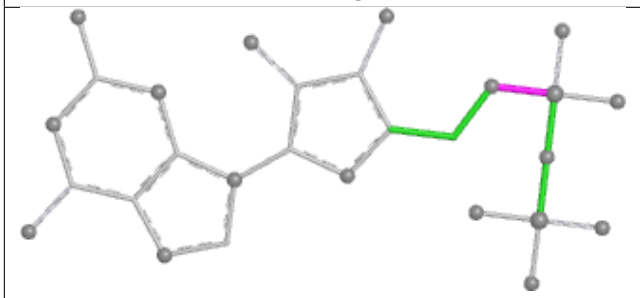
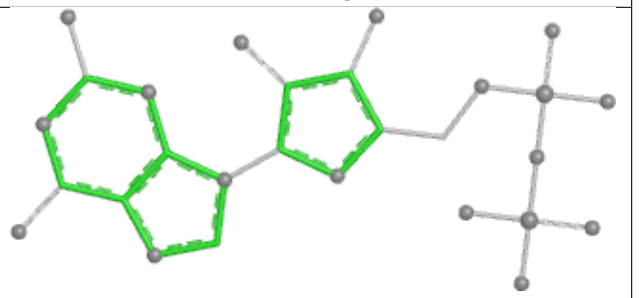
Ligand GDP LH 501



Ligand GTP TG 501



Ligand GDP JJ 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP FH 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

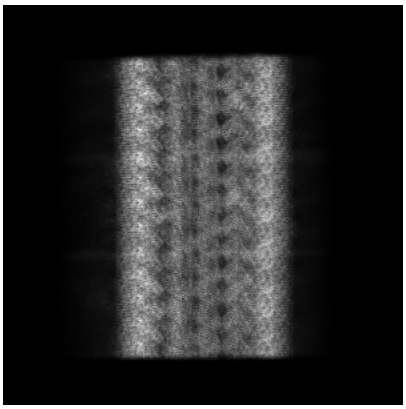
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-40619. These allow visual inspection of the internal detail of the map and identification of artifacts.

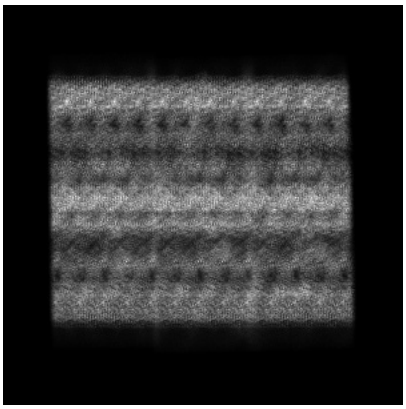
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

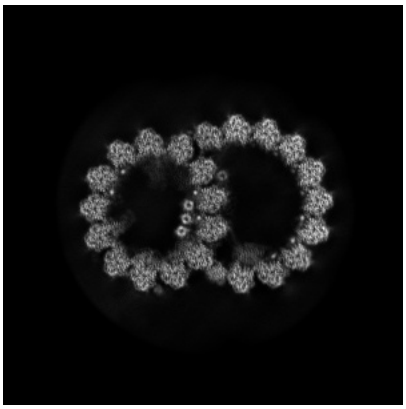
6.1.1 Primary map



X

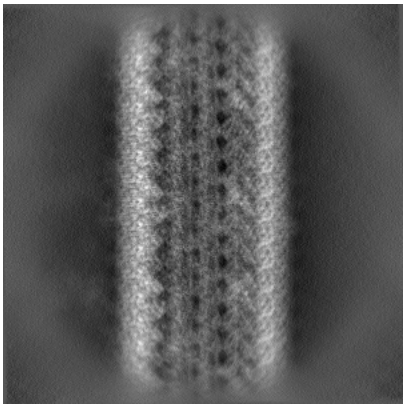


Y

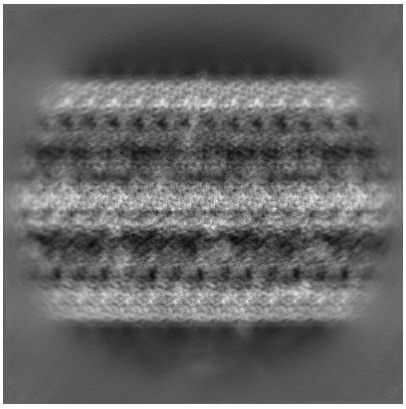


Z

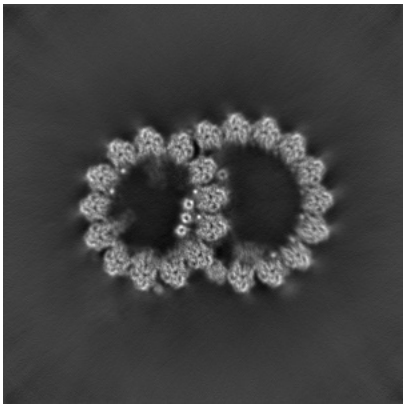
6.1.2 Raw map



X



Y

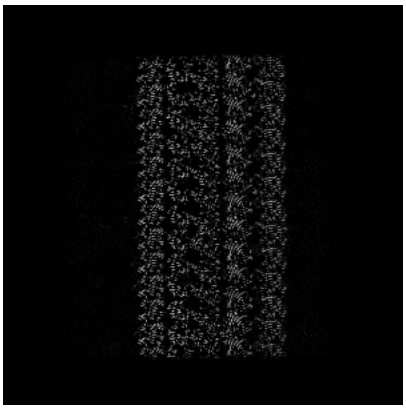


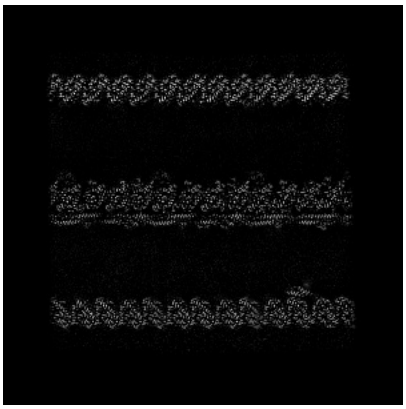
Z

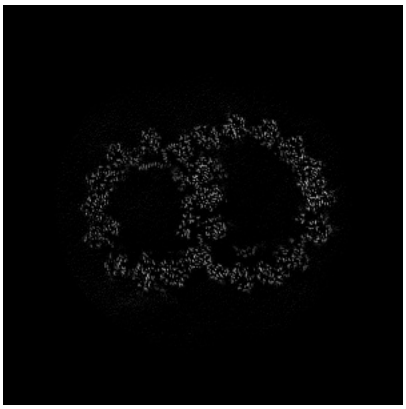
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

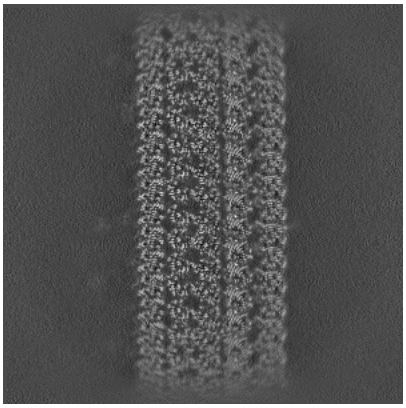
6.2.1 Primary map

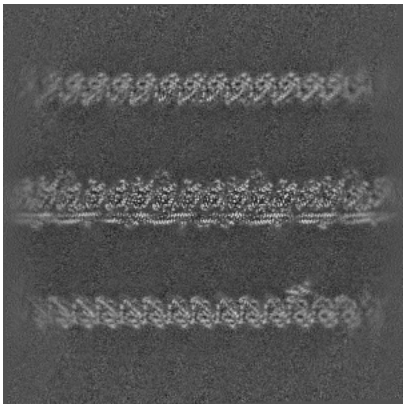

X Index: 256

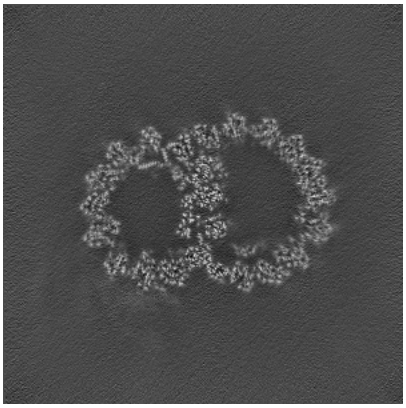

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

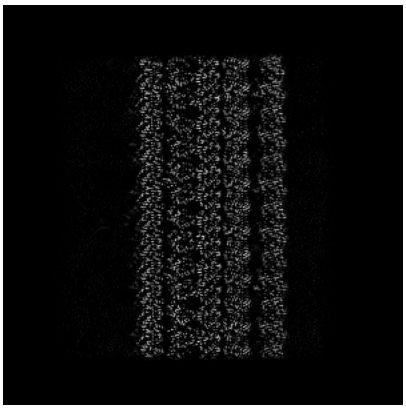

Y Index: 256


Z Index: 256

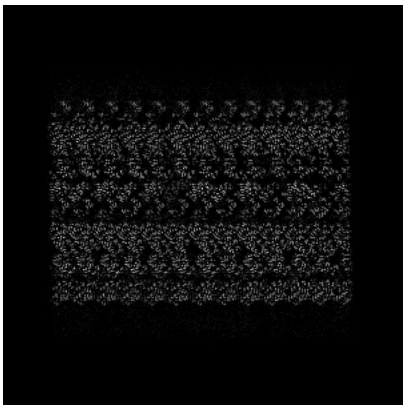
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

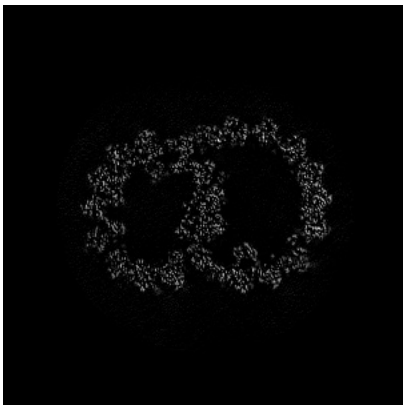
6.3.1 Primary map



X Index: 258

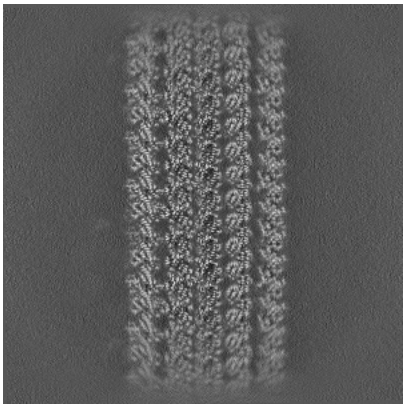


Y Index: 174

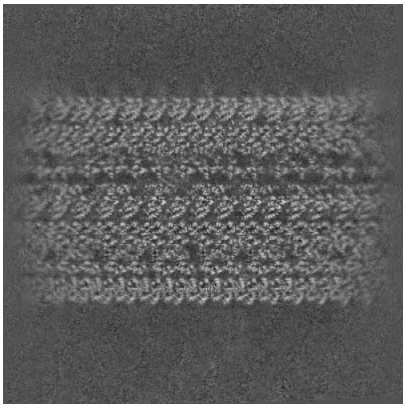


Z Index: 385

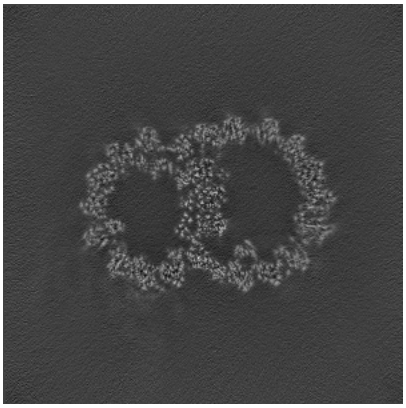
6.3.2 Raw map



X Index: 264



Y Index: 177

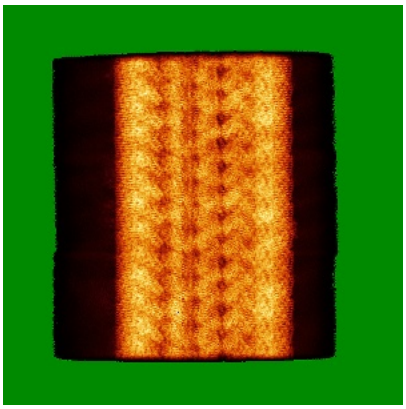


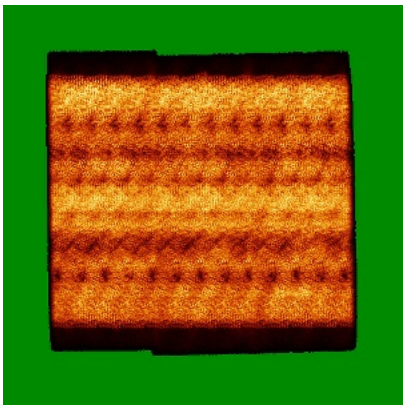
Z Index: 260

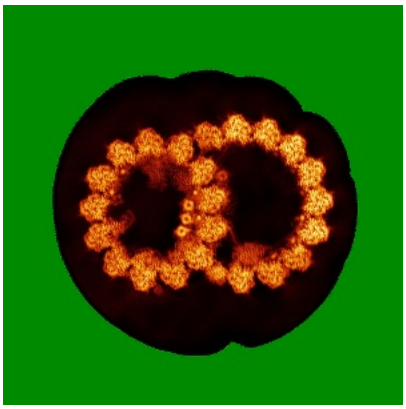
The images above show the largest variance slices of the map in three orthogonal directions.

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

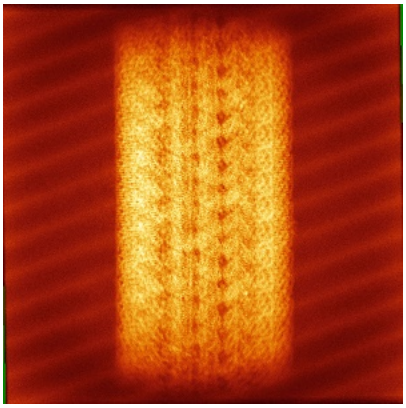
6.4.1 Primary map

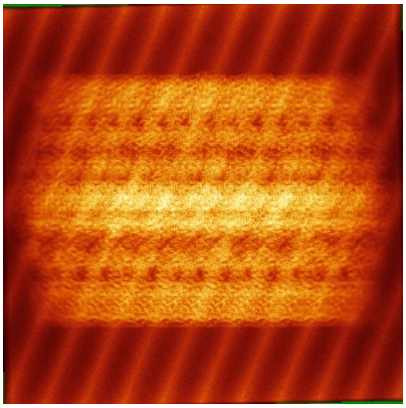

X

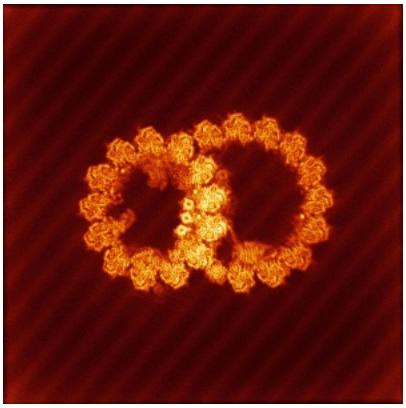

Y


Z

6.4.2 Raw map


X

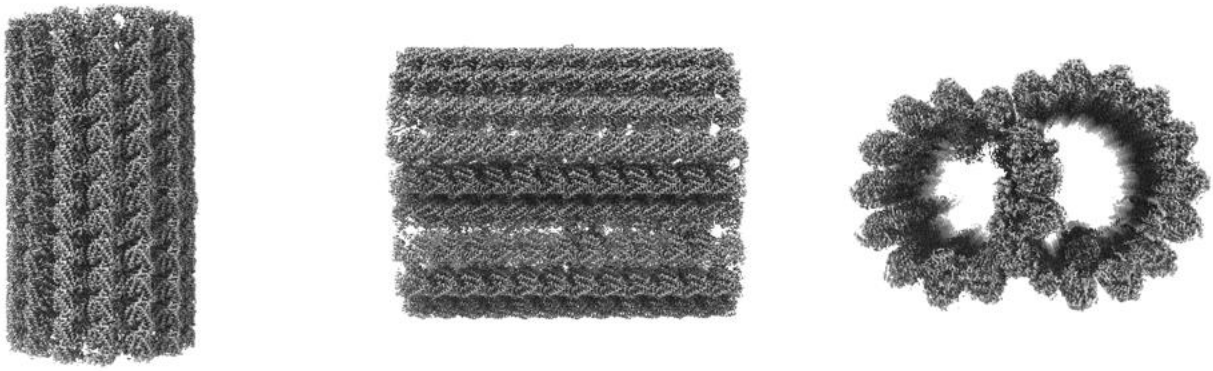

Y


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)

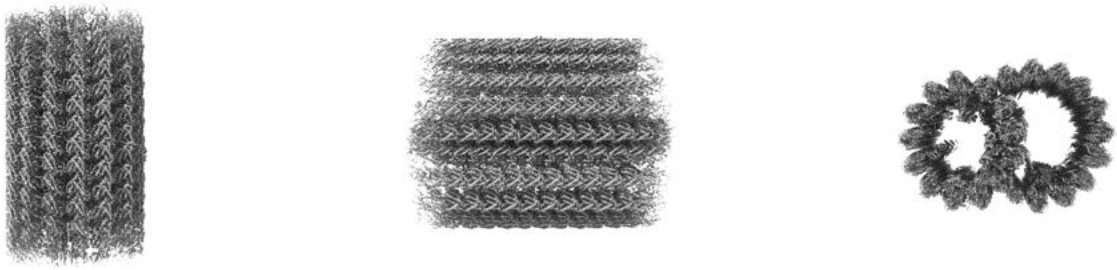
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.63. 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.

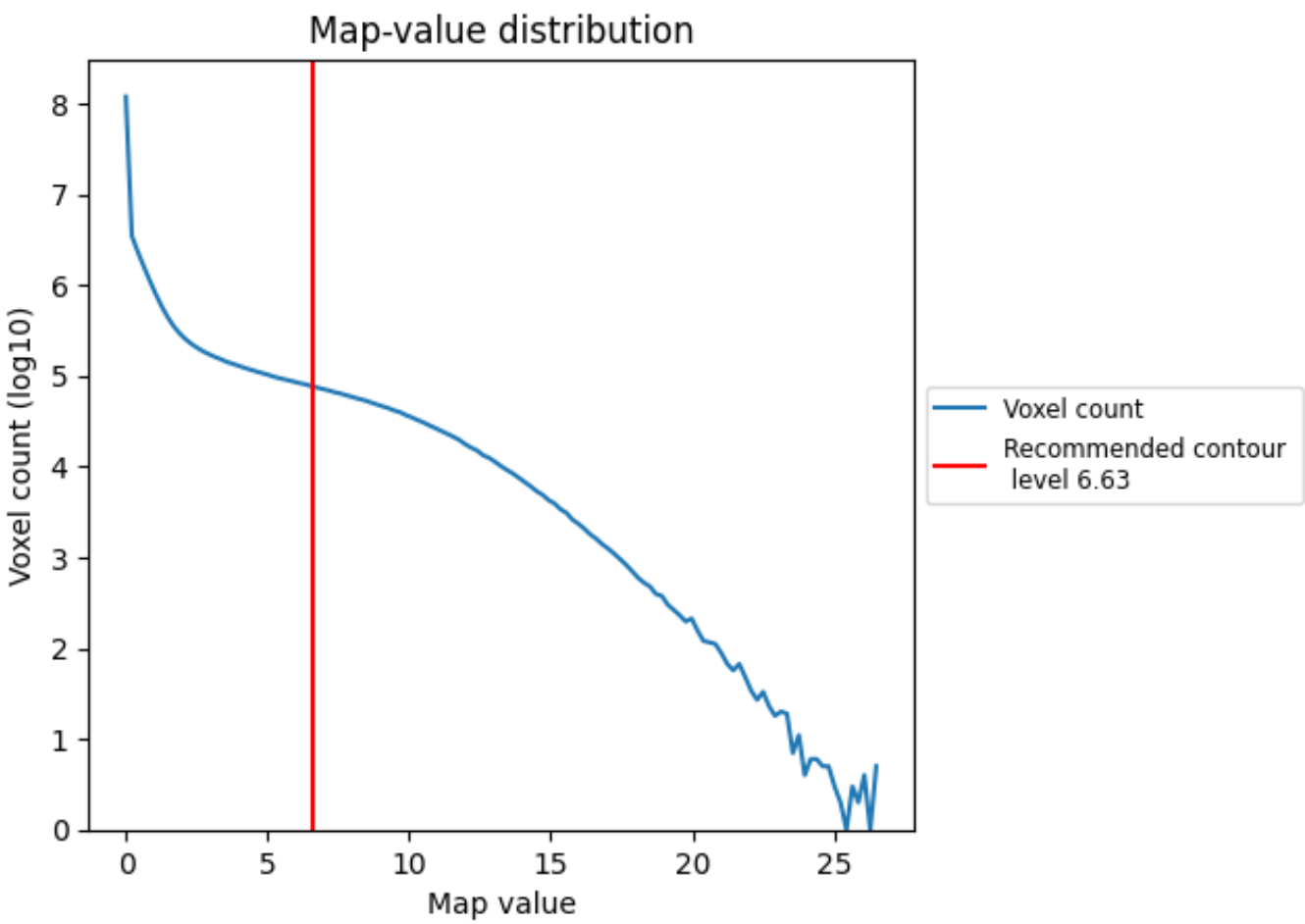
6.6 Mask visualisation (i)

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

7 Map analysis (i)

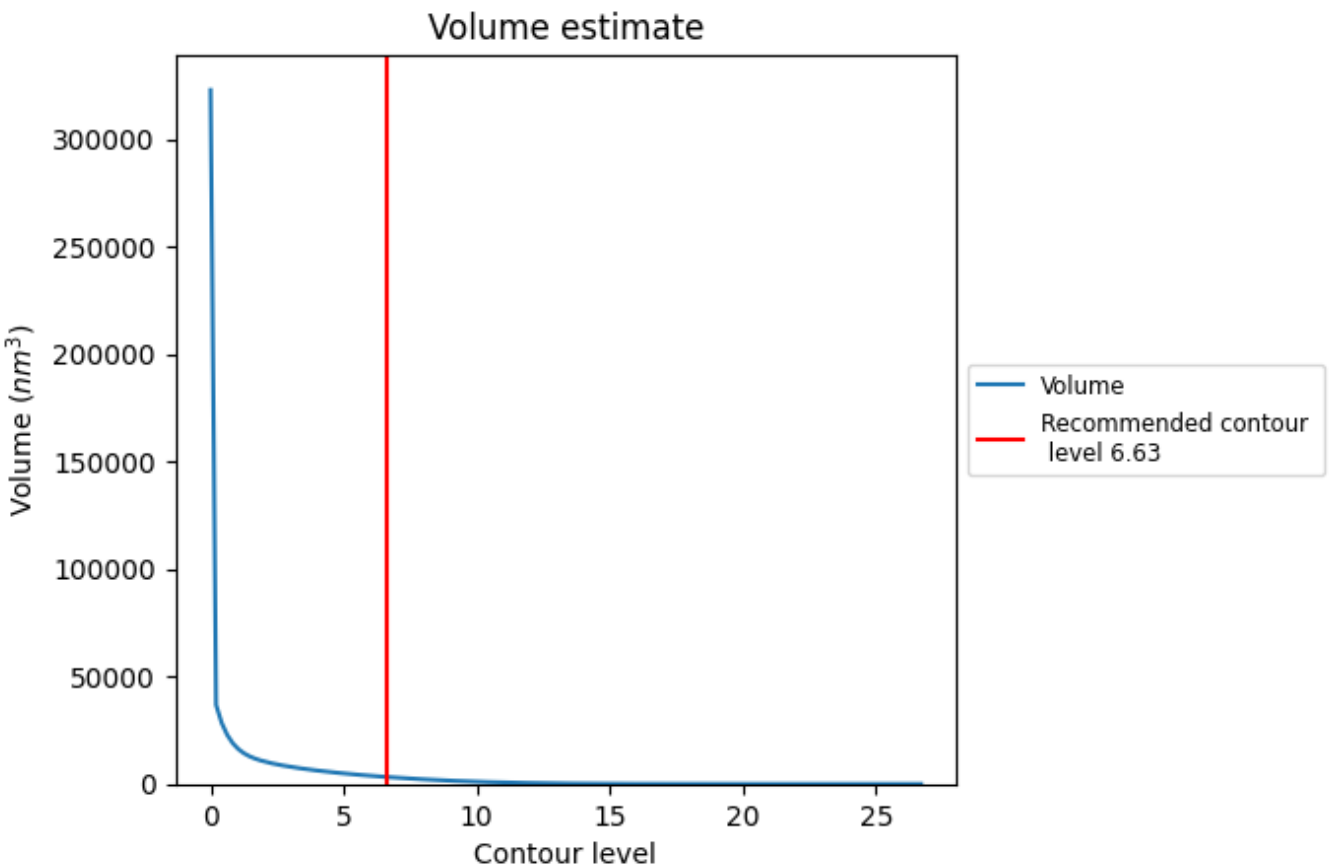
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

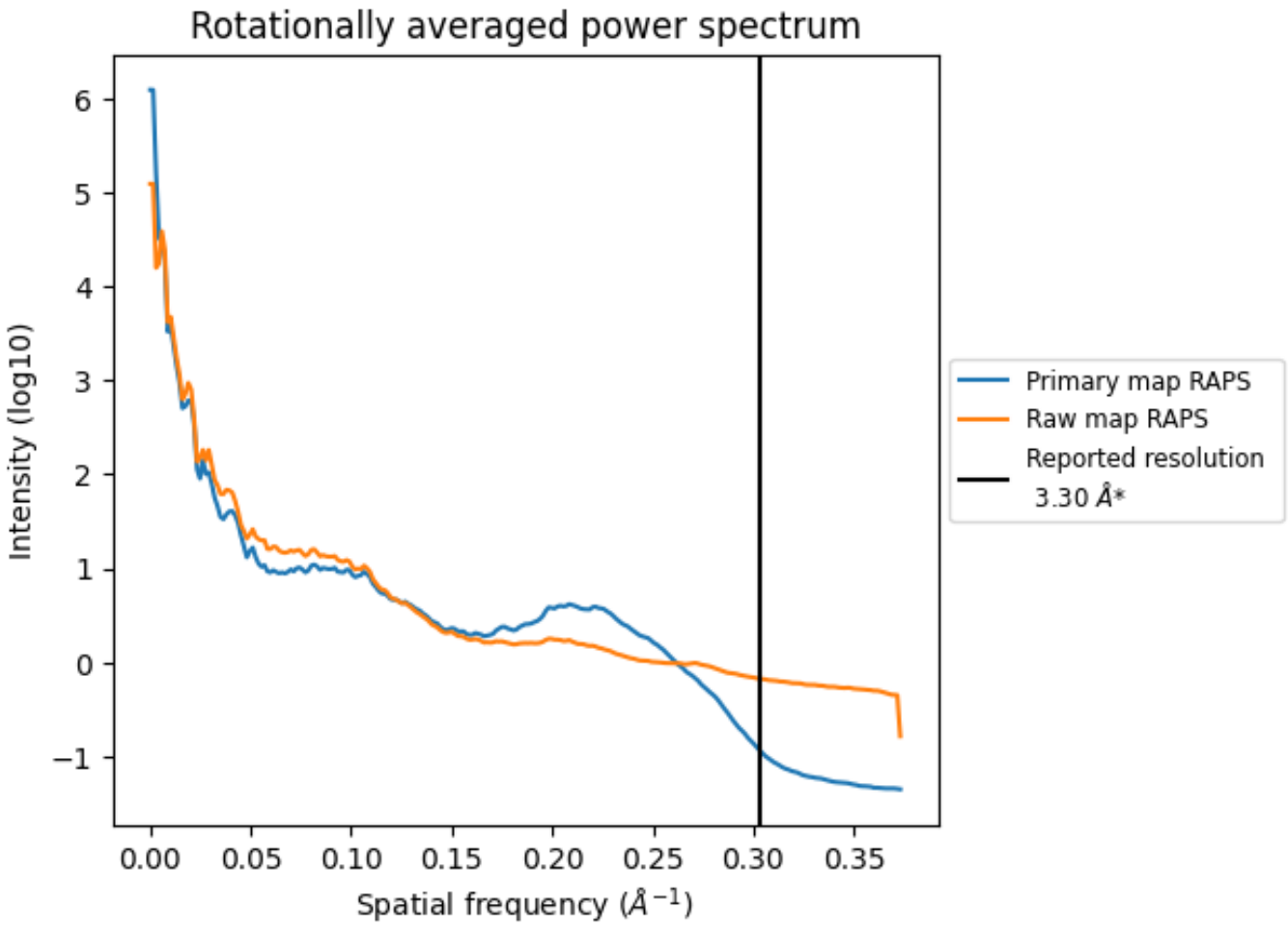
7.2 Volume estimate (i)



The volume at the recommended contour level is 3228 nm^3; this corresponds to an approximate mass of 2916 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)

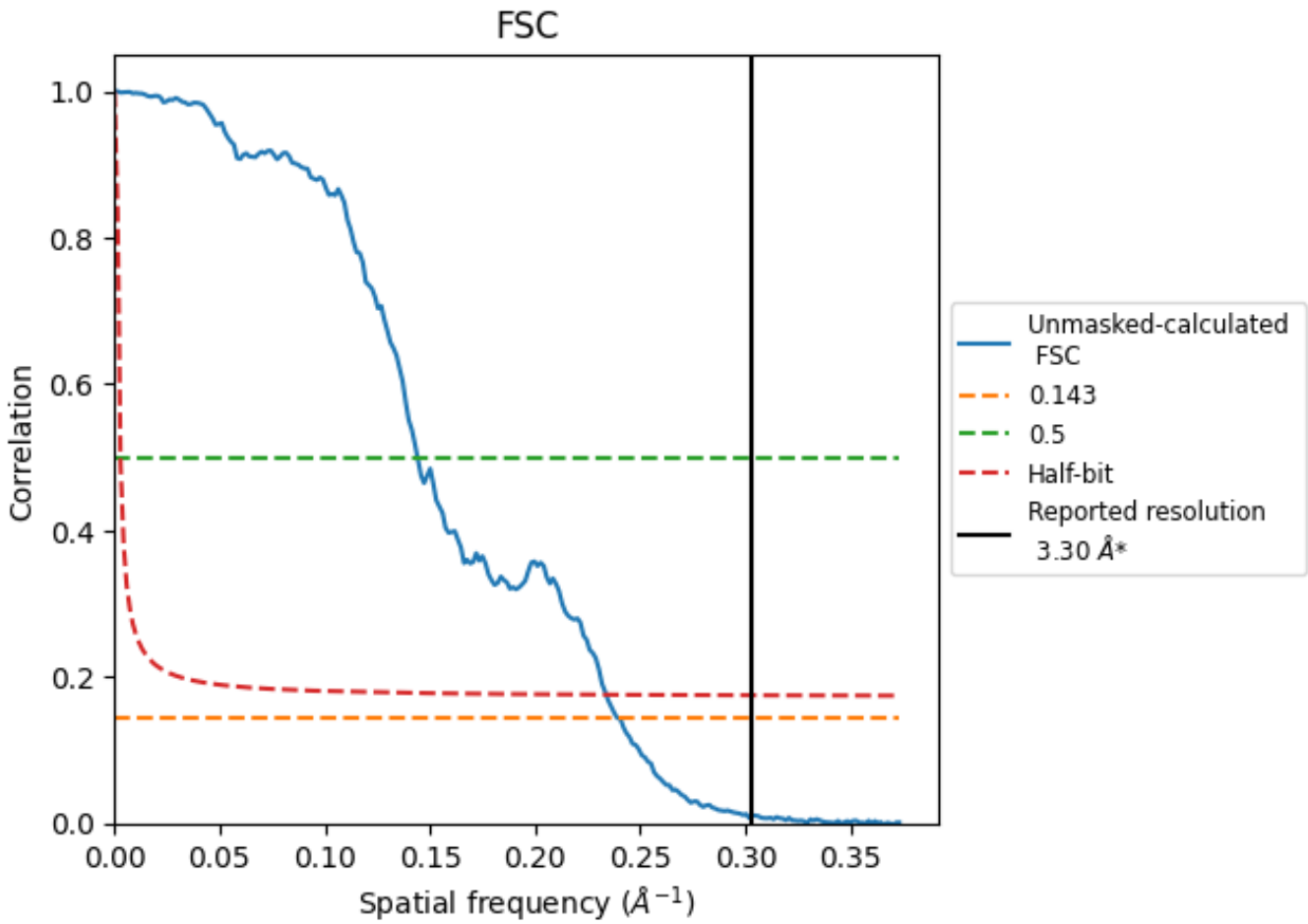


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

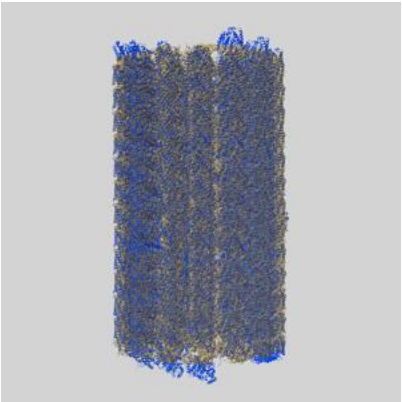
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.18	6.94	4.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 3.3 by more than 10 %

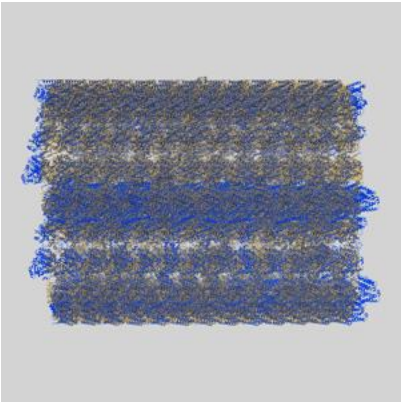
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-40619 and PDB model 8SNB. Per-residue inclusion information can be found in section 3 on page 71.

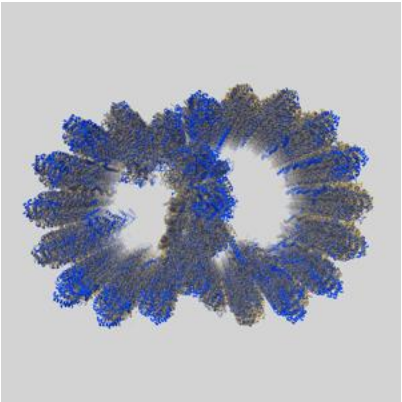
9.1 Map-model overlay (i)



X



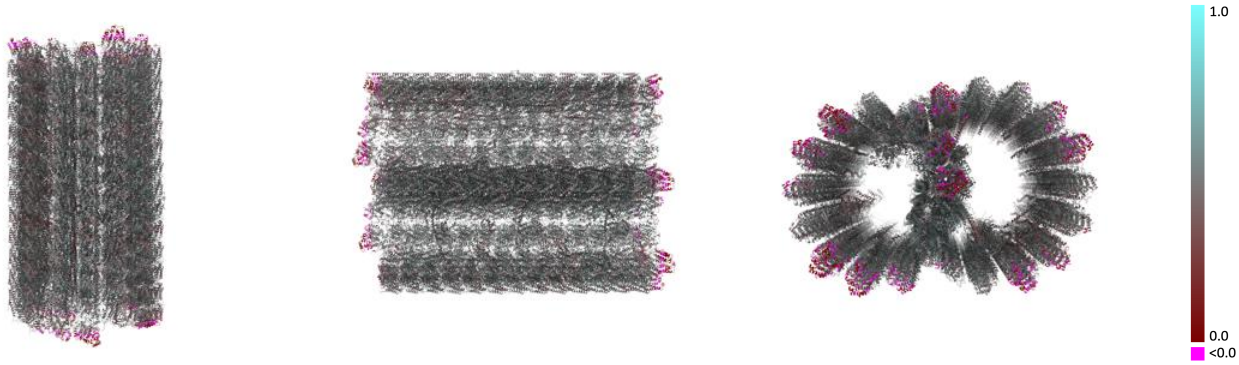
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.63 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.

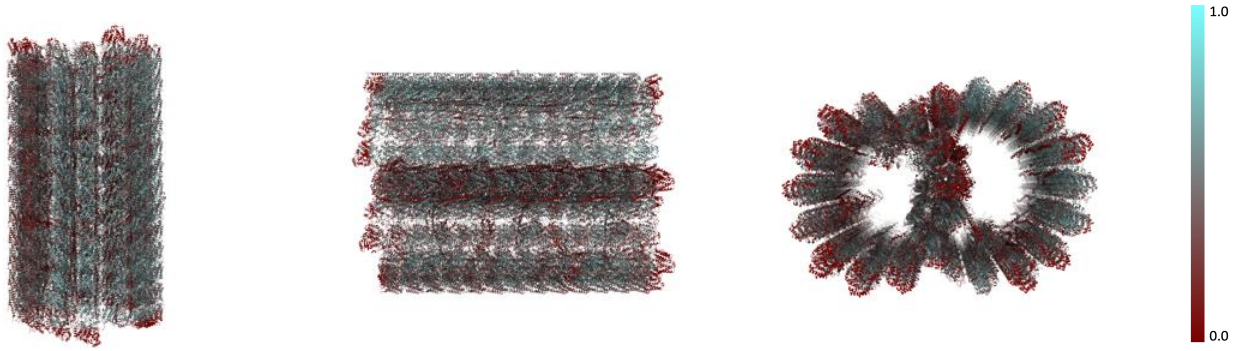
9.2 Q-score mapped to coordinate model (i)



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.

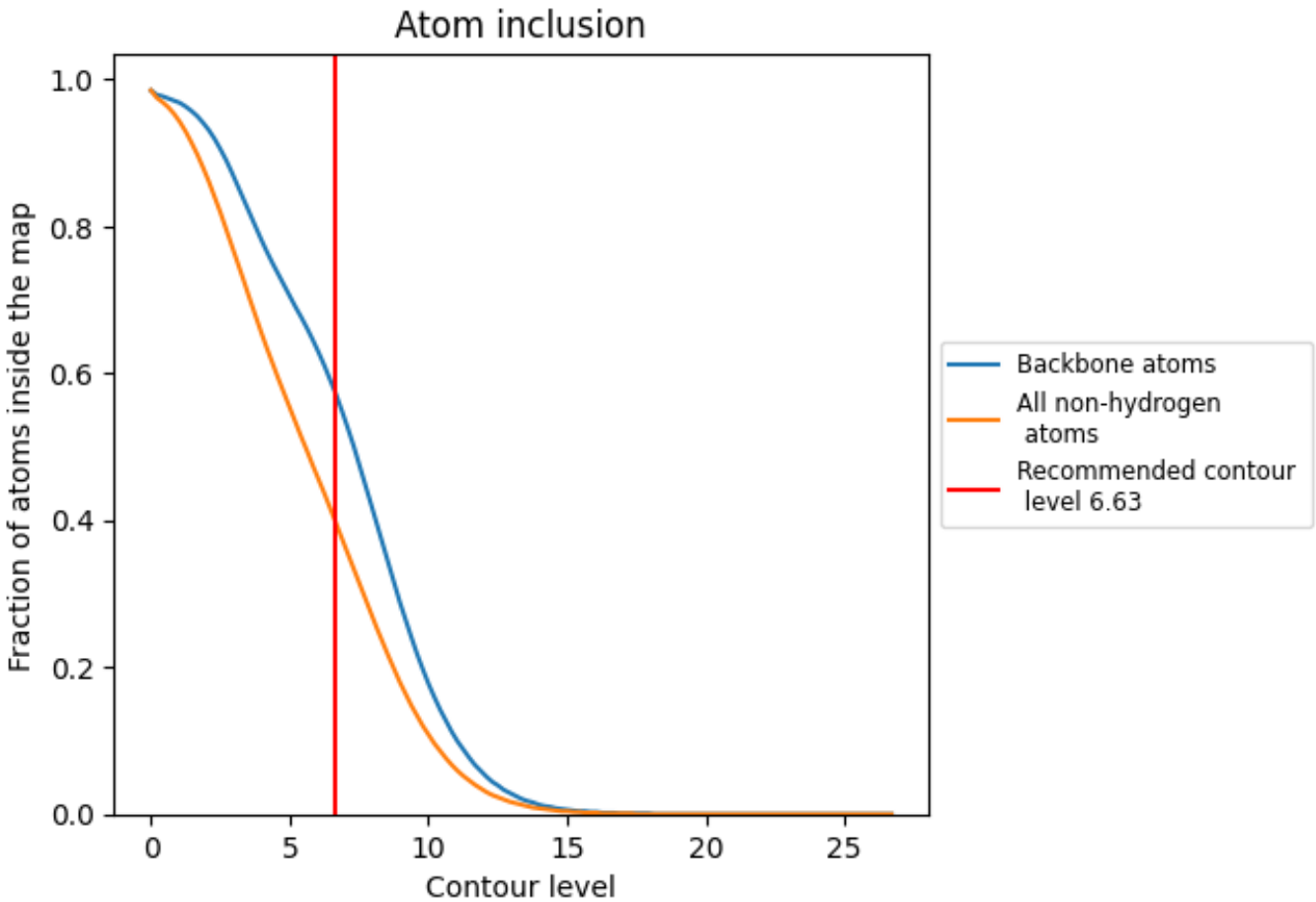
9.3 Atom inclusion mapped to coordinate model (i)



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 (6.63).

9.4 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 40% 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 (6.63) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4000	0.4660
1A	0.2300	0.4870
1B	0.2370	0.4500
1E	0.1060	0.4740
1F	0.0650	0.4450
1G	0.1040	0.4840
1H	0.0330	0.4580
1K	0.0000	0.4050
1L	0.0000	0.4140
1M	0.0000	0.4350
1P	0.3380	0.4850
1Q	0.2620	0.4250
1T	0.3330	0.4780
1U	0.3860	0.4800
1V	0.3120	0.4780
1W	0.3130	0.4720
1Y	0.1950	0.4020
1a	0.1090	0.4400
1b	0.0630	0.4220
1d	0.0350	0.4010
1f	0.3110	0.3900
1g	0.2520	0.3900
1i	0.2200	0.4110
1j	0.2320	0.4330
1l	0.0030	0.3890
1m	0.0130	0.3910
1o	0.2770	0.4580
1p	0.3900	0.4540
1q	0.3040	0.4170
1r	0.3070	0.4490
1v	0.0270	0.4260
1w	0.0140	0.3970
1x	0.0040	0.3490
1y	0.0040	0.3610
1z	0.0060	0.3450

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Chain	Atom inclusion	Q-score
2A	0.2450	0.4620
2B	0.2510	0.4430
2C	0.2320	0.4520
2D	0.2460	0.4260
2G	0.3030	0.4950
2J	0.0790	0.4560
2K	0.1610	0.4810
2L	0.2380	0.4920
2O	0.2750	0.4660
2R	0.3660	0.4520
2S	0.2590	0.4370
2V	0.3270	0.4920
2W	0.3440	0.4920
2a	0.0140	0.3200
3A	0.4710	0.5070
3B	0.4630	0.4870
3C	0.3300	0.4660
3D	0.3340	0.4640
3E	0.4550	0.5060
3F	0.3670	0.4770
3G	0.4810	0.5060
3J	0.2750	0.4500
3K	0.1310	0.4050
3N	0.3440	0.4080
3O	0.3370	0.4220
3R	0.2060	0.4740
3S	0.2230	0.4720
3T	0.2020	0.4670
3W	0.1430	0.3880
3X	0.2380	0.3920
3Y	0.2550	0.4370
3Z	0.2560	0.4150
4A	0.3310	0.4840
4B	0.3870	0.4830
4C	0.3550	0.4820
4F	0.3350	0.4370
4G	0.3810	0.4700
4J	0.3330	0.4700
4K	0.2700	0.4560
4N	0.2530	0.4710
4O	0.0480	0.4180
4P	0.0730	0.4320

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Chain	Atom inclusion	Q-score
4Q	0.0850	0.4150
4T	0.0030	0.4390
4U	0.0010	0.4270
4V	0.0000	0.3900
4Y	0.3690	0.5020
5A	0.0620	0.4830
5B	0.2180	0.4670
5E	0.2560	0.4580
5F	0.3250	0.4680
5G	0.3060	0.4430
5H	0.3360	0.4390
5I	0.1130	0.3900
5J	0.2820	0.4330
5K	0.3680	0.4210
5L	0.4200	0.4410
5M	0.2700	0.4390
5N	0.3410	0.4330
5O	0.0530	0.4630
6A	0.4290	0.5010
6B	0.0300	0.4660
6C	0.3150	0.4820
6D	0.4400	0.4990
6E	0.4580	0.5100
6F	0.4260	0.4940
6I	0.3260	0.4550
6J	0.2770	0.4490
6M	0.3810	0.5150
6N	0.3090	0.4940
6Q	0.3950	0.4880
6R	0.3190	0.5020
6U	0.3730	0.4970
6V	0.4340	0.5060
6W	0.4200	0.4920
6X	0.4200	0.4900
7A	0.3180	0.4640
7B	0.1530	0.4100
7C	0.3290	0.4680
7D	0.3300	0.4600
7G	0.3840	0.4800
7H	0.3790	0.4780
7I	0.3090	0.4650
7M	0.3950	0.5270

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Chain	Atom inclusion	Q-score
7N	0.3650	0.5030
7Q	0.3120	0.4820
7R	0.1320	0.4600
7U	0.1270	0.4100
7V	0.1810	0.4140
7Y	0.2980	0.4570
7Z	0.1020	0.3970
8A	0.2820	0.4570
8D	0.4450	0.5040
8E	0.3870	0.4870
8F	0.4200	0.5110
8G	0.3990	0.4920
8J	0.4570	0.5040
8K	0.4180	0.5030
8L	0.4290	0.4880
8M	0.4160	0.4860
8N	0.4230	0.5350
8Q	0.4940	0.5320
8R	0.4470	0.4910
8S	0.4310	0.4880
8T	0.4700	0.4910
8U	0.4800	0.4980
8X	0.0360	0.4510
8Y	0.1000	0.4650
8Z	0.0320	0.4450
9A	0.2910	0.4670
9D	0.1900	0.4420
9G	0.3320	0.4640
9J	0.1040	0.4530
9M	0.2020	0.4350
9N	0.2620	0.4730
9O	0.0270	0.2600
9R	0.4140	0.5090
9T	0.2940	0.4910
9V	0.0060	0.3600
9W	0.0020	0.4150
9Y	0.0430	0.4620
9Z	0.0200	0.4280
AA	0.4710	0.5110
AB	0.4640	0.5090
AC	0.4480	0.5000
AD	0.4700	0.4990

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Chain	Atom inclusion	Q-score
AE	0.4800	0.5100
AF	0.4620	0.4970
AG	0.4400	0.5010
AH	0.4930	0.5080
AI	0.5090	0.5180
AJ	0.5120	0.5120
AK	0.3500	0.4750
AL	0.4950	0.5140
AM	0.2850	0.3990
BA	0.4360	0.4940
BB	0.4030	0.4790
BC	0.4320	0.4850
BD	0.4270	0.4780
BE	0.4230	0.4810
BF	0.3750	0.4640
BG	0.3610	0.4660
BH	0.4300	0.4770
BI	0.4120	0.4790
BJ	0.4150	0.4750
BK	0.2310	0.3620
BL	0.4190	0.4900
BM	0.3650	0.4560
CA	0.4850	0.4970
CB	0.4500	0.4900
CC	0.4620	0.4880
CD	0.4690	0.4910
CE	0.4820	0.4920
CF	0.4280	0.4780
CG	0.3650	0.4730
CH	0.4710	0.4880
CI	0.4630	0.4870
CJ	0.4080	0.4710
CK	0.1490	0.2580
CL	0.4520	0.4870
CM	0.3900	0.4770
DA	0.4060	0.4820
DB	0.3530	0.4740
DC	0.4220	0.4880
DD	0.3950	0.4800
DE	0.4260	0.4800
DF	0.3760	0.4750
DG	0.3250	0.4640

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Chain	Atom inclusion	Q-score
DH	0.3500	0.4720
DI	0.3740	0.4750
DJ	0.3870	0.4770
DK	0.0420	0.1280
DL	0.3750	0.4760
DM	0.3640	0.4740
EA	0.3920	0.4700
EB	0.3970	0.4730
EC	0.3680	0.4790
ED	0.3540	0.4680
EE	0.3790	0.4840
EF	0.3870	0.4720
EG	0.3450	0.4720
EH	0.3180	0.4590
EI	0.3410	0.4660
EJ	0.4210	0.4790
EK	0.3900	0.4810
EL	0.1180	0.2590
EM	0.3060	0.4670
FA	0.4480	0.4700
FB	0.4290	0.4770
FC	0.4600	0.4820
FD	0.3720	0.4530
FE	0.4310	0.4680
FF	0.4560	0.4760
FG	0.4200	0.4720
FH	0.3260	0.4480
FI	0.4010	0.4620
FJ	0.4490	0.4750
FK	0.4270	0.4740
FL	0.2420	0.3820
FM	0.3010	0.4200
GA	0.4280	0.4790
GB	0.4800	0.4920
GC	0.4690	0.4840
GD	0.3460	0.4480
GE	0.4050	0.4670
GF	0.4630	0.4790
GG	0.4460	0.4760
GH	0.3470	0.4600
GI	0.4150	0.4700
GJ	0.4230	0.4860

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Chain	Atom inclusion	Q-score
GK	0.4470	0.4830
GL	0.3110	0.4540
GM	0.2270	0.3320
HA	0.4190	0.4800
HB	0.4890	0.4930
HC	0.4590	0.4830
HD	0.3390	0.4560
HE	0.3940	0.4760
HF	0.4700	0.4900
HG	0.4680	0.4860
HH	0.3890	0.4720
HI	0.4460	0.4800
HJ	0.4790	0.4940
HK	0.5190	0.4990
HL	0.3460	0.4700
HM	0.1070	0.2130
IA	0.3780	0.4810
IB	0.4680	0.5000
IC	0.4230	0.4890
ID	0.4020	0.4810
IE	0.3060	0.4640
IF	0.4610	0.4990
IG	0.4440	0.4970
IH	0.3460	0.4750
II	0.4200	0.4940
IJ	0.4330	0.4920
IK	0.4500	0.4950
IL	0.3010	0.4750
IM	0.0910	0.2470
JA	0.4540	0.5000
JB	0.4600	0.5000
JC	0.4920	0.5010
JD	0.3820	0.4920
JE	0.4320	0.4950
JF	0.4410	0.5030
JG	0.3920	0.4940
JH	0.4660	0.5000
JI	0.4120	0.4940
JJ	0.4820	0.5080
JK	0.4260	0.5000
JL	0.2230	0.3830
JM	0.3500	0.4610

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Chain	Atom inclusion	Q-score
KA	0.4680	0.5060
KB	0.4850	0.5020
KC	0.4670	0.5020
KD	0.4420	0.4950
KE	0.4500	0.5030
KF	0.4780	0.5060
KG	0.4720	0.5040
KH	0.4630	0.5020
KI	0.4190	0.5120
KJ	0.4190	0.5080
KK	0.4810	0.5110
KL	0.3550	0.4840
KM	0.2640	0.3640
LA	0.4810	0.5140
LB	0.4700	0.5120
LC	0.4440	0.5070
LD	0.4740	0.5150
LE	0.4480	0.5130
LF	0.4690	0.5120
LG	0.4610	0.5190
LH	0.4940	0.5280
LI	0.4850	0.5250
LJ	0.4970	0.5270
LK	0.4710	0.5140
LL	0.4710	0.5180
LM	0.1310	0.2360
MA	0.4690	0.5140
MB	0.4590	0.5060
MC	0.4390	0.5080
MD	0.4740	0.5140
ME	0.4700	0.5120
MF	0.4690	0.5130
MG	0.4620	0.5210
MH	0.5050	0.5330
MI	0.5460	0.5330
MJ	0.4740	0.5200
MK	0.1520	0.2610
ML	0.4450	0.5090
MM	0.4610	0.5140
NA	0.4130	0.4870
NB	0.3610	0.4700
NC	0.3490	0.4630

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Chain	Atom inclusion	Q-score
ND	0.3990	0.4810
NE	0.3950	0.4830
NF	0.4040	0.4840
NG	0.2760	0.4680
NH	0.3810	0.4770
NI	0.3540	0.4740
NJ	0.2800	0.4600
NK	0.1300	0.2640
NL	0.3850	0.4740
NM	0.3970	0.4710
OA	0.5550	0.4990
OB	0.4890	0.4820
OC	0.4970	0.4780
OD	0.5200	0.4870
OE	0.5470	0.4960
OF	0.5540	0.4930
OG	0.4940	0.4720
OH	0.5670	0.4880
OI	0.5420	0.4820
OJ	0.4680	0.4590
OK	0.1240	0.1660
OL	0.5340	0.4840
OM	0.5140	0.4830
PA	0.5550	0.4900
PB	0.4630	0.4690
PC	0.4740	0.4640
PD	0.5420	0.4880
PE	0.5530	0.4970
PF	0.5330	0.4870
PG	0.4690	0.4640
PH	0.5100	0.4720
PI	0.5150	0.4750
PJ	0.4370	0.4520
PK	0.2450	0.3020
PL	0.4430	0.4630
PM	0.5200	0.4790
QA	0.5610	0.4840
QB	0.4710	0.4620
QC	0.5120	0.4750
QD	0.5360	0.4970
QE	0.5360	0.4940
QF	0.5200	0.4930

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Chain	Atom inclusion	Q-score
QG	0.5070	0.4660
QH	0.5130	0.4530
QI	0.5720	0.4680
QJ	0.5360	0.4650
QK	0.4440	0.4230
QL	0.3330	0.3730
QM	0.5630	0.4820
RA	0.5430	0.4770
RB	0.4930	0.4590
RC	0.5310	0.4730
RD	0.5190	0.4880
RE	0.5470	0.4960
RF	0.5410	0.4890
RG	0.5090	0.4730
RH	0.5100	0.4550
RI	0.5250	0.4650
RJ	0.5600	0.4730
RK	0.4960	0.4590
RL	0.1930	0.2530
RM	0.5290	0.4710
SA	0.5380	0.4760
SB	0.5090	0.4660
SC	0.5360	0.4770
SD	0.5440	0.4870
SE	0.5670	0.4930
SF	0.5430	0.4880
SG	0.5280	0.4810
SH	0.5080	0.4590
SI	0.5700	0.4820
SJ	0.5600	0.4840
SK	0.5570	0.4820
SL	0.1120	0.1610
SM	0.4960	0.4630
TA	0.5300	0.4670
TB	0.5290	0.4730
TC	0.5400	0.4750
TD	0.5310	0.4680
TE	0.5420	0.4800
TF	0.5600	0.4820
TG	0.5200	0.4760
TH	0.4940	0.4550
TI	0.5370	0.4740

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Chain	Atom inclusion	Q-score
TJ	0.5920	0.4850
TK	0.5710	0.4830
TL	0.2170	0.2830
TM	0.4470	0.4510
UA	0.3960	0.4450
UB	0.4010	0.4550
UC	0.3840	0.4500
UD	0.3490	0.4330
UE	0.3570	0.4470
UF	0.3640	0.4440
UG	0.3500	0.4510
UH	0.2920	0.4110
UI	0.3790	0.4580
UJ	0.3850	0.4590
UK	0.4470	0.4610
UL	0.2150	0.3800
UM	0.2520	0.3640
VA	0.3930	0.4560
VB	0.4350	0.4730
VC	0.4350	0.4660
VD	0.4020	0.4600
VE	0.3960	0.4680
VF	0.4160	0.4740
VG	0.4140	0.4710
VH	0.3290	0.4460
VI	0.3720	0.4680
VJ	0.3670	0.4710
VK	0.4080	0.4780
VL	0.3370	0.4640
VM	0.2240	0.2990
WA	0.4190	0.4750
WB	0.4720	0.4820
WC	0.4770	0.4900
WD	0.4330	0.4760
WE	0.3980	0.4730
WF	0.4640	0.4840
WG	0.4550	0.4770
WH	0.3940	0.4770
WI	0.4590	0.4940
WJ	0.4870	0.4900
WK	0.4690	0.4920
WL	0.4600	0.4890