wwPDB EM Validation Summary Report (i)

Mar 6, 2026 – 02:18 AM UTC

PDB ID	:	8OTZ / pdb_00008otz
EMDB ID	:	EMD-17187
Title	:	48-nm repeat of the native axonemal doublet microtubule from bovine sperm
Authors	:	Leung, M.R.; Zeng, J.; Zhang, R.; Zeev-Ben-Mordehai, T.
Deposited on	:	2023-04-21
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

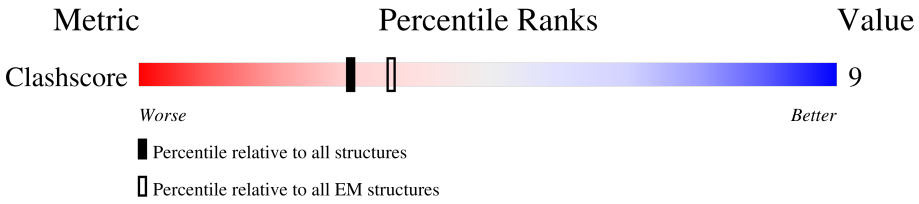
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

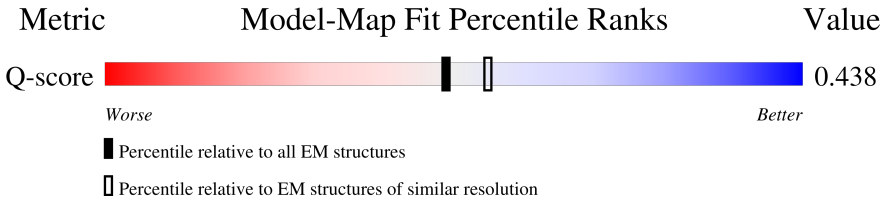
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	0	232	16% · 83%
1	V	232	5% 61% 17% · 21%
2	0A	224	11% 54% 15% · 30%
2	0C	224	17% 51% 18% 30%
2	0E	224	25% 50% 20% 30%
2	0G	224	17% 60% 9% 30%

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Mol	Chain	Length	Quality of chain
2	0W	224	13% 62% 7% 30%
2	0Y	224	12% 50% 19% 30%
2	0a	224	10% 54% 16% 30%
2	0c	224	17% 53% 16% 30%
2	0e	224	5% 56% 13% 31%
2	0g	224	11% 54% 15% 30%
2	0i	224	15% 46% 21% 30%
2	0k	224	17% 51% 19% 30%
2	CT	224	9% 50% 20% 30%
2	CU	224	10% 47% 22% 31%
2	CV	224	24% 49% 21% 30%
2	CX	224	7% 49% 21% 30%
2	CY	224	16% 53% 16% 30%
2	CZ	224	10% 59% 10% 30%
2	Ca	224	10% 56% 13% 30%
2	Cb	224	8% 49% 21% 30%
2	Cc	224	9% 54% 15% 30%
2	Cd	224	15% 52% 17% 30%
2	Ce	224	26% 56% 12% 31%
2	Cf	224	21% 51% 18% 31%
2	Cg	224	15% 53% 16% 30%
2	Ch	224	13% 59% 10% 30%
2	Ci	224	12% 51% 18% 30%
2	Cj	224	17% 54% 16% 31%
2	Ck	224	23% 48% 21% 30%

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Mol	Chain	Length	Quality of chain
3	1	273	61% 62% 16% 21%
3	2	273	74% 75% 20% 5%
3	x	273	61% 70% 25% 5%
4	3	275	19% 51% 14% 35%
4	y	275	21% 57% 8% 35%
4	z	275	19% 53% 12% 35%
5	A	176	16% 6% 78%
5	B	176	34% 18% 48%
5	C	176	6% 37% 15% 48%
6	A0	274	6% 34% 12% 53%
6	BN	274	22% 7% 71%
7	A1	254	29% 69% 24% 6%
7	A2	254	13% 6% 81%
7	A3	254	27% 89% 7%
7	A4	254	12% 37% 7% 56%
7	A5	254	17% 56% 6% 39%
7	A6	254	15% 81%
7	A7	254	11% 63% 26% 11%
7	A8	254	9% 47% 17% 33%
7	A9	254	8% 37% 6% 56%
7	Au	254	21% 6% 72%
7	Av	254	9% 42% 15% 42%
7	Aw	254	9% 41% 9% 49%
7	Ay	254	9% 54% 17% 28%
7	Az	254	12% 83%

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Mol	Chain	Length	Quality of chain
8	AA	450	78% 20%
8	AC	450	81% 17%
8	AE	450	78% 20%
8	AG	450	82% 15%
8	AI	450	83% 15%
8	AK	450	79% 18%
8	AM	450	82% 16%
8	BA	450	71% 25% 5%
8	BC	450	76% 21%
8	BE	450	76% 19%
8	BG	450	5% 76% 21%
8	BI	450	74% 21% 5%
8	BK	450	73% 24%
8	BM	450	75% 20%
8	CA	450	20% 74% 24%
8	CC	450	9% 74% 23%
8	CE	450	7% 74% 23%
8	CG	450	10% 75% 21%
8	CI	450	7% 80% 17%
8	CK	450	9% 74% 23%
8	CM	450	8% 76% 21%
8	DA	450	21% 60% 24% 16%
8	DC	450	12% 70% 25% 5%
8	DE	450	8% 70% 25% 5%
8	DG	450	10% 75% 21%

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Mol	Chain	Length	Quality of chain
8	DI	450	9% 70% 25% 5%
8	DK	450	10% 71% 24% 5%
8	DM	450	12% 69% 26% 5%
8	EC	450	14% 69% 27%
8	EE	450	12% 76% 22%
8	EG	450	8% 74% 23%
8	EI	450	8% 75% 22%
8	EK	450	13% 71% 26%
8	EM	450	11% 71% 24% 5%
8	FC	450	9% 73% 23% 5%
8	FE	450	6% 72% 21% 6%
8	FG	450	5% 70% 26%
8	FI	450	6% 66% 28% 6%
8	FK	450	5% 72% 23% 5%
8	FM	450	5% 80% 16% 5%
8	GC	450	8% 77% 20%
8	GE	450	6% 79% 17%
8	GG	450	7% 75% 20%
8	GI	450	6% 74% 23%
8	GK	450	75% 20%
8	GM	450	7% 78% 20%
8	HC	450	6% 79% 17% 5%
8	HE	450	75% 20% 5%
8	HG	450	6% 78% 18%
8	HI	450	7% 77% 18%

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Mol	Chain	Length	Quality of chain
8	HK	450	73% 22%
8	HM	450	6% 82% 14%
8	HO	450	7% 65% 20% 14%
8	IC	450	78% 18%
8	IE	450	80% 16%
8	IG	450	78% 19%
8	II	450	5% 76% 20%
8	IK	450	72% 23%
8	IM	450	83% 14%
8	IO	450	74% 21% 5%
8	JC	450	6% 79% 18%
8	JE	450	80% 16%
8	JG	450	79% 16% 5%
8	JI	450	79% 16% 5%
8	JK	450	78% 19%
8	JM	450	79% 16%
8	KC	450	78% 18%
8	KE	450	82% 14%
8	KG	450	75% 20%
8	KI	450	76% 19% 5%
8	KK	450	86% 10%
8	KM	450	87% 9%
8	KO	450	76% 15% 9%
8	LC	450	77% 21%
8	LE	450	92% 7%

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Mol	Chain	Length	Quality of chain
8	LG	450	83% 15%
8	LI	450	6% 86% 13%
8	LK	450	84% 14%
8	LM	450	82% 14%
8	MC	450	83% 14%
8	ME	450	77% 18% 5%
8	MG	450	78% 18%
8	MI	450	80% 16%
8	MK	450	80% 18%
8	MM	450	78% 18%
8	NA	450	11% 76% 19% 5%
8	NC	450	13% 70% 24% 5%
8	NE	450	9% 78% 18%
8	NG	450	11% 75% 21%
8	NI	450	12% 74% 20% 5%
8	NK	450	16% 74% 21% 5%
8	OA	450	8% 75% 20% 5%
8	OC	450	8% 68% 27% 5%
8	OE	450	6% 72% 24%
8	OG	450	8% 74% 22%
8	OI	450	10% 72% 24%
8	OK	450	7% 73% 23%
8	PA	450	9% 76% 19%
8	PC	450	10% 69% 27%
8	PE	450	10% 70% 26%

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Mol	Chain	Length	Quality of chain
8	PG	450	13% 71% 25%
8	PI	450	8% 69% 26% 5%
8	PK	450	7% 74% 21% 5%
8	PM	450	9% 73% 22%
8	QA	450	18% 74% 20% 5%
8	QC	450	17% 67% 28% 5%
8	QE	450	14% 67% 29%
8	QG	450	16% 68% 28%
8	QI	450	9% 66% 29% 5%
8	QK	450	16% 69% 26%
8	QM	450	13% 68% 28%
8	RA	450	18% 66% 29% 5%
8	RC	450	12% 70% 26%
8	RE	450	10% 68% 27% 5%
8	RG	450	15% 70% 26%
8	RI	450	11% 67% 28%
8	RK	450	15% 72% 24%
8	RM	450	18% 68% 27% 5%
8	SA	450	18% 72% 23% 5%
8	SC	450	9% 67% 29%
8	SE	450	68% 28%
8	SG	450	9% 72% 24%
8	SI	450	8% 72% 23% 5%
8	SK	450	11% 72% 24%
8	SM	450	10% 68% 27%

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Mol	Chain	Length	Quality of chain
8	TC	450	6% 72% 23% 5%
8	TE	450	5% 70% 26%
8	TG	450	7% 76% 19% 5%
8	TI	450	6% 75% 20%
8	TK	450	7% 71% 24%
8	TM	450	8% 74% 21%
8	UC	450	12% 79% 16%
8	UE	450	11% 77% 18%
8	UG	450	10% 81% 15%
8	UI	450	12% 77% 19%
8	UK	450	9% 74% 22%
8	UM	450	10% 76% 19% 5%
8	VC	450	9% 75% 21%
8	VE	450	10% 72% 24%
8	VG	450	10% 73% 25%
8	VI	450	11% 71% 24% 5%
8	VK	450	9% 70% 27%
8	VM	450	10% 79% 17%
8	WC	450	13% 73% 24%
8	WE	450	8% 74% 21%
8	WG	450	10% 74% 23%
8	WI	450	7% 69% 26% 5%
8	WK	450	7% 73% 24%
8	WM	450	7% 75% 21%
9	AB	445	82% 16%

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Mol	Chain	Length	Quality of chain
9	AD	445	74% 23%
9	AF	445	75% 23%
9	AH	445	77% 21%
9	AJ	445	79% 19%
9	AL	445	76% 21%
9	BB	445	73% 22%
9	BD	445	74% 21%
9	BF	445	5% 73% 23%
9	BH	445	79% 17%
9	BJ	445	76% 20%
9	BL	445	72% 23%
9	CB	445	10% 73% 23%
9	CD	445	9% 74% 22%
9	CF	445	8% 76% 20%
9	CH	445	10% 71% 24%
9	CJ	445	6% 72% 24%
9	CL	445	8% 74% 21%
9	DB	445	18% 67% 29%
9	DD	445	12% 71% 24%
9	DF	445	7% 71% 24%
9	DH	445	10% 65% 30%
9	DJ	445	6% 68% 28%
9	DL	445	8% 73% 22%
9	DN	445	16% 67% 20% 13%
9	EB	445	21% 69% 26%

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Mol	Chain	Length	Quality of chain
9	ED	445	12% 72% 24%
9	EF	445	7% 72% 24%
9	EH	445	11% 71% 24%
9	EJ	445	73% 22%
9	EL	445	9% 76% 19%
9	EN	445	15% 76% 20%
9	FB	445	14% 71% 24%
9	FD	445	7% 75% 21%
9	FF	445	75% 21%
9	FH	445	75% 20%
9	FJ	445	75% 19%
9	FL	445	6% 74% 22%
9	FN	445	9% 75% 20%
9	GB	445	12% 78% 18%
9	GD	445	8% 80% 15%
9	GF	445	6% 77% 18%
9	GH	445	6% 74% 22%
9	GJ	445	5% 78% 18%
9	GL	445	6% 73% 22%
9	GN	445	9% 79% 17%
9	HB	445	16% 78% 18%
9	HD	445	76% 20%
9	HF	445	5% 74% 22%
9	HH	445	7% 79% 17%
9	HJ	445	73% 23%

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Mol	Chain	Length	Quality of chain
9	HL	445	5% 75% 20%
9	HN	445	7% 78% 18%
9	IB	445	11% 65% 17% 17%
9	ID	445	78% 18%
9	IF	445	76% 20%
9	IH	445	72% 24%
9	IJ	445	74% 22%
9	IL	445	6% 76% 20%
9	IN	445	73% 22%
9	JB	445	74% 22%
9	JD	445	73% 23%
9	JF	445	77% 19%
9	JH	445	76% 19%
9	JJ	445	76% 20%
9	JL	445	73% 22%
9	JN	445	79% 17%
9	KB	445	7% 73% 18% 9%
9	KD	445	74% 22%
9	KF	445	78% 18%
9	KH	445	78% 18%
9	KJ	445	80% 16%
9	KL	445	79% 18%
9	KN	445	80% 16%
9	LB	445	81% 17%
9	LD	445	77% 19%

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Mol	Chain	Length	Quality of chain
9	LF	445	82% 16%
9	LH	445	81% 16%
9	LJ	445	84% 14%
9	LL	445	77% 19%
9	LN	445	78% 21%
9	MB	445	77% 18%
9	MD	445	79% 17%
9	MF	445	75% 21%
9	MH	445	79% 17%
9	MJ	445	78% 18%
9	ML	445	79% 17%
9	MN	445	77% 19%
9	N0	445	11% 69% 26%
9	NB	445	13% 78% 18%
9	ND	445	7% 74% 21%
9	NF	445	12% 72% 23%
9	NH	445	10% 72% 24%
9	NJ	445	14% 76% 21%
9	NL	445	13% 76% 20%
9	O0	445	12% 67% 21% 12%
9	OB	445	7% 76% 20%
9	OD	445	7% 73% 22% 5%
9	OF	445	7% 70% 26%
9	OH	445	7% 72% 24%
9	OJ	445	9% 74% 21%

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Mol	Chain	Length	Quality of chain
9	OL	445	6% 72% 23% 5%
9	PB	445	6% 71% 24%
9	PD	445	10% 69% 27%
9	PF	445	12% 69% 27%
9	PH	445	11% 73% 23%
9	PJ	445	10% 66% 30%
9	PL	445	6% 73% 22%
9	QB	445	11% 68% 28%
9	QD	445	12% 69% 27%
9	QF	445	14% 65% 31%
9	QH	445	15% 66% 29%
9	QJ	445	11% 63% 32%
9	QL	445	11% 64% 32%
9	RB	445	10% 66% 30%
9	RD	445	12% 67% 28%
9	RF	445	13% 71% 25%
9	RH	445	13% 68% 28%
9	RJ	445	10% 64% 31%
9	RL	445	12% 65% 30%
9	SB	445	9% 71% 24%
9	SD	445	9% 70% 26%
9	SF	445	7% 70% 26%
9	SH	445	6% 73% 22%
9	SJ	445	7% 69% 27%
9	SL	445	9% 72% 24%

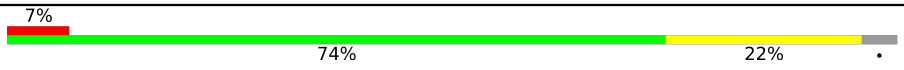
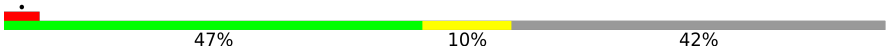
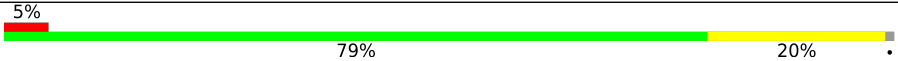
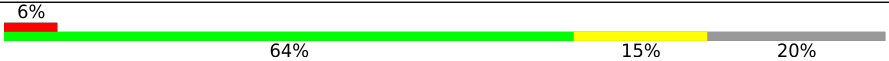
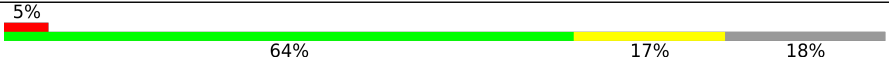
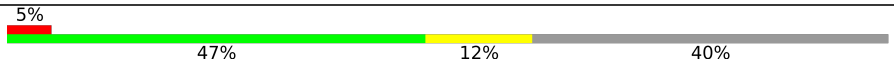
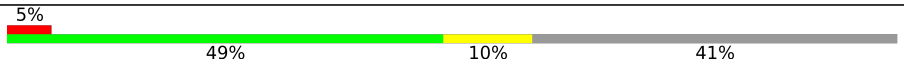
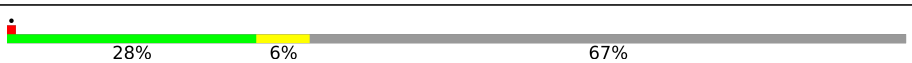
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Mol	Chain	Length	Quality of chain
9	TB	445	11% 73% 22%
9	TD	445	7% 75% 21%
9	TF	445	5% 73% 22%
9	TH	445	5% 72% 24%
9	TJ	445	72% 24%
9	TL	445	6% 70% 25%
9	UB	445	13% 71% 25%
9	UD	445	12% 72% 23%
9	UF	445	9% 71% 24%
9	UH	445	11% 74% 22%
9	UJ	445	8% 70% 25%
9	UL	445	12% 73% 23%
9	UN	445	15% 73% 23%
9	VB	445	12% 75% 21%
9	VD	445	10% 71% 24%
9	VF	445	6% 72% 23%
9	VH	445	9% 73% 23%
9	VJ	445	10% 69% 27%
9	VL	445	9% 72% 24%
9	VN	445	11% 70% 26%
9	WB	445	13% 71% 24%
9	WD	445	6% 69% 27%
9	WF	445	6% 75% 21%
9	WH	445	7% 76% 19%
9	WJ	445	6% 71% 24%

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Mol	Chain	Length	Quality of chain
9	WL	445	
9	WN	445	
10	AP	196	
10	AQ	196	
10	AR	196	
10	AS	196	
11	AT	514	
11	AU	514	
12	AV	377	
12	AW	377	
13	Aa	733	
13	Ab	733	
13	Ac	733	
13	Ad	733	
14	Al	320	
14	Am	320	
14	An	320	
14	Ao	320	
14	B7	320	
14	BY	320	
14	BZ	320	
14	Ba	320	
14	Bb	320	
14	Bc	320	
14	Bd	320	

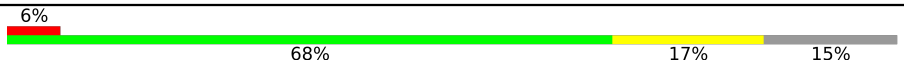
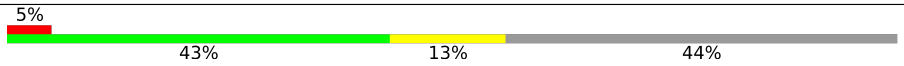
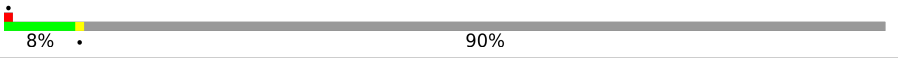
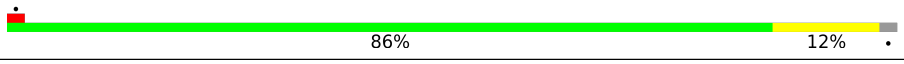
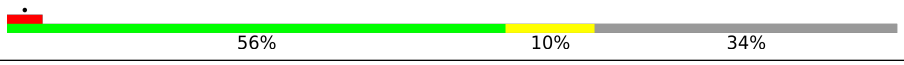
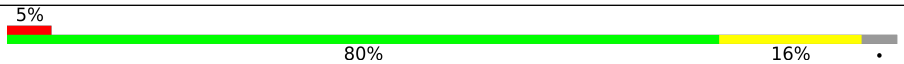
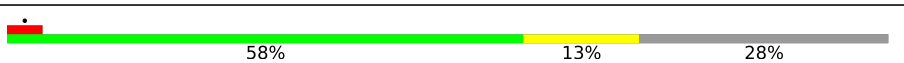
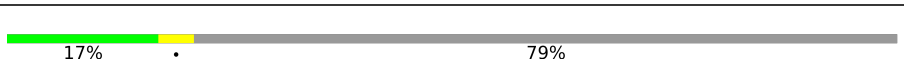
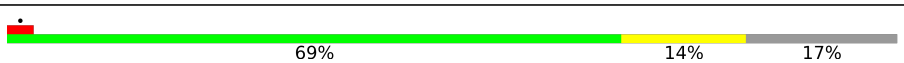
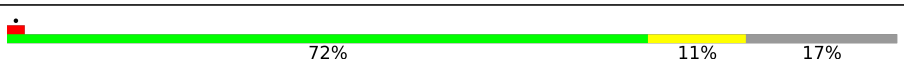
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Mol	Chain	Length	Quality of chain
14	Be	320	28% 6% 67%
14	CN	320	21% 5% 74%
14	CO	320	22% 6% 73%
15	Ap	201	52% 12% 35%
15	Aq	201	33% 11% 56%
15	Ar	201	58% 17% 24%
16	At	303	8% 22% 11% 67%
16	Ax	303	13% 28% 11% 61%
17	B0	304	13% 85%
17	B1	304	9% 88%
17	B2	304	12% 87%
17	B3	304	8% 91%
17	B4	304	11% 87%
17	B8	304	12% 87%
17	B9	304	10% 88%
17	CQ	304	12% 85%
17	CR	304	11% 87%
17	CS	304	11% 88%
18	B5	259	12% 81% 12% 6%
18	B6	259	14% 79% 17%
18	By	259	7% 50% 12% 38%
18	Bz	259	12% 79% 15% 6%
19	BO	500	37% 8% 55%
19	BP	500	8% 69% 14% 16%
19	BQ	500	5% 62% 12% 27%

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Mol	Chain	Length	Quality of chain
19	BR	500	
20	BS	428	
20	BT	428	
21	BU	377	
21	BV	377	
21	Bi	377	
21	Bj	377	
21	Bk	377	
22	BW	196	
22	BX	196	
23	Bf	136	
23	Bg	136	
24	Bh	120	
25	Bl	477	
25	Bm	477	
25	Bn	477	
25	Bo	477	
25	Bp	477	
26	Bq	338	
26	Bu	338	
27	Br	495	
27	Bs	495	
28	C0	490	
28	C2	490	
28	C3	490	

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Mol	Chain	Length	Quality of chain
28	C4	490	59% 11% 30%
28	C5	490	38% 8% 54%
28	C6	490	7% 92%
28	C7	490	77% 10% 13%
28	C8	490	74% 12% 13%
28	C9	490	64% 13% 22%
28	DO	490	22% 74%
28	F2	490	77% 8% 15%
28	F3	490	71% 14% 15%
28	F4	490	68% 10% 21%
28	F5	490	20% 78%
28	F6	490	20% 5% 74%
29	C1	489	55% 12% 33%
29	Cz	489	7% 49% 11% 39%
29	D0	489	11% 86%
29	D1	489	58% 15% 27%
29	D2	489	66% 13% 21%
29	D3	489	66% 13% 21%
29	D4	489	5% 66% 13% 21%
29	D5	489	5% 60% 14% 26%
29	D6	489	26% 70%
29	D7	489	12% 85%
29	D8	489	69% 10% 21%
29	D9	489	27% 6% 67%
29	DP	489	36% 5% 58%

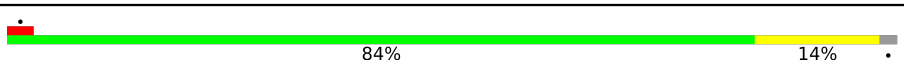
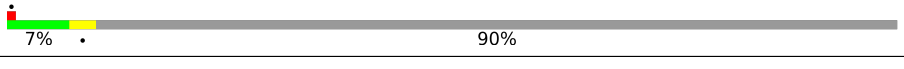
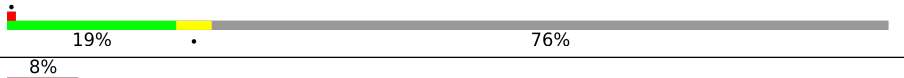
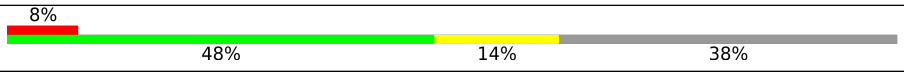
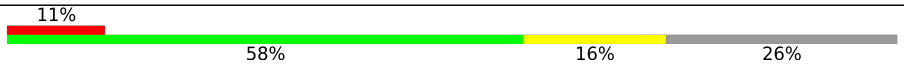
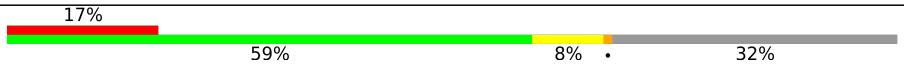
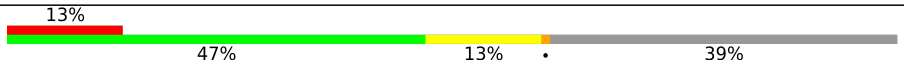
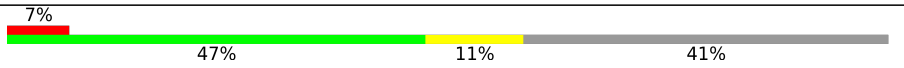
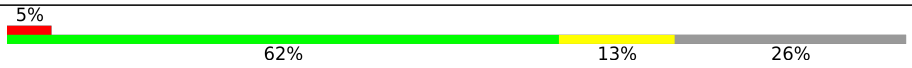
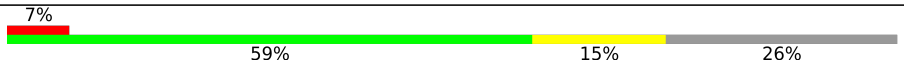
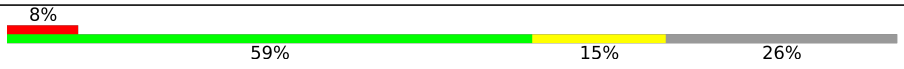
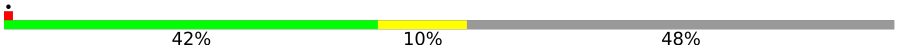
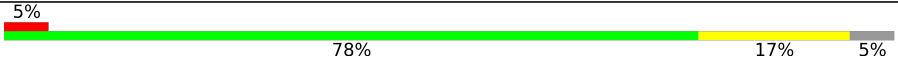
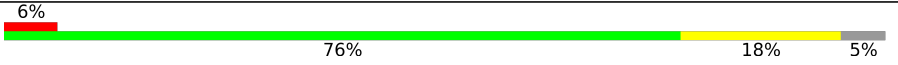
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Mol	Chain	Length	Quality of chain
29	DQ	489	5% 49% 10% 40%
29	DR	489	15% 45% 8% 47%
29	DS	489	8% 40% 12% 47%
29	DT	489	27% 7% 66%
29	DU	489	49% 12% 39%
29	DV	489	6% 49% 13% 38%
29	DW	489	6% 46% 15% 38%
29	DX	489	12% 38% 8% 53%
29	EA	489	69% 12% 18%
29	EO	489	6% 70% 12% 19%
29	EP	489	59% 14% 26%
29	EQ	489	26% 10% 64%
29	ER	489	9% 91%
30	CW	484	27% 6% 66%
31	Cl	440	24% 5% 71%
32	Cm	418	80% 15% 5%
32	Cn	418	85% 10% 5%
32	Co	418	71% 11% 17%
32	Cp	418	41% 8% 50%
33	Cq	430	85% 13%
33	Cr	430	83% 13%
33	Cs	430	34% 9% 57%
33	Ct	430	76% 14% 10%
33	Cu	430	75% 13% 13%
33	Cv	430	82% 16%

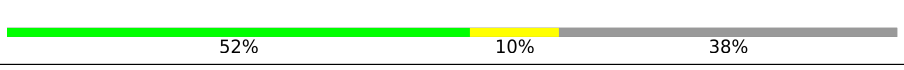
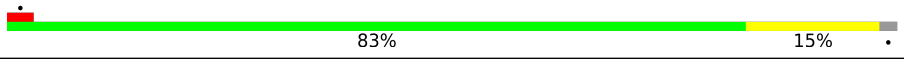
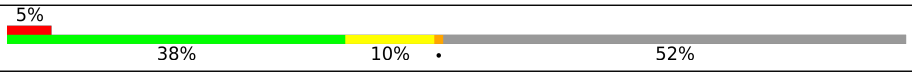
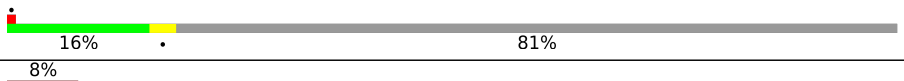
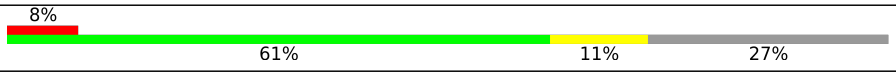
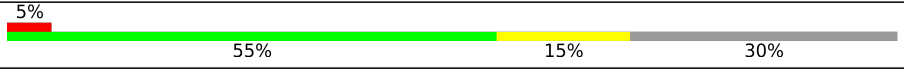
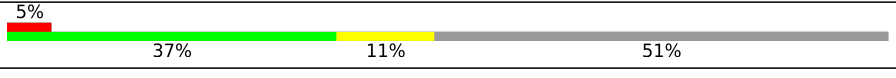
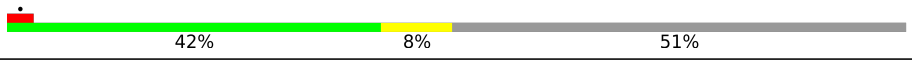
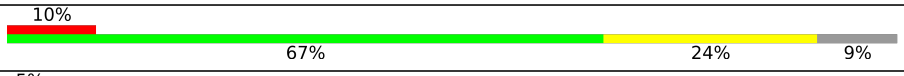
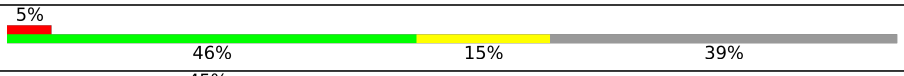
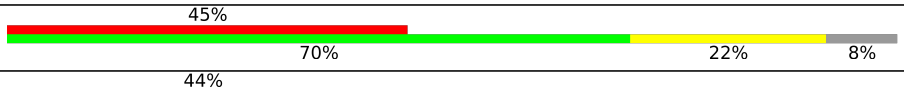
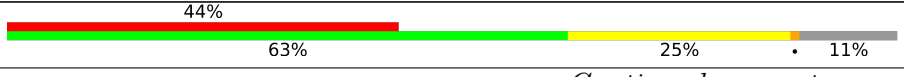
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Mol	Chain	Length	Quality of chain
33	Cw	430	
33	Cx	430	
33	Cy	430	
34	D	138	
35	DY	216	
35	DZ	216	
35	Da	216	
35	Ee	216	
36	Db	192	
36	Dc	192	
36	Dd	192	
37	De	272	
38	Df	180	
38	Dg	180	
38	Dh	180	
39	Di	133	
39	Dj	133	
39	Dk	133	
39	Dl	133	
40	Dm	131	
41	Dn	450	
42	E	877	
42	F	877	
43	E1	208	
43	E2	208	

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Mol	Chain	Length	Quality of chain
43	E3	208	
43	E4	208	
44	ES	447	
44	ET	447	
44	EU	447	
44	EV	447	
44	EW	447	
44	EX	447	
44	EY	447	
44	EZ	447	
45	G	584	
46	H	547	
46	o	547	
47	I	640	
47	X	640	
47	Y	640	
48	J	235	
48	K	235	
48	L	235	
48	M	235	
49	K1	135	
50	L1	147	
50	L2	147	
51	N	154	
51	O	154	

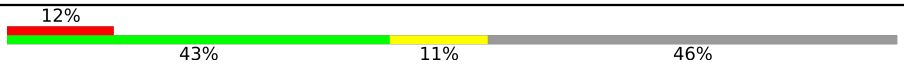
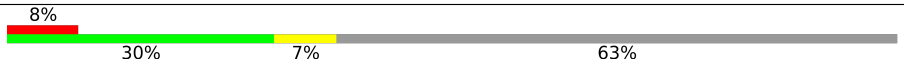
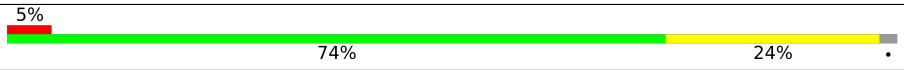
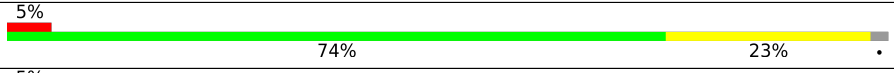
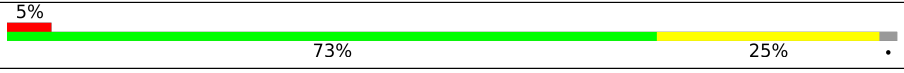
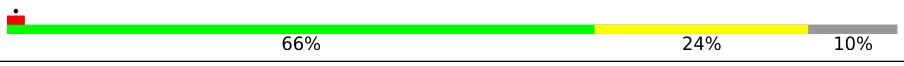
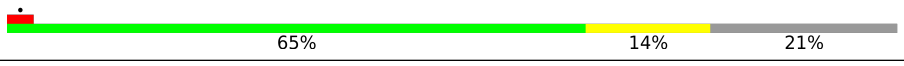
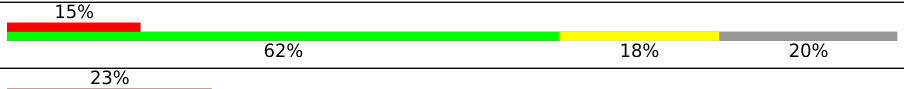
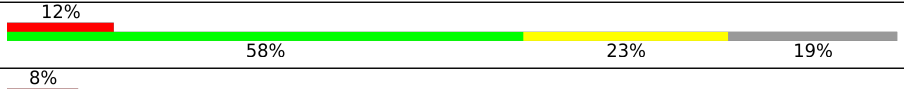
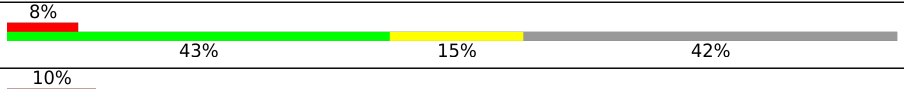
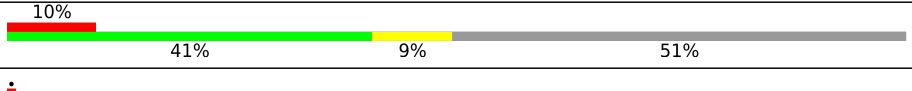
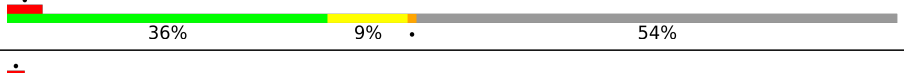
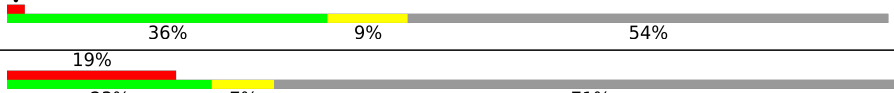
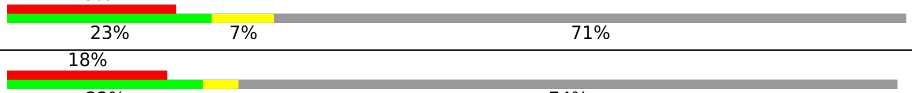
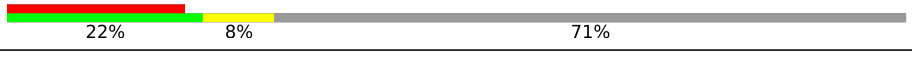
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Mol	Chain	Length	Quality of chain
52	P	137	9% 55% 20% 23%
53	Q	169	51% 11% 37%
54	R	284	37% 12% 51%
54	S	284	40% 9% 51%
54	T	284	43% 6% 51%
54	U	284	29% 5% 66%
55	W	309	26% 30% 10% 60%
56	XG	193	6% 69% 25% 6%
56	XH	193	65% 30% 6%
56	XI	193	59% 35% 6%
56	XJ	193	5% 67% 27% 6%
56	XK	193	5% 70% 24% 6%
56	XL	193	5% 68% 26% 6%
56	XM	193	8% 72% 20% 7%
57	YG	257	50% 65% 17% 18%
57	YH	257	6% 68% 16% 15%
57	YI	257	5% 62% 23% 15%
57	YJ	257	5% 68% 17% 15%
57	YK	257	72% 13% 15%
57	YL	257	8% 66% 18% 15%
58	Z	164	48% 63% 9% 29%
58	p	164	24% 27% 5% 67%
58	q	164	47% 46% 12% 41%
59	a	549	6% 27% 7% 66%
59	b	549	14% 43% 16% 40%

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Mol	Chain	Length	Quality of chain
59	c	549	
59	d	549	
60	e	623	
60	f	623	
60	g	623	
61	h	101	
62	i	321	
62	j	321	
63	k	196	
63	l	196	
63	m	196	
63	n	196	
64	ke	197	
65	r	170	
65	s	170	
65	t	170	
66	u	438	
66	v	438	
66	w	438	

2 Entry composition (i)

There are 69 unique types of molecules in this entry. The entry contains 1456841 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 Cilia- and flagella-associated protein 95.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	40	Total	C	N	O	S	0	0
			330	205	63	61	1		
1	V	183	Total	C	N	O	S	0	0
			1487	932	258	288	9		

- Molecule 2 is a protein called Sperm acrosome associated 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0A	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0C	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0E	157	Total	C	N	O	S	0	0
			1260	787	225	237	11		
2	0G	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0W	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0Y	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0a	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0c	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0e	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	0g	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0i	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0k	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	CT	157	Total	C	N	O	S	0	0
			1260	787	225	237	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CU	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	CV	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	CX	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	CY	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	CZ	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Ca	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Cb	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Cc	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Cd	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Ce	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	Cf	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	Cg	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Ch	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Ci	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Cj	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	Ck	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		

- Molecule 3 is a protein called Testis specific serine kinase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	216	Total	C	N	O	S	0	0
			1700	1076	317	301	6		
3	2	258	Total	C	N	O	S	0	0
			2027	1292	370	357	8		
3	x	258	Total	C	N	O	S	0	0
			2027	1292	370	357	8		

- Molecule 4 is a protein called EF-hand domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	178	Total	C	N	O	S	0	0
			1469	941	252	265	11		
4	y	178	Total	C	N	O	S	0	0
			1469	941	252	265	11		
4	z	178	Total	C	N	O	S	0	0
			1469	941	252	265	11		

- Molecule 5 is a protein called ATP6V1F neighbor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	39	Total	C	N	O	S	0	0
			338	216	64	56	2		
5	B	91	Total	C	N	O	S	0	0
			751	486	129	132	4		
5	C	91	Total	C	N	O	S	0	0
			751	486	129	132	4		

- Molecule 6 is a protein called Outer dense fiber of sperm tails 3 like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A0	130	Total	C	N	O	S	0	0
			1017	656	177	175	9		
6	BN	79	Total	C	N	O	S	0	0
			614	386	121	103	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A1	239	Total	C	N	O	S	0	0
			1828	1173	321	324	10		
7	A2	49	Total	C	N	O	S	0	0
			385	252	72	60	1		
7	A3	244	Total	C	N	O		0	0
			1200	712	244	244			
7	A4	111	Total	C	N	O		0	0
			546	324	111	111			
7	A5	155	Total	C	N	O		0	0
			762	452	155	155			
7	A6	49	Total	C	N	O	S	0	0
			369	235	63	67	4		
7	A7	226	Total	C	N	O	S	0	0
			1726	1110	305	303	8		

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Mol	Chain	Residues	Atoms	AltConf	Trace
7	A8	169	Total C N O S 1281 815 222 237 7	0	0
7	A9	112	Total C N O S 879 573 156 147 3	0	0
7	Au	71	Total C N O S 540 344 93 99 4	0	0
7	Av	148	Total C N O S 1126 717 195 207 7	0	0
7	Aw	129	Total C N O S 1009 652 182 172 3	0	0
7	Ay	183	Total C N O S 1412 909 250 248 5	0	0
7	Az	42	Total C N O S 313 201 53 56 3	0	0

- Molecule 8 is a protein called Tubulin alpha-3 chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	AA	438	Total C N O S 3413 2161 581 650 21	0	0
8	AC	440	Total C N O S 3428 2171 583 652 22	0	0
8	AE	440	Total C N O S 3428 2171 583 652 22	0	0
8	AG	440	Total C N O S 3428 2171 583 652 22	0	0
8	AI	440	Total C N O S 3428 2171 583 652 22	0	0
8	AK	440	Total C N O S 3428 2171 583 652 22	0	0
8	AM	439	Total C N O S 3421 2166 582 651 22	0	0
8	BA	429	Total C N O S 3355 2128 571 635 21	0	0
8	BC	438	Total C N O S 3415 2163 581 649 22	0	0
8	BE	430	Total C N O S 3363 2133 572 636 22	0	0
8	BG	439	Total C N O S 3421 2166 582 651 22	0	0
8	BI	429	Total C N O S 3357 2130 571 634 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	BK	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
8	BM	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	CA	437	Total	C	N	O	S	0	0
			3407	2158	580	648	21		
8	CC	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
8	CE	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
8	CG	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
8	CI	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
8	CK	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
8	CM	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
8	DA	380	Total	C	N	O	S	0	0
			2965	1881	509	556	19		
8	DC	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
8	DE	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
8	DG	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
8	DI	428	Total	C	N	O	S	0	0
			3348	2124	570	632	22		
8	DK	427	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
8	DM	427	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
8	EC	434	Total	C	N	O	S	0	0
			3392	2150	577	643	22		
8	EE	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
8	EG	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
8	EI	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
8	EK	437	Total	C	N	O	S	0	0
			3413	2162	580	649	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	EM	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
8	FC	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	FE	424	Total	C	N	O	S	0	0
			3323	2110	566	625	22		
8	FG	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	FI	425	Total	C	N	O	S	0	0
			3325	2109	567	627	22		
8	FK	428	Total	C	N	O	S	0	0
			3350	2125	570	633	22		
8	FM	429	Total	C	N	O	S	0	0
			3356	2128	571	635	22		
8	GC	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
8	GE	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
8	GG	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		
8	GI	436	Total	C	N	O	S	0	0
			3398	2154	578	644	22		
8	GK	430	Total	C	N	O	S	0	0
			3364	2132	572	638	22		
8	GM	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
8	HC	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	HE	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	HG	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
8	HI	430	Total	C	N	O	S	0	0
			3362	2134	572	634	22		
8	HK	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
8	HM	434	Total	C	N	O	S	0	0
			3393	2150	577	644	22		
8	HO	387	Total	C	N	O	S	0	0
			3035	1925	518	571	21		
8	IC	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	IE	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	IG	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
8	II	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
8	IK	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
8	IM	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
8	IO	428	Total	C	N	O	S	0	0
			3348	2124	570	632	22		
8	JC	433	Total	C	N	O	S	0	0
			3382	2144	575	641	22		
8	JE	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	JG	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
8	JI	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	JK	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
8	JM	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	KC	434	Total	C	N	O	S	0	0
			3389	2146	576	645	22		
8	KE	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
8	KG	430	Total	C	N	O	S	0	0
			3361	2132	572	635	22		
8	KI	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
8	KK	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
8	KM	434	Total	C	N	O	S	0	0
			3383	2143	576	642	22		
8	KO	411	Total	C	N	O	S	0	0
			3229	2048	548	611	22		
8	LC	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
8	LE	445	Total	C	N	O	S	0	0
			3465	2192	588	663	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	LG	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
8	LI	445	Total	C	N	O	S	0	0
			3465	2192	588	663	22		
8	LK	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
8	LM	436	Total	C	N	O	S	0	0
			3404	2157	578	647	22		
8	MC	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
8	ME	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	MG	432	Total	C	N	O	S	0	0
			3377	2140	574	641	22		
8	MI	431	Total	C	N	O	S	0	0
			3369	2136	573	638	22		
8	MK	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
8	MM	437	Total	C	N	O	S	0	0
			3407	2158	580	648	21		
8	NA	426	Total	C	N	O	S	0	0
			3333	2117	568	627	21		
8	NC	427	Total	C	N	O	S	0	0
			3343	2123	569	629	22		
8	NE	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	NG	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	NI	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	NK	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	OA	428	Total	C	N	O	S	0	0
			3349	2125	570	633	21		
8	OC	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	OE	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
8	OG	432	Total	C	N	O	S	0	0
			3375	2139	574	640	22		
8	OI	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	OK	430	Total	C	N	O	S	0	0
			3365	2134	572	637	22		
8	PA	430	Total	C	N	O	S	0	0
			3363	2132	572	638	21		
8	PC	434	Total	C	N	O	S	0	0
			3385	2144	576	643	22		
8	PE	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
8	PG	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		
8	PI	427	Total	C	N	O	S	0	0
			3341	2121	569	630	21		
8	PK	429	Total	C	N	O	S	0	0
			3355	2129	571	633	22		
8	PM	431	Total	C	N	O	S	0	0
			3369	2136	573	638	22		
8	QA	428	Total	C	N	O	S	0	0
			3347	2124	570	632	21		
8	QC	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
8	QE	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	QG	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
8	QI	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
8	QK	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	QM	431	Total	C	N	O	S	0	0
			3369	2136	573	638	22		
8	RA	429	Total	C	N	O	S	0	0
			3355	2128	571	635	21		
8	RC	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
8	RE	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	RG	432	Total	C	N	O	S	0	0
			3376	2141	574	639	22		
8	RI	432	Total	C	N	O	S	0	0
			3376	2141	574	639	22		
8	RK	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	RM	428	Total	C	N	O	S	0	0
			3348	2124	570	632	22		
8	SA	428	Total	C	N	O	S	0	0
			3349	2125	570	633	21		
8	SC	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	SE	431	Total	C	N	O	S	0	0
			3372	2138	573	639	22		
8	SG	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
8	SI	426	Total	C	N	O	S	0	0
			3341	2121	567	631	22		
8	SK	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
8	SM	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	TC	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	TE	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
8	TG	429	Total	C	N	O	S	0	0
			3355	2129	571	633	22		
8	TI	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	TK	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
8	TM	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	UC	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
8	UE	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
8	UG	432	Total	C	N	O	S	0	0
			3375	2139	574	640	22		
8	UI	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
8	UK	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
8	UM	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	VC	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	VE	430	Total	C	N	O	S	0	0
			3365	2134	573	636	22		
8	VG	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
8	VI	428	Total	C	N	O	S	0	0
			3350	2125	570	633	22		
8	VK	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
8	VM	432	Total	C	N	O	S	0	0
			3377	2140	574	641	22		
8	WC	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
8	WE	430	Total	C	N	O	S	0	0
			3361	2132	572	635	22		
8	WG	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
8	WI	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
8	WK	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
8	WM	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		

- Molecule 9 is a protein called Tubulin beta-4B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AB	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
9	AD	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
9	AF	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
9	AH	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
9	AJ	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
9	AL	431	Total	C	N	O	S	0	0
			3383	2124	579	655	25		
9	BB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	BD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	BF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	BH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	BJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	BL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
9	CB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	CD	425	Total	C	N	O	S	0	0
			3339	2100	572	641	26		
9	CF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	CH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	CJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	CL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
9	DB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	DD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	DF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	DH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	DJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	DL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
9	DN	387	Total	C	N	O	S	0	0
			3035	1911	519	582	23		
9	EB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	ED	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	EF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	EH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	EJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	EL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
9	EN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	FB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	FD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	FF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	FH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	FJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	FL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
9	FN	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	GB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	GD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	GF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	GH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	GJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	GL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
9	GN	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	HB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	HD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	HF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	HH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	HJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	HL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
9	HN	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	IB	368	Total	C	N	O	S	0	0
			2892	1817	499	553	23		
9	ID	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	IF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	IH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	IJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	IL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	IN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	JB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	JD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	JF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	JH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	JJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	JL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	JN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	KB	403	Total	C	N	O	S	0	0
			3165	1989	539	613	24		
9	KD	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	KF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	KH	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	KJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	KL	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	KN	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	LB	437	Total	C	N	O	S	0	0
			3433	2155	585	667	26		
9	LD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	LF	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
9	LH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	LJ	437	Total	C	N	O	S	0	0
			3433	2155	585	667	26		
9	LL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	LN	437	Total	C	N	O	S	0	0
			3433	2155	585	667	26		
9	MB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	MD	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	MF	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	MH	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	MJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	ML	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	MN	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
9	N0	425	Total	C	N	O	S	0	0
			3339	2100	572	641	26		
9	NB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	ND	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	NF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	NH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	NJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	NL	425	Total	C	N	O	S	0	0
			3339	2100	572	641	26		
9	O0	391	Total	C	N	O	S	0	0
			3078	1937	526	592	23		
9	OB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	OD	424	Total	C	N	O	S	0	0
			3327	2091	571	639	26		
9	OF	425	Total	C	N	O	S	0	0
			3339	2100	572	641	26		
9	OH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	OJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	OL	424	Total	C	N	O	S	0	0
			3327	2091	571	639	26		
9	PB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	PD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	PF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	PH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	PJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	PL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
9	QB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	QD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	QF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	QH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	QJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	QL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	RB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	RD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	RF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	RH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	RJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	RL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	SB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	SD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	SF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	SH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	SJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	SL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	TB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	TD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	TF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	TH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	TJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	TL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	UB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	UD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	UF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	UH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	UJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	UL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	UN	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
9	VB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	VD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	VF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	VH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
9	VJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	VL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	VN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	WB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	WD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	WF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	WH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	WJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	WL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
9	WN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

- Molecule 10 is a protein called Protein Flattop.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AP	117	Total	C	N	O	S	0	0
			920	586	168	164	2		
10	AQ	117	Total	C	N	O	S	0	0
			920	586	168	164	2		
10	AR	95	Total	C	N	O	S	0	0
			735	470	137	126	2		
10	AS	117	Total	C	N	O	S	0	0
			920	586	168	164	2		

- Molecule 11 is a protein called Cilia- and flagella-associated protein 53.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AT	297	Total	C	N	O	S	0	0
			2521	1541	478	489	13		
11	AU	217	Total	C	N	O	S	0	0
			1855	1127	350	364	14		

- Molecule 12 is a protein called Nucleoside diphosphate kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AV	366	Total	C	N	O	S	0	0
			2901	1853	491	536	21		
12	AW	372	Total	C	N	O	S	0	0
			2947	1880	499	546	22		

- Molecule 13 is a protein called EF-hand domain-containing family member C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Aa	585	Total	C	N	O	S	0	0
			4829	3100	812	892	25		
13	Ab	598	Total	C	N	O	S	0	0
			4935	3171	827	912	25		
13	Ac	600	Total	C	N	O	S	0	0
			4948	3179	831	913	25		
13	Ad	512	Total	C	N	O	S	0	0
			4235	2727	705	782	21		

- Molecule 14 is a protein called Family with sequence similarity 166 member A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Al	43	Total	C	N	O	S	0	0
			338	217	58	62	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	Am	43	Total	C	N	O	S	0	0
			338	217	58	62	1		
14	An	43	Total	C	N	O	S	0	0
			338	217	58	62	1		
14	Ao	67	Total	C	N	O	S	0	0
			573	379	96	95	3		
14	B7	86	Total	C	N	O	S	0	0
			686	443	117	122	4		
14	BY	106	Total	C	N	O	S	0	0
			866	553	155	152	6		
14	BZ	106	Total	C	N	O	S	0	0
			866	553	155	152	6		
14	Ba	191	Total	C	N	O	S	0	0
			1587	1026	281	271	9		
14	Bb	191	Total	C	N	O	S	0	0
			1587	1026	281	271	9		
14	Bc	190	Total	C	N	O	S	0	0
			1575	1017	280	269	9		
14	Bd	106	Total	C	N	O	S	0	0
			866	553	155	152	6		
14	Be	106	Total	C	N	O	S	0	0
			866	553	155	152	6		
14	CN	84	Total	C	N	O	S	0	0
			670	431	115	120	4		
14	CO	87	Total	C	N	O	S	0	0
			697	449	121	123	4		

- Molecule 15 is a protein called Protein FAM166C.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ap	130	Total	C	N	O	S	0	0
			1101	710	202	187	2		
15	Aq	88	Total	C	N	O	S	0	0
			766	493	146	126	1		
15	Ar	152	Total	C	N	O	S	0	0
			1257	809	228	218	2		

- Molecule 16 is a protein called Outer dense fiber of sperm tails 3B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	At	100	Total	C	N	O	S	0	0
			772	495	138	135	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ax	119	Total	C	N	O	S	0	0
			914	590	179	142	3		

- Molecule 17 is a protein called Spermatid-specific manchette-related protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B0	45	Total	C	N	O		0	0
			367	240	59	68			
17	B1	37	Total	C	N	O		0	0
			300	198	46	56			
17	B2	41	Total	C	N	O	S	0	0
			307	190	56	55	6		
17	B3	26	Total	C	N	O	S	0	0
			200	124	35	37	4		
17	B4	39	Total	C	N	O	S	0	0
			305	188	57	54	6		
17	B8	41	Total	C	N	O	S	0	0
			320	196	62	56	6		
17	B9	38	Total	C	N	O		0	0
			307	202	47	58			
17	CQ	45	Total	C	N	O		0	0
			367	240	59	68			
17	CR	39	Total	C	N	O		0	0
			316	208	49	59			
17	CS	38	Total	C	N	O		0	0
			307	202	47	58			

- Molecule 18 is a protein called Enkurin.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B5	244	Total	C	N	O	S	0	0
			2008	1283	348	369	8		
18	B6	248	Total	C	N	O	S	0	0
			2040	1306	352	374	8		
18	By	160	Total	C	N	O	S	0	0
			1316	833	228	250	5		
18	Bz	244	Total	C	N	O	S	0	0
			2008	1283	348	369	8		

- Molecule 19 is a protein called Coiled-coil domain-containing protein 105.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BO	227	Total	C	N	O	S	1	0
			1817	1123	346	332	16		
19	BP	418	Total	C	N	O	S	1	0
			3394	2101	651	616	26		
19	BQ	367	Total	C	N	O	S	1	0
			2989	1843	580	545	21		
19	BR	427	Total	C	N	O	S	1	0
			3465	2147	665	627	26		

- Molecule 20 is a protein called Protein phosphatase 1 regulatory subunit 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BS	151	Total	C	N	O	S	0	0
			1192	756	212	223	1		
20	BT	240	Total	C	N	O	S	0	0
			1886	1193	327	362	4		

- Molecule 21 is a protein called RIB43A-like with coiled-coils protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BU	36	Total	C	N	O	S	0	0
			307	192	64	50	1		
21	BV	371	Total	C	N	O	S	0	0
			3087	1881	602	589	15		
21	Bi	43	Total	C	N	O	S	0	0
			352	214	68	67	3		
21	Bj	247	Total	C	N	O	S	0	0
			2029	1233	393	393	10		
21	Bk	174	Total	C	N	O	S	0	0
			1444	876	285	276	7		

- Molecule 22 is a protein called Cilia- and flagella-associated protein 107.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BW	189	Total	C	N	O	S	0	0
			1586	1022	284	279	1		
22	BX	50	Total	C	N	O		0	0
			424	272	73	79			

- Molecule 23 is a protein called Piercer of microtubule wall 1 protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
23	Bf	62	Total C N O S 508 324 87 93 4	0	0
23	Bg	115	Total C N O S 950 602 168 175 5	0	0

- Molecule 24 is a protein called Piercer of microtubule wall 2 protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
24	Bh	96	Total C N O S 775 496 130 142 7	0	0

- Molecule 25 is a protein called Stabilizer of axonemal microtubules 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
25	Bl	127	Total C N O 635 381 127 127	0	0
25	Bm	128	Total C N O 640 384 128 128	0	0
25	Bn	138	Total C N O 690 414 138 138	0	0
25	Bo	143	Total C N O 715 429 143 143	0	0
25	Bp	163	Total C N O 815 489 163 163	0	0

- Molecule 26 is a protein called Stabilizer of axonemal microtubules 3.

Mol	Chain	Residues	Atoms	AltConf	Trace
26	Bq	100	Total C N O 782 505 139 138	0	0
26	Bu	147	Total C N O S 1177 755 219 202 1	0	0

- Molecule 27 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
27	Br	165	Total C N O S 1380 842 259 272 7	0	0
27	Bs	355	Total C N O S 3042 1886 556 583 17	0	0

- Molecule 28 is a protein called Tektin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C0	105	Total	C	N	O	S	0	0
			851	527	155	166	3		
28	C2	407	Total	C	N	O	S	0	0
			3314	2044	605	649	16		
28	C3	407	Total	C	N	O	S	0	0
			3314	2044	605	649	16		
28	C4	342	Total	C	N	O	S	0	0
			2779	1715	505	545	14		
28	C5	226	Total	C	N	O	S	0	0
			1843	1145	331	354	13		
28	C6	41	Total	C	N	O	S	0	0
			352	218	65	68	1		
28	C7	425	Total	C	N	O	S	0	0
			3454	2128	630	678	18		
28	C8	424	Total	C	N	O	S	0	0
			3446	2124	629	675	18		
28	C9	381	Total	C	N	O	S	0	0
			3089	1897	568	609	15		
28	DO	127	Total	C	N	O	S	0	0
			1041	632	197	209	3		
28	F2	418	Total	C	N	O	S	0	0
			3411	2107	621	667	16		
28	F3	417	Total	C	N	O	S	0	0
			3400	2102	616	666	16		
28	F4	387	Total	C	N	O	S	0	0
			3141	1931	577	618	15		
28	F5	108	Total	C	N	O	S	0	0
			873	540	159	171	3		
28	F6	127	Total	C	N	O	S	0	0
			1047	643	194	208	2		

- Molecule 29 is a protein called Tektin-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	C1	330	Total	C	N	O	S	0	0
			2710	1677	498	513	22		
29	Cz	297	Total	C	N	O	S	0	0
			2435	1509	445	461	20		
29	D0	69	Total	C	N	O	S	0	0
			569	351	107	106	5		
29	D1	358	Total	C	N	O	S	0	0
			2933	1802	545	560	26		
29	D2	387	Total	C	N	O	S	0	0
			3169	1945	592	603	29		

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Mol	Chain	Residues	Atoms					AltConf	Trace
29	D3	386	Total	C	N	O	S	0	0
			3160	1939	590	602	29		
29	D4	385	Total	C	N	O	S	0	0
			3152	1936	587	601	28		
29	D5	362	Total	C	N	O	S	0	0
			2961	1818	552	564	27		
29	D6	148	Total	C	N	O	S	0	0
			1209	733	227	239	10		
29	D7	73	Total	C	N	O	S	0	0
			603	374	111	113	5		
29	D8	387	Total	C	N	O	S	0	0
			3169	1945	592	603	29		
29	D9	160	Total	C	N	O	S	0	0
			1305	789	247	258	11		
29	DP	204	Total	C	N	O	S	0	0
			1668	1010	317	327	14		
29	DQ	293	Total	C	N	O	S	0	0
			2411	1481	450	459	21		
29	DR	261	Total	C	N	O	S	0	0
			2151	1327	399	407	18		
29	DS	257	Total	C	N	O	S	0	0
			2118	1308	392	401	17		
29	DT	165	Total	C	N	O	S	0	0
			1373	874	240	249	10		
29	DU	300	Total	C	N	O	S	0	0
			2497	1547	463	466	21		
29	DV	301	Total	C	N	O	S	0	0
			2502	1550	464	467	21		
29	DW	301	Total	C	N	O	S	0	0
			2502	1550	464	467	21		
29	DX	229	Total	C	N	O	S	0	0
			1897	1171	354	357	15		
29	EA	399	Total	C	N	O	S	0	0
			3259	2006	604	618	31		
29	EO	398	Total	C	N	O	S	0	0
			3251	2000	603	617	31		
29	EP	360	Total	C	N	O	S	0	0
			2940	1805	544	563	28		
29	EQ	178	Total	C	N	O	S	0	0
			1458	909	265	270	14		
29	ER	44	Total	C	N	O	S	0	0
			358	217	68	68	5		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	245	ASP	GLU	variant	UNP Q2YDI7
Cz	245	ASP	GLU	variant	UNP Q2YDI7
D0	245	ASP	GLU	variant	UNP Q2YDI7
D1	245	ASP	GLU	variant	UNP Q2YDI7
D2	245	ASP	GLU	variant	UNP Q2YDI7
D3	245	ASP	GLU	variant	UNP Q2YDI7
D4	245	ASP	GLU	variant	UNP Q2YDI7
D5	245	ASP	GLU	variant	UNP Q2YDI7
D6	245	ASP	GLU	variant	UNP Q2YDI7
D7	245	ASP	GLU	variant	UNP Q2YDI7
D8	245	ASP	GLU	variant	UNP Q2YDI7
D9	245	ASP	GLU	variant	UNP Q2YDI7
DP	245	ASP	GLU	variant	UNP Q2YDI7
DQ	245	ASP	GLU	variant	UNP Q2YDI7
DR	245	ASP	GLU	variant	UNP Q2YDI7
DS	245	ASP	GLU	variant	UNP Q2YDI7
DT	245	ASP	GLU	variant	UNP Q2YDI7
DU	245	ASP	GLU	variant	UNP Q2YDI7
DV	245	ASP	GLU	variant	UNP Q2YDI7
DW	245	ASP	GLU	variant	UNP Q2YDI7
DX	245	ASP	GLU	variant	UNP Q2YDI7
EA	245	ASP	GLU	variant	UNP Q2YDI7
EO	245	ASP	GLU	variant	UNP Q2YDI7
EP	245	ASP	GLU	variant	UNP Q2YDI7
EQ	245	ASP	GLU	variant	UNP Q2YDI7
ER	245	ASP	GLU	variant	UNP Q2YDI7

- Molecule 30 is a protein called Sperm-associated antigen 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CW	163	Total	C	N	O	S	0	0
			1319	827	236	249	7		

- Molecule 31 is a protein called Spermatogenesis-associated protein 48.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Cl	127	Total	C	N	O	S	0	0
			977	615	168	190	4		

- Molecule 32 is a protein called Tektin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Cm	396	Total	C	N	O	S	0	0
			3264	2032	594	629	9		
32	Cn	399	Total	C	N	O	S	0	0
			3286	2047	598	632	9		
32	Co	345	Total	C	N	O	S	0	0
			2845	1776	512	549	8		
32	Cp	208	Total	C	N	O	S	0	0
			1690	1058	306	319	7		

- Molecule 33 is a protein called Tektin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Cq	421	Total	C	N	O	S	0	0
			3427	2114	632	667	14		
33	Cr	415	Total	C	N	O	S	0	0
			3386	2087	626	659	14		
33	Cs	183	Total	C	N	O	S	0	0
			1496	915	282	293	6		
33	Ct	387	Total	C	N	O	S	0	0
			3147	1943	575	614	15		
33	Cu	376	Total	C	N	O	S	0	0
			3055	1887	556	598	14		
33	Cv	422	Total	C	N	O	S	0	0
			3436	2120	634	668	14		
33	Cw	422	Total	C	N	O	S	0	0
			3436	2120	634	668	14		
33	Cx	199	Total	C	N	O	S	0	0
			1611	987	302	316	6		
33	Cy	44	Total	C	N	O	S	0	0
			365	224	71	68	2		

- Molecule 34 is a protein called Uncharacterized protein C1orf100 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D	62	Total	C	N	O	S	0	0
			537	344	94	98	1		

- Molecule 35 is a protein called TEPP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	DY	38	Total	C	N	O	S	0	0
			308	187	53	63	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
35	DZ	51	Total	C	N	O	S	0	0
			416	250	82	79	5		
35	Da	134	Total	C	N	O	S	0	0
			1095	704	194	193	4		
35	Ee	45	Total	C	N	O	S	0	0
			386	248	71	66	1		

- Molecule 36 is a protein called Uncharacterized protein MGC137036.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Db	52	Total	C	N	O	S	0	0
			450	290	81	78	1		
36	Dc	51	Total	C	N	O	S	0	0
			442	284	80	77	1		
36	Dd	47	Total	C	N	O	S	0	0
			406	262	72	71	1		

- Molecule 37 is a protein called Testis expressed 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	De	66	Total	C	N	O	S	0	0
			545	343	97	101	4		

- Molecule 38 is a protein called Testis-expressed sequence 37 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Df	133	Total	C	N	O	S	0	0
			1060	685	176	196	3		
38	Dg	123	Total	C	N	O	S	0	0
			981	629	167	181	4		
38	Dh	109	Total	C	N	O	S	0	0
			873	561	143	166	3		

- Molecule 39 is a protein called Testis-expressed protein 43.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Di	78	Total	C	N	O	S	0	0
			632	405	120	102	5		
39	Dj	99	Total	C	N	O	S	0	0
			806	513	154	133	6		
39	Dk	99	Total	C	N	O	S	0	0
			806	513	154	133	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
39	Dl	99	Total	C	N	O	S	0	0
			806	513	154	133	6		

- Molecule 40 is a protein called Testis expressed 49.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Dm	87	Total	C	N	O	S	0	0
			725	458	136	127	4		

- Molecule 41 is a protein called Theg spermatid protein like.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Dn	56	Total	C	N	O	S	0	0
			468	289	97	81	1		

- Molecule 42 is a protein called EF-hand domain-containing family member B.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	E	148	Total	C	N	O	S	0	0
			1181	742	206	230	3		
42	F	455	Total	C	N	O	S	0	0
			3679	2344	655	667	13		

- Molecule 43 is a protein called Tektin bundle interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	E1	197	Total	C	N	O	S	1	0
			1648	1052	300	292	4		
43	E2	197	Total	C	N	O	S	1	0
			1648	1052	300	292	4		
43	E3	197	Total	C	N	O	S	0	0
			1641	1047	299	291	4		
43	E4	145	Total	C	N	O	S	1	0
			1221	782	222	214	3		

- Molecule 44 is a protein called Tektin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	ES	425	Total	C	N	O	S	0	0
			3483	2143	653	672	15		
44	ET	278	Total	C	N	O	S	0	0
			2273	1404	416	445	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
44	EU	329	Total	C	N	O	S	0	0
			2692	1660	501	517	14		
44	EV	425	Total	C	N	O	S	0	0
			3483	2143	653	672	15		
44	EW	319	Total	C	N	O	S	0	0
			2601	1601	482	504	14		
44	EX	436	Total	C	N	O	S	0	0
			3560	2192	665	687	16		
44	EY	311	Total	C	N	O	S	0	0
			2552	1578	476	486	12		
44	EZ	443	Total	C	N	O	S	0	0
			3615	2228	673	698	16		

- Molecule 45 is a protein called Chromosome 7 open reading frame 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	G	282	Total	C	N	O	S	0	0
			2317	1475	409	427	6		

- Molecule 46 is a protein called Cilia- and flagella- associated protein 210.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	H	102	Total	C	N	O	S	0	0
			848	533	146	166	3		
46	o	397	Total	C	N	O	S	0	0
			3401	2106	640	644	11		

- Molecule 47 is a protein called EF-hand domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	I	447	Total	C	N	O	S	0	0
			3689	2376	623	676	14		
47	X	448	Total	C	N	O	S	0	0
			3692	2385	621	672	14		
47	Y	454	Total	C	N	O	S	0	0
			3743	2416	631	682	14		

- Molecule 48 is a protein called Uncharacterized protein C10orf82 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	J	116	Total	C	N	O	S	0	0
			951	599	178	165	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
48	K	116	Total	C	N	O	S	0	0
			951	599	178	165	9		
48	L	108	Total	C	N	O	S	0	0
			891	562	167	155	7		
48	M	89	Total	C	N	O	S	0	0
			728	459	135	127	7		

- Molecule 49 is a protein called Cilia- and flagella-associated protein 144.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	K1	116	Total	C	N	O	S	0	0
			992	627	186	177	2		

- Molecule 50 is a protein called Chromosome 20 C5orf49 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	L1	134	Total	C	N	O	S	0	0
			1090	685	208	195	2		
50	L2	90	Total	C	N	O	S	0	0
			743	467	137	137	2		

- Molecule 51 is a protein called Chromosome 19 C17orf98 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	N	142	Total	C	N	O	S	0	0
			1173	737	232	199	5		
51	O	137	Total	C	N	O	S	0	0
			1134	715	222	194	3		

- Molecule 52 is a protein called Chromosome 13 C20orf85 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	P	105	Total	C	N	O	S	0	0
			870	564	151	153	2		

- Molecule 53 is a protein called Cilia- and flagella-associated protein 68.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Q	107	Total	C	N	O	S	0	0
			919	584	160	170	5		

- Molecule 54 is a protein called Cilia and flagella associated protein 77.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	R	140	Total	C	N	O	S	0	0
			1162	731	225	200	6		
54	S	140	Total	C	N	O	S	0	0
			1162	731	225	200	6		
54	T	140	Total	C	N	O	S	0	0
			1165	734	226	199	6		
54	U	97	Total	C	N	O	S	0	0
			818	518	155	141	4		

- Molecule 55 is a protein called UPF0602 protein C4orf47 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	W	124	Total	C	N	O	S	0	0
			990	626	176	185	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	199	PRO	THR	variant	UNP Q2T9M0

- Molecule 56 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	XG	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
56	XH	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
56	XI	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
56	XJ	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
56	XK	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
56	XL	181	Total	C	N	O	S	0	0
			1503	963	264	269	7		
56	XM	180	Total	C	N	O	S	0	0
			1494	958	262	267	7		

- Molecule 57 is a protein called Parkin coregulated gene protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	YG	210	Total	C	N	O	S	0	0
			1706	1108	288	301	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
57	YH	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
57	YI	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
57	YJ	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
57	YK	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
57	YL	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		

- Molecule 58 is a protein called CFAP97 domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Z	117	Total	C	N	O	S	0	0
			1014	632	205	175	2		
58	p	54	Total	C	N	O	S	0	0
			459	294	88	76	1		
58	q	96	Total	C	N	O	S	0	0
			829	510	169	148	2		

- Molecule 59 is a protein called Cilia- and flagella-associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	a	185	Total	C	N	O	S	0	0
			1559	959	297	294	9		
59	b	327	Total	C	N	O	S	0	0
			2814	1700	563	539	12		
59	c	297	Total	C	N	O	S	0	0
			2525	1544	478	487	16		
59	d	203	Total	C	N	O	S	0	0
			1728	1048	349	326	5		

- Molecule 60 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	e	610	Total	C	N	O	S	0	0
			4722	2990	823	877	32		
60	f	609	Total	C	N	O	S	0	0
			4713	2985	822	874	32		
60	g	609	Total	C	N	O	S	0	0
			4713	2985	822	874	32		

- Molecule 61 is a protein called Cilia- and flagella-associated protein 141.

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

- Molecule 62 is a protein called Cilia- and flagella-associated protein 161.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	i	255	Total	C	N	O	S	0	0
			2055	1302	369	373	11		
62	j	268	Total	C	N	O	S	0	0
			2158	1367	386	394	11		

- Molecule 63 is a protein called Dual specificity phosphatase 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	k	157	Total	C	N	O	S	0	0
			1245	797	207	230	11		
63	l	137	Total	C	N	O	S	0	0
			1098	706	185	199	8		
63	m	159	Total	C	N	O	S	0	0
			1263	807	211	234	11		
63	n	114	Total	C	N	O	S	0	0
			908	587	147	167	7		

- Molecule 64 is a protein called Uncharacterized protein C4orf45 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	ke	97	Total	C	N	O	S	0	0
			796	516	138	141	1		

- Molecule 65 is a protein called Cilia- and flagella-associated protein 276.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	r	77	Total	C	N	O	0	0
			615	386	113	116		
65	s	78	Total	C	N	O	0	0
			624	391	115	118		
65	t	78	Total	C	N	O	0	0
			624	391	115	118		

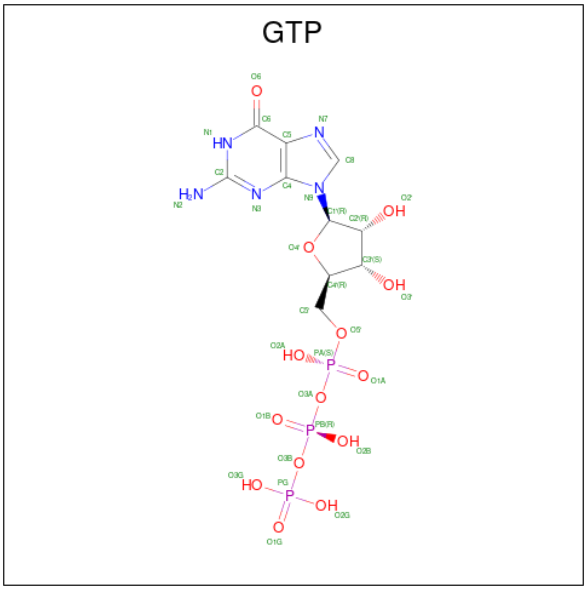
- Molecule 66 is a protein called EF-hand calcium-binding domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	u	128	Total	C	N	O	S	0	0
			1081	697	188	192	4		
66	v	113	Total	C	N	O	S	0	0
			957	620	164	170	3		
66	w	128	Total	C	N	O	S	0	0
			1081	697	188	192	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	290	ALA	GLU	variant	UNP Q2T9P0
u	303	SER	THR	variant	UNP Q2T9P0
v	290	ALA	GLU	variant	UNP Q2T9P0
v	303	SER	THR	variant	UNP Q2T9P0
w	290	ALA	GLU	variant	UNP Q2T9P0
w	303	SER	THR	variant	UNP Q2T9P0

- Molecule 67 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
67	AA	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	AC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	AD	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	AG	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
67	AH	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	AK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	AM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	BA	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	BC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	BG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	BI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	BK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	BM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	CA	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	CB	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	CD	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	CG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	CH	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	CJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	CL	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	DA	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	DC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	DE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	DF	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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Mol	Chain	Residues	Atoms					AltConf
67	HC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	HE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	HG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	HI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	HK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	HL	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	HN	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	IC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	IE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	IG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	II	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	IK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	IM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	IN	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	JC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	JE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	JG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	JI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	JK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	JM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	KC	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
67	KE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	KG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	KI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	KK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	KM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	KO	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	LC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	LE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	LG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	LI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	LK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	LM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	MC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	ME	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	MG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	MI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	MK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	MM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	NA	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	NB	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	NE	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
67	NF	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	NI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	NK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	O0	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	OC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	OE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	OF	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	OH	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	OK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	PA	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	PC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	PD	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	PG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	PI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	PK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	PM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	QA	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	QC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	QE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	QG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	QI	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
67	QK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	QM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	RA	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	RB	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	RE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	RG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	RI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	RK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	RM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	SA	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	SC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	SE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	SF	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	SI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	SK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	SM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	TC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	TE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	TG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	TI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	TK	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
67	TM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	UC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	UE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	UG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	UI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	UK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	UM	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	VC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	VE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	VG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	VI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	VK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	VL	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	WC	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	WE	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	WG	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	WI	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	WK	1	Total	C	N	O	P	0
			32	10	5	14	3	
67	WM	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 68 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
68	AA	1	Total Mg 1 1	0
68	AC	1	Total Mg 1 1	0
68	AE	1	Total Mg 1 1	0
68	AG	1	Total Mg 1 1	0
68	AI	1	Total Mg 1 1	0
68	AK	1	Total Mg 1 1	0
68	AM	1	Total Mg 1 1	0
68	BA	1	Total Mg 1 1	0
68	BC	1	Total Mg 1 1	0
68	BE	1	Total Mg 1 1	0
68	BG	1	Total Mg 1 1	0
68	BI	1	Total Mg 1 1	0
68	BK	1	Total Mg 1 1	0
68	BM	1	Total Mg 1 1	0
68	CA	1	Total Mg 1 1	0
68	CC	1	Total Mg 1 1	0
68	CE	1	Total Mg 1 1	0
68	CG	1	Total Mg 1 1	0
68	CI	1	Total Mg 1 1	0
68	CK	1	Total Mg 1 1	0
68	CM	1	Total Mg 1 1	0
68	DA	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
68	DC	1	Total Mg 1 1	0
68	DE	1	Total Mg 1 1	0
68	DG	1	Total Mg 1 1	0
68	DI	1	Total Mg 1 1	0
68	DK	1	Total Mg 1 1	0
68	DM	1	Total Mg 1 1	0
68	EC	1	Total Mg 1 1	0
68	EE	1	Total Mg 1 1	0
68	EG	1	Total Mg 1 1	0
68	EI	1	Total Mg 1 1	0
68	EJ	1	Total Mg 1 1	0
68	EM	1	Total Mg 1 1	0
68	FC	1	Total Mg 1 1	0
68	FE	1	Total Mg 1 1	0
68	FG	1	Total Mg 1 1	0
68	FI	1	Total Mg 1 1	0
68	FK	1	Total Mg 1 1	0
68	FM	1	Total Mg 1 1	0
68	GC	1	Total Mg 1 1	0
68	GE	1	Total Mg 1 1	0
68	GG	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
68	GI	1	Total Mg 1 1	0
68	GK	1	Total Mg 1 1	0
68	GM	1	Total Mg 1 1	0
68	HC	1	Total Mg 1 1	0
68	HE	1	Total Mg 1 1	0
68	HG	1	Total Mg 1 1	0
68	HI	1	Total Mg 1 1	0
68	HK	1	Total Mg 1 1	0
68	HM	1	Total Mg 1 1	0
68	HO	1	Total Mg 1 1	0
68	IC	1	Total Mg 1 1	0
68	IE	1	Total Mg 1 1	0
68	IG	1	Total Mg 1 1	0
68	II	1	Total Mg 1 1	0
68	IK	1	Total Mg 1 1	0
68	IM	1	Total Mg 1 1	0
68	IO	1	Total Mg 1 1	0
68	JC	1	Total Mg 1 1	0
68	JE	1	Total Mg 1 1	0
68	JG	1	Total Mg 1 1	0
68	JI	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
68	JK	1	Total Mg 1 1	0
68	JM	1	Total Mg 1 1	0
68	KC	1	Total Mg 1 1	0
68	KE	1	Total Mg 1 1	0
68	KG	1	Total Mg 1 1	0
68	KI	1	Total Mg 1 1	0
68	KK	1	Total Mg 1 1	0
68	KM	1	Total Mg 1 1	0
68	KN	1	Total Mg 1 1	0
68	LC	1	Total Mg 1 1	0
68	LE	1	Total Mg 1 1	0
68	LG	1	Total Mg 1 1	0
68	LI	1	Total Mg 1 1	0
68	LK	1	Total Mg 1 1	0
68	LL	1	Total Mg 1 1	0
68	MC	1	Total Mg 1 1	0
68	ME	1	Total Mg 1 1	0
68	MG	1	Total Mg 1 1	0
68	MI	1	Total Mg 1 1	0
68	MK	1	Total Mg 1 1	0
68	MM	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
68	NA	1	Total Mg 1 1	0
68	NC	1	Total Mg 1 1	0
68	NE	1	Total Mg 1 1	0
68	NG	1	Total Mg 1 1	0
68	NI	1	Total Mg 1 1	0
68	NK	1	Total Mg 1 1	0
68	OA	1	Total Mg 1 1	0
68	OC	1	Total Mg 1 1	0
68	OE	1	Total Mg 1 1	0
68	OG	1	Total Mg 1 1	0
68	OI	1	Total Mg 1 1	0
68	OK	1	Total Mg 1 1	0
68	PA	1	Total Mg 1 1	0
68	PC	1	Total Mg 1 1	0
68	PE	1	Total Mg 1 1	0
68	PG	1	Total Mg 1 1	0
68	PH	1	Total Mg 1 1	0
68	PK	1	Total Mg 1 1	0
68	PM	1	Total Mg 1 1	0
68	QA	1	Total Mg 1 1	0
68	QC	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
68	QE	1	Total Mg 1 1	0
68	QG	1	Total Mg 1 1	0
68	QI	1	Total Mg 1 1	0
68	QK	1	Total Mg 1 1	0
68	QM	1	Total Mg 1 1	0
68	RA	1	Total Mg 1 1	0
68	RC	1	Total Mg 1 1	0
68	RE	1	Total Mg 1 1	0
68	RG	1	Total Mg 1 1	0
68	RI	1	Total Mg 1 1	0
68	RK	1	Total Mg 1 1	0
68	RM	1	Total Mg 1 1	0
68	SA	1	Total Mg 1 1	0
68	SC	1	Total Mg 1 1	0
68	SE	1	Total Mg 1 1	0
68	SG	1	Total Mg 1 1	0
68	SI	1	Total Mg 1 1	0
68	SK	1	Total Mg 1 1	0
68	SM	1	Total Mg 1 1	0
68	TC	1	Total Mg 1 1	0
68	TE	1	Total Mg 1 1	0

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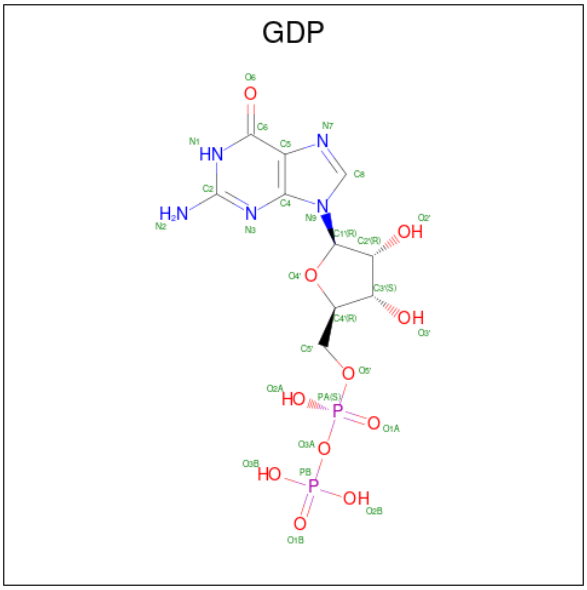
Mol	Chain	Residues	Atoms	AltConf
68	TG	1	Total Mg 1 1	0
68	TH	1	Total Mg 1 1	0
68	TK	1	Total Mg 1 1	0
68	TM	1	Total Mg 1 1	0
68	UC	1	Total Mg 1 1	0
68	UE	1	Total Mg 1 1	0
68	UG	1	Total Mg 1 1	0
68	UI	1	Total Mg 1 1	0
68	UK	1	Total Mg 1 1	0
68	UM	1	Total Mg 1 1	0
68	VC	1	Total Mg 1 1	0
68	VE	1	Total Mg 1 1	0
68	VG	1	Total Mg 1 1	0
68	VI	1	Total Mg 1 1	0
68	VK	1	Total Mg 1 1	0
68	VM	1	Total Mg 1 1	0
68	WC	1	Total Mg 1 1	0
68	WE	1	Total Mg 1 1	0
68	WG	1	Total Mg 1 1	0
68	WI	1	Total Mg 1 1	0
68	WK	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
68	WM	1	Total	Mg	0
			1	1	

- Molecule 69 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

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Mol	Chain	Residues	Atoms					AltConf
69	BJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	BL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	CB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	CF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	CH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	CJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	CL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	DB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	DD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	DF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	DH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	DJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	DL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	DN	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	EB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	ED	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	EF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	EH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	EJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	EL	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
69	EN	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	FB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	FD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	FF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	FH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	FJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	FL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	FN	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	GB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	GD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	GF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	GH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	GJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	GL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	GN	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	HB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	HD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	HF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	HH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	HJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	HL	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
69	HN	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	IB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	ID	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	IF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	IH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	IJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	IL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	IN	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	JB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	JD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	JF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	JH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	JJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	JL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	JN	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	KB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	KD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	KF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	KH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	KJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	KL	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
69	KN	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	LB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	LD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	LF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	LH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	LJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	LL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	LN	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	MB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	MD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	MF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	MH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	MJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	ML	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	MN	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	N0	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	NB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	ND	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	NF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	NH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	NJ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
69	NL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	O0	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	OB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	OD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	OF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	OH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	OJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	OL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	PB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	PD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	PF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	PH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	PJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	PL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	QB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	QD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	QF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	QH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	QJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	QL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	RB	1	Total	C	N	O	P	0
			28	10	5	11	2	

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

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Mol	Chain	Residues	Atoms					AltConf
69	UJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	UL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	UN	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	VB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	VD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	VF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	VH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	VJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	VL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	VN	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	WB	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	WD	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	WF	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	WH	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	WJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	WL	1	Total	C	N	O	P	0
			28	10	5	11	2	
69	WN	1	Total	C	N	O	P	0
			28	10	5	11	2	

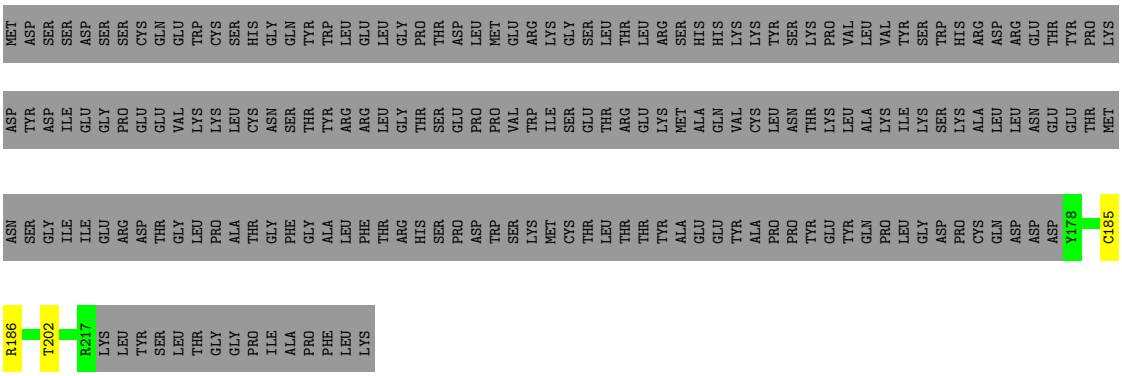
3 Residue-property plots (i)

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: Cilia- and flagella-associated protein 95

Chain 0:

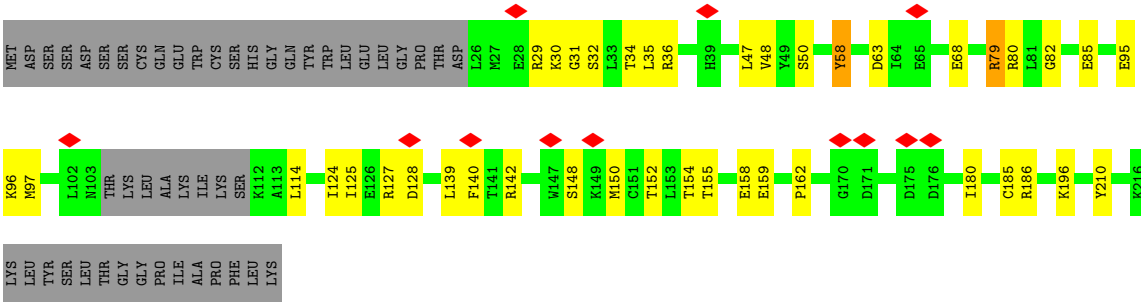




• Molecule 1: Cilia- and flagella-associated protein 95

Chain V:

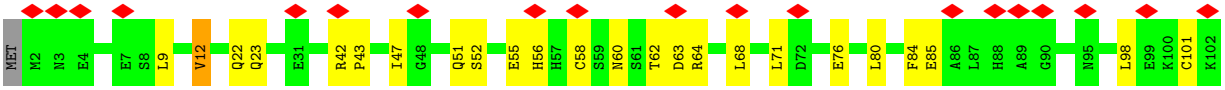


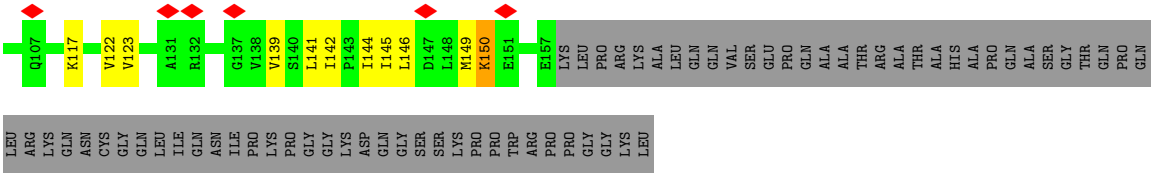


• Molecule 2: Sperm acrosome associated 9

Chain 0A:



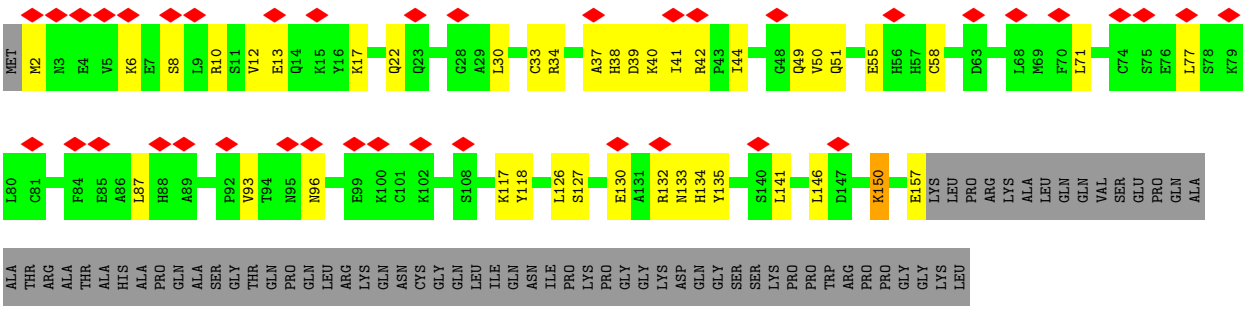




• Molecule 2: Sperm acrosome associated 9

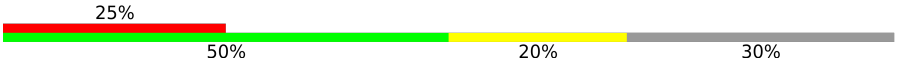
Chain 0C:

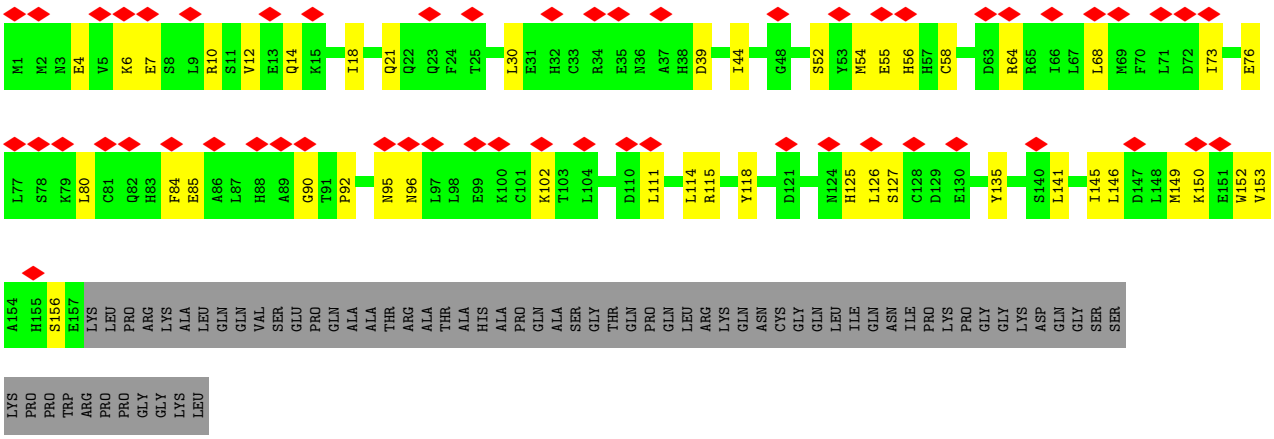




• Molecule 2: Sperm acrosome associated 9

Chain 0E:

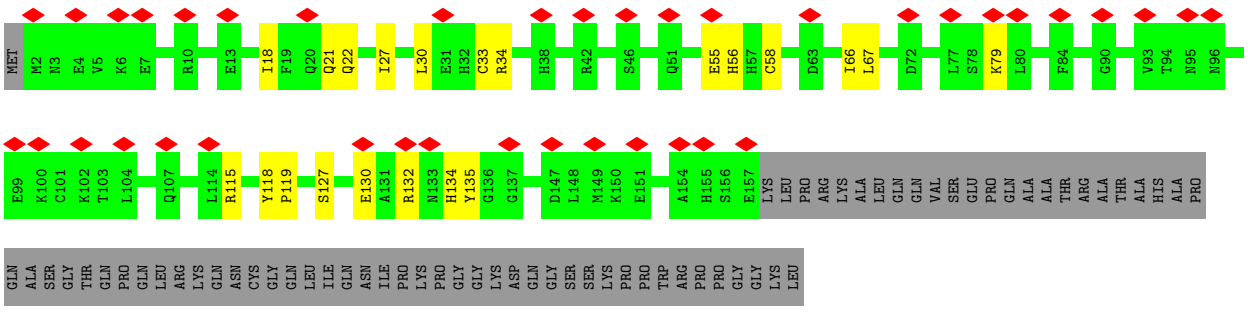




• Molecule 2: Sperm acrosome associated 9

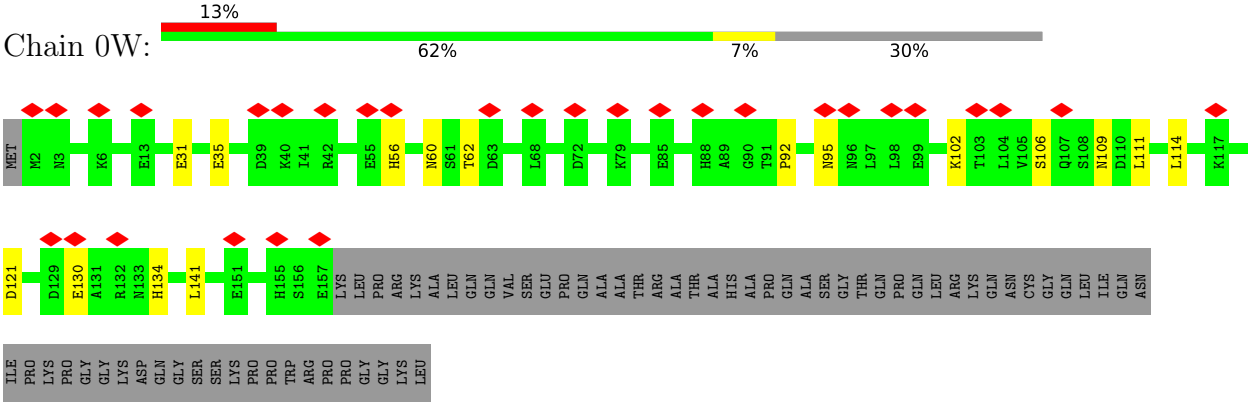
Chain 0G:





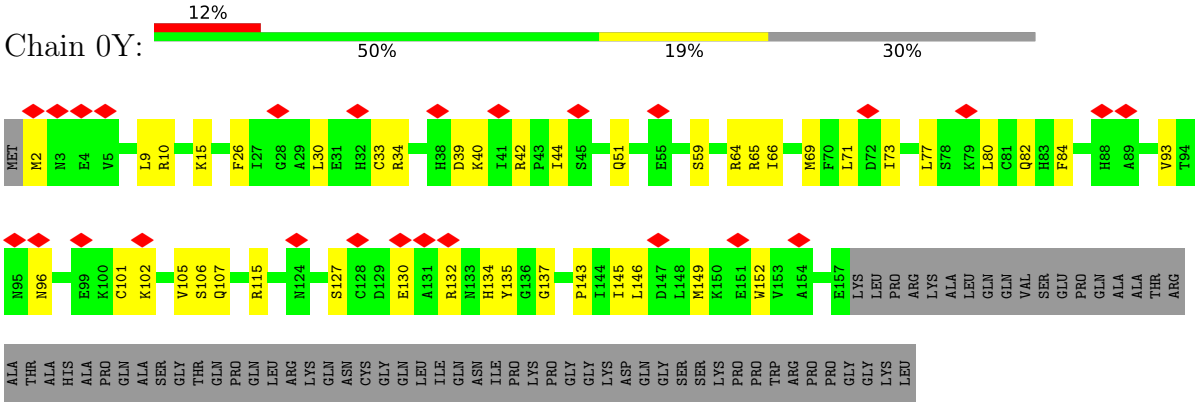
• Molecule 2: Sperm acrosome associated 9

Chain 0W:



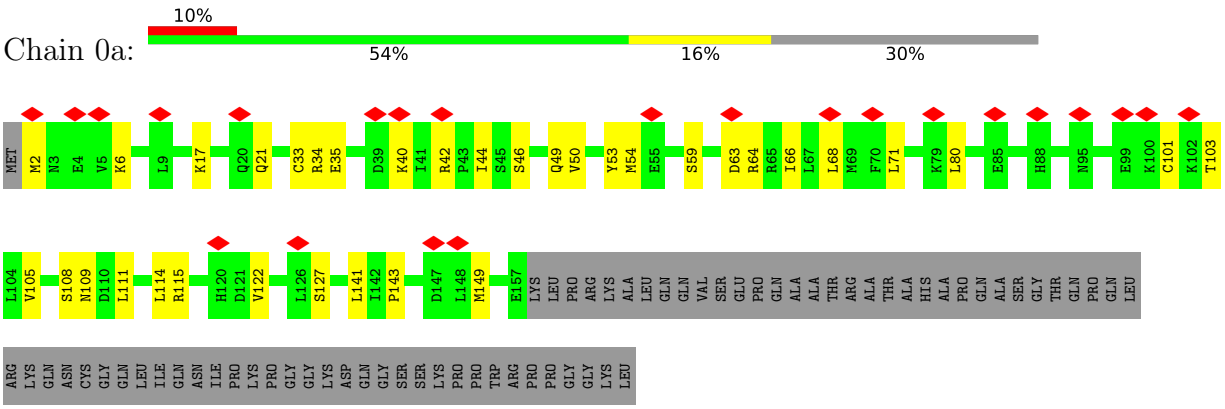
• Molecule 2: Sperm acrosome associated 9

Chain 0Y:



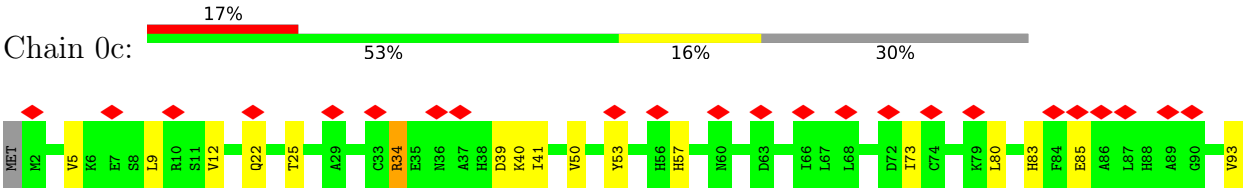
• Molecule 2: Sperm acrosome associated 9

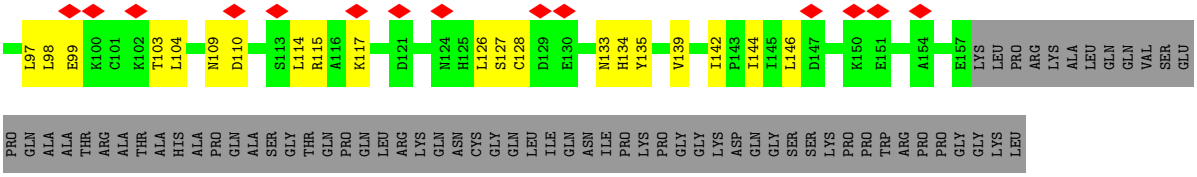
Chain 0a:



• Molecule 2: Sperm acrosome associated 9

Chain 0c:

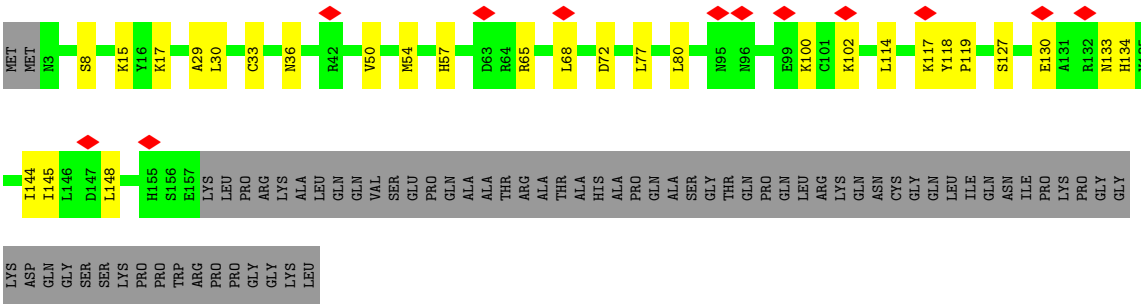




• Molecule 2: Sperm acrosome associated 9

Chain 0e:

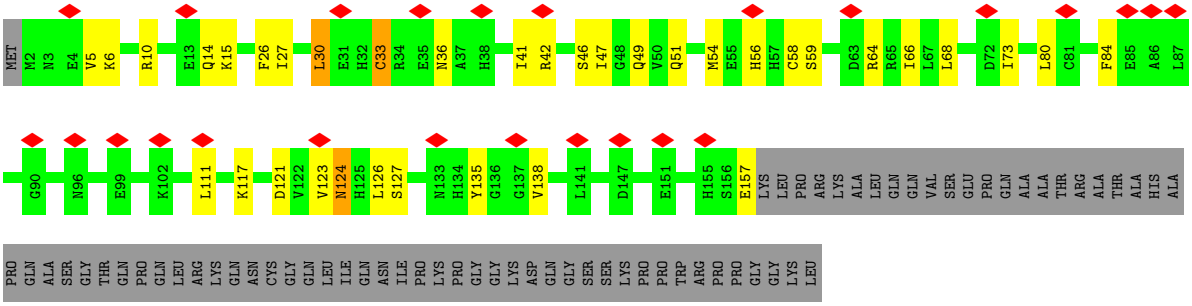




• Molecule 2: Sperm acrosome associated 9

Chain 0g:

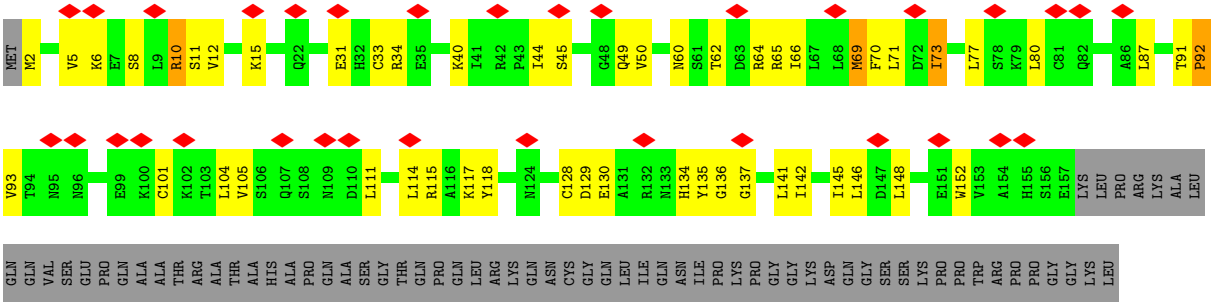




• Molecule 2: Sperm acrosome associated 9

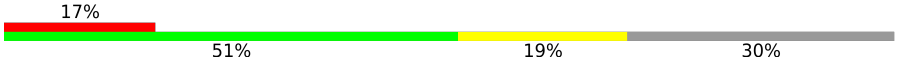
Chain 0i:

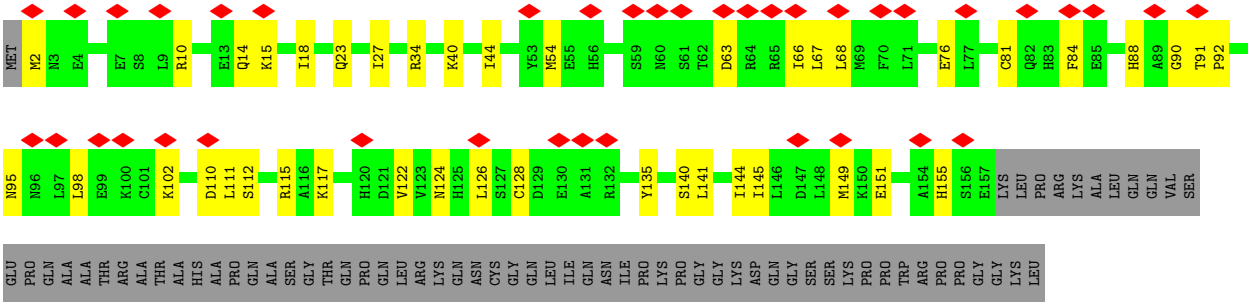




• Molecule 2: Sperm acrosome associated 9

Chain 0k:

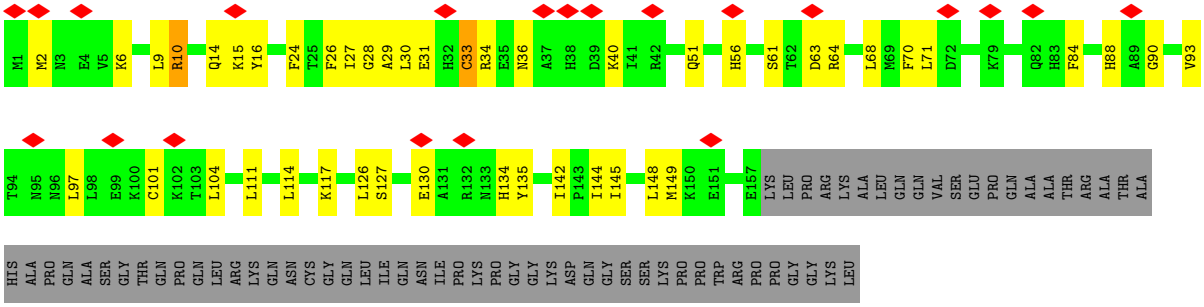




• Molecule 2: Sperm acrosome associated 9

Chain CT:

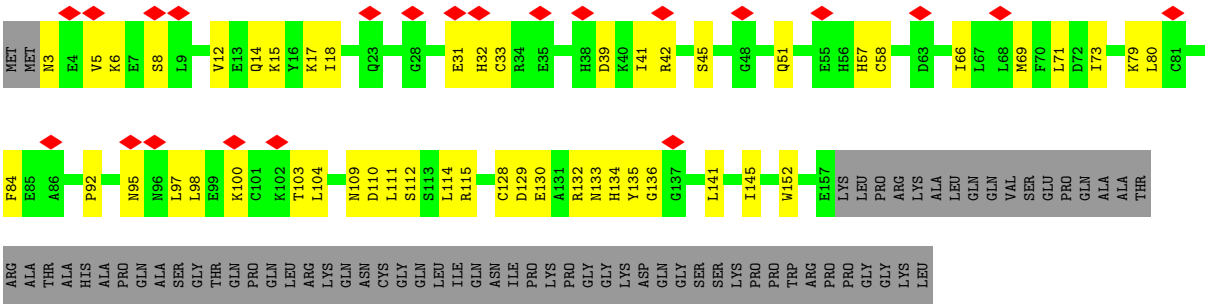




• Molecule 2: Sperm acrosome associated 9

Chain CU:

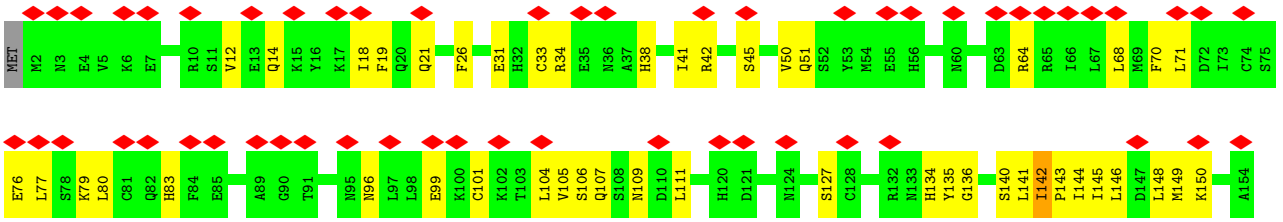


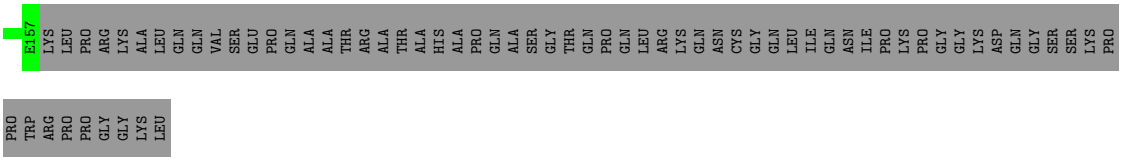


• Molecule 2: Sperm acrosome associated 9

Chain CV:

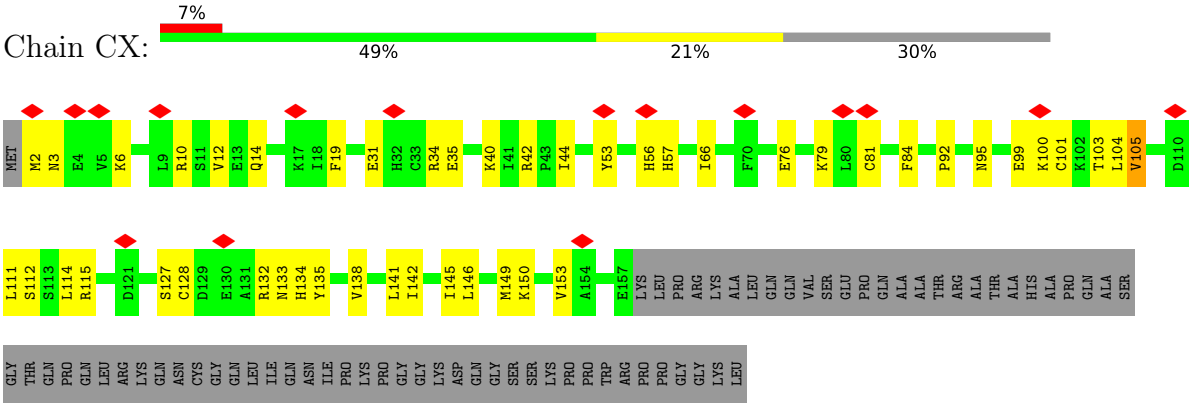






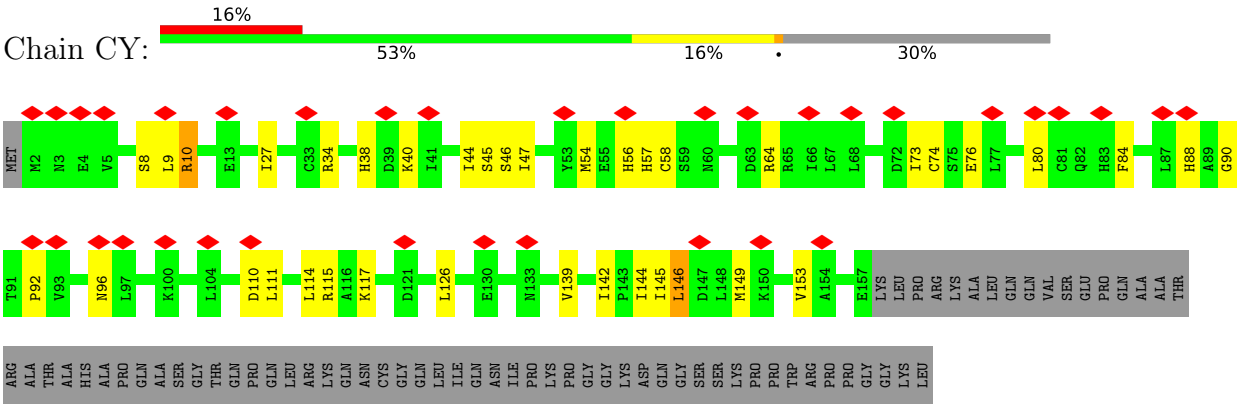
• Molecule 2: Sperm acrosome associated 9

Chain CX:



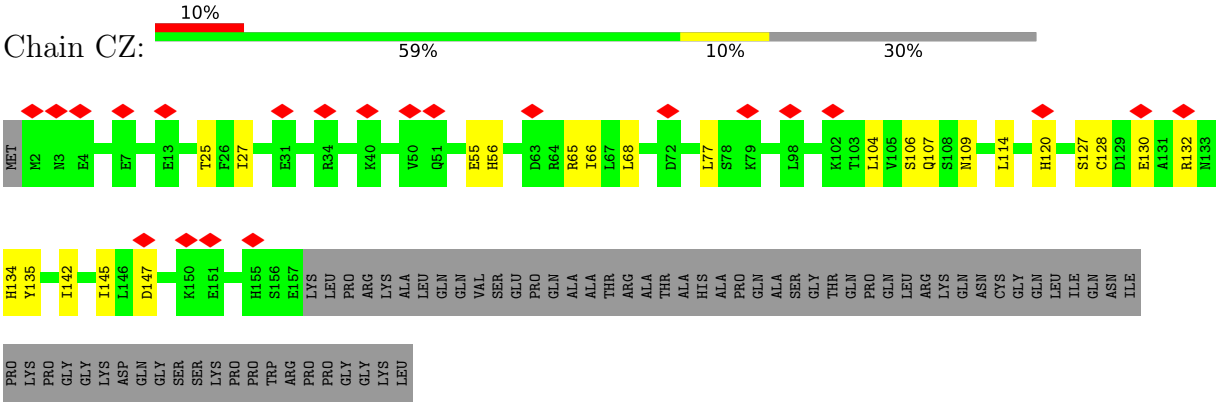
• Molecule 2: Sperm acrosome associated 9

Chain CY:



• Molecule 2: Sperm acrosome associated 9

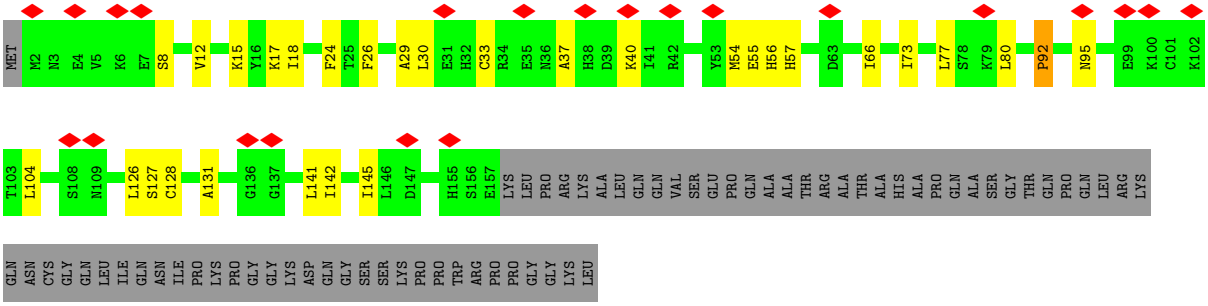
Chain CZ:



• Molecule 2: Sperm acrosome associated 9

Chain Ca:

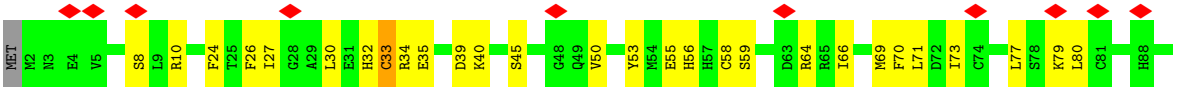


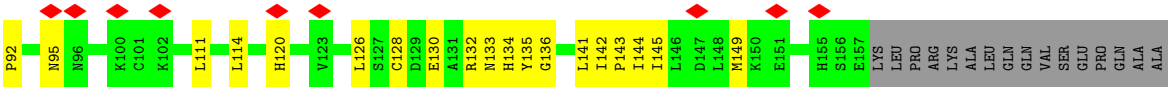


• Molecule 2: Sperm acrosome associated 9

Chain Cb:





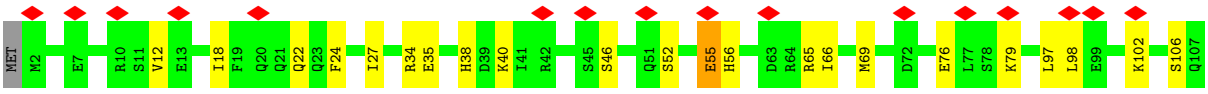


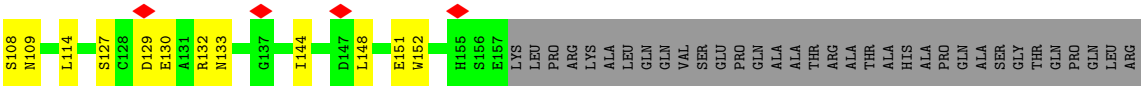


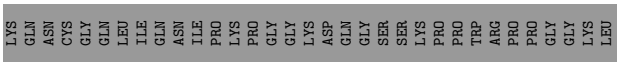
• Molecule 2: Sperm acrosome associated 9

Chain Cc:





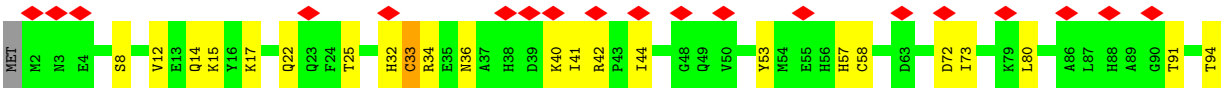


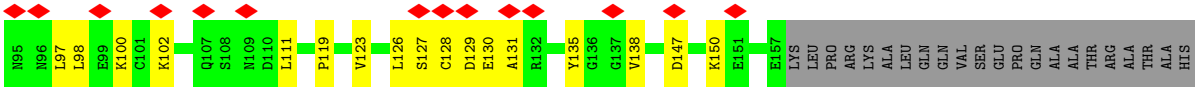


• Molecule 2: Sperm acrosome associated 9

Chain Cd:



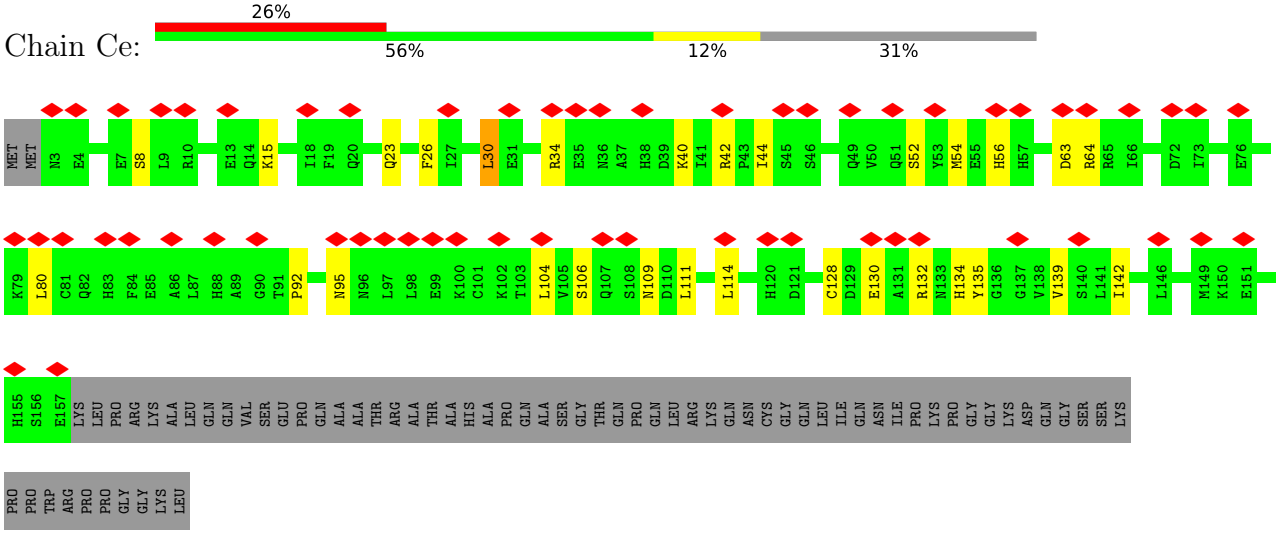






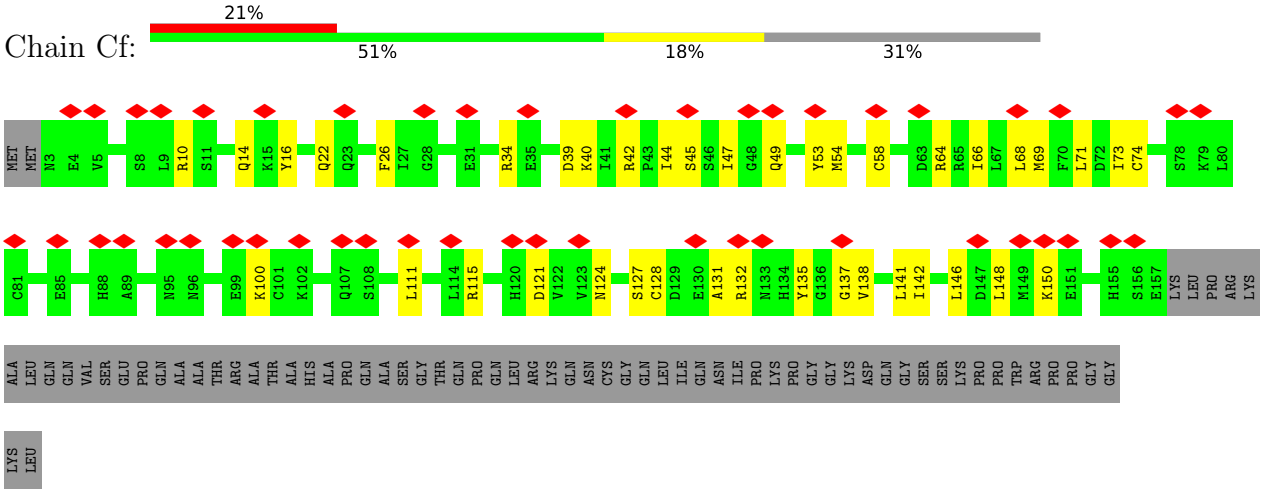
• Molecule 2: Sperm acrosome associated 9

Chain Ce:



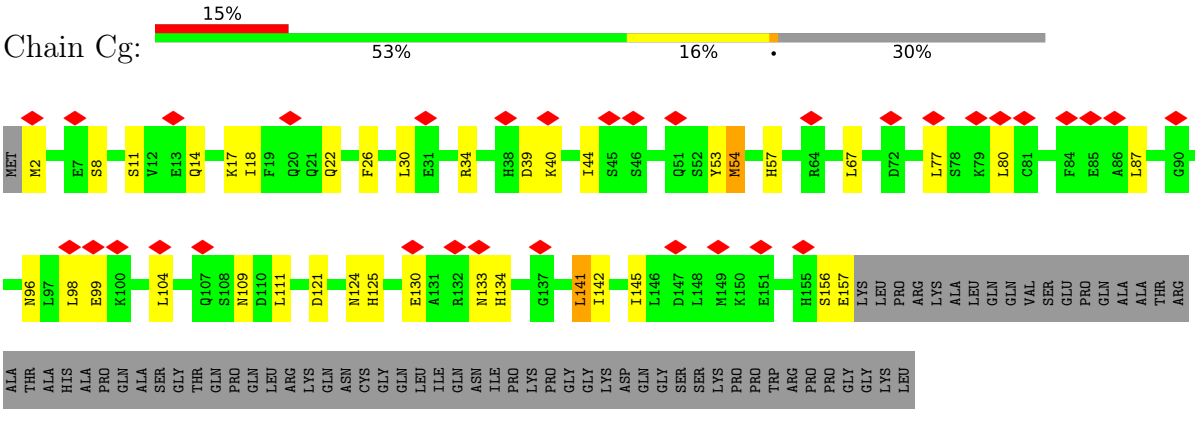
• Molecule 2: Sperm acrosome associated 9

Chain Cf:



• Molecule 2: Sperm acrosome associated 9

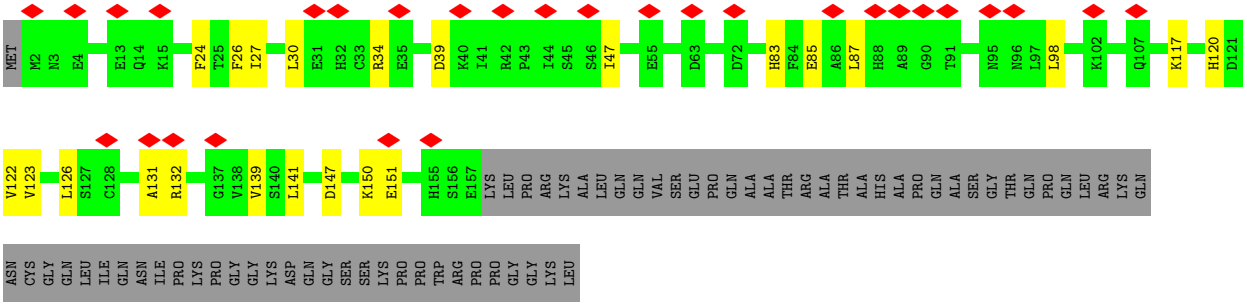
Chain Cg:



• Molecule 2: Sperm acrosome associated 9

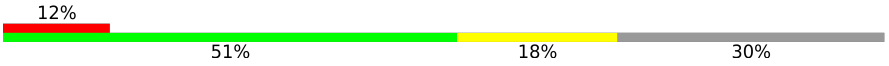
Chain Ch:

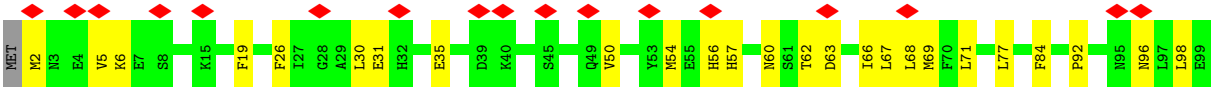


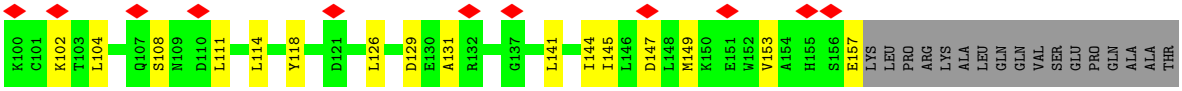


• Molecule 2: Sperm acrosome associated 9

Chain Ci:





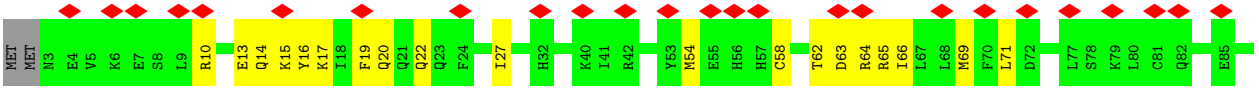


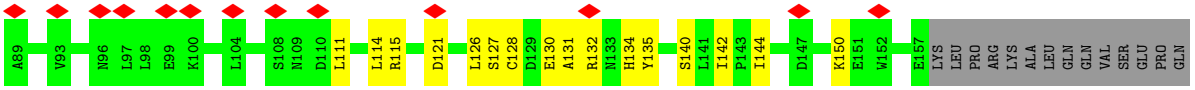


• Molecule 2: Sperm acrosome associated 9

Chain Cj:





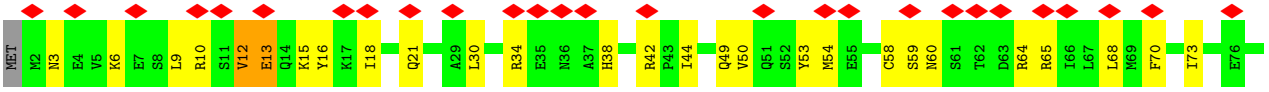


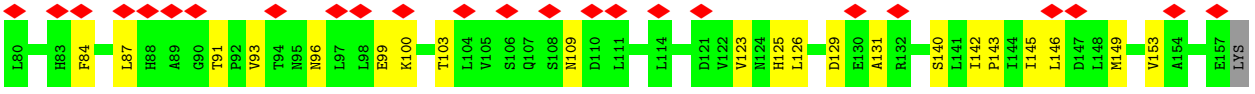


• Molecule 2: Sperm acrosome associated 9

Chain Ck:







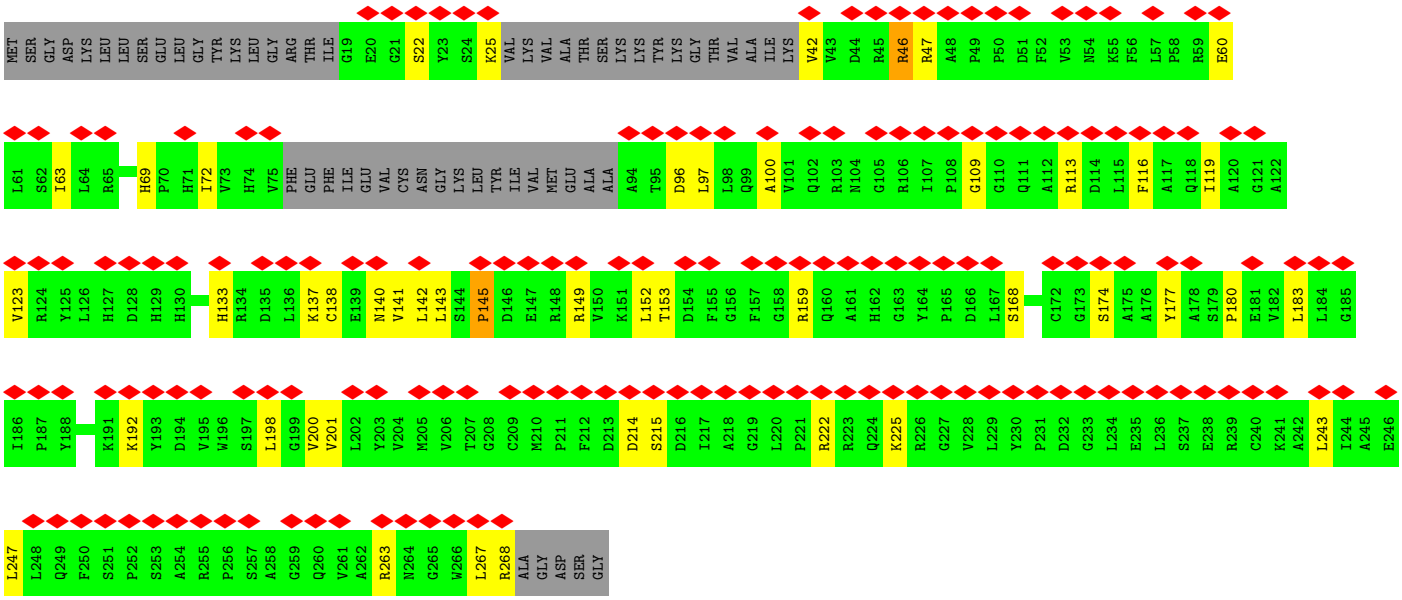




• Molecule 3: Testis specific serine kinase 6

Chain 1:

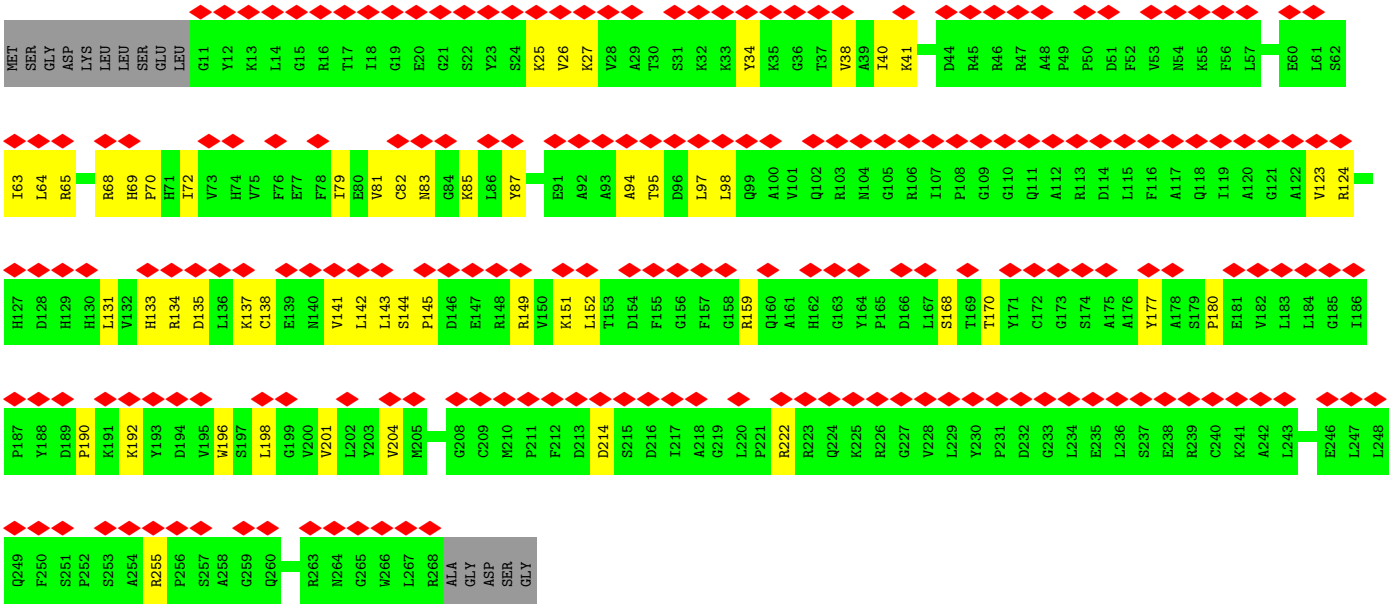




• Molecule 3: Testis specific serine kinase 6

Chain 2:

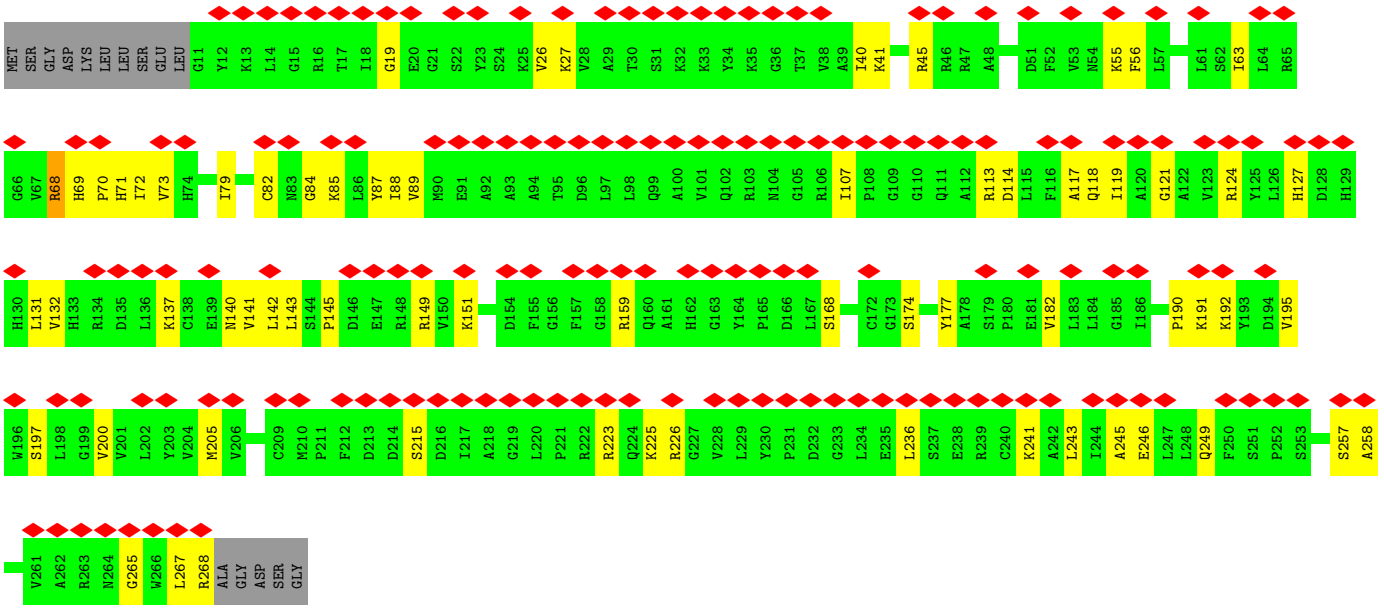




• Molecule 3: Testis specific serine kinase 6

Chain x:

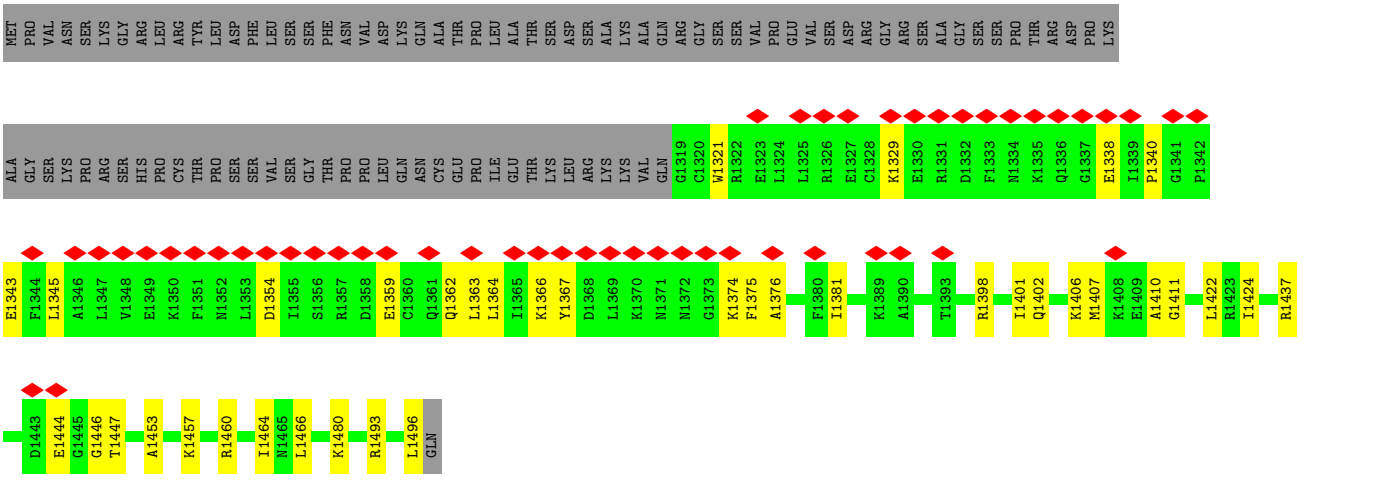




• Molecule 4: EF-hand domain-containing protein

Chain 3:

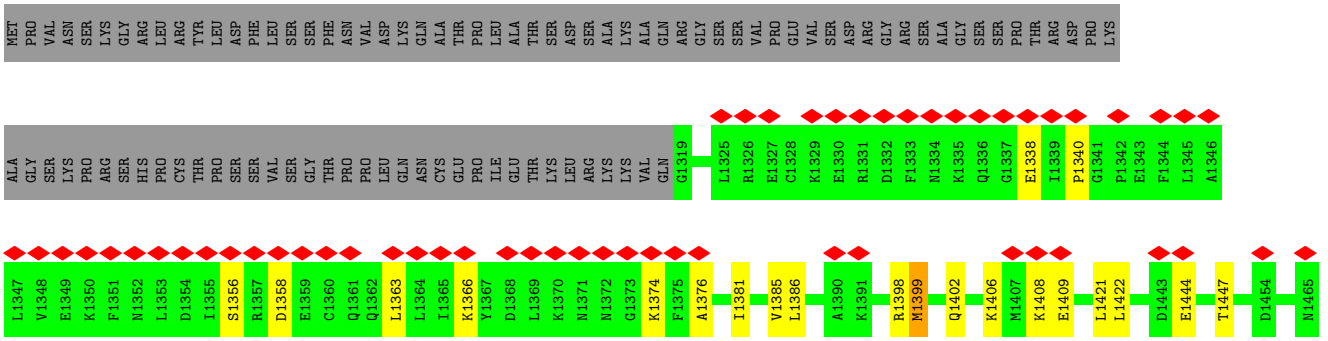


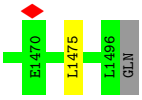


• Molecule 4: EF-hand domain-containing protein

Chain y:



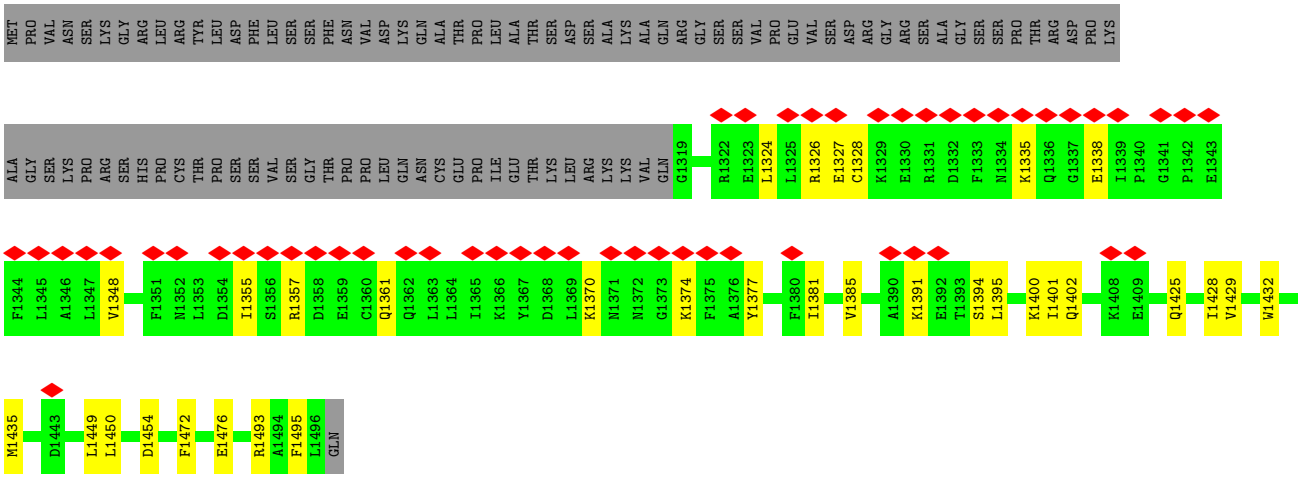




• Molecule 4: EF-hand domain-containing protein

Chain z:

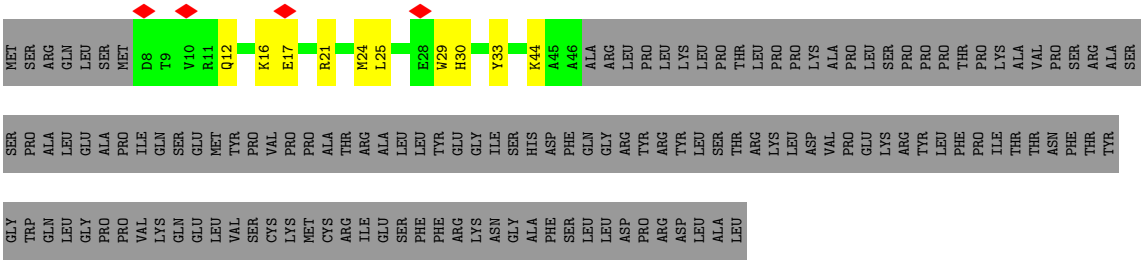




• Molecule 5: ATP6V1F neighbor

Chain A:

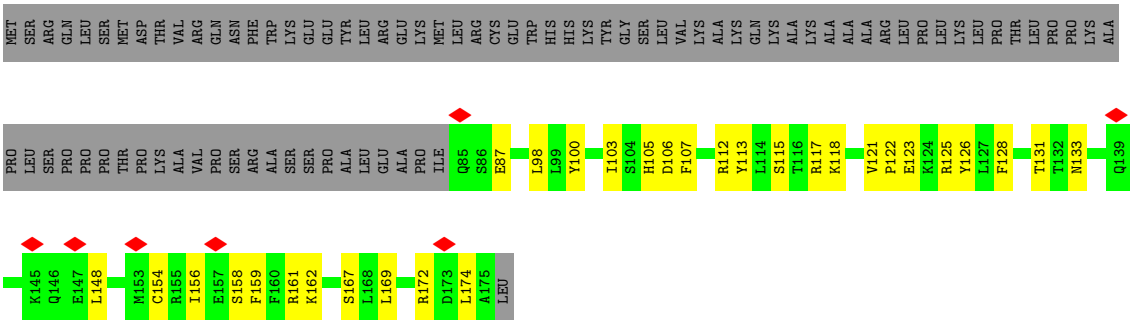




• Molecule 5: ATP6V1F neighbor

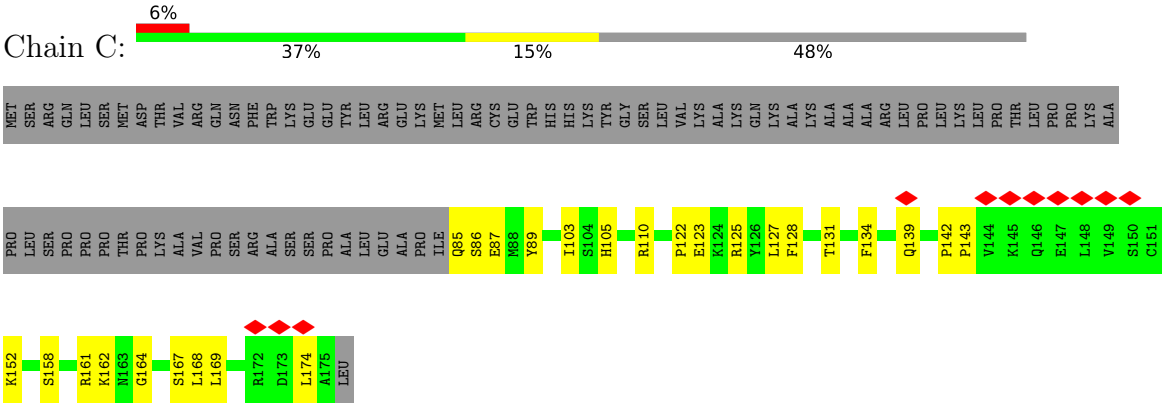
Chain B:





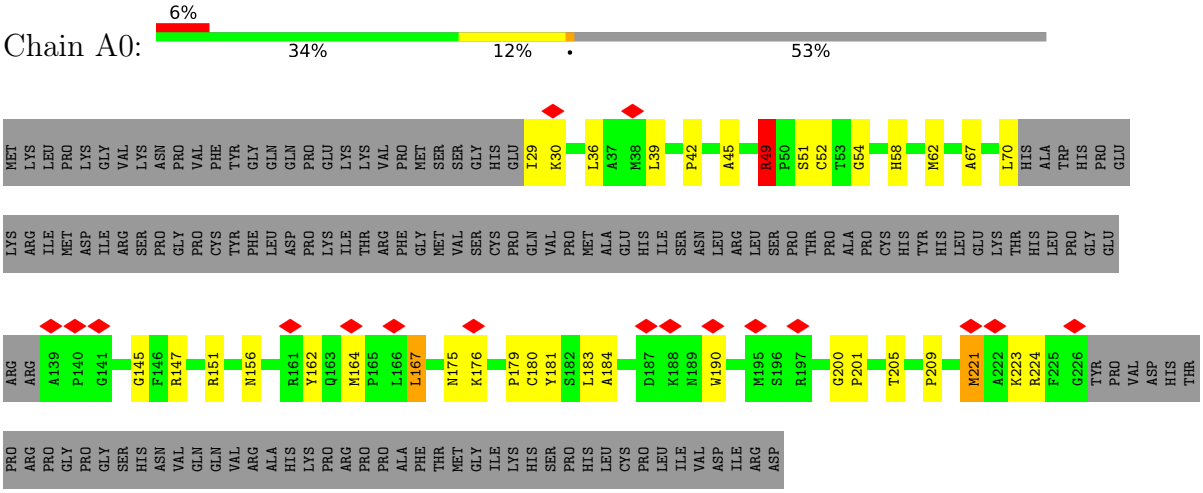
• Molecule 5: ATP6V1F neighbor

Chain C:



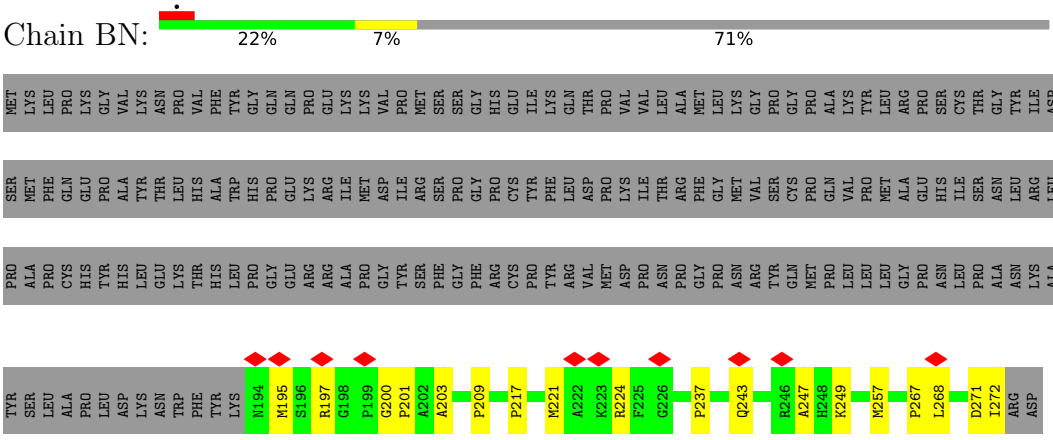
• Molecule 6: Outer dense fiber of sperm tails 3 like 1

Chain A0:



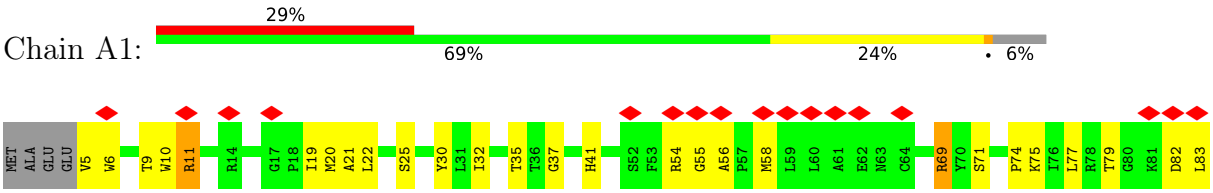
• Molecule 6: Outer dense fiber of sperm tails 3 like 1

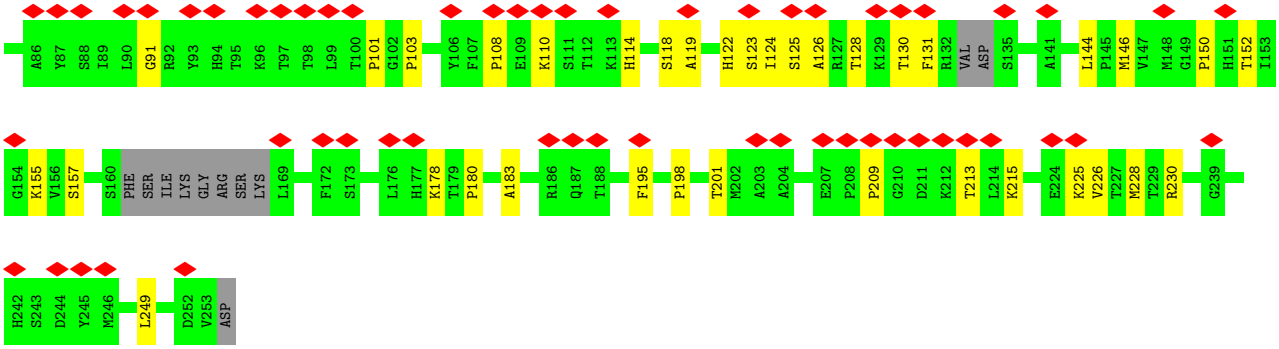
Chain BN:



• Molecule 7: Outer dense fiber of sperm tails 3

Chain A1:

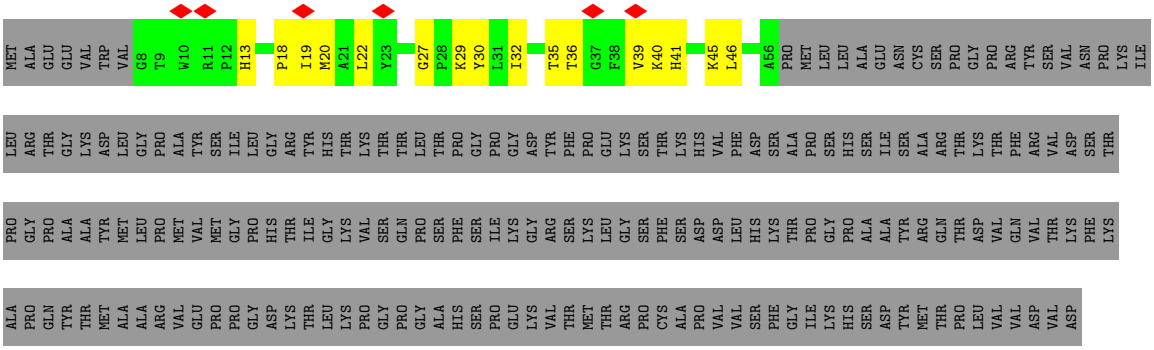




• Molecule 7: Outer dense fiber of sperm tails 3

Chain A2:

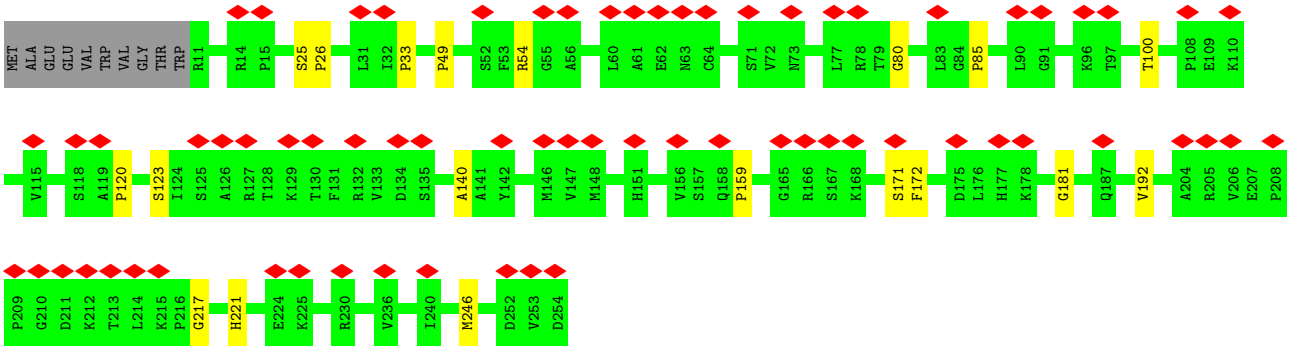




• Molecule 7: Outer dense fiber of sperm tails 3

Chain A3:

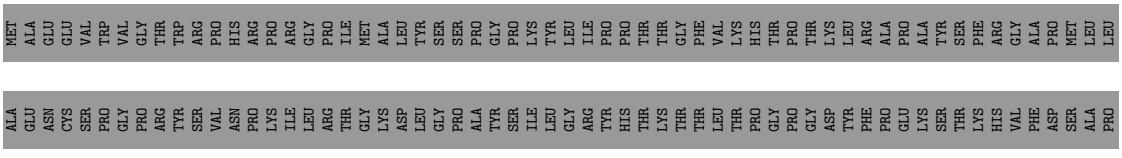


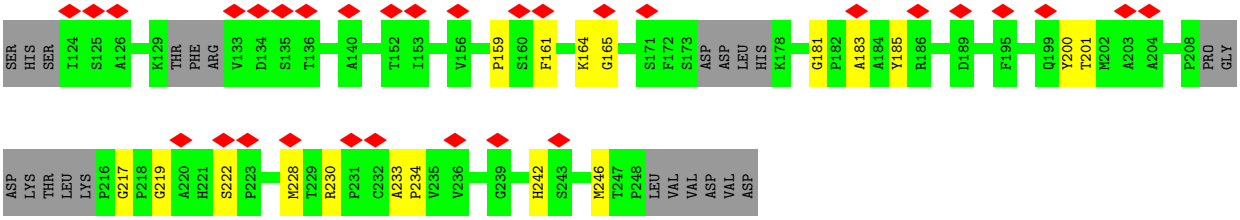


• Molecule 7: Outer dense fiber of sperm tails 3

Chain A4:



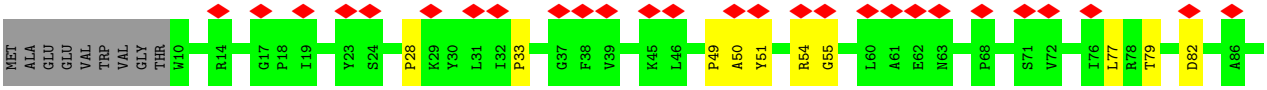


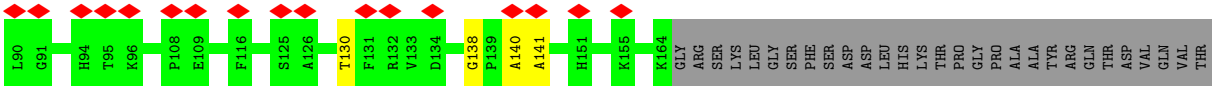


• Molecule 7: Outer dense fiber of sperm tails 3

Chain A5:











• Molecule 7: Outer dense fiber of sperm tails 3

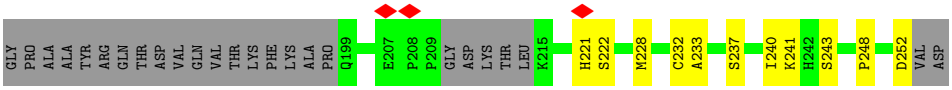
Chain A6:







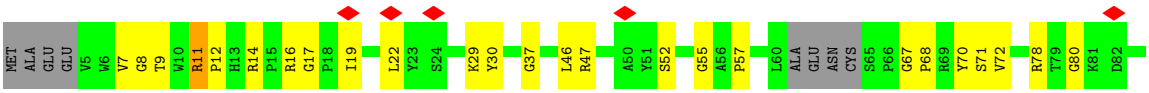


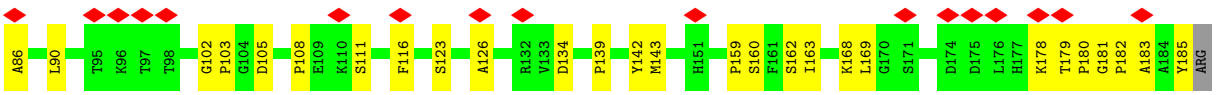


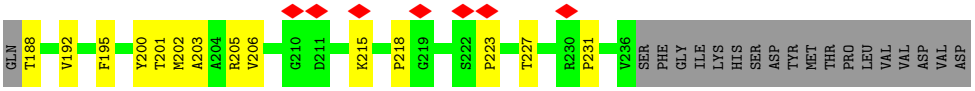
• Molecule 7: Outer dense fiber of sperm tails 3

Chain A7:





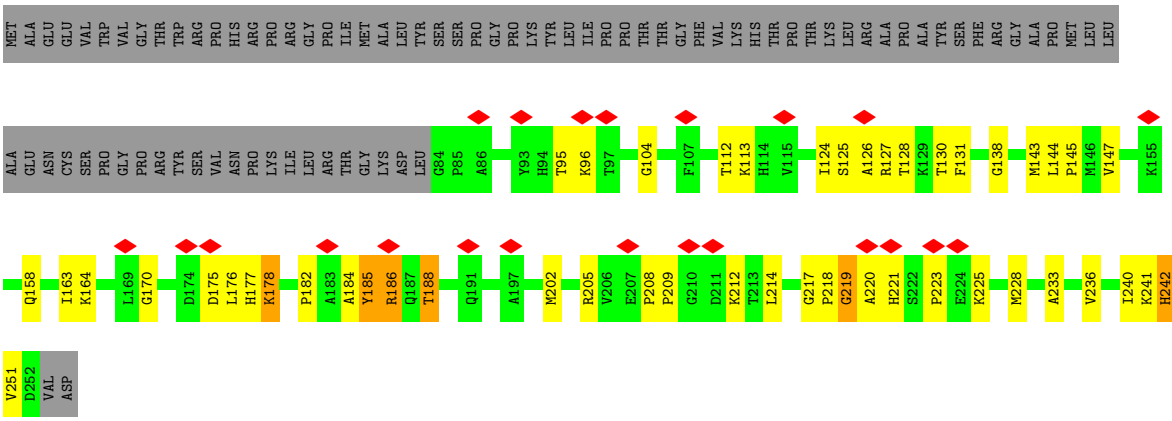




• Molecule 7: Outer dense fiber of sperm tails 3

Chain A8:

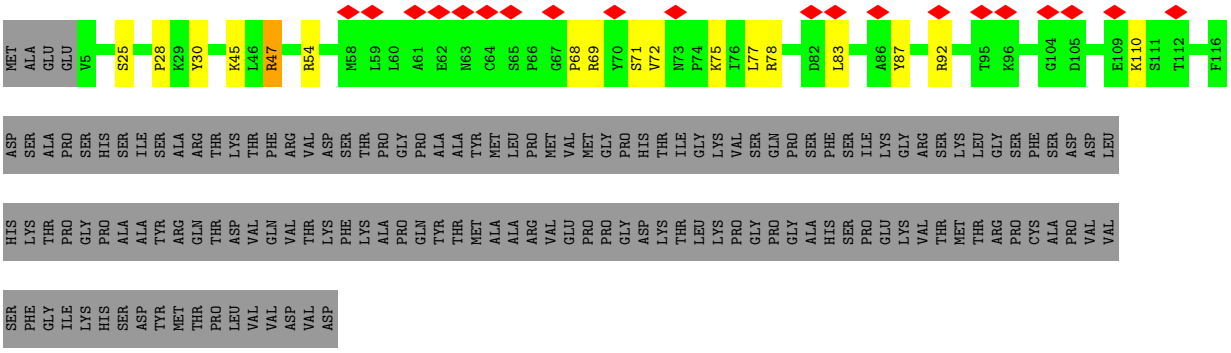




• Molecule 7: Outer dense fiber of sperm tails 3

Chain A9:

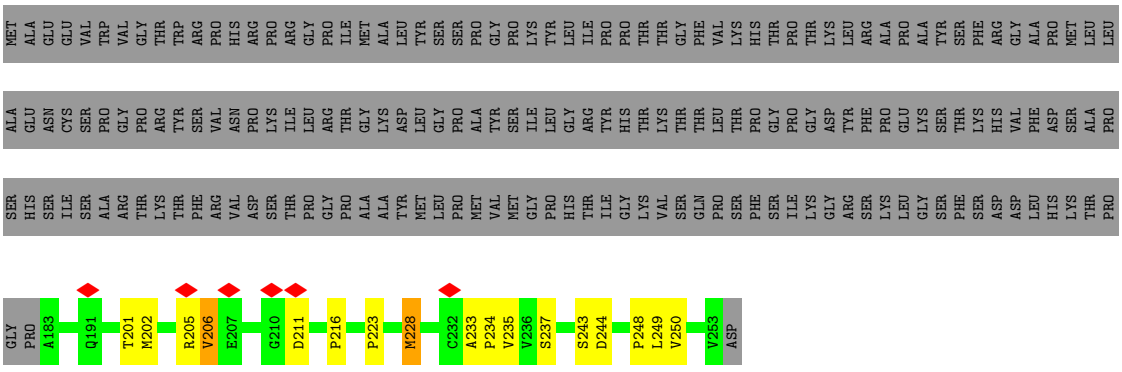




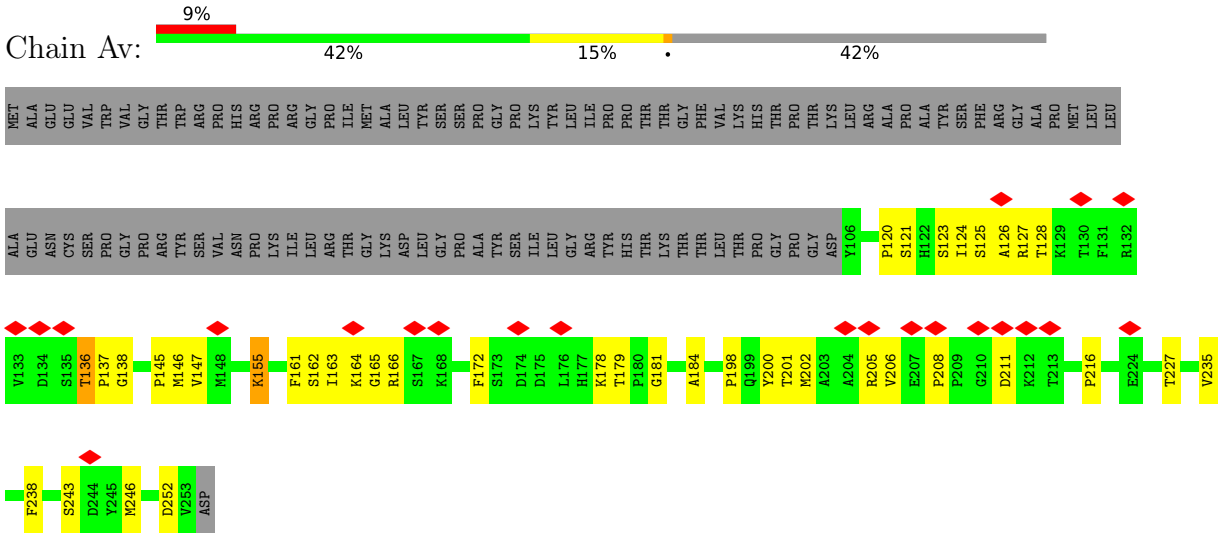
• Molecule 7: Outer dense fiber of sperm tails 3

Chain Au:

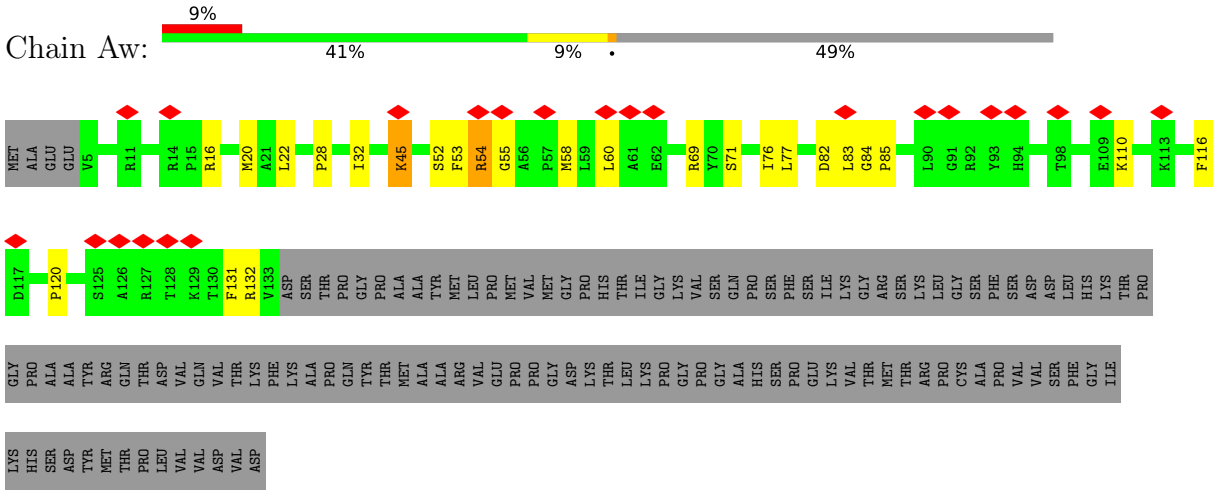




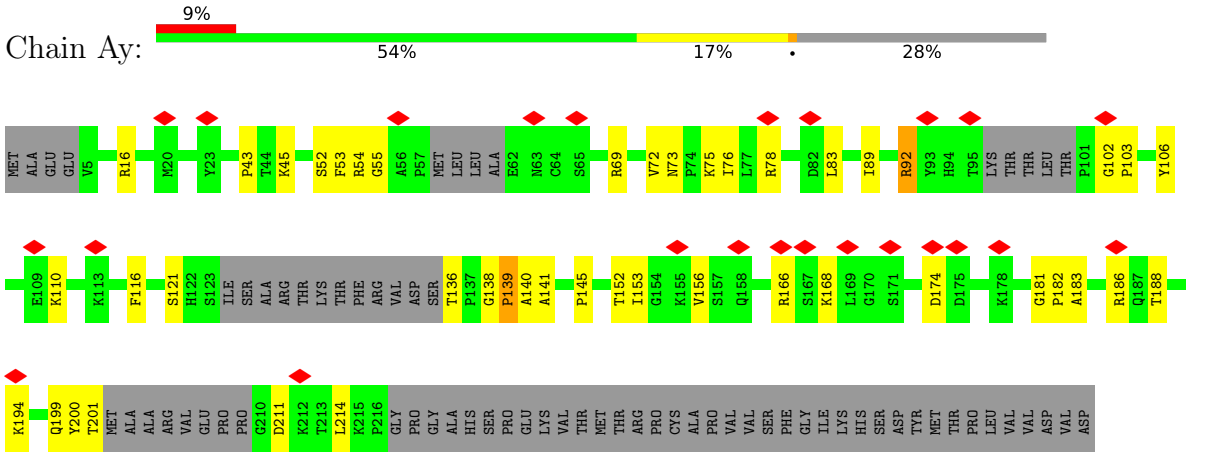
• Molecule 7: Outer dense fiber of sperm tails 3



• Molecule 7: Outer dense fiber of sperm tails 3

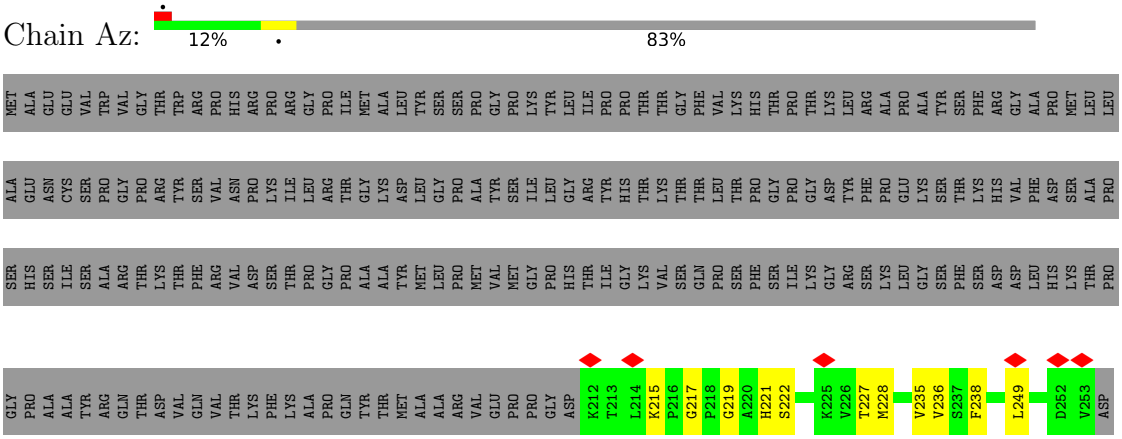


• Molecule 7: Outer dense fiber of sperm tails 3



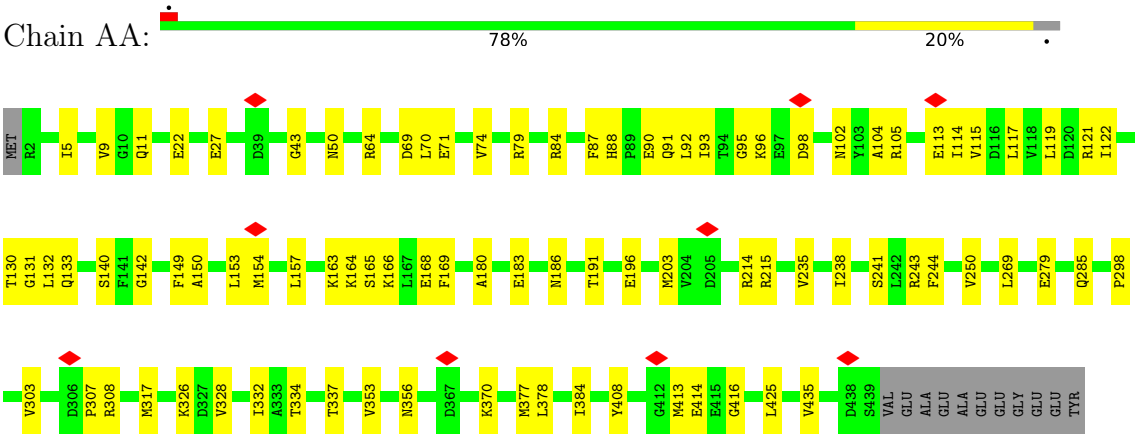
• Molecule 7: Outer dense fiber of sperm tails 3

Chain Az:



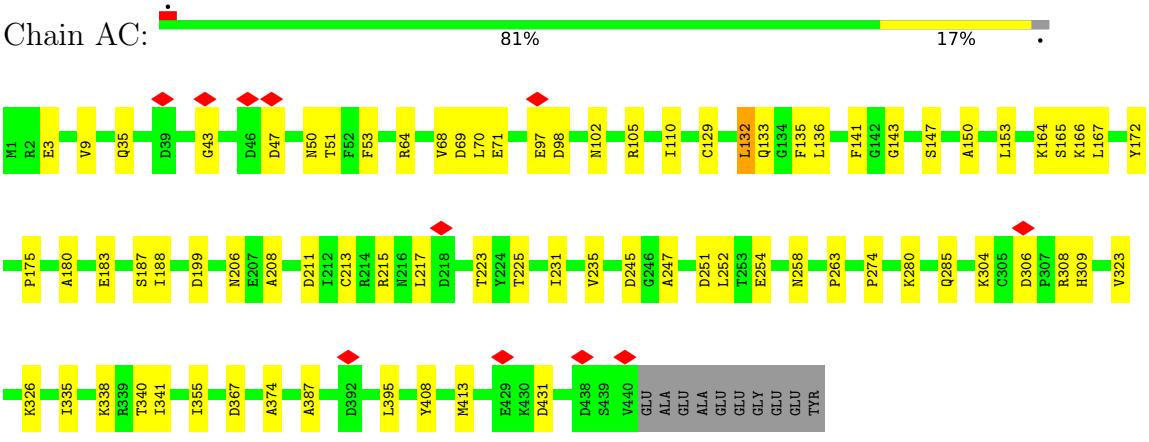
• Molecule 8: Tubulin alpha-3 chain

Chain AA:



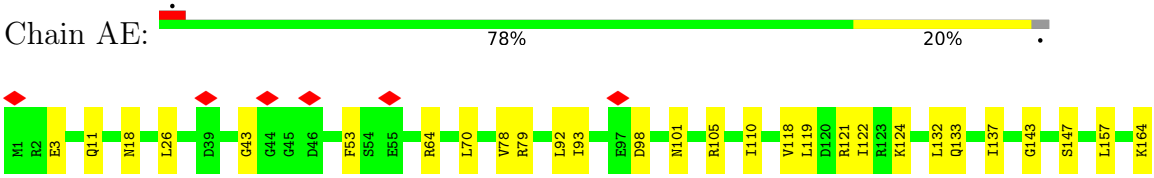
• Molecule 8: Tubulin alpha-3 chain

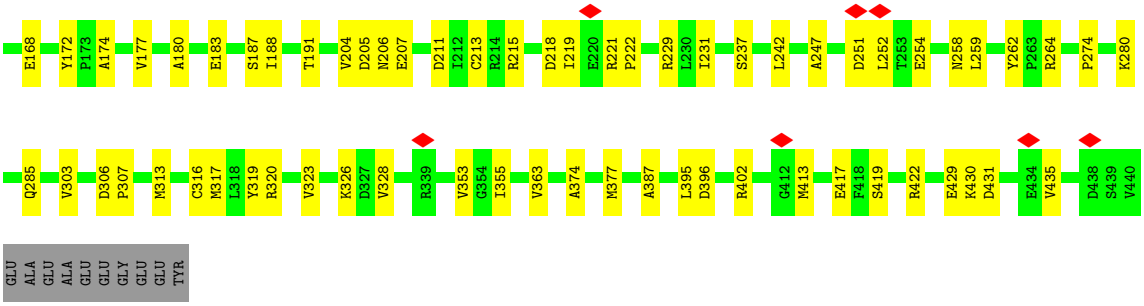
Chain AC:



• Molecule 8: Tubulin alpha-3 chain

Chain AE:

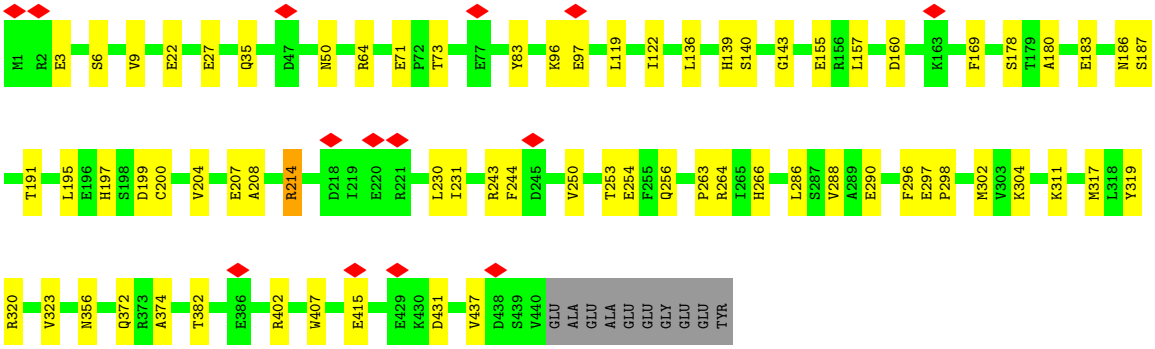




• Molecule 8: Tubulin alpha-3 chain

Chain AG:

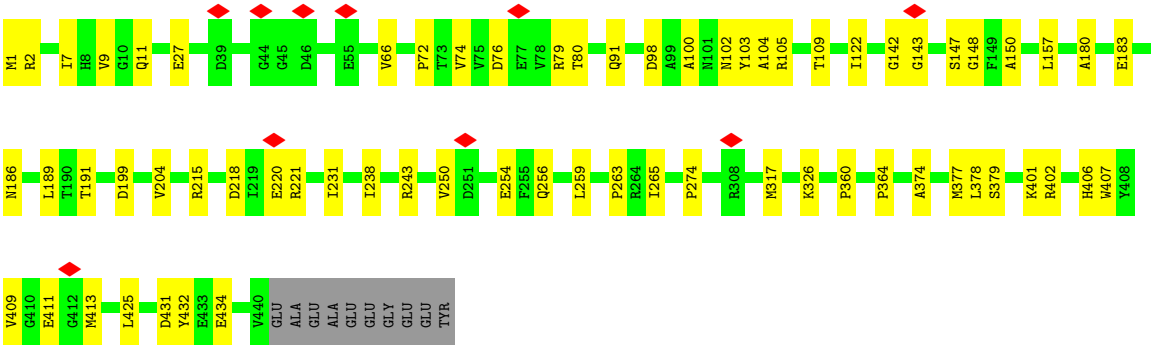




• Molecule 8: Tubulin alpha-3 chain

Chain AI:

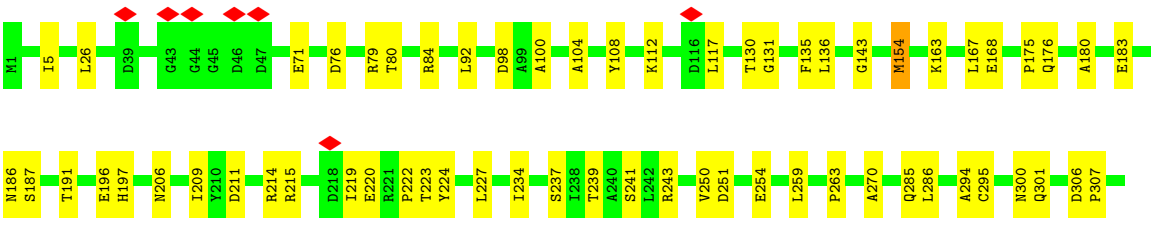


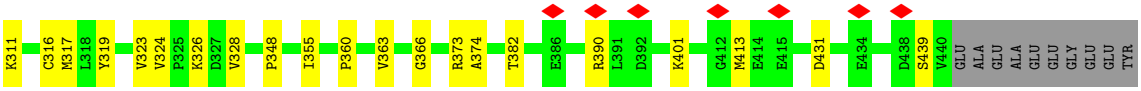


• Molecule 8: Tubulin alpha-3 chain

Chain AK:







• Molecule 8: Tubulin alpha-3 chain

Chain AM:





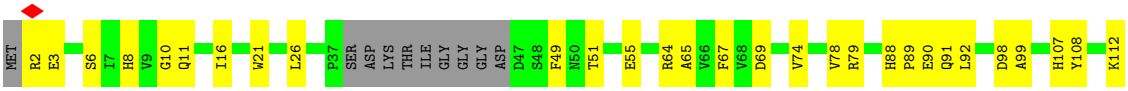


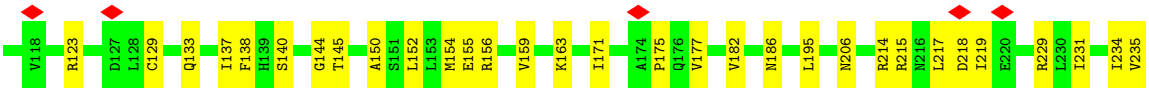


• Molecule 8: Tubulin alpha-3 chain

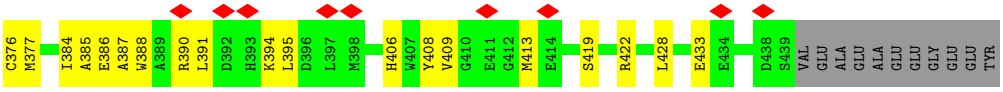
Chain BA:







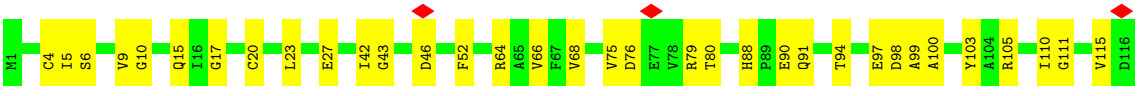


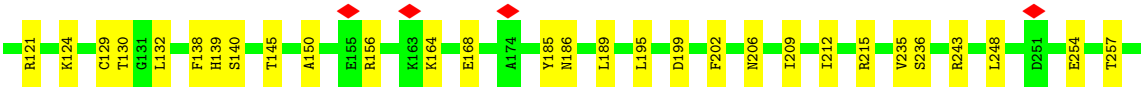


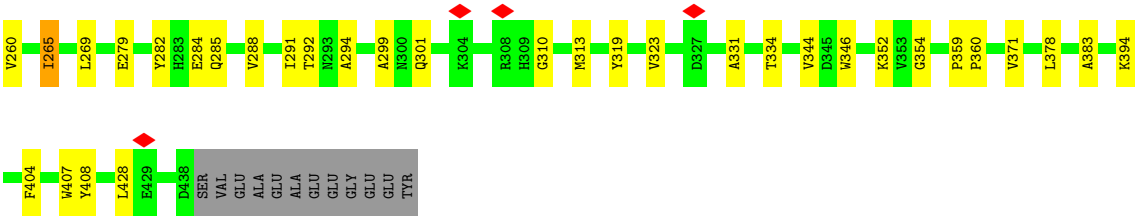
• Molecule 8: Tubulin alpha-3 chain

Chain BC:





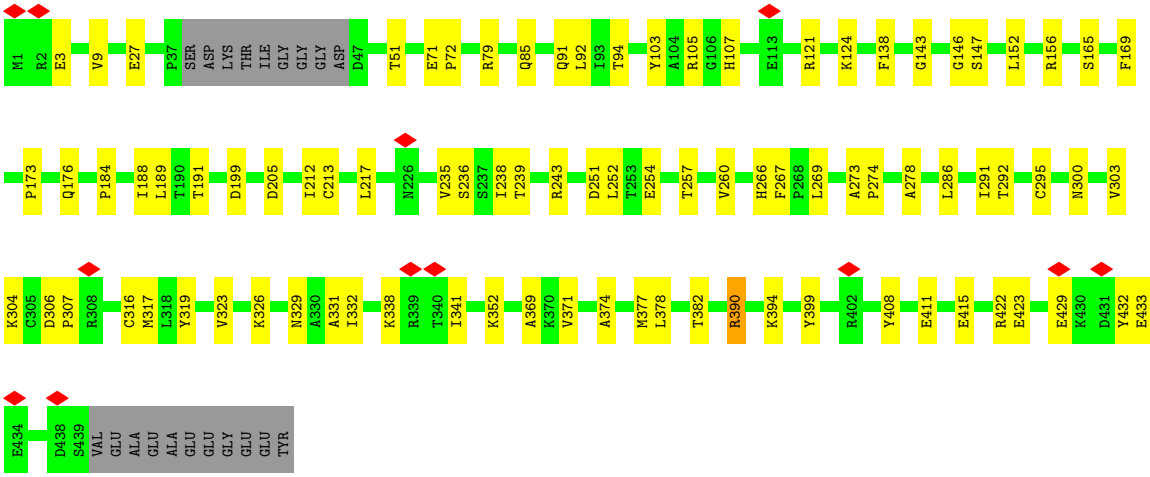




• Molecule 8: Tubulin alpha-3 chain

Chain BE:

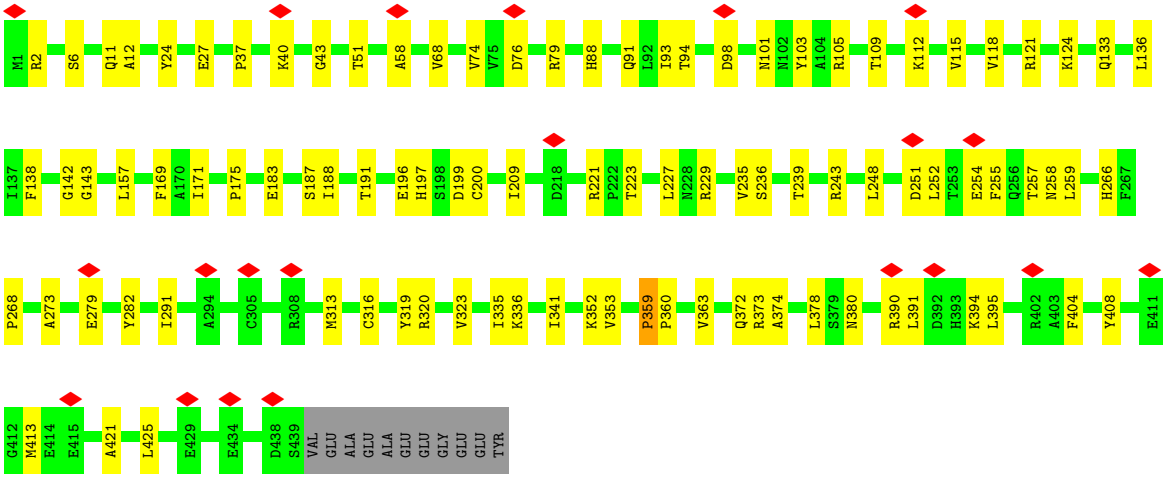




• Molecule 8: Tubulin alpha-3 chain

Chain BG:

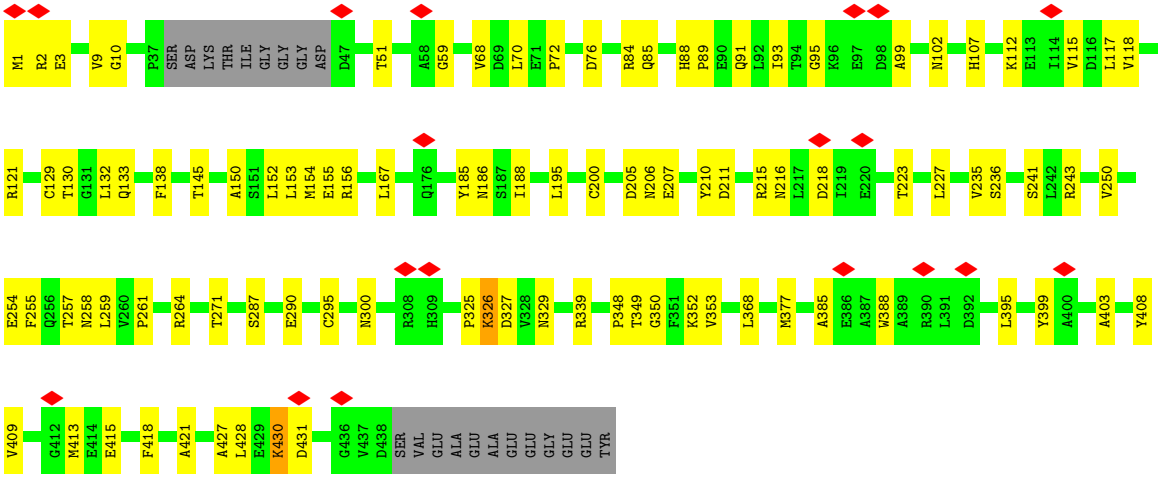




• Molecule 8: Tubulin alpha-3 chain

Chain BI:

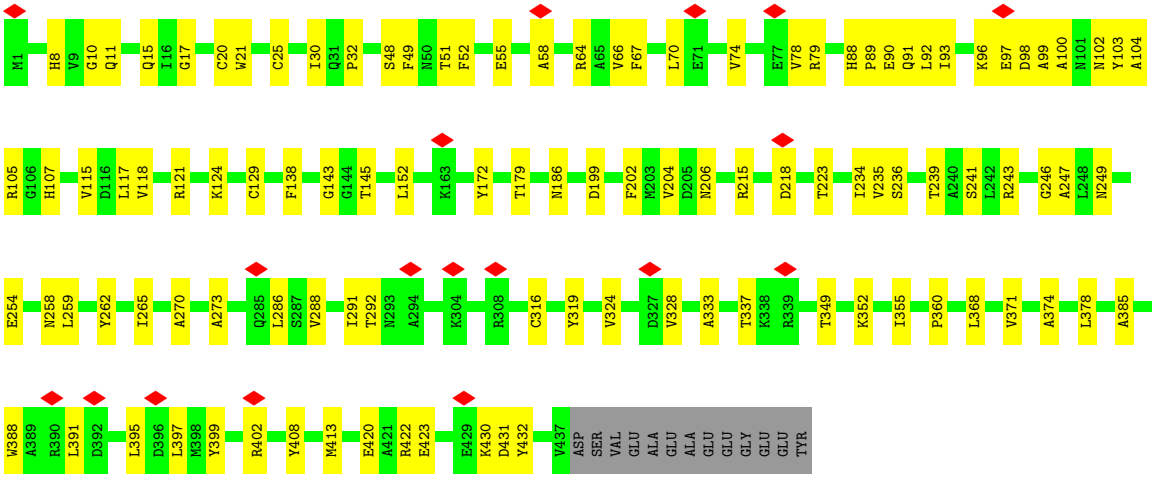




• Molecule 8: Tubulin alpha-3 chain

Chain BK:

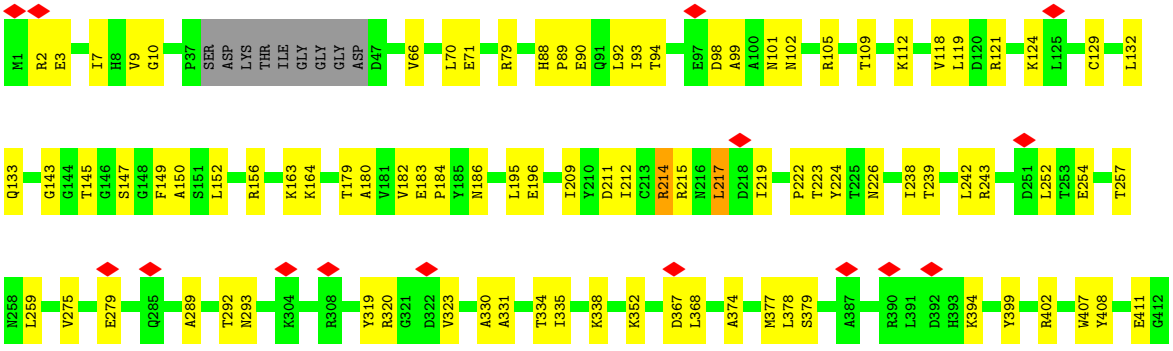


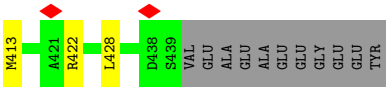


• Molecule 8: Tubulin alpha-3 chain

Chain BM:



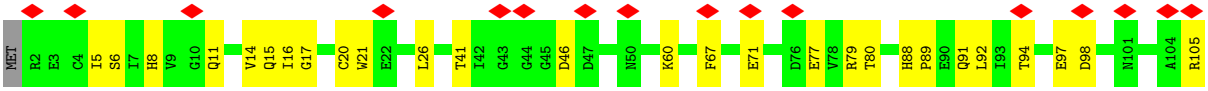


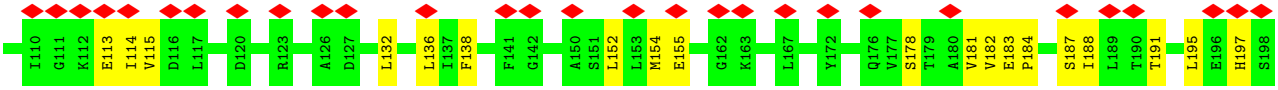


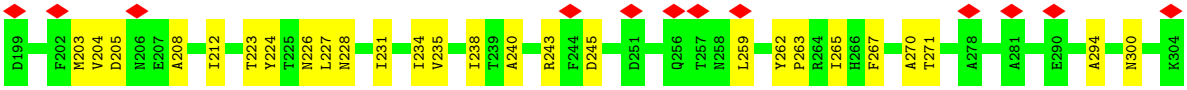
• Molecule 8: Tubulin alpha-3 chain

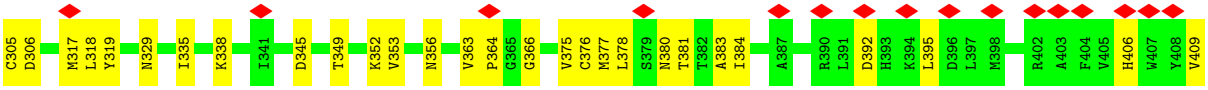
Chain CA:

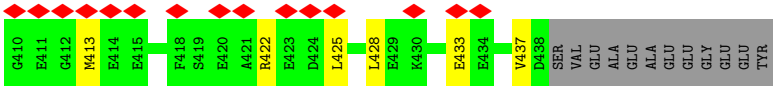








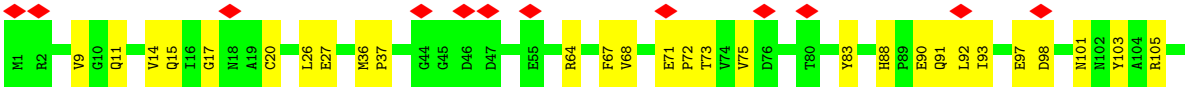


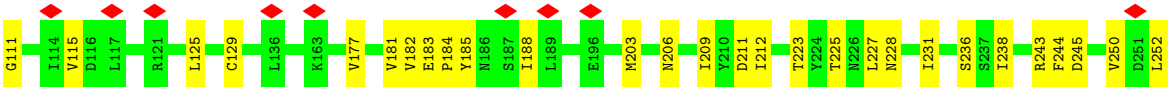


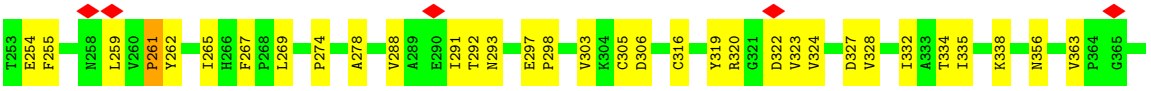
• Molecule 8: Tubulin alpha-3 chain

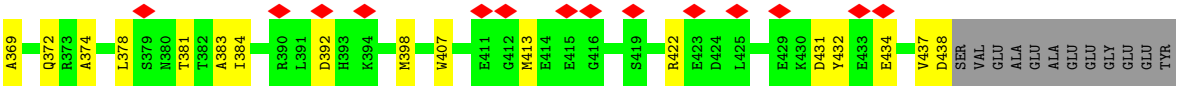
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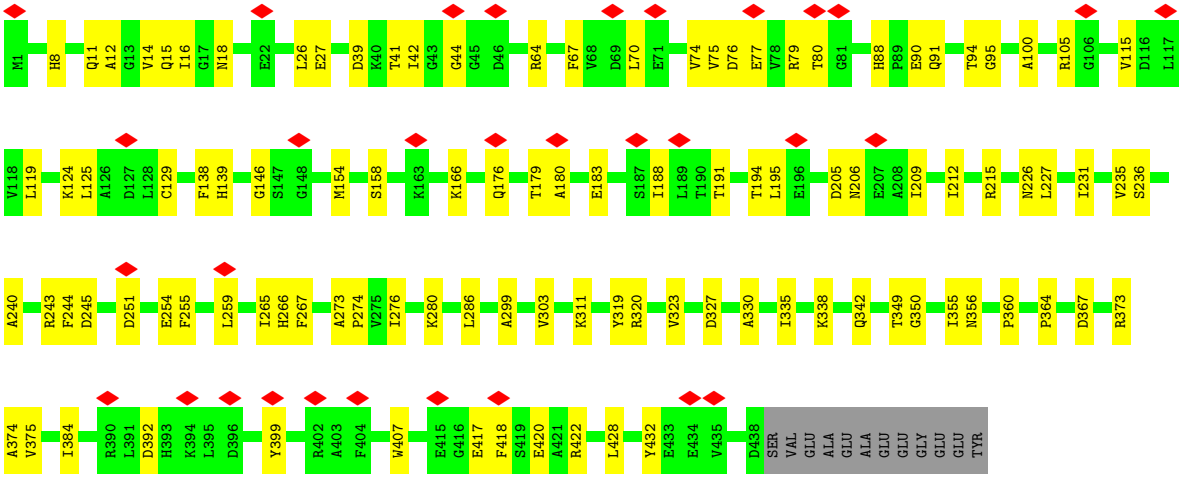




• Molecule 8: Tubulin alpha-3 chain

Chain CE:

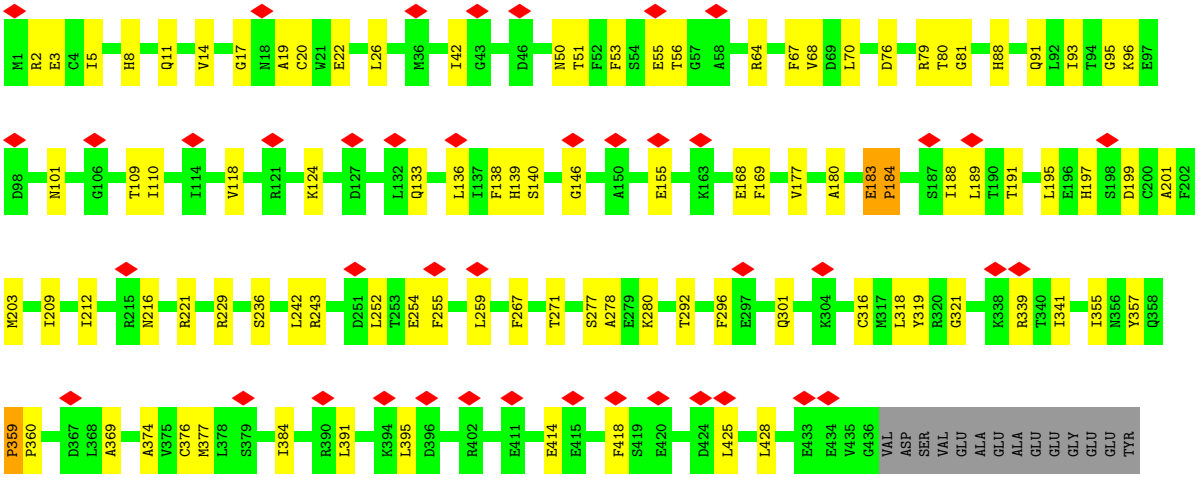




• Molecule 8: Tubulin alpha-3 chain

Chain CG:

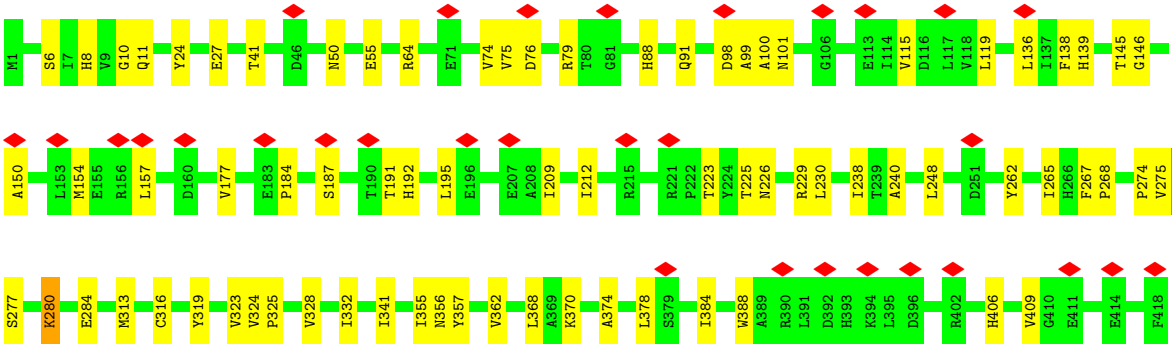


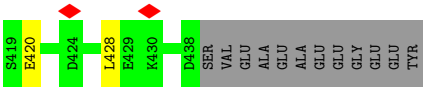


• Molecule 8: Tubulin alpha-3 chain

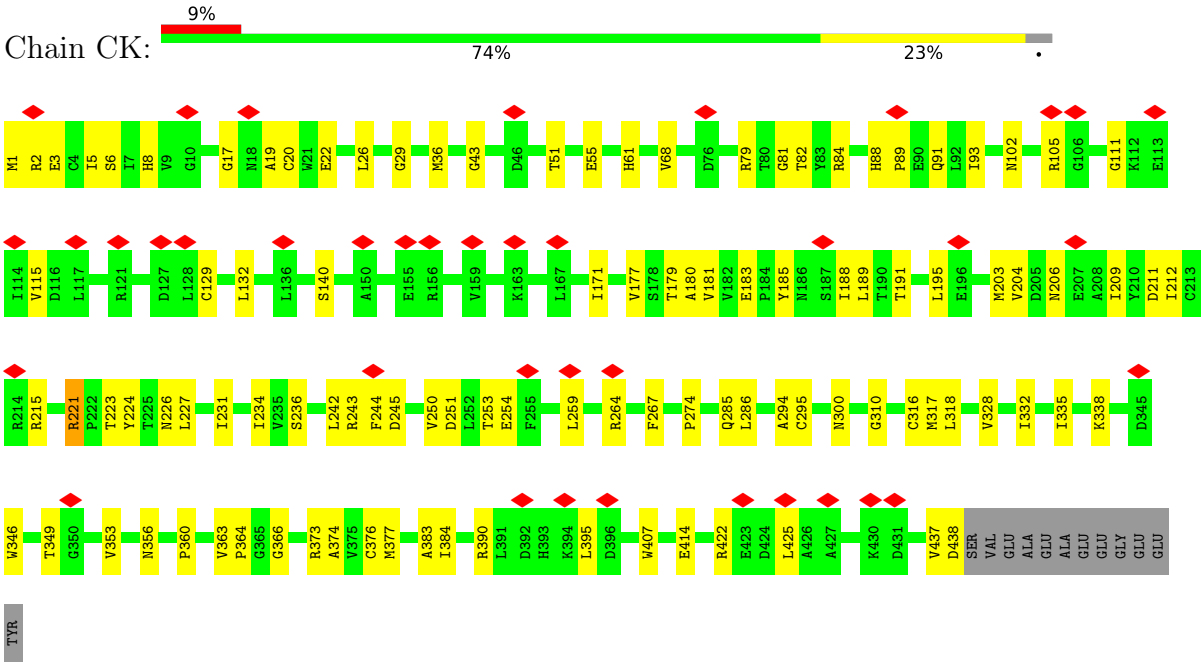
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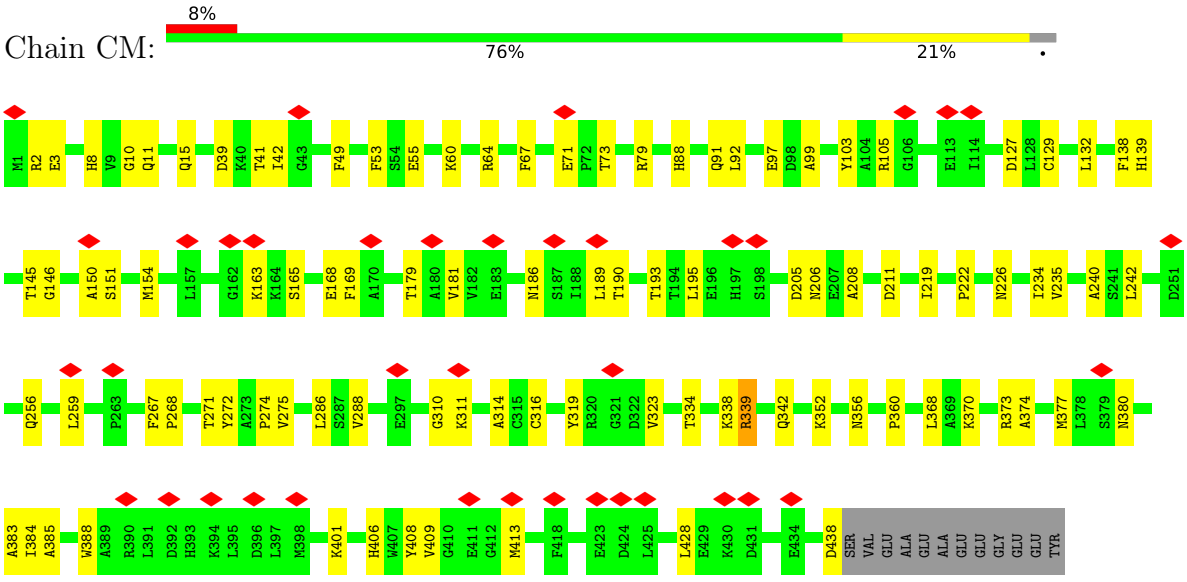




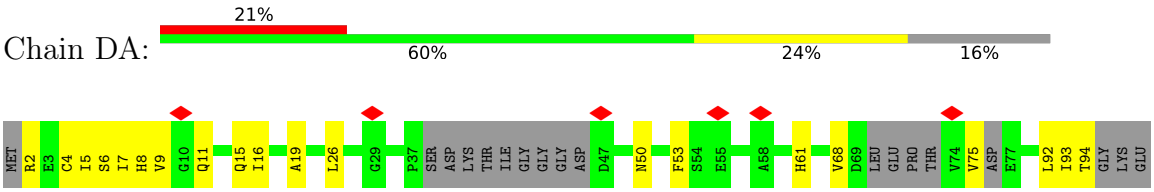
• Molecule 8: Tubulin alpha-3 chain

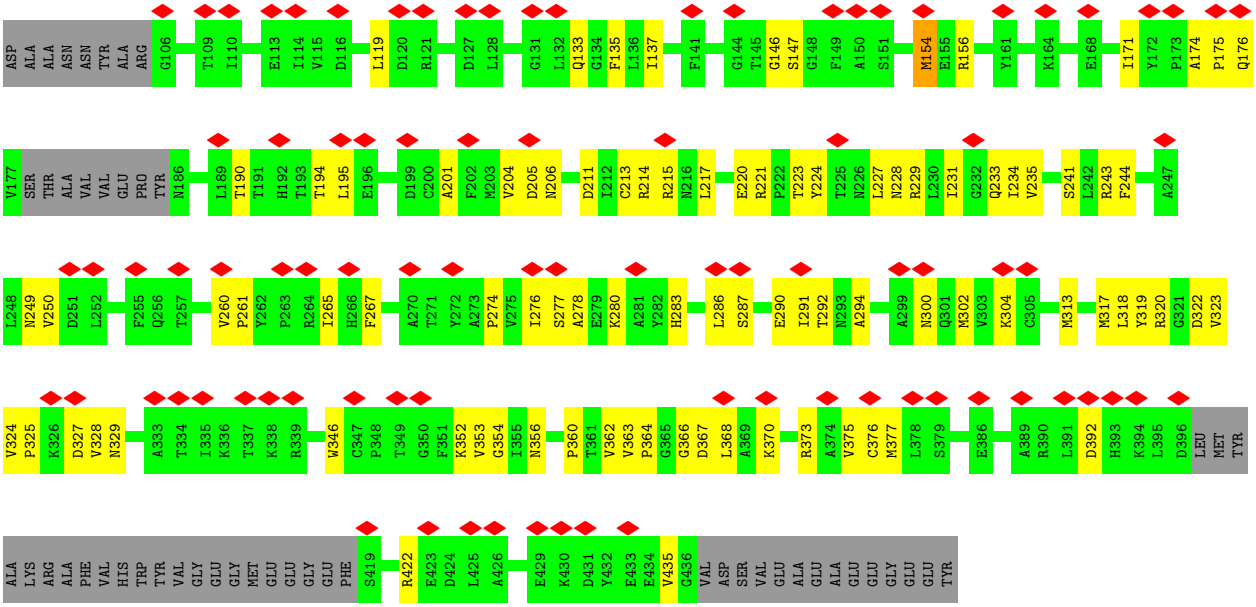


• Molecule 8: Tubulin alpha-3 chain



• Molecule 8: Tubulin alpha-3 chain

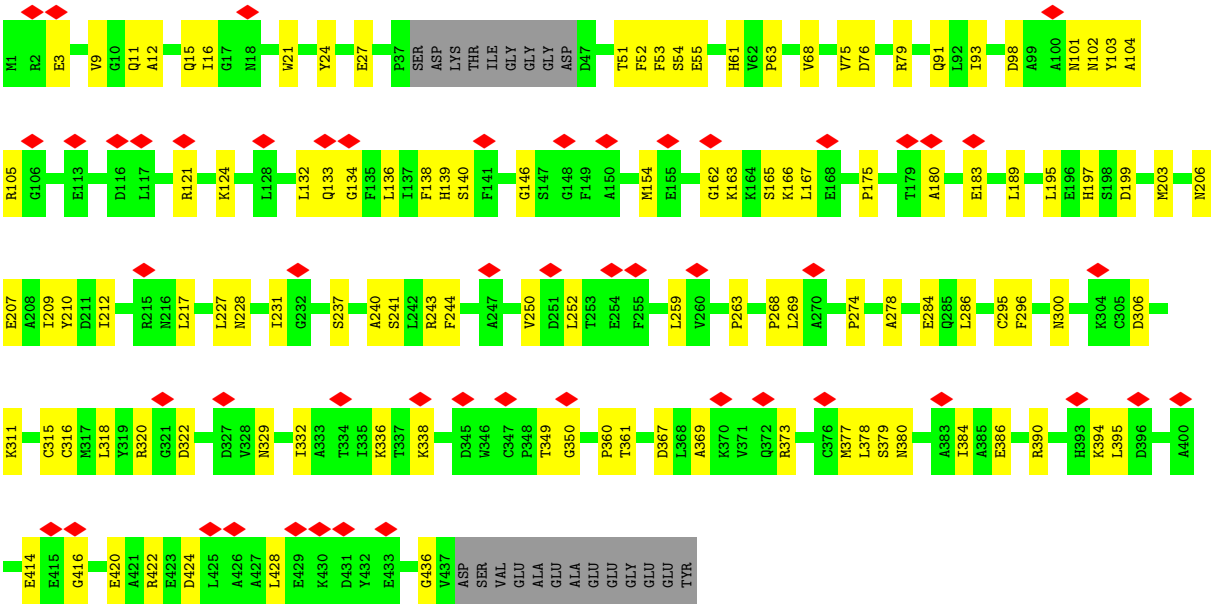




• Molecule 8: Tubulin alpha-3 chain

Chain DC:

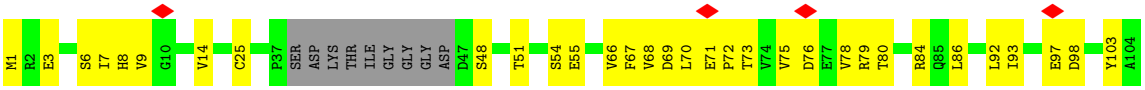


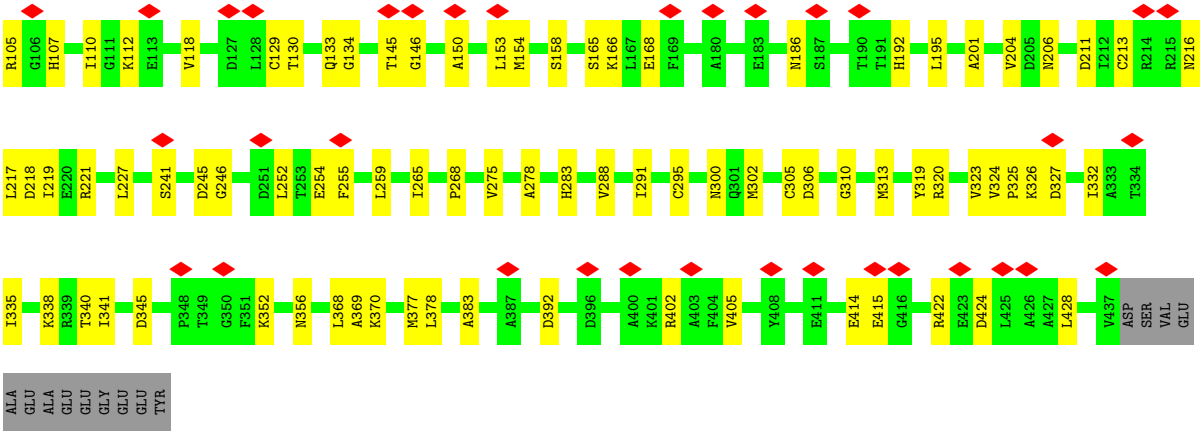


• Molecule 8: Tubulin alpha-3 chain

Chain DE:



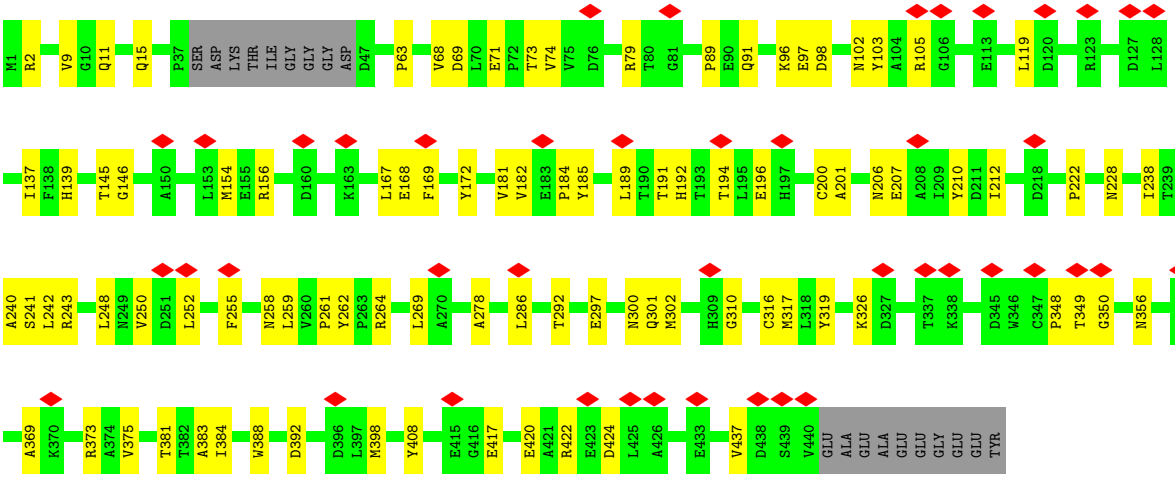




• Molecule 8: Tubulin alpha-3 chain

Chain DG:

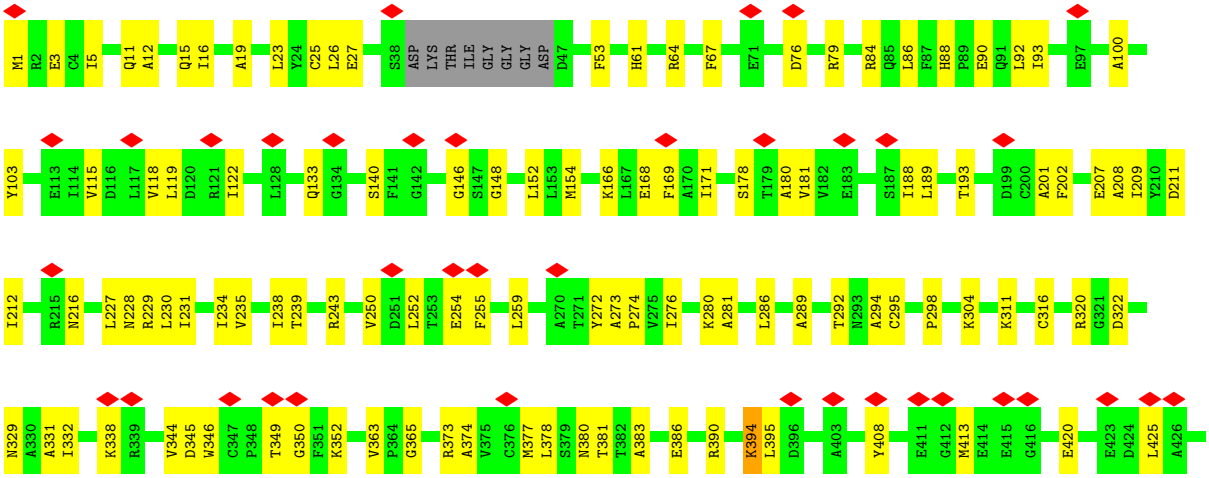


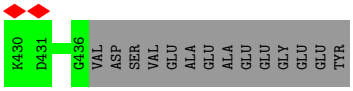


• Molecule 8: Tubulin alpha-3 chain

Chain DI:



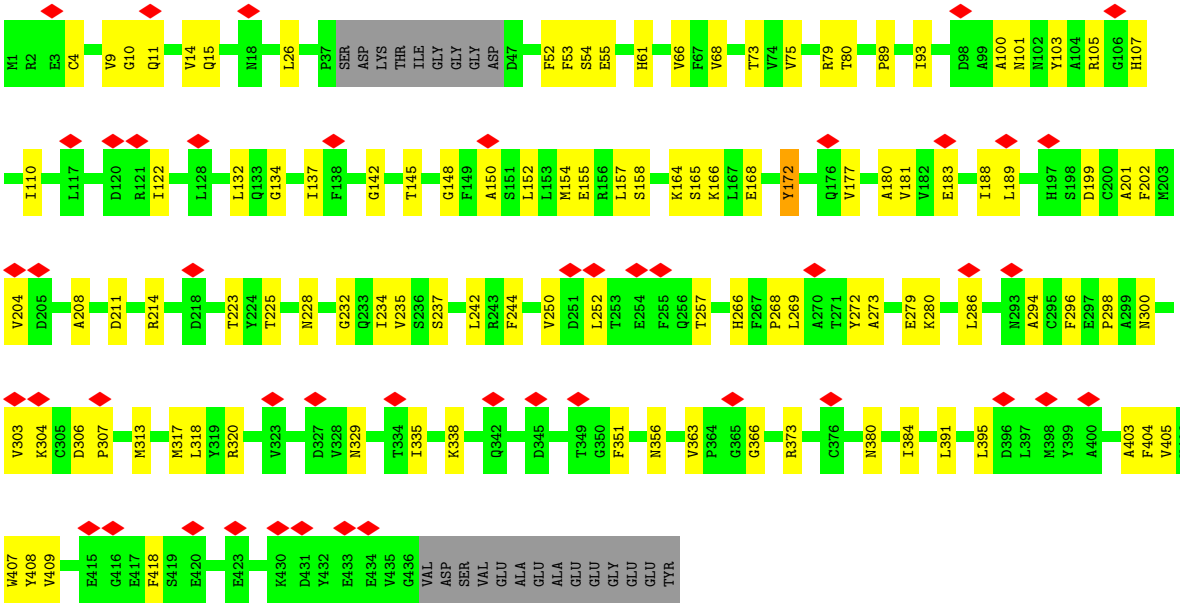




• Molecule 8: Tubulin alpha-3 chain

Chain DK:

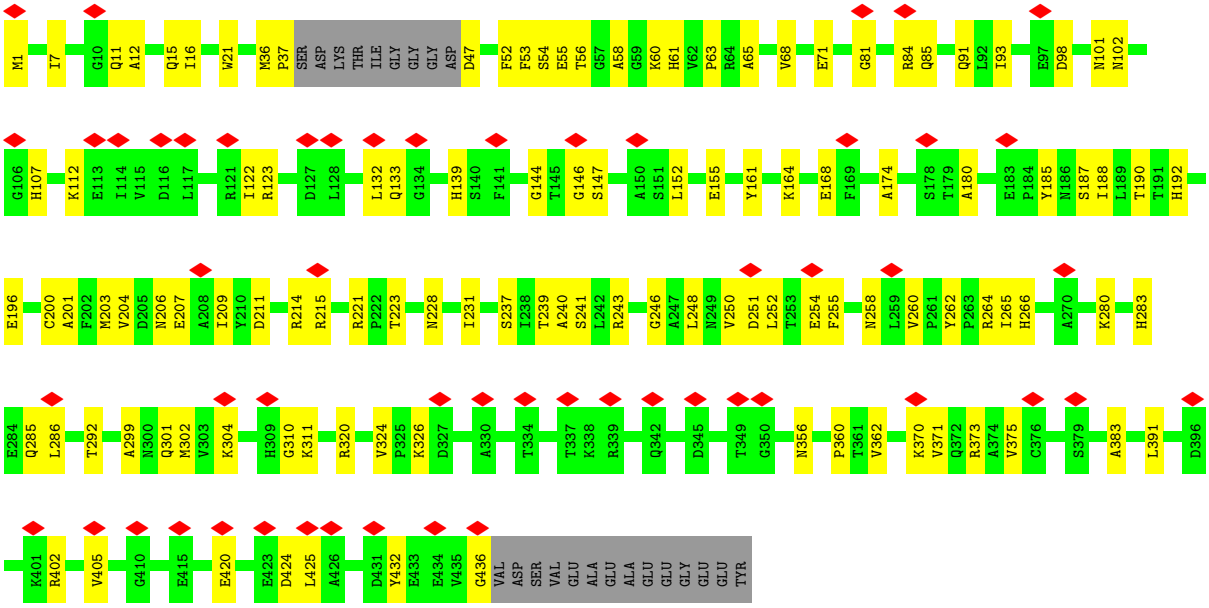




• Molecule 8: Tubulin alpha-3 chain

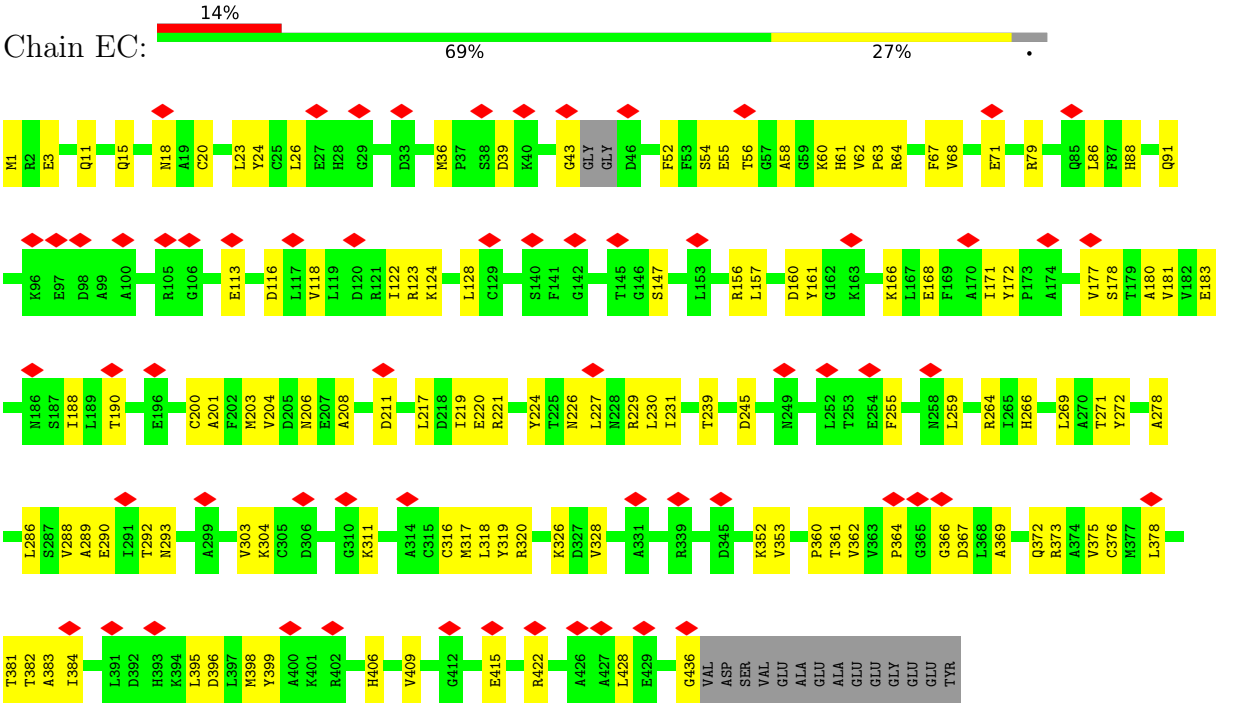
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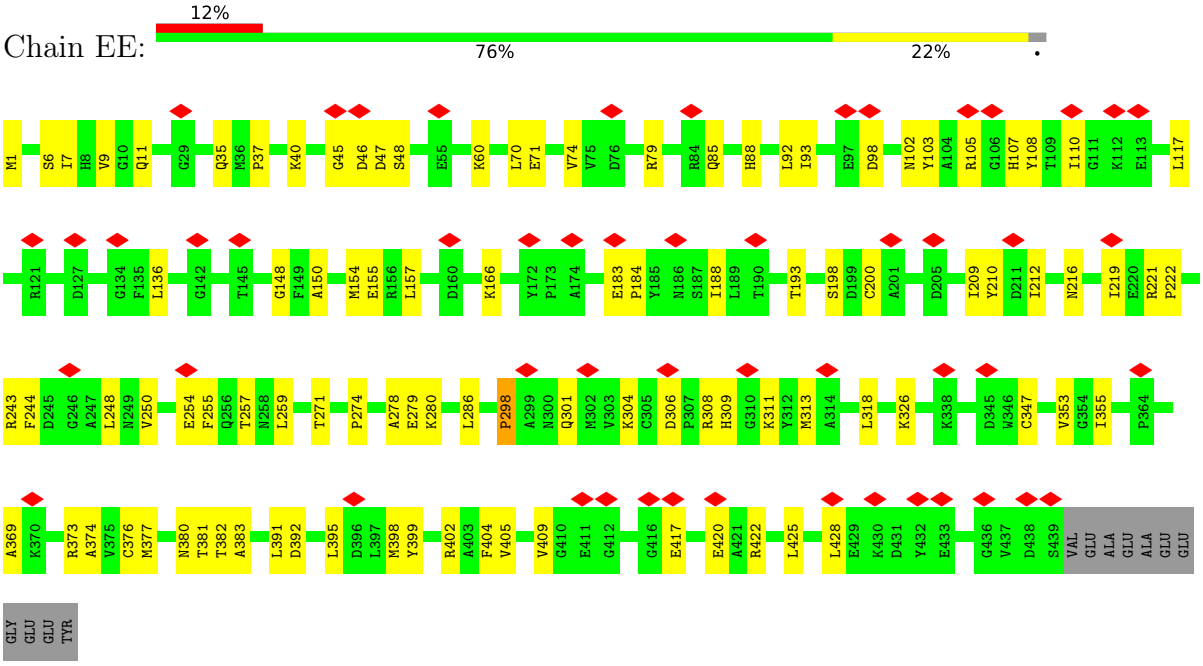
• Molecule 8: Tubulin alpha-3 chain

Chain EC:



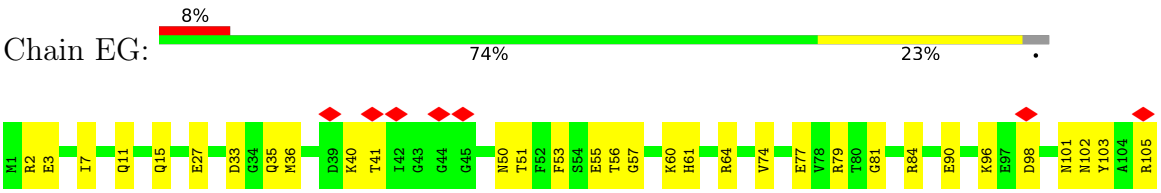
• Molecule 8: Tubulin alpha-3 chain

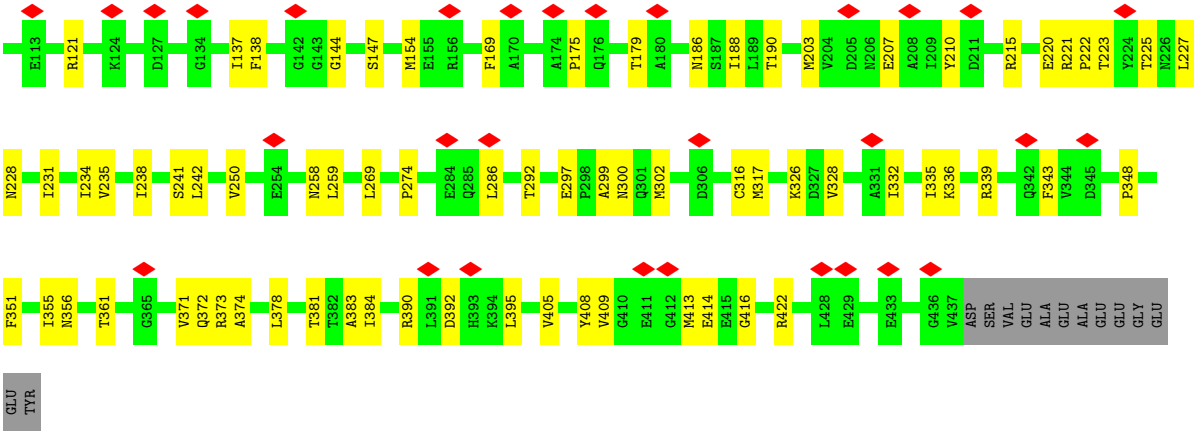
Chain EE:



• Molecule 8: Tubulin alpha-3 chain

Chain EG:

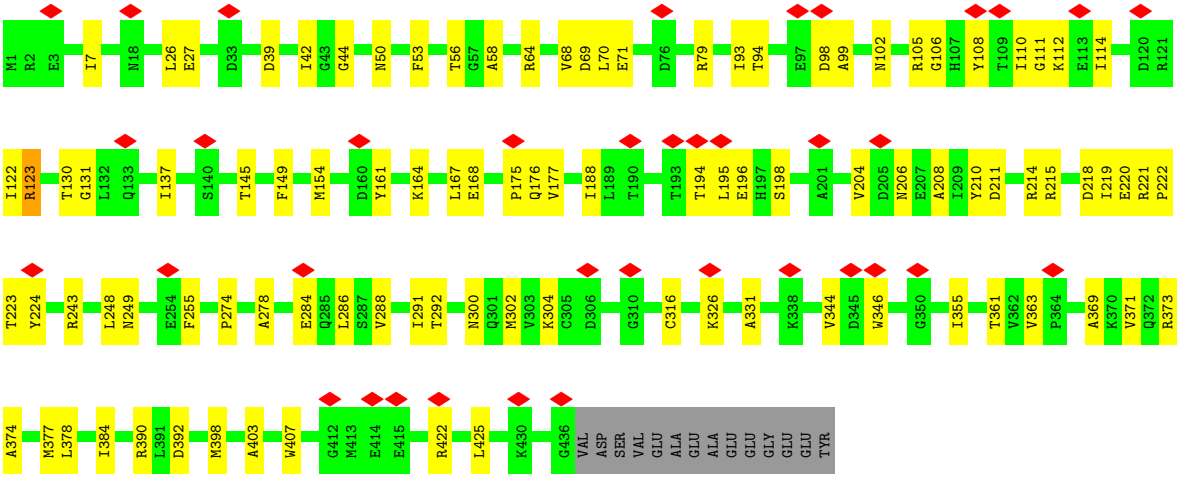




• Molecule 8: Tubulin alpha-3 chain

Chain EI:

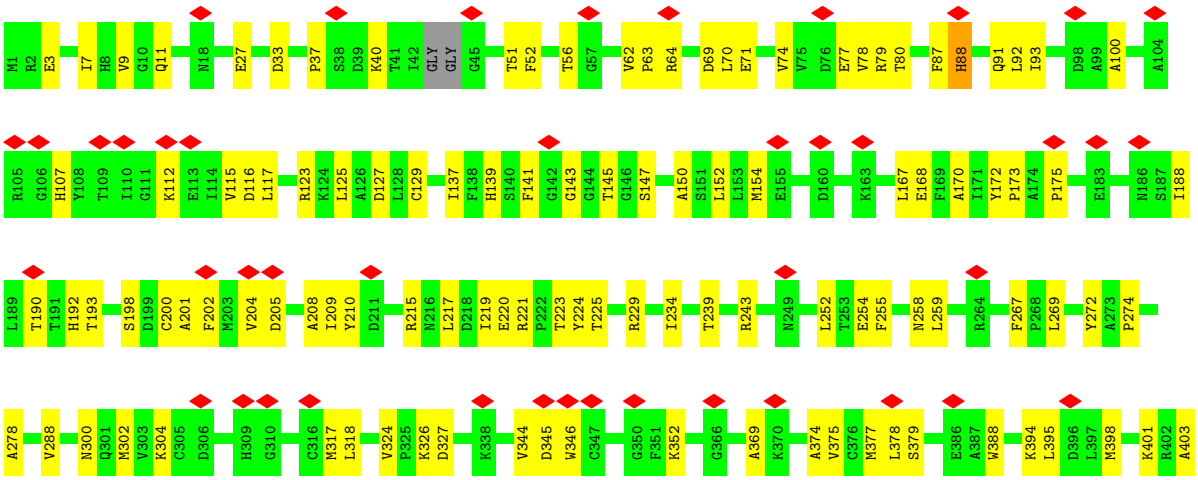


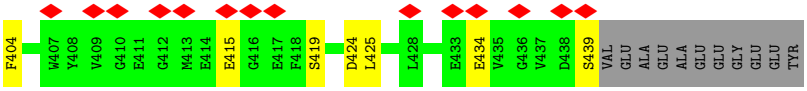


• Molecule 8: Tubulin alpha-3 chain

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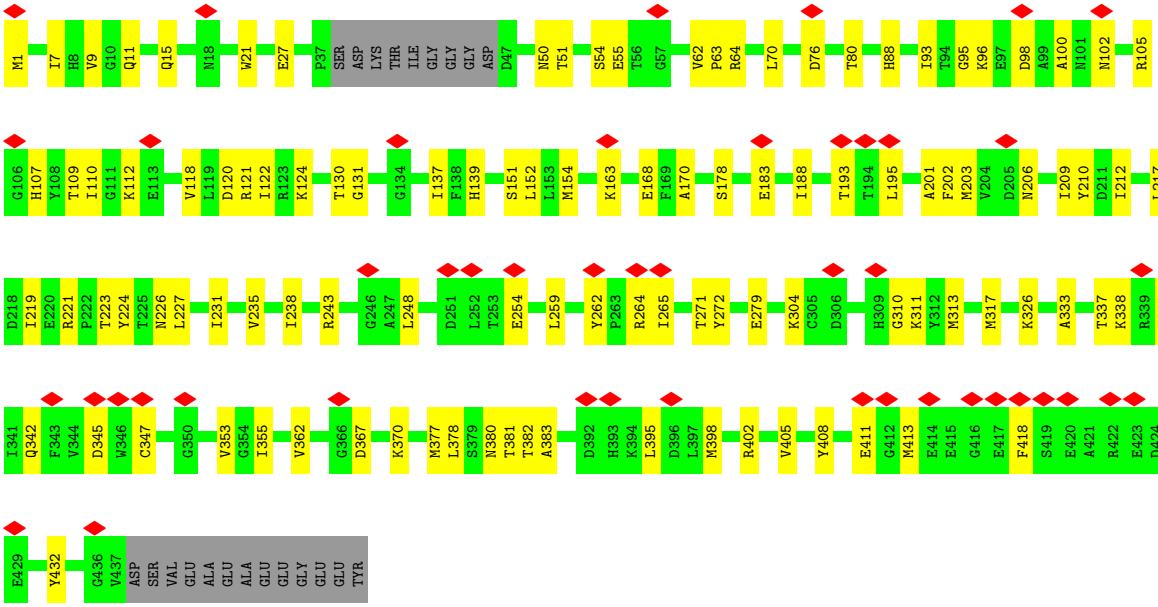




• Molecule 8: Tubulin alpha-3 chain

Chain EM:

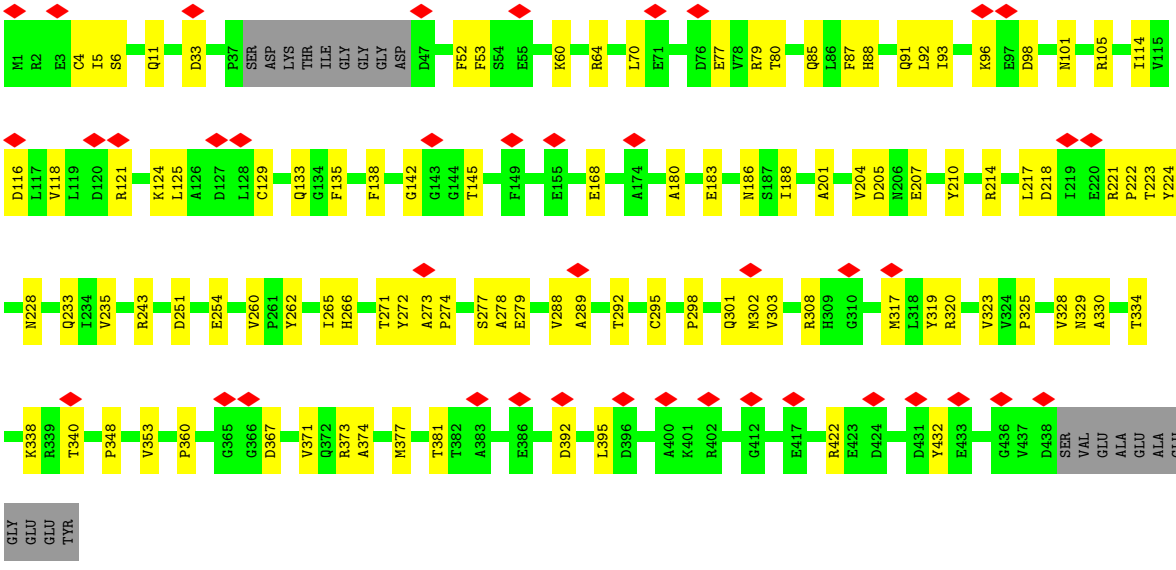




• Molecule 8: Tubulin alpha-3 chain

Chain FC:

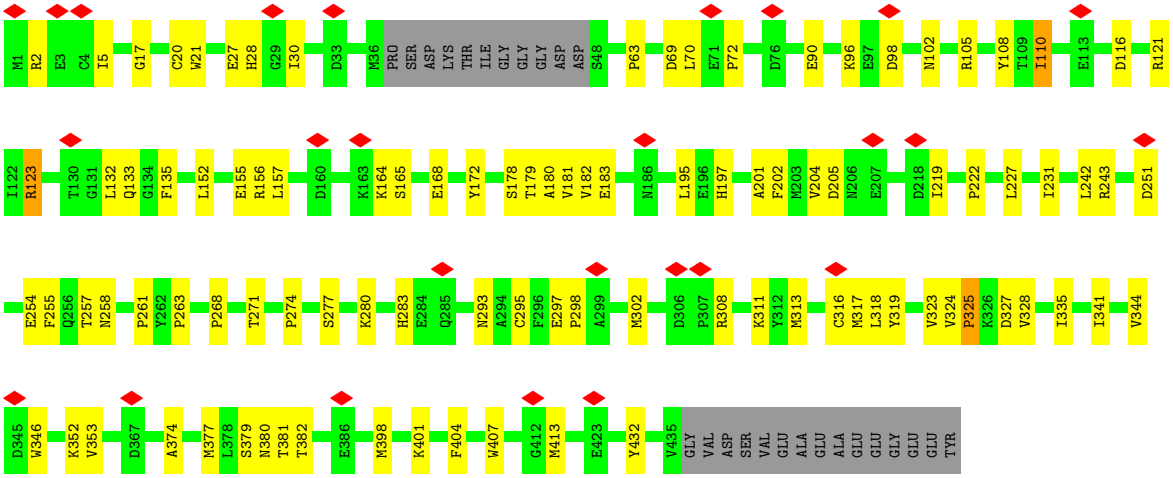




• Molecule 8: Tubulin alpha-3 chain

Chain FE:

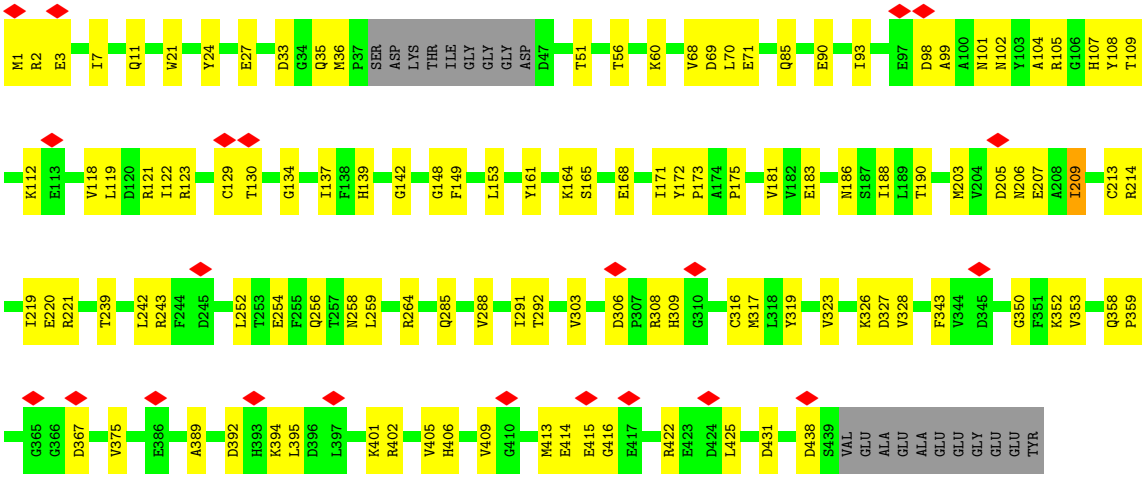




• Molecule 8: Tubulin alpha-3 chain

Chain FG:

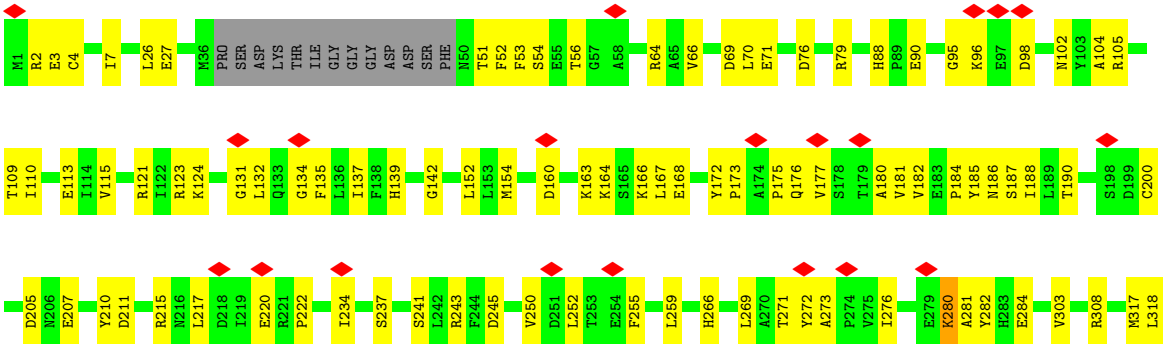


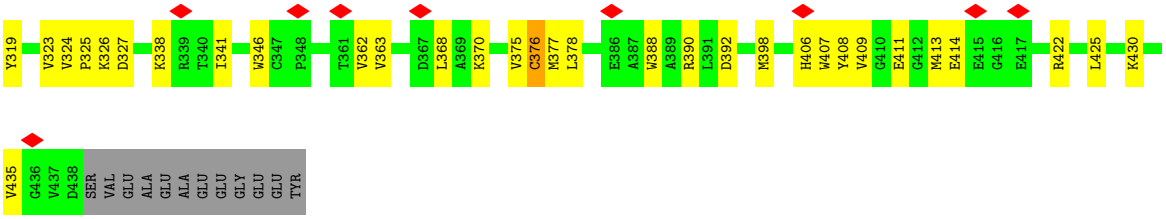


• Molecule 8: Tubulin alpha-3 chain

Chain FI:



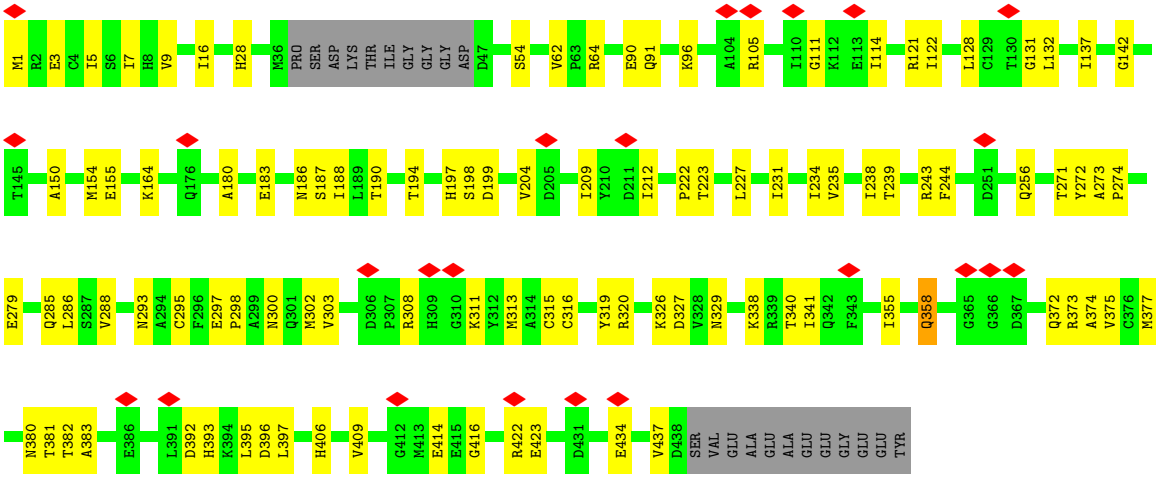




• Molecule 8: Tubulin alpha-3 chain

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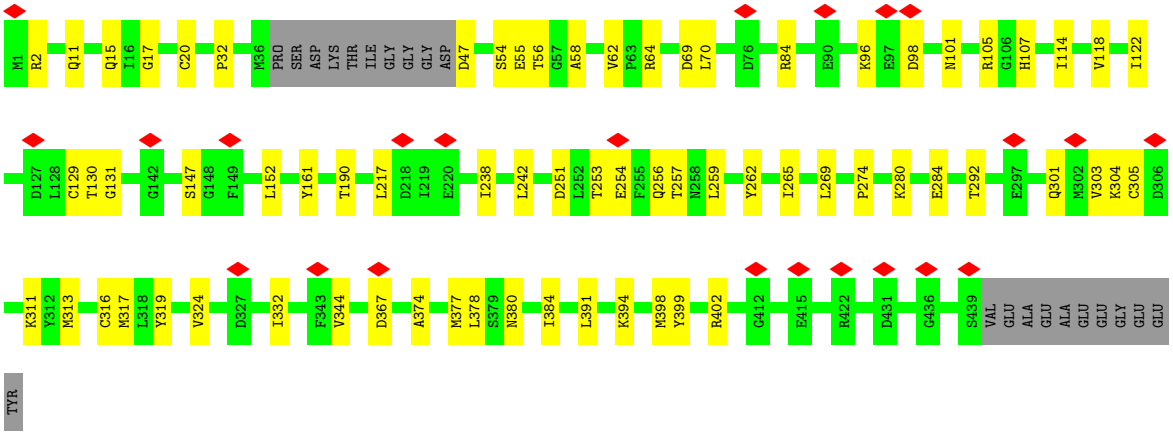




• Molecule 8: Tubulin alpha-3 chain

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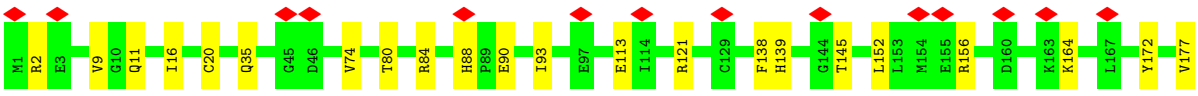


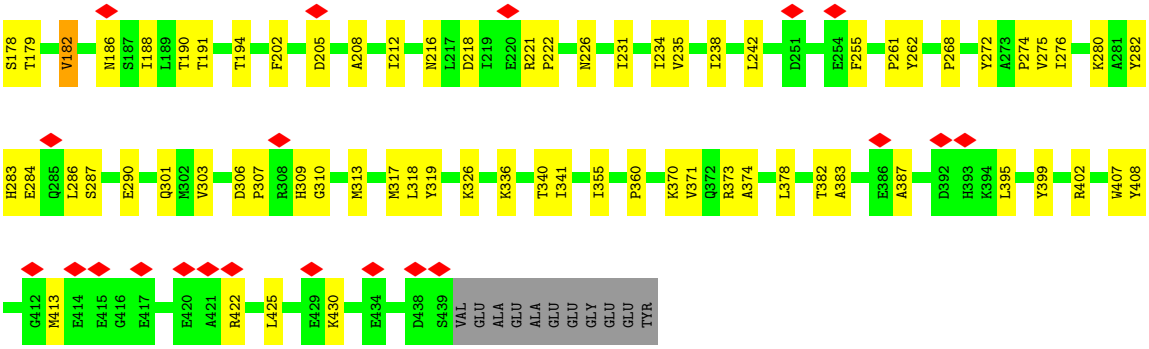


• Molecule 8: Tubulin alpha-3 chain

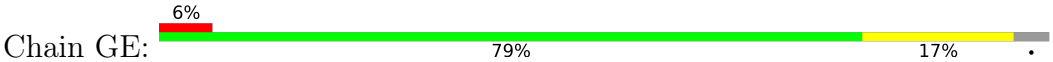
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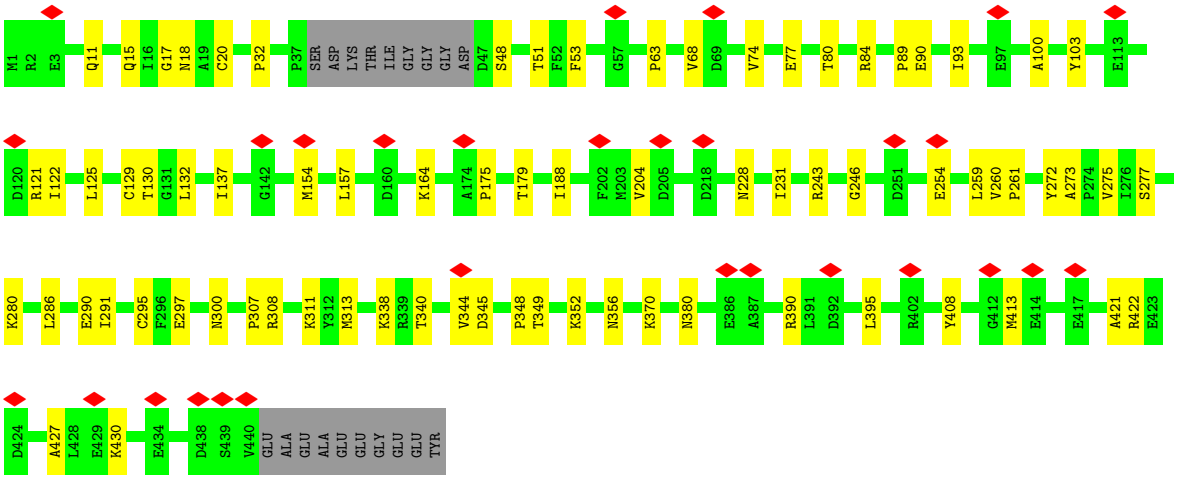




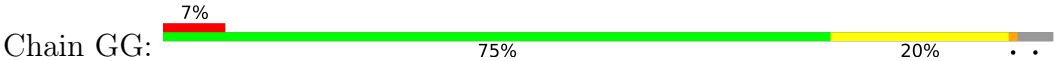


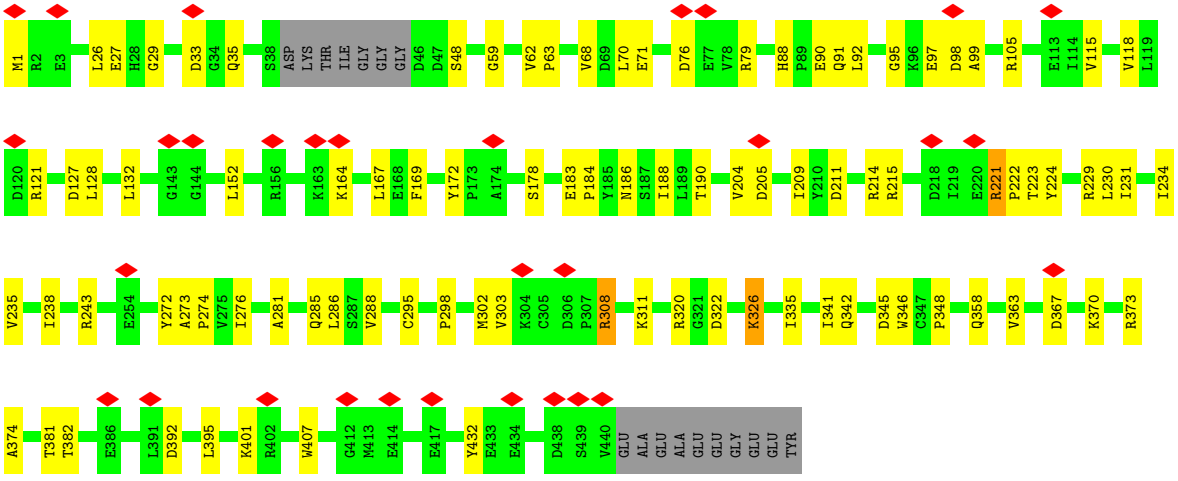
• Molecule 8: Tubulin alpha-3 chain





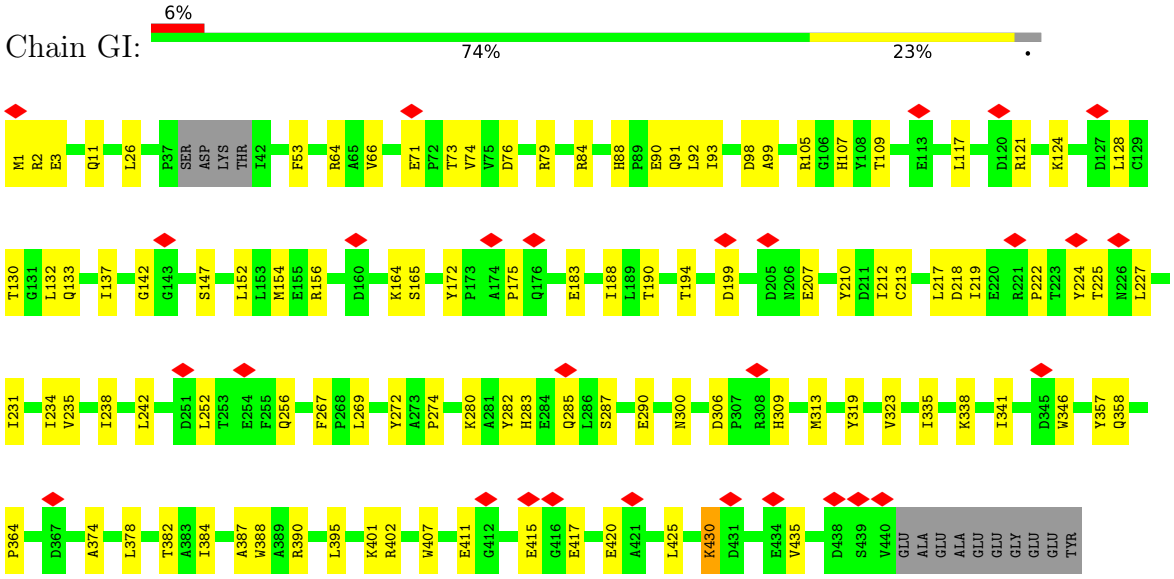
• Molecule 8: Tubulin alpha-3 chain





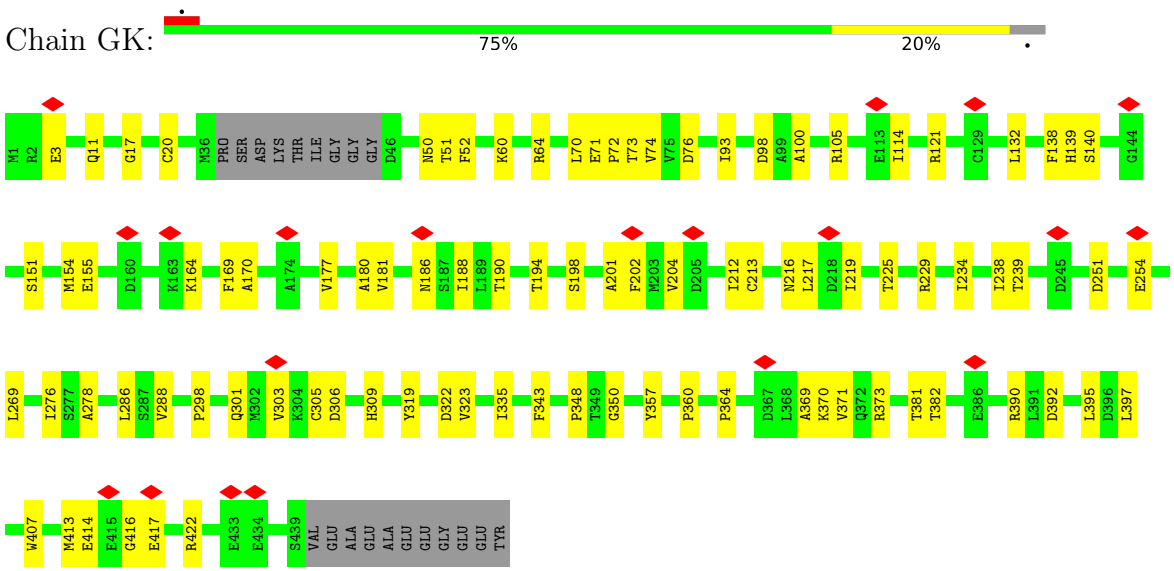
• Molecule 8: Tubulin alpha-3 chain

Chain GI:



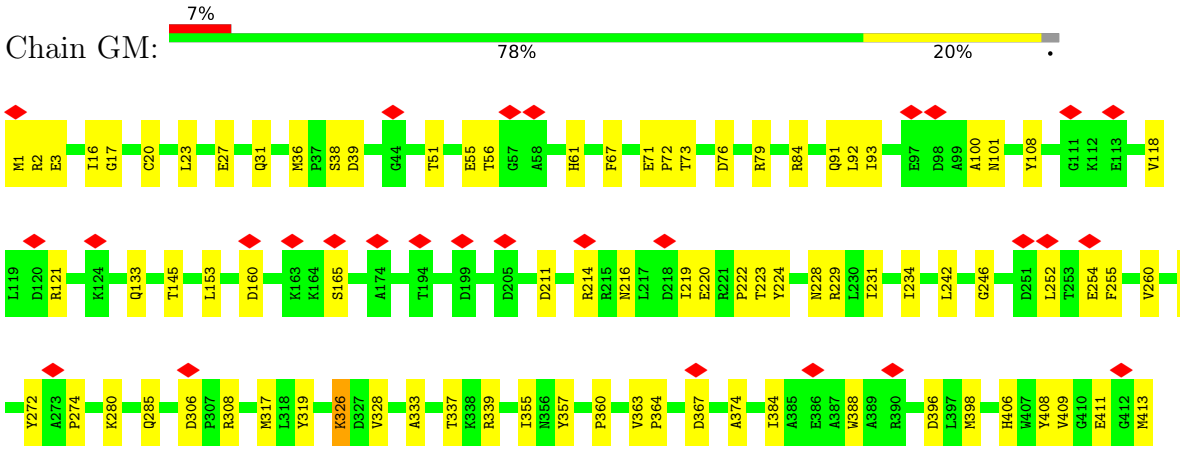
• Molecule 8: Tubulin alpha-3 chain

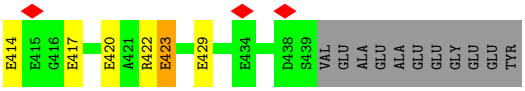
Chain GK:



• Molecule 8: Tubulin alpha-3 chain

Chain GM:

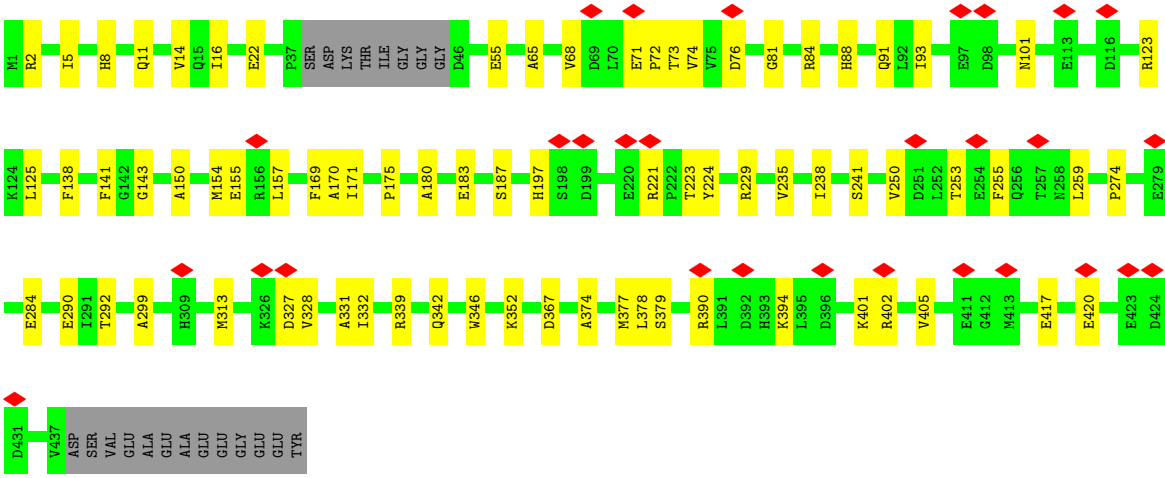




• Molecule 8: Tubulin alpha-3 chain

Chain HC:

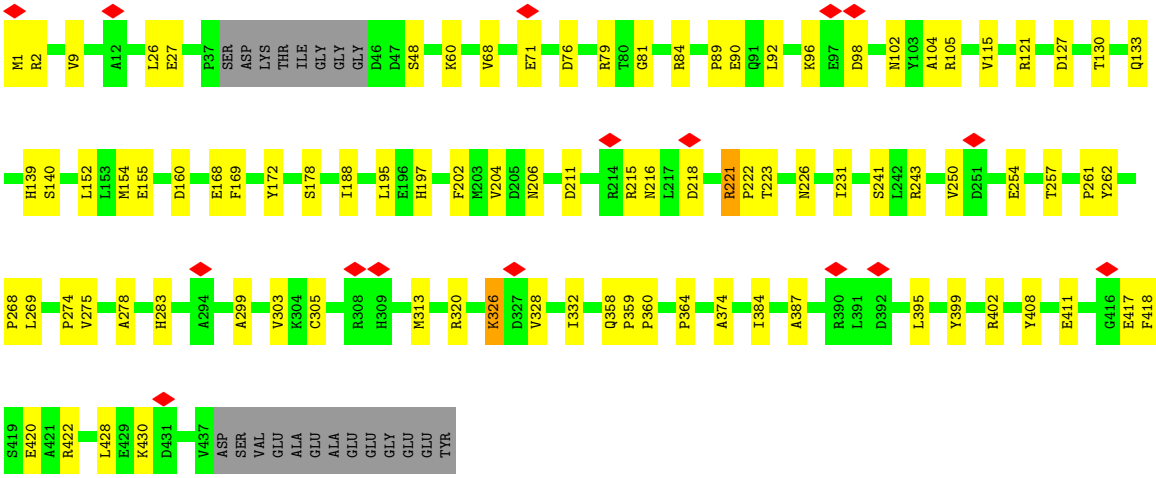




• Molecule 8: Tubulin alpha-3 chain

Chain HE:

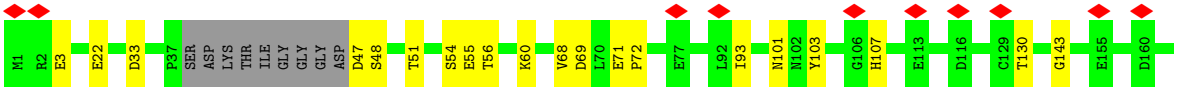


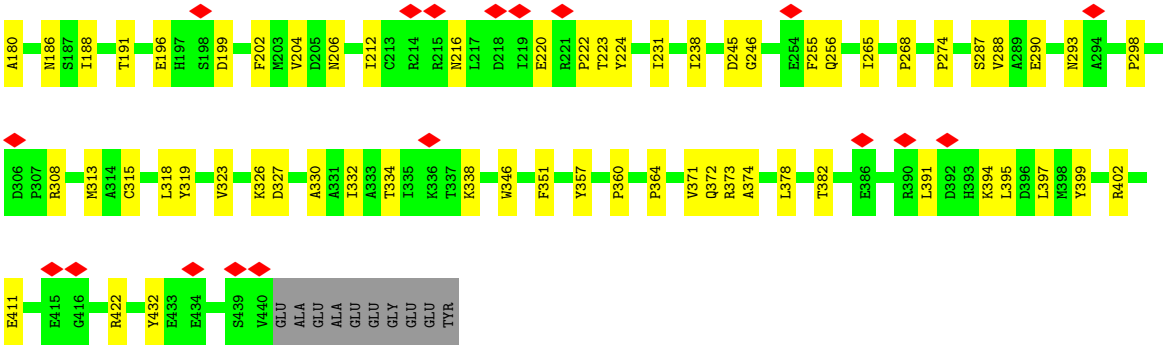


• Molecule 8: Tubulin alpha-3 chain

Chain HG:



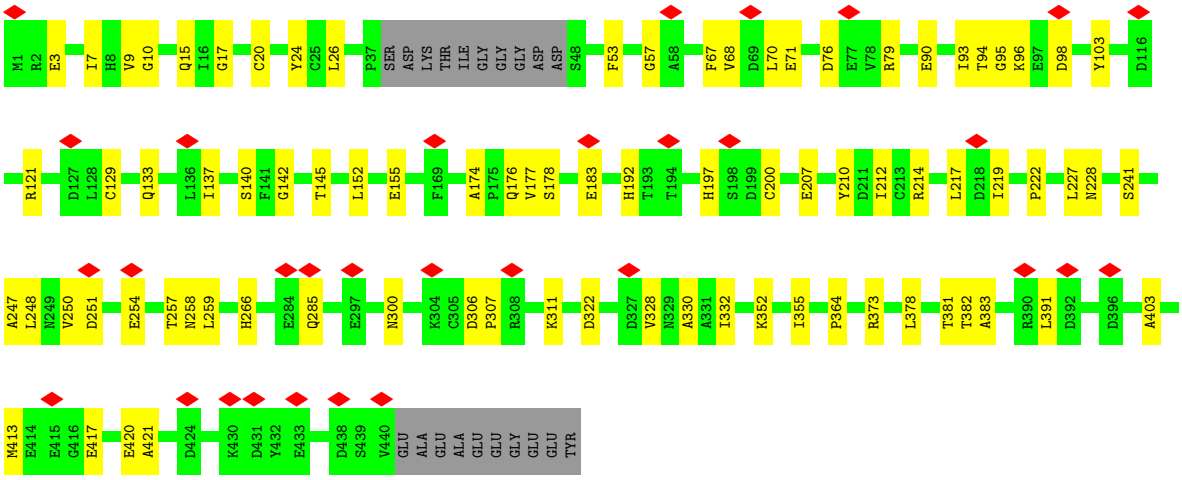




• Molecule 8: Tubulin alpha-3 chain

Chain HI:

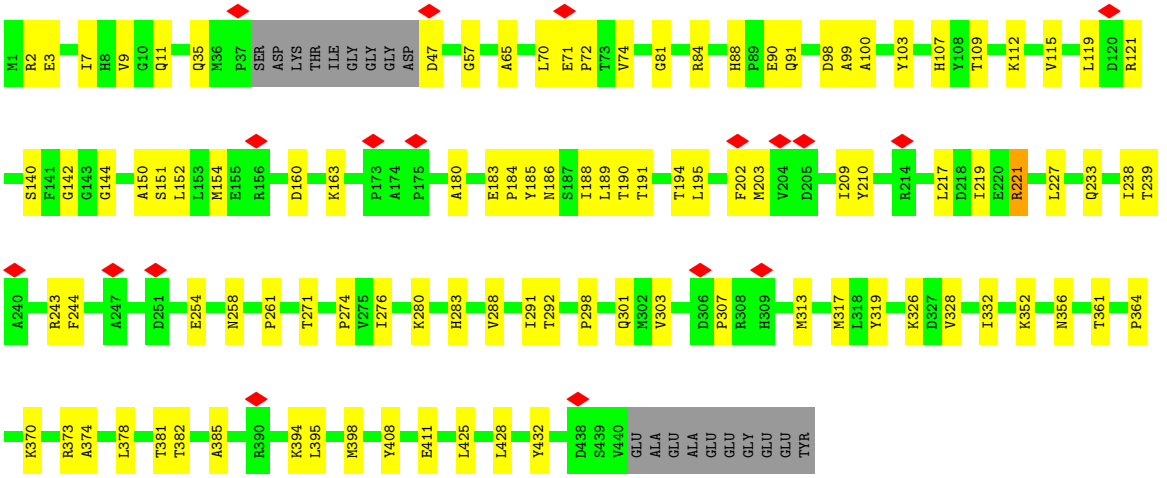




• Molecule 8: Tubulin alpha-3 chain

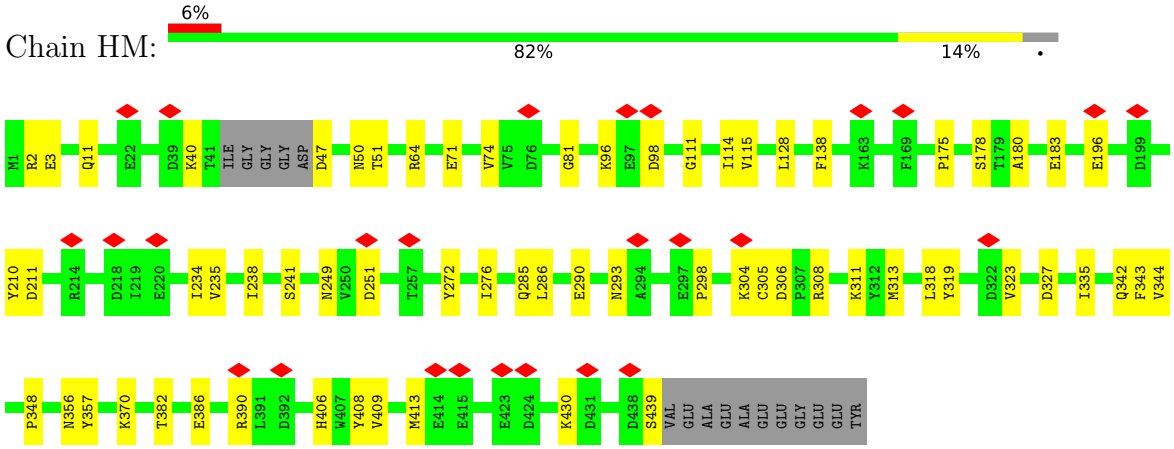
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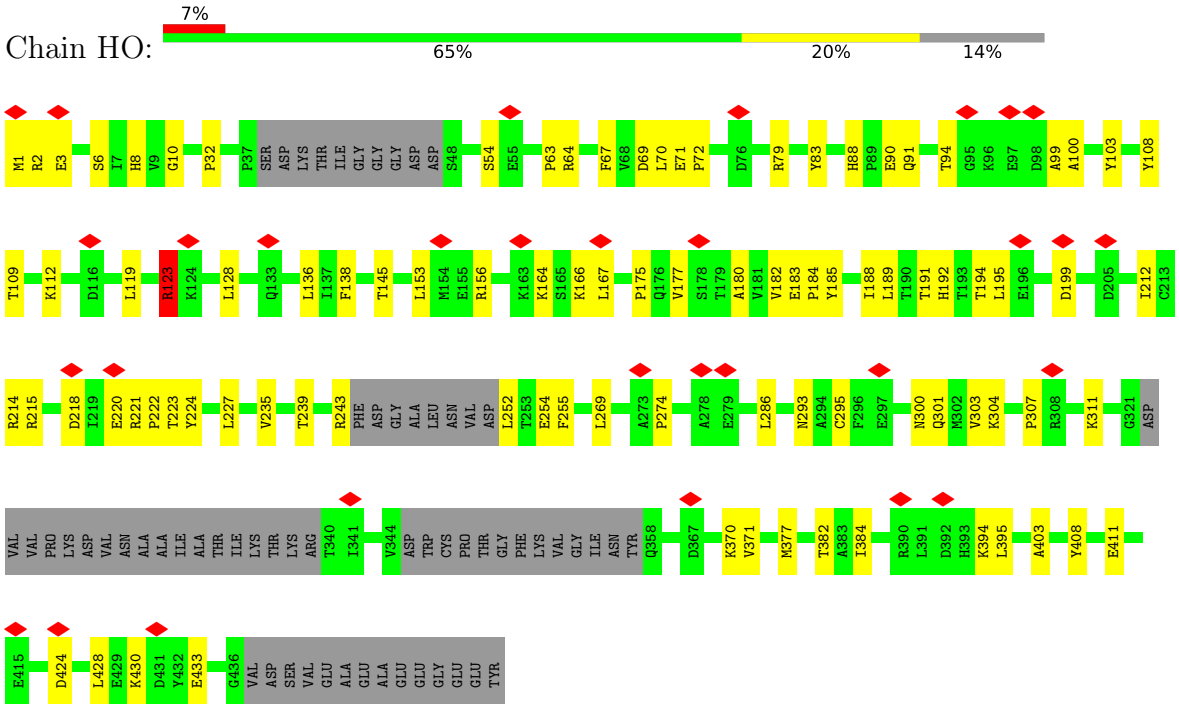
• Molecule 8: Tubulin alpha-3 chain

Chain HM:



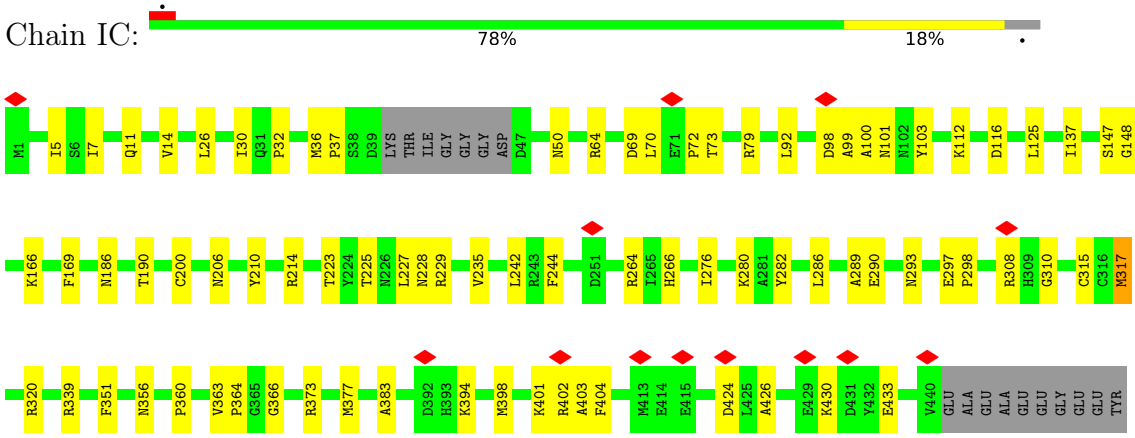
• Molecule 8: Tubulin alpha-3 chain

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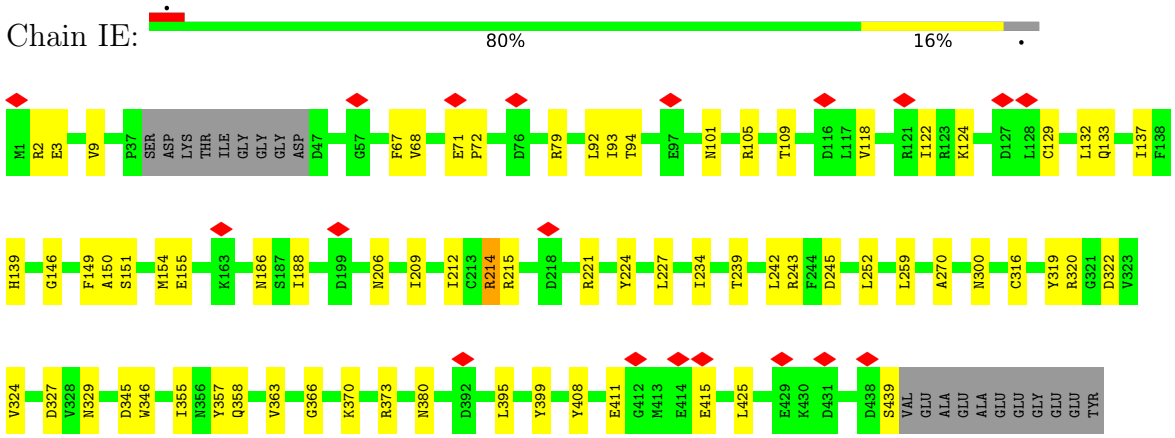
• Molecule 8: Tubulin alpha-3 chain

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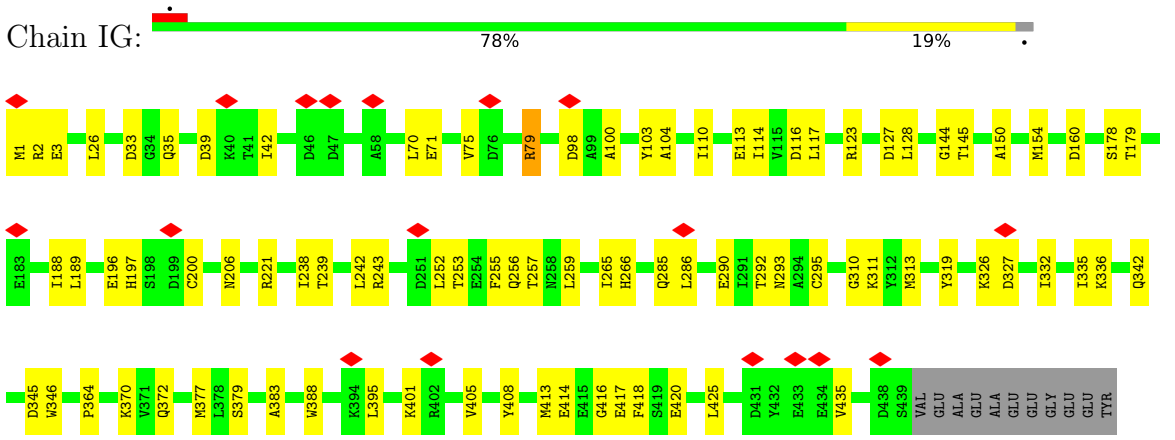
• Molecule 8: Tubulin alpha-3 chain

Chain IE:



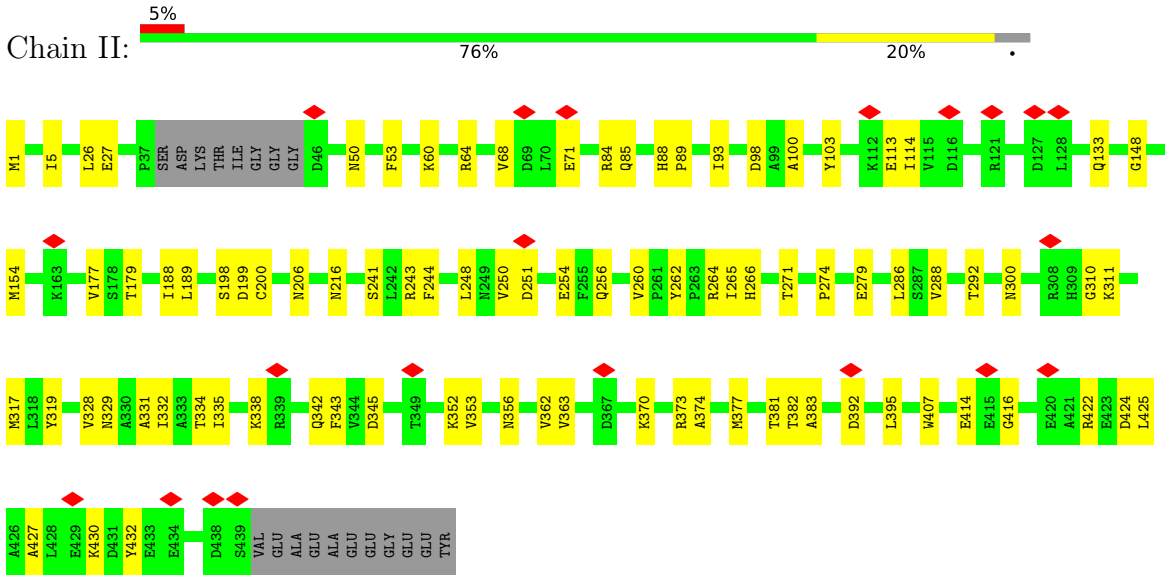
• Molecule 8: Tubulin alpha-3 chain

Chain IG:



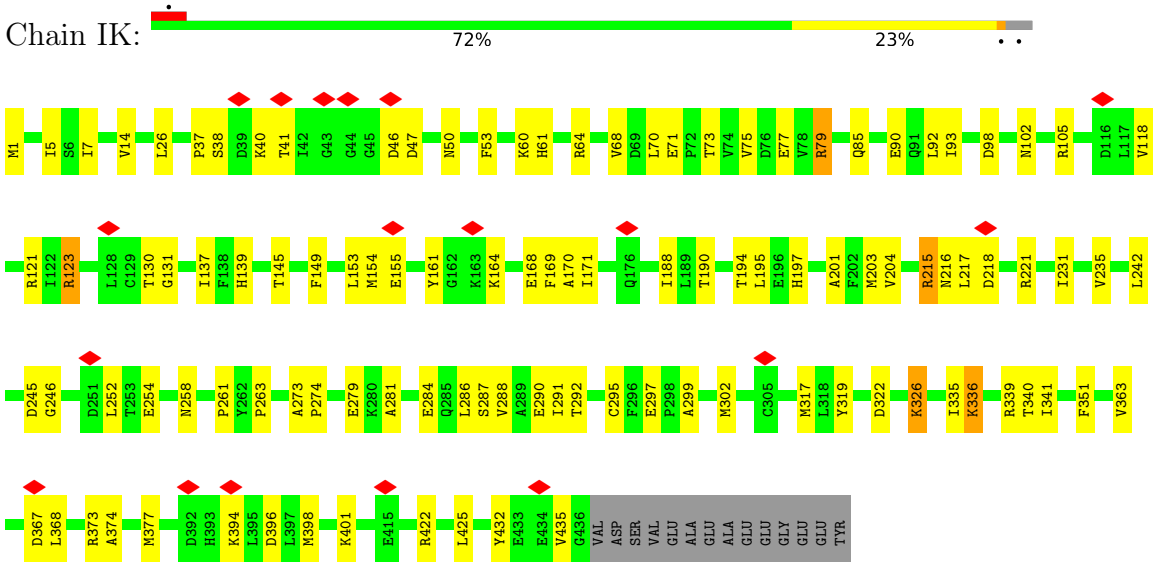
• Molecule 8: Tubulin alpha-3 chain

Chain II:



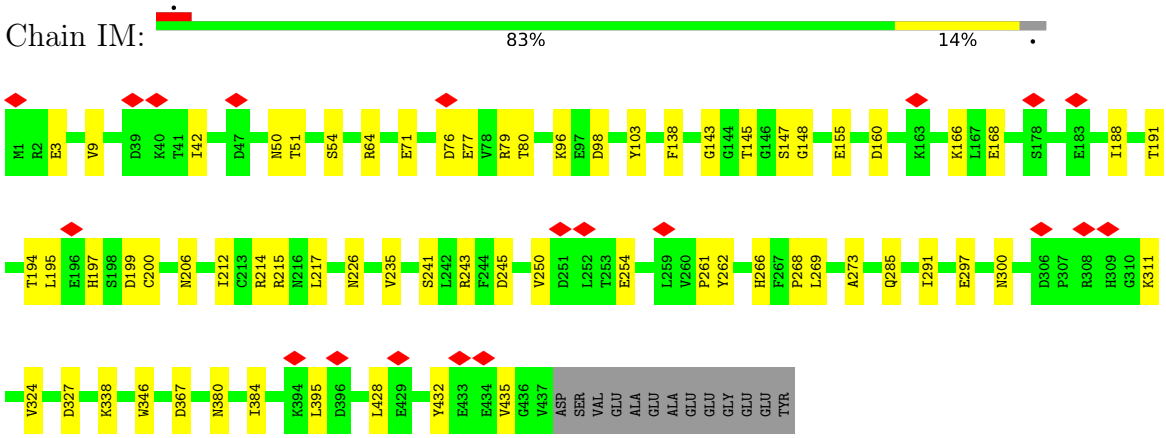
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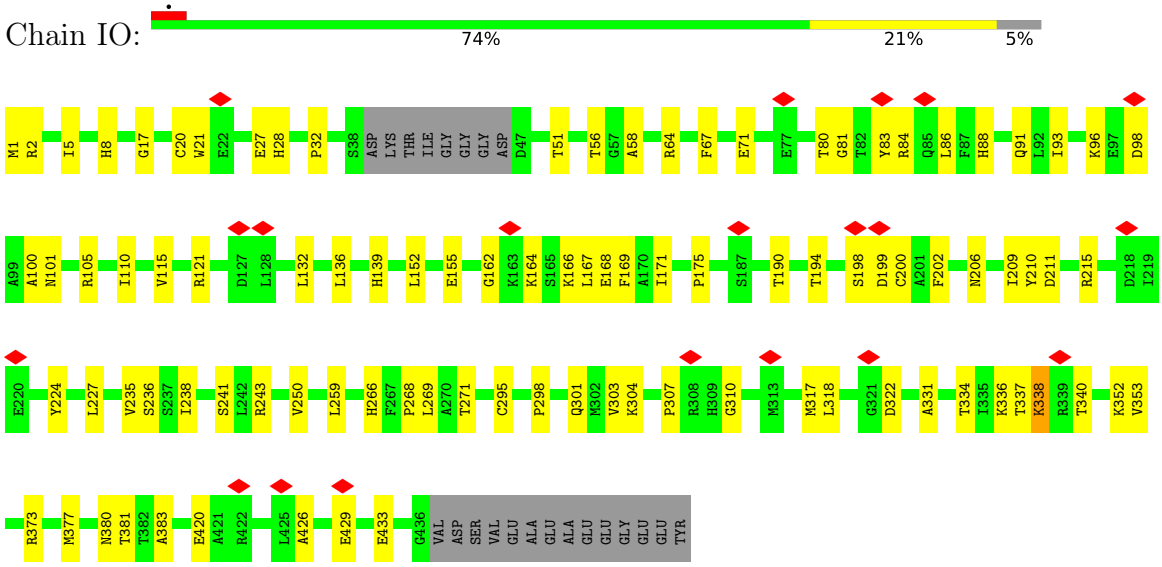
• Molecule 8: Tubulin alpha-3 chain

Chain IM:



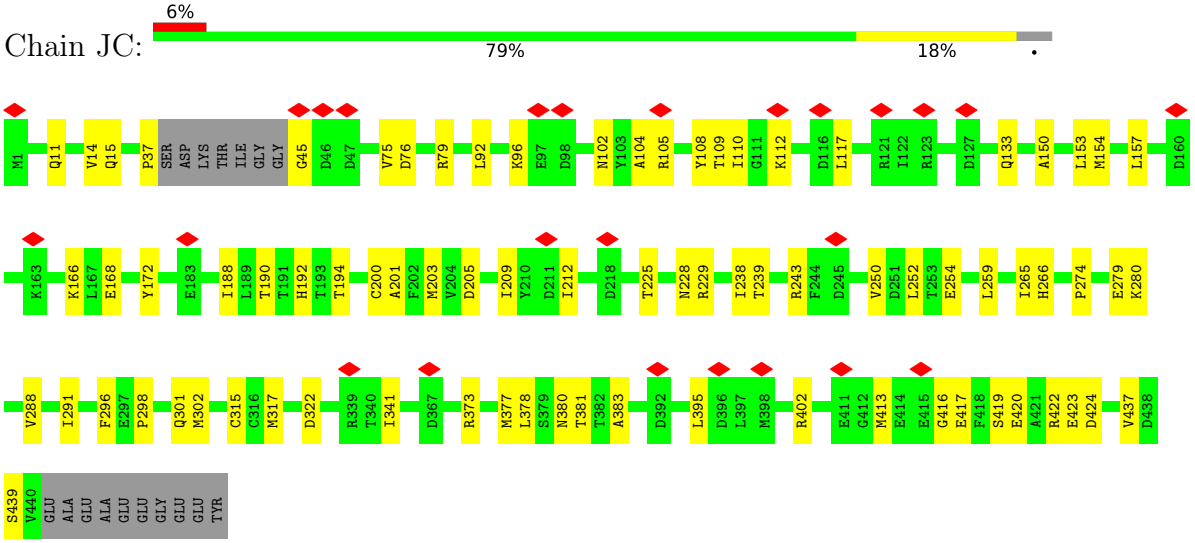
• Molecule 8: Tubulin alpha-3 chain

Chain IO:



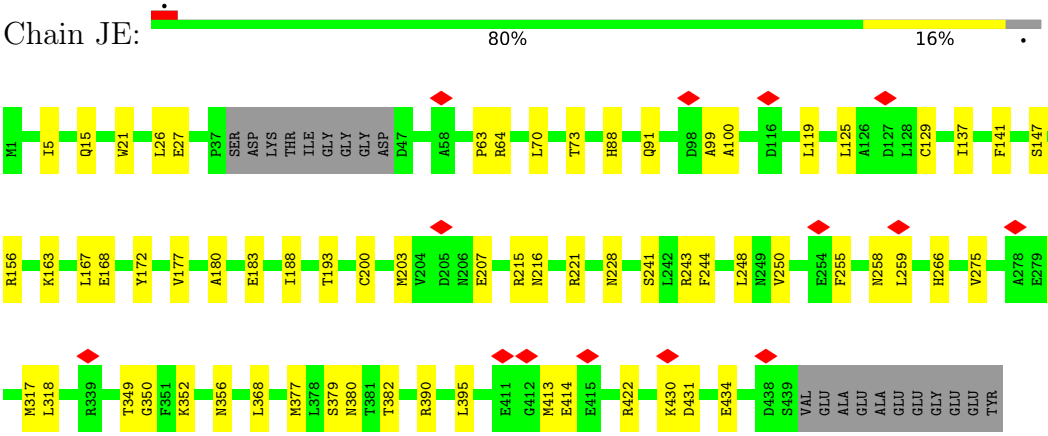
• Molecule 8: Tubulin alpha-3 chain

Chain JC:



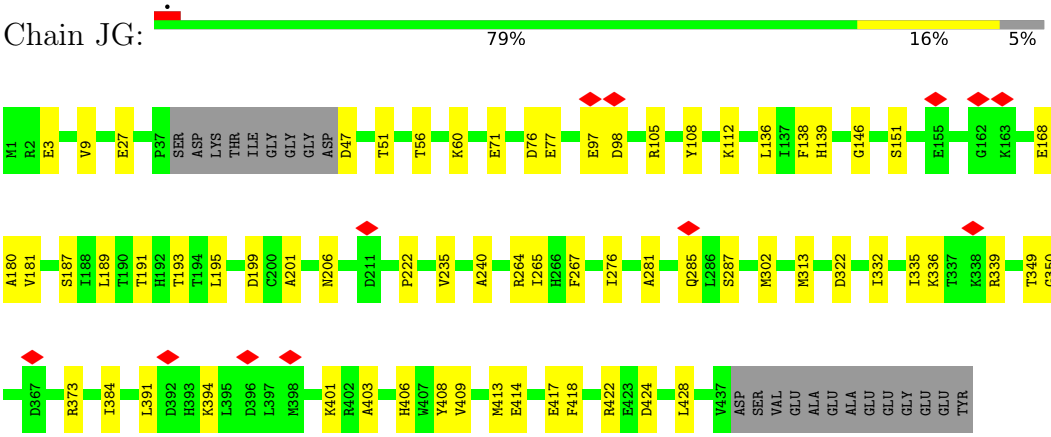
• Molecule 8: Tubulin alpha-3 chain

Chain JE:



• Molecule 8: Tubulin alpha-3 chain

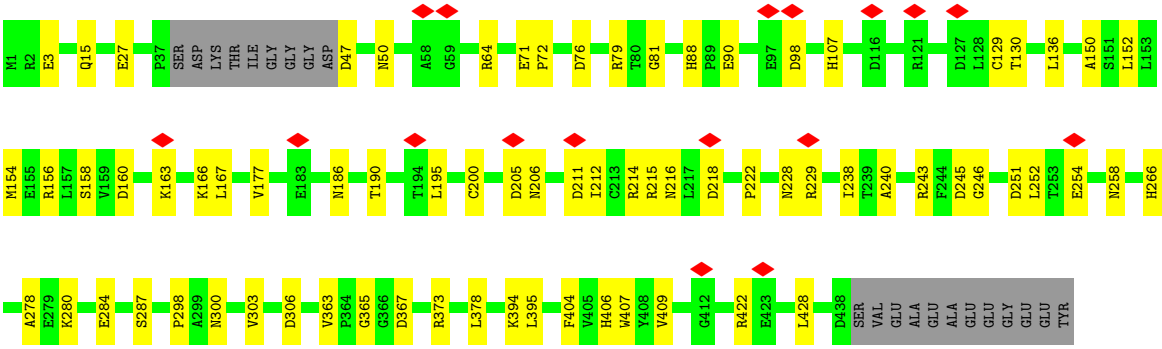
Chain JG:



• Molecule 8: Tubulin alpha-3 chain

Chain JI:

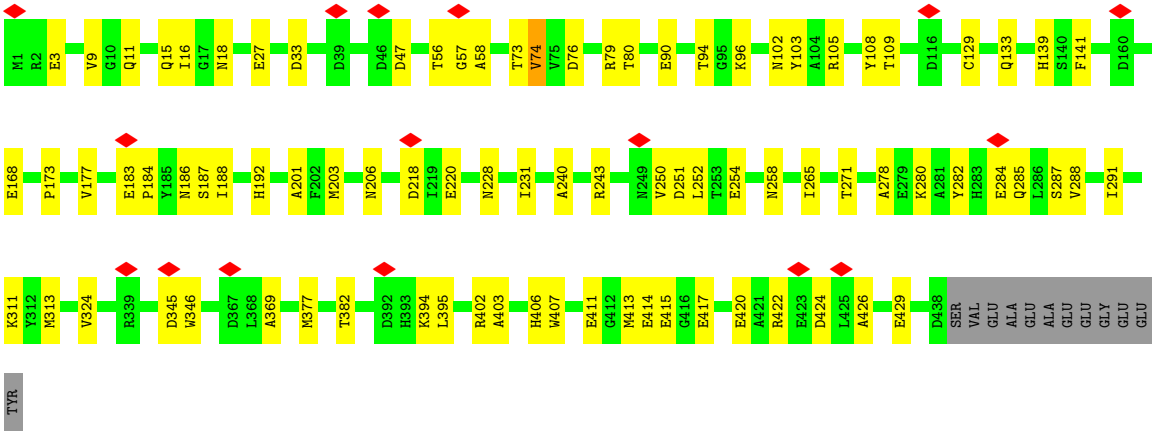




• Molecule 8: Tubulin alpha-3 chain

Chain JK:

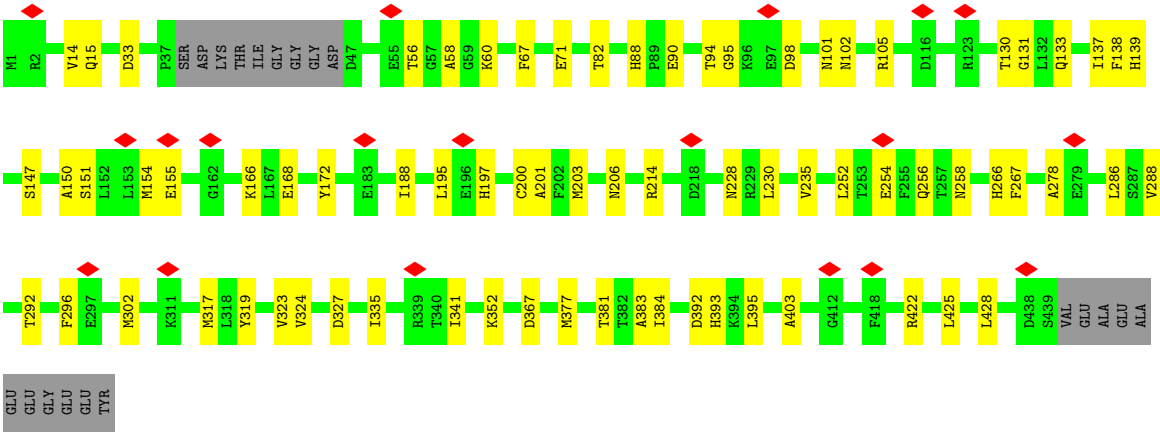




• Molecule 8: Tubulin alpha-3 chain

Chain JM:

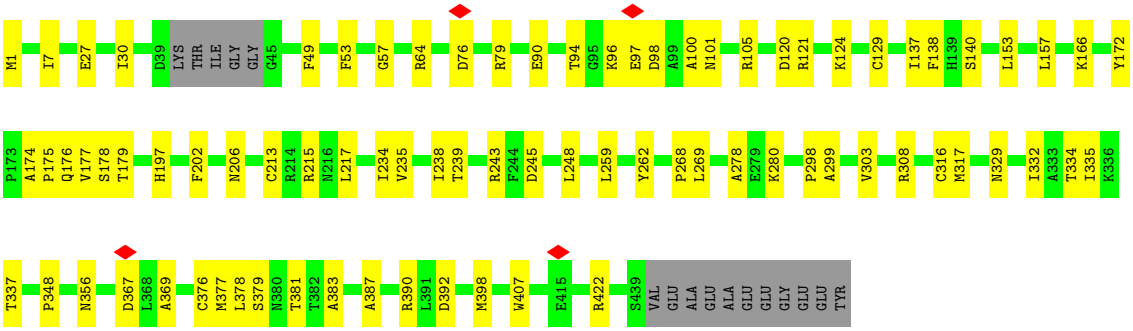




• Molecule 8: Tubulin alpha-3 chain

Chain KC:

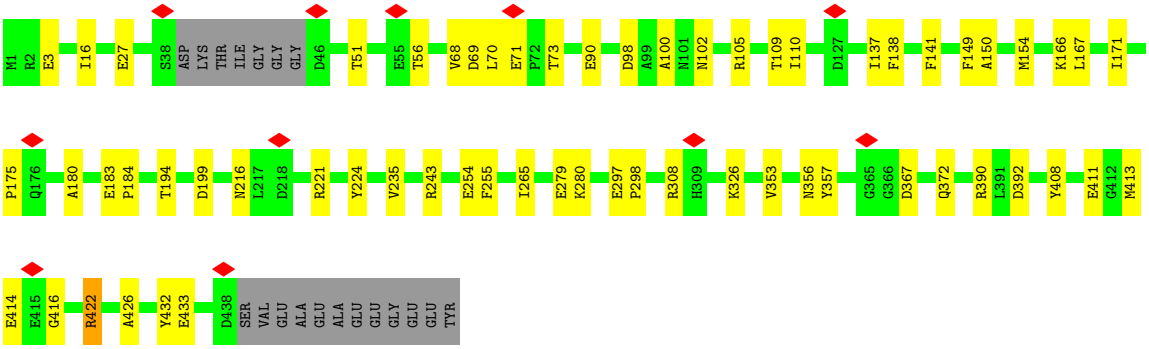




• Molecule 8: Tubulin alpha-3 chain

Chain KE:

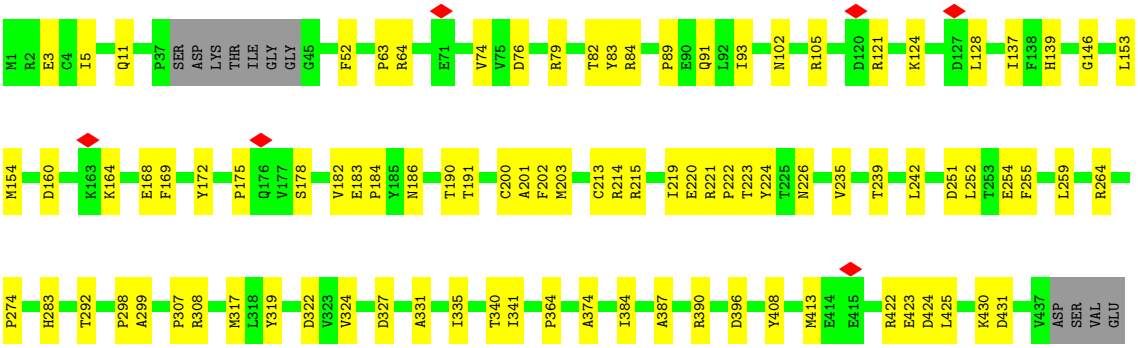




• Molecule 8: Tubulin alpha-3 chain

Chain KG:





• Molecule 8: Tubulin alpha-3 chain

Chain KI:



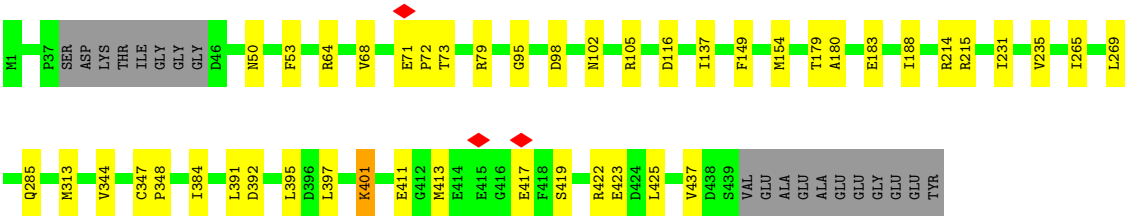




• Molecule 8: Tubulin alpha-3 chain

Chain KK:

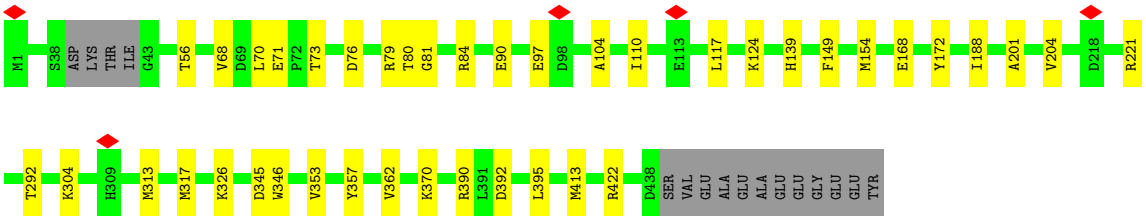




• Molecule 8: Tubulin alpha-3 chain

Chain KM:

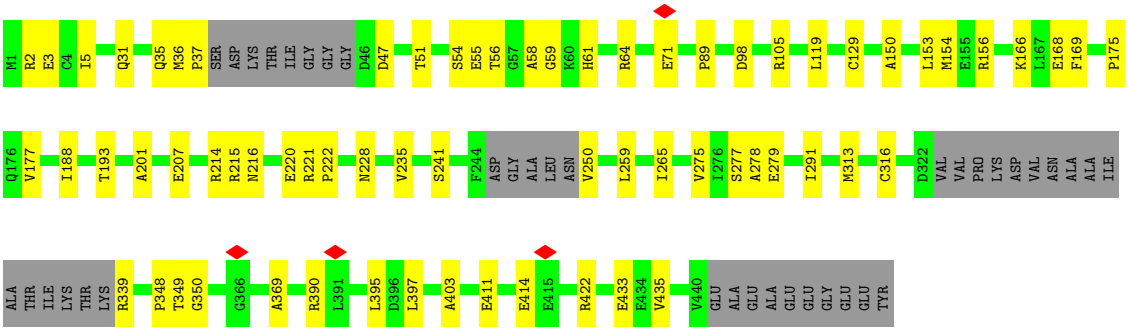




• Molecule 8: Tubulin alpha-3 chain

Chain KO:

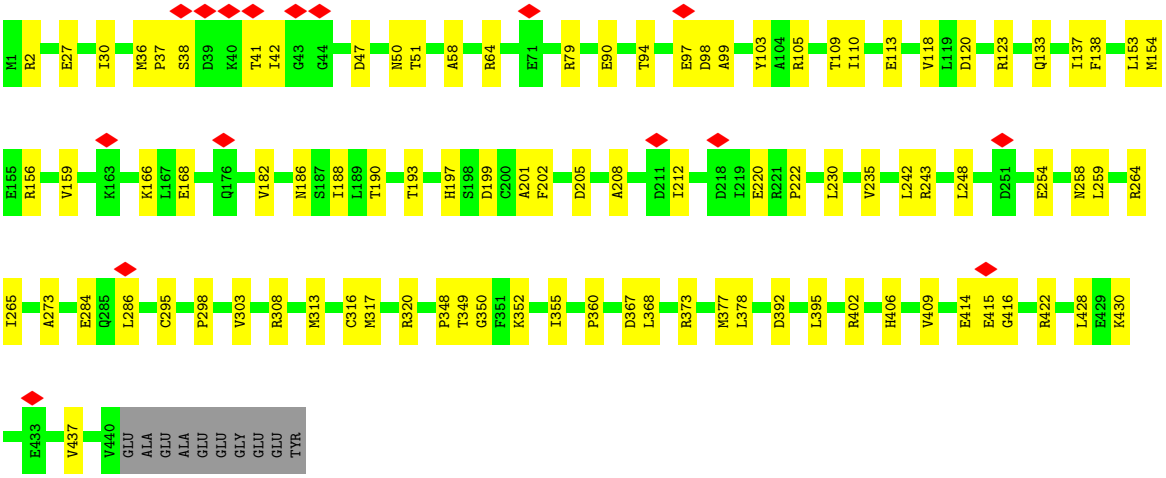




• Molecule 8: Tubulin alpha-3 chain

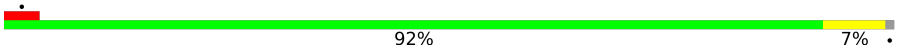
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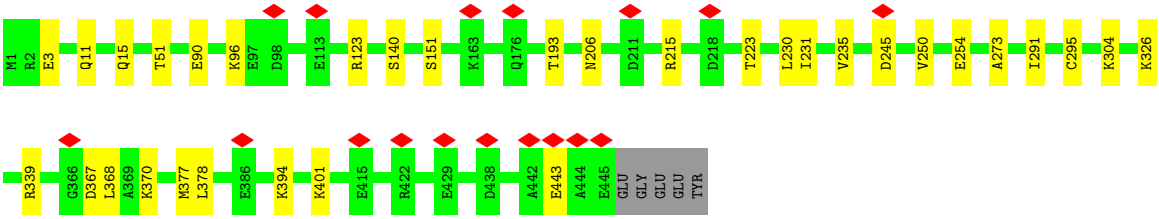




• Molecule 8: Tubulin alpha-3 chain

Chain LE:

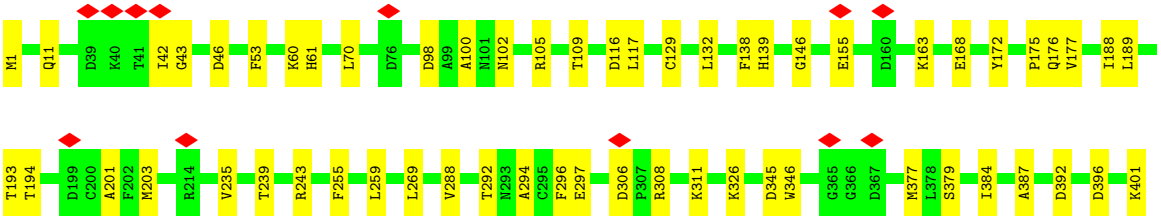




• Molecule 8: Tubulin alpha-3 chain

Chain LG:

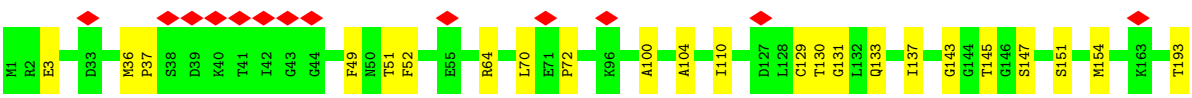


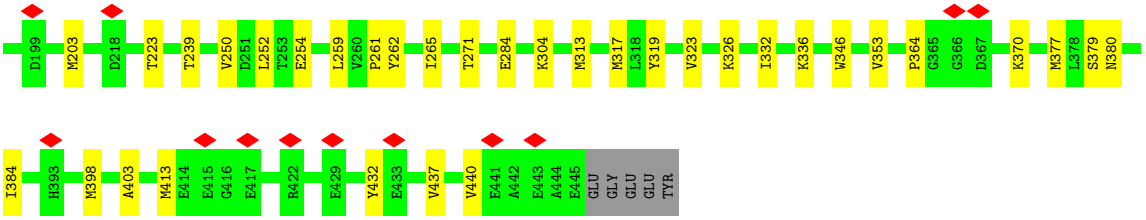


• Molecule 8: Tubulin alpha-3 chain

Chain LI:



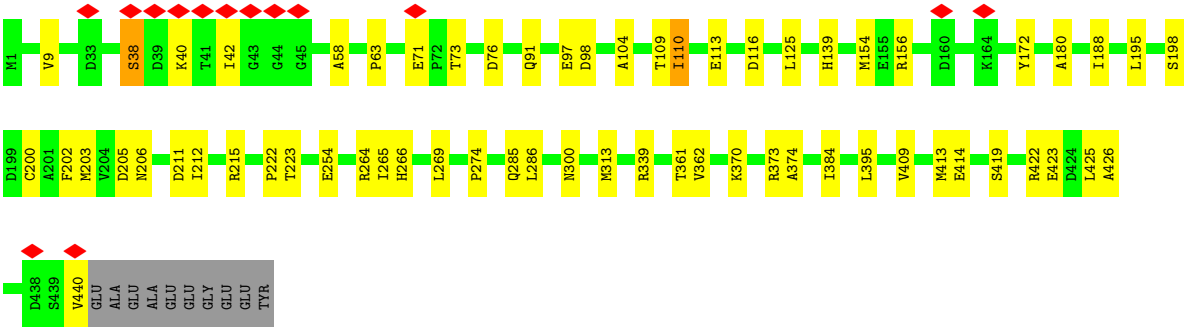




• Molecule 8: Tubulin alpha-3 chain

Chain LK:

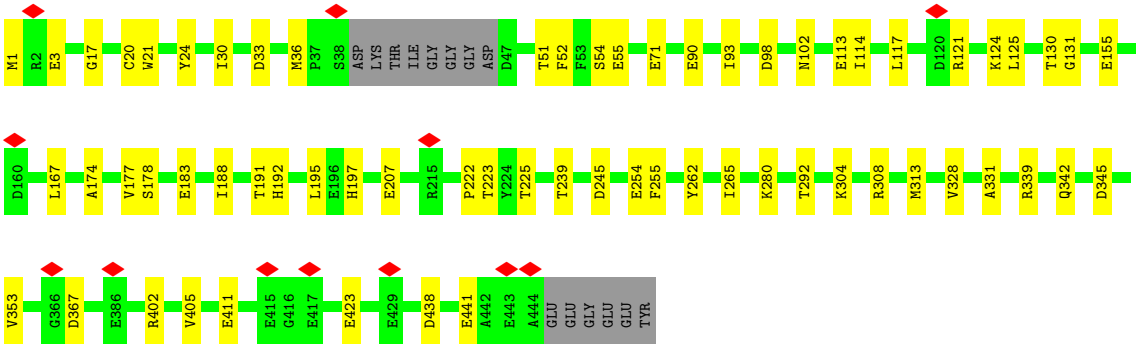




• Molecule 8: Tubulin alpha-3 chain

Chain LM:

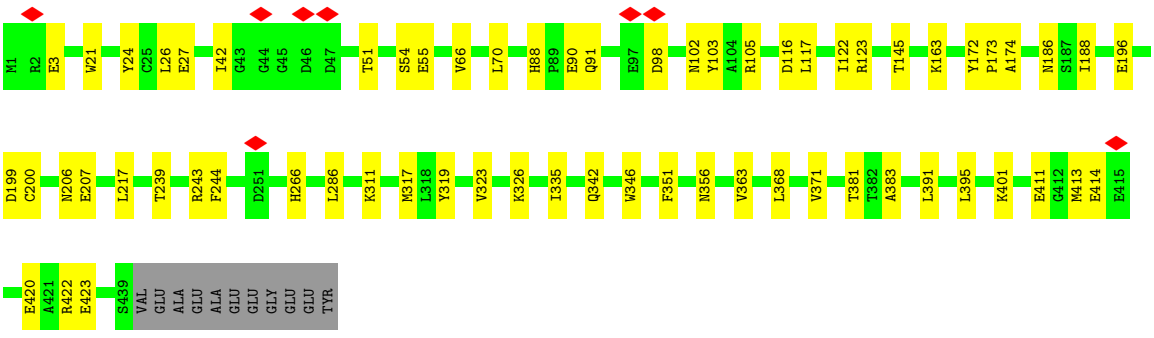




• Molecule 8: Tubulin alpha-3 chain

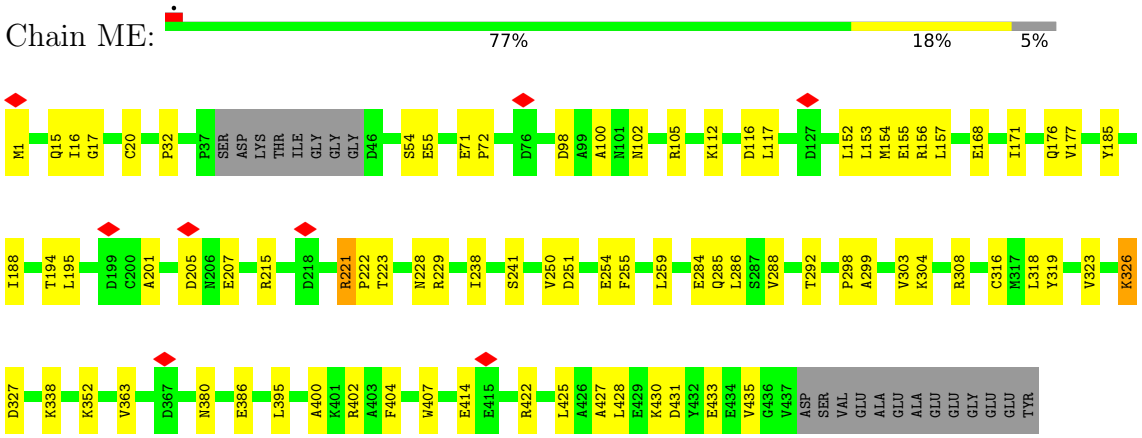
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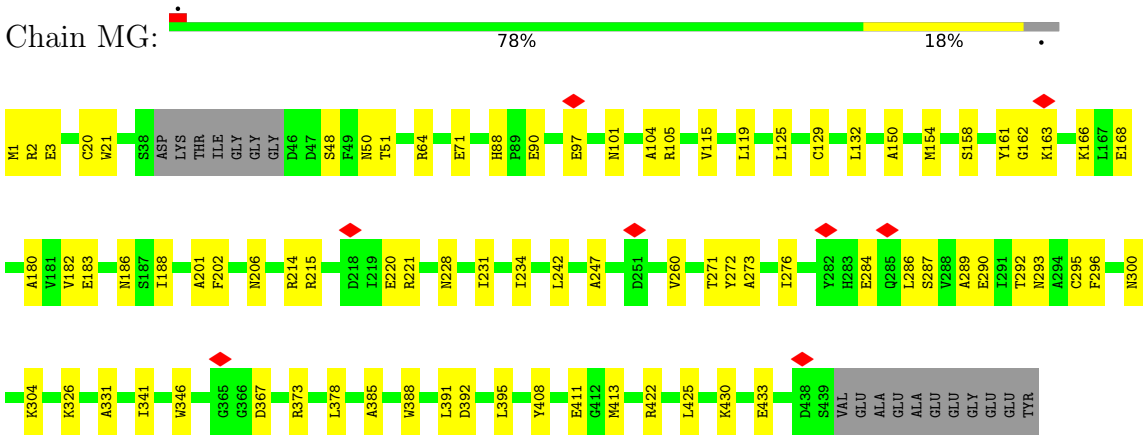
• Molecule 8: Tubulin alpha-3 chain

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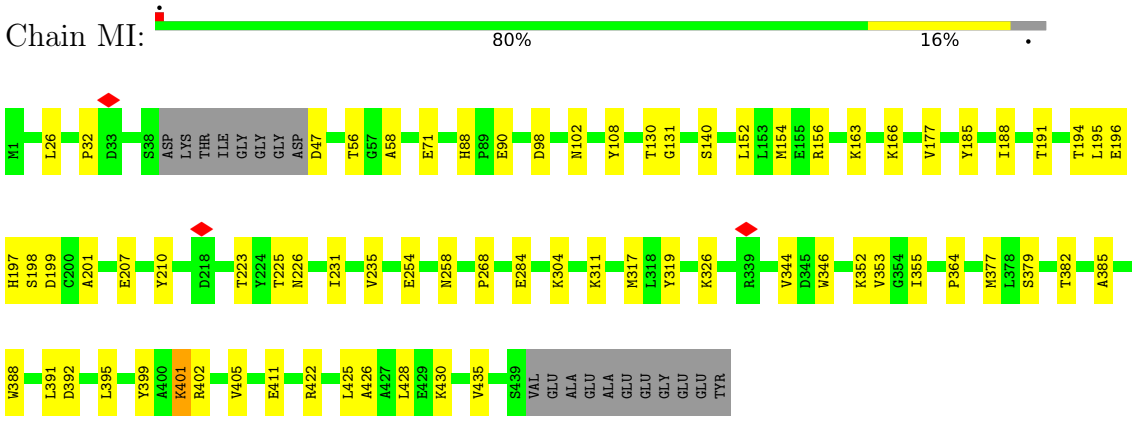
• Molecule 8: Tubulin alpha-3 chain

Chain MG:



• Molecule 8: Tubulin alpha-3 chain

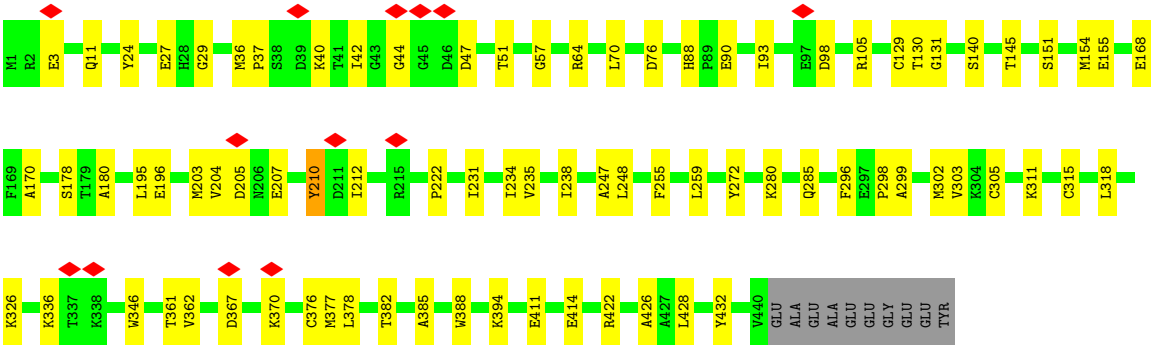
Chain MI:



• Molecule 8: Tubulin alpha-3 chain

Chain MK:

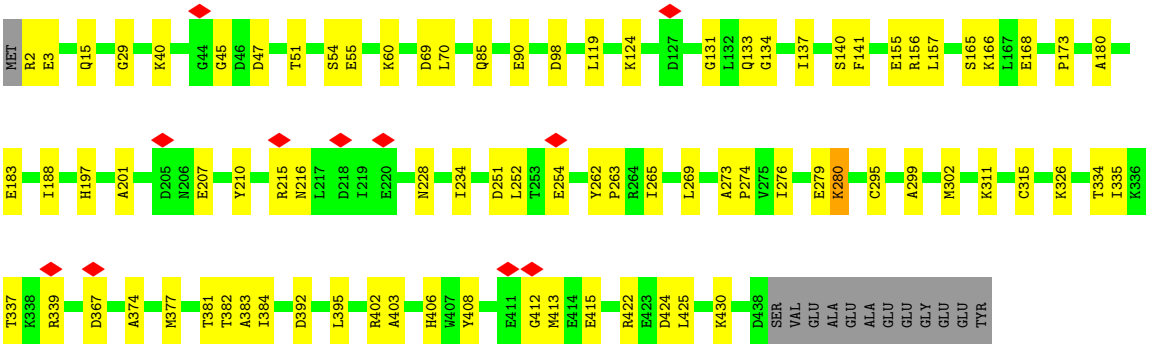




• Molecule 8: Tubulin alpha-3 chain

Chain MM:

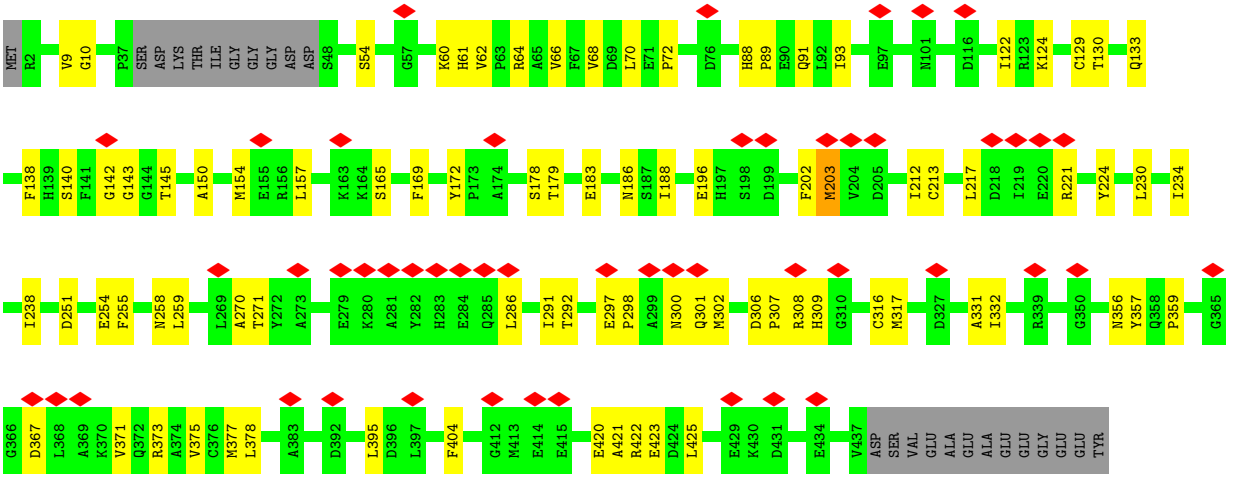




• Molecule 8: Tubulin alpha-3 chain

Chain NA:

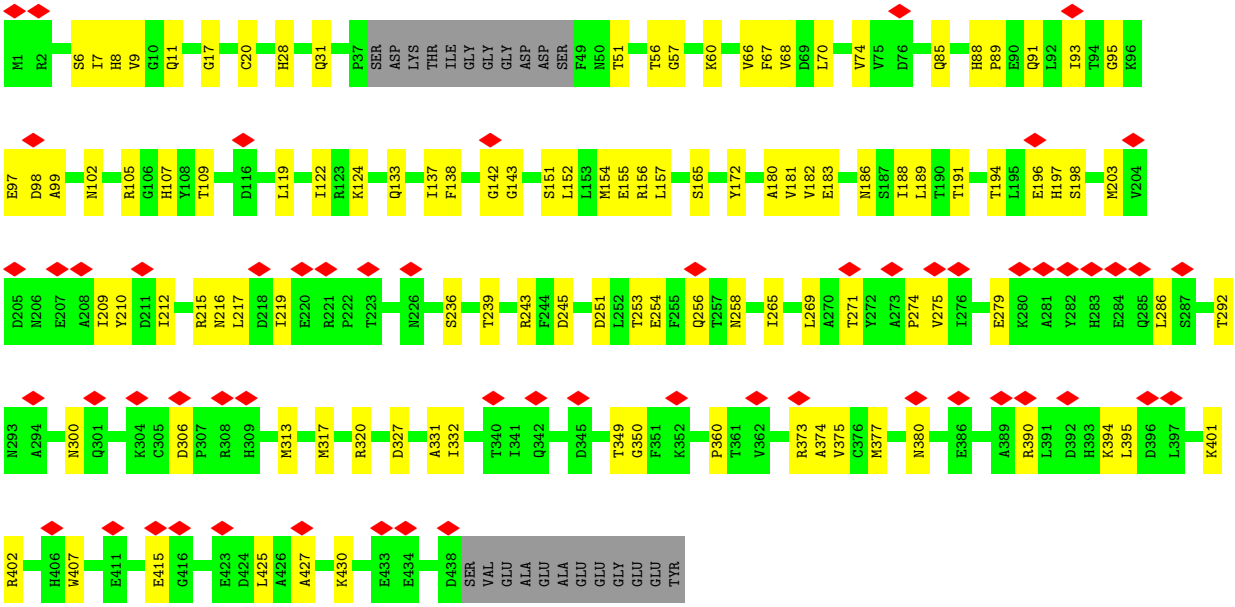




• Molecule 8: Tubulin alpha-3 chain

Chain NC:

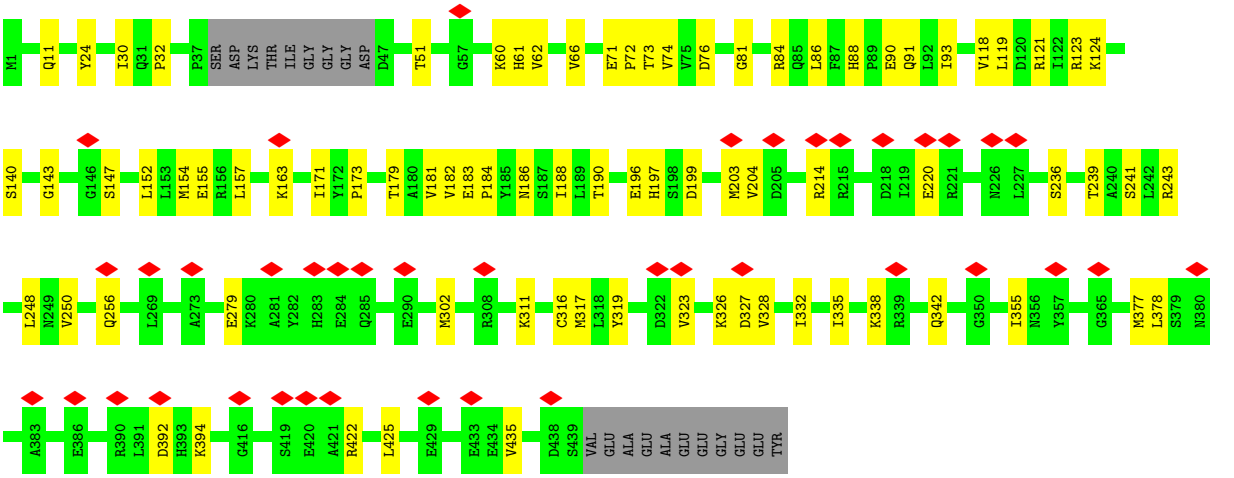




• Molecule 8: Tubulin alpha-3 chain

Chain NE:

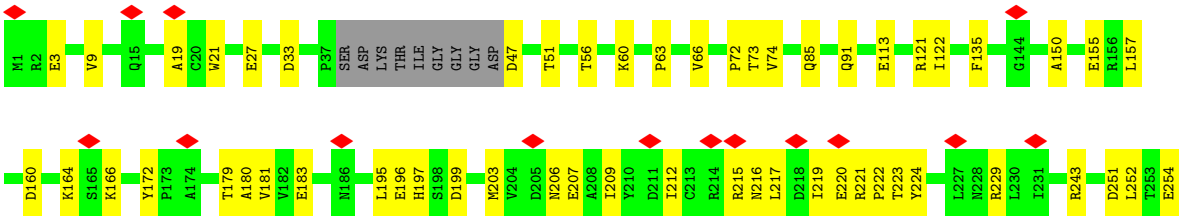


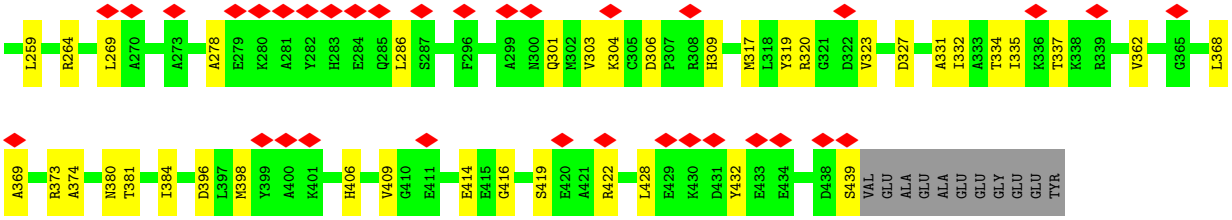


• Molecule 8: Tubulin alpha-3 chain

Chain NG:



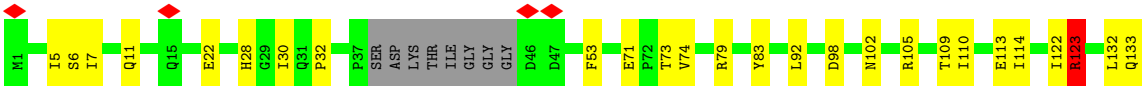


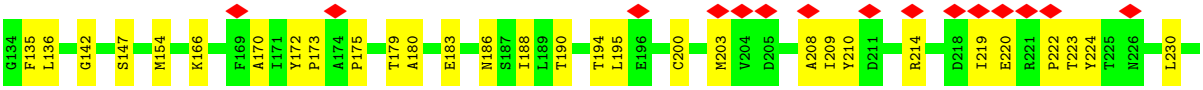


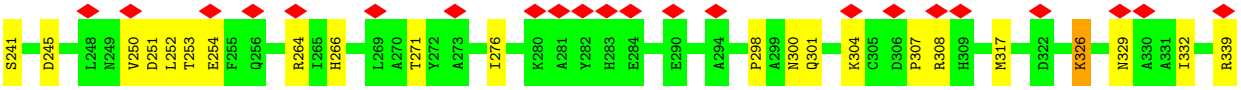
• Molecule 8: Tubulin alpha-3 chain

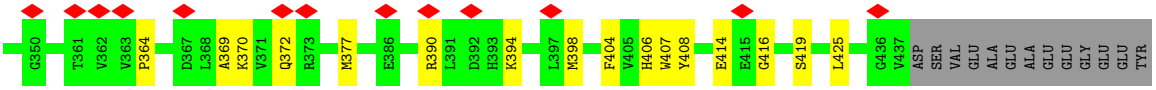
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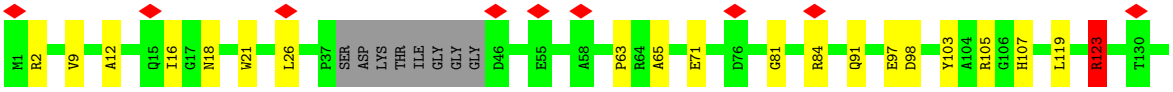


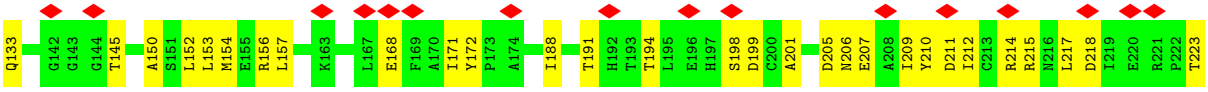


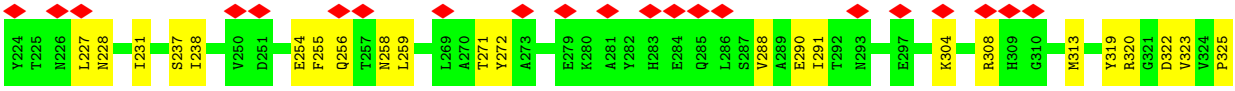
• Molecule 8: Tubulin alpha-3 chain

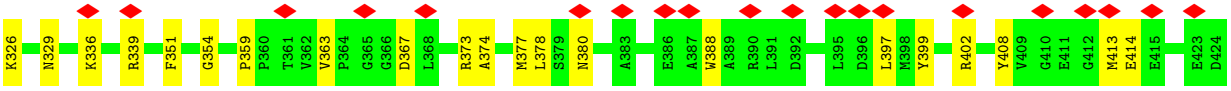
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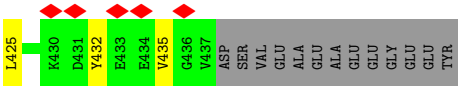






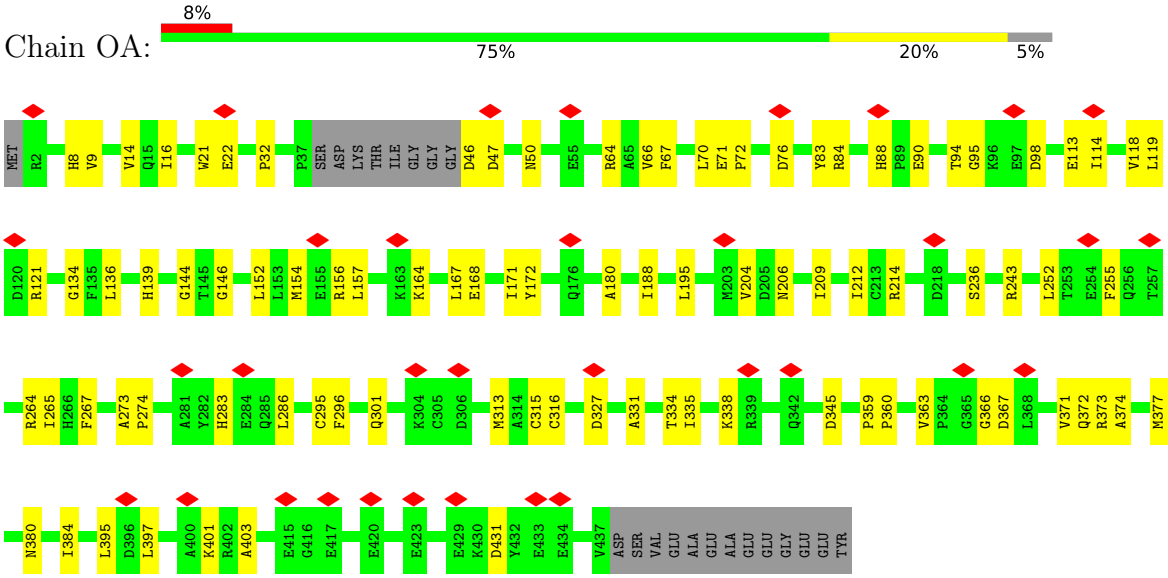






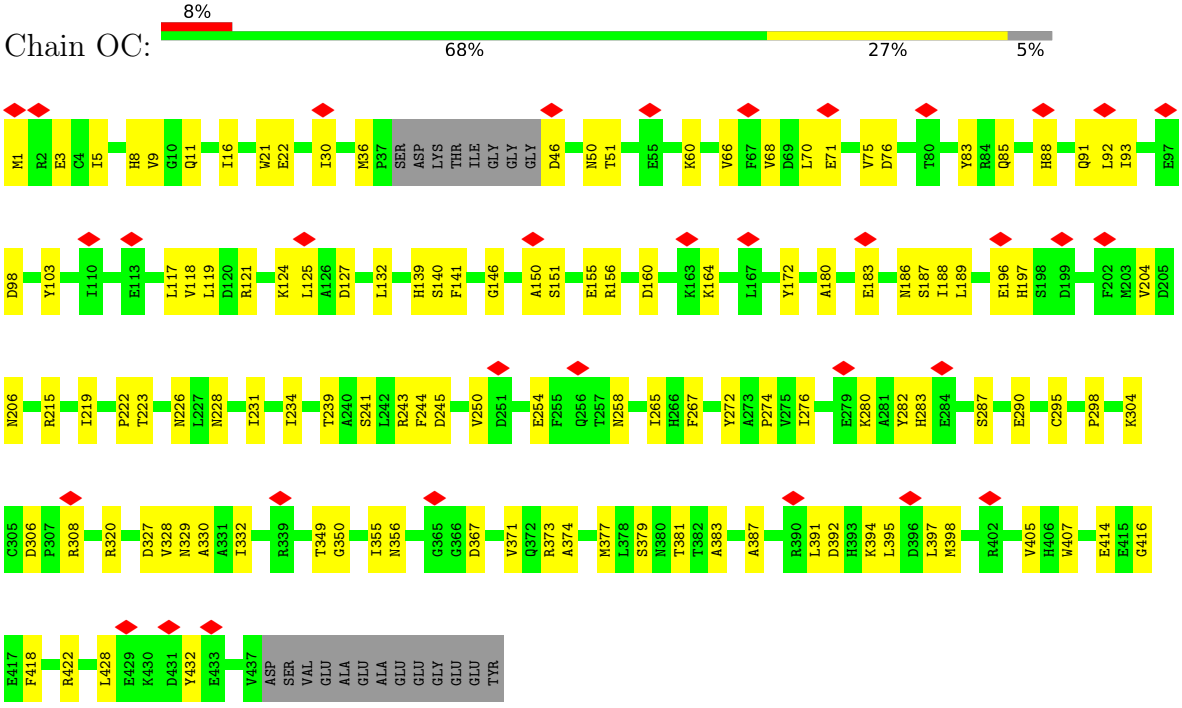
• Molecule 8: Tubulin alpha-3 chain

Chain OA:



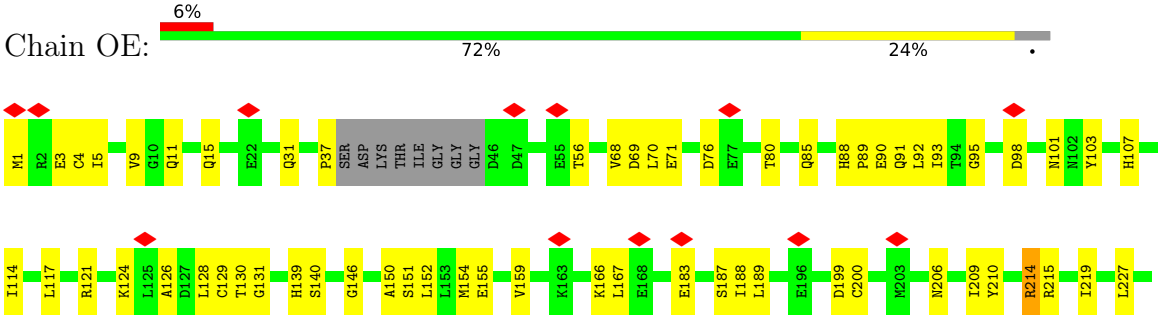
• Molecule 8: Tubulin alpha-3 chain

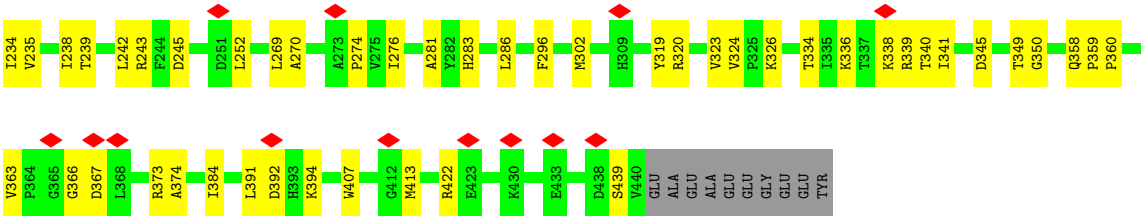
Chain OC:



• Molecule 8: Tubulin alpha-3 chain

Chain OE:

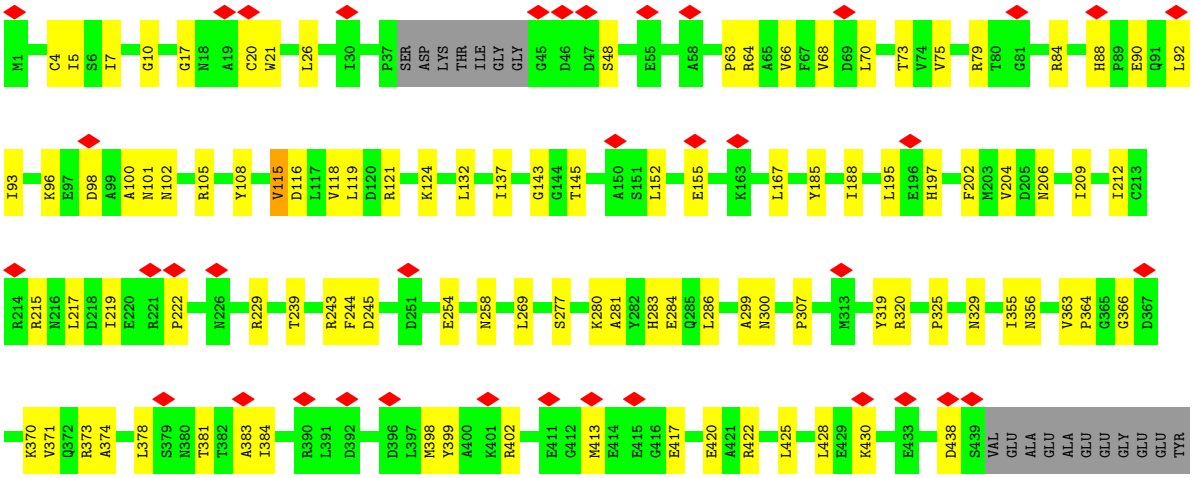




• Molecule 8: Tubulin alpha-3 chain

Chain OG:

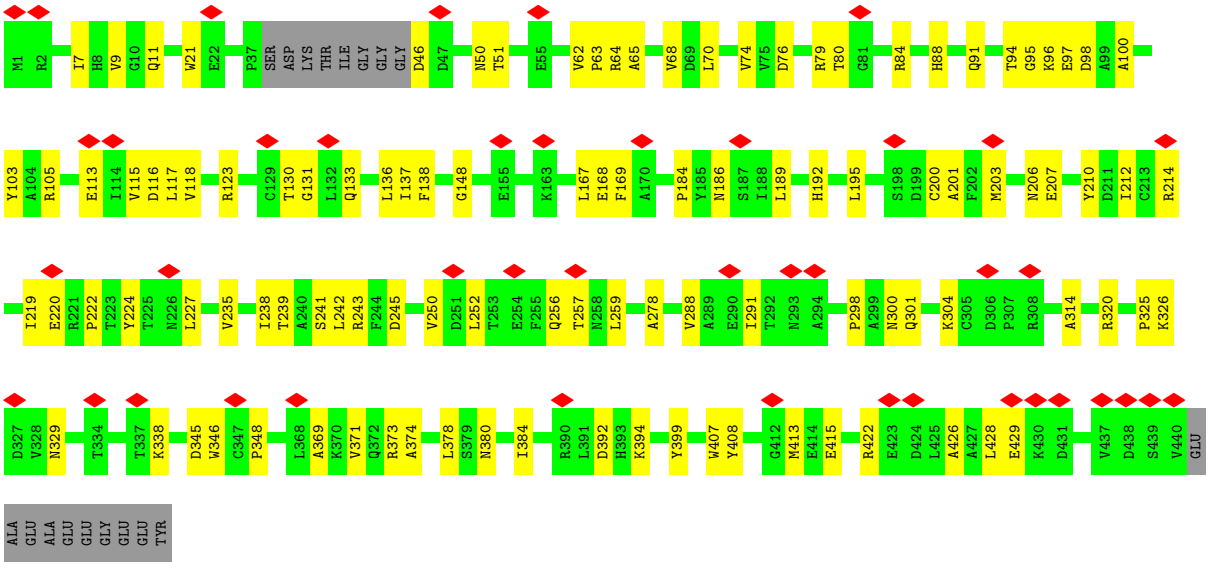




• Molecule 8: Tubulin alpha-3 chain

Chain OI:

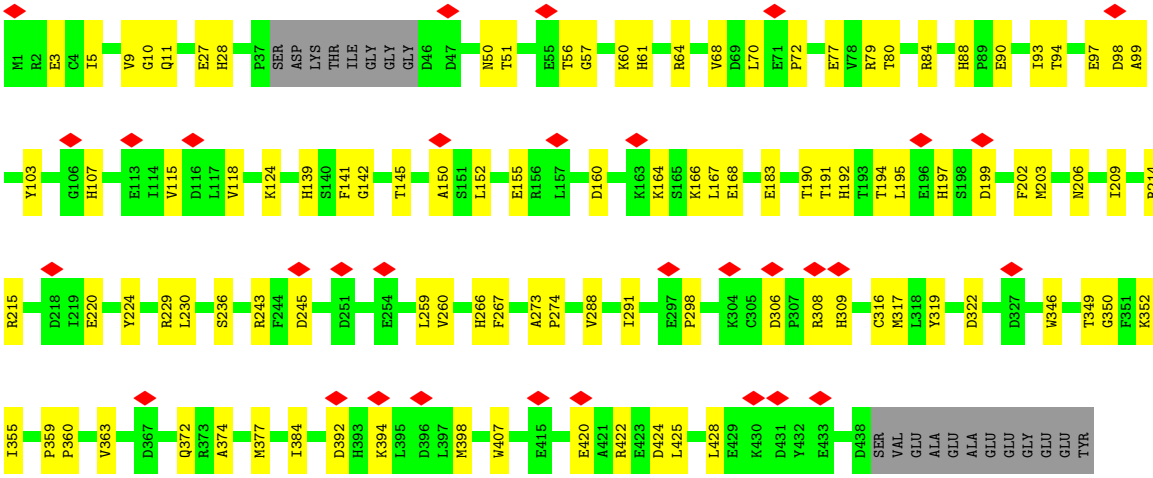




• Molecule 8: Tubulin alpha-3 chain

Chain OK:

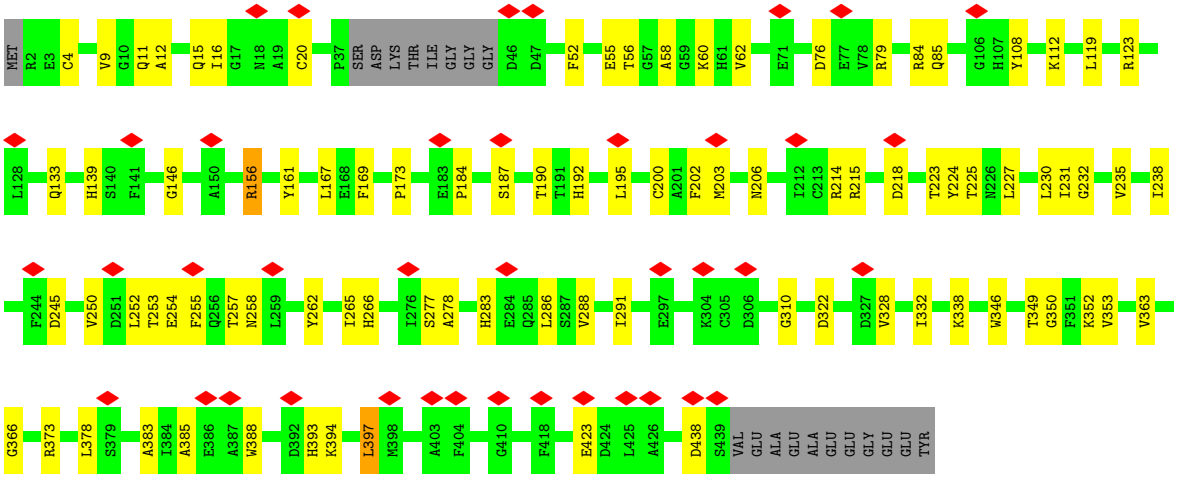




• Molecule 8: Tubulin alpha-3 chain

Chain PA:

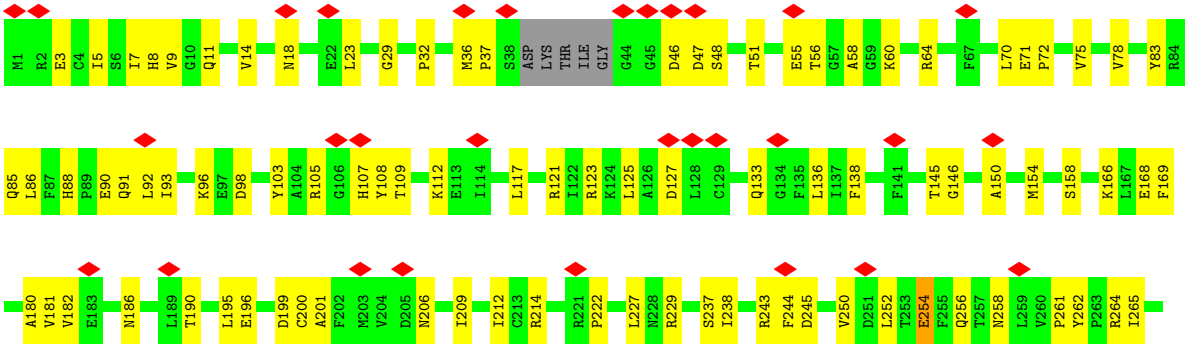


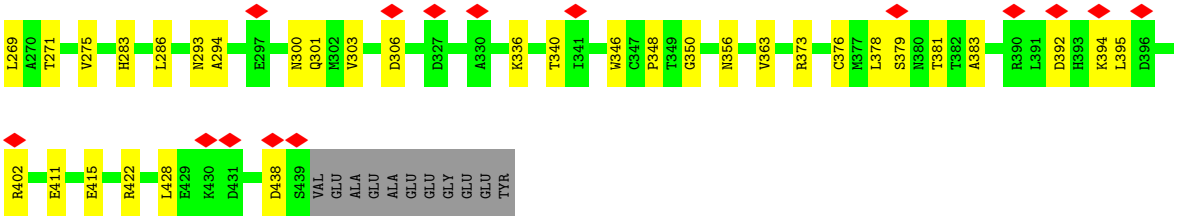


• Molecule 8: Tubulin alpha-3 chain

Chain PC:



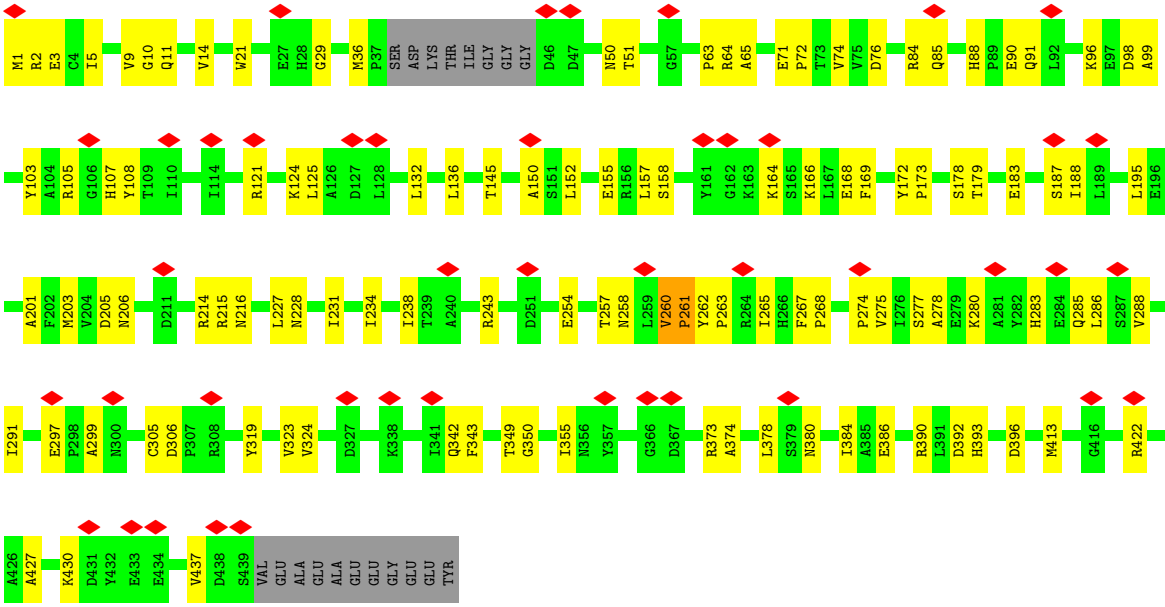




• Molecule 8: Tubulin alpha-3 chain

Chain PE:

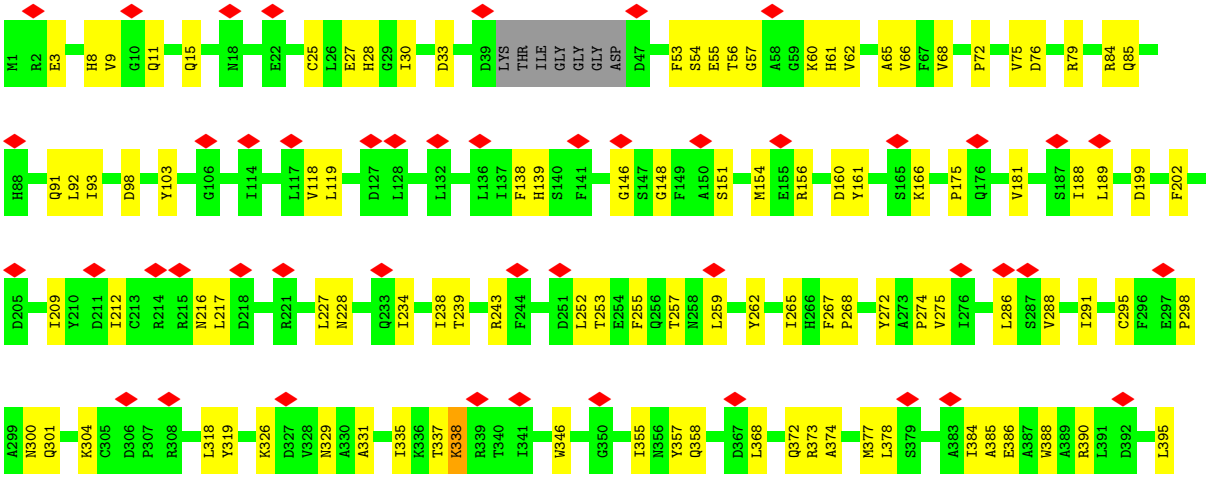


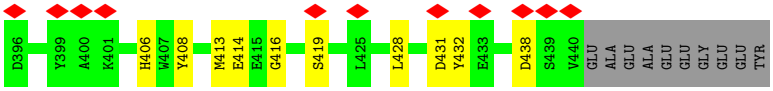


• Molecule 8: Tubulin alpha-3 chain

Chain PG:



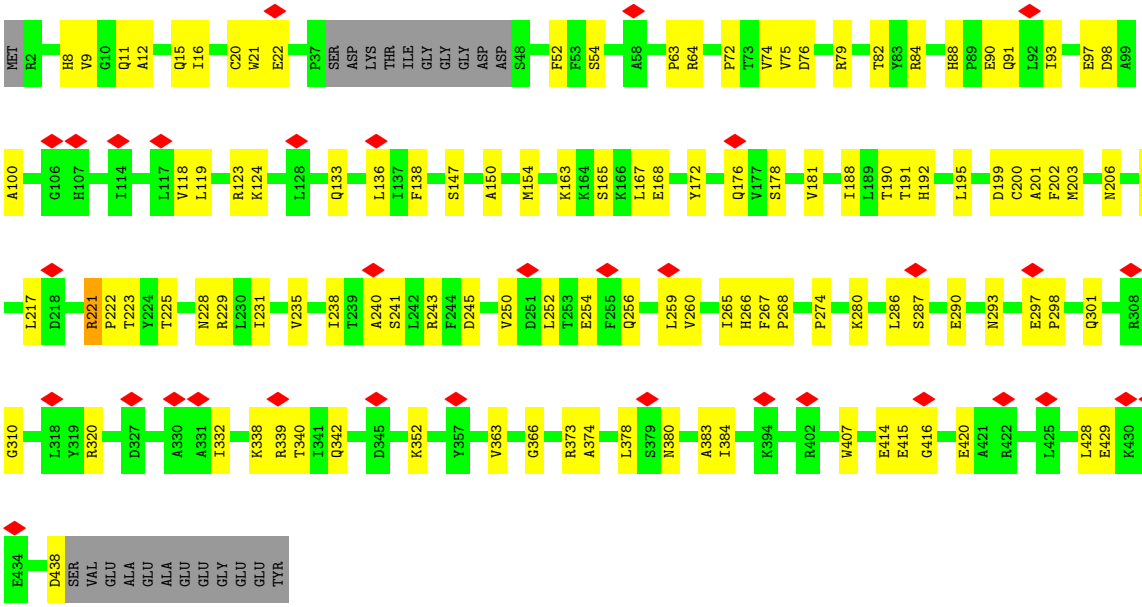




• Molecule 8: Tubulin alpha-3 chain

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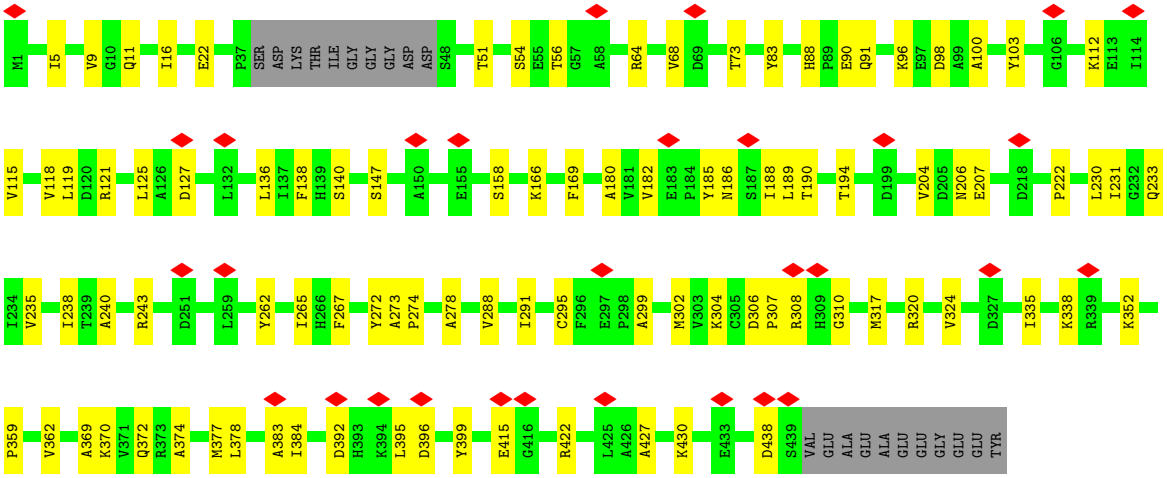




• Molecule 8: Tubulin alpha-3 chain

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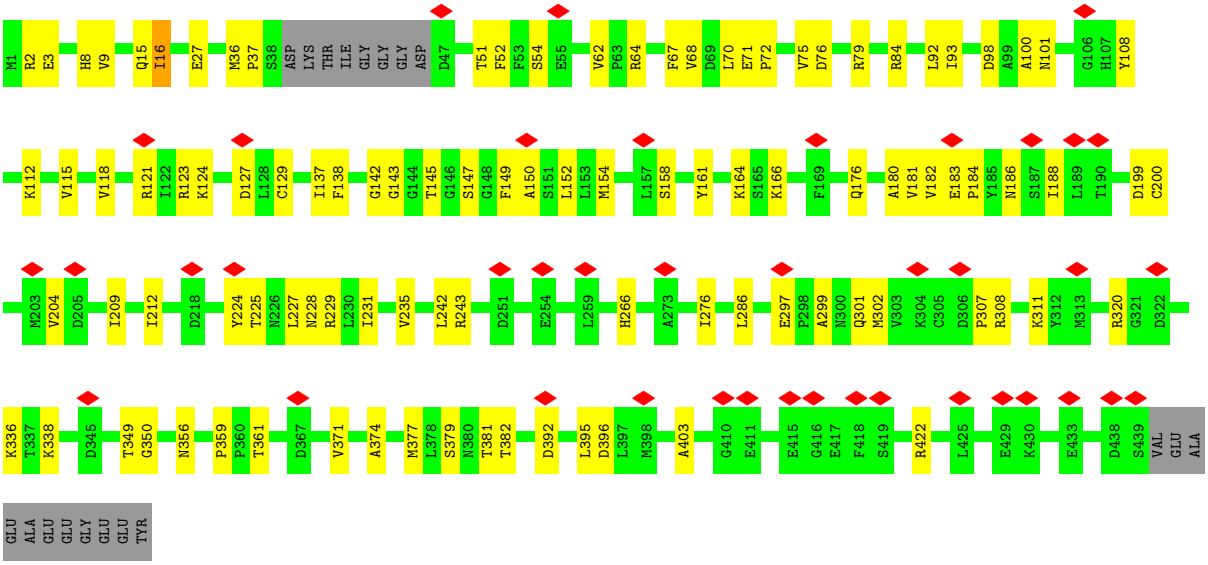




• Molecule 8: Tubulin alpha-3 chain

Chain PM:

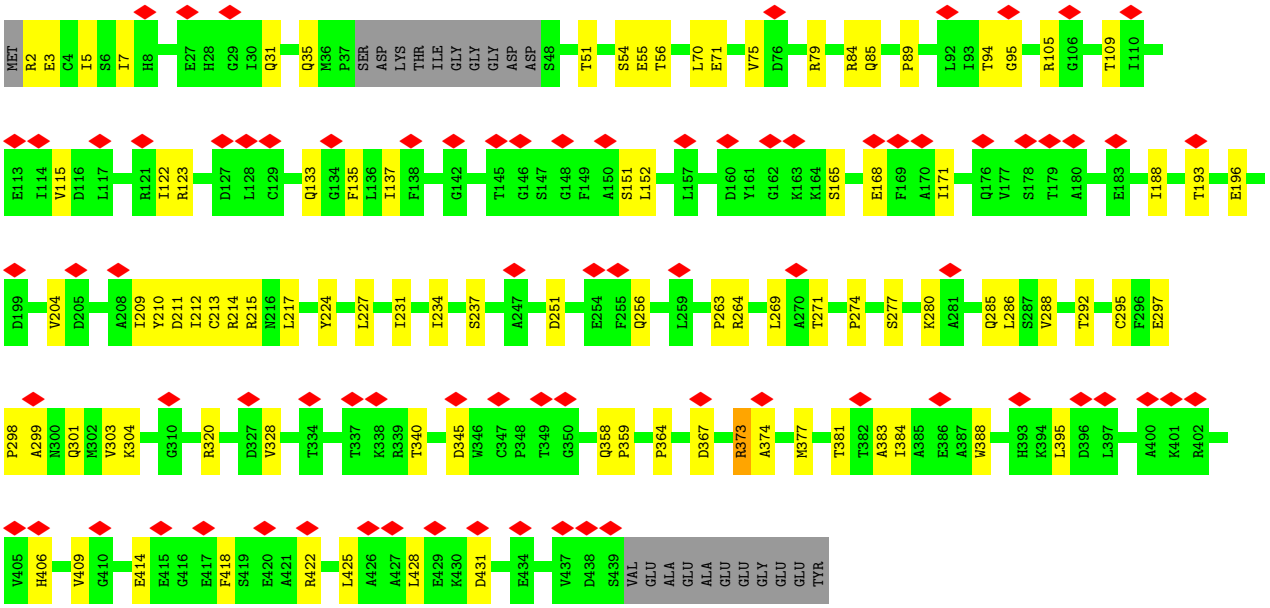




• Molecule 8: Tubulin alpha-3 chain

Chain QA:

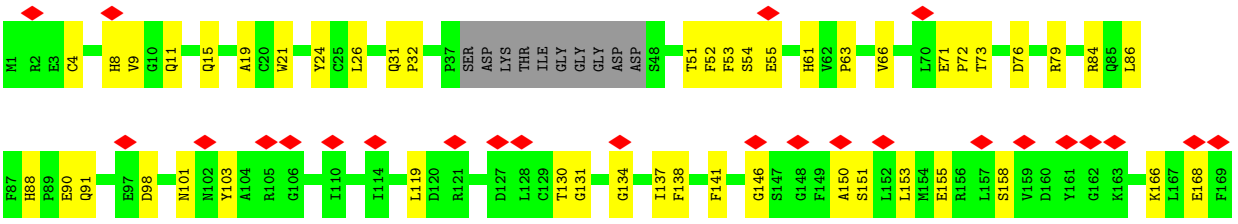


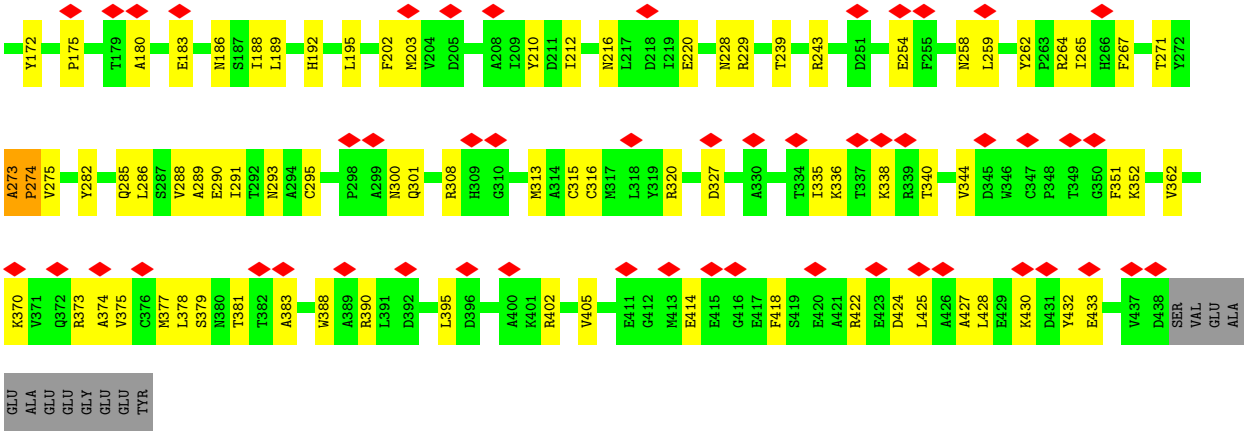


• Molecule 8: Tubulin alpha-3 chain

Chain QC:



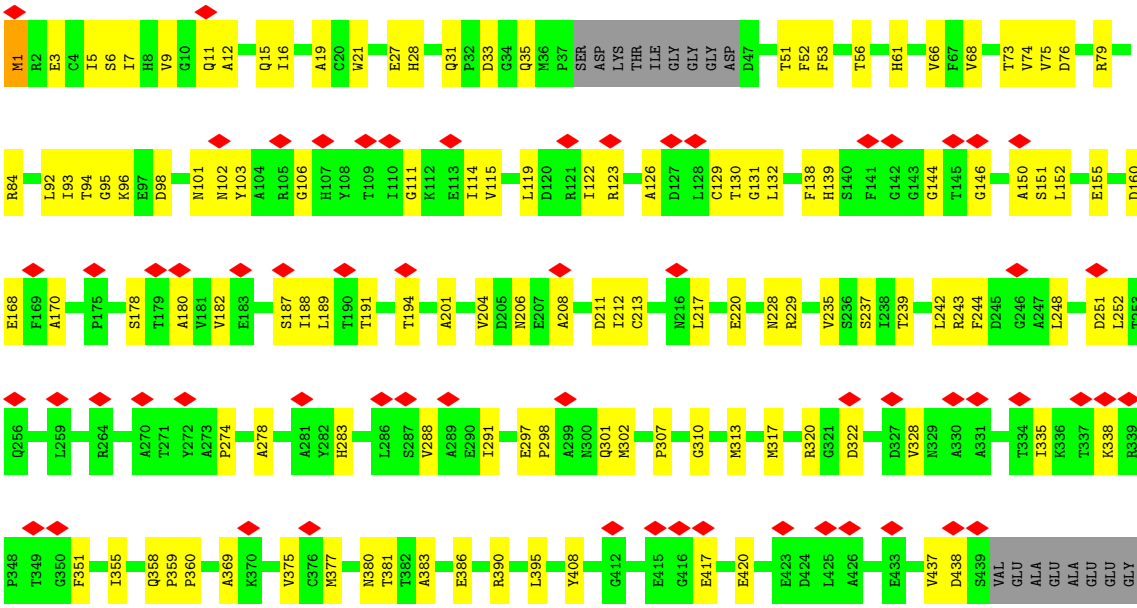




• Molecule 8: Tubulin alpha-3 chain

Chain QE:

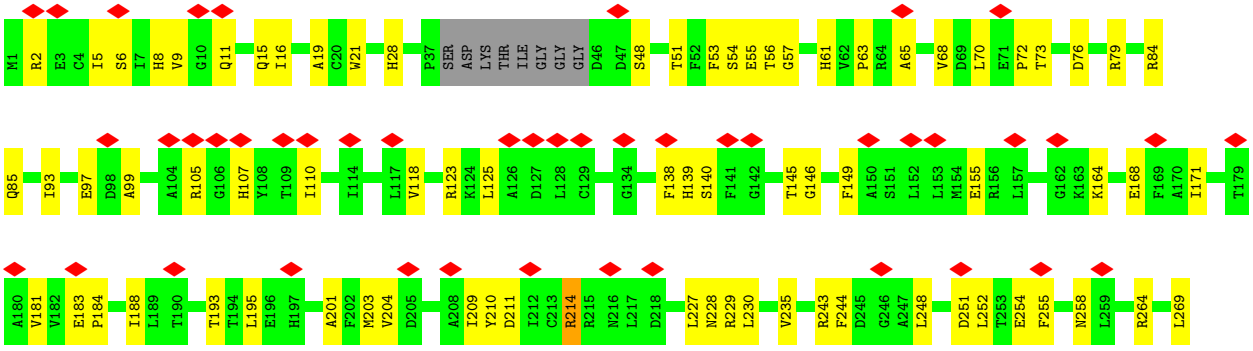


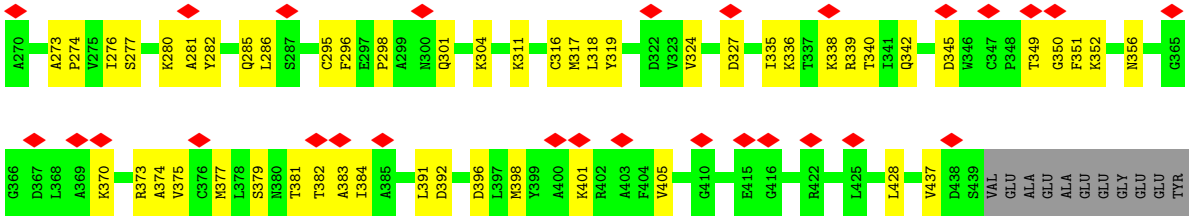


• Molecule 8: Tubulin alpha-3 chain

Chain QG:



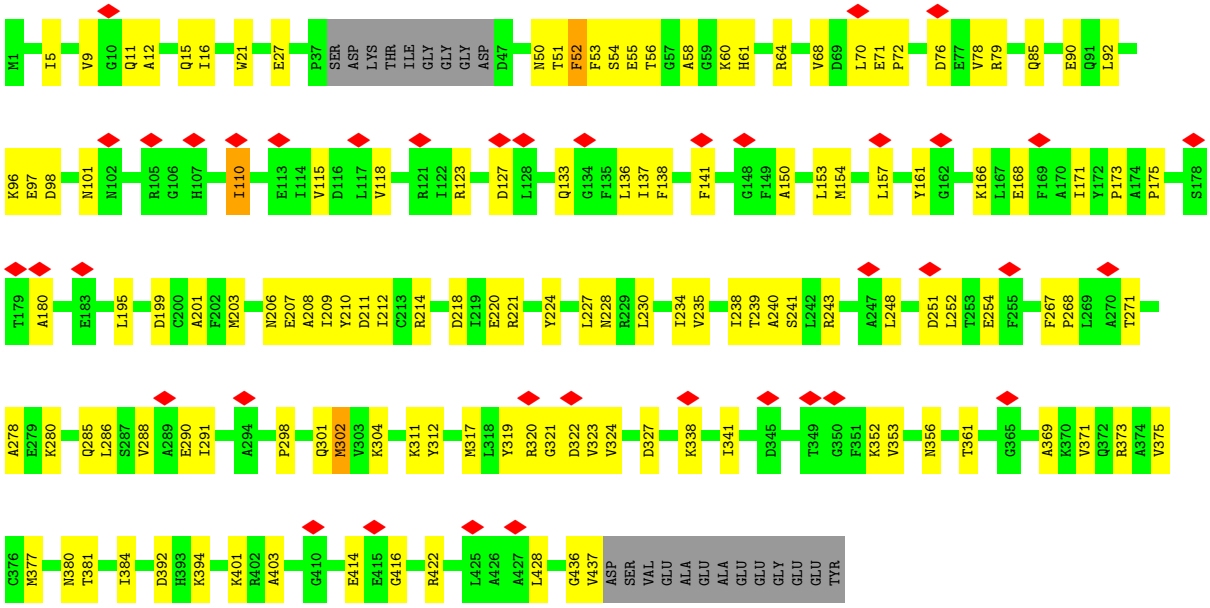




• Molecule 8: Tubulin alpha-3 chain

Chain QI:

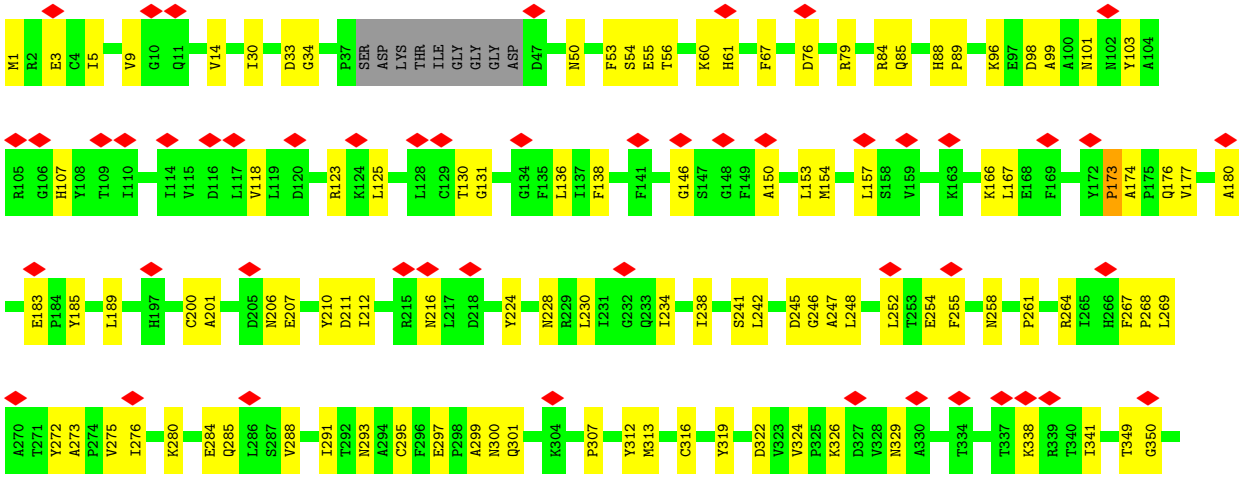


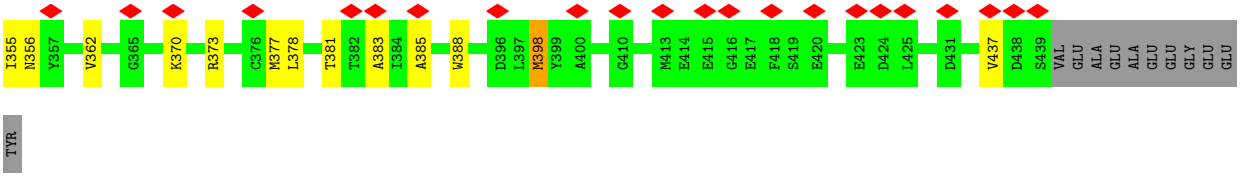


• Molecule 8: Tubulin alpha-3 chain

Chain QK:



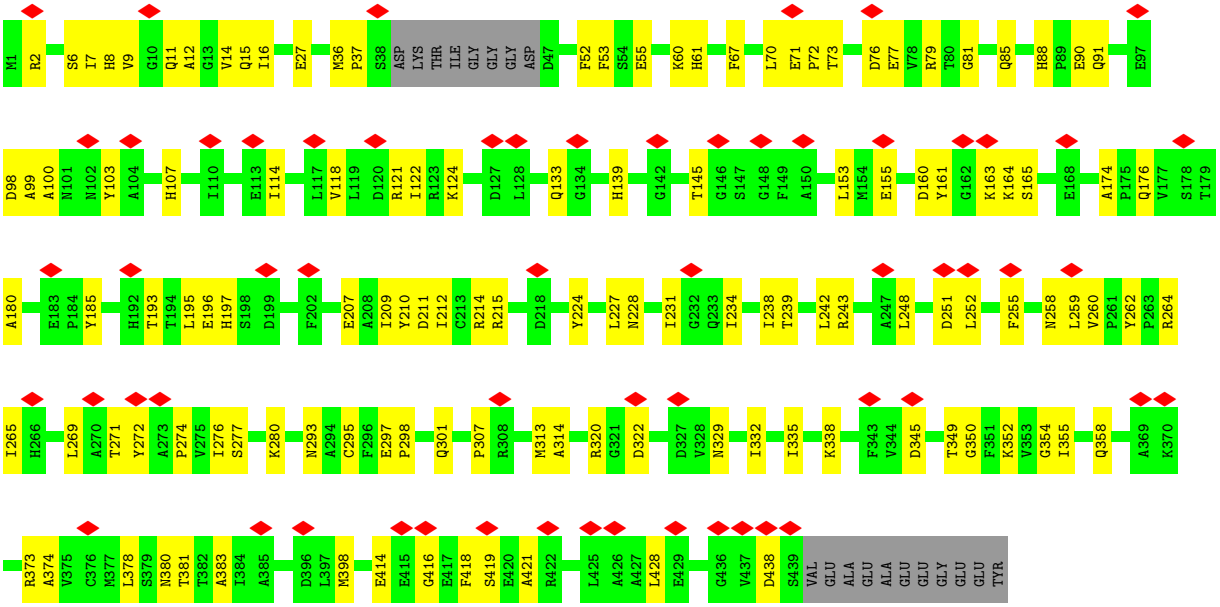




• Molecule 8: Tubulin alpha-3 chain

Chain QM:

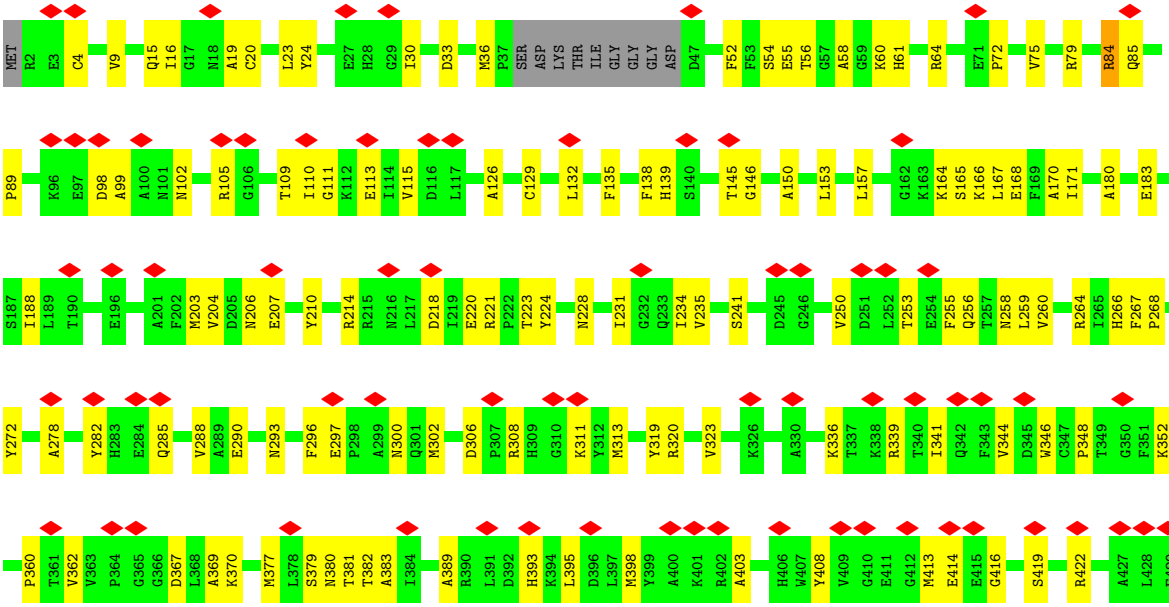


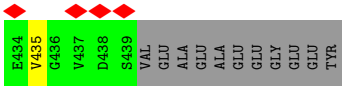


• Molecule 8: Tubulin alpha-3 chain

Chain RA:

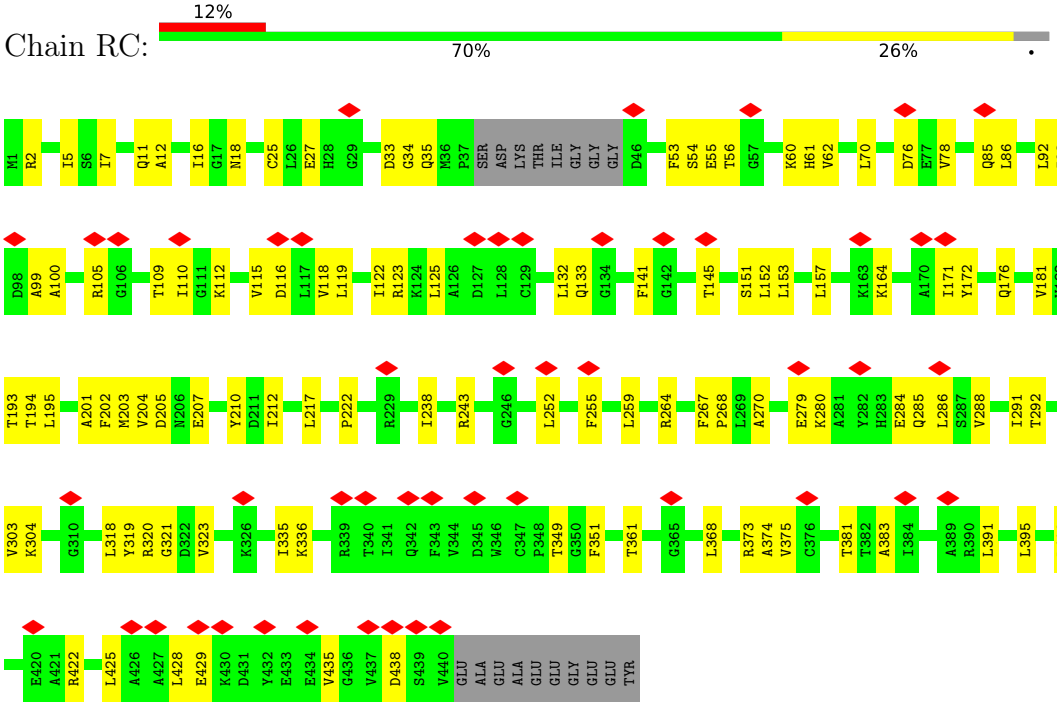






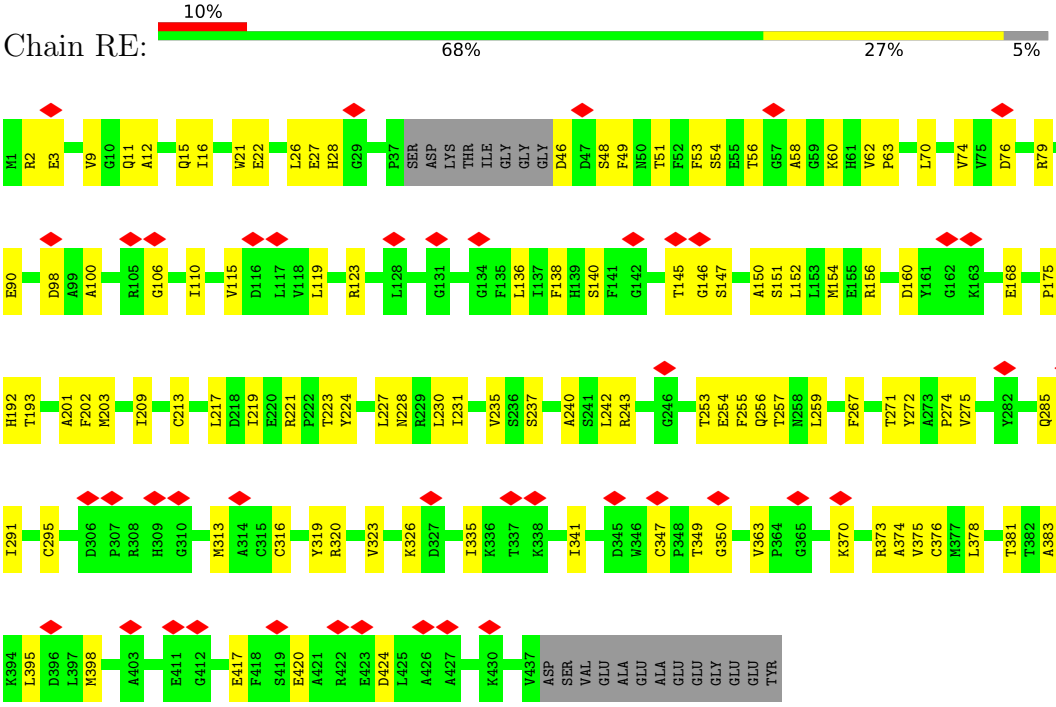
• Molecule 8: Tubulin alpha-3 chain

Chain RC:



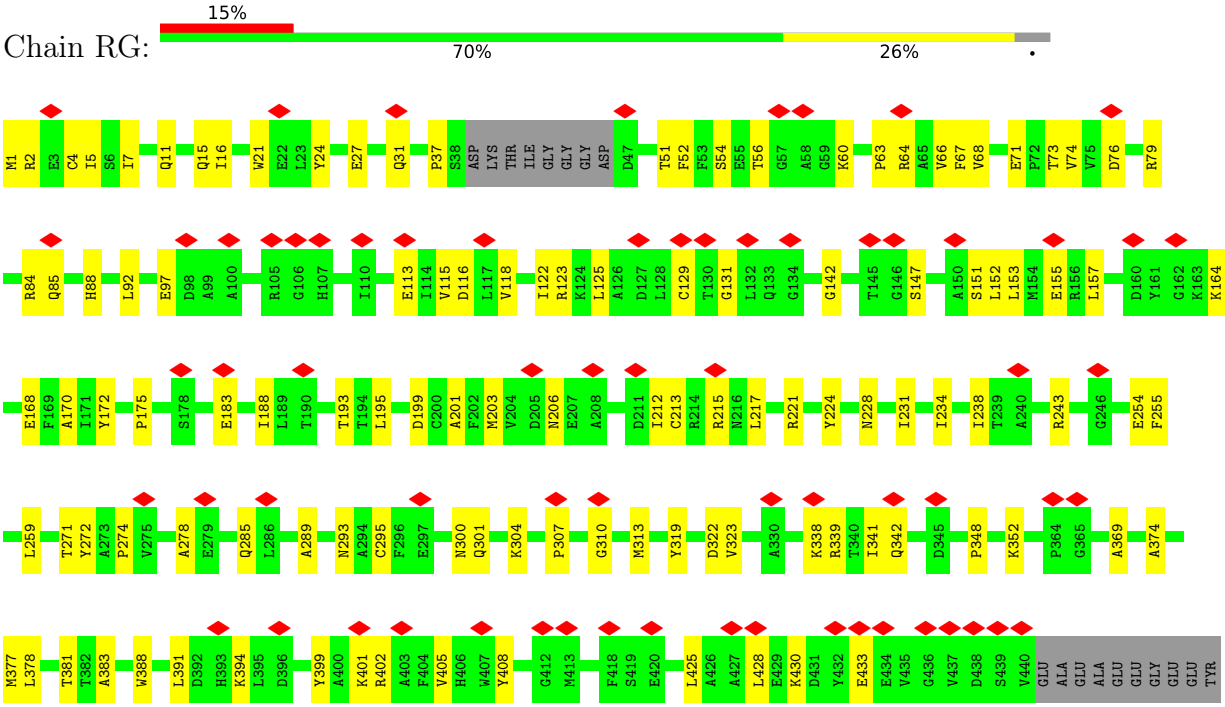
• Molecule 8: Tubulin alpha-3 chain

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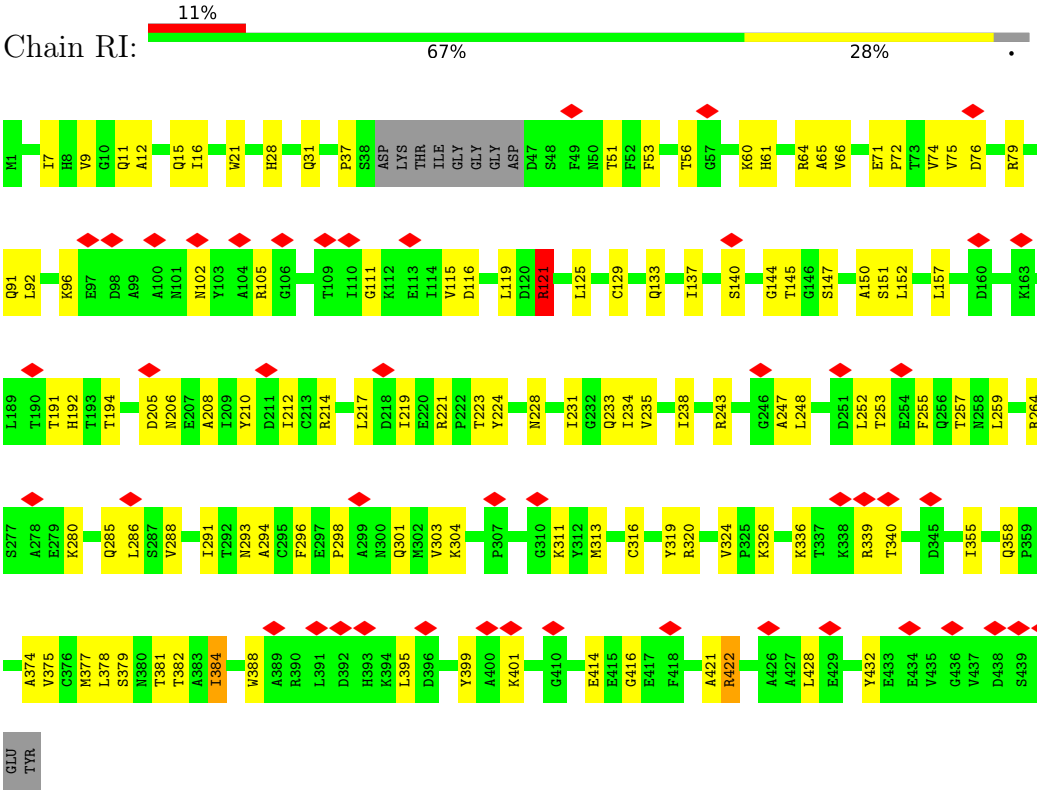
• Molecule 8: Tubulin alpha-3 chain

Chain RG:



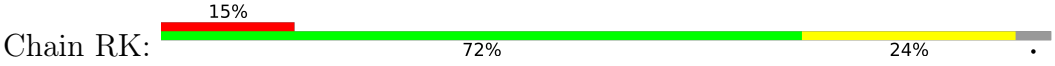
• Molecule 8: Tubulin alpha-3 chain

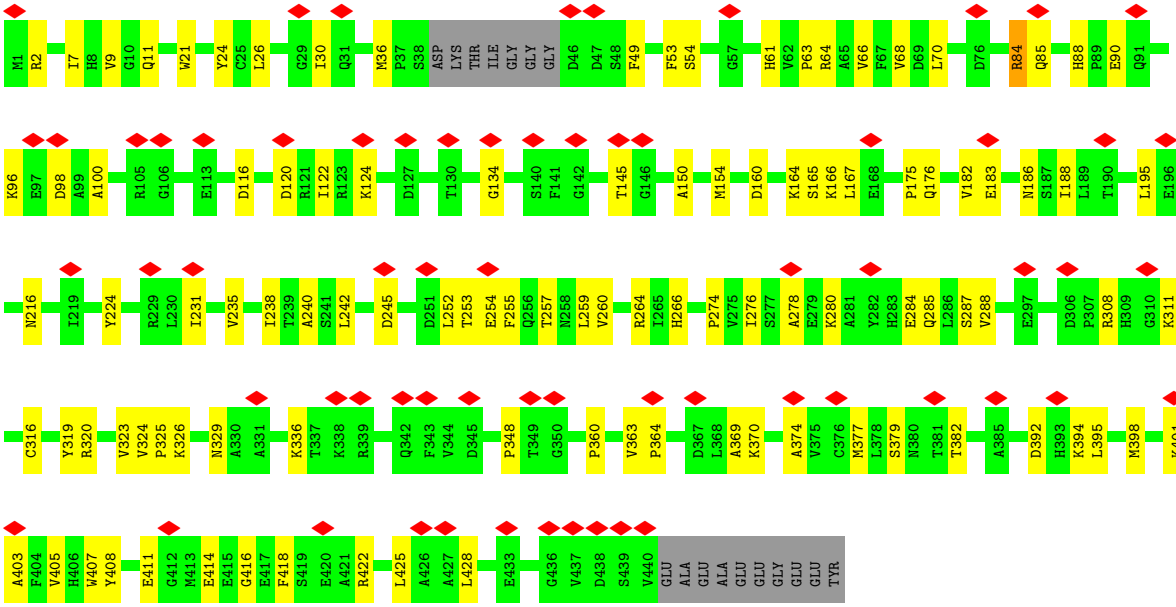
Chain RI:



• Molecule 8: Tubulin alpha-3 chain

Chain RK:

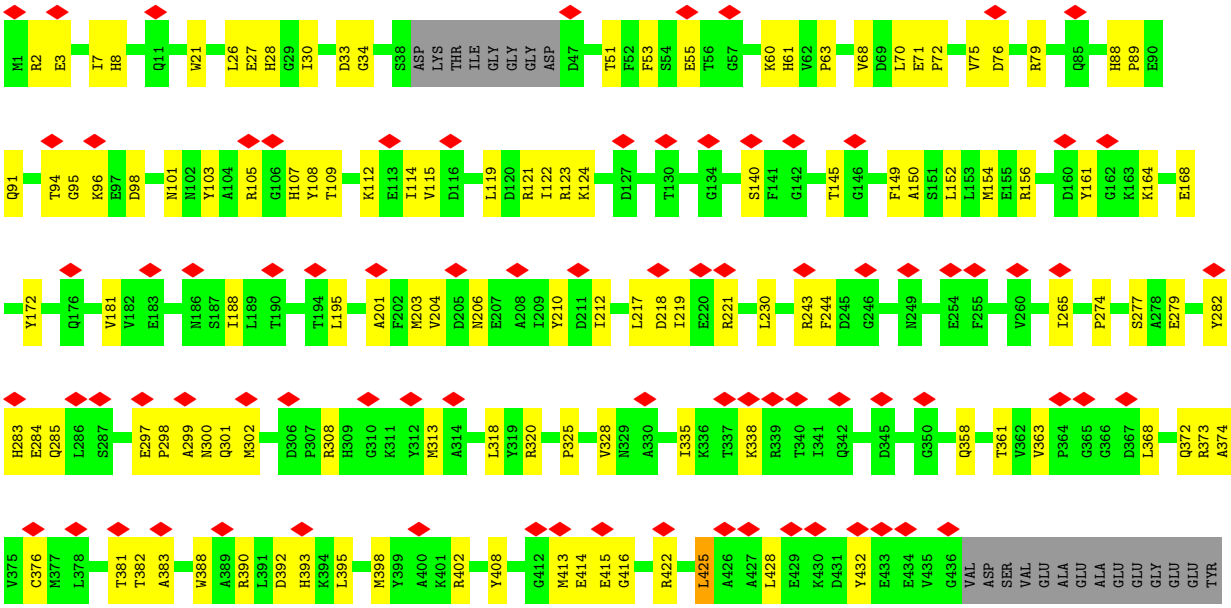




• Molecule 8: Tubulin alpha-3 chain

Chain RM:

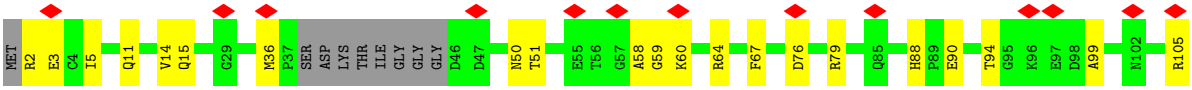


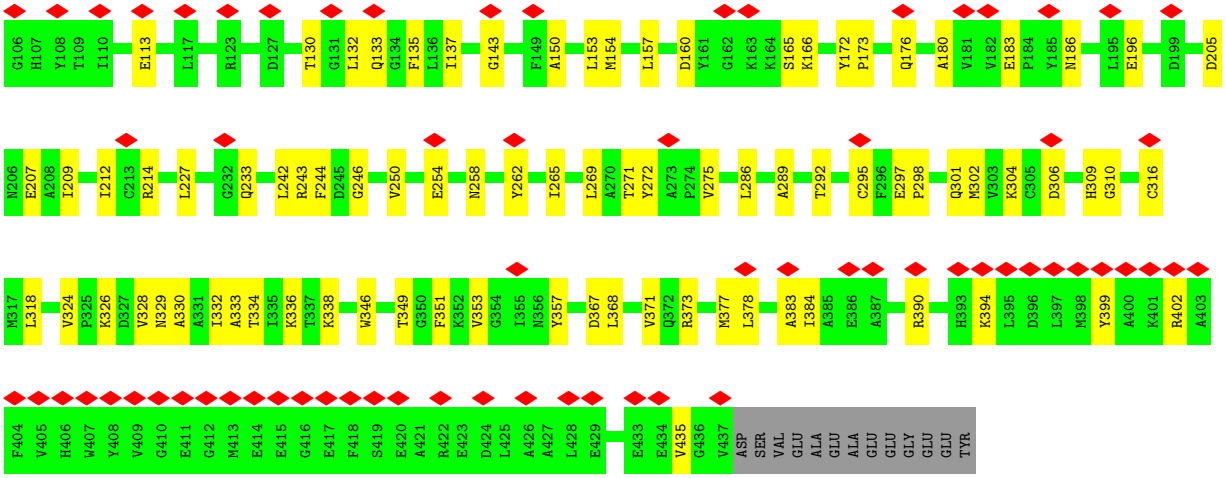


• Molecule 8: Tubulin alpha-3 chain

Chain SA:



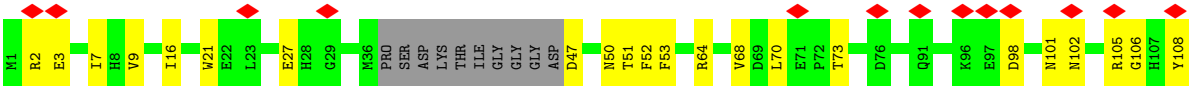


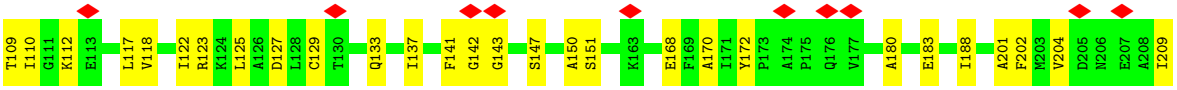


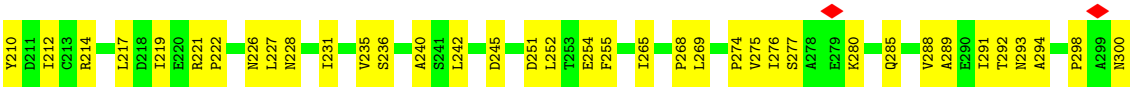
• Molecule 8: Tubulin alpha-3 chain

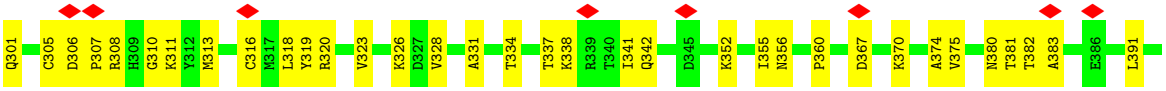
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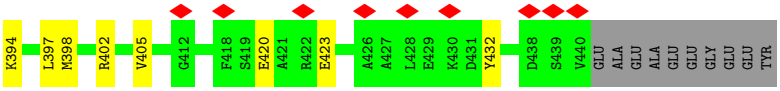








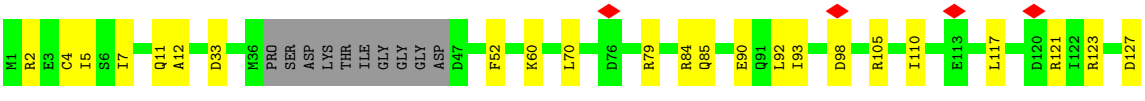


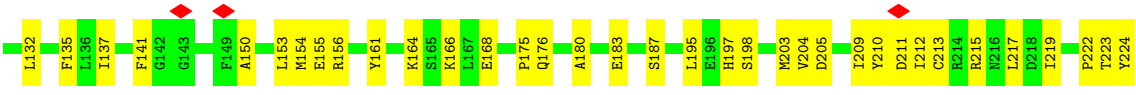


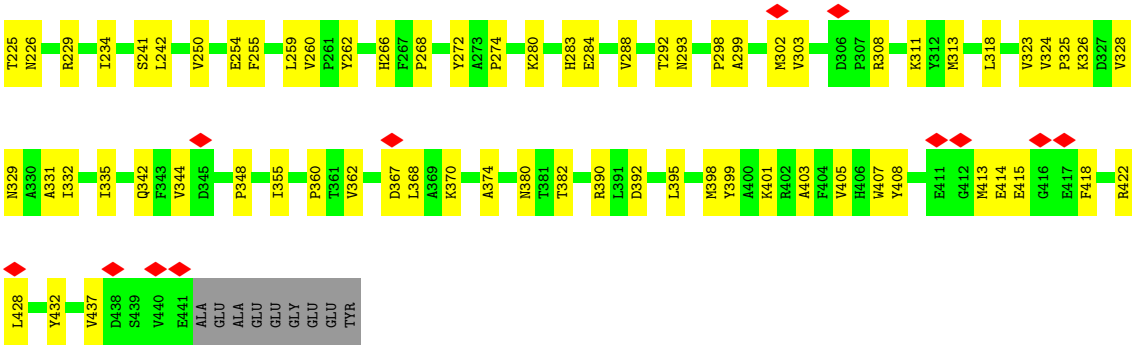
• Molecule 8: Tubulin alpha-3 chain

Chain SE:





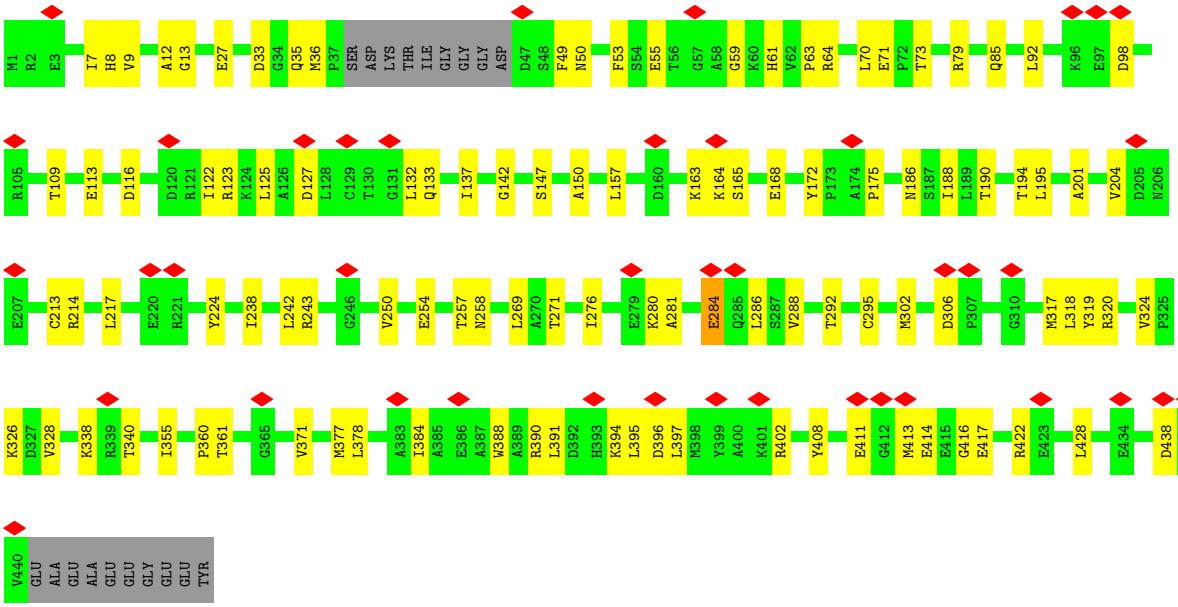




• Molecule 8: Tubulin alpha-3 chain

Chain SG:

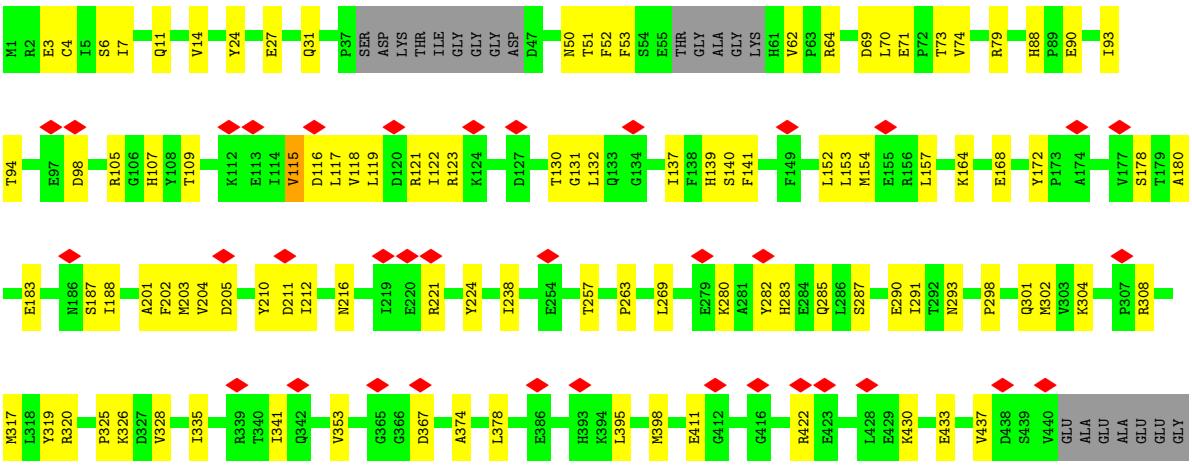




• Molecule 8: Tubulin alpha-3 chain

Chain SI:

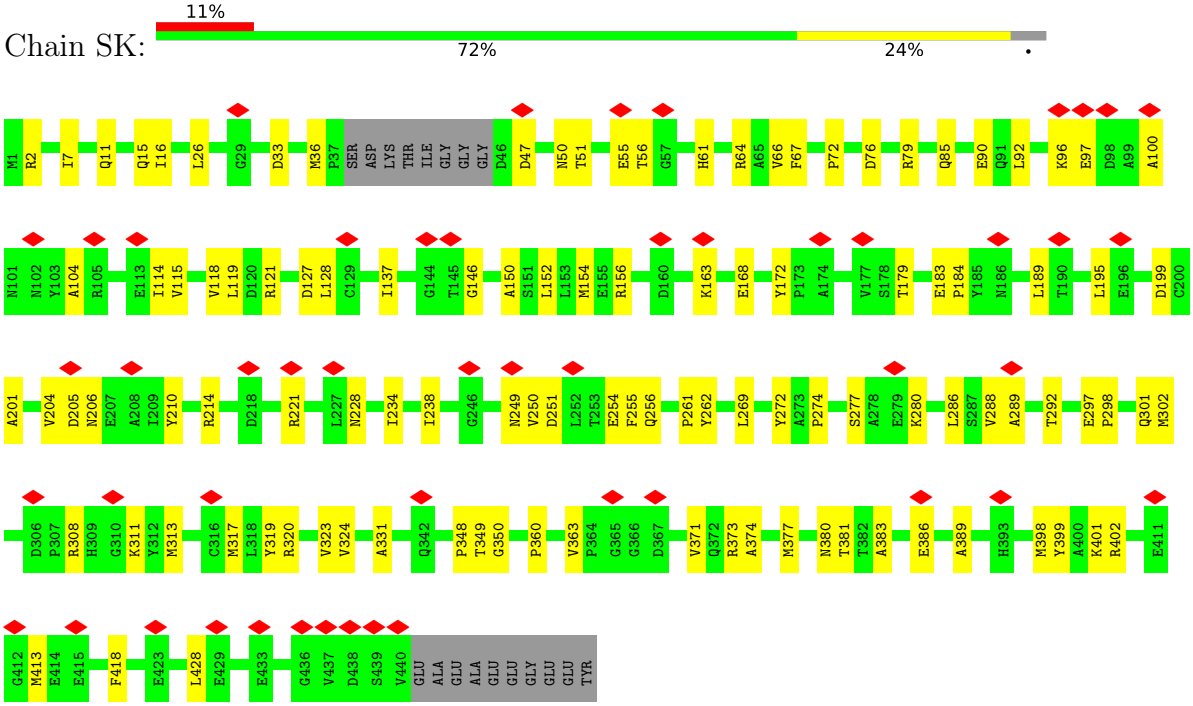






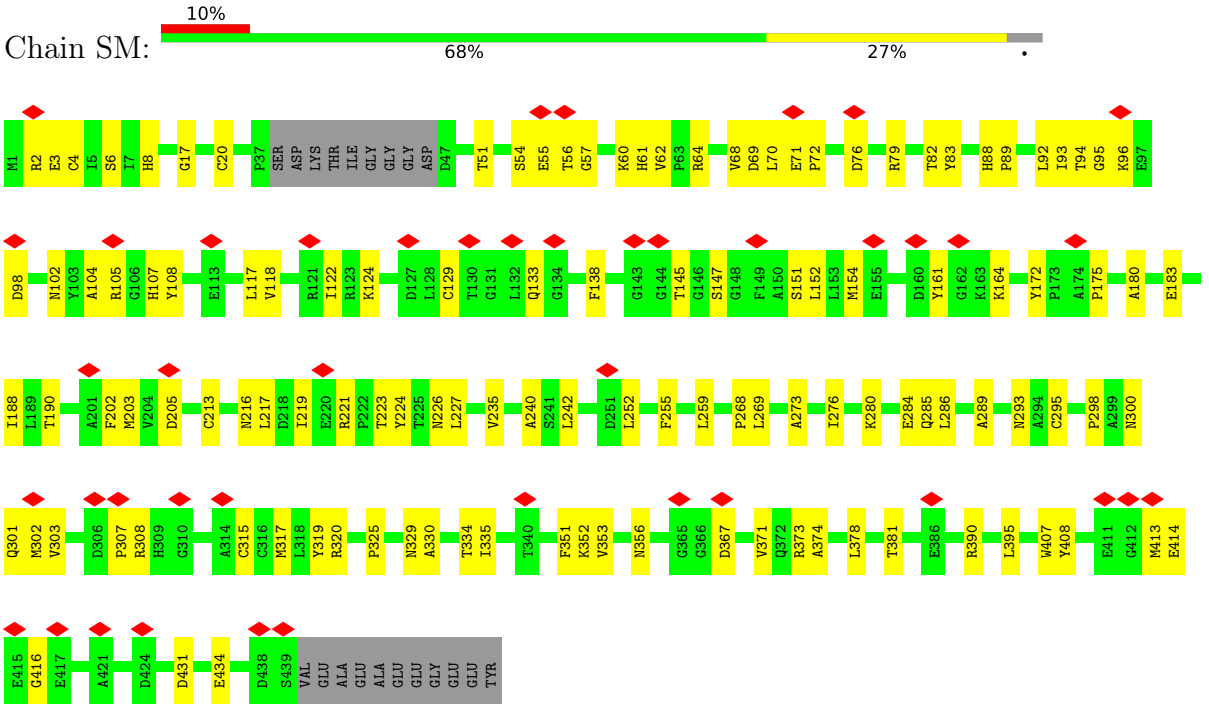
• Molecule 8: Tubulin alpha-3 chain

Chain SK:



• Molecule 8: Tubulin alpha-3 chain

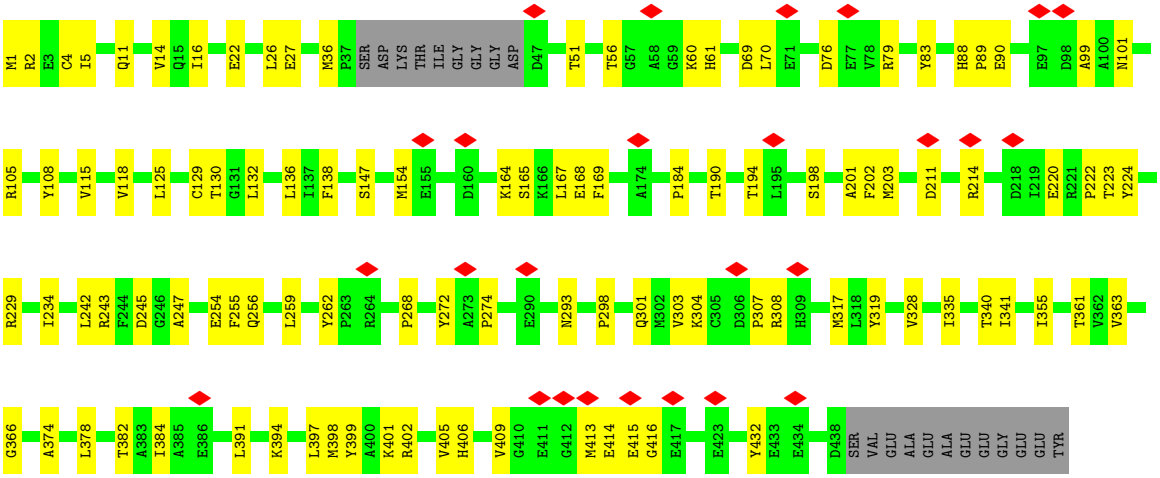
Chain SM:



• Molecule 8: Tubulin alpha-3 chain

Chain TC:

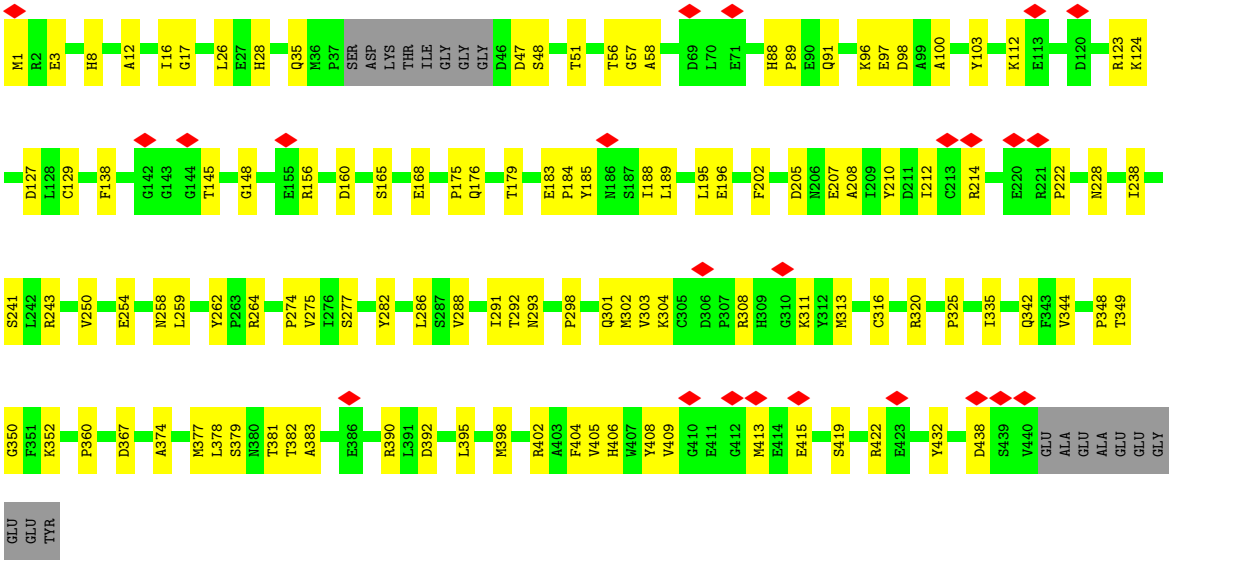




• Molecule 8: Tubulin alpha-3 chain

Chain TE:

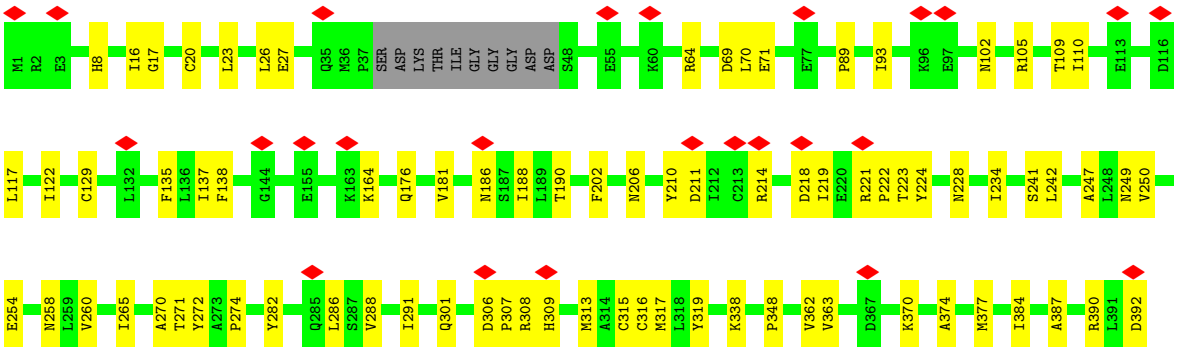


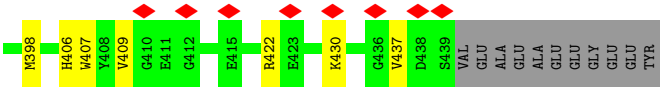


• Molecule 8: Tubulin alpha-3 chain

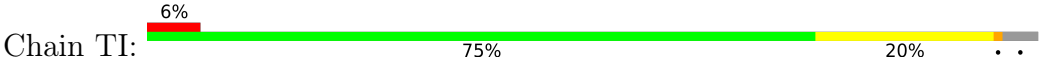
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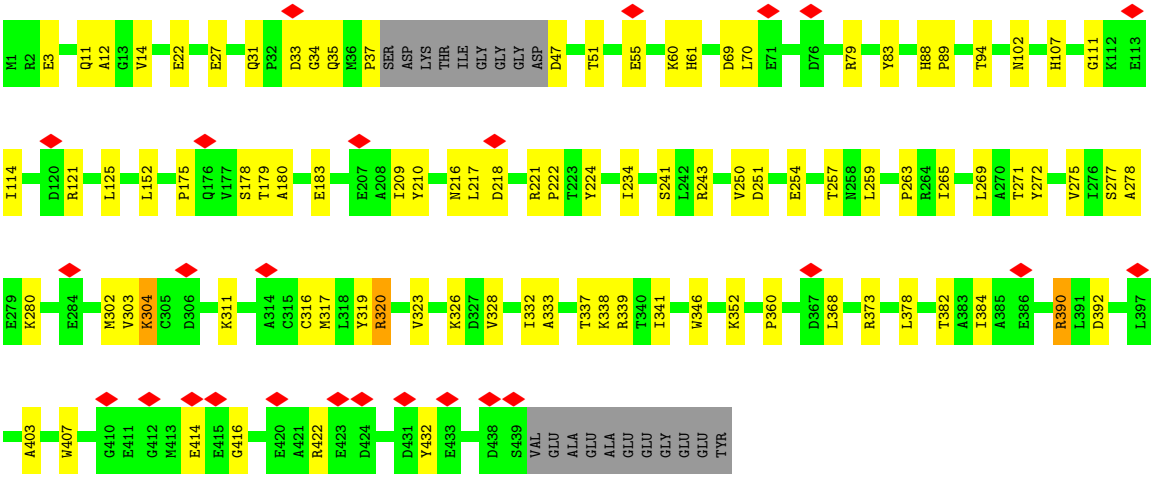






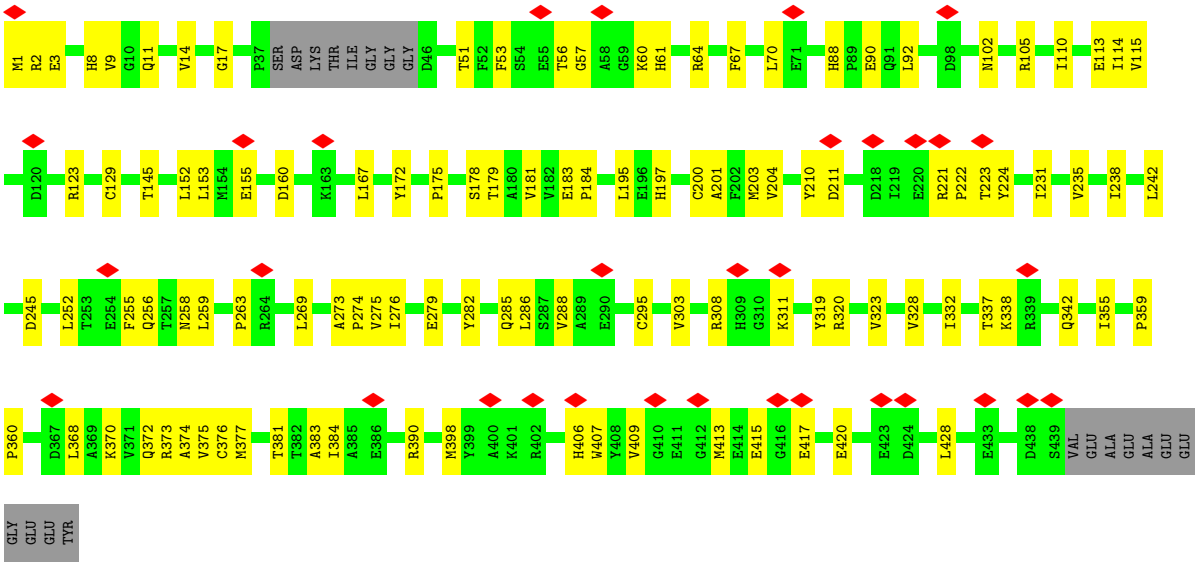
• Molecule 8: Tubulin alpha-3 chain



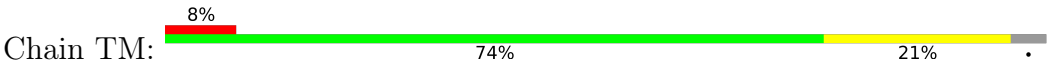


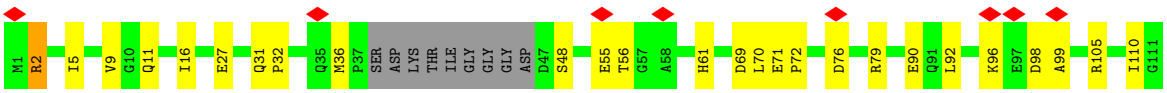
• Molecule 8: Tubulin alpha-3 chain

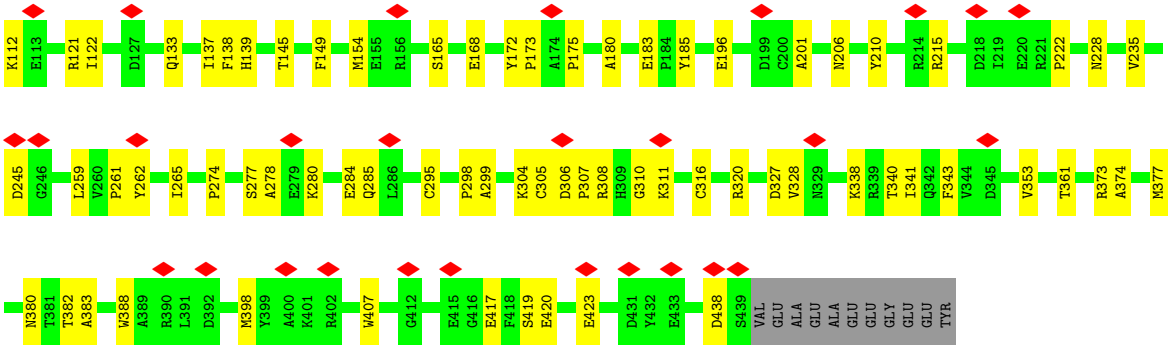




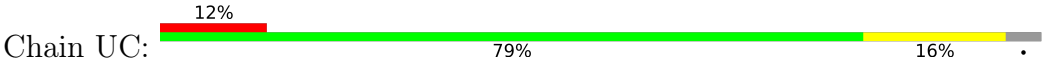
• Molecule 8: Tubulin alpha-3 chain

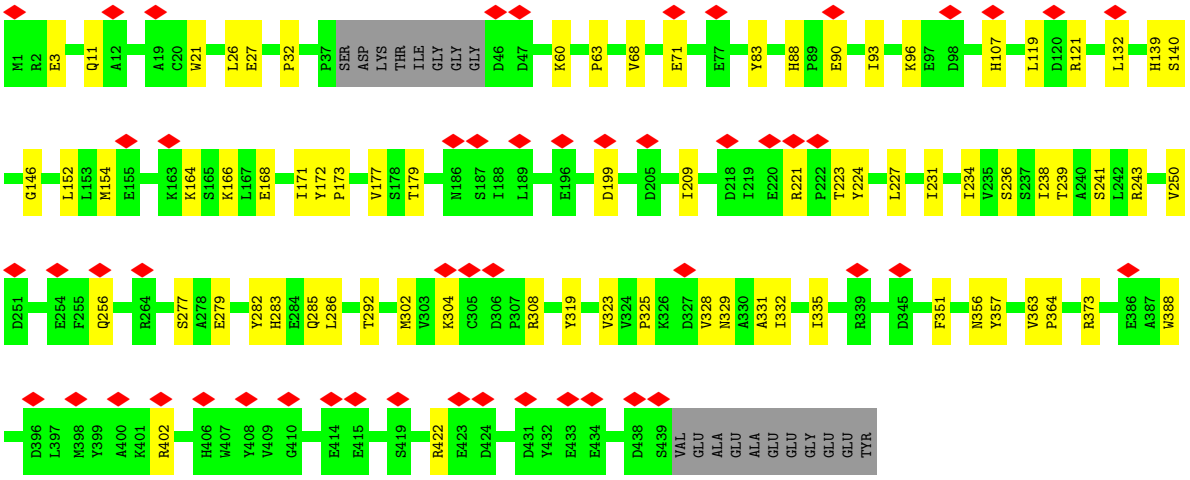




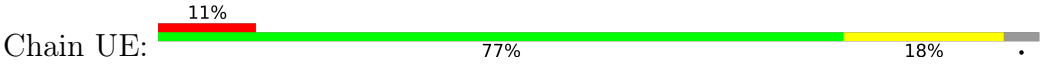


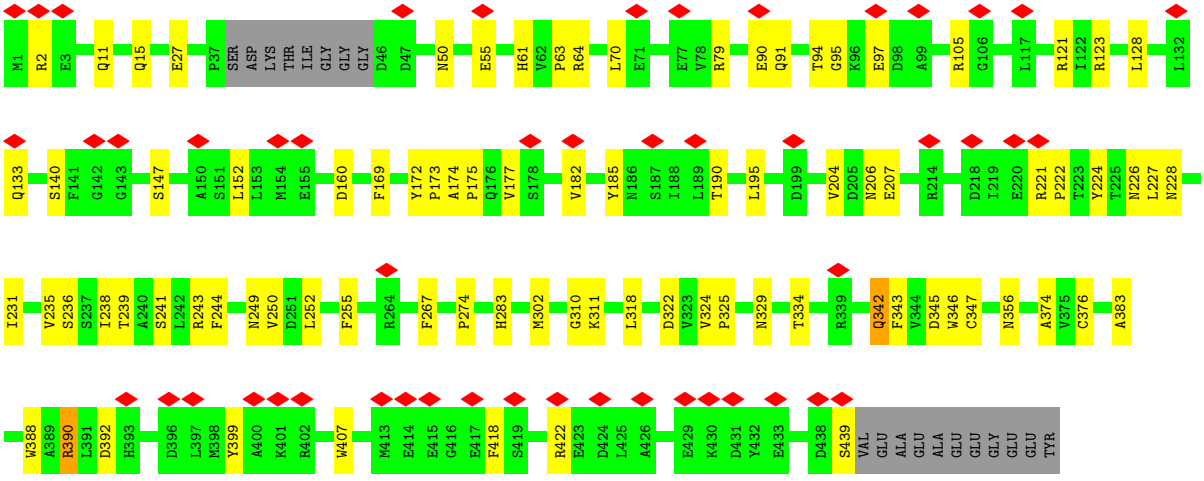
• Molecule 8: Tubulin alpha-3 chain





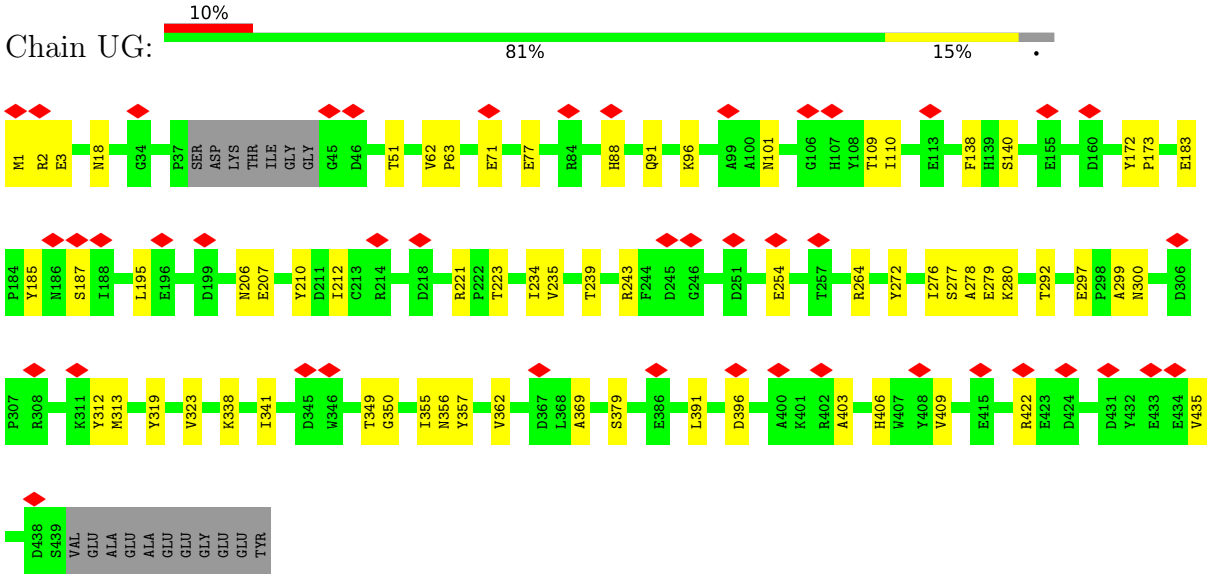
• Molecule 8: Tubulin alpha-3 chain





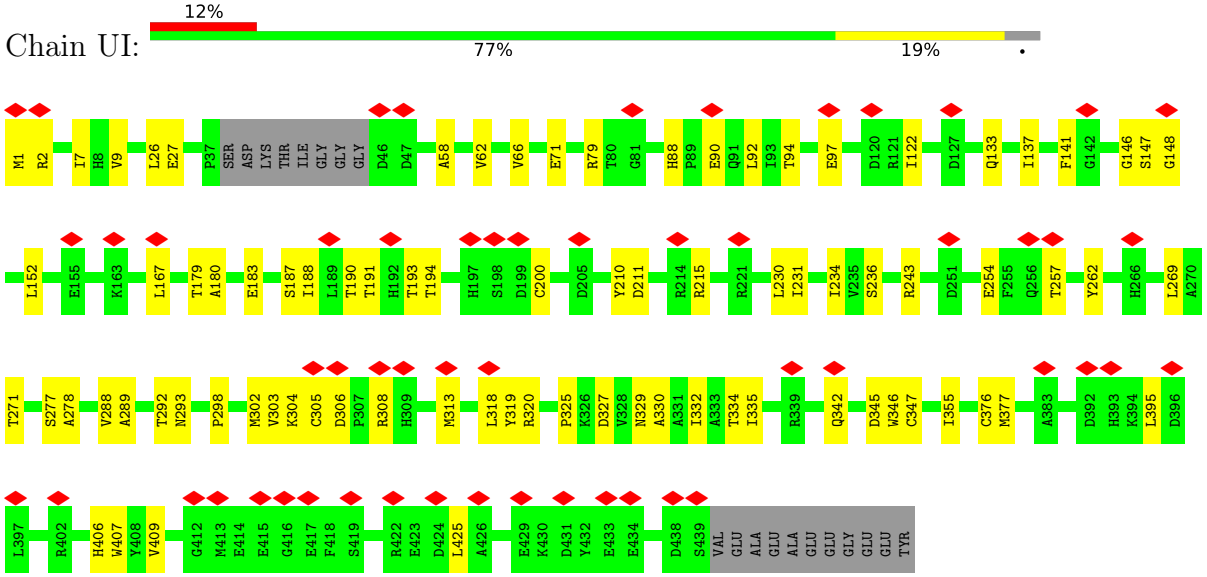
• Molecule 8: Tubulin alpha-3 chain

Chain UG:



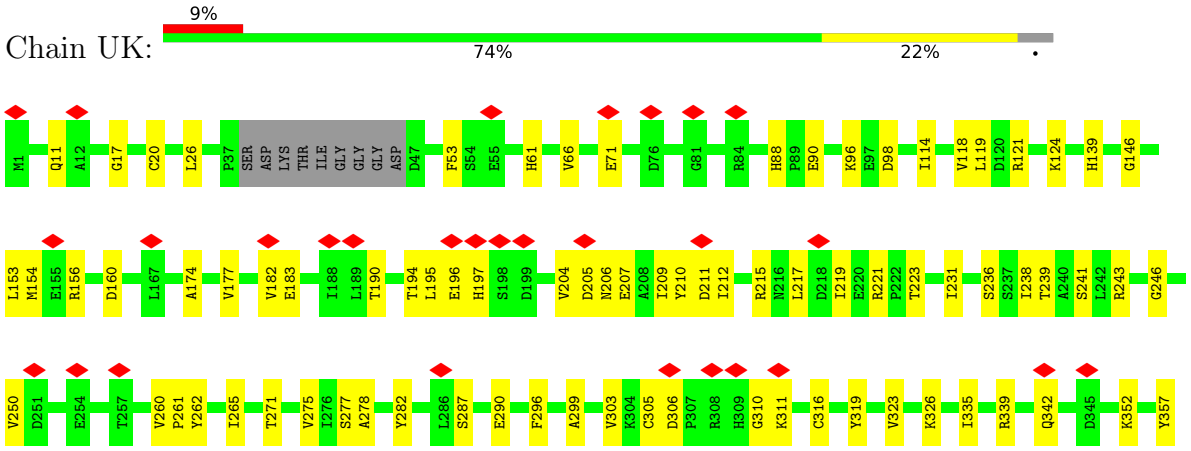
• Molecule 8: Tubulin alpha-3 chain

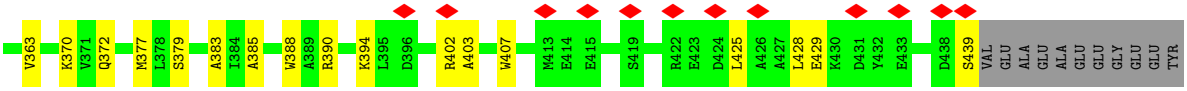
Chain UI:



• Molecule 8: Tubulin alpha-3 chain

Chain UK:

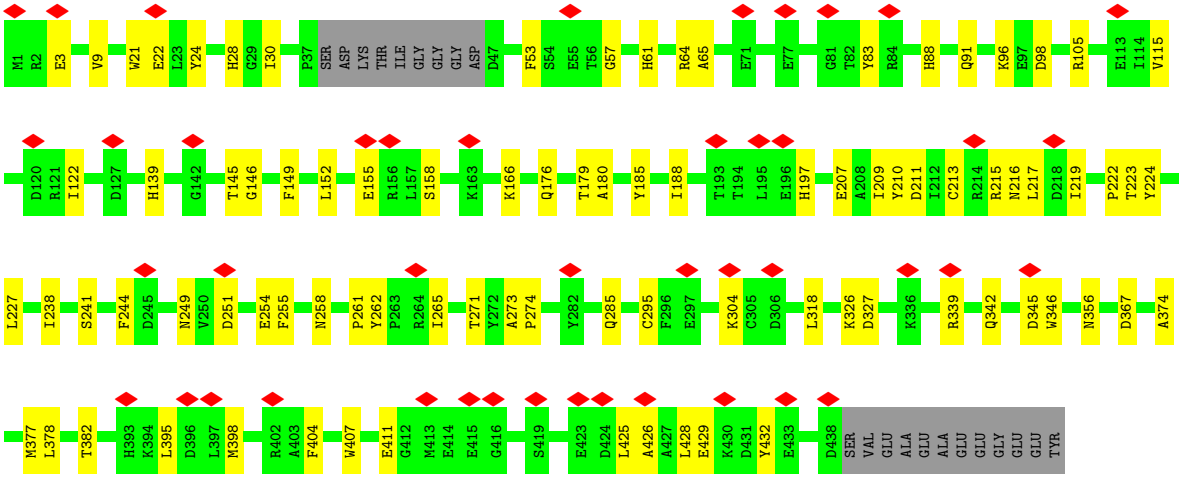




• Molecule 8: Tubulin alpha-3 chain

Chain UM:

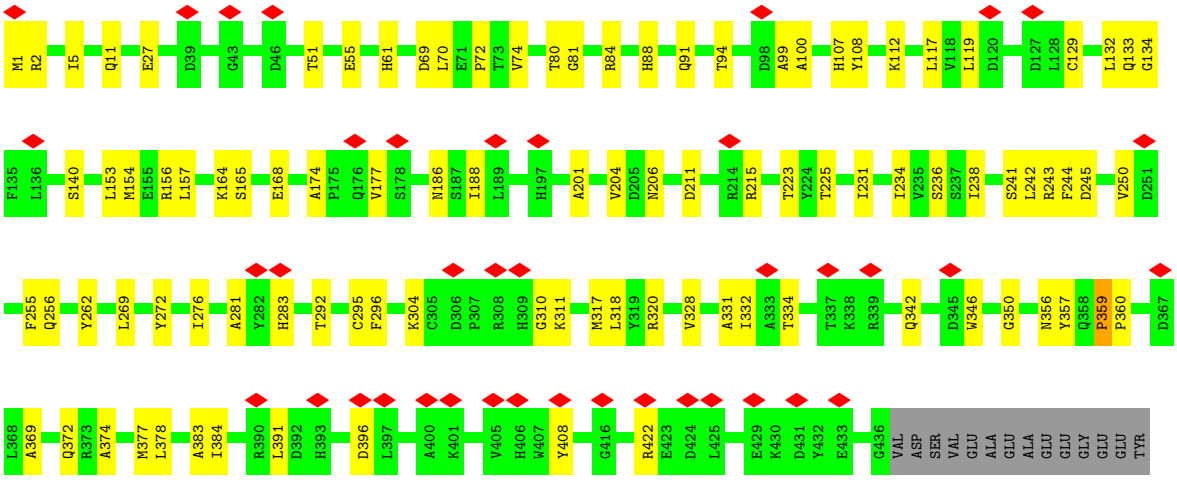




• Molecule 8: Tubulin alpha-3 chain

Chain VC:

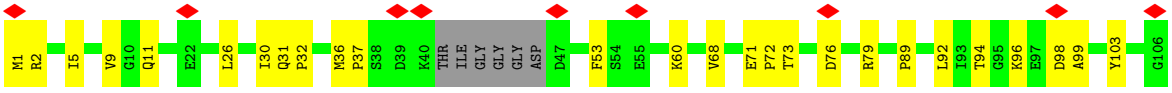


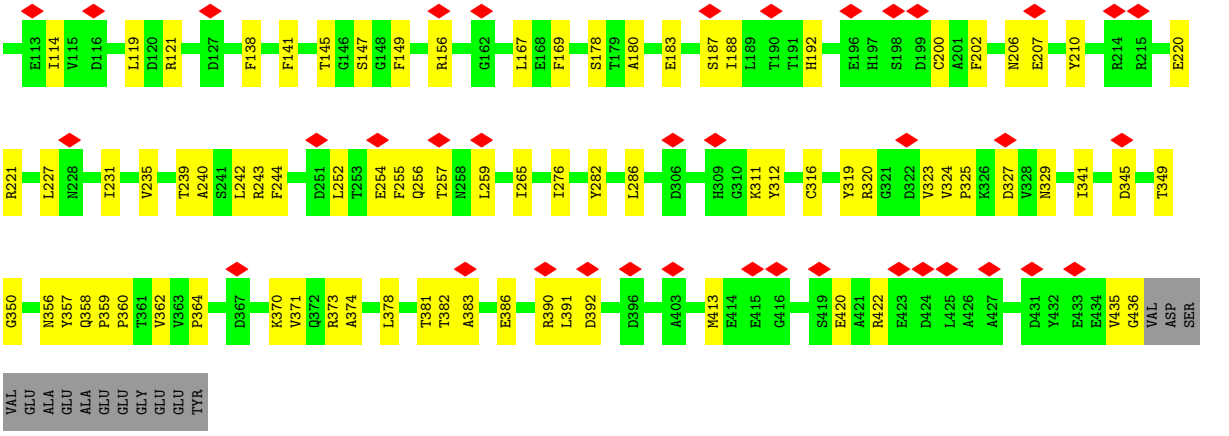


• Molecule 8: Tubulin alpha-3 chain

Chain VE:



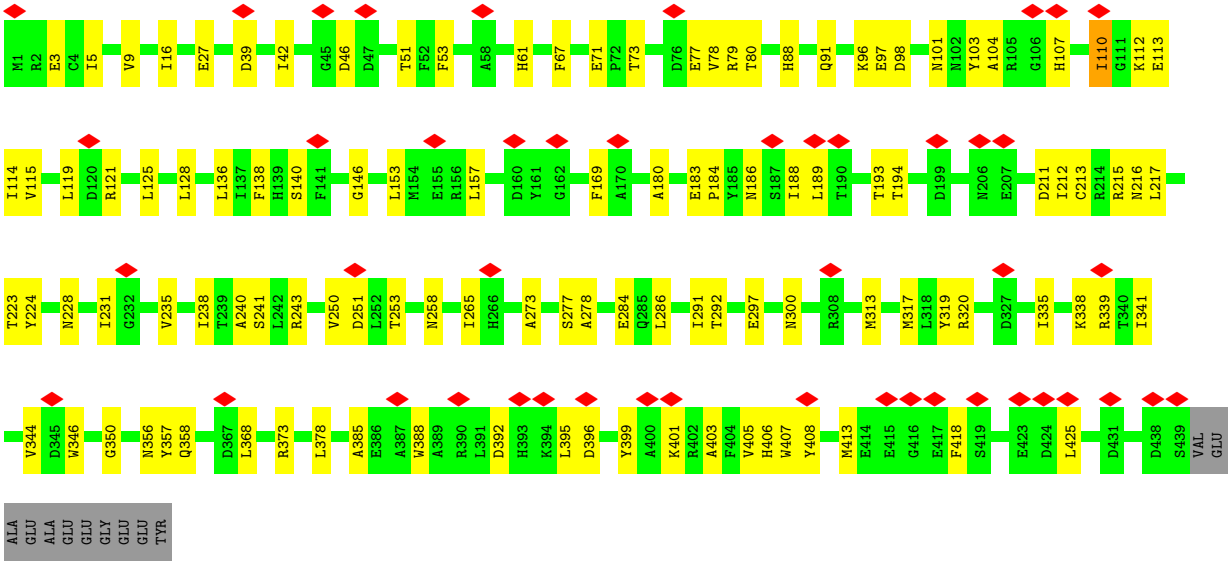




• Molecule 8: Tubulin alpha-3 chain

Chain VG:

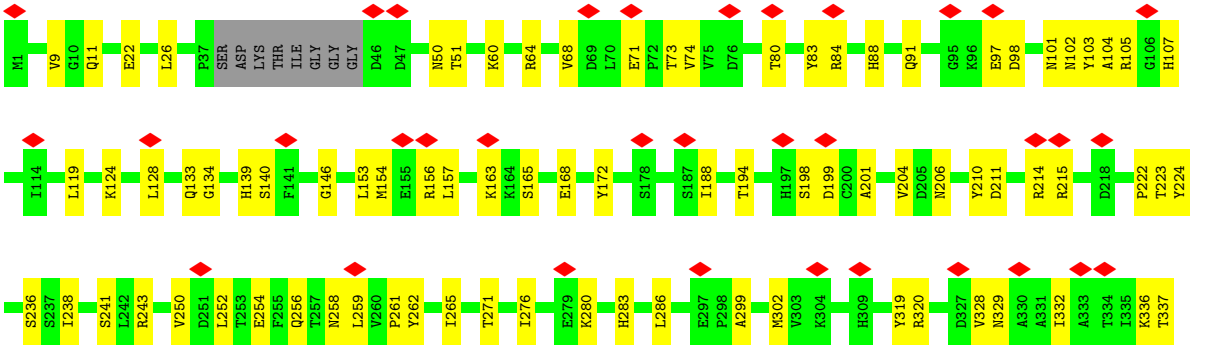


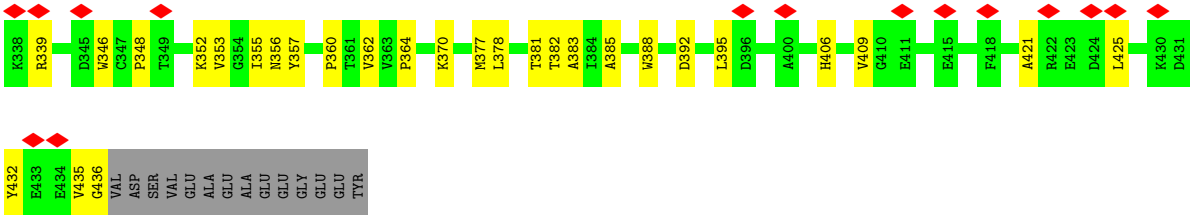


• Molecule 8: Tubulin alpha-3 chain

Chain VI:

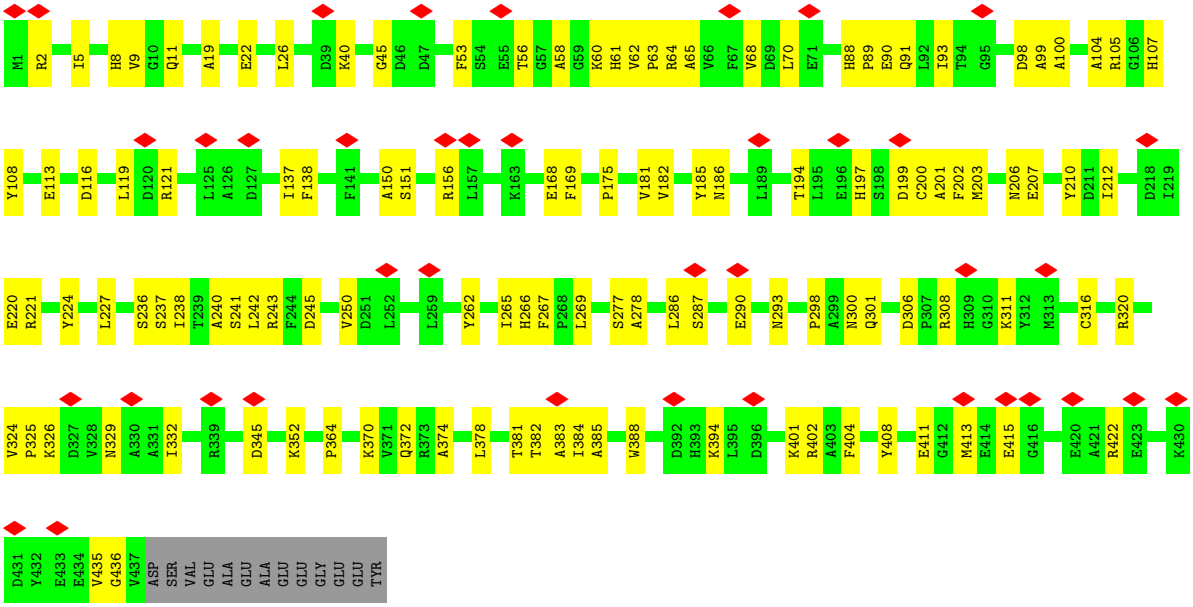




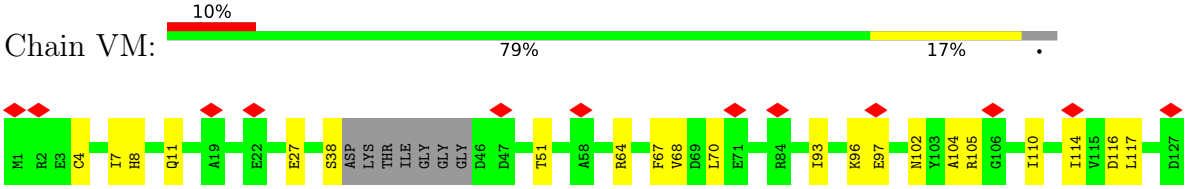


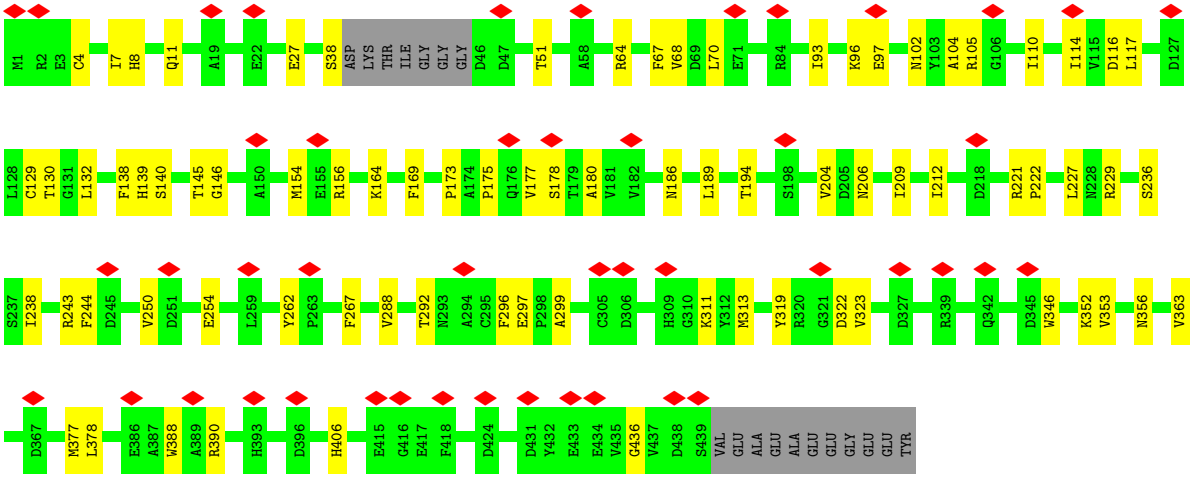
• Molecule 8: Tubulin alpha-3 chain





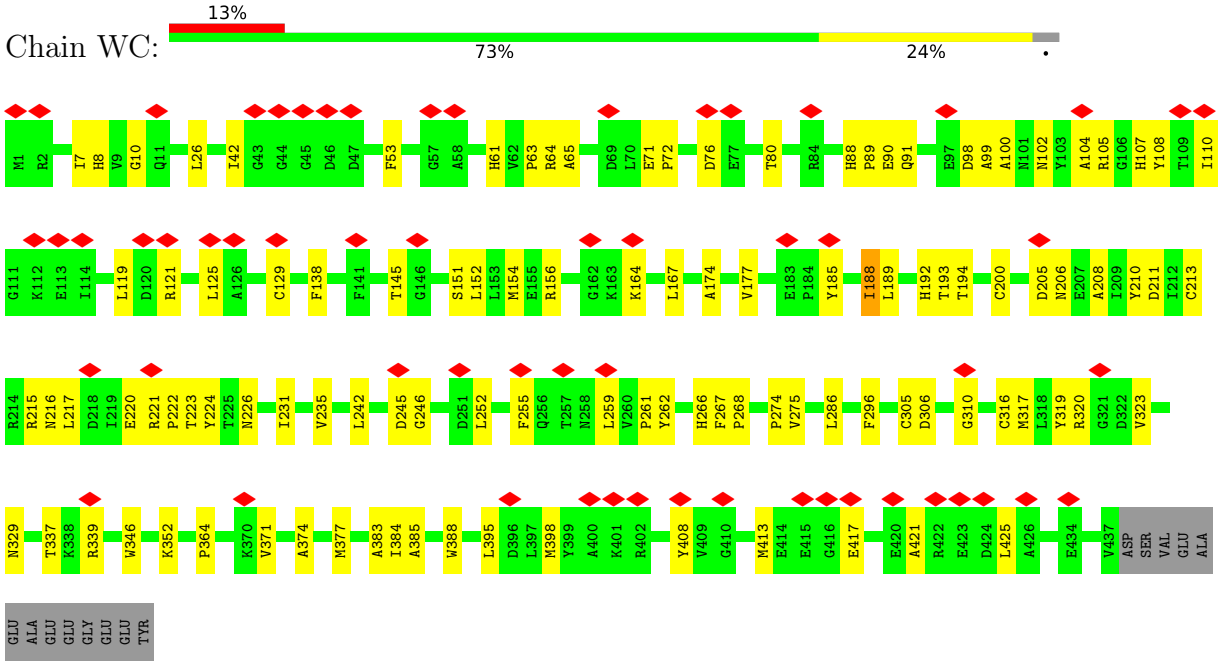
• Molecule 8: Tubulin alpha-3 chain





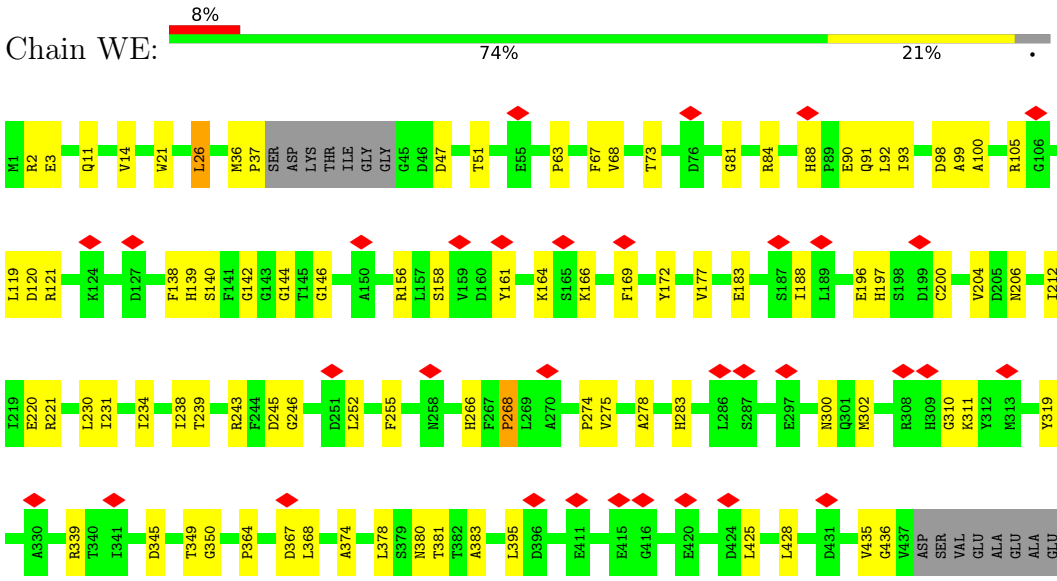
• Molecule 8: Tubulin alpha-3 chain

Chain WC:



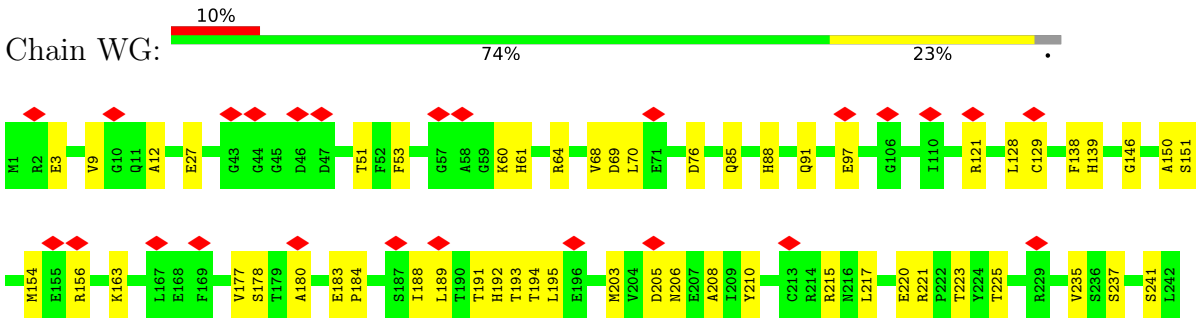
• Molecule 8: Tubulin alpha-3 chain

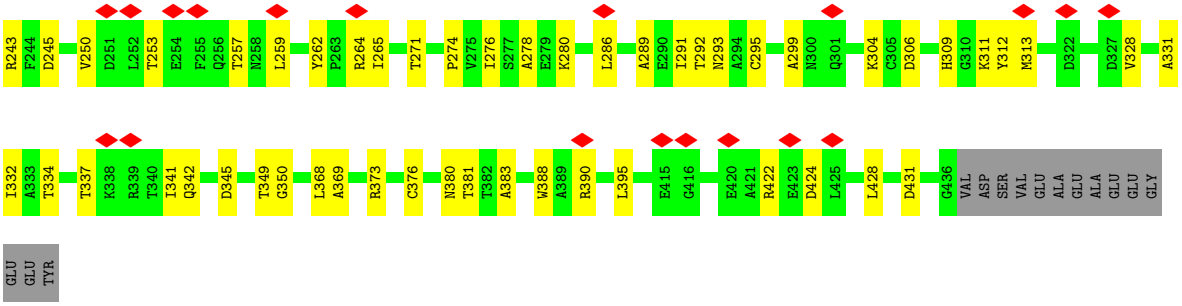
Chain WE:



• Molecule 8: Tubulin alpha-3 chain

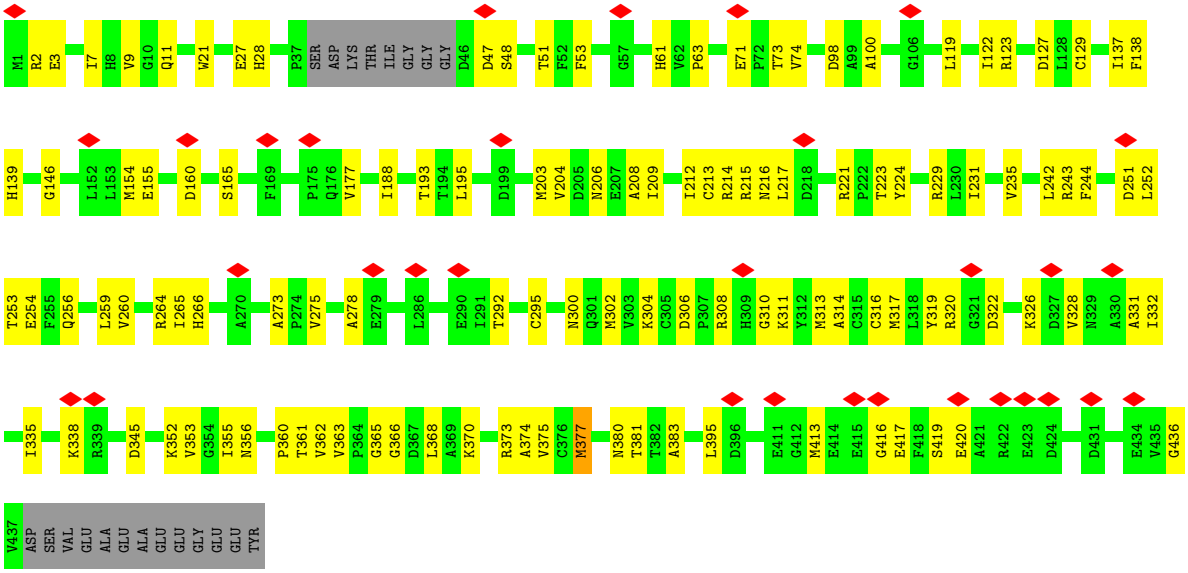
Chain WG:



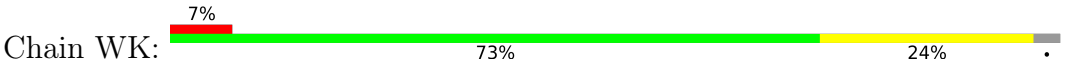


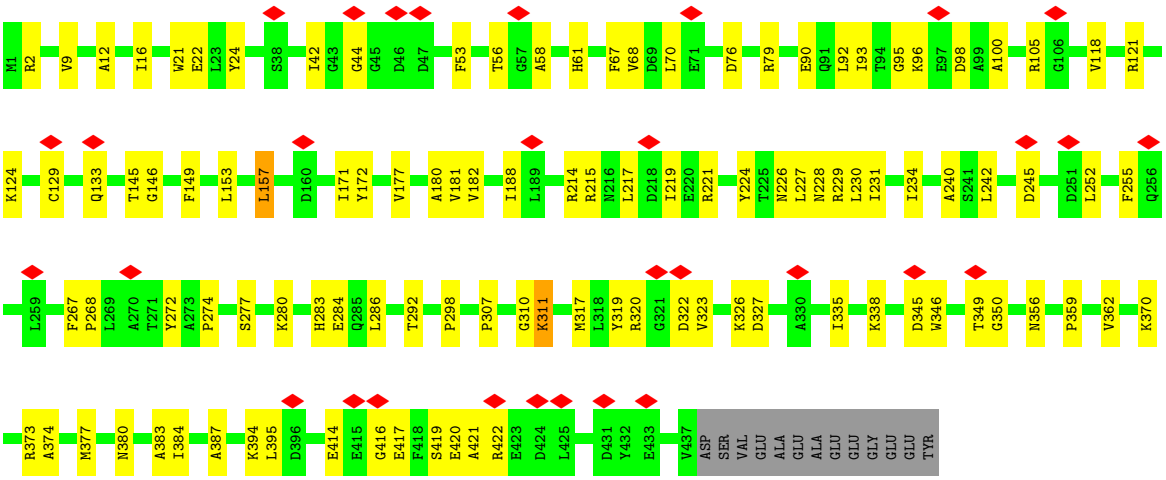
• Molecule 8: Tubulin alpha-3 chain





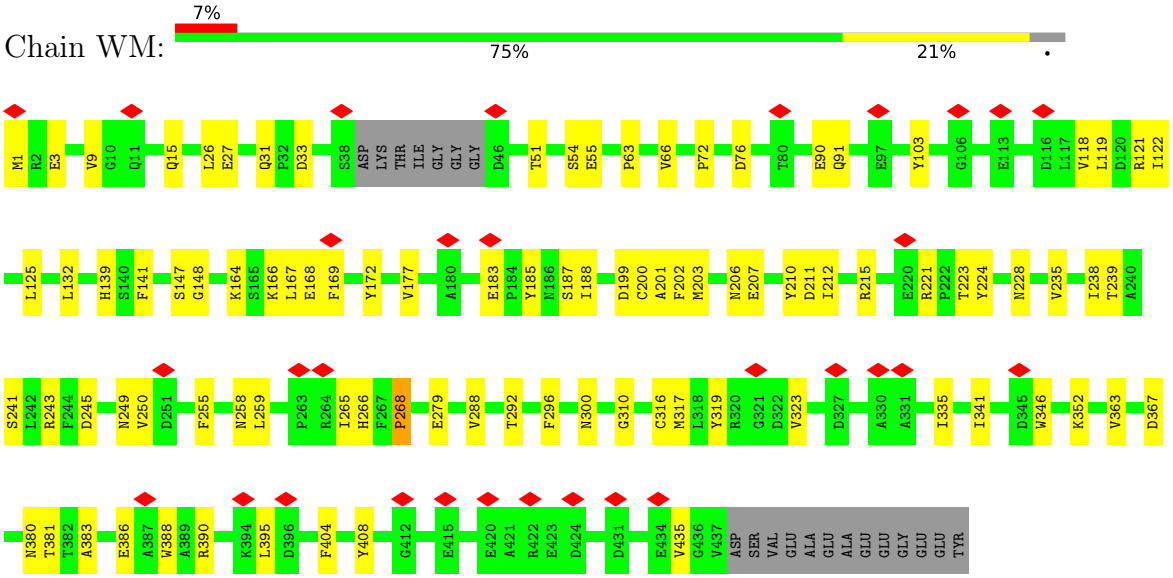
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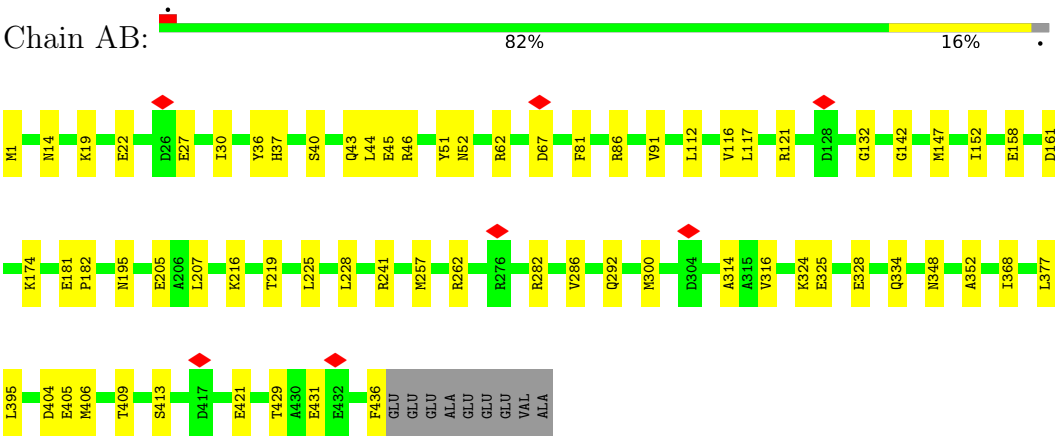
• Molecule 8: Tubulin alpha-3 chain

Chain WM:



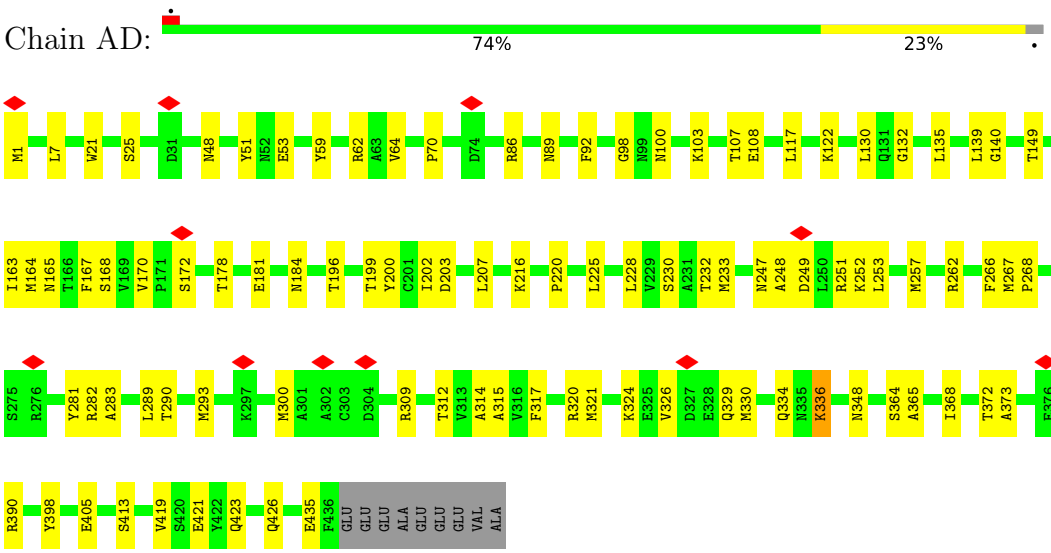
• Molecule 9: Tubulin beta-4B chain

Chain AB:



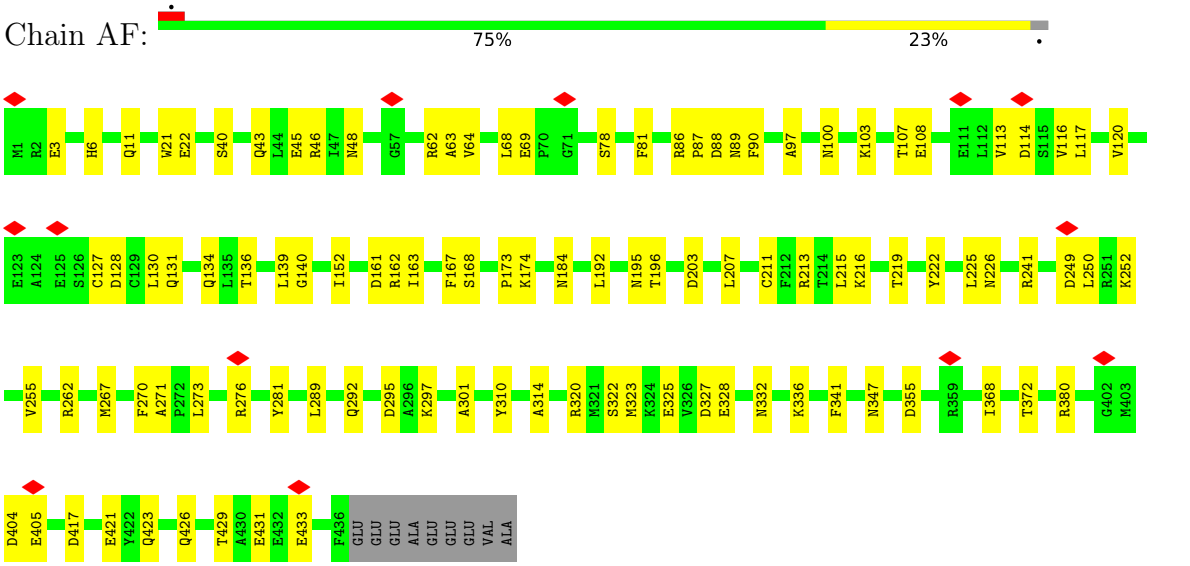
• Molecule 9: Tubulin beta-4B chain

Chain AD:



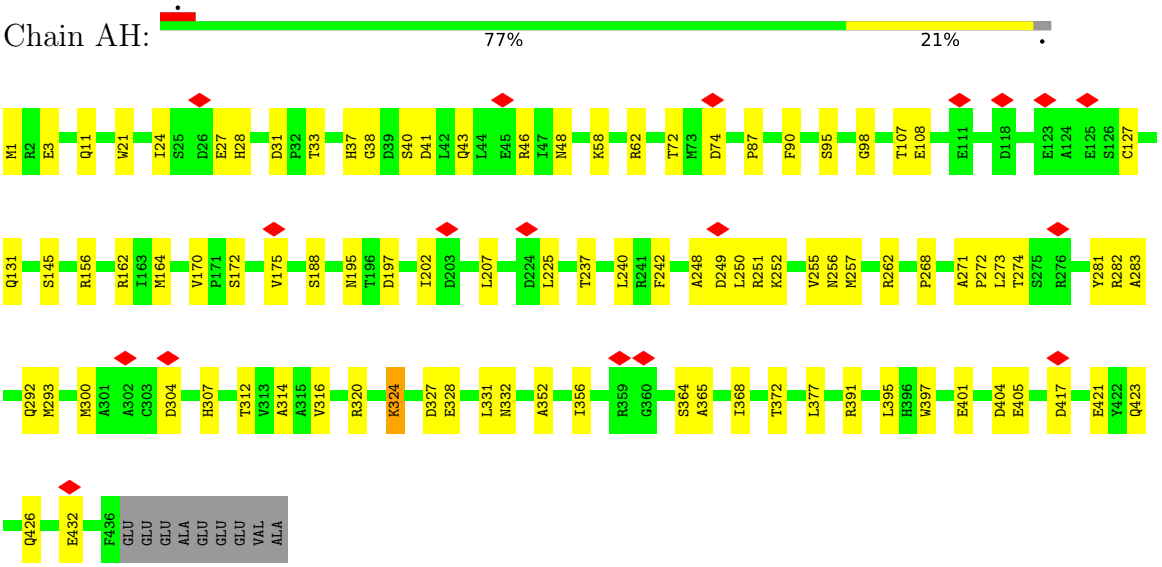
• Molecule 9: Tubulin beta-4B chain

Chain AF:



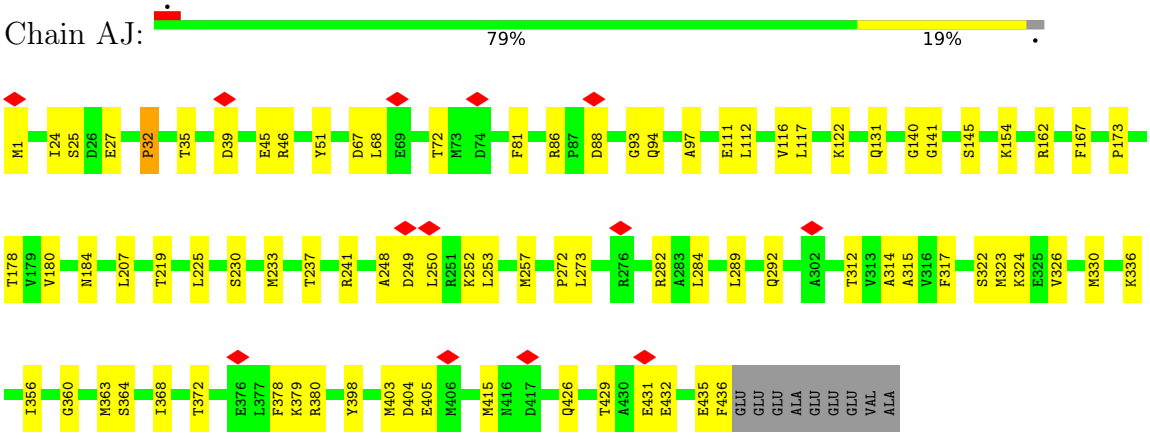
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Chain AH:



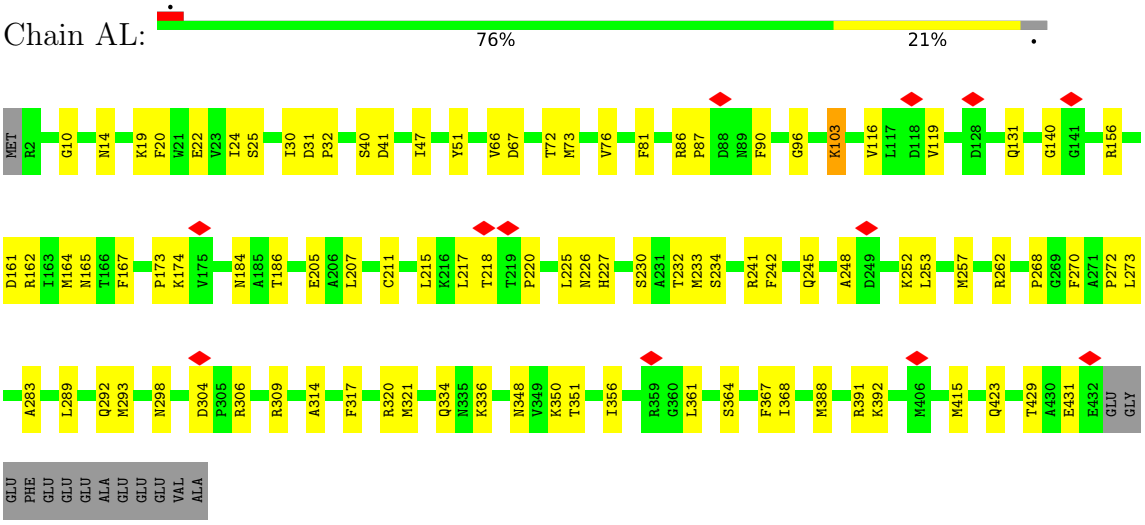
• Molecule 9: Tubulin beta-4B chain

Chain AJ:



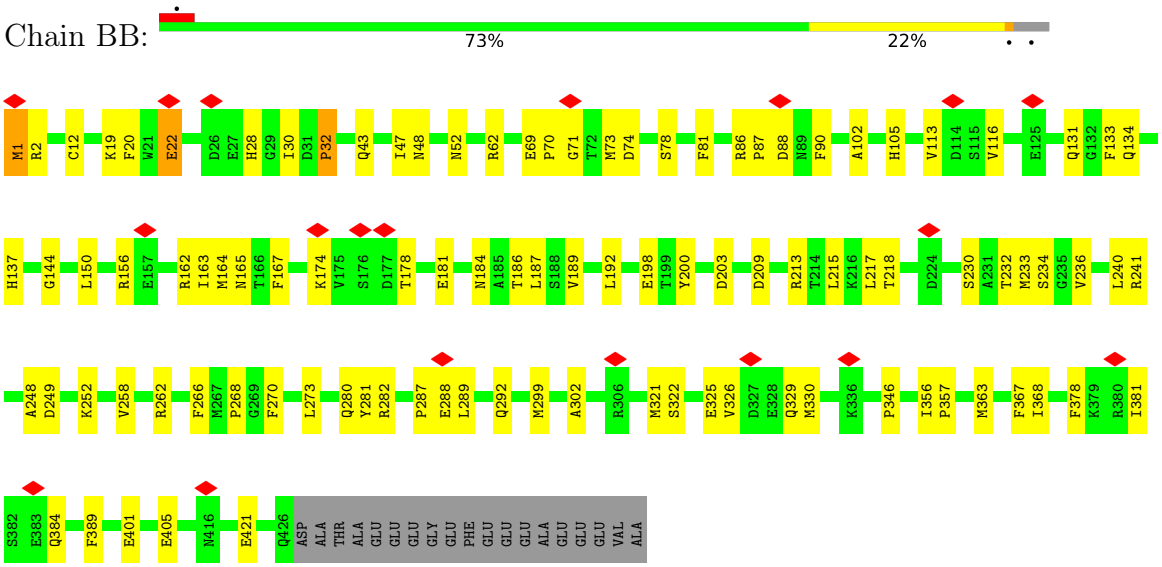
• Molecule 9: Tubulin beta-4B chain

Chain AL:



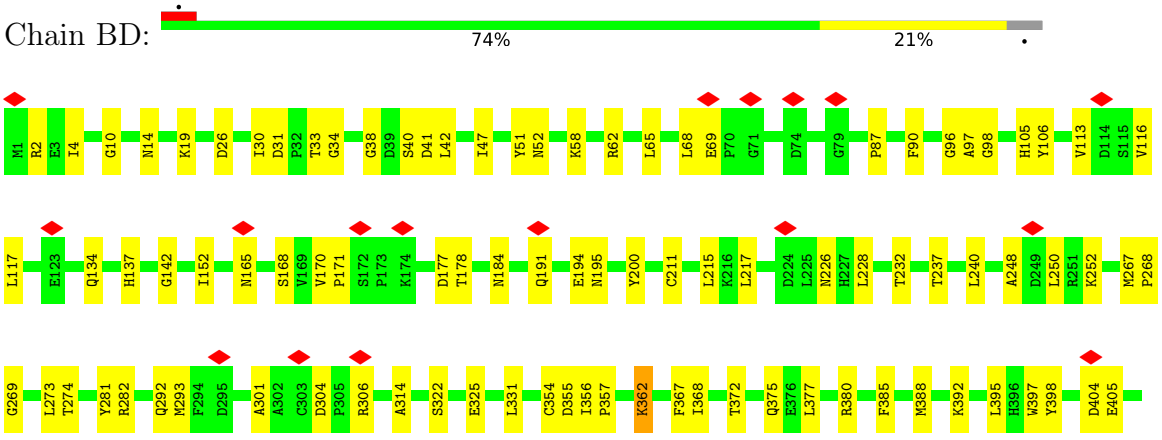
• Molecule 9: Tubulin beta-4B chain

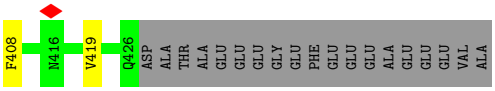
Chain BB:



• Molecule 9: Tubulin beta-4B chain

Chain BD:

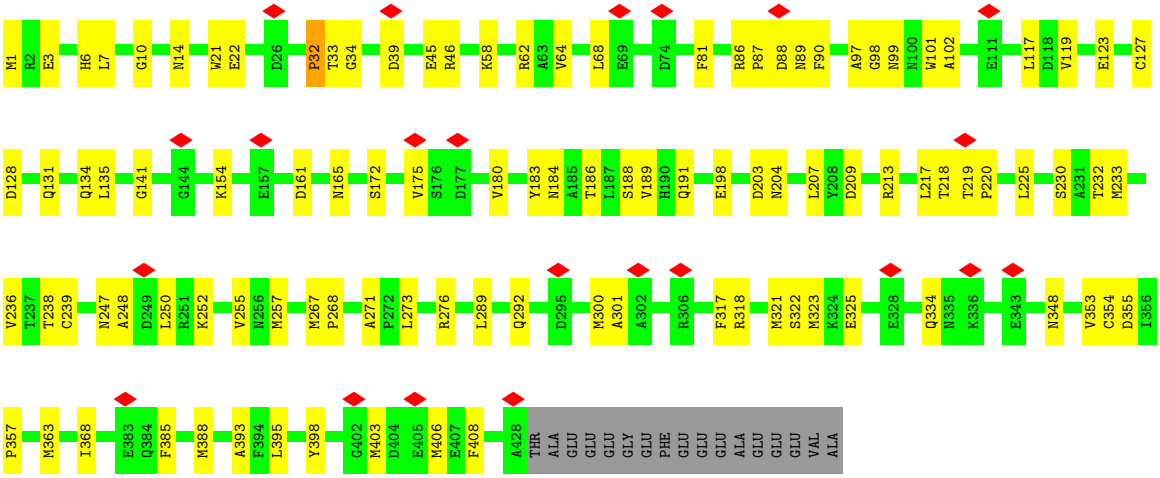




• Molecule 9: Tubulin beta-4B chain

Chain BF:

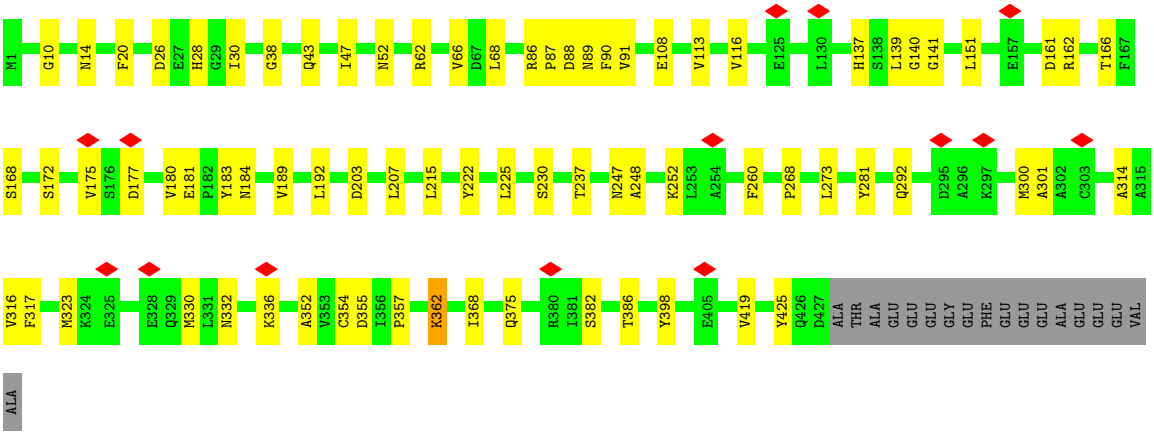




• Molecule 9: Tubulin beta-4B chain

Chain BH:

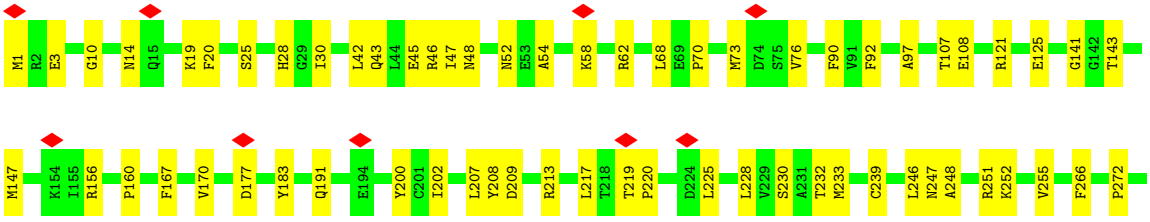


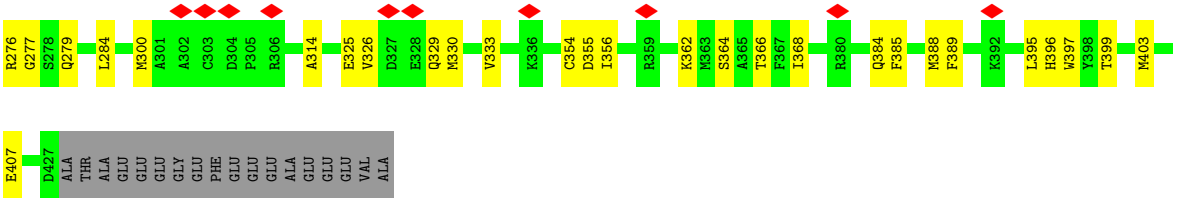


• Molecule 9: Tubulin beta-4B chain

Chain BJ:



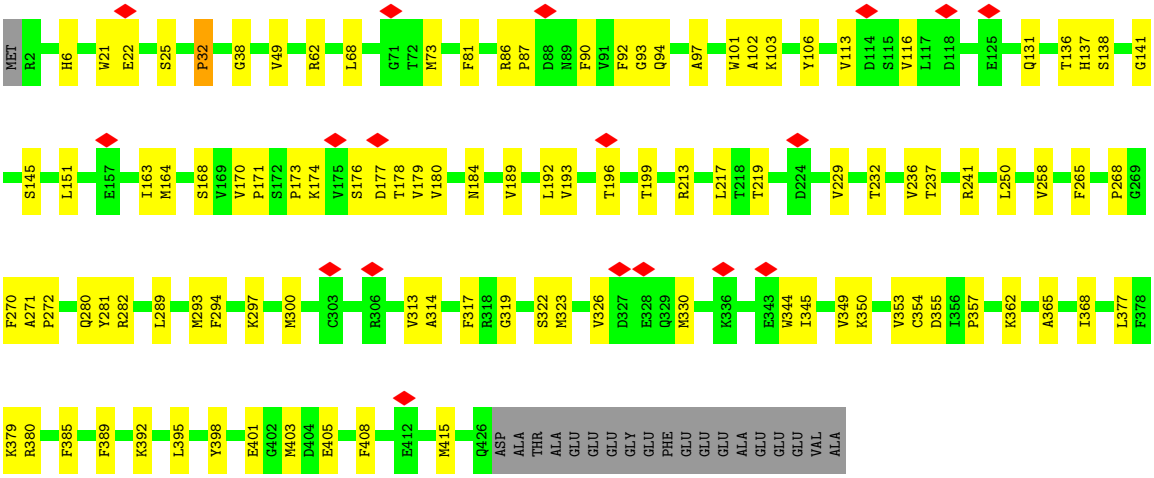




• Molecule 9: Tubulin beta-4B chain

Chain BL:

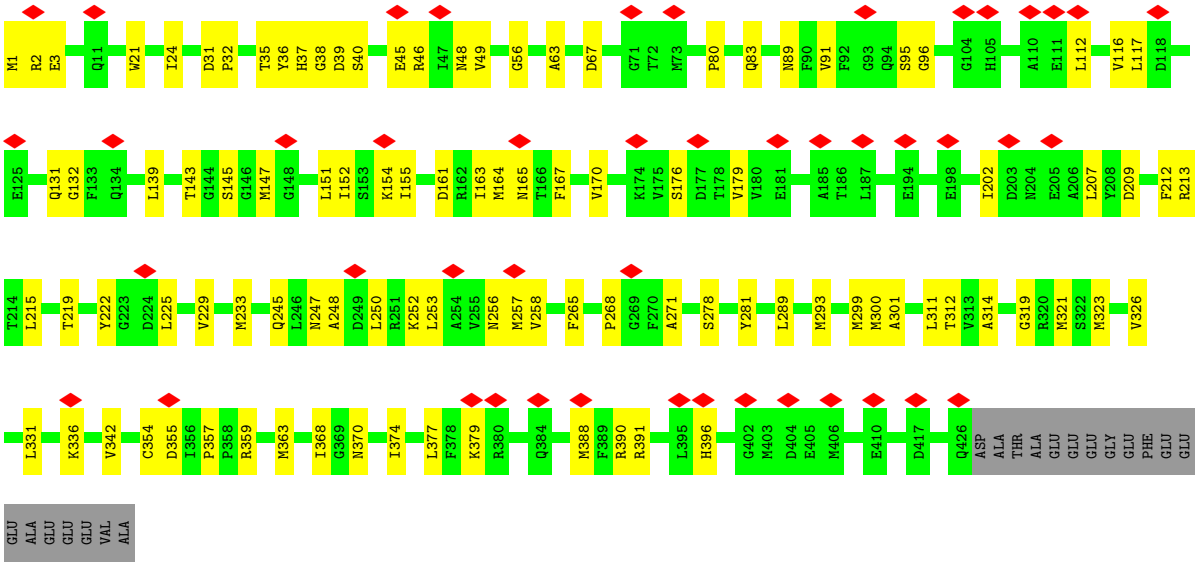




• Molecule 9: Tubulin beta-4B chain

Chain CB:

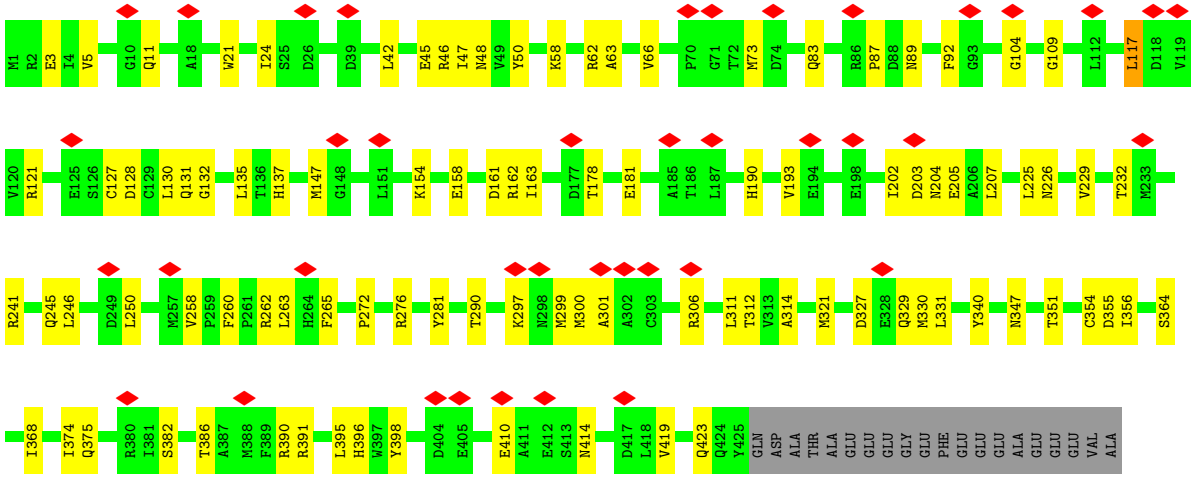




• Molecule 9: Tubulin beta-4B chain

Chain CD:

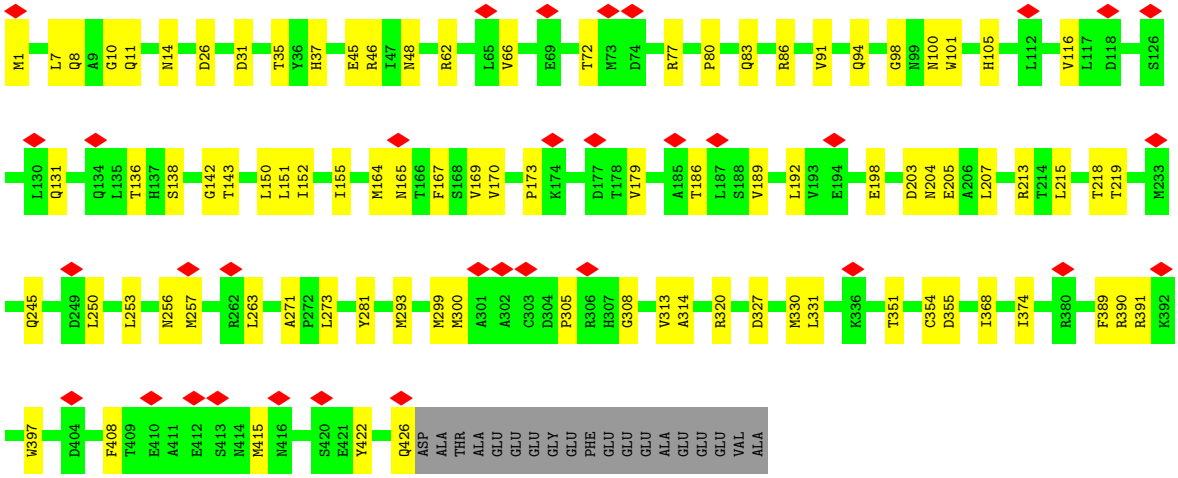




• Molecule 9: Tubulin beta-4B chain

Chain CF:

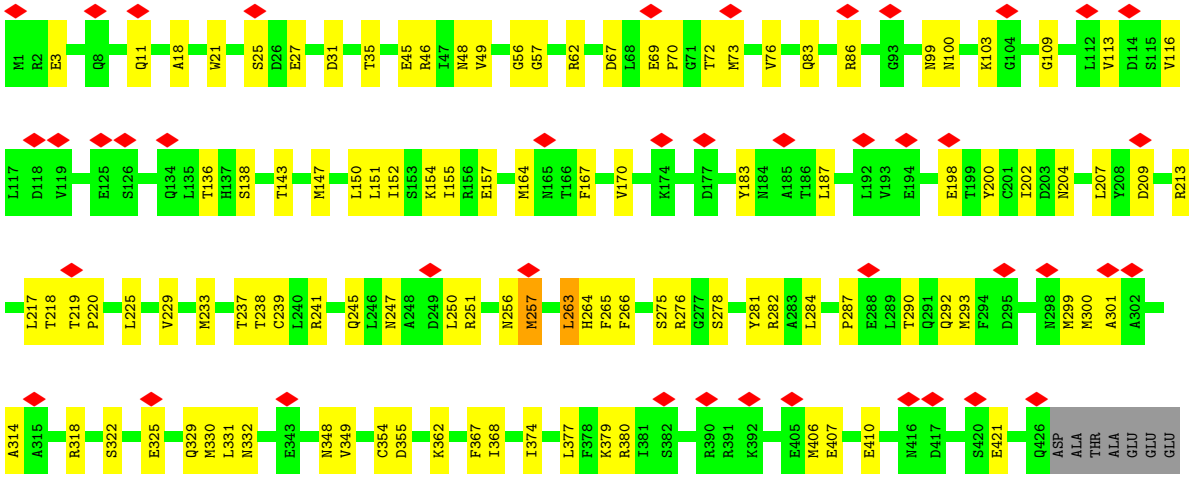




• Molecule 9: Tubulin beta-4B chain

Chain CH:



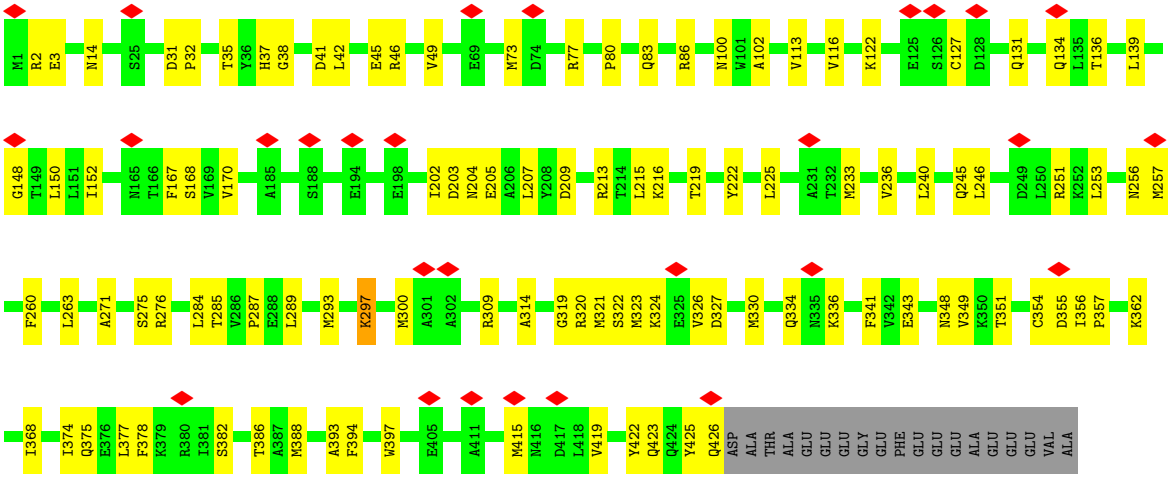




• Molecule 9: Tubulin beta-4B chain

Chain CJ:

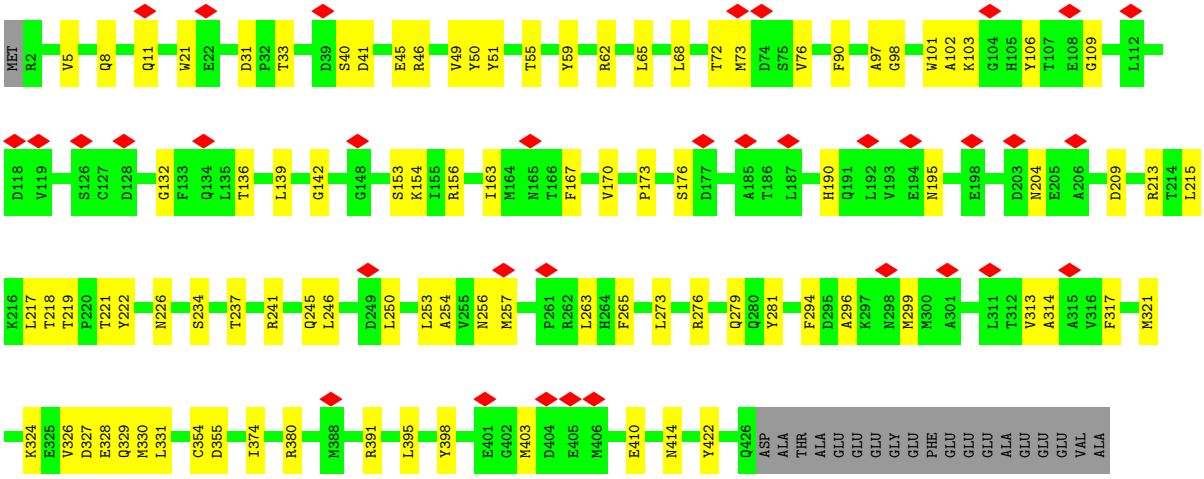




• Molecule 9: Tubulin beta-4B chain

Chain CL:

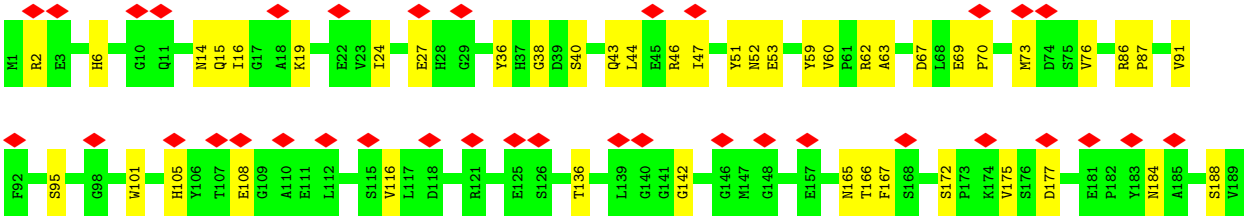


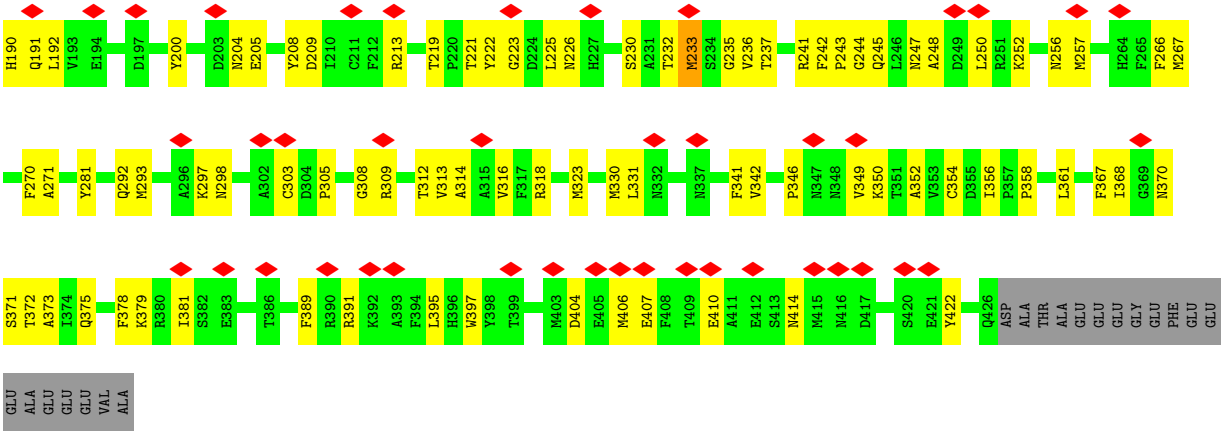


• Molecule 9: Tubulin beta-4B chain

Chain DB:



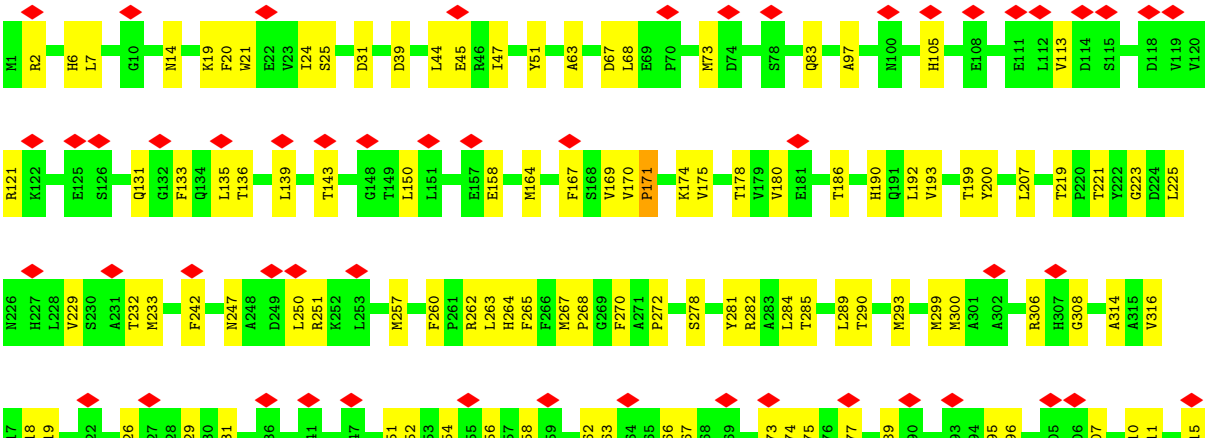




• Molecule 9: Tubulin beta-4B chain

Chain DD:

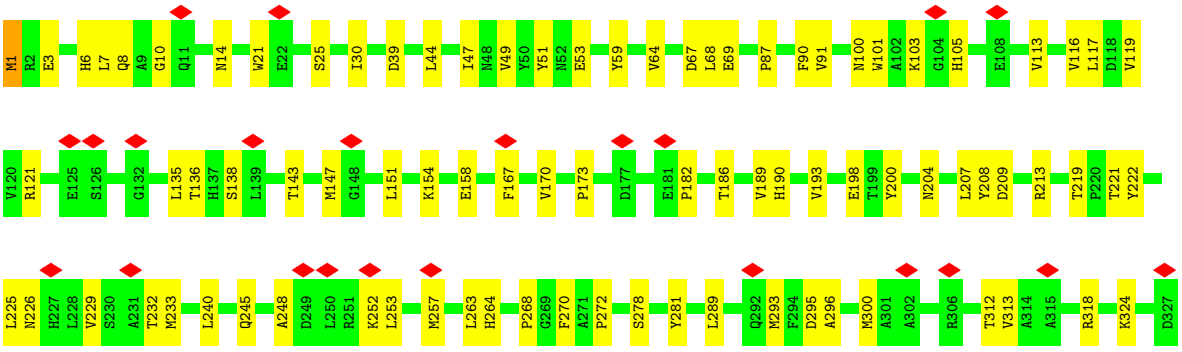


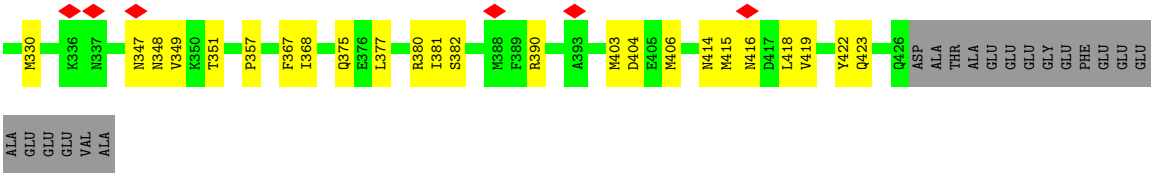


• Molecule 9: Tubulin beta-4B chain

Chain DF:



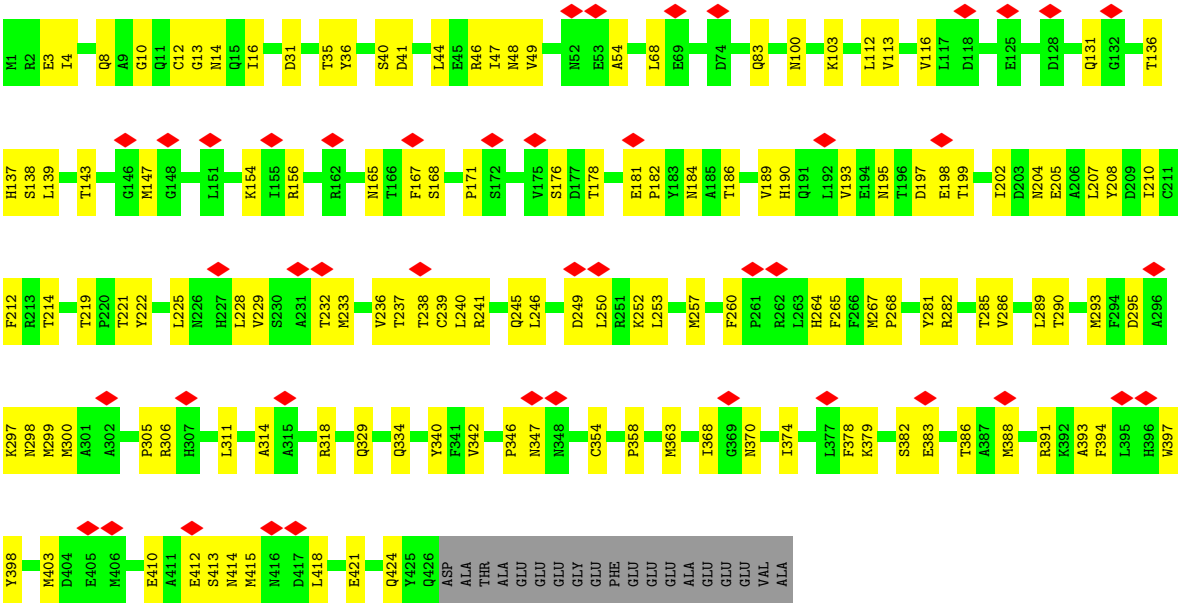




• Molecule 9: Tubulin beta-4B chain

Chain DH:

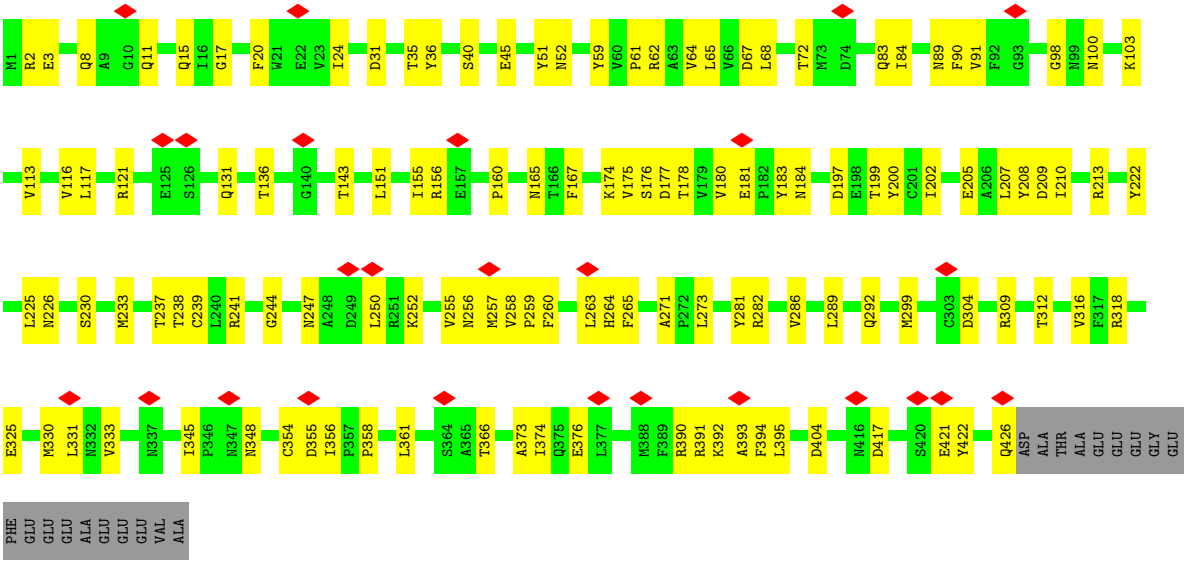




• Molecule 9: Tubulin beta-4B chain

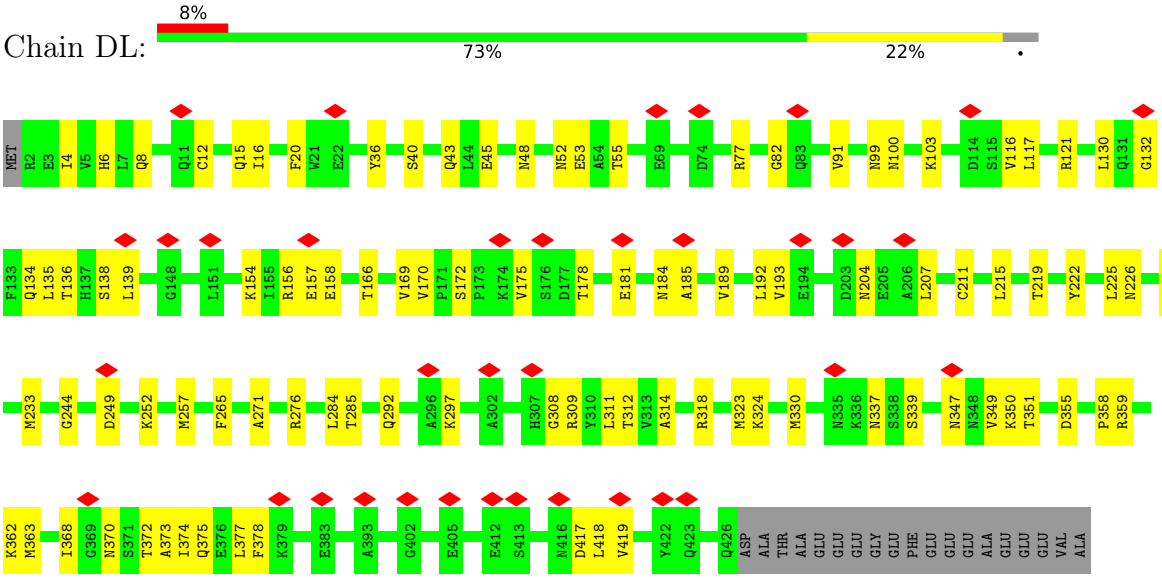
Chain DJ:





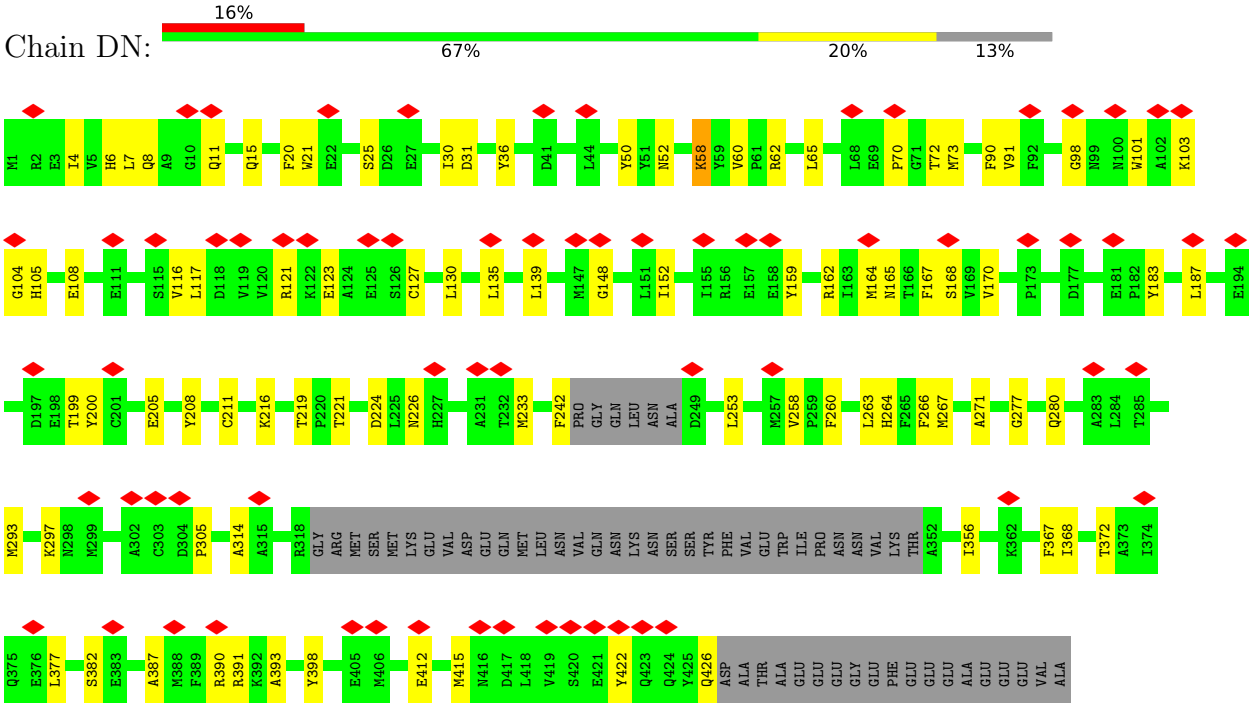
• Molecule 9: Tubulin beta-4B chain

Chain DL:



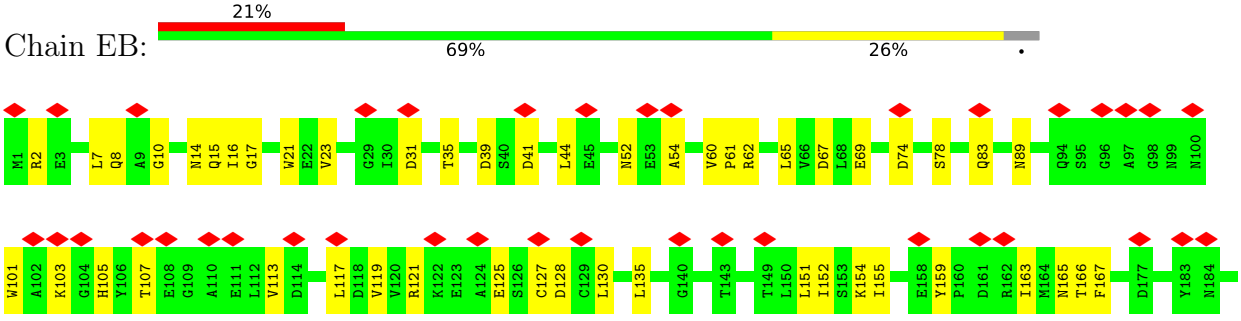
• Molecule 9: Tubulin beta-4B chain

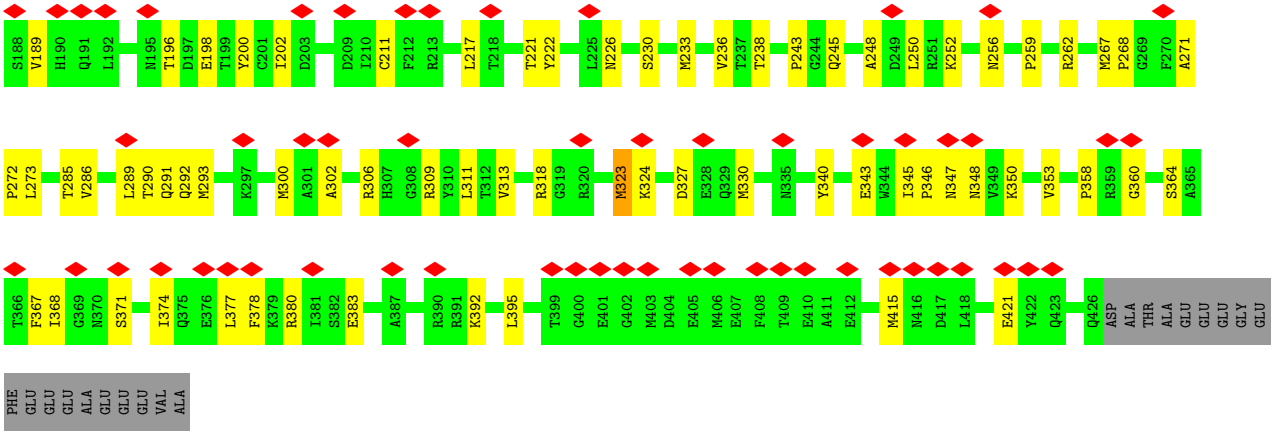
Chain DN:



• Molecule 9: Tubulin beta-4B chain

Chain EB:

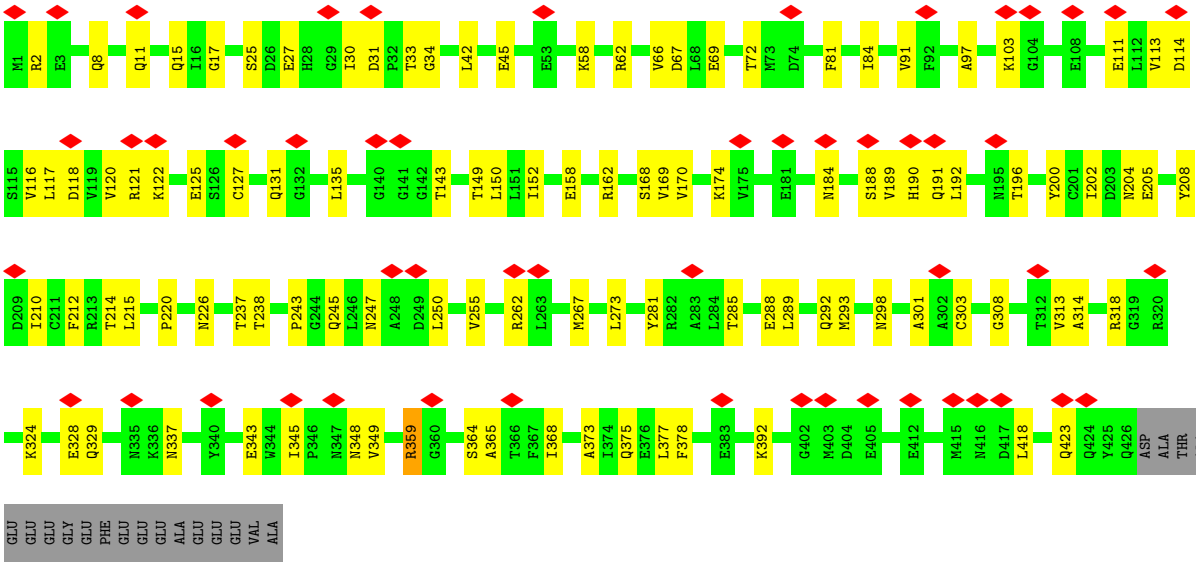




• Molecule 9: Tubulin beta-4B chain

Chain ED:

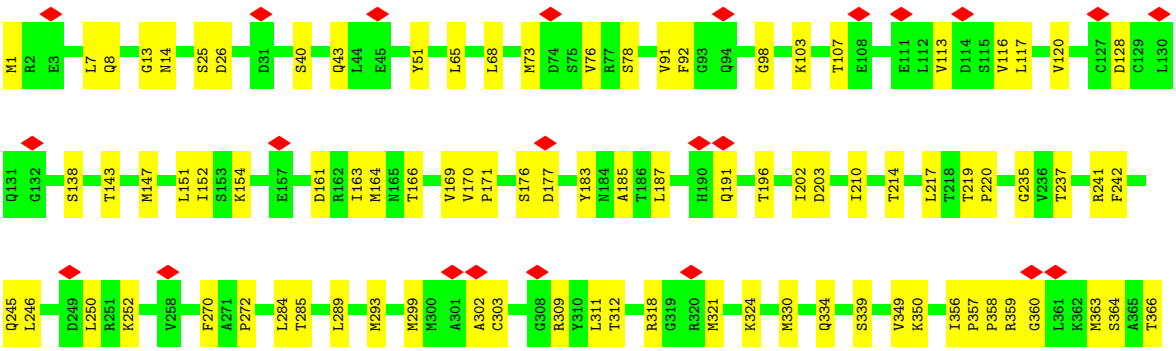


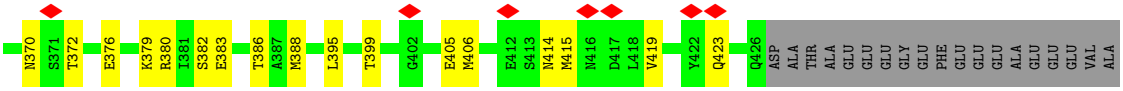


• Molecule 9: Tubulin beta-4B chain

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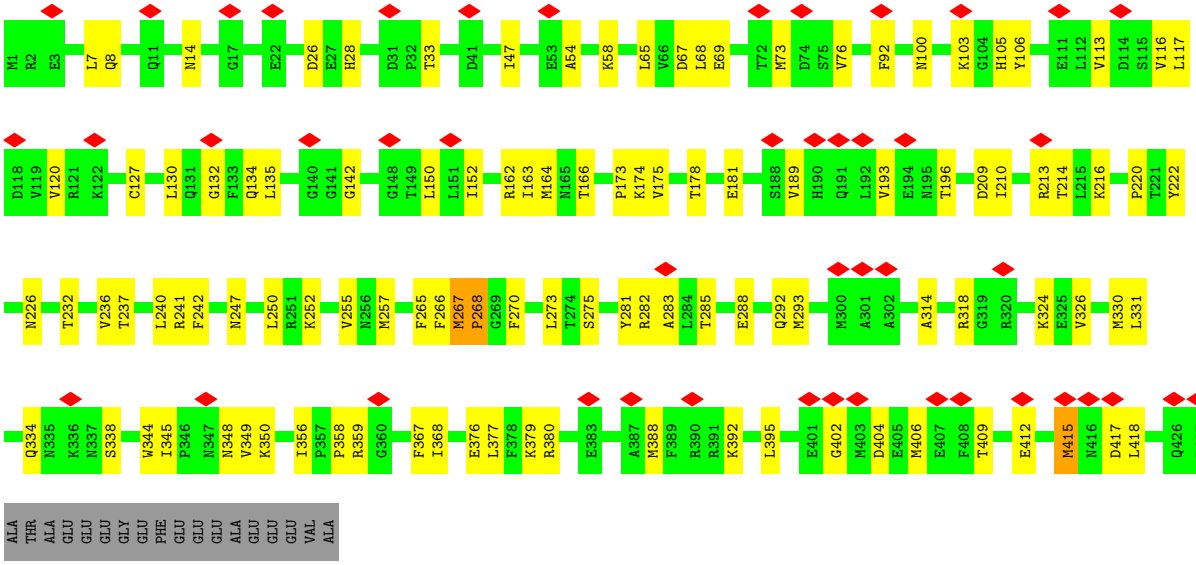




• Molecule 9: Tubulin beta-4B chain

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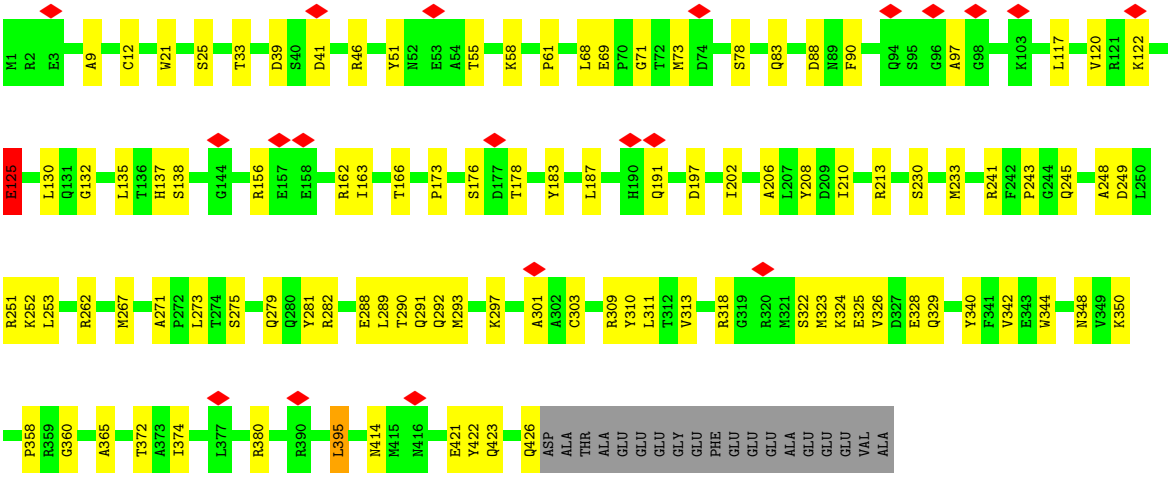




• Molecule 9: Tubulin beta-4B chain

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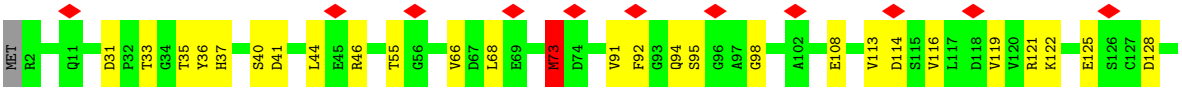


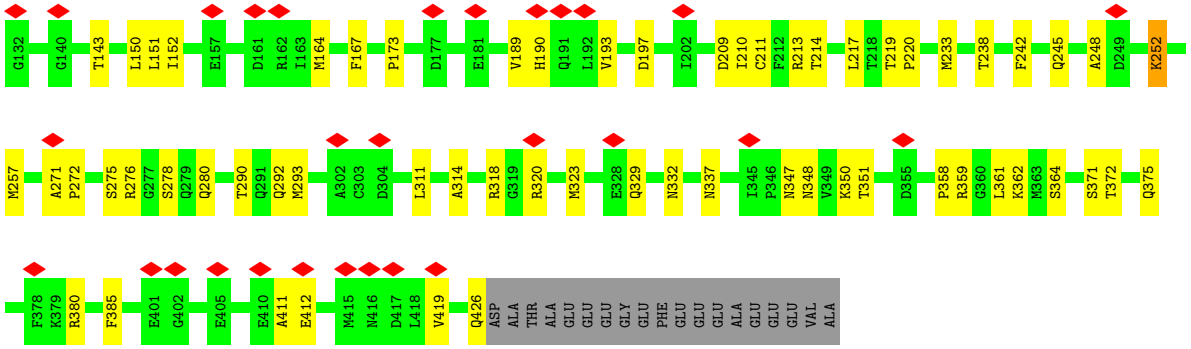


• Molecule 9: Tubulin beta-4B chain

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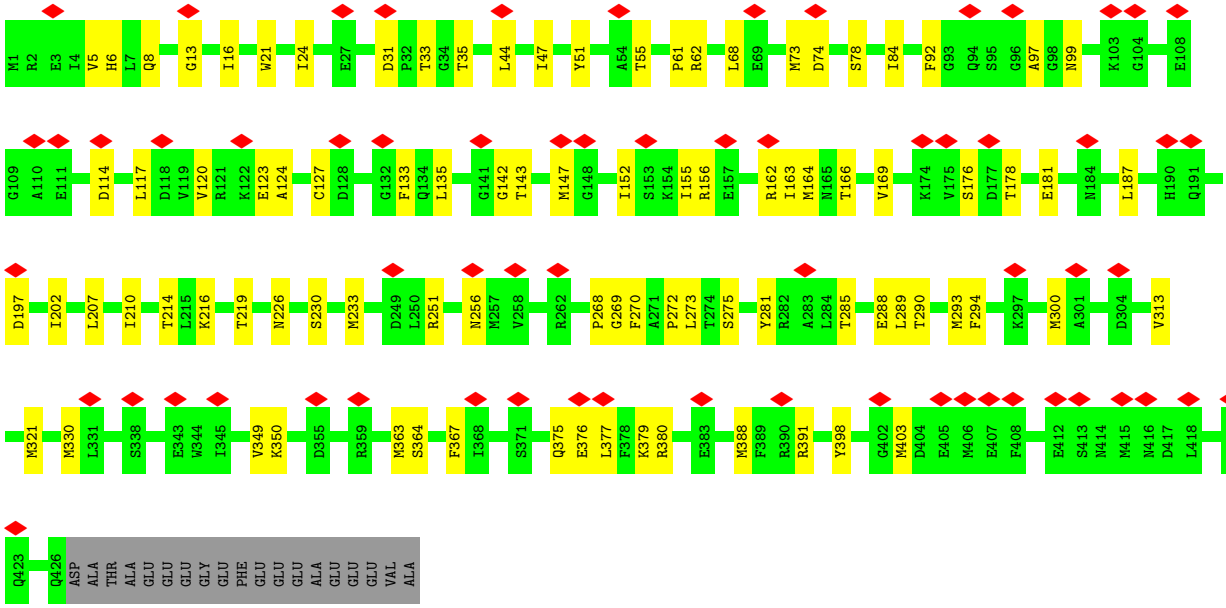




• Molecule 9: Tubulin beta-4B chain

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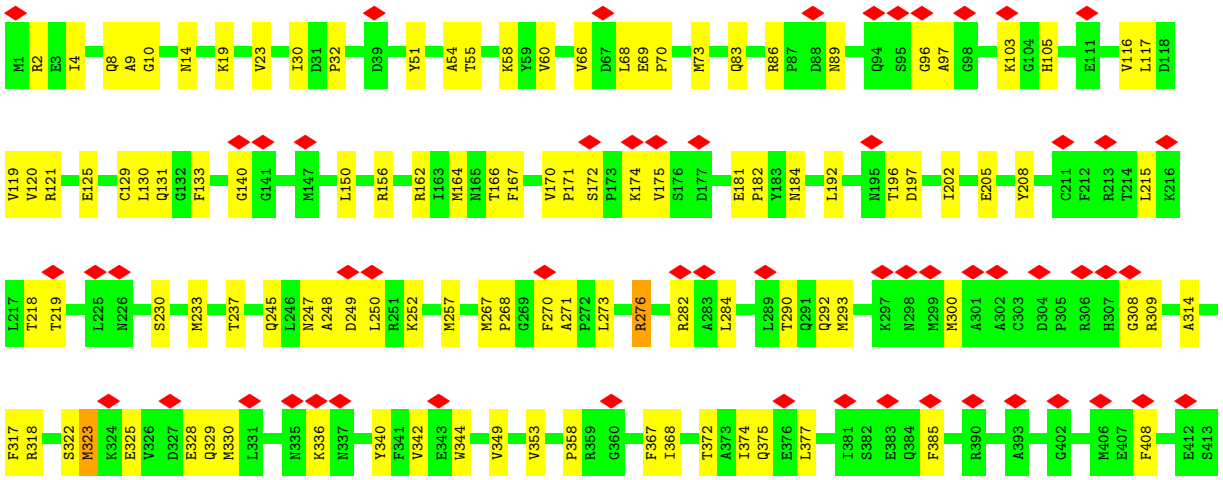


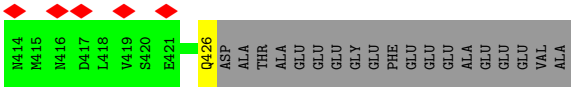


• Molecule 9: Tubulin beta-4B chain

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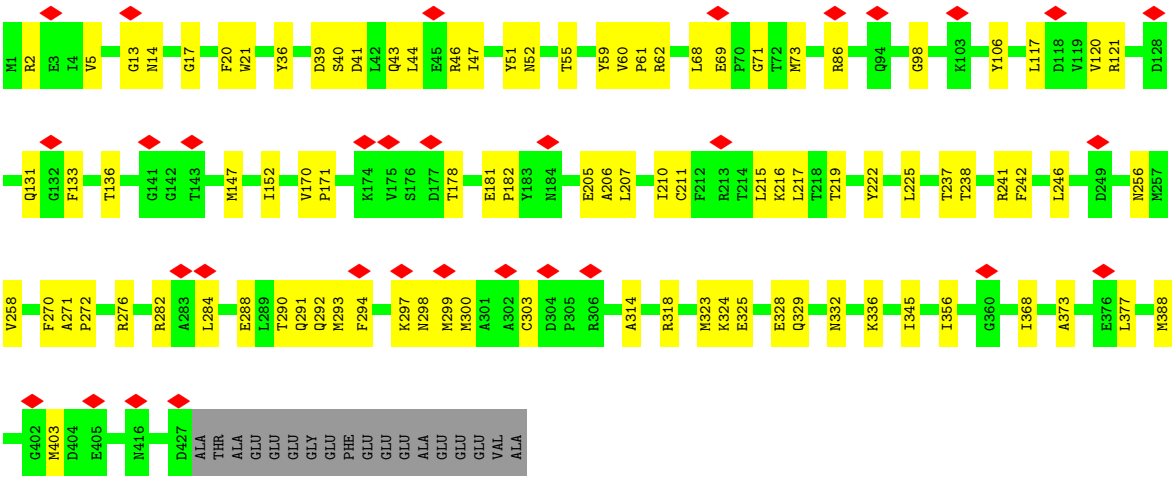




• Molecule 9: Tubulin beta-4B chain

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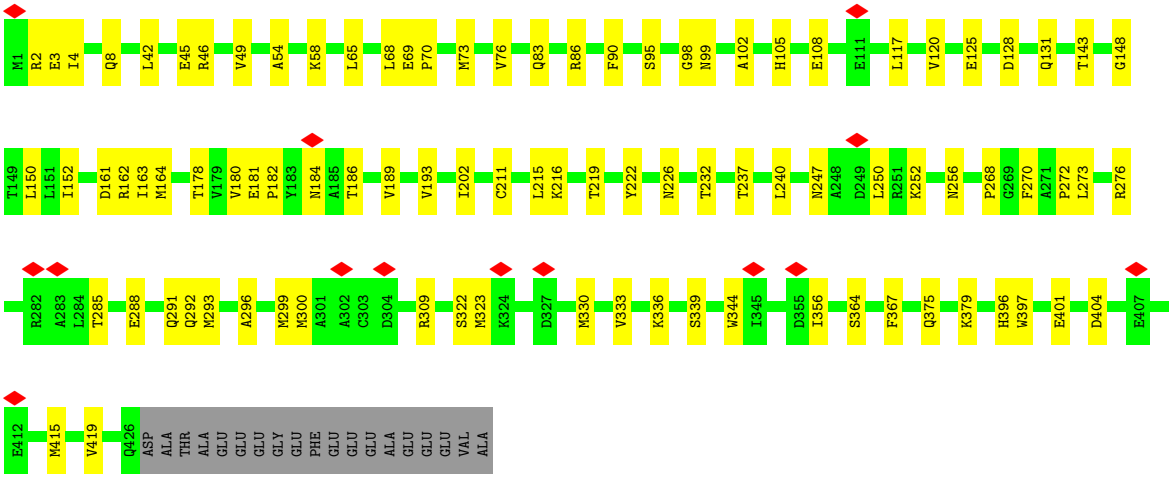




• Molecule 9: Tubulin beta-4B chain

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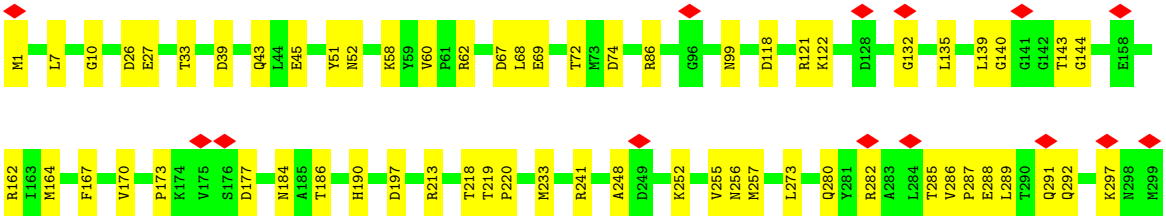


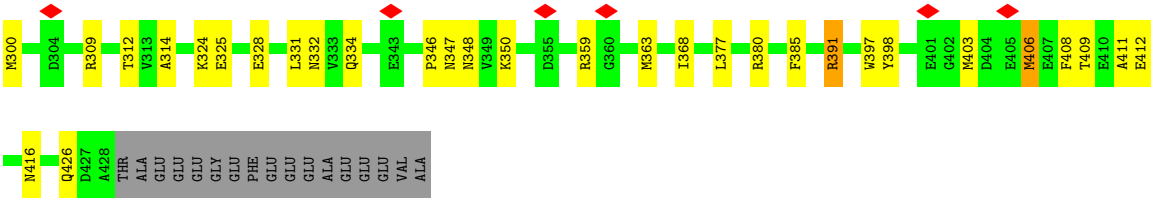


• Molecule 9: Tubulin beta-4B chain

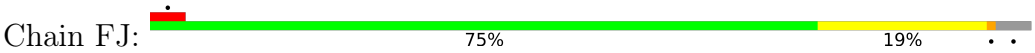
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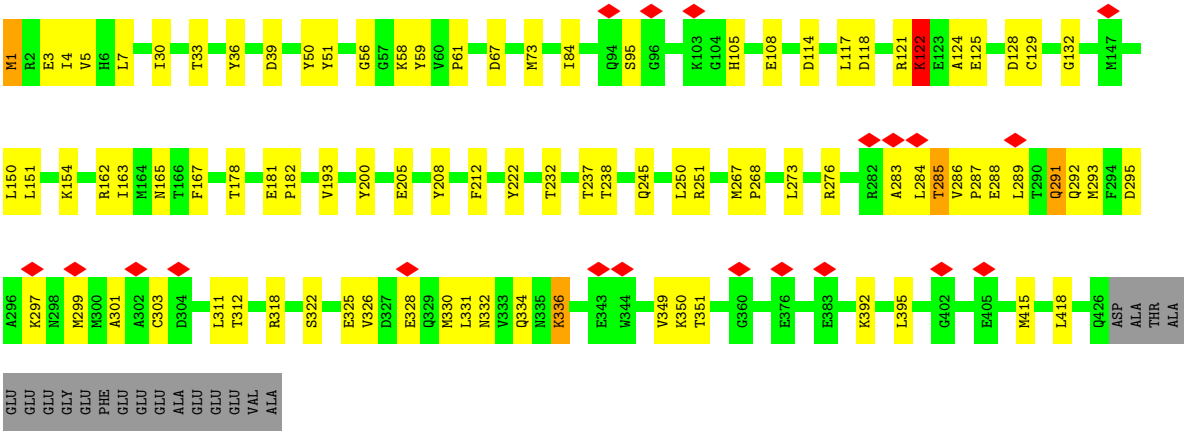




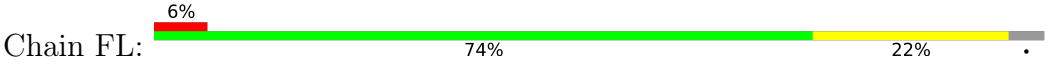


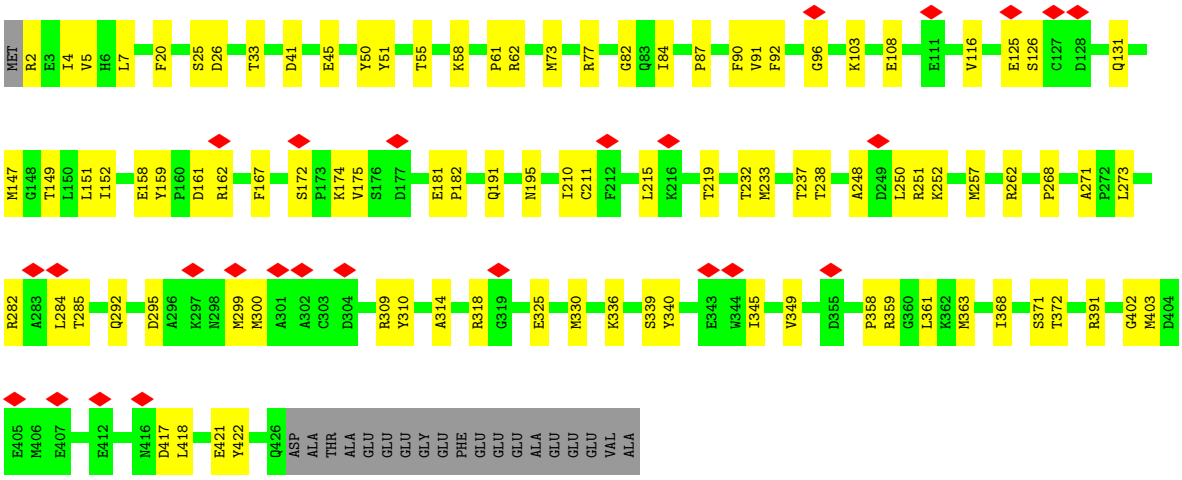
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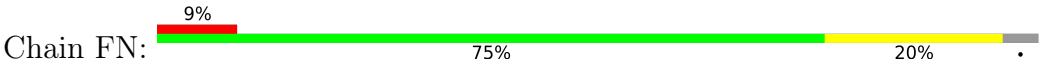


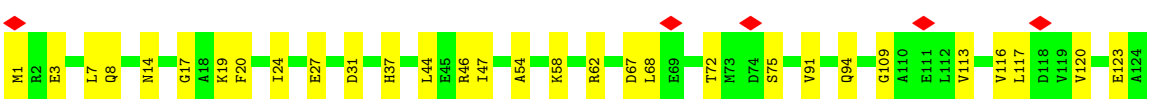
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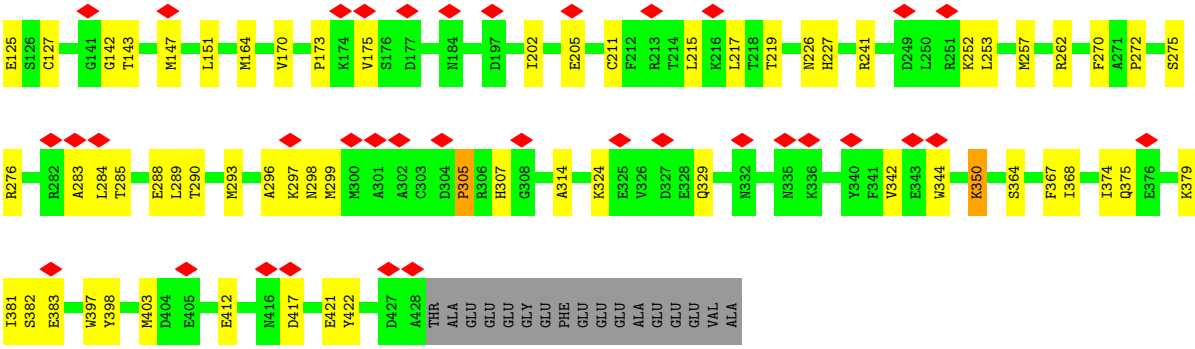




• Molecule 9: Tubulin beta-4B chain



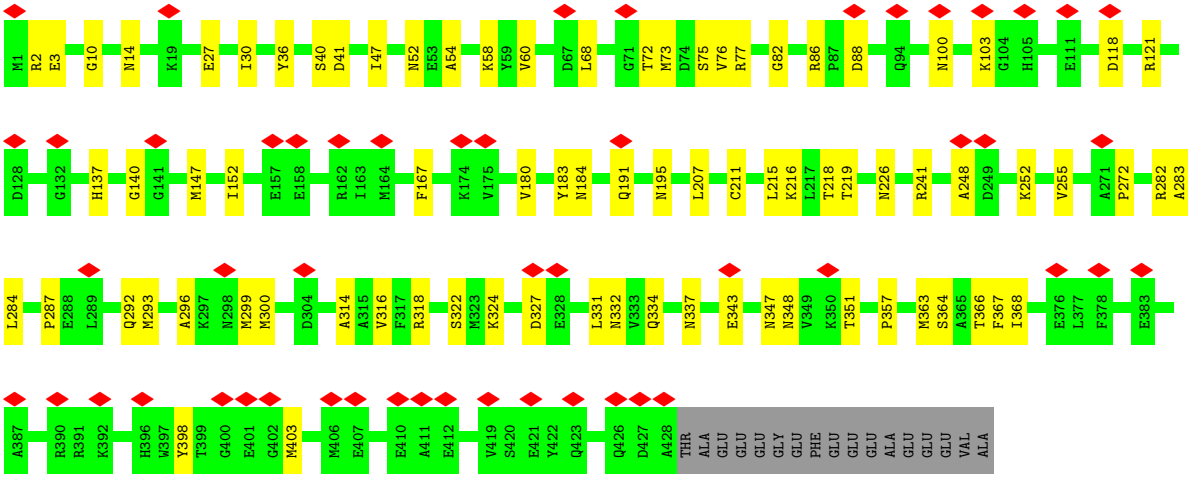




• Molecule 9: Tubulin beta-4B chain

Chain GB:

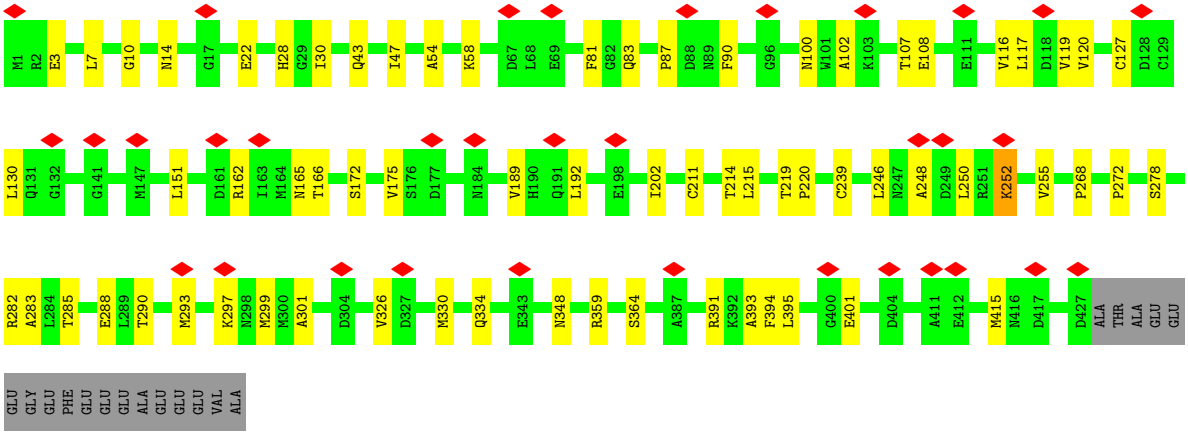




• Molecule 9: Tubulin beta-4B chain

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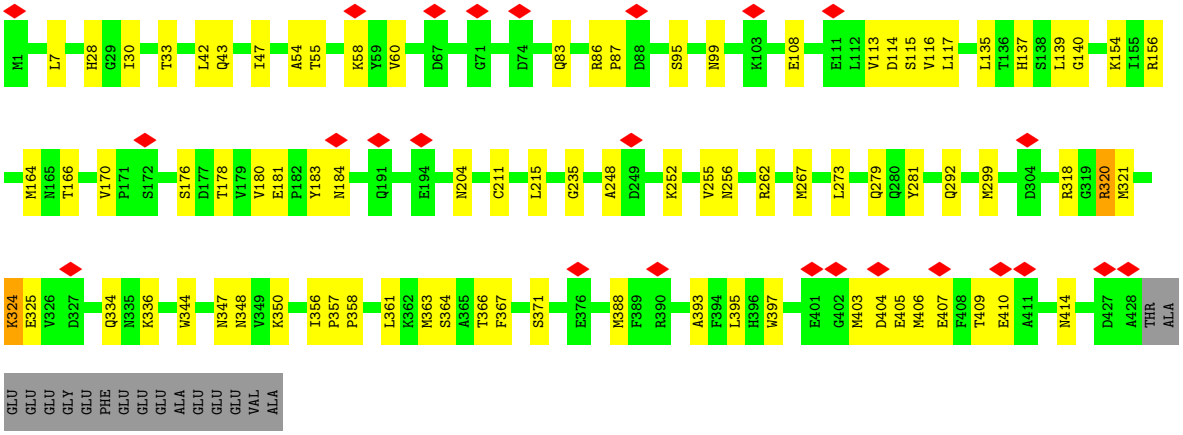




• Molecule 9: Tubulin beta-4B chain

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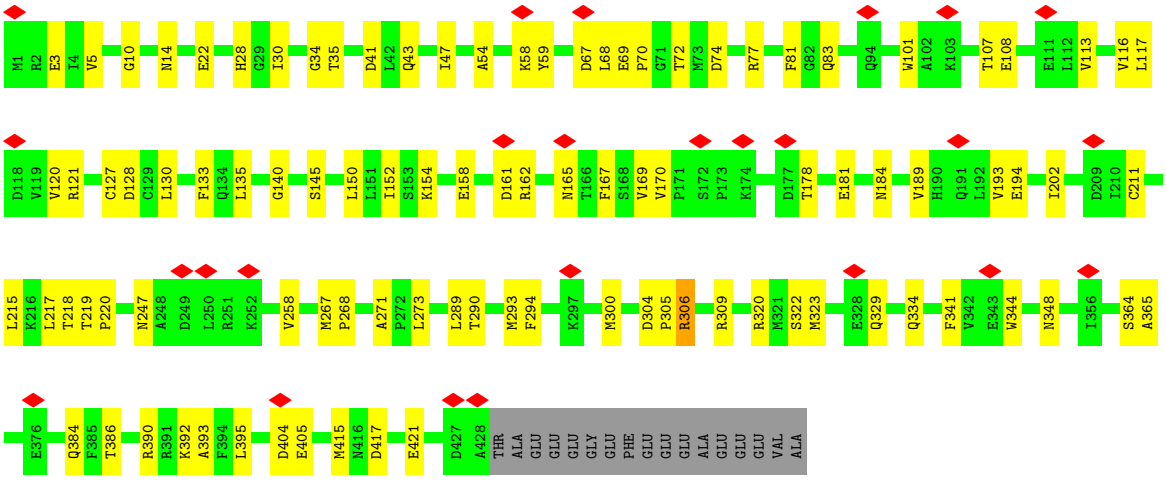




• Molecule 9: Tubulin beta-4B chain

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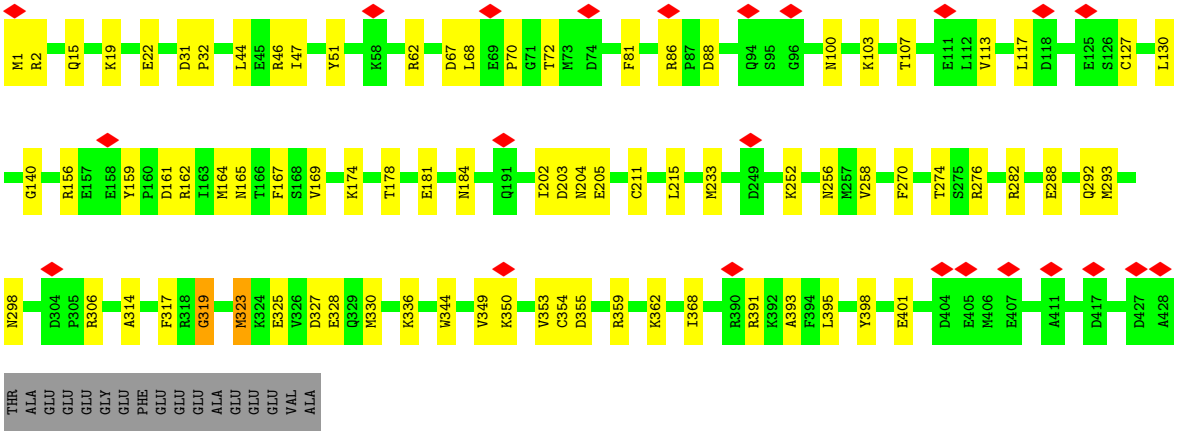




• Molecule 9: Tubulin beta-4B chain

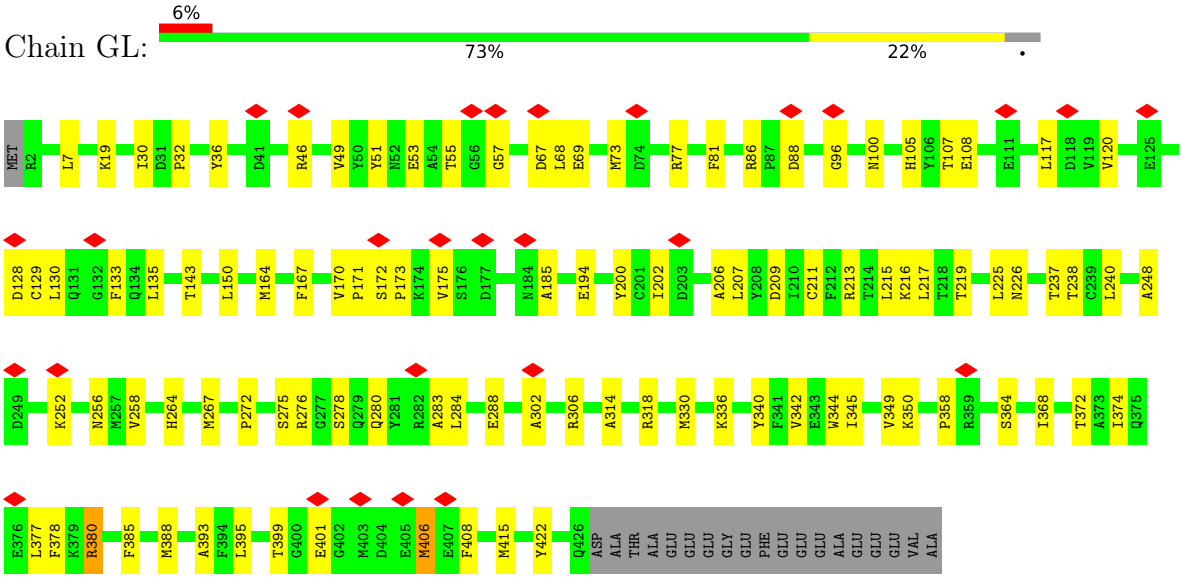
Chain GJ:





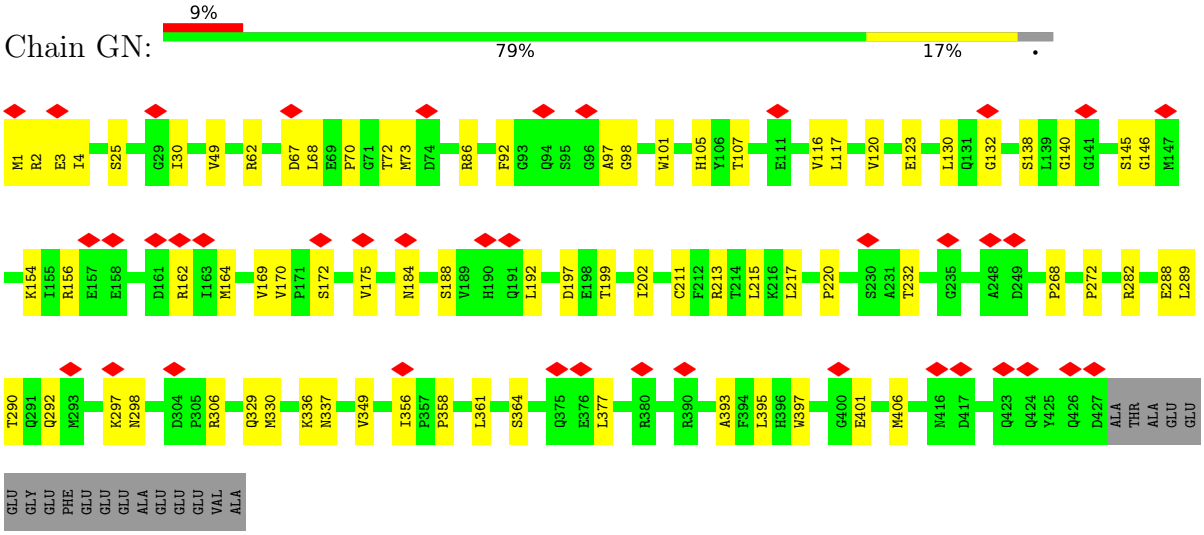
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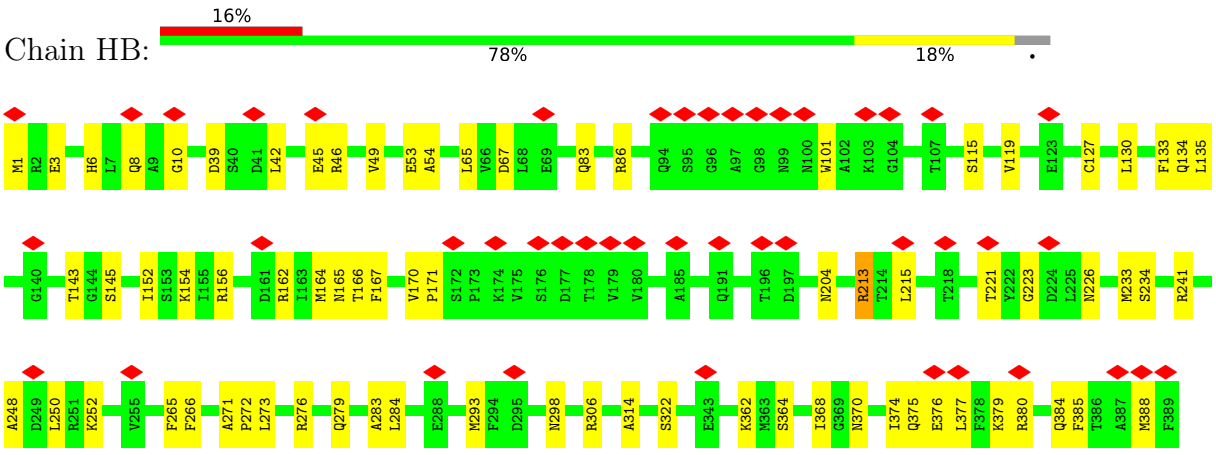
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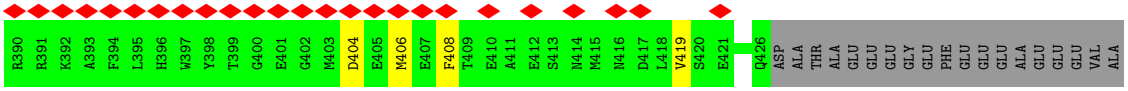
Chain GN:



• Molecule 9: Tubulin beta-4B chain

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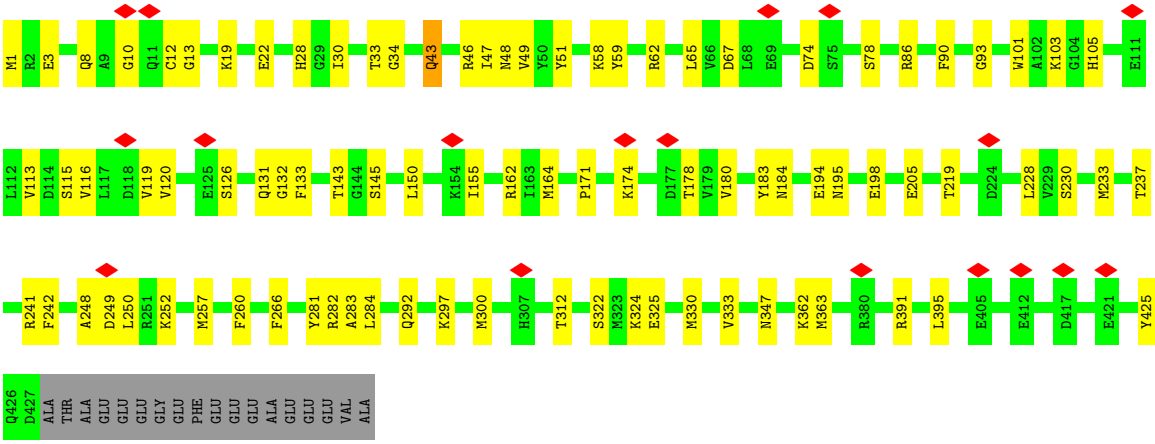




• Molecule 9: Tubulin beta-4B chain

Chain HD:

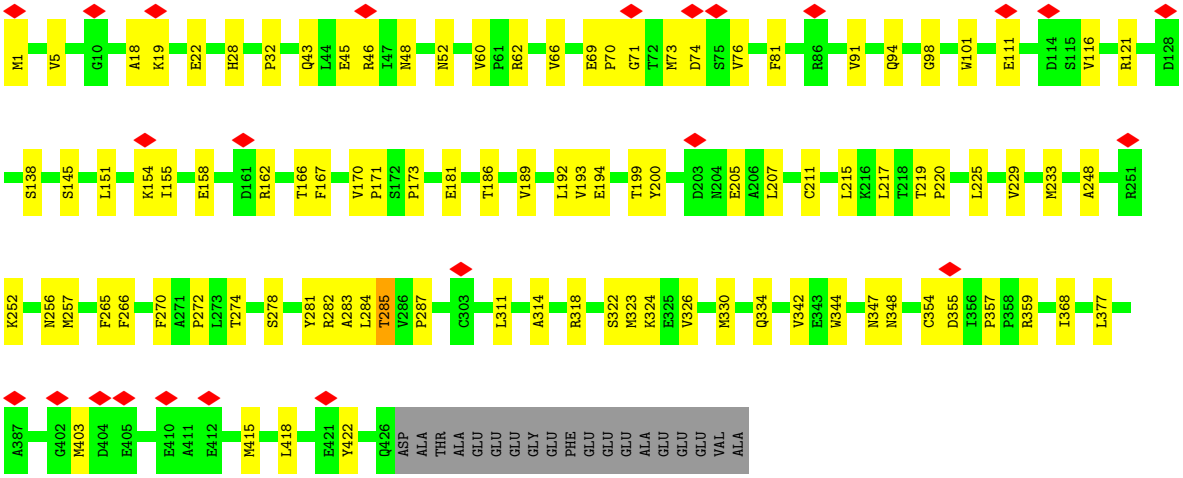




• Molecule 9: Tubulin beta-4B chain

Chain HF:

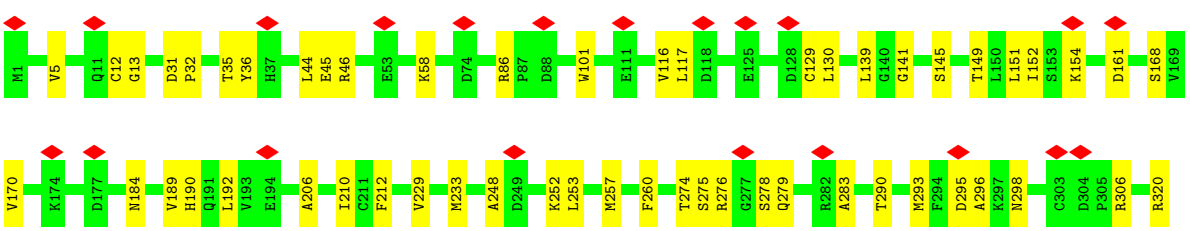


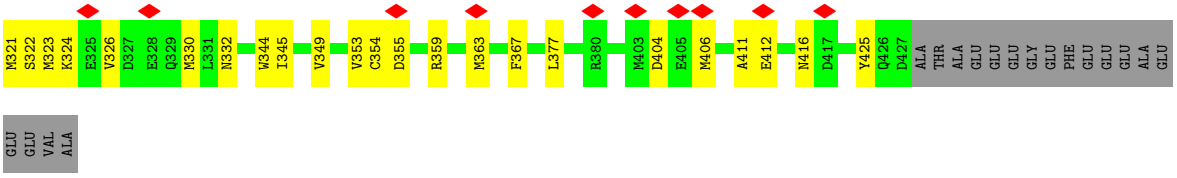


• Molecule 9: Tubulin beta-4B chain

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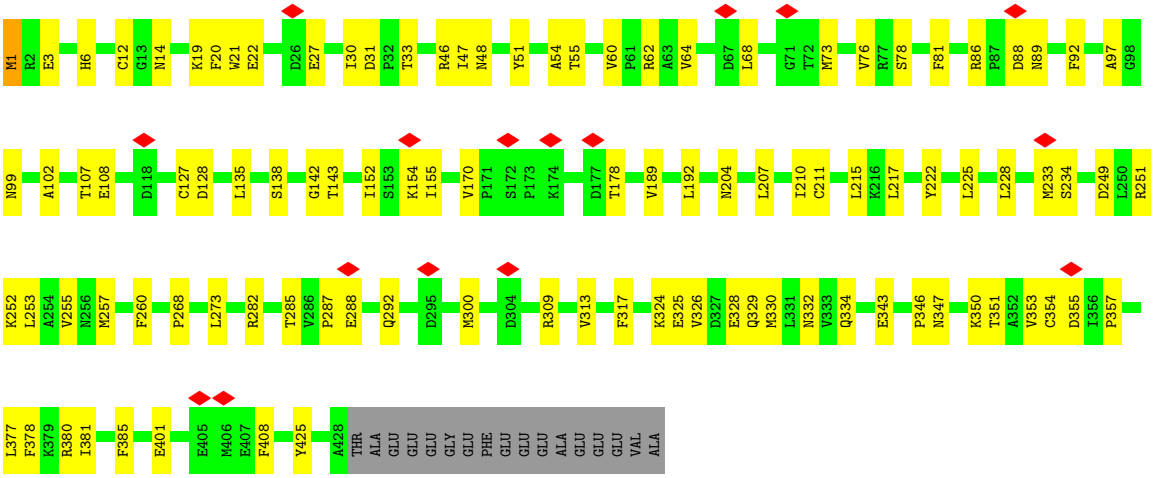




• Molecule 9: Tubulin beta-4B chain

Chain HJ:

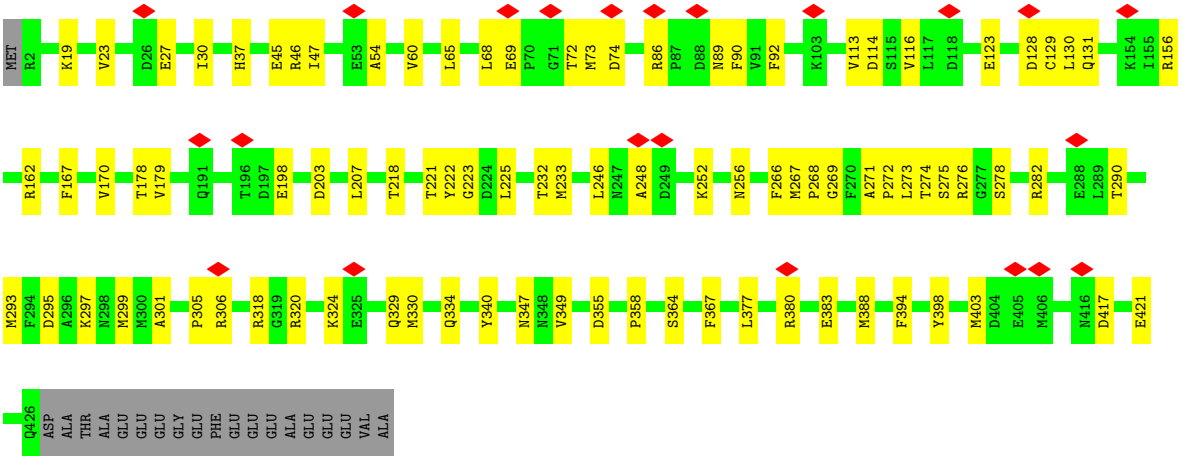




• Molecule 9: Tubulin beta-4B chain

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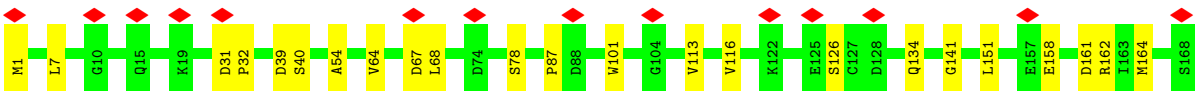


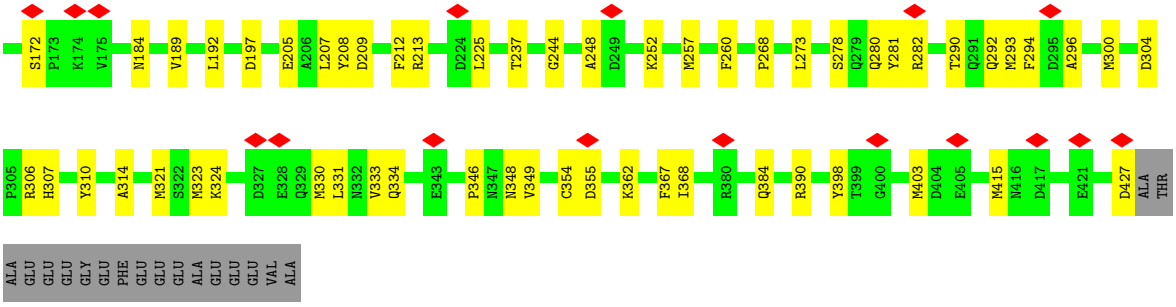


• Molecule 9: Tubulin beta-4B chain

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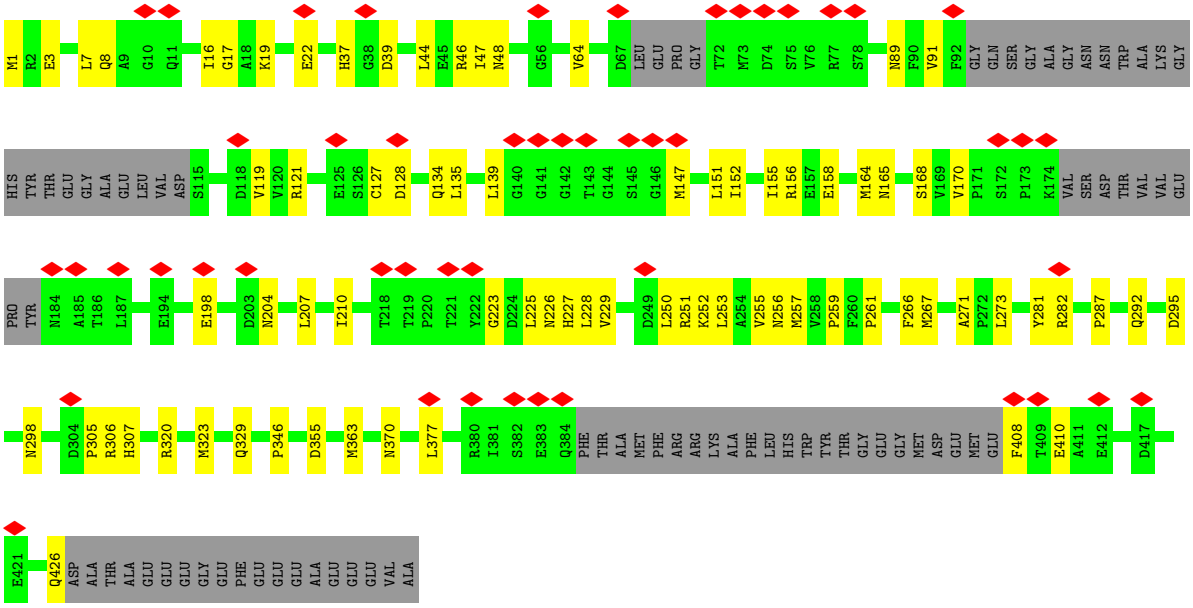




• Molecule 9: Tubulin beta-4B chain

Chain IB:

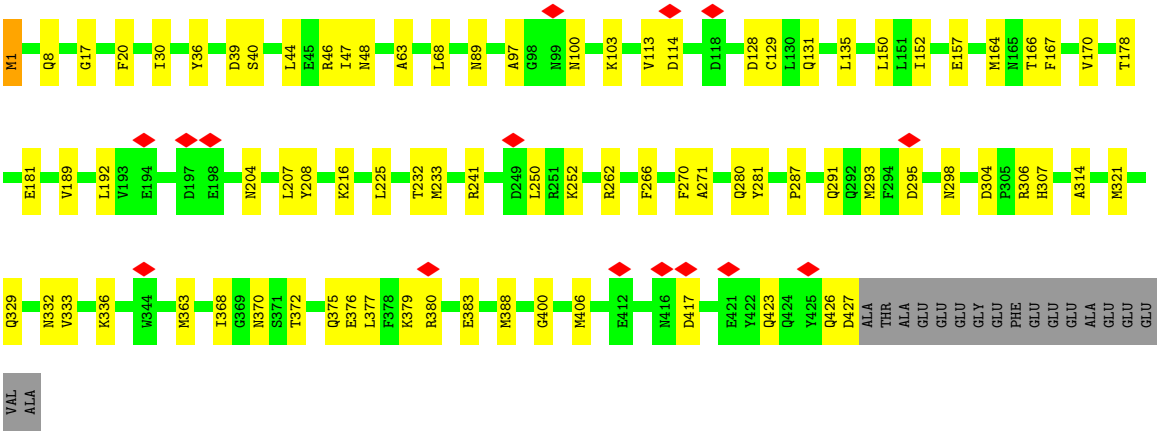




• Molecule 9: Tubulin beta-4B chain

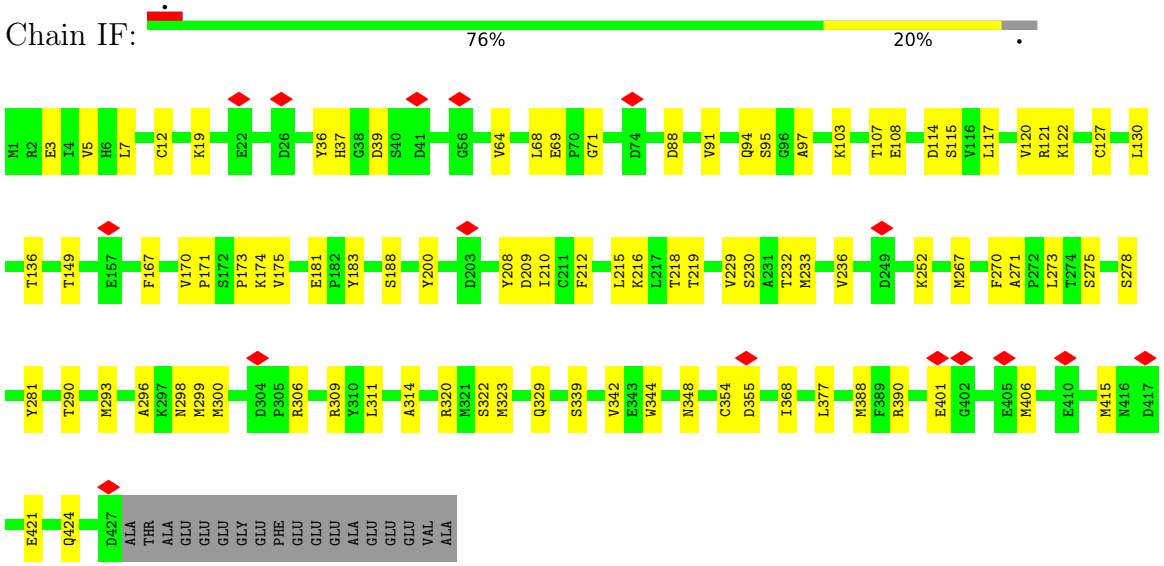
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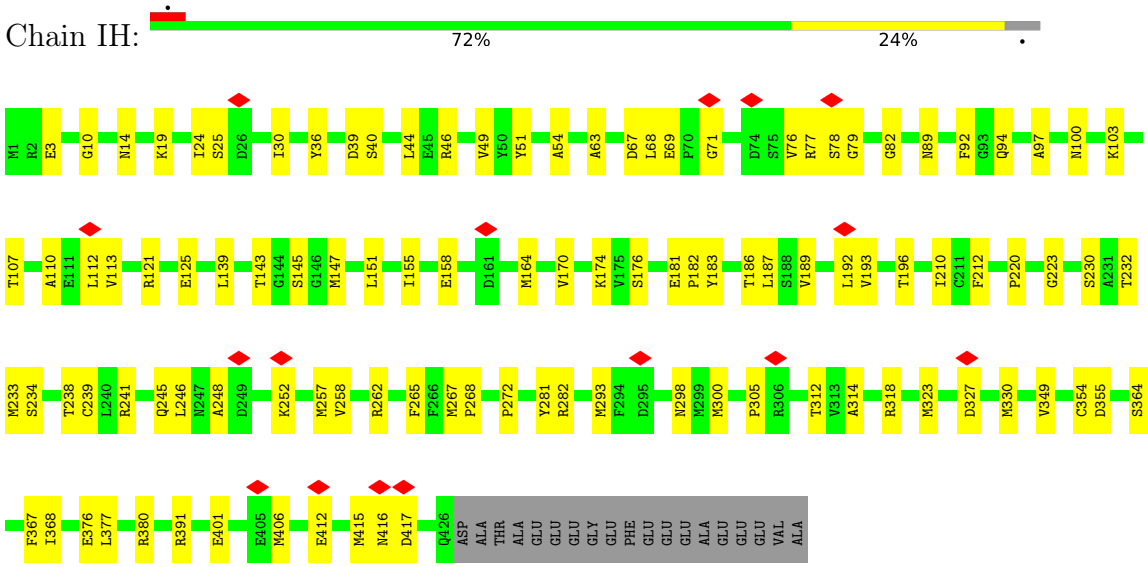
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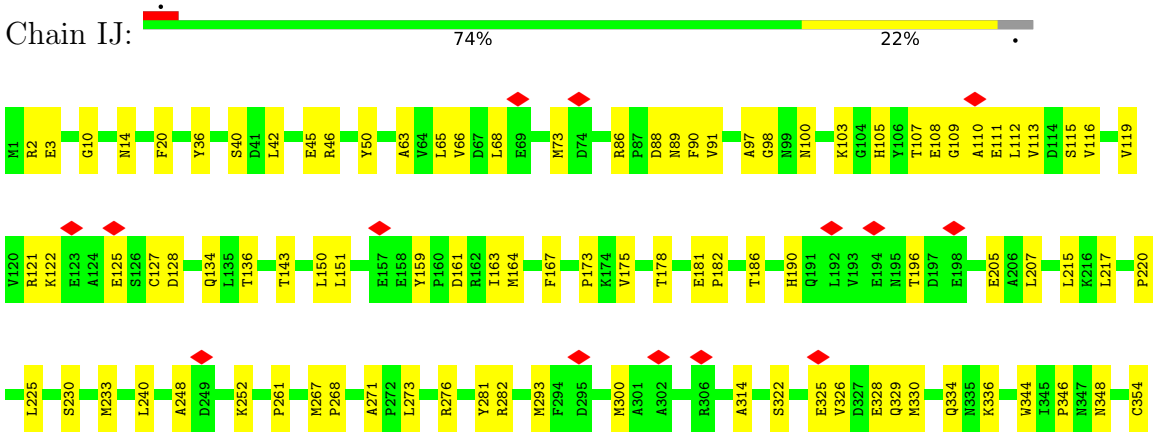
• Molecule 9: Tubulin beta-4B chain

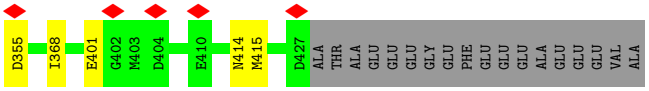
Chain IH:



• Molecule 9: Tubulin beta-4B chain

Chain IJ:

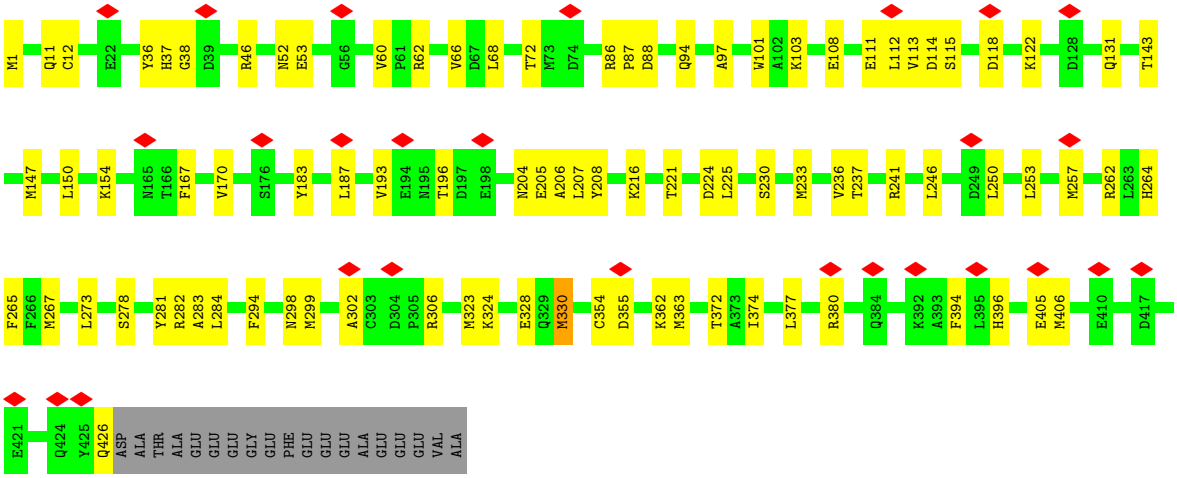




• Molecule 9: Tubulin beta-4B chain

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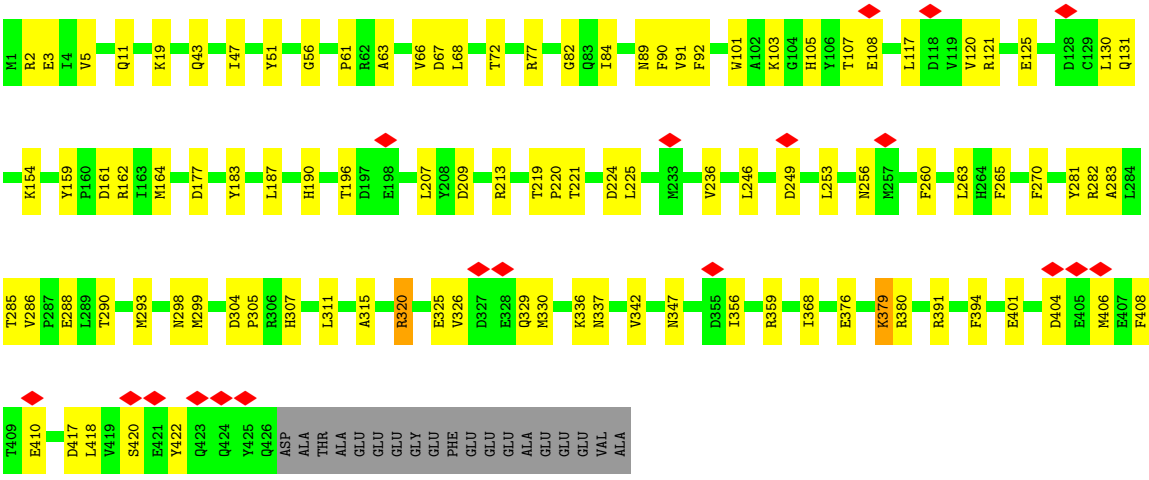




• Molecule 9: Tubulin beta-4B chain

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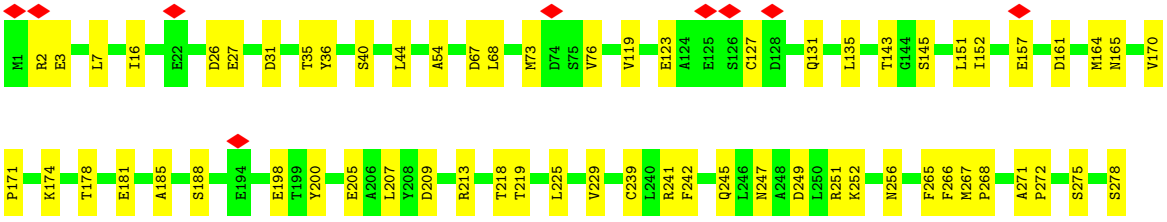


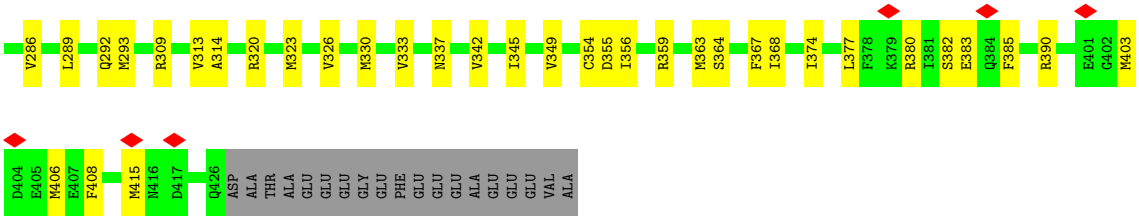


• Molecule 9: Tubulin beta-4B chain

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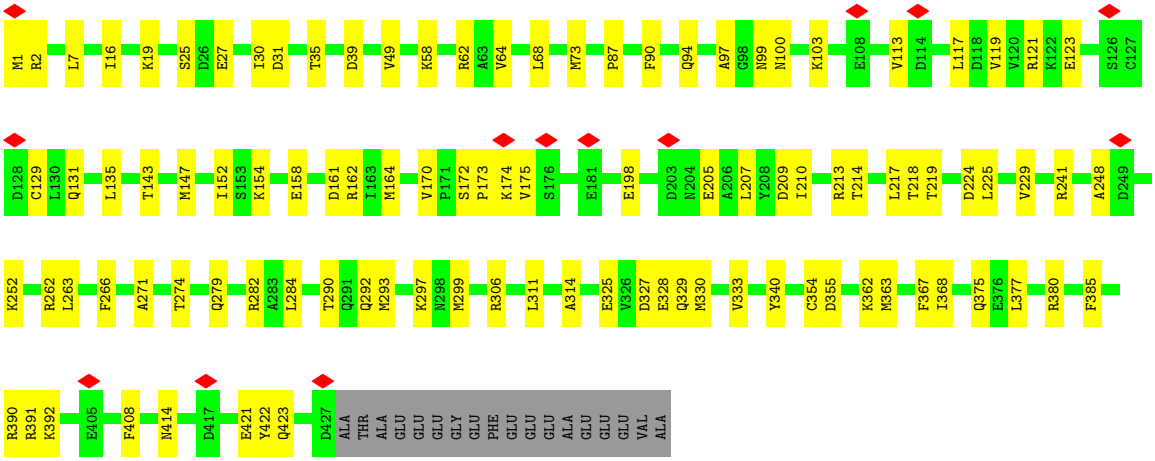




• Molecule 9: Tubulin beta-4B chain

Chain JD:

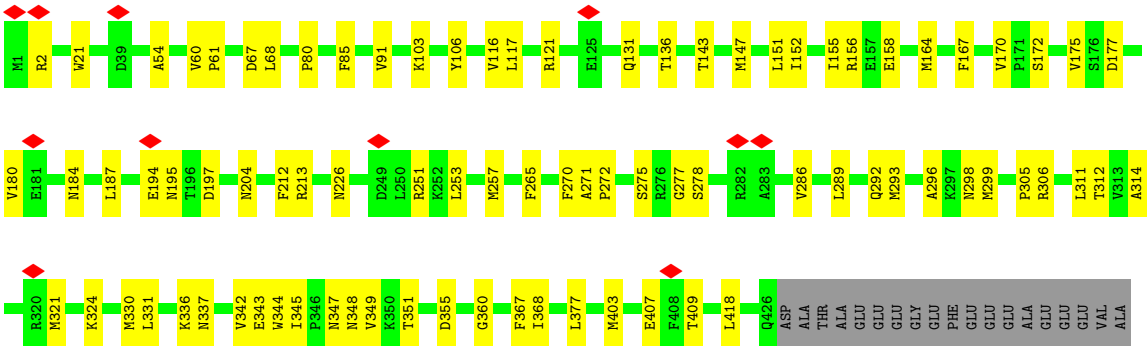




• Molecule 9: Tubulin beta-4B chain

Chain JF:

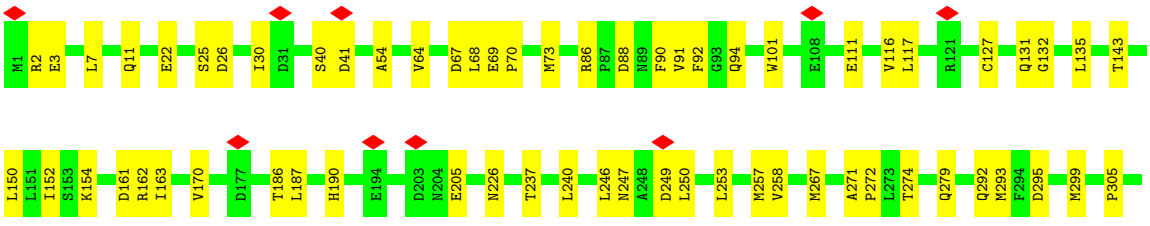


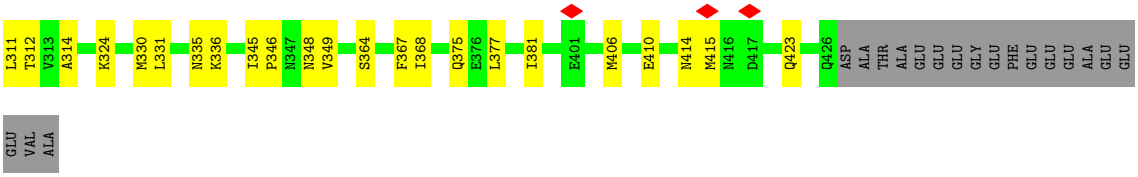


• Molecule 9: Tubulin beta-4B chain

Chain JH:



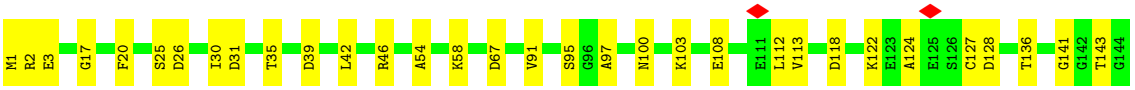


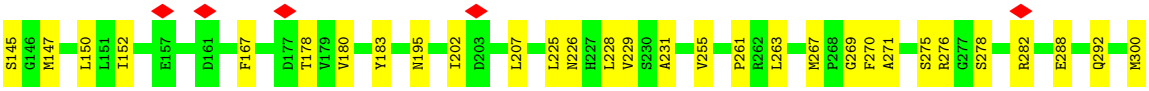


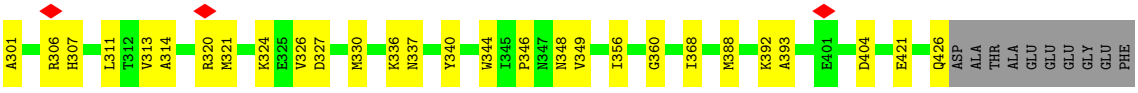
• Molecule 9: Tubulin beta-4B chain

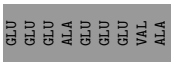
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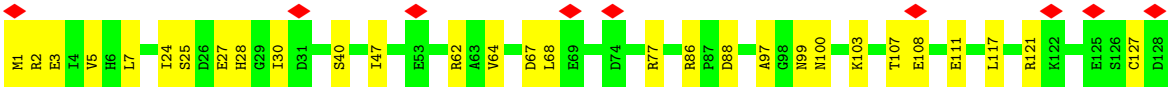


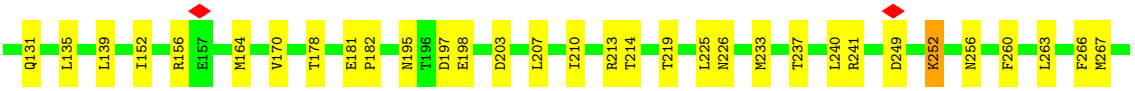


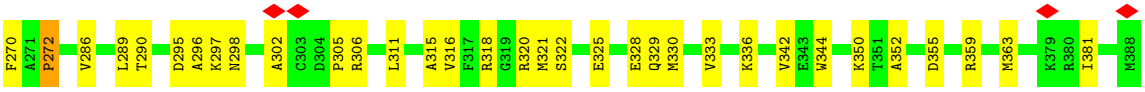
• Molecule 9: Tubulin beta-4B chain

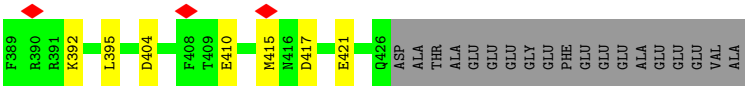
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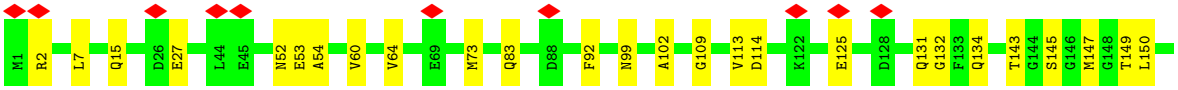


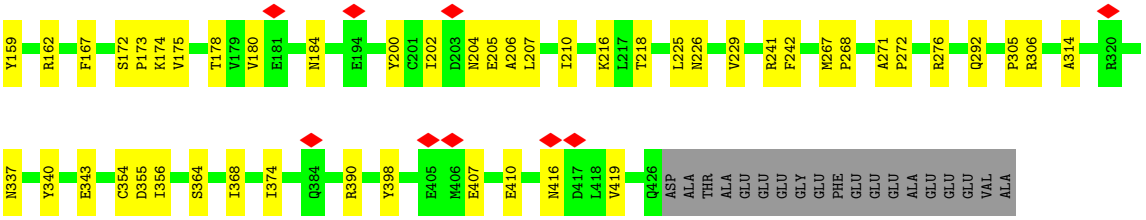


• Molecule 9: Tubulin beta-4B chain

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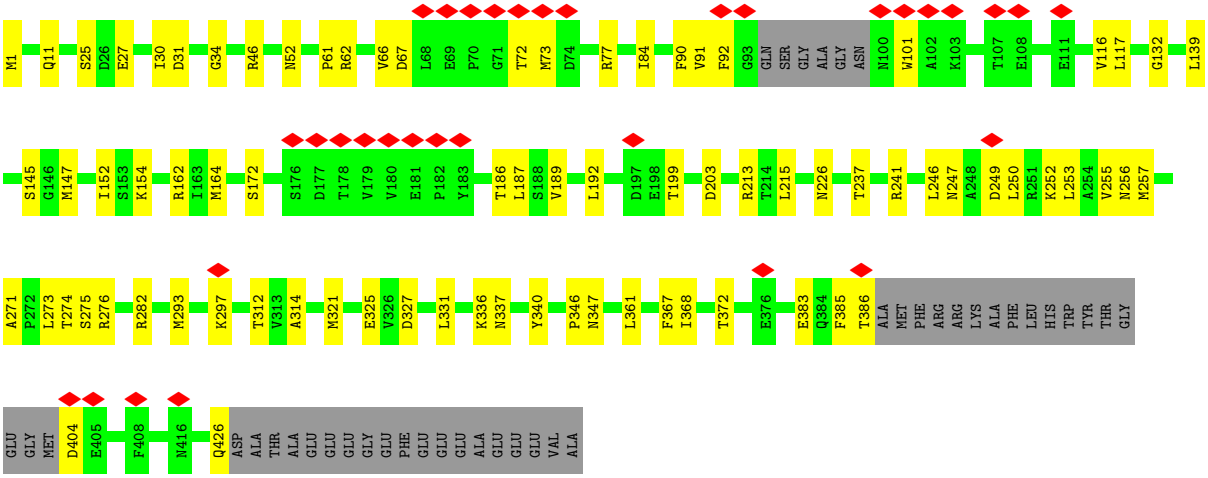




• Molecule 9: Tubulin beta-4B chain

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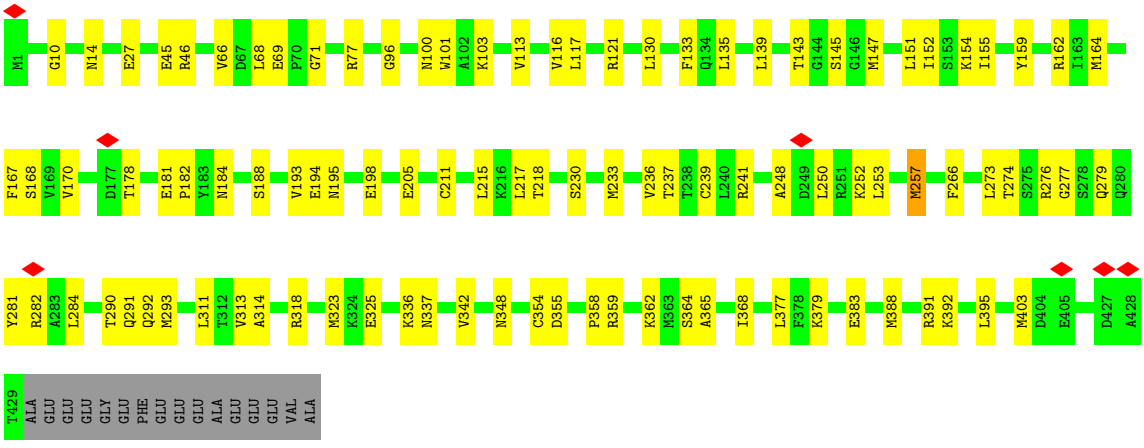




• Molecule 9: Tubulin beta-4B chain

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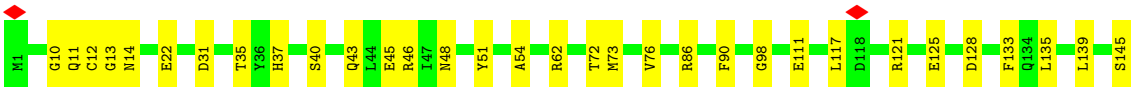


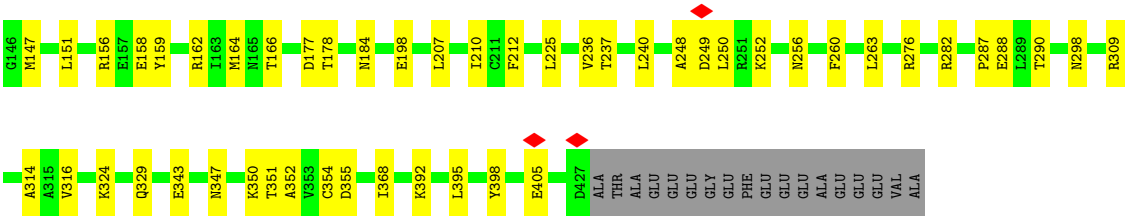


• Molecule 9: Tubulin beta-4B chain

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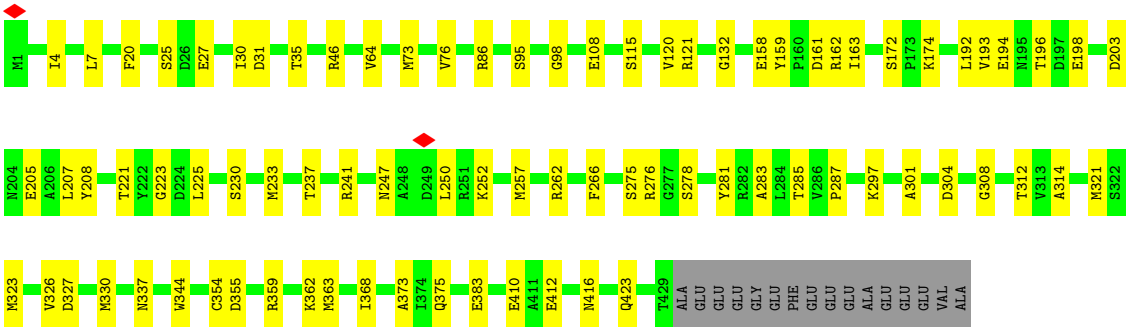




• Molecule 9: Tubulin beta-4B chain

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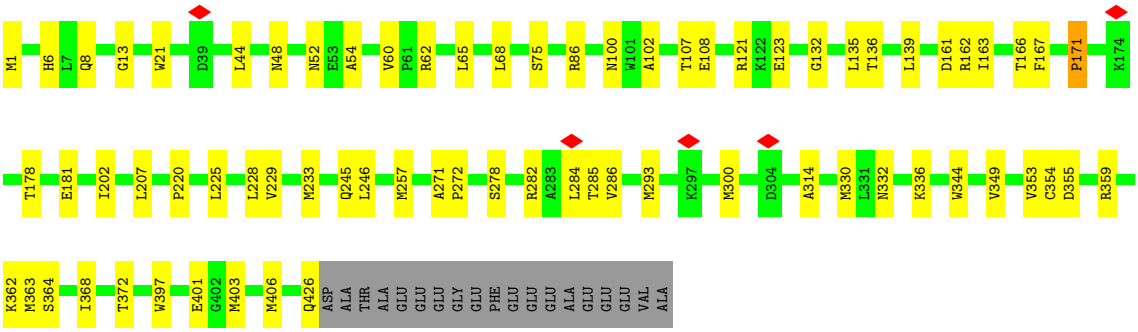




• Molecule 9: Tubulin beta-4B chain

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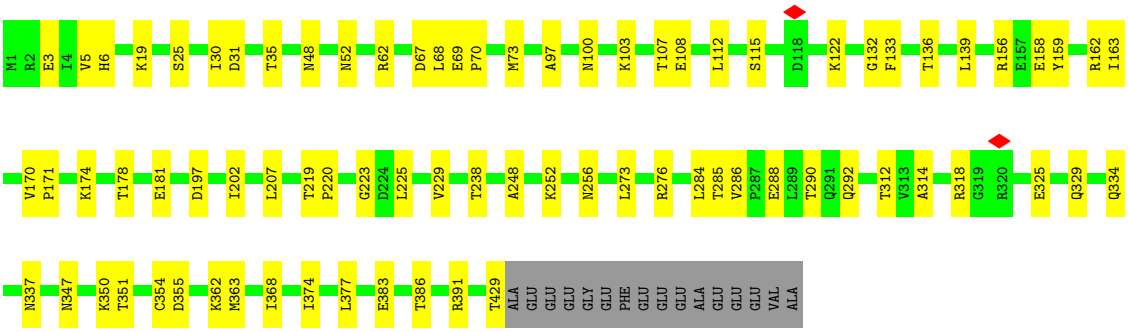




• Molecule 9: Tubulin beta-4B chain

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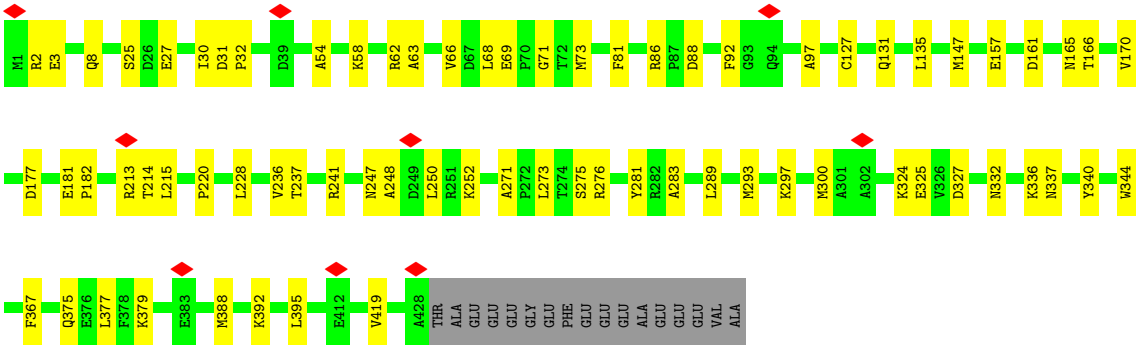




• Molecule 9: Tubulin beta-4B chain

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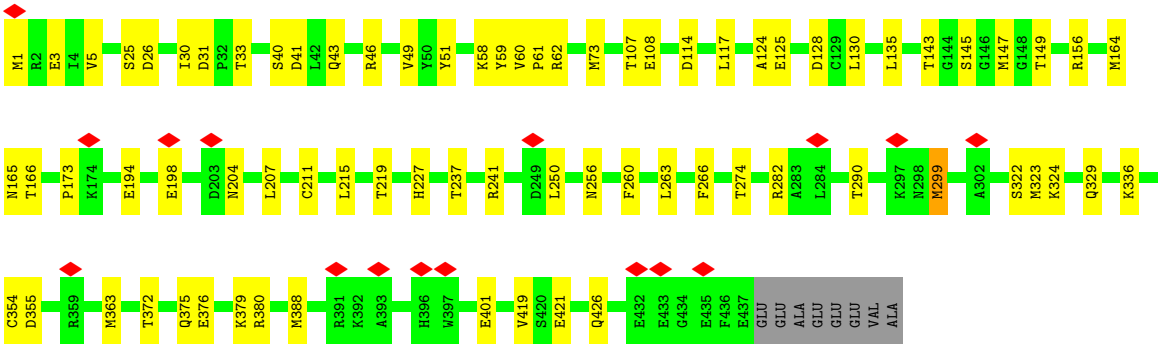




• Molecule 9: Tubulin beta-4B chain

Chain LB:

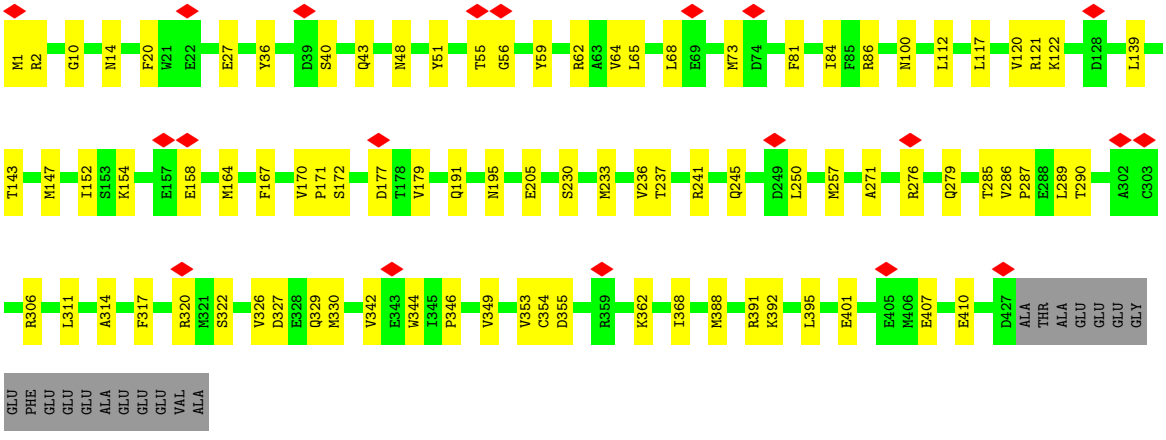




• Molecule 9: Tubulin beta-4B chain

Chain LD:

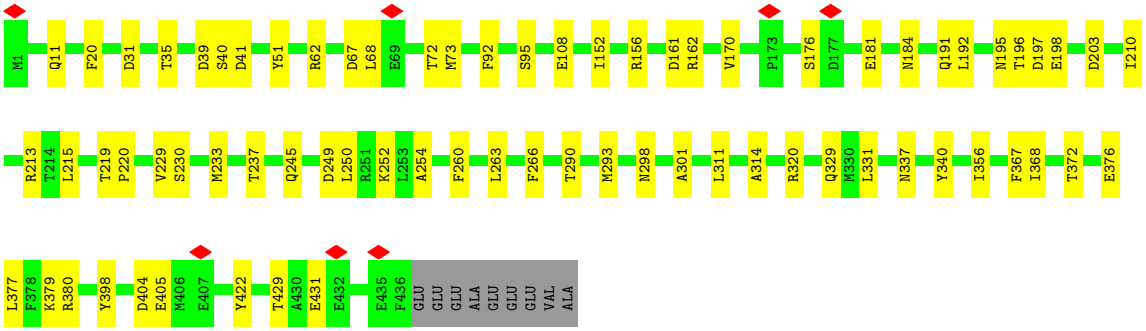




• Molecule 9: Tubulin beta-4B chain

Chain LF:

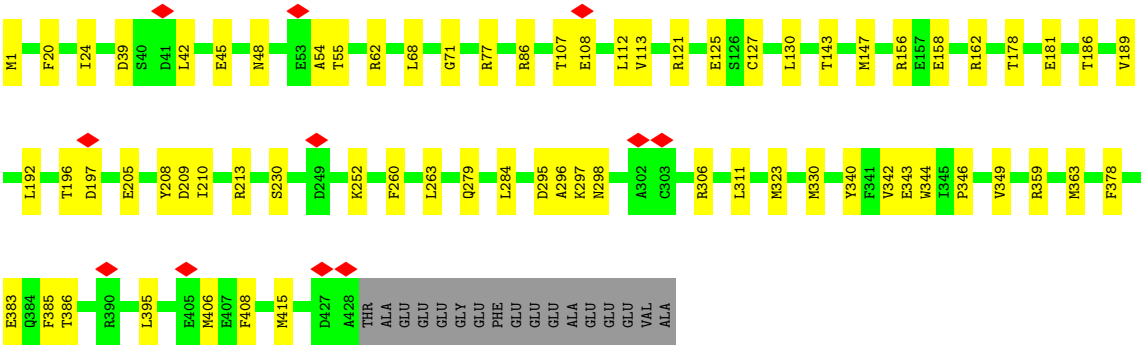




• Molecule 9: Tubulin beta-4B chain

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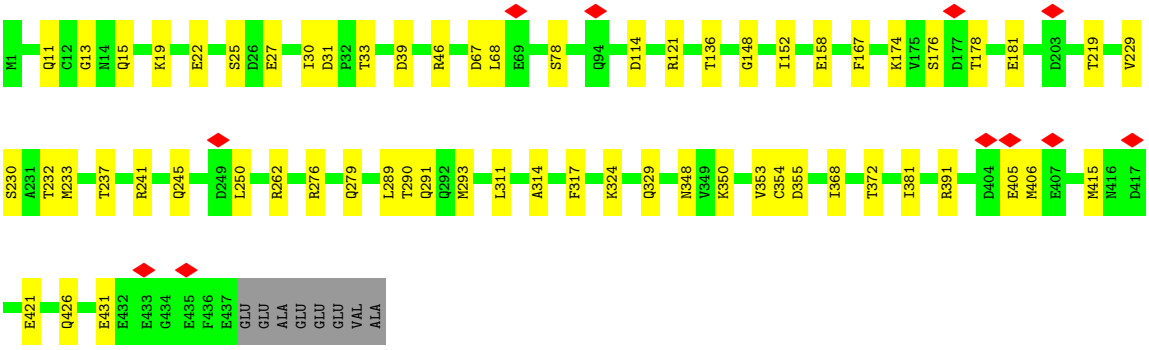




• Molecule 9: Tubulin beta-4B chain

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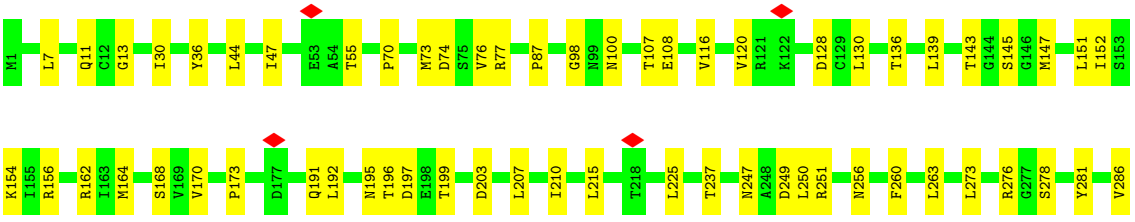


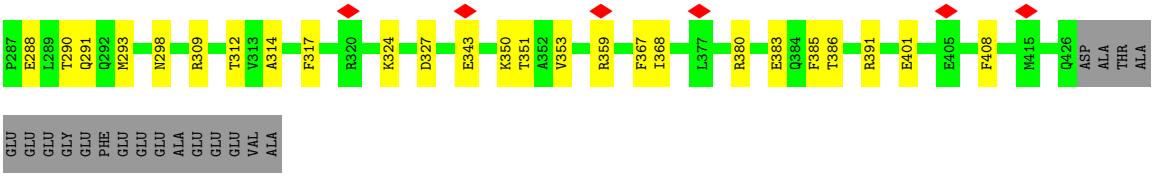


• Molecule 9: Tubulin beta-4B chain

Chain LL:

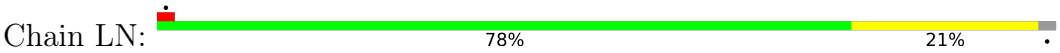


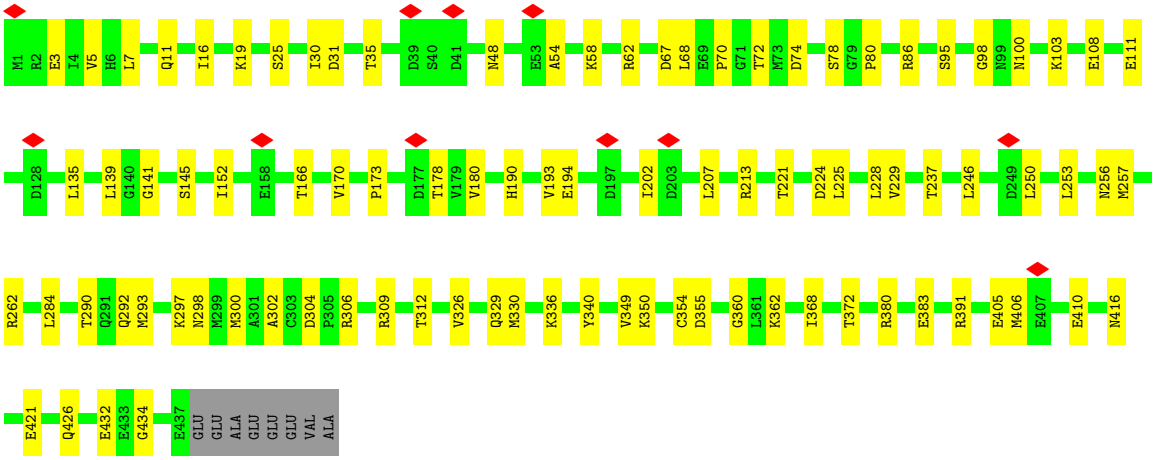




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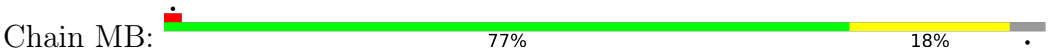
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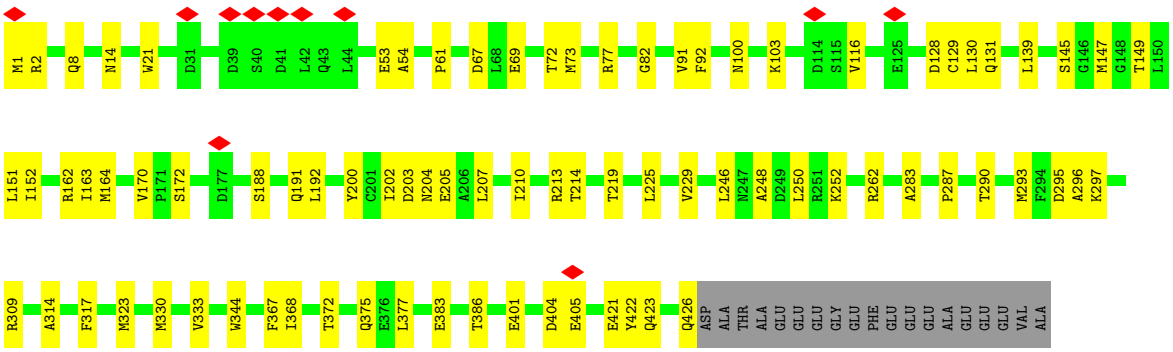




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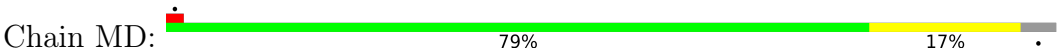
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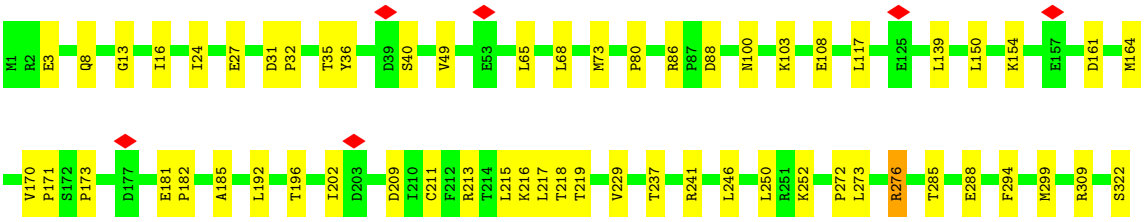


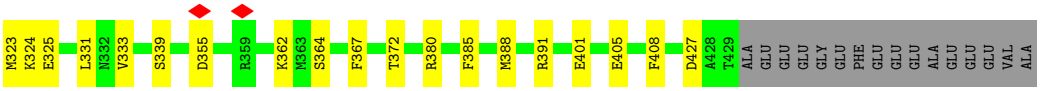


• Molecule 9: Tubulin beta-4B chain

Chain MD:



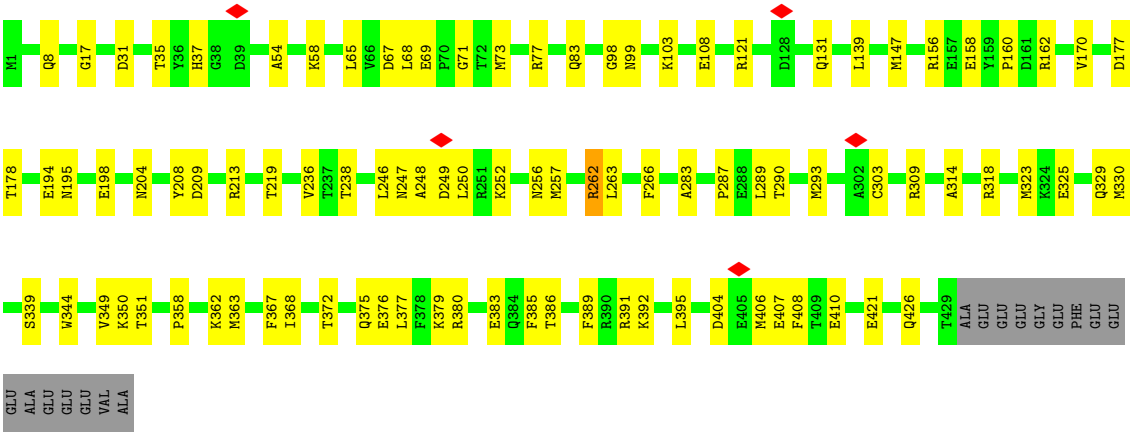




• Molecule 9: Tubulin beta-4B chain

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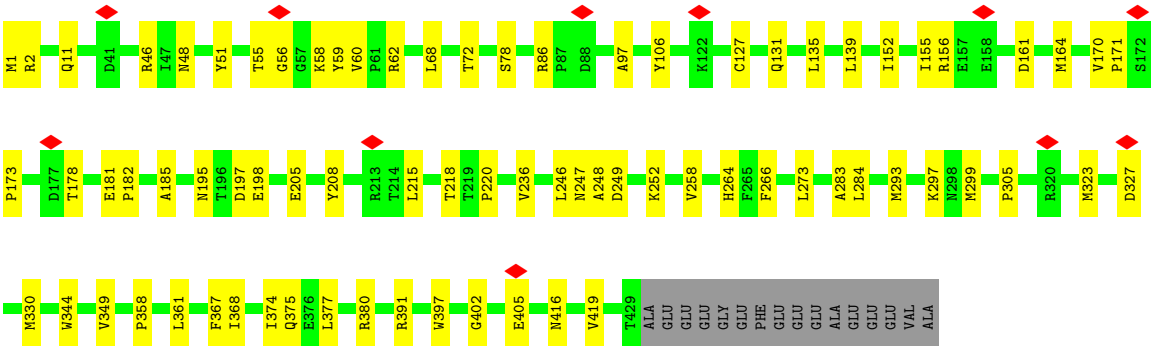




• Molecule 9: Tubulin beta-4B chain

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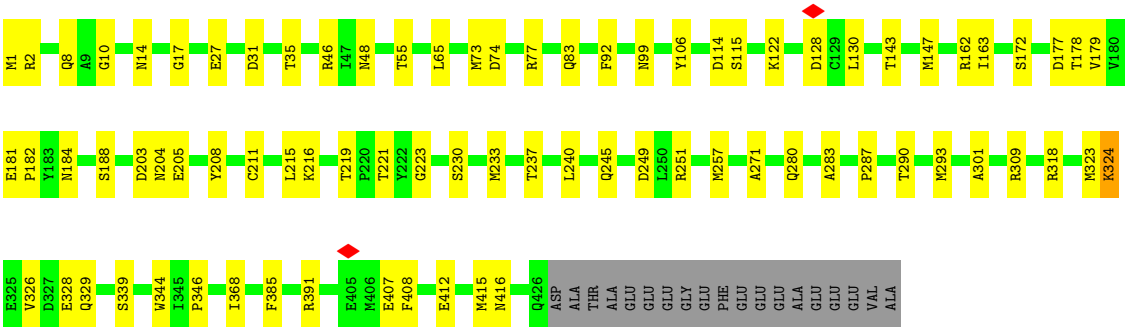




• Molecule 9: Tubulin beta-4B chain

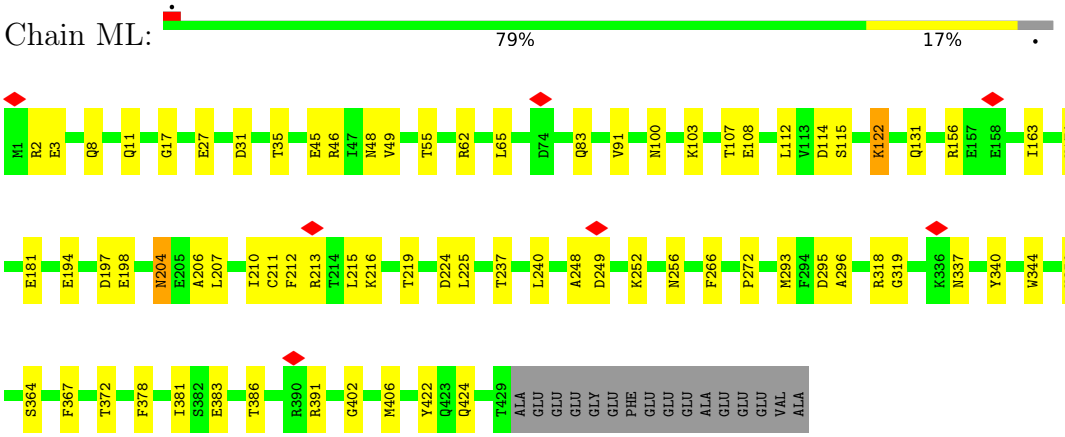
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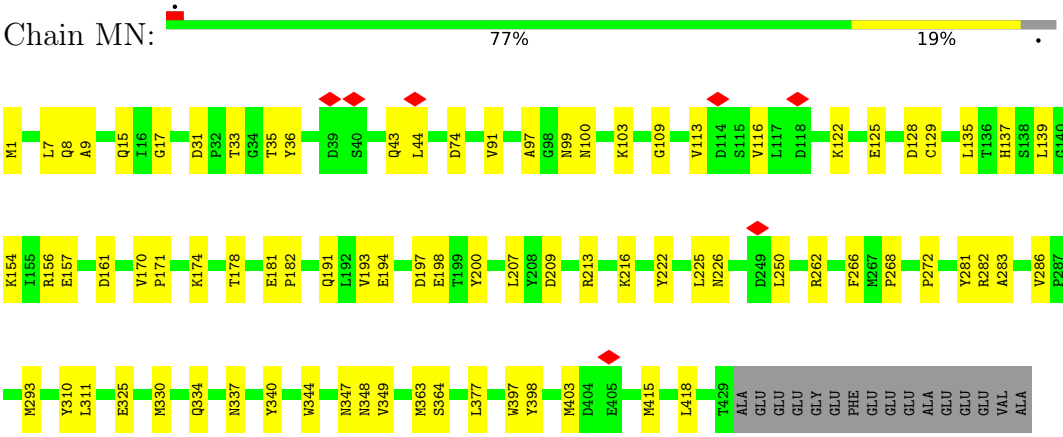
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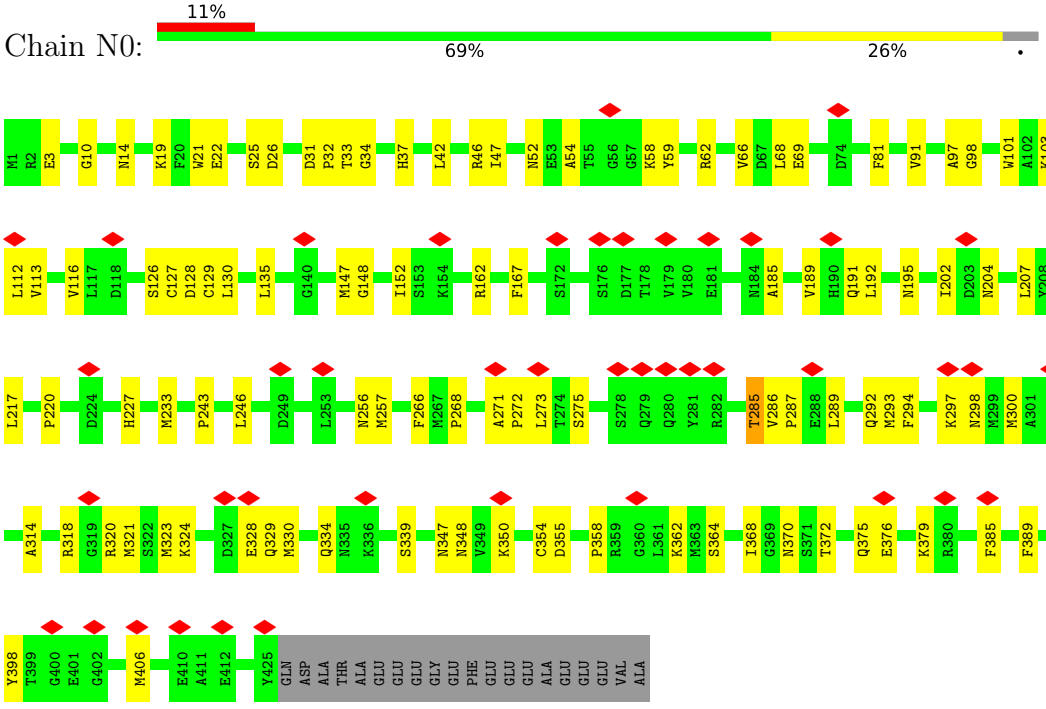
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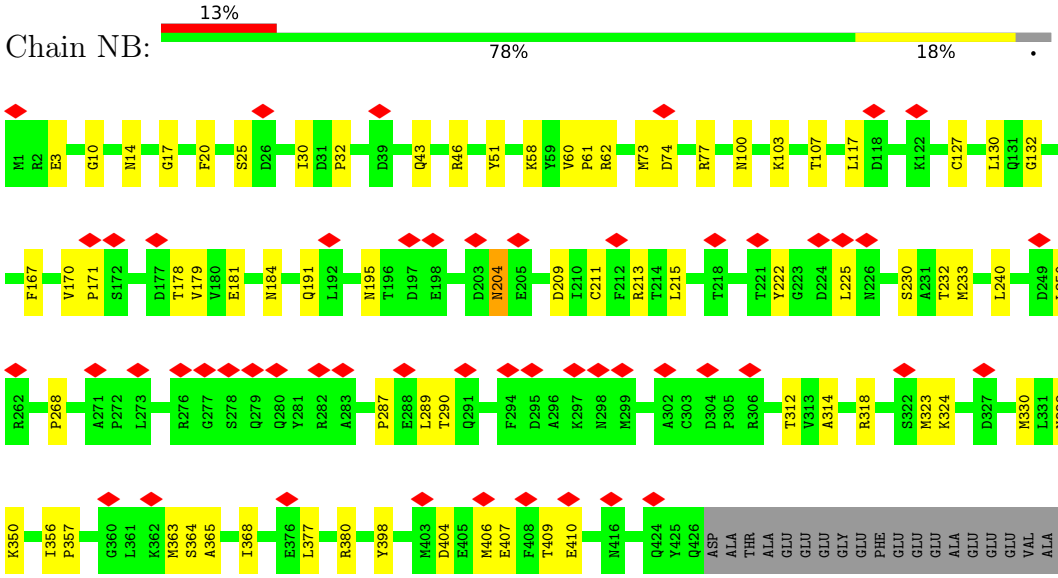
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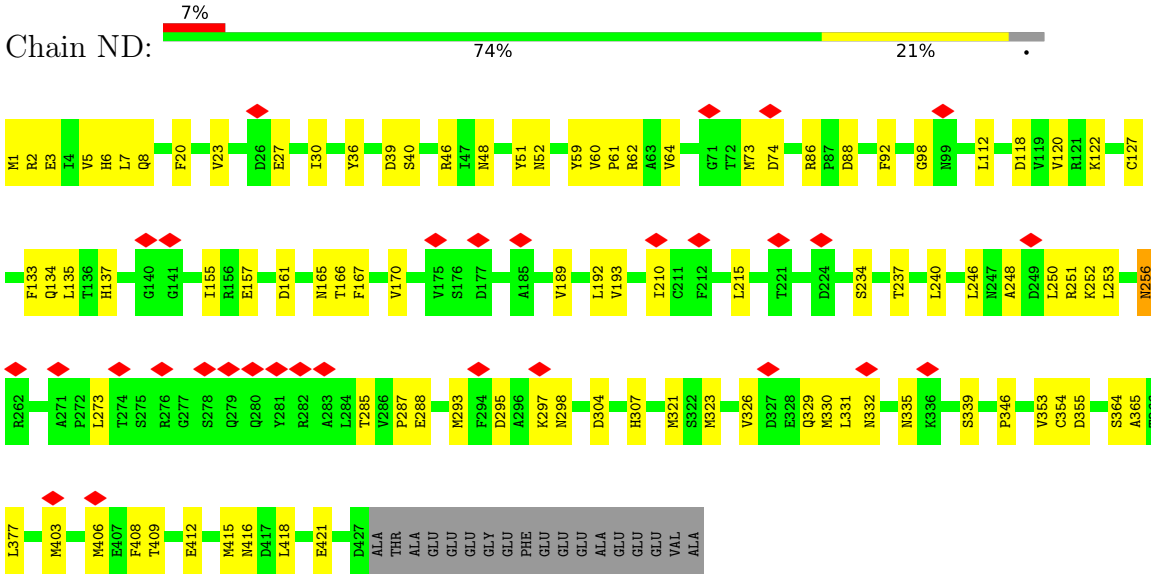
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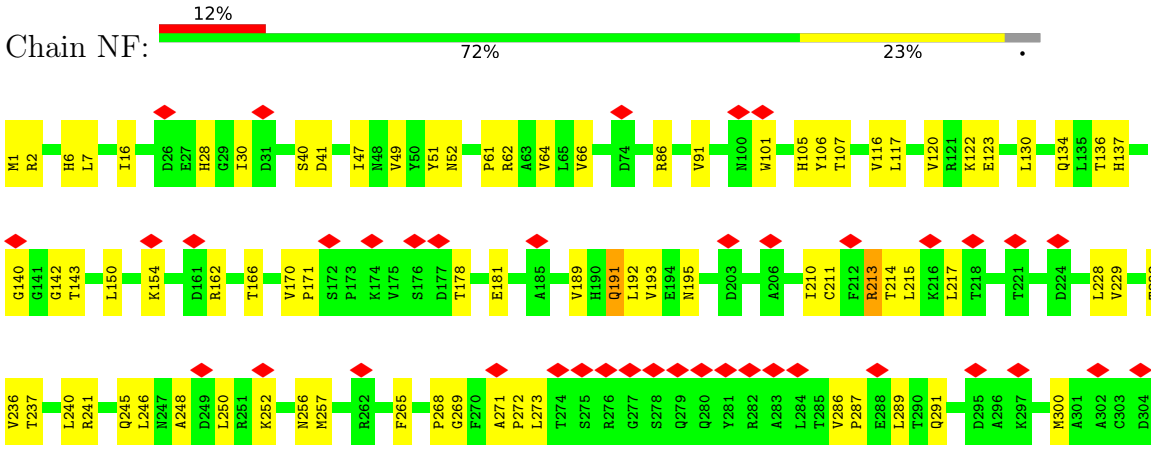
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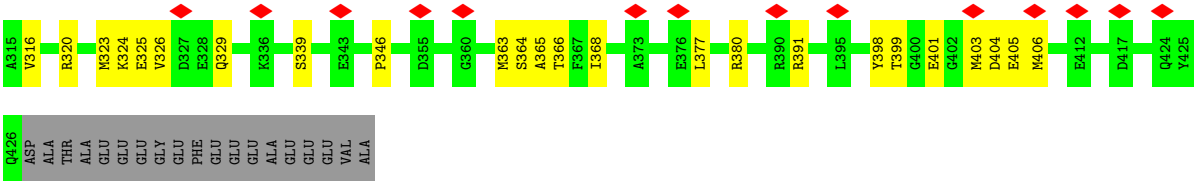
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• Molecule 9: Tubulin beta-4B chain

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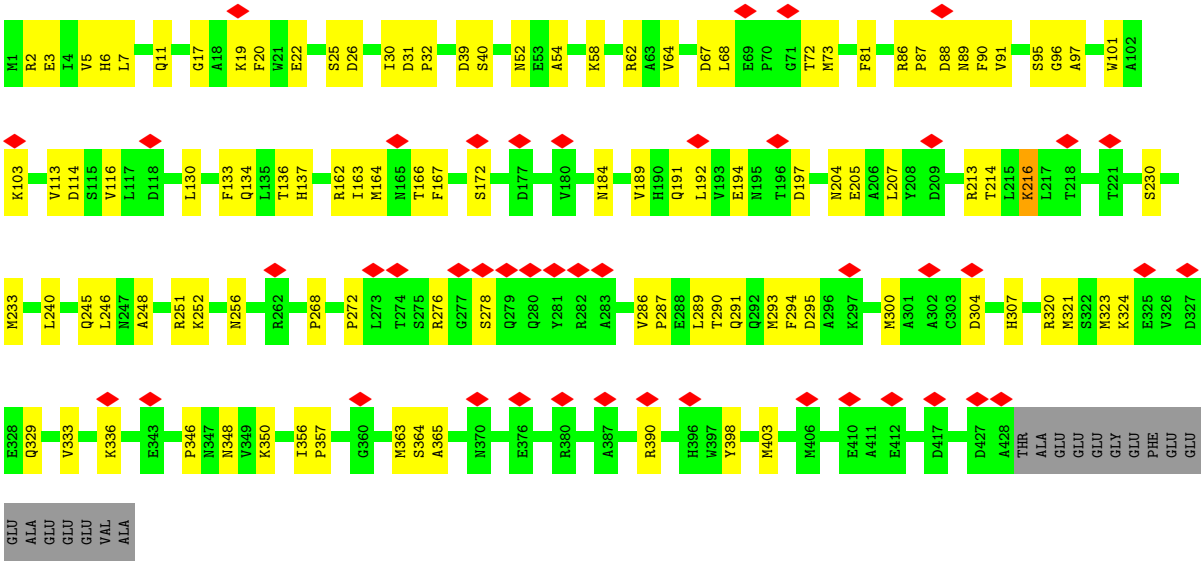




• Molecule 9: Tubulin beta-4B chain

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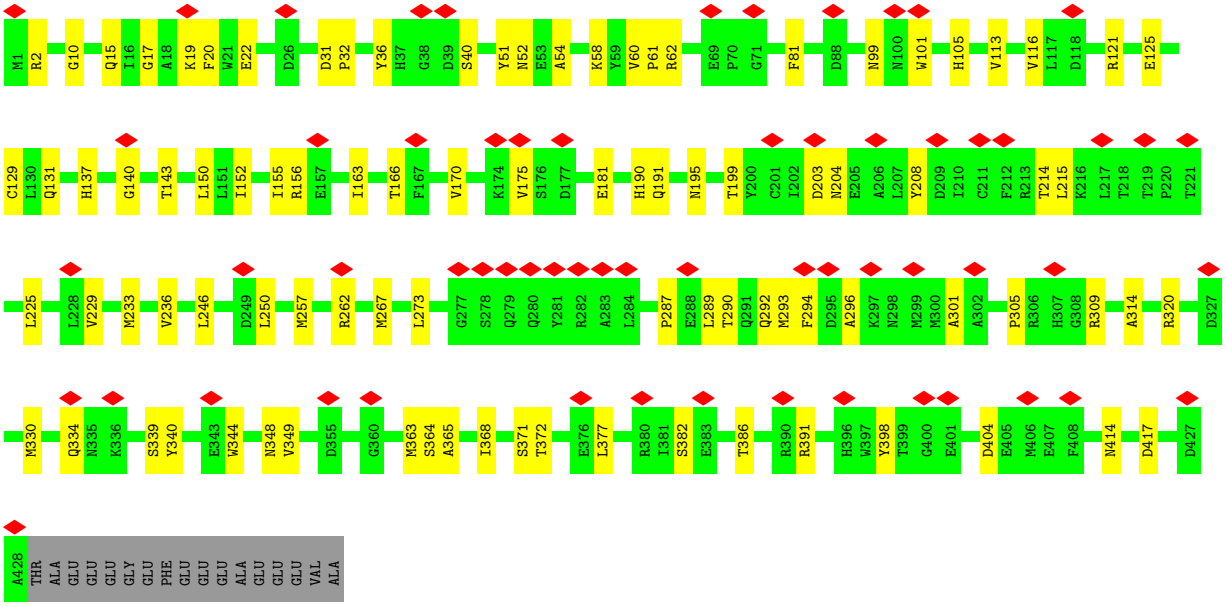




• Molecule 9: Tubulin beta-4B chain

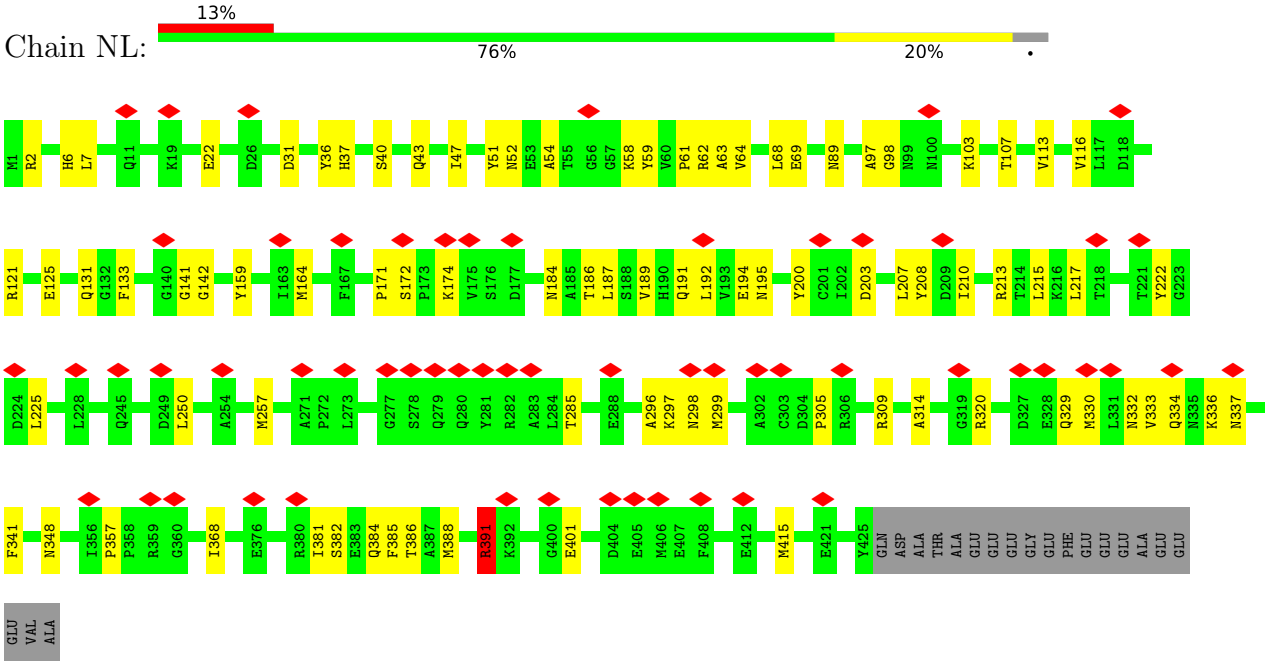
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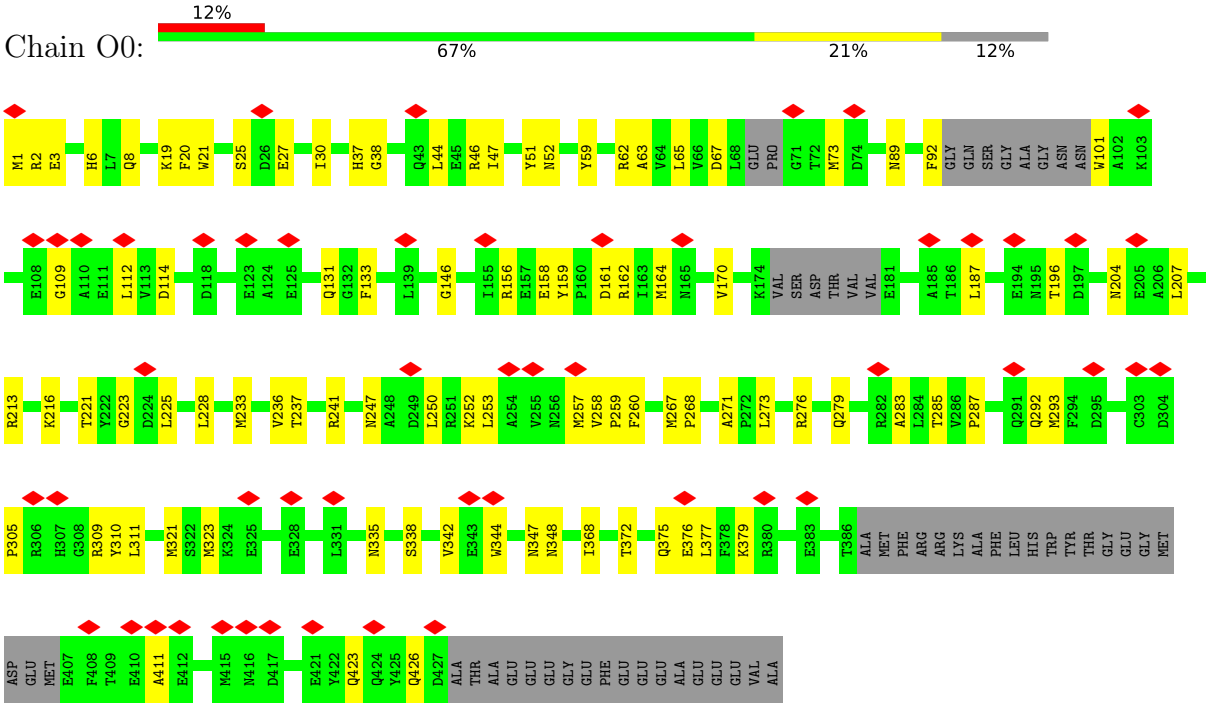
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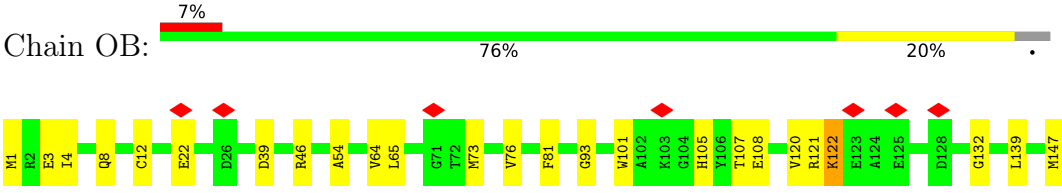
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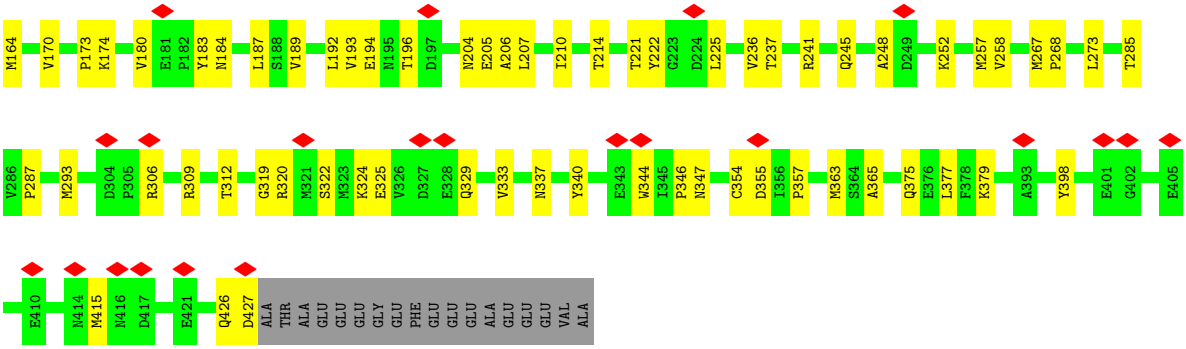
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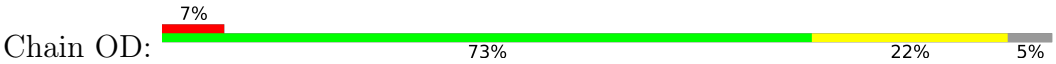
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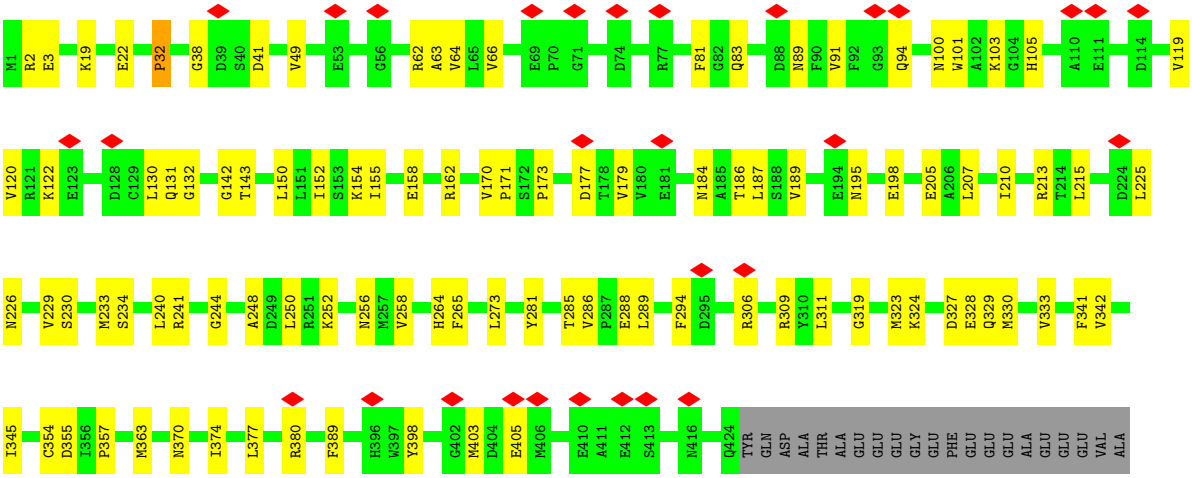
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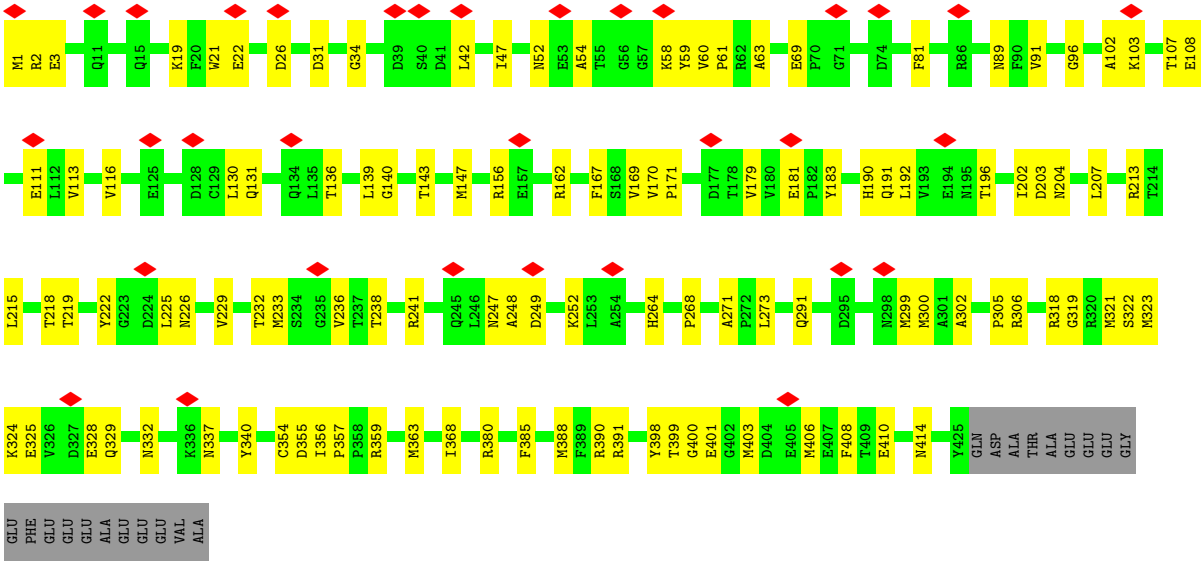
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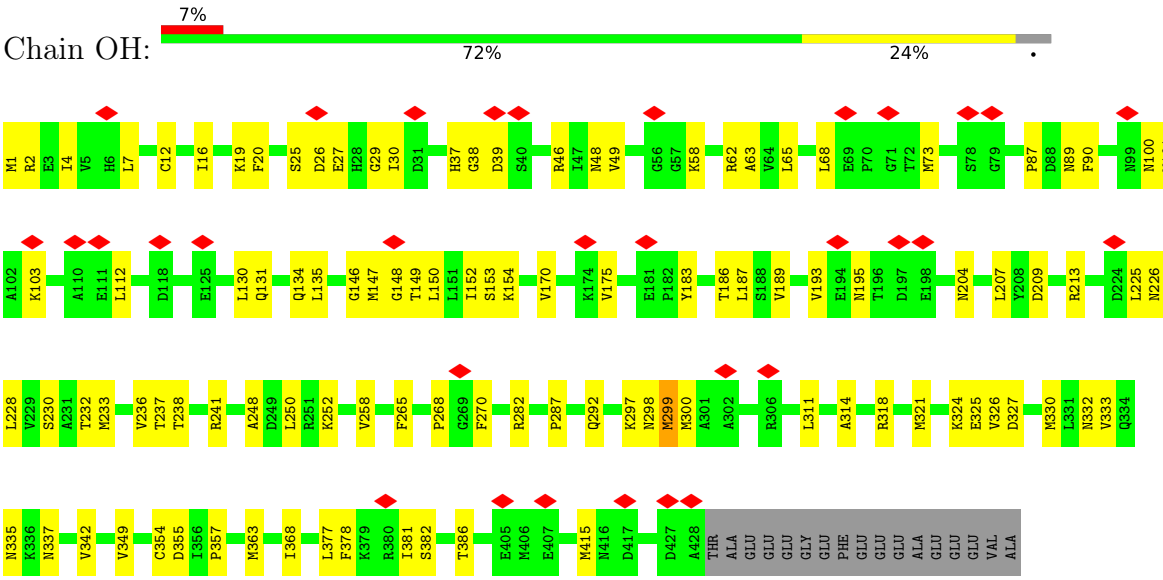
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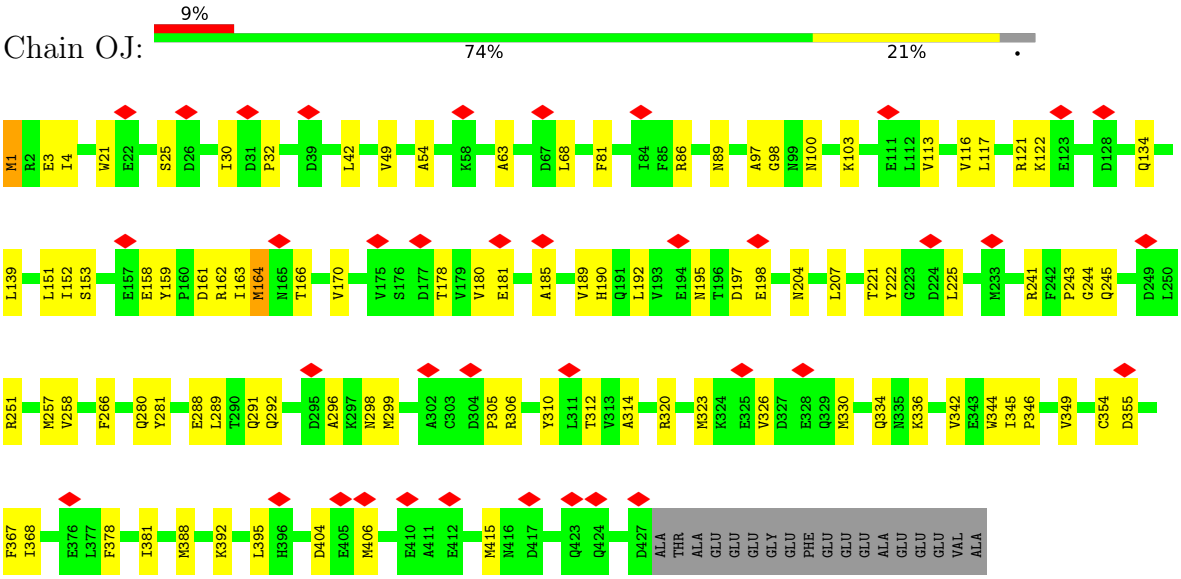
• Molecule 9: Tubulin beta-4B chain

Chain OH:



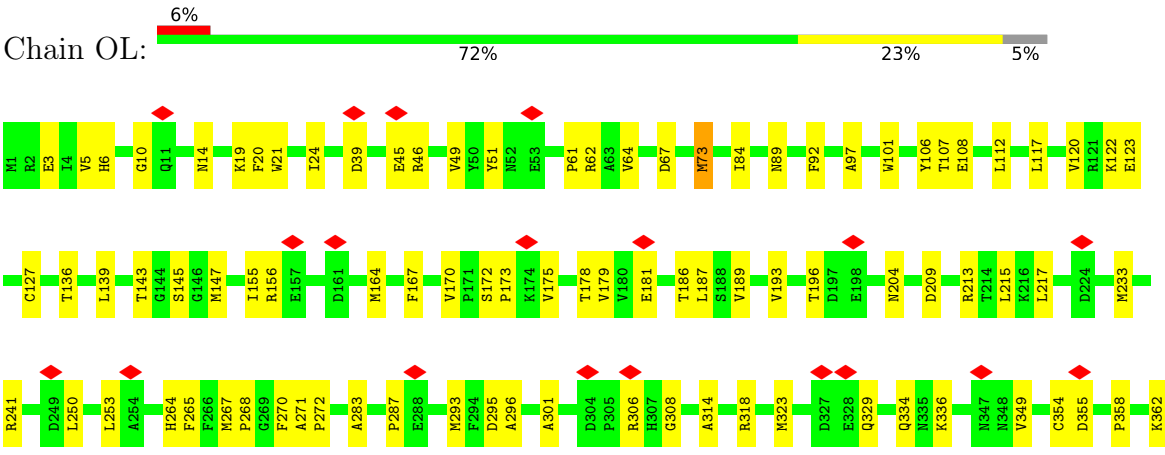
• Molecule 9: Tubulin beta-4B chain

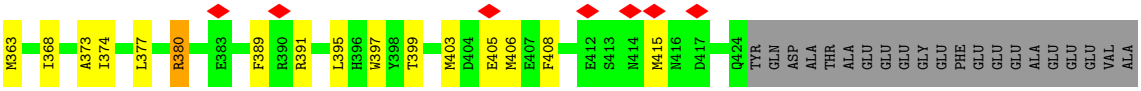
Chain OJ:



• Molecule 9: Tubulin beta-4B chain

Chain OL:

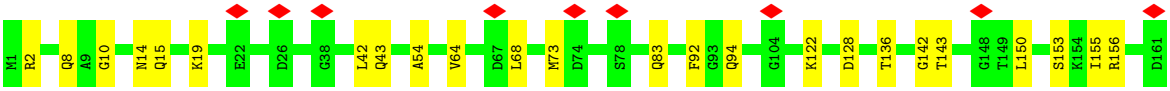


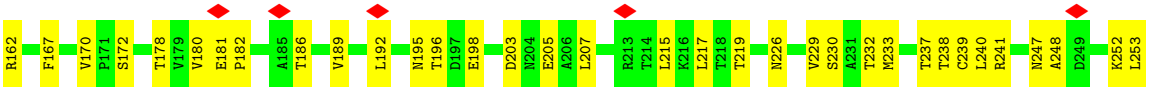


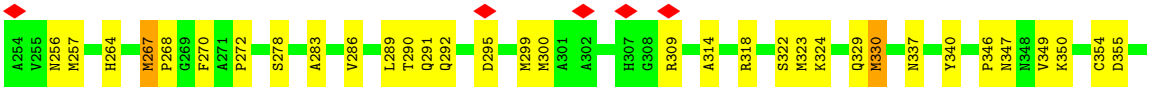
• Molecule 9: Tubulin beta-4B chain

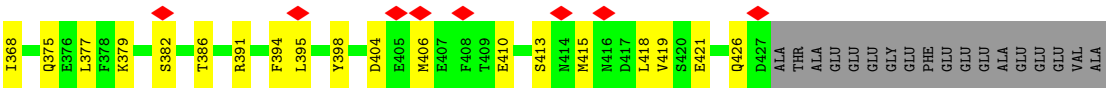
Chain PB:







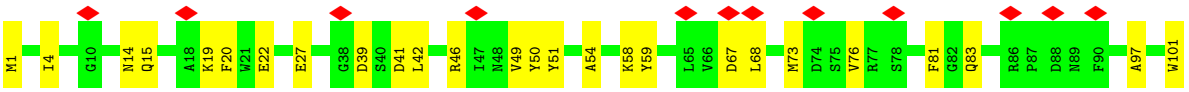


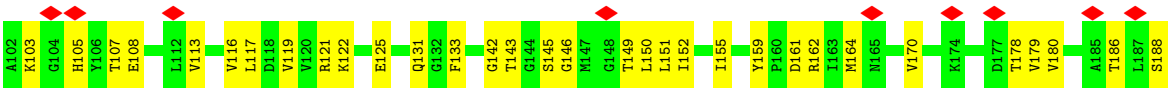


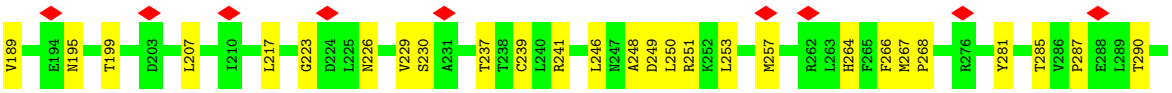
• Molecule 9: Tubulin beta-4B chain

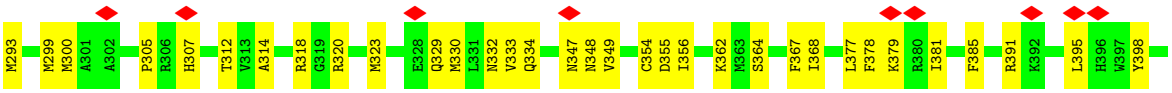
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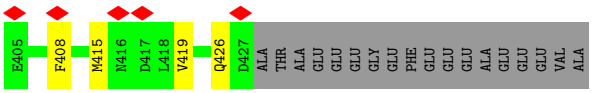








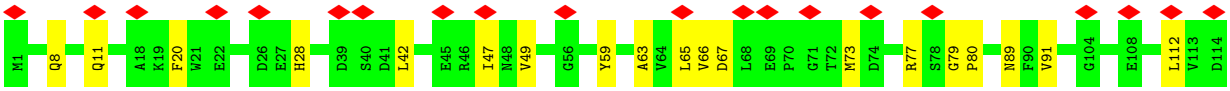


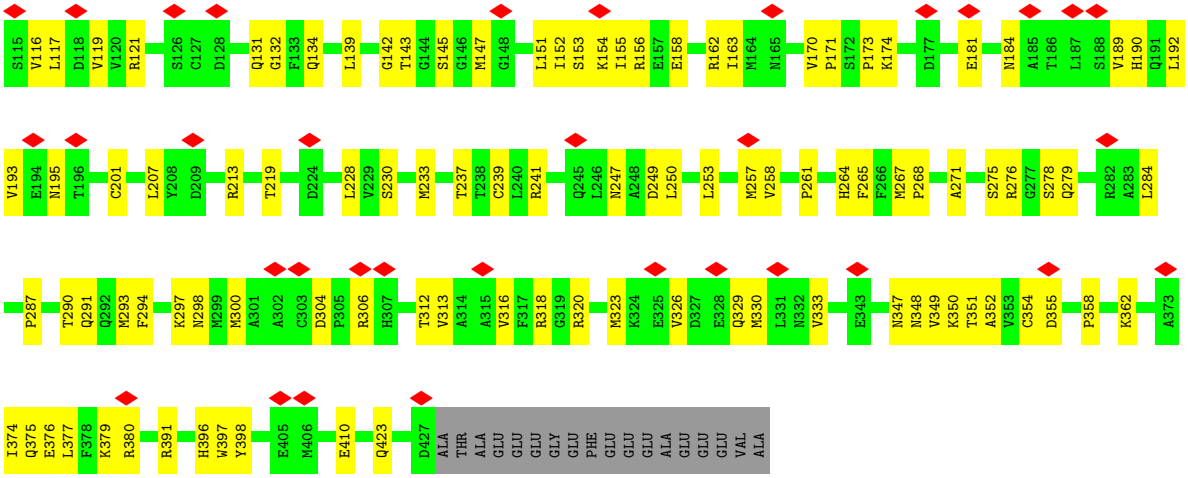


• Molecule 9: Tubulin beta-4B chain

Chain PF:



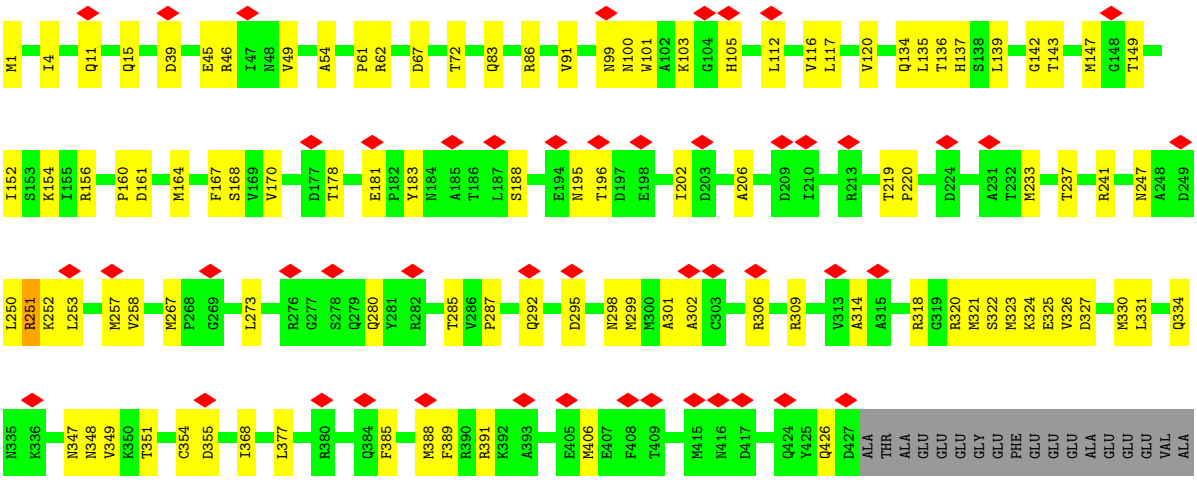




• Molecule 9: Tubulin beta-4B chain

Chain PH:

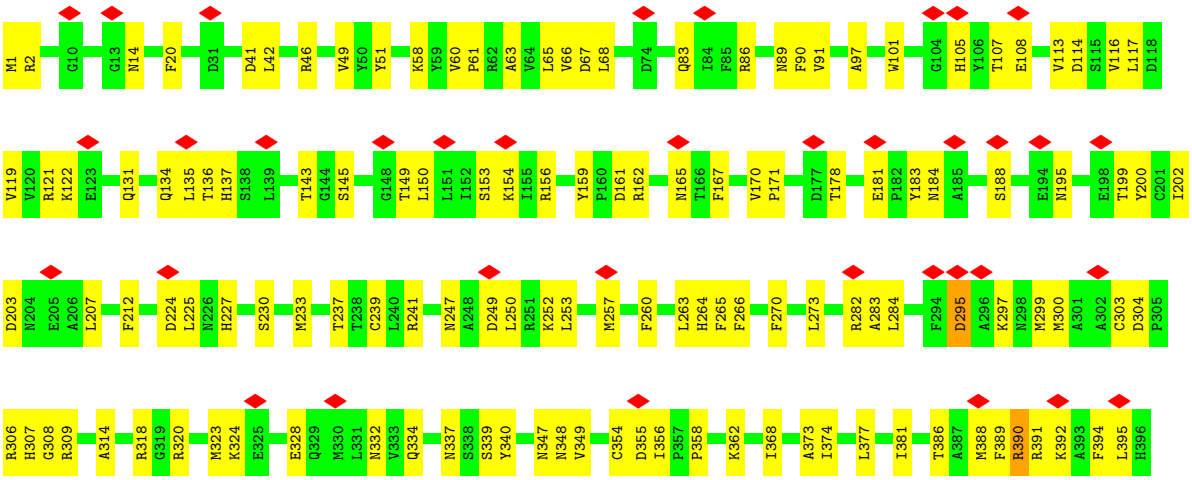


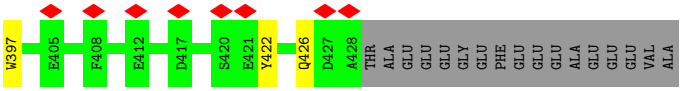


• Molecule 9: Tubulin beta-4B chain

Chain PJ:



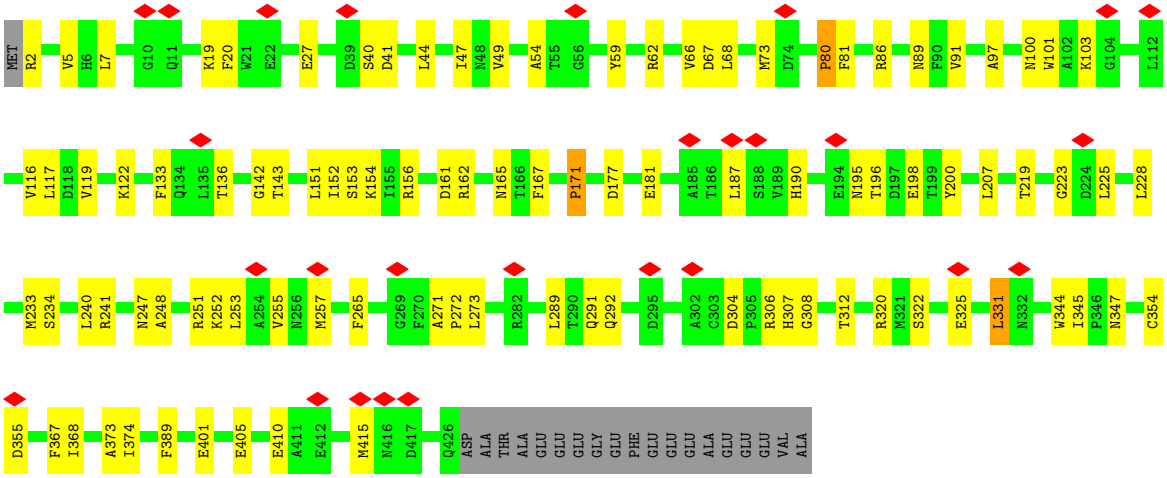




• Molecule 9: Tubulin beta-4B chain

Chain PL:

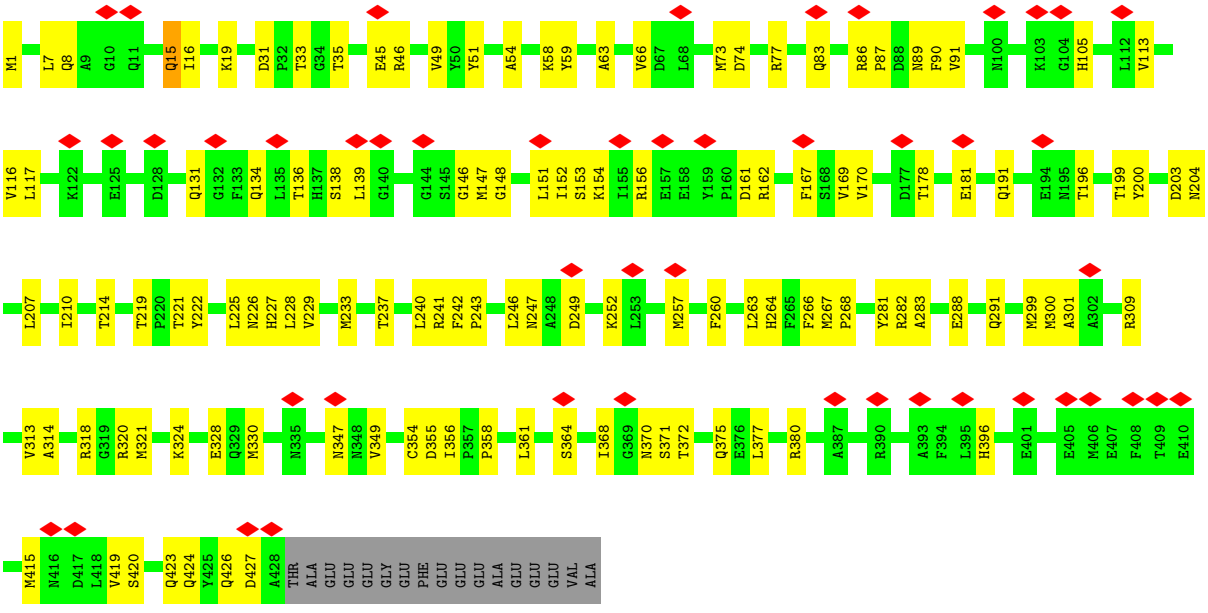




• Molecule 9: Tubulin beta-4B chain

Chain QB:

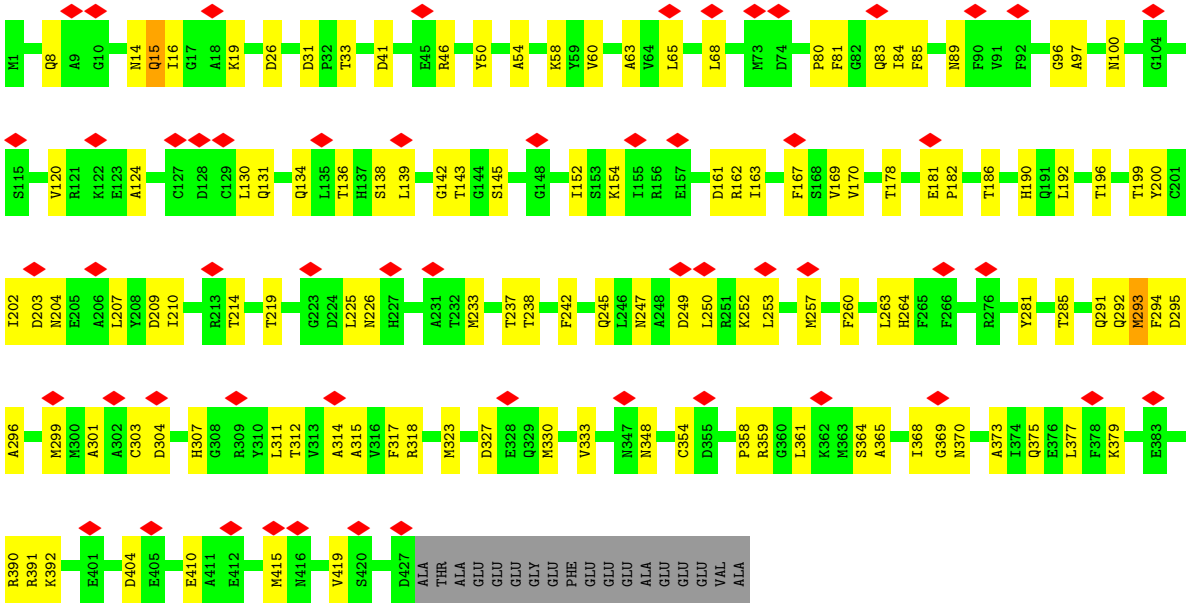




• Molecule 9: Tubulin beta-4B chain

Chain QD:

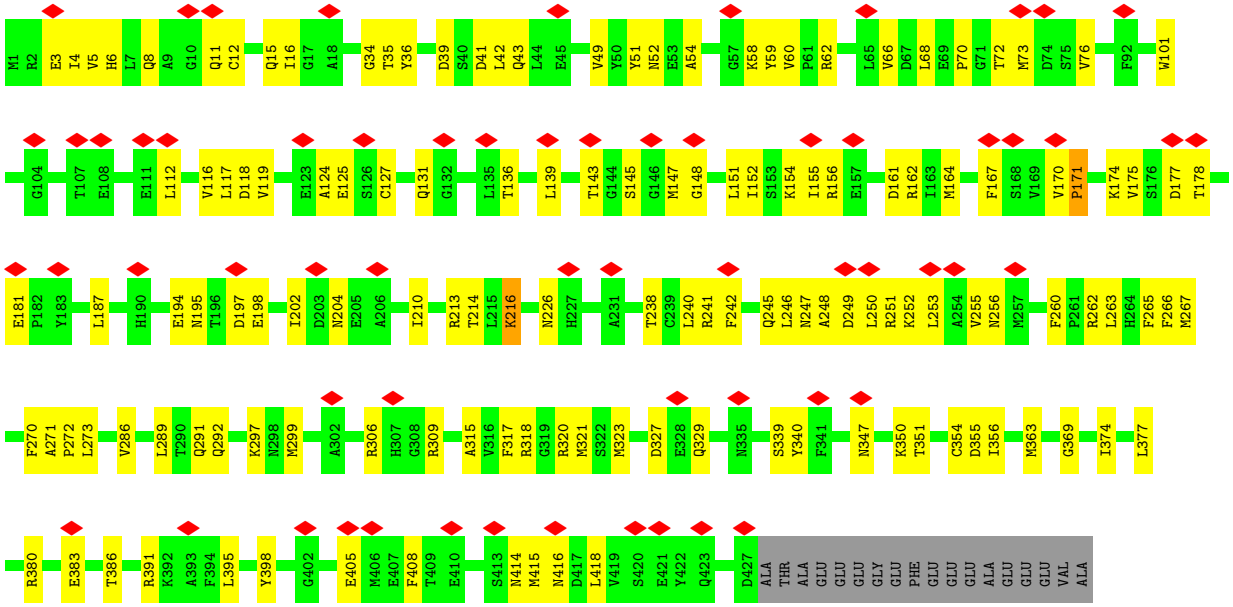




• Molecule 9: Tubulin beta-4B chain

Chain QF:

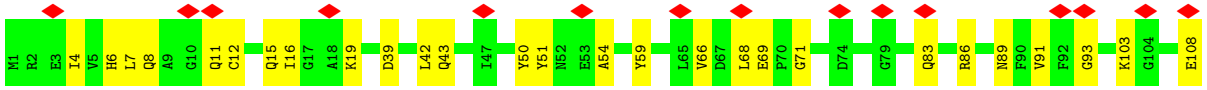


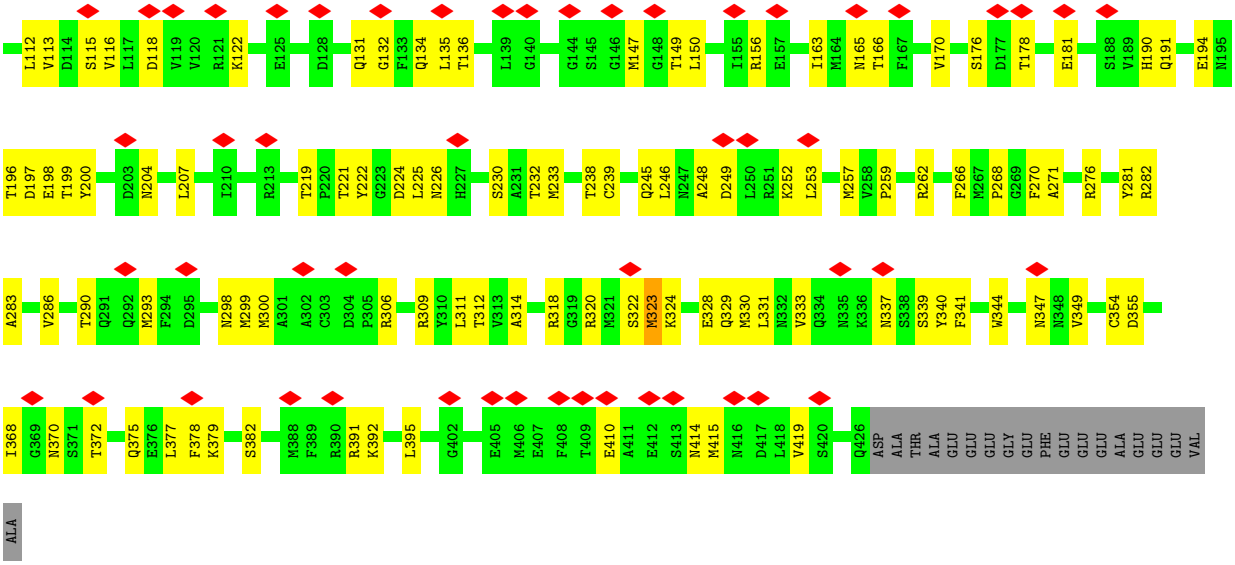


• Molecule 9: Tubulin beta-4B chain

Chain QH:



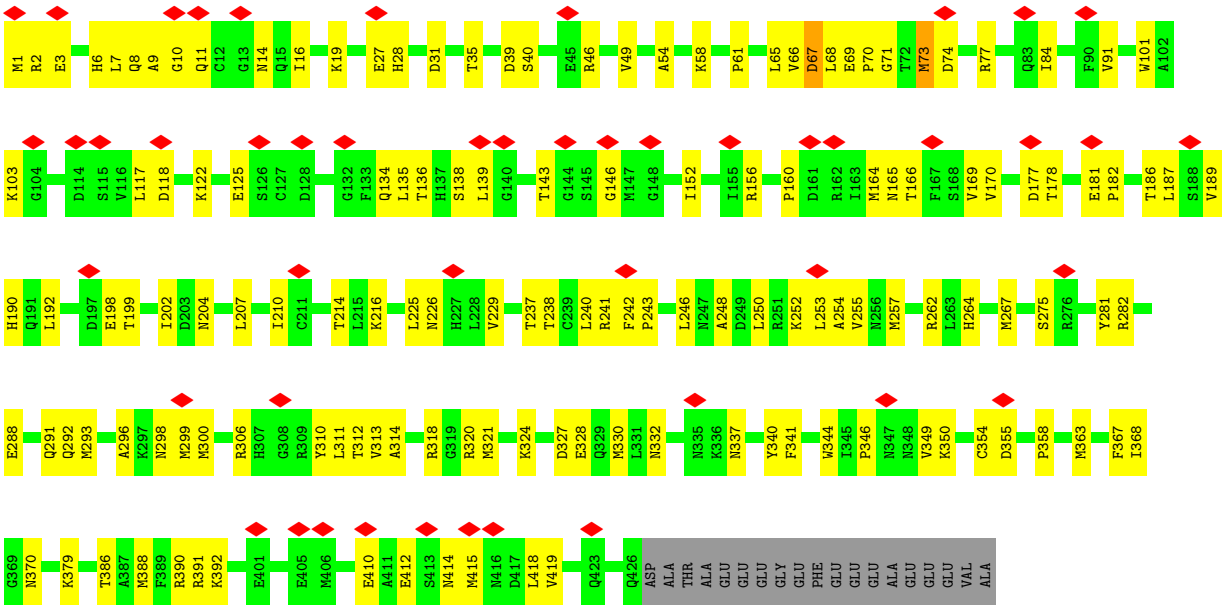




• Molecule 9: Tubulin beta-4B chain

Chain QJ:

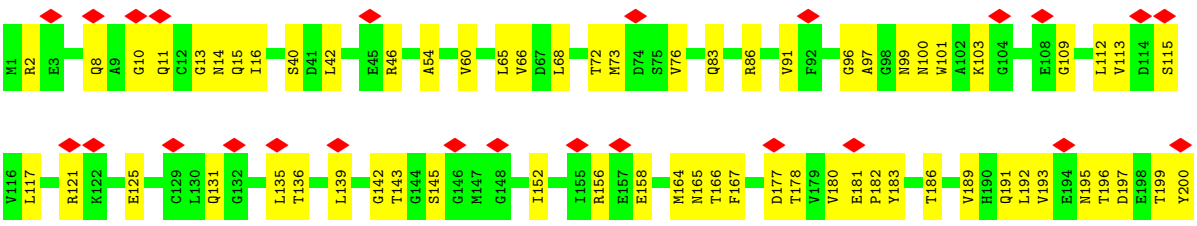


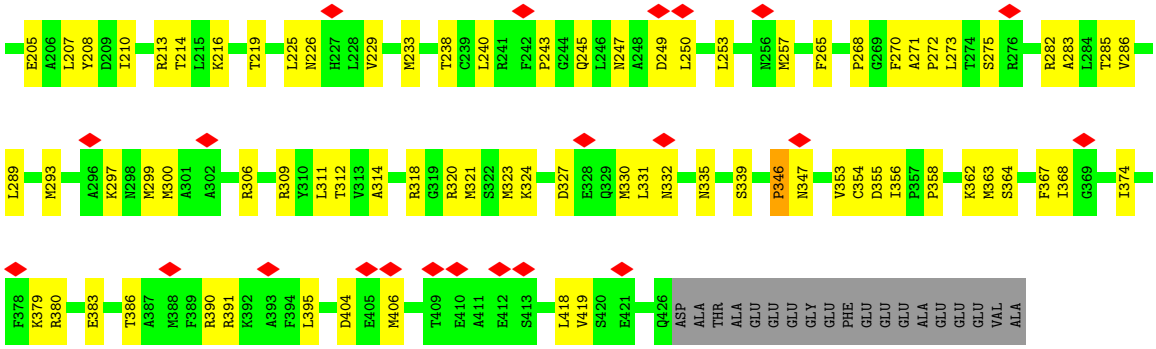


• Molecule 9: Tubulin beta-4B chain

Chain QL:



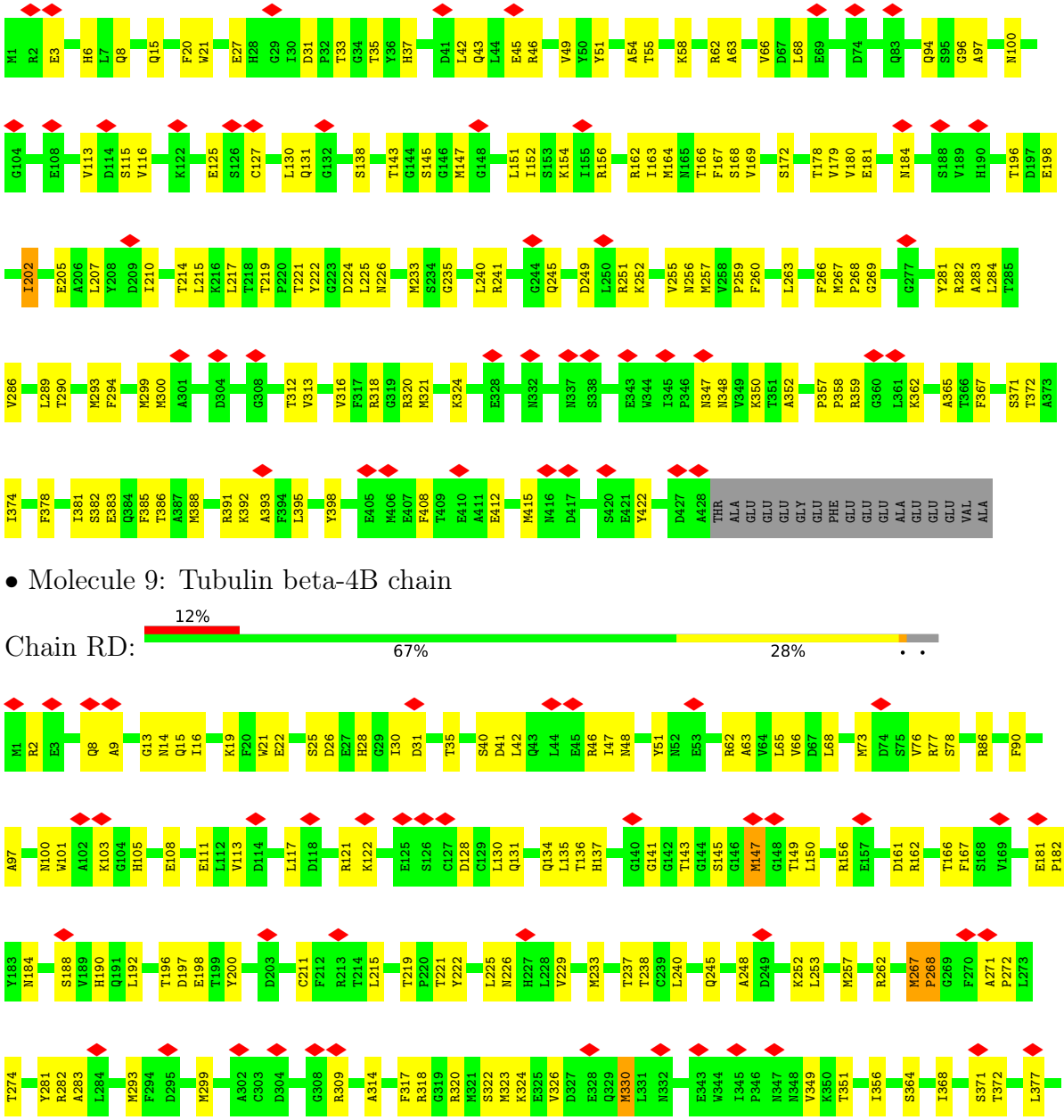




• Molecule 9: Tubulin beta-4B chain

Chain RB:





• Molecule 9: Tubulin beta-4B chain

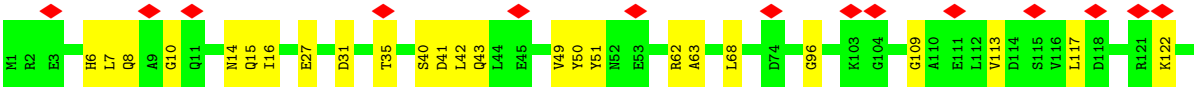
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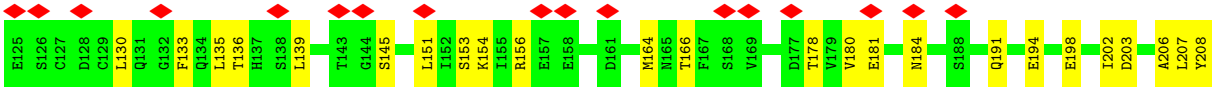


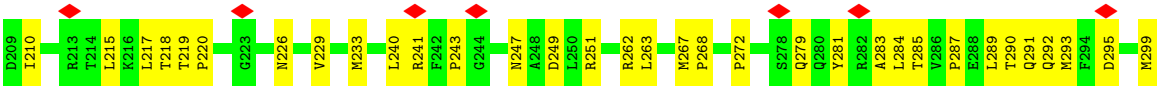
• Molecule 9: Tubulin beta-4B chain

Chain RF:

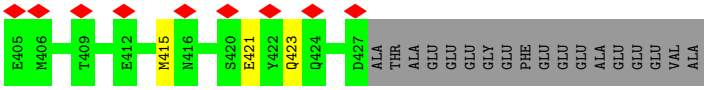








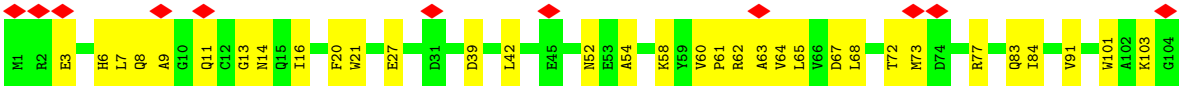


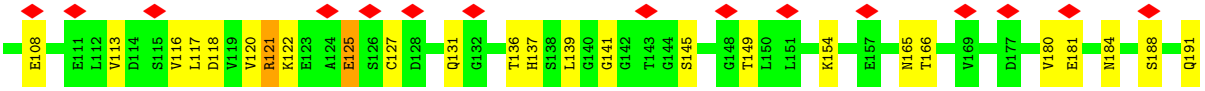


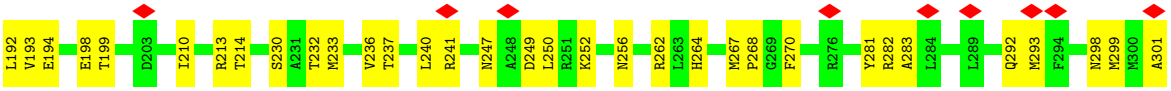
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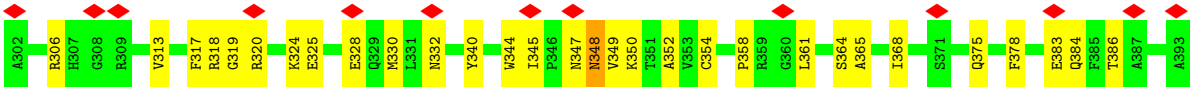
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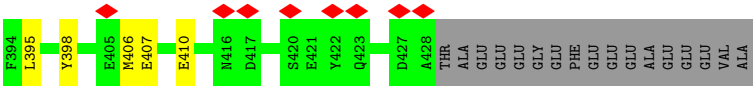








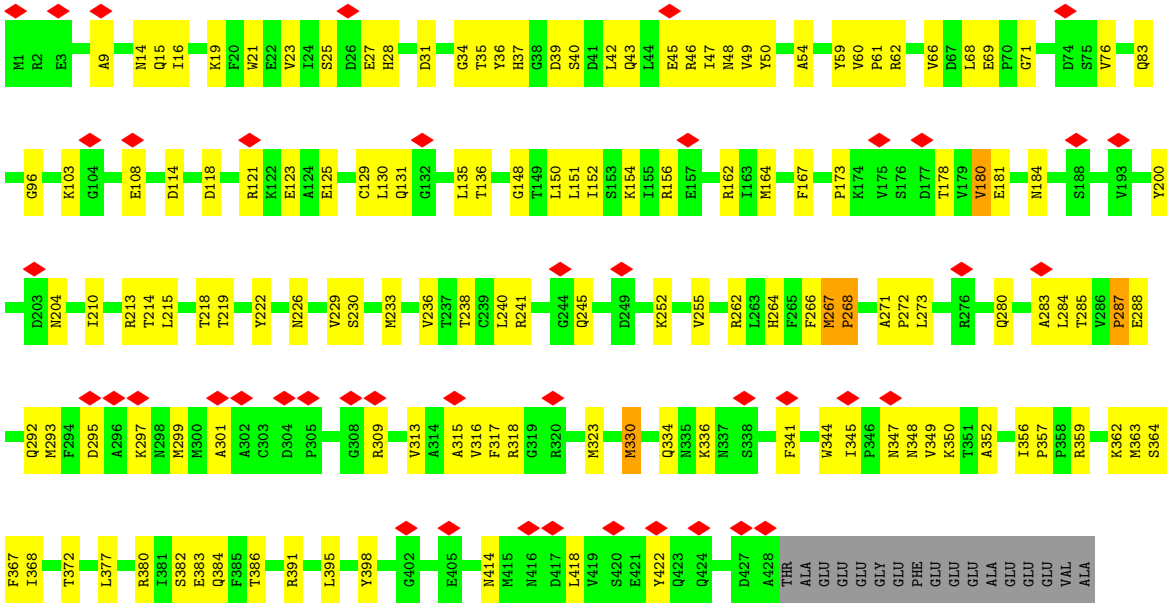




• Molecule 9: Tubulin beta-4B chain

Chain RJ:

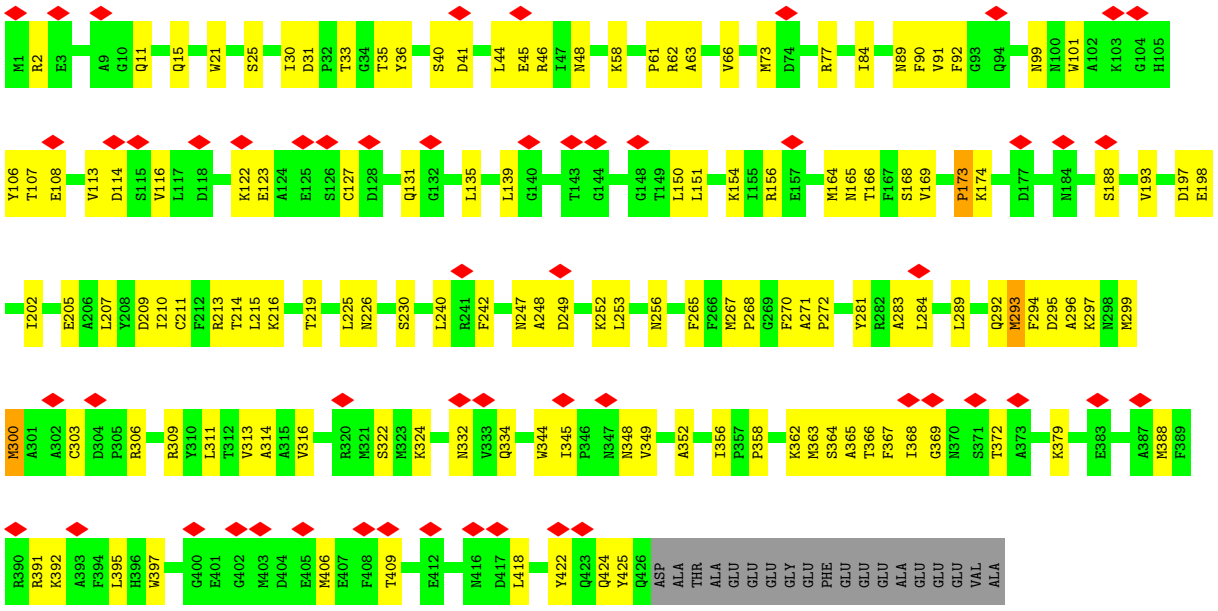




• Molecule 9: Tubulin beta-4B chain

Chain RL:

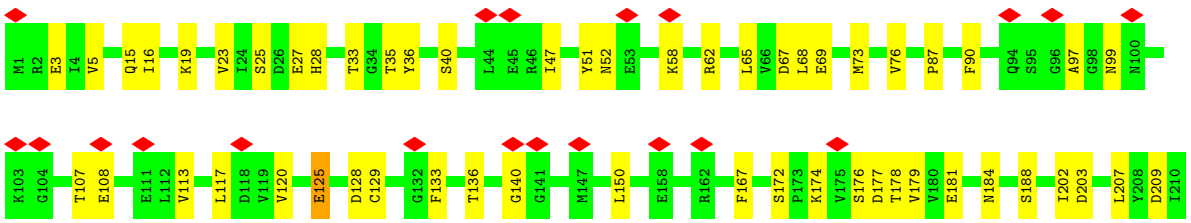


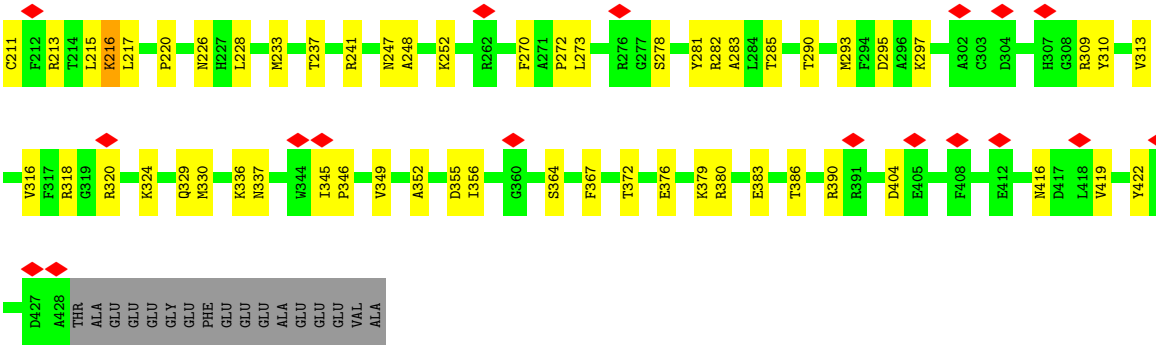


• Molecule 9: Tubulin beta-4B chain

Chain SB:



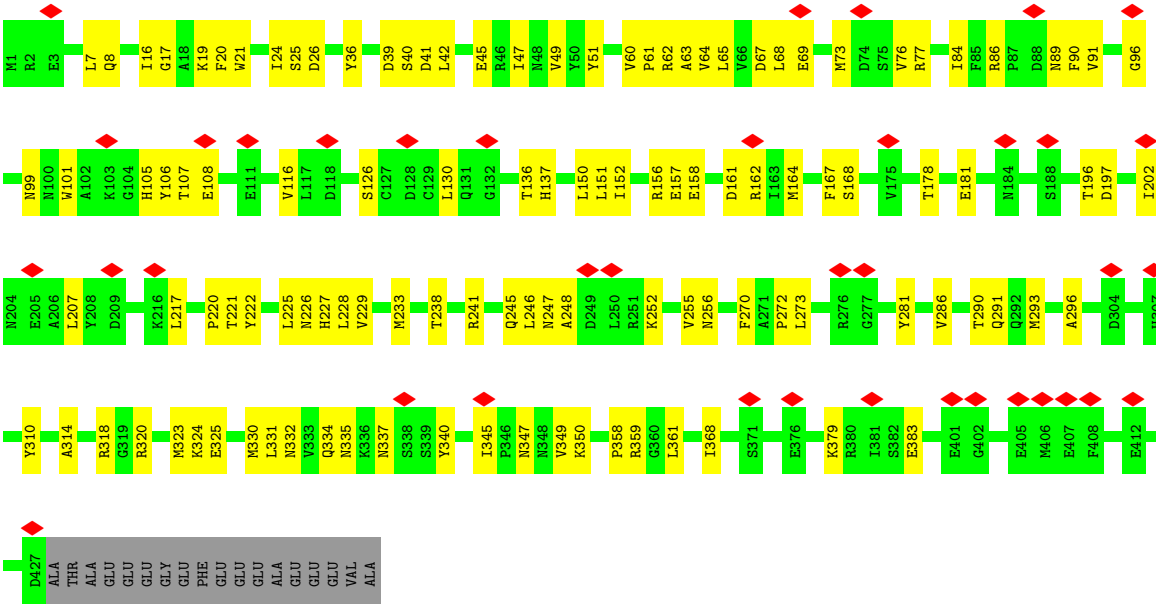




• Molecule 9: Tubulin beta-4B chain

Chain SD:

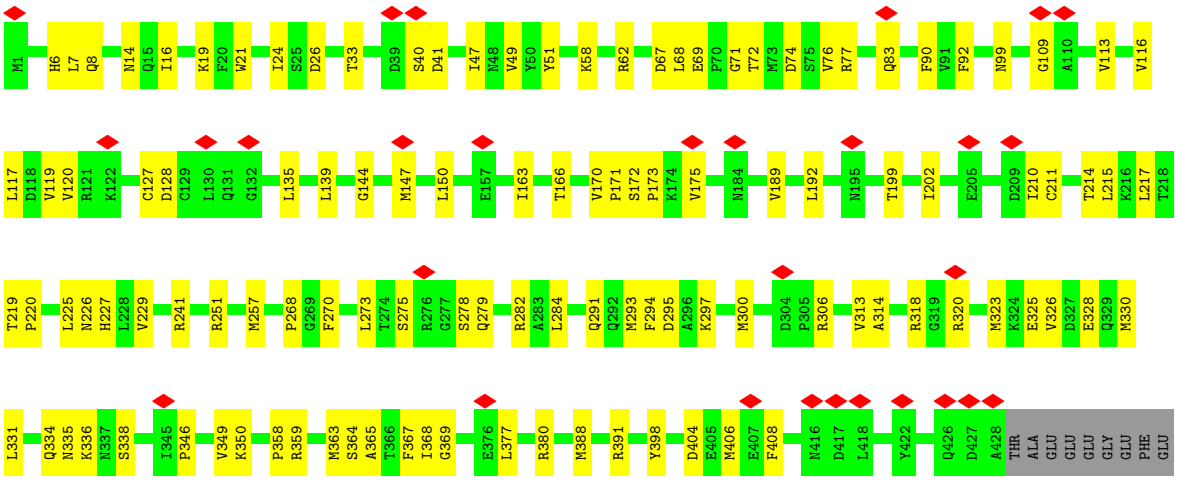




• Molecule 9: Tubulin beta-4B chain

Chain SF:



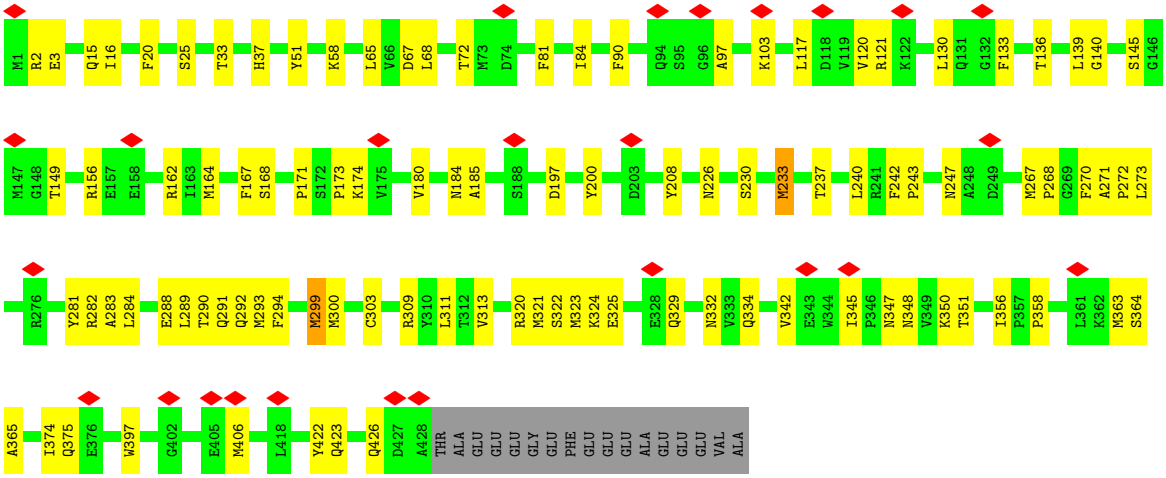




• Molecule 9: Tubulin beta-4B chain

Chain SH:

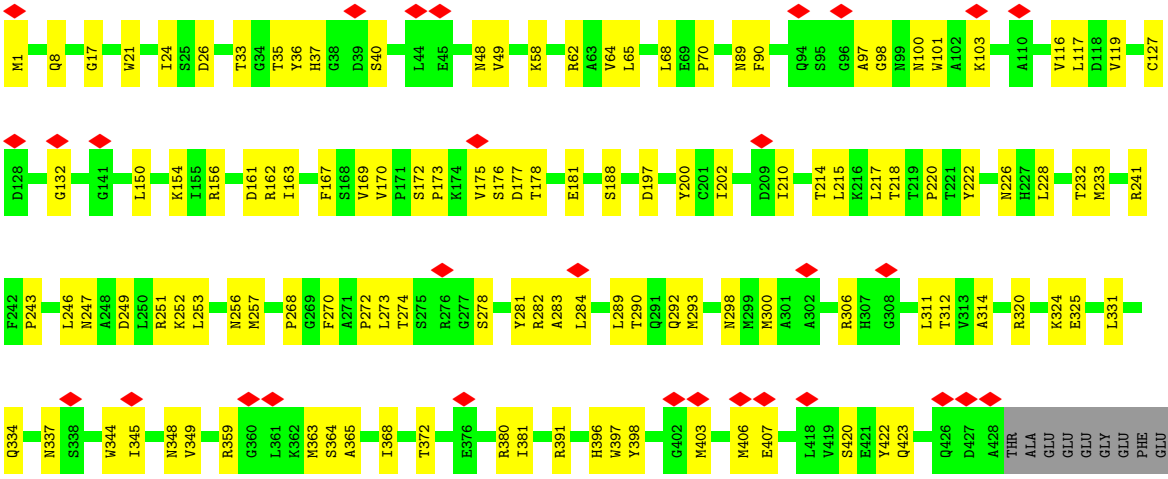




• Molecule 9: Tubulin beta-4B chain

Chain SJ:



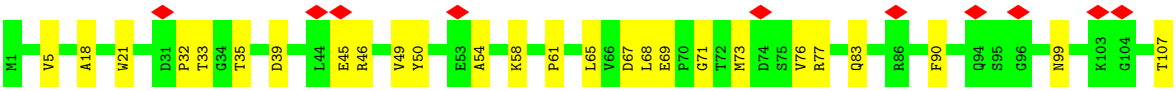


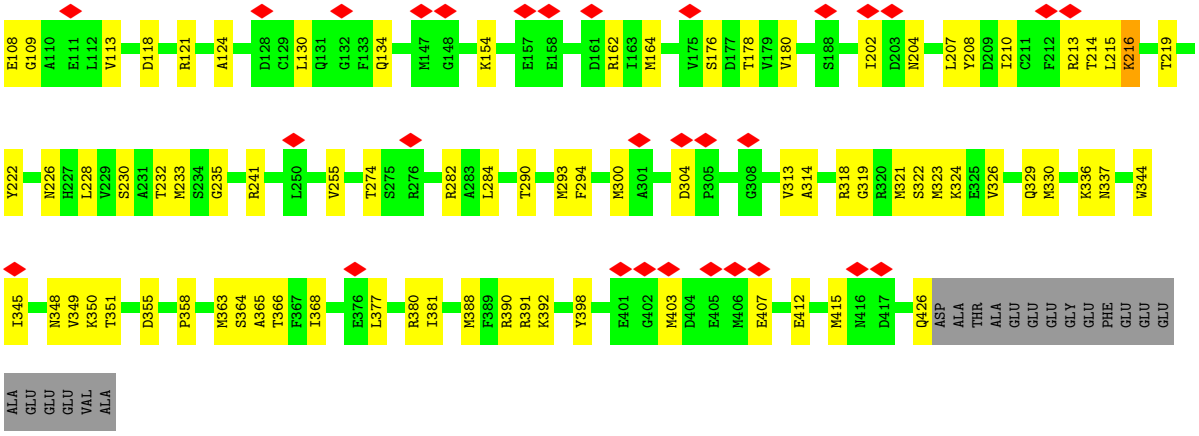


• Molecule 9: Tubulin beta-4B chain

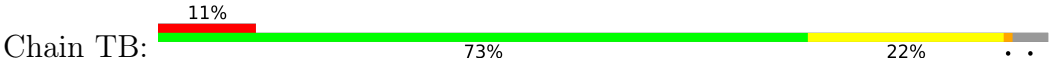
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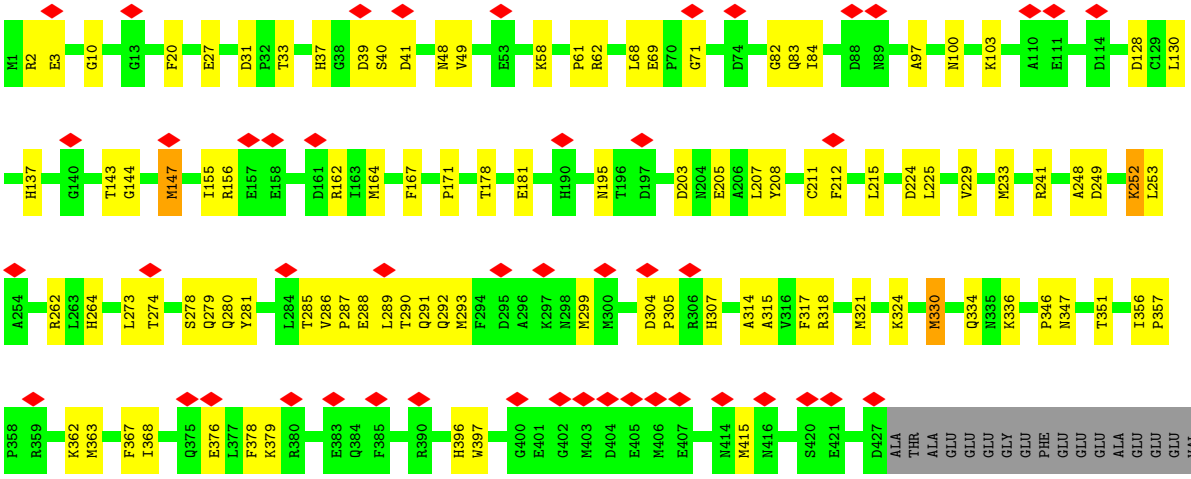




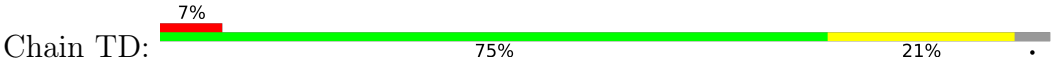


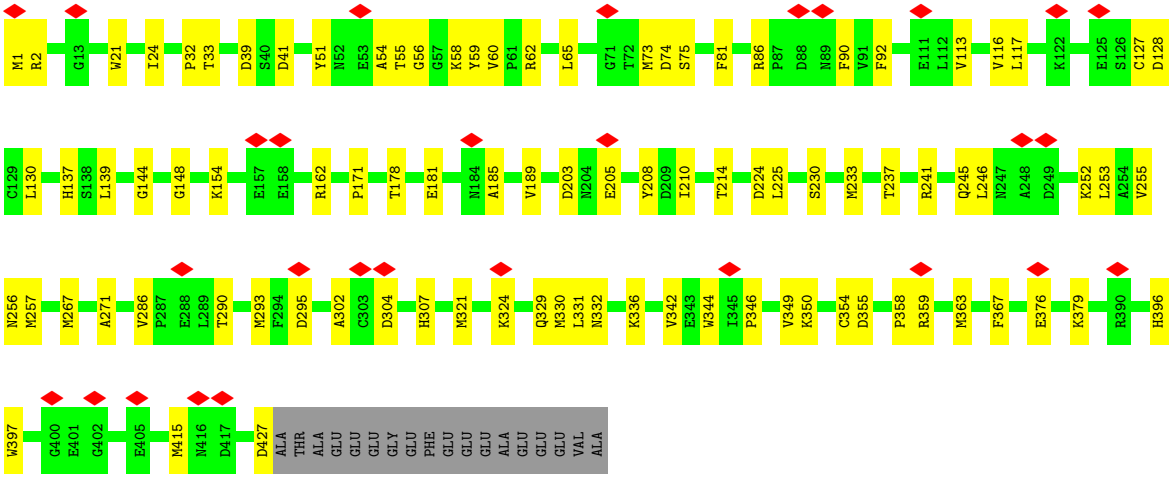
• Molecule 9: Tubulin beta-4B chain





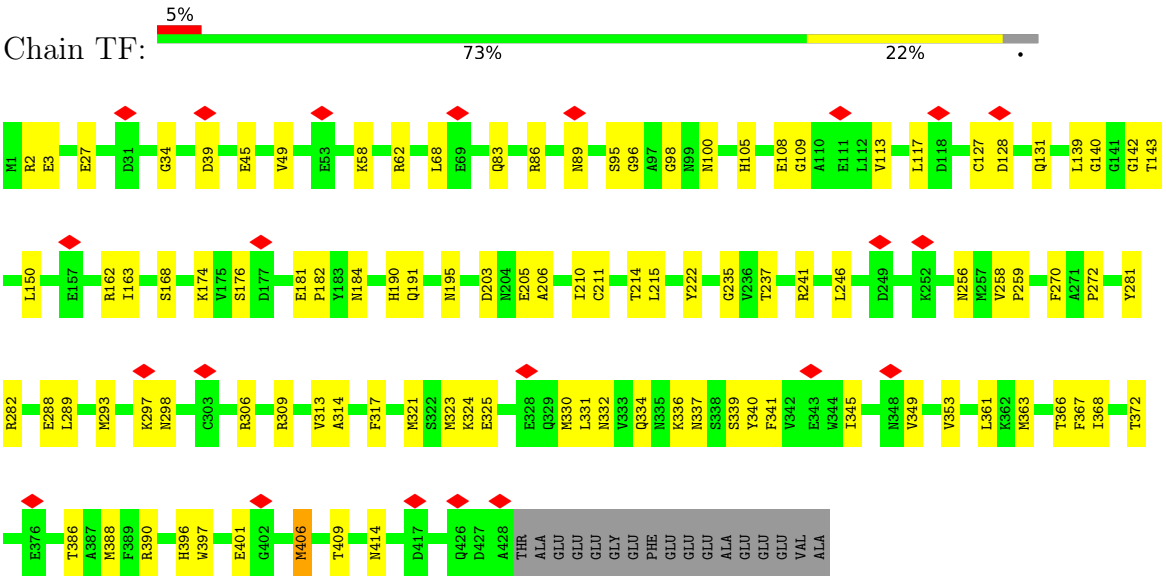
• Molecule 9: Tubulin beta-4B chain





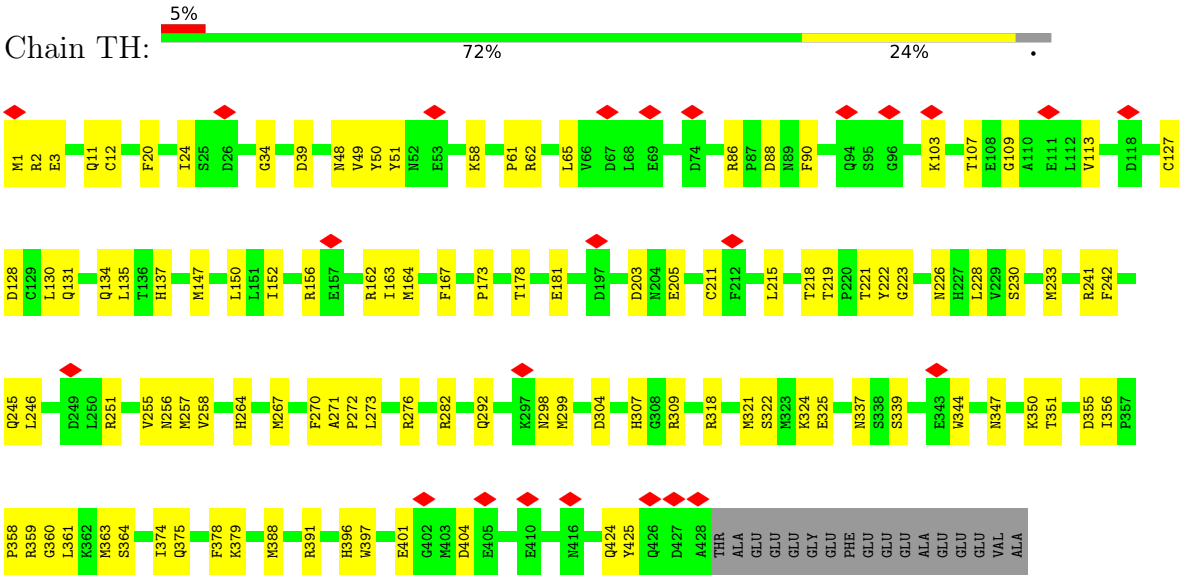
• Molecule 9: Tubulin beta-4B chain

Chain TF:



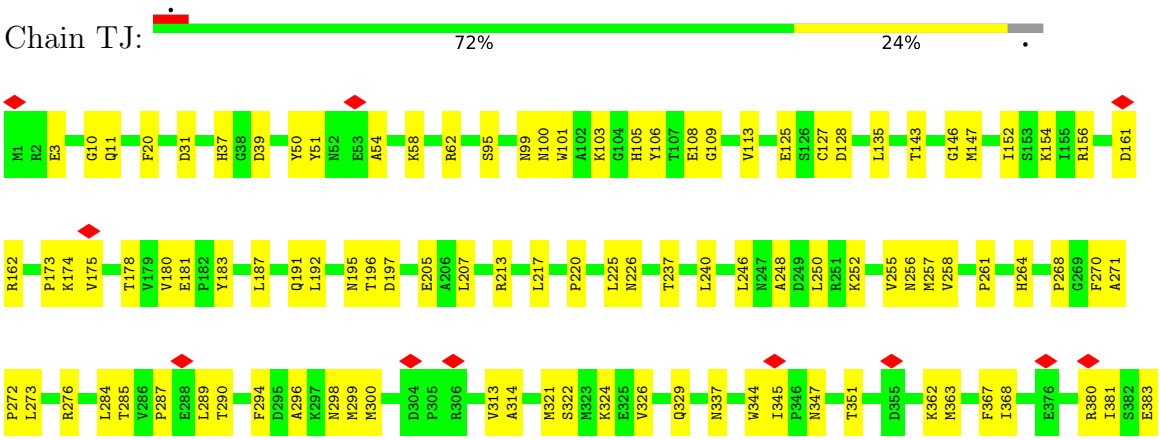
• Molecule 9: Tubulin beta-4B chain

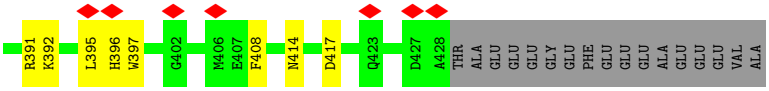
Chain TH:



• Molecule 9: Tubulin beta-4B chain

Chain TJ:

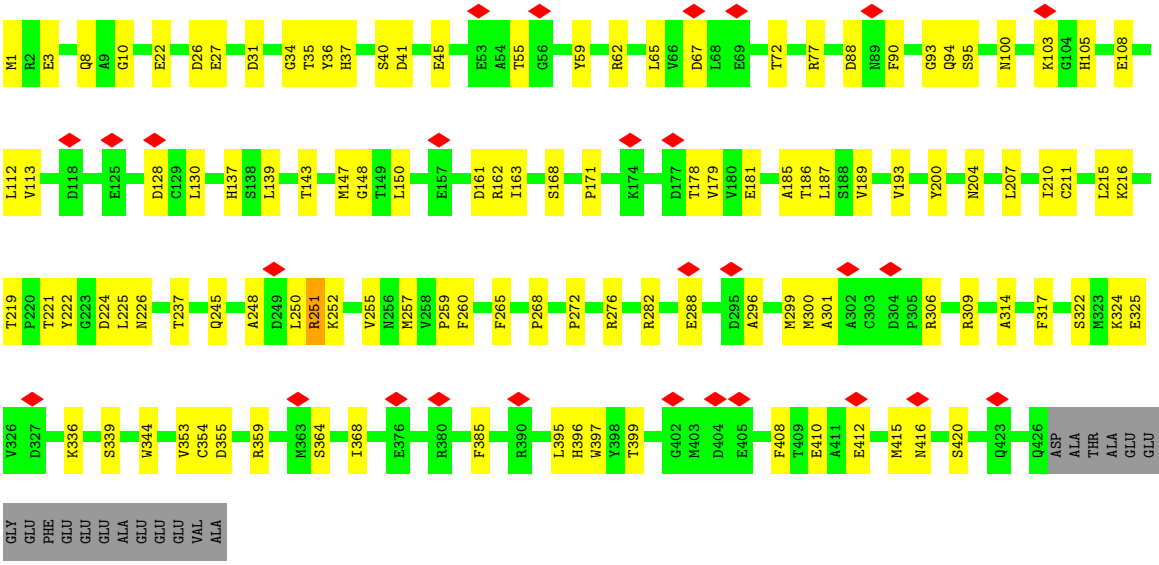




• Molecule 9: Tubulin beta-4B chain

Chain TL:

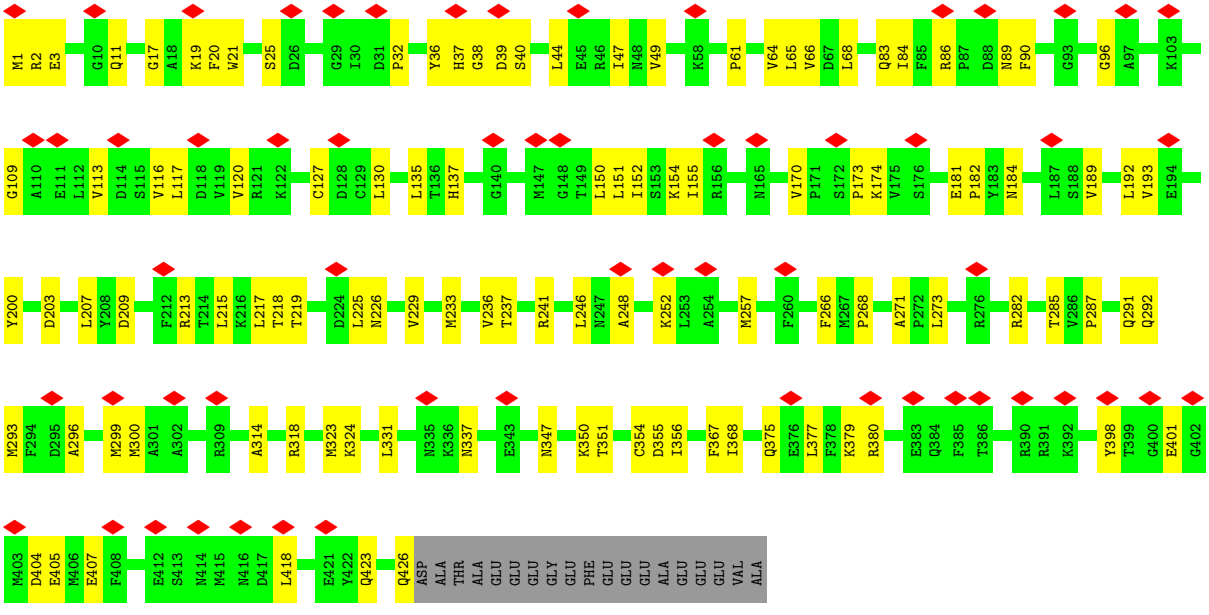




• Molecule 9: Tubulin beta-4B chain

Chain UB:

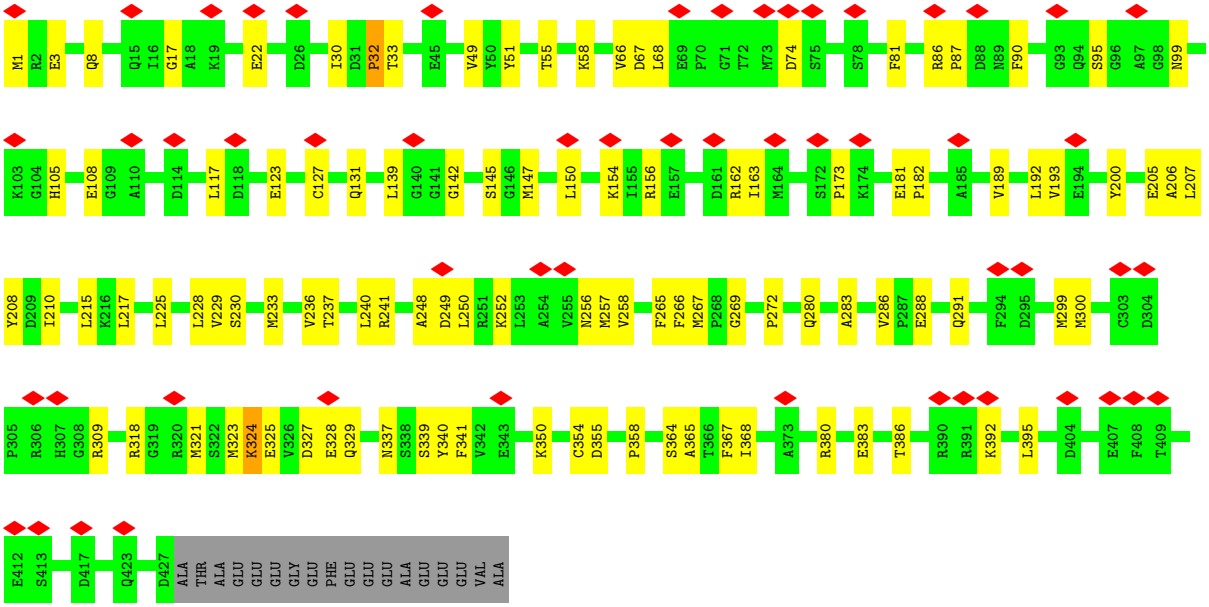




• Molecule 9: Tubulin beta-4B chain

Chain UD:

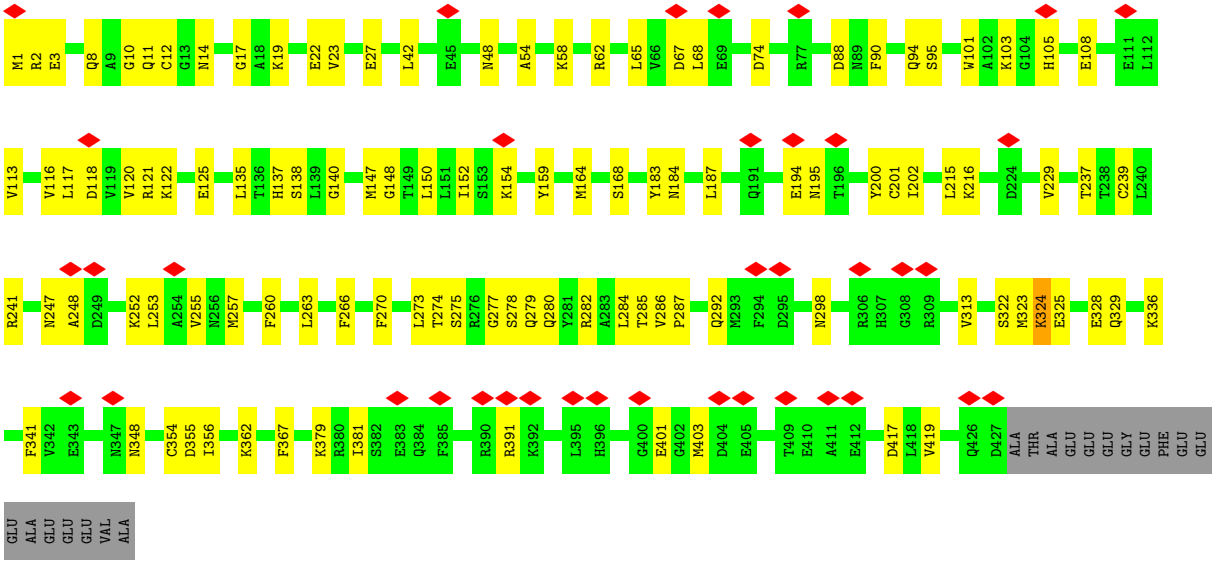




• Molecule 9: Tubulin beta-4B chain

Chain UF:

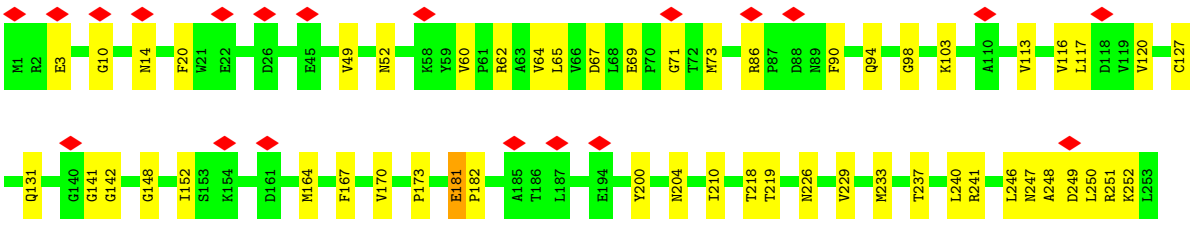


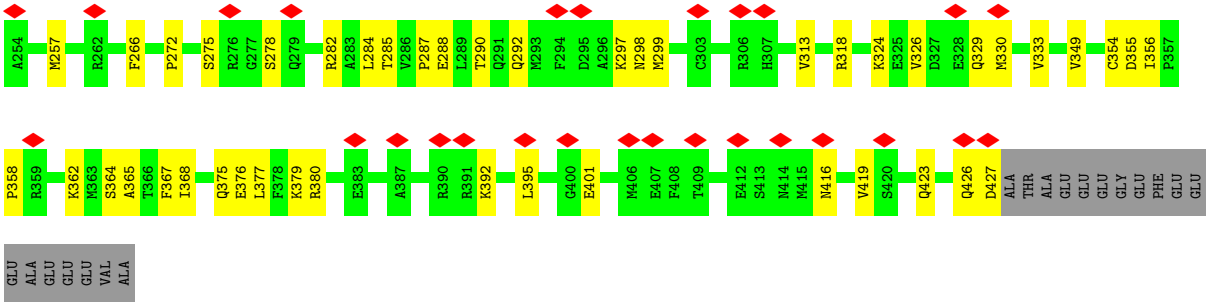


• Molecule 9: Tubulin beta-4B chain

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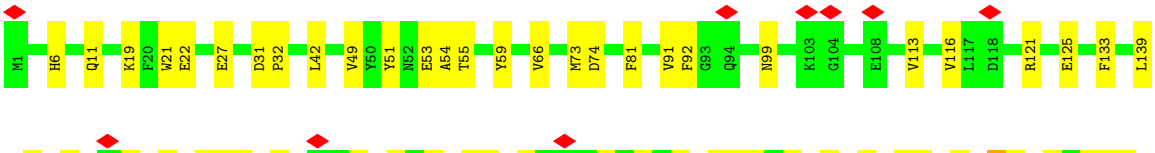




• Molecule 9: Tubulin beta-4B chain

Chain UJ:

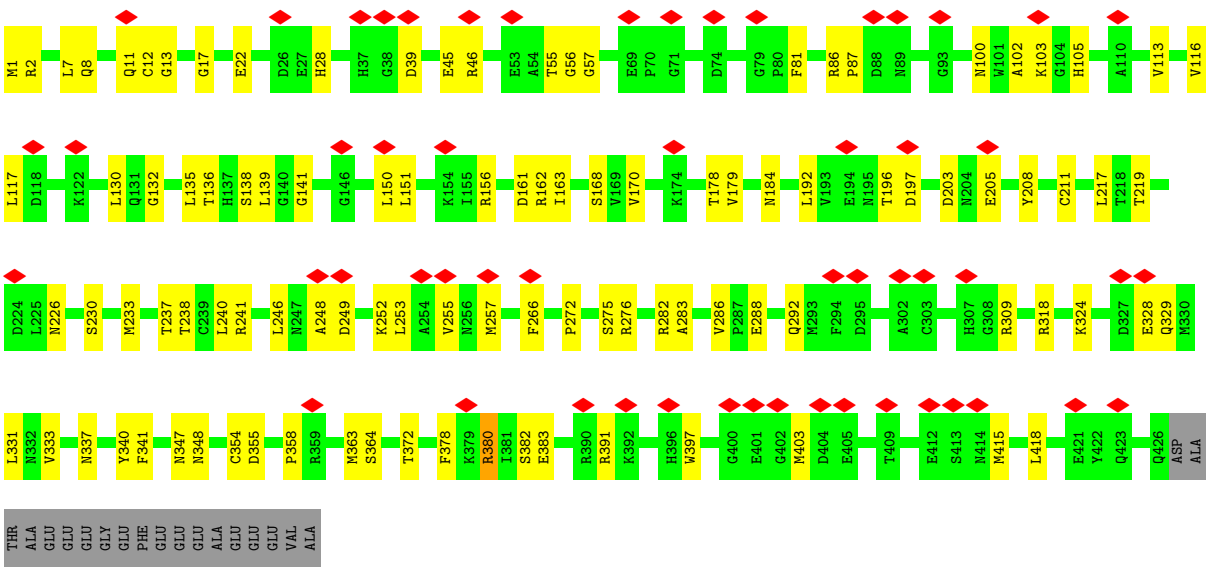




• Molecule 9: Tubulin beta-4B chain

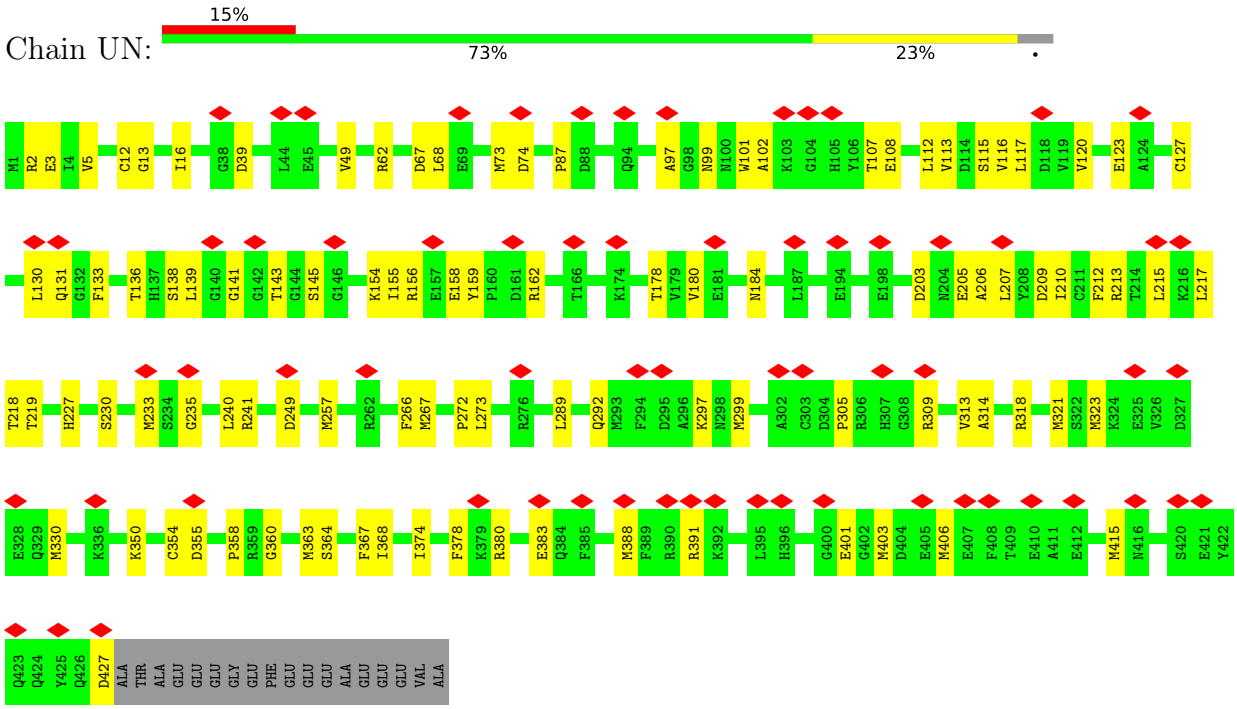
Chain UL:





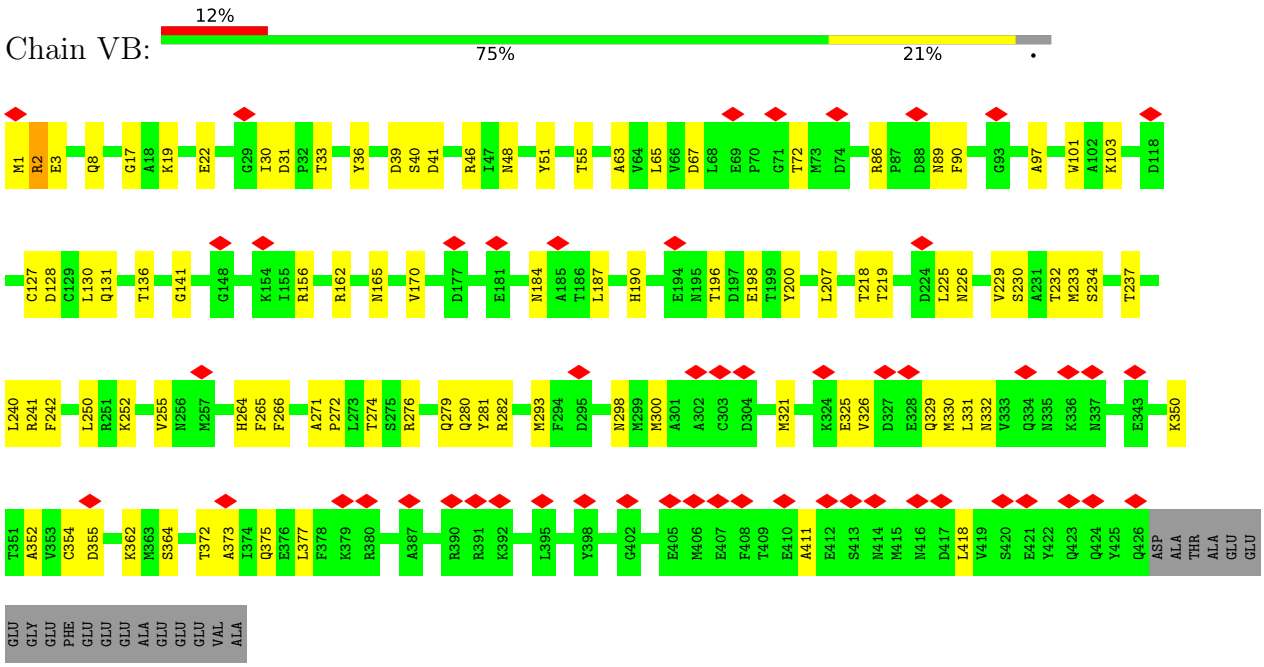
• Molecule 9: Tubulin beta-4B chain

Chain UN:



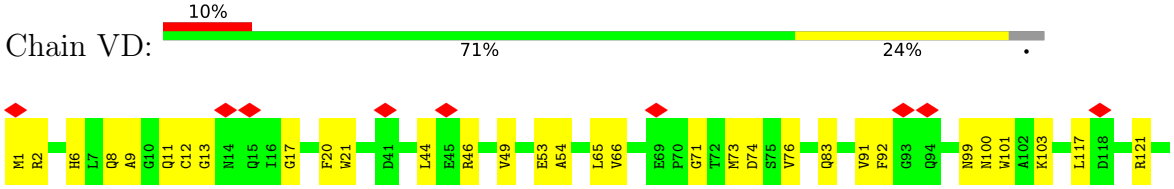
• Molecule 9: Tubulin beta-4B chain

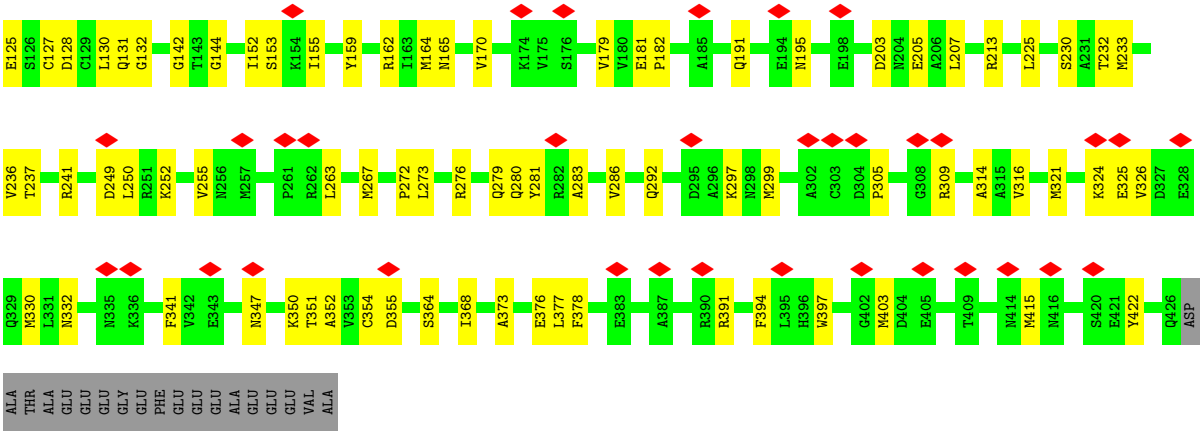
Chain VB:



• Molecule 9: Tubulin beta-4B chain

Chain VD:

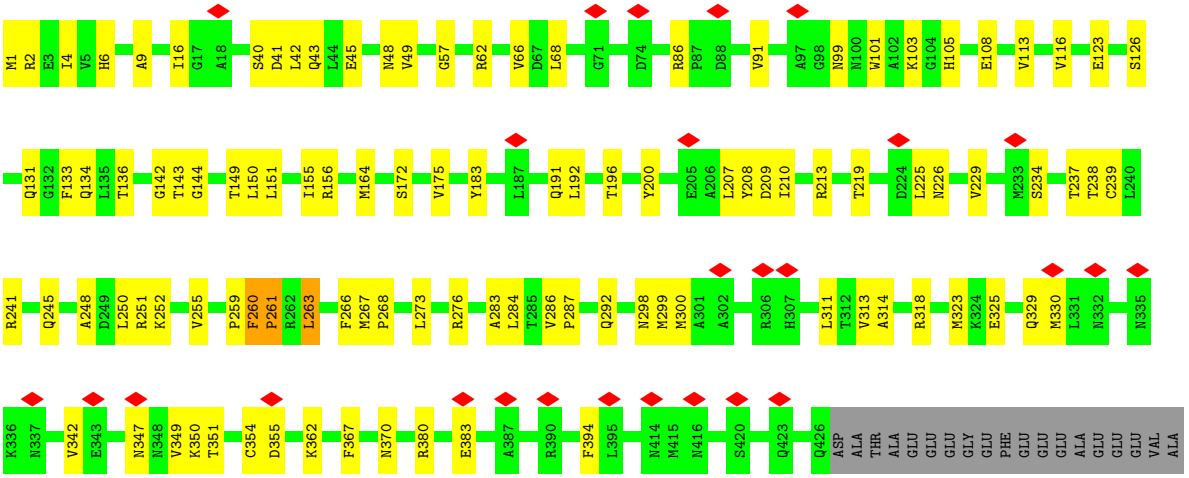




• Molecule 9: Tubulin beta-4B chain

Chain VF:

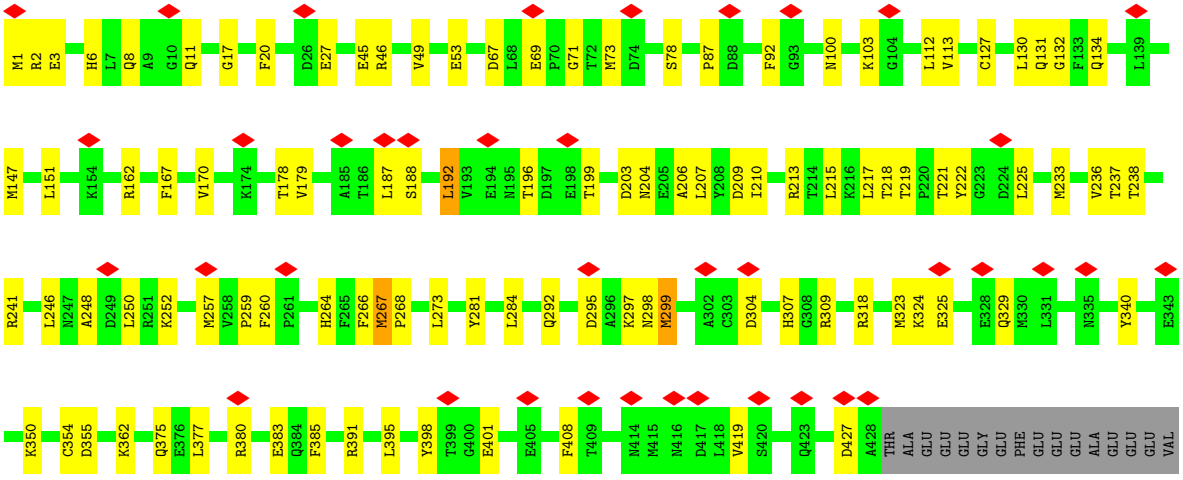




• Molecule 9: Tubulin beta-4B chain

Chain VH:



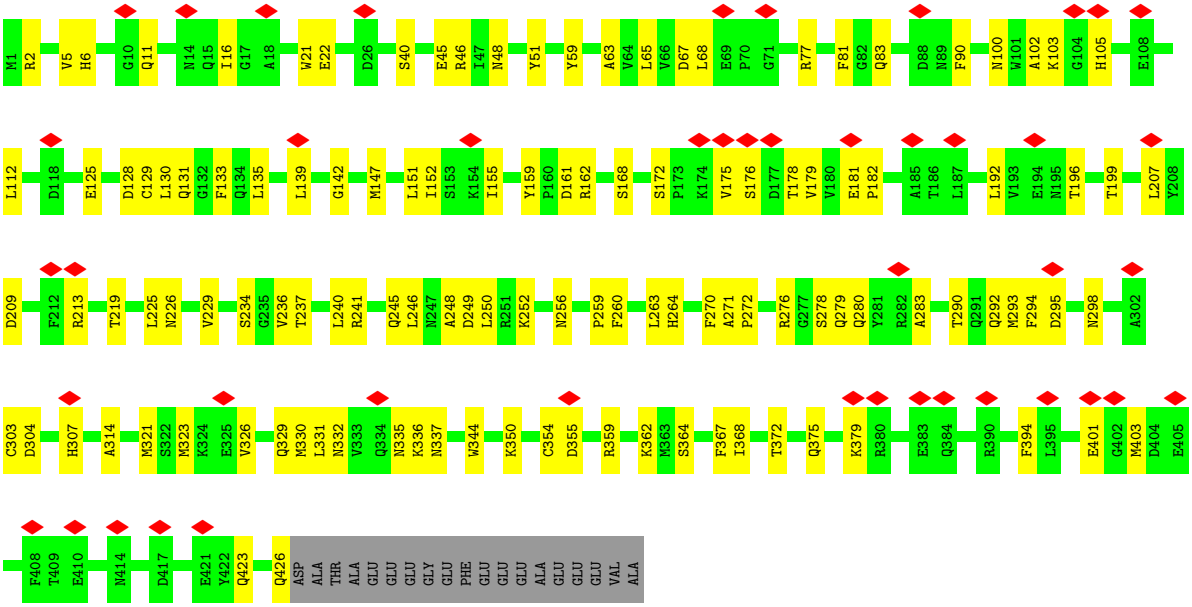




• Molecule 9: Tubulin beta-4B chain

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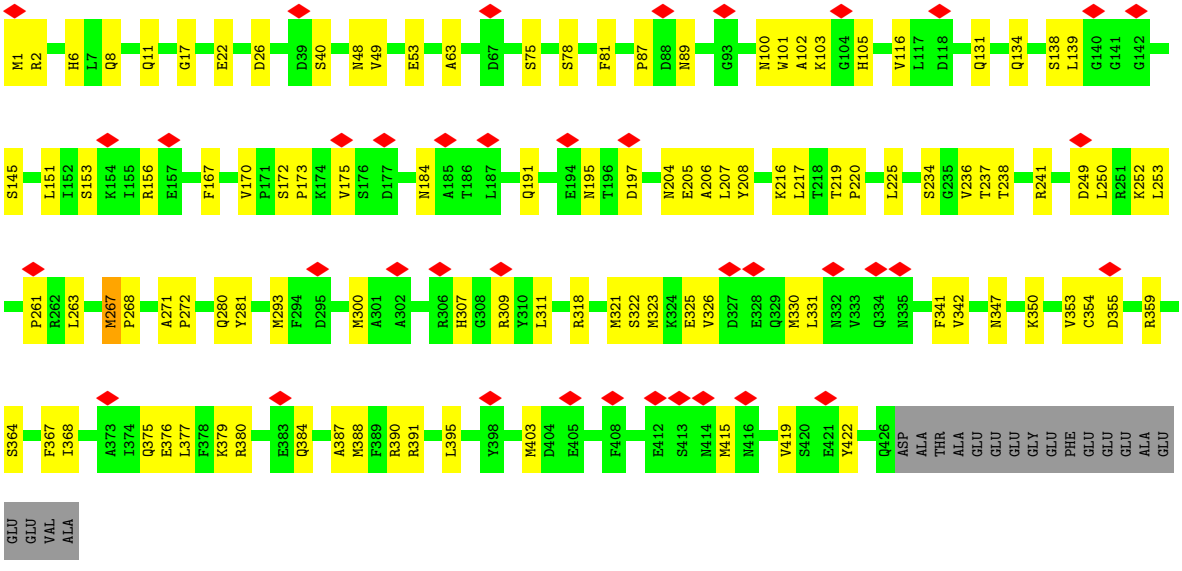




• Molecule 9: Tubulin beta-4B chain

Chain VL:

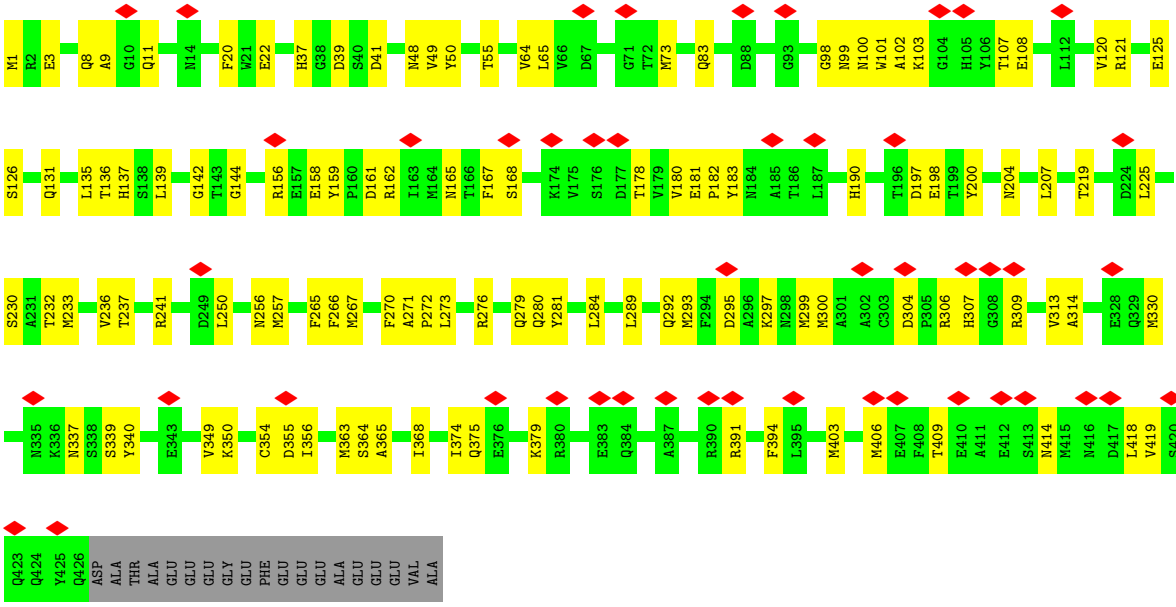




• Molecule 9: Tubulin beta-4B chain

Chain VN:

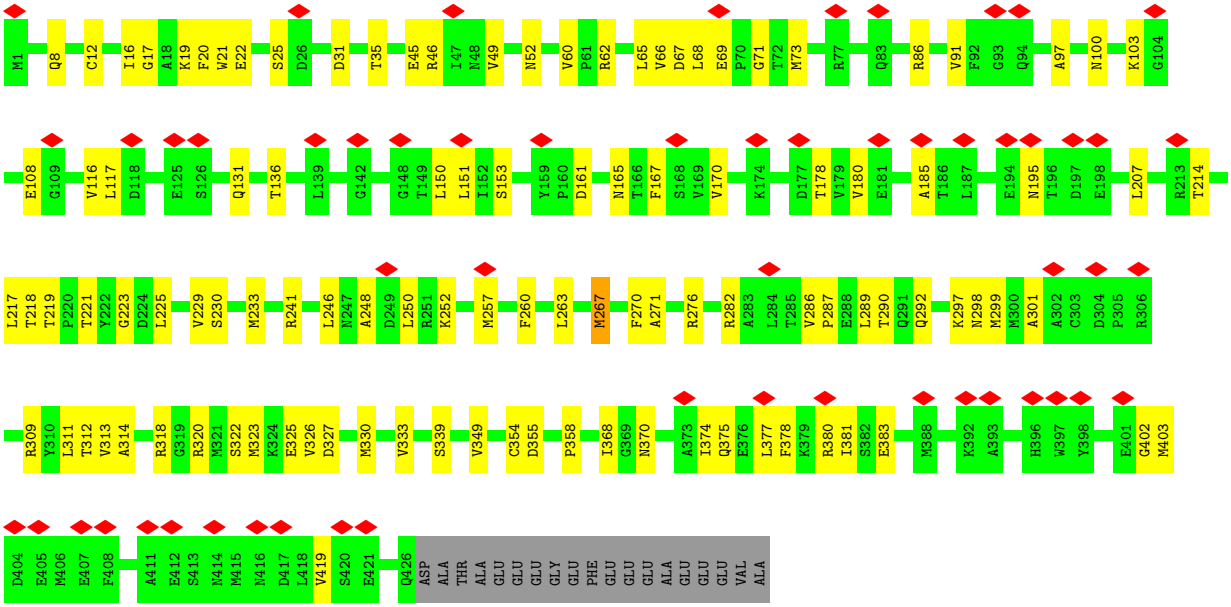




• Molecule 9: Tubulin beta-4B chain

Chain WB:

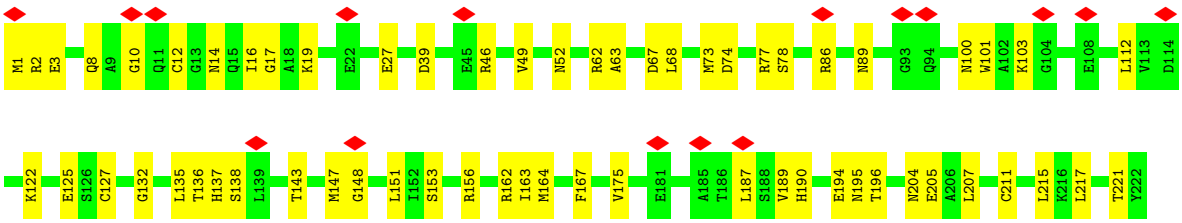


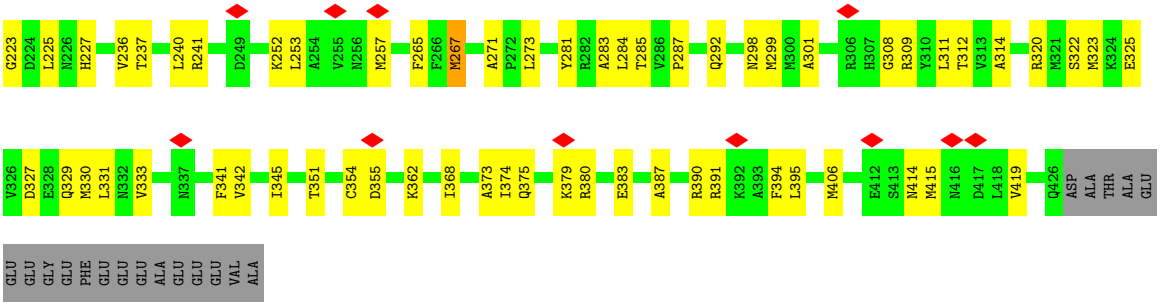


• Molecule 9: Tubulin beta-4B chain

Chain WD:



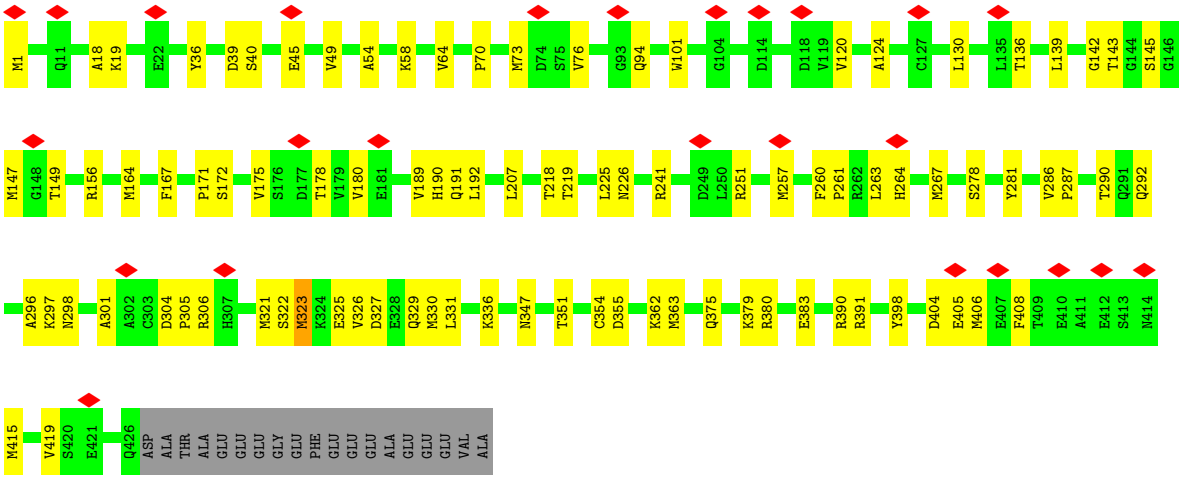




• Molecule 9: Tubulin beta-4B chain

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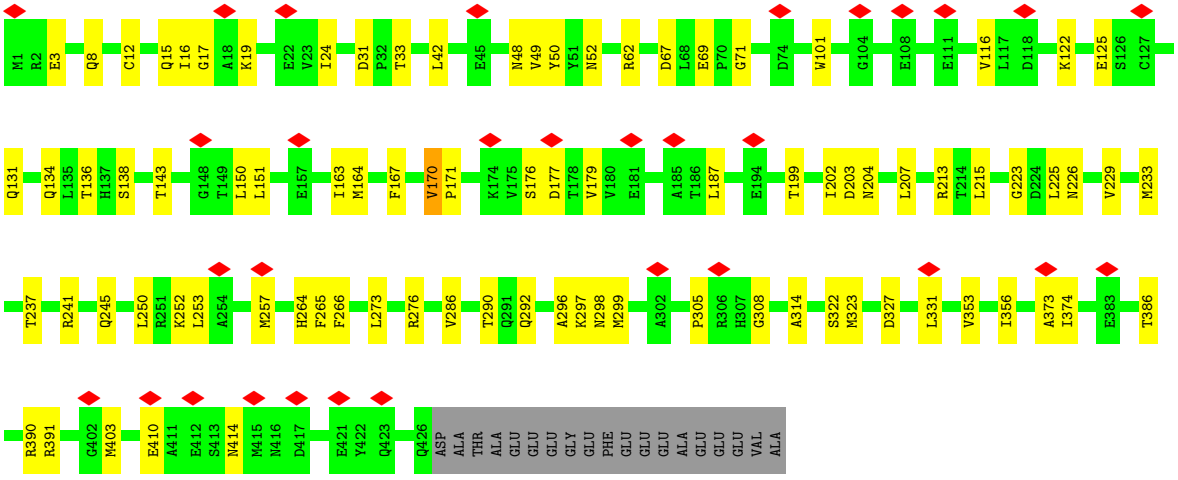




• Molecule 9: Tubulin beta-4B chain

Chain WH:

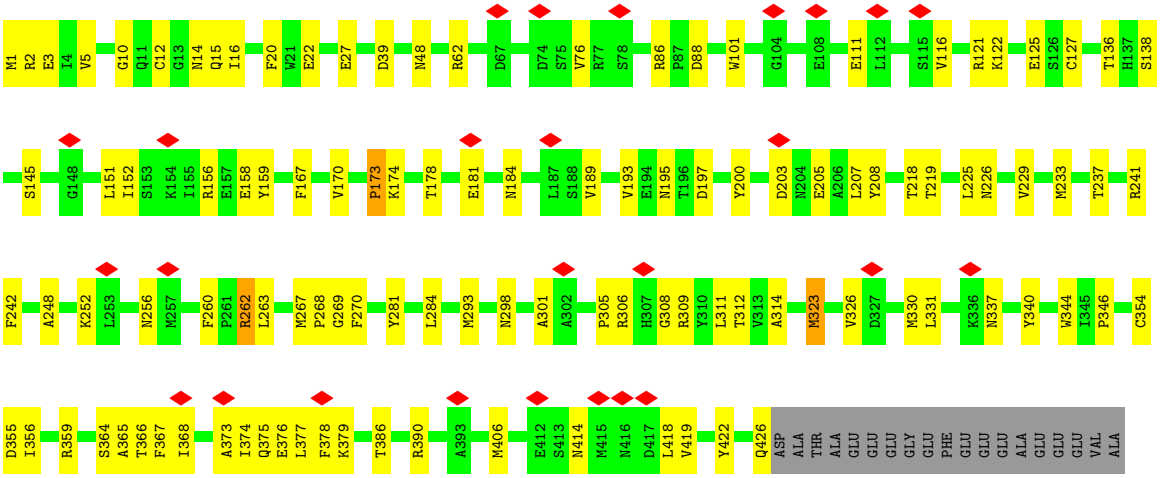




• Molecule 9: Tubulin beta-4B chain

Chain WJ:

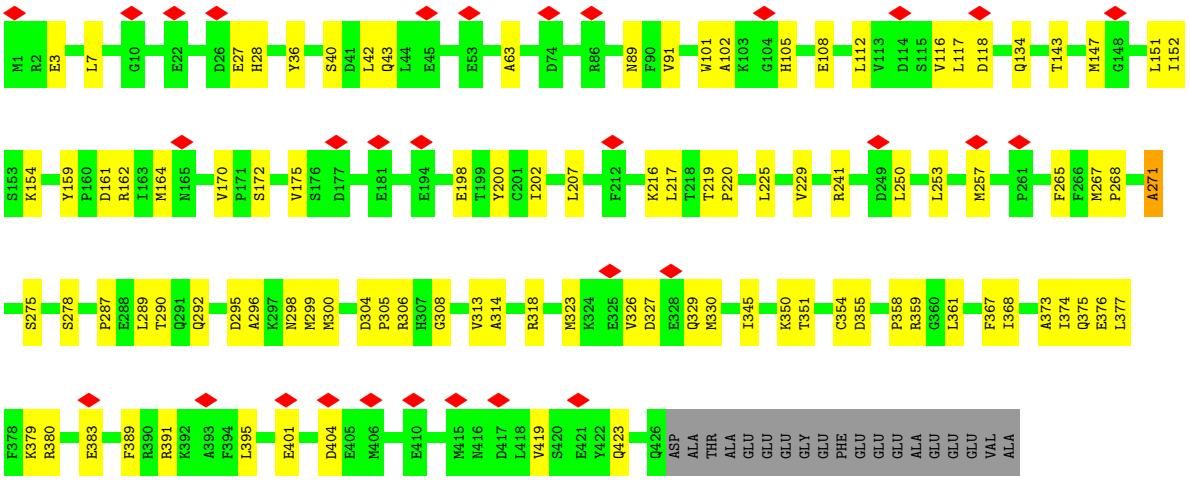




• Molecule 9: Tubulin beta-4B chain

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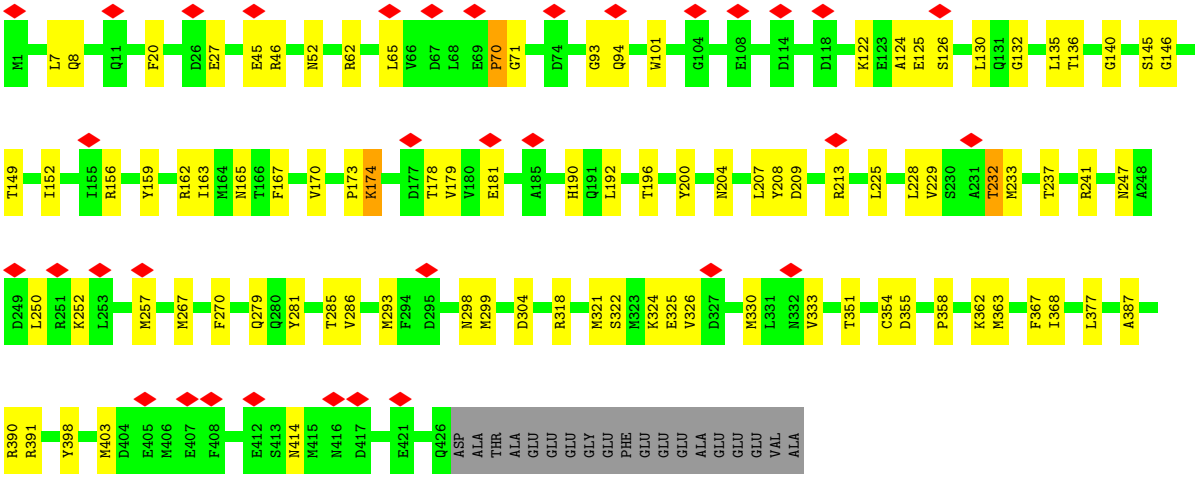




• Molecule 9: Tubulin beta-4B chain

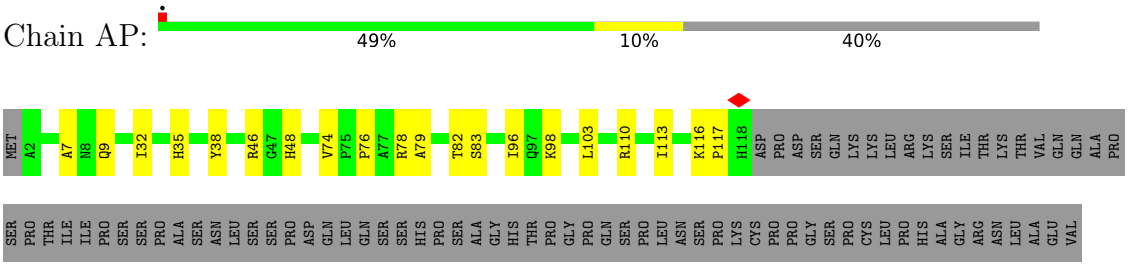
Chain WN:





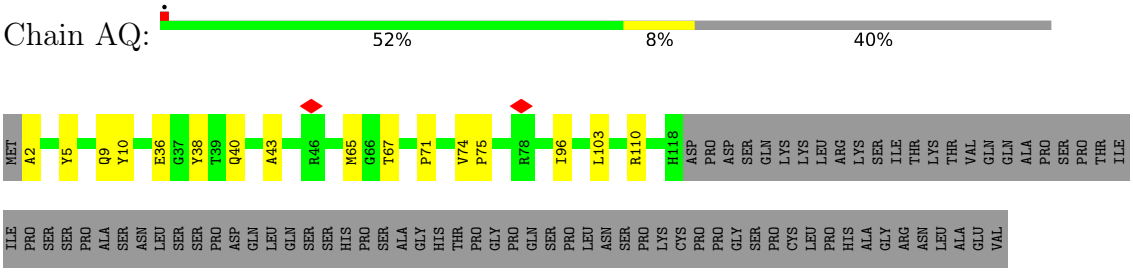
• Molecule 10: Protein Flattop

Chain AP:



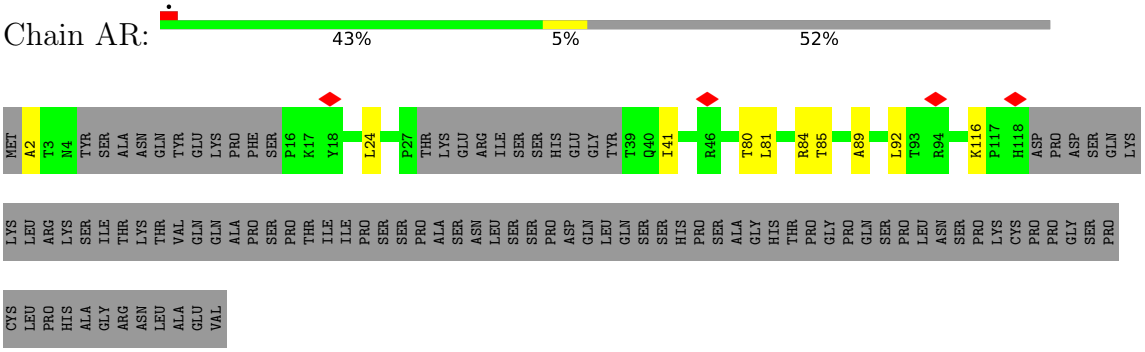
• Molecule 10: Protein Flattop

Chain AQ:



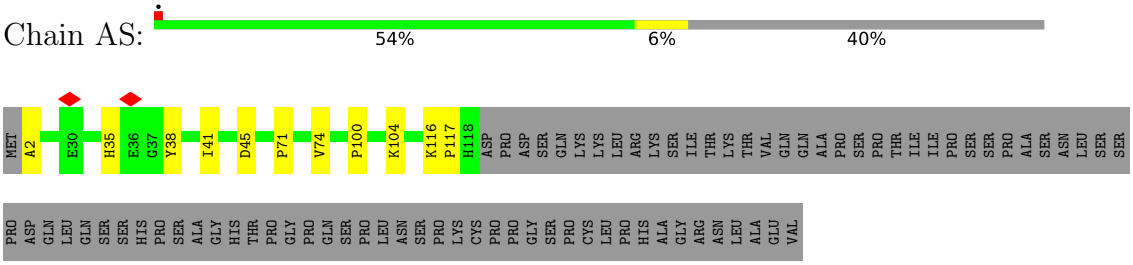
• Molecule 10: Protein Flattop

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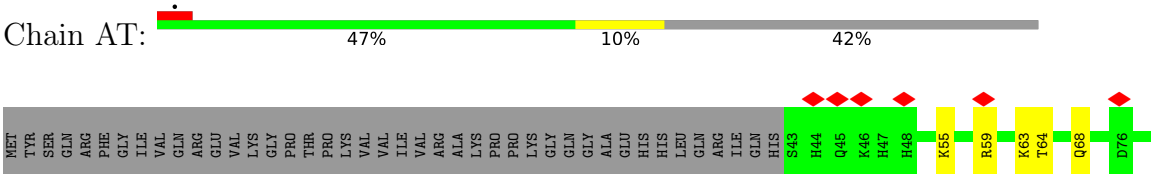
• Molecule 10: Protein Flattop

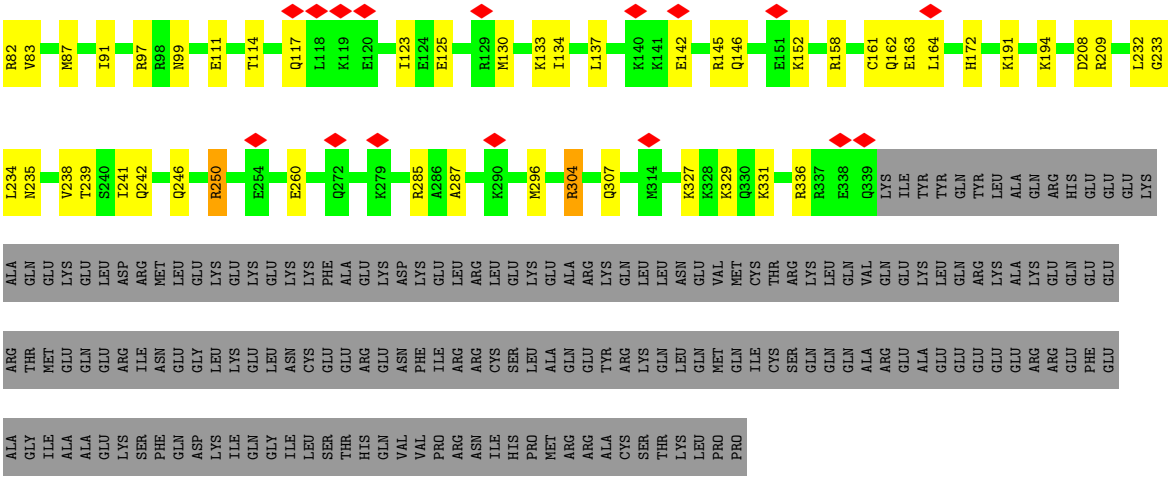
Chain AS:



• Molecule 11: Cilia- and flagella-associated protein 53

Chain AT:

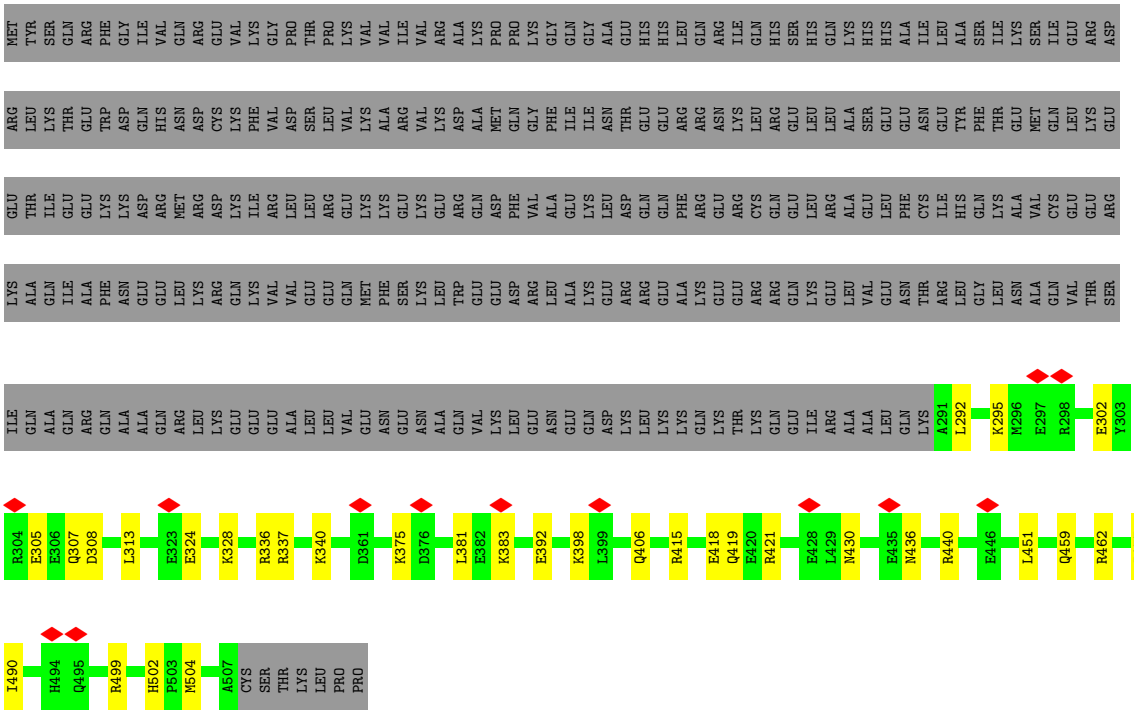




• Molecule 11: Cilia- and flagella-associated protein 53

Chain AU:

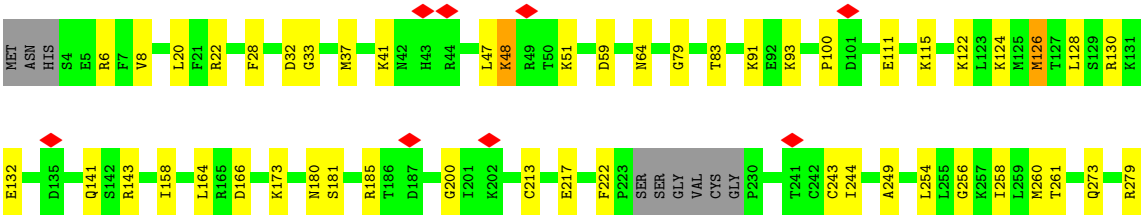


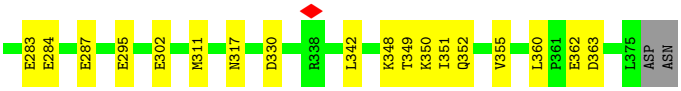


• Molecule 12: Nucleoside diphosphate kinase 7

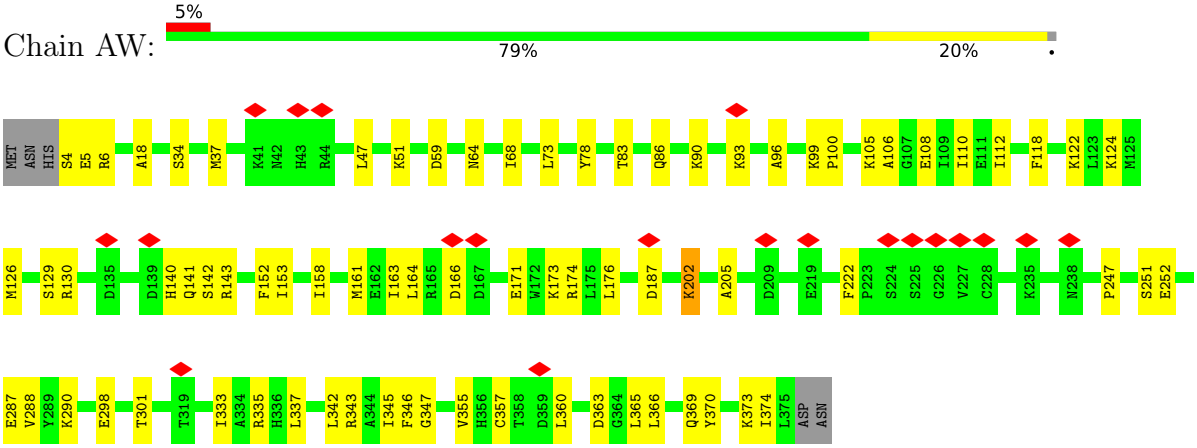
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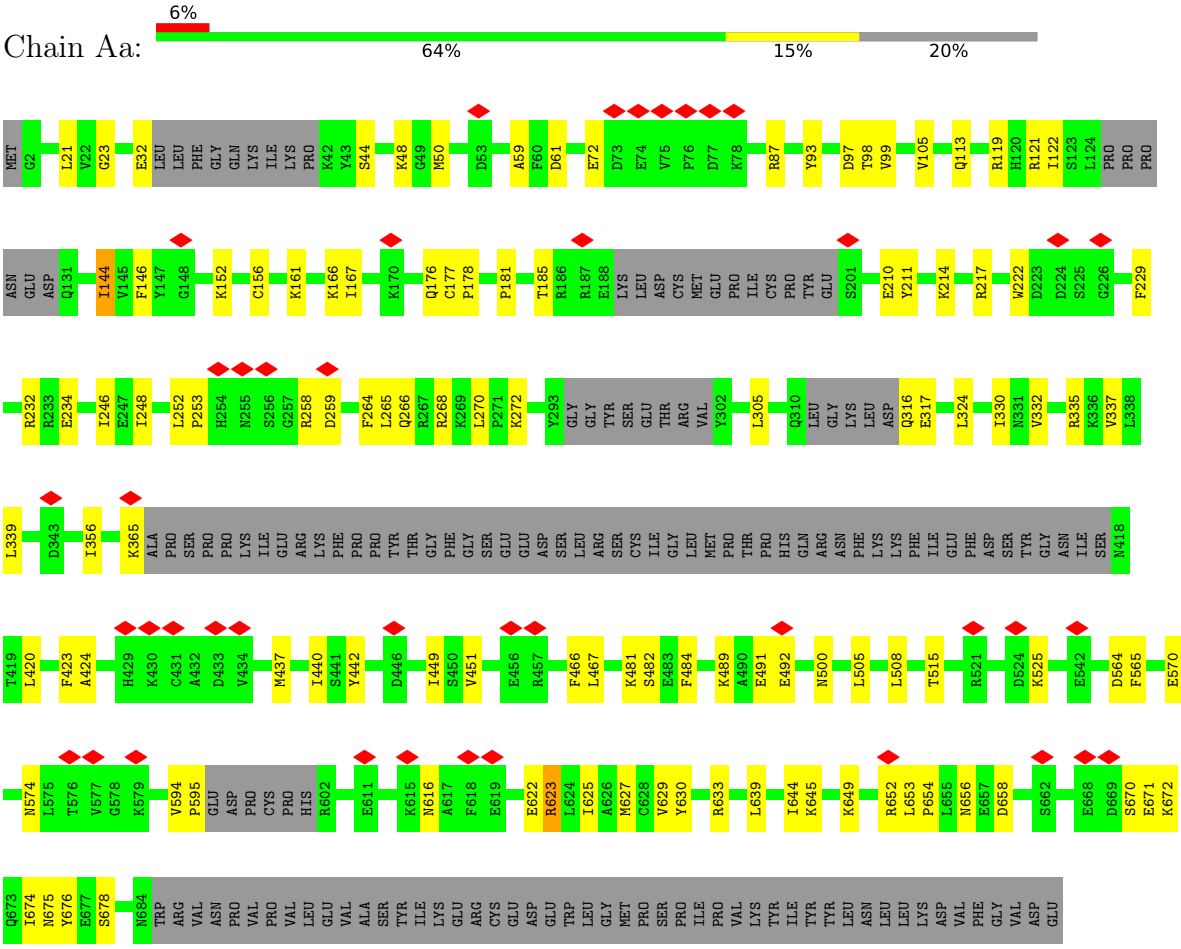




• Molecule 12: Nucleoside diphosphate kinase 7

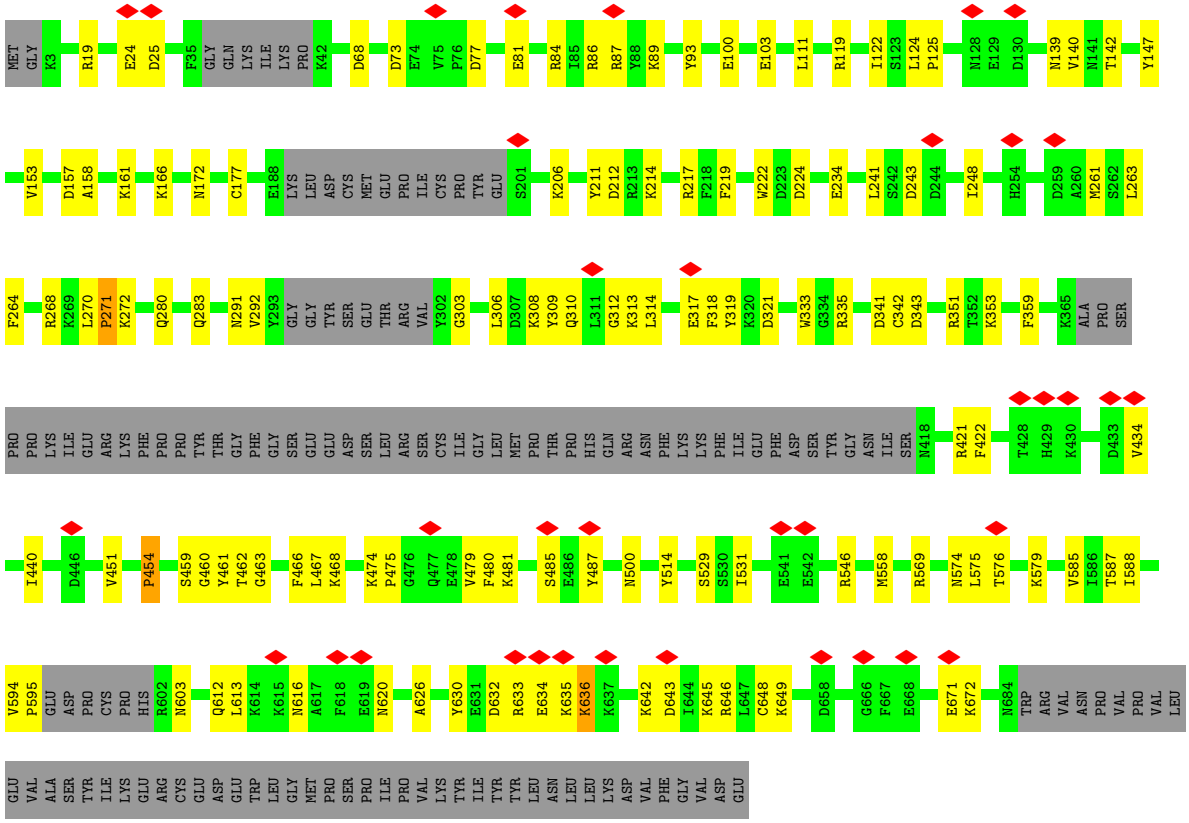


• Molecule 13: EF-hand domain-containing family member C2



• Molecule 13: EF-hand domain-containing family member C2

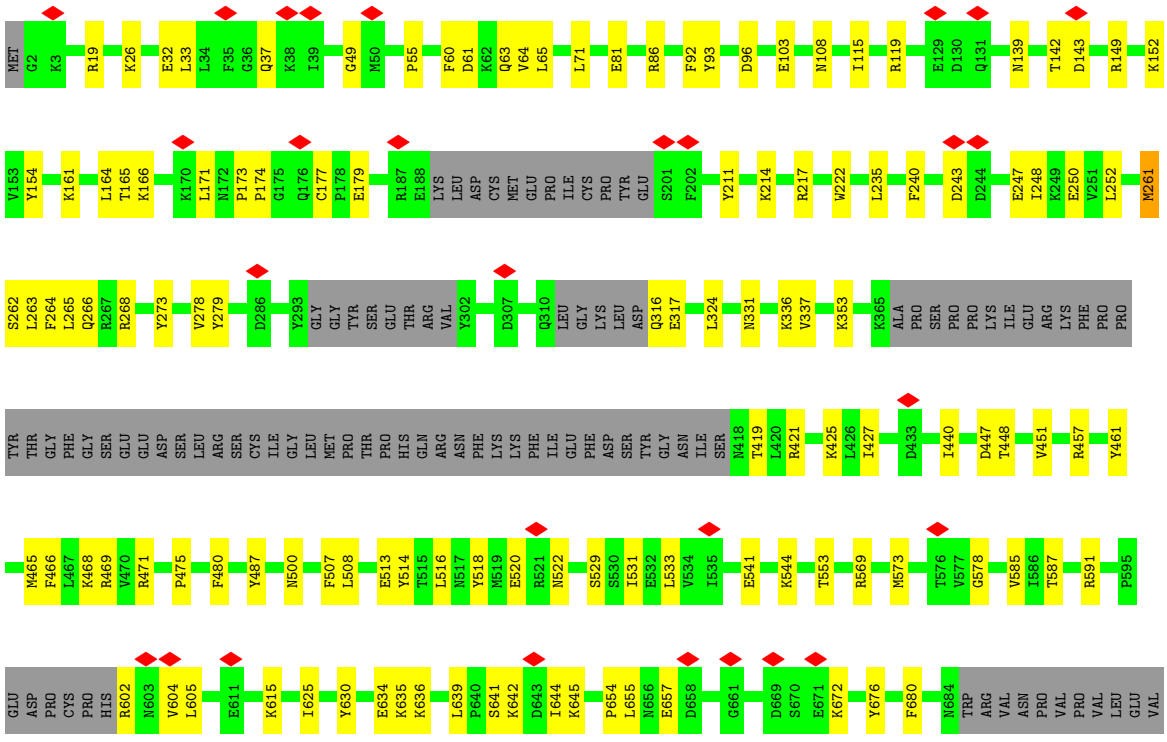




• Molecule 13: EF-hand domain-containing family member C2

Chain Ac:



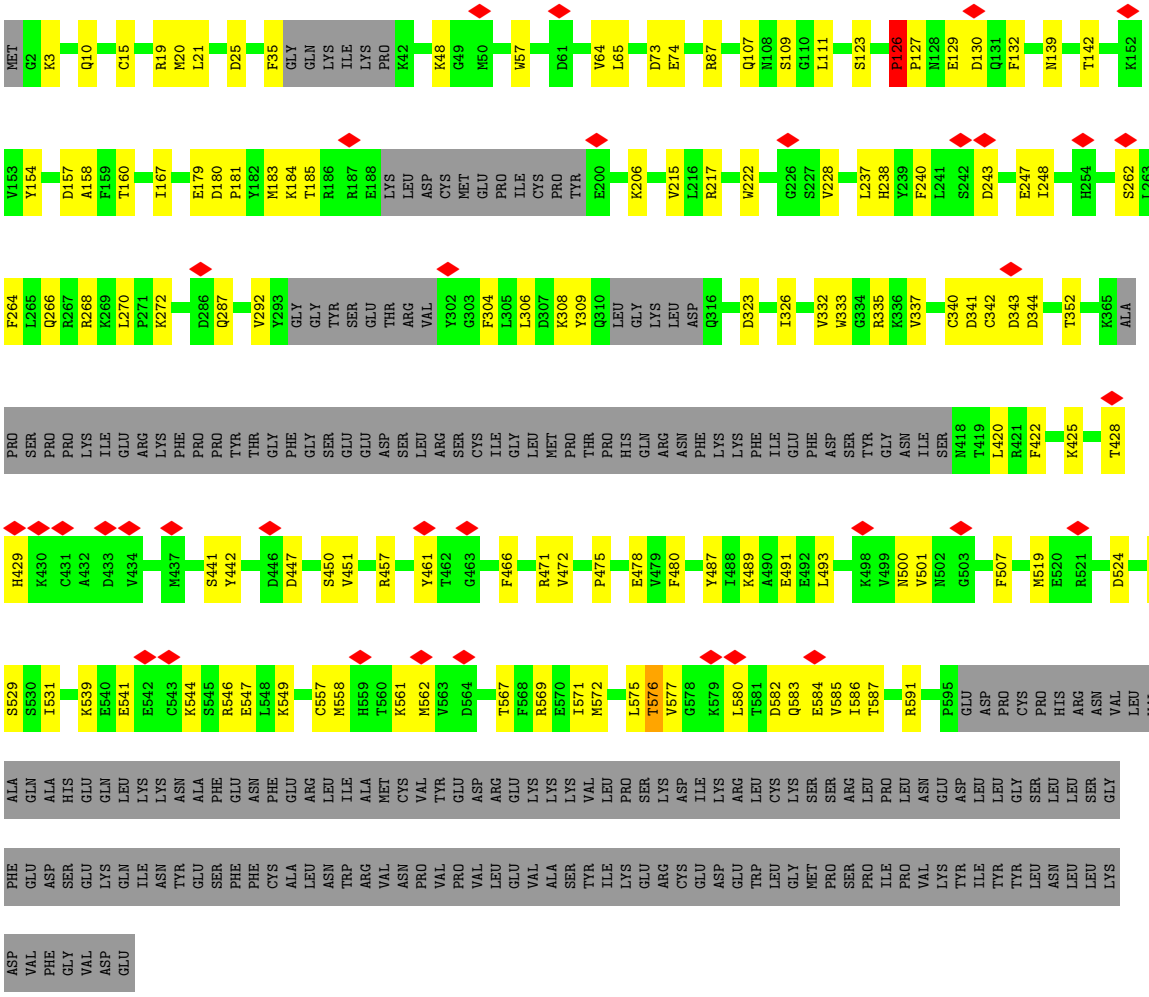




• Molecule 13: EF-hand domain-containing family member C2

Chain Ad:

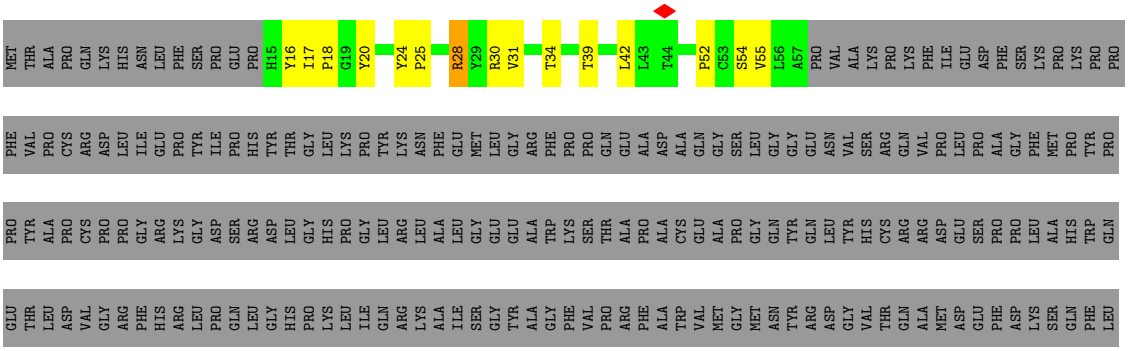


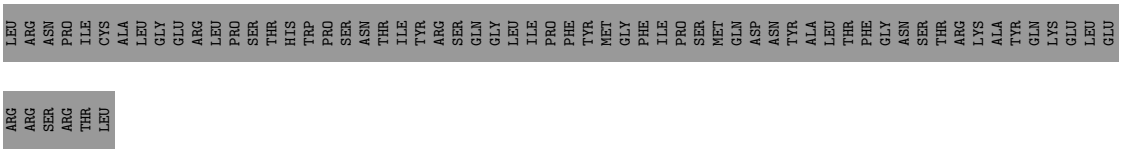


• Molecule 14: Family with sequence similarity 166 member A

Chain Al:



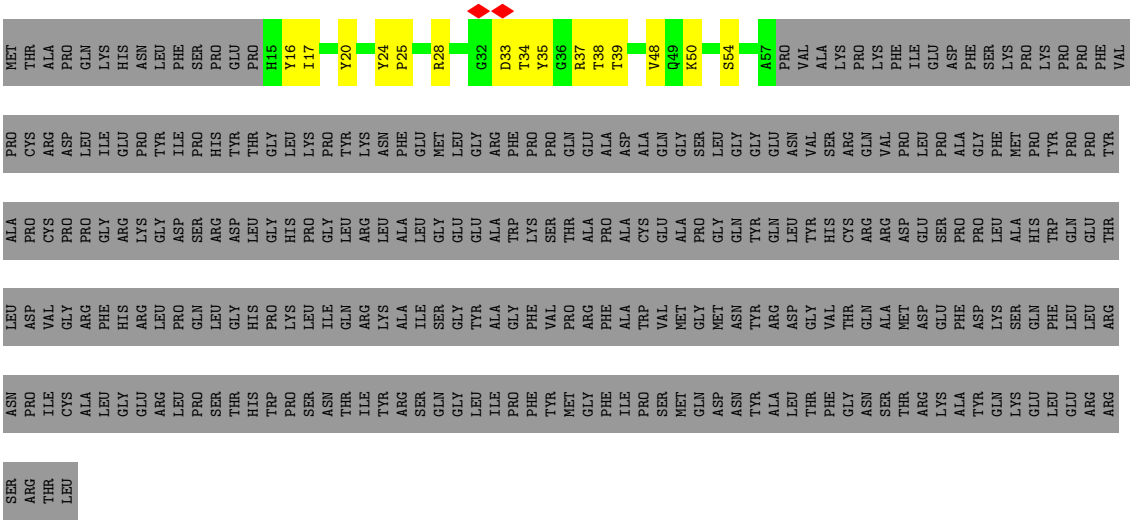




• Molecule 14: Family with sequence similarity 166 member A

Chain Am:

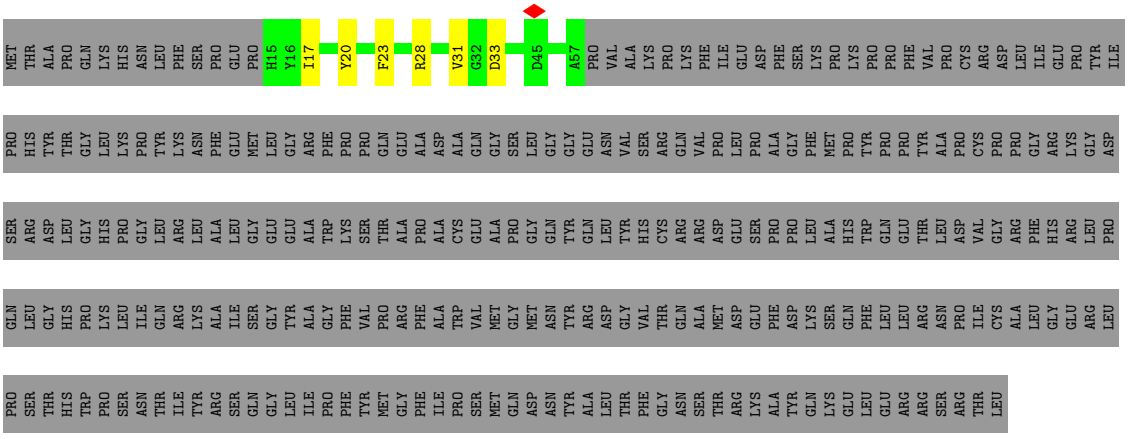




• Molecule 14: Family with sequence similarity 166 member A

Chain An:



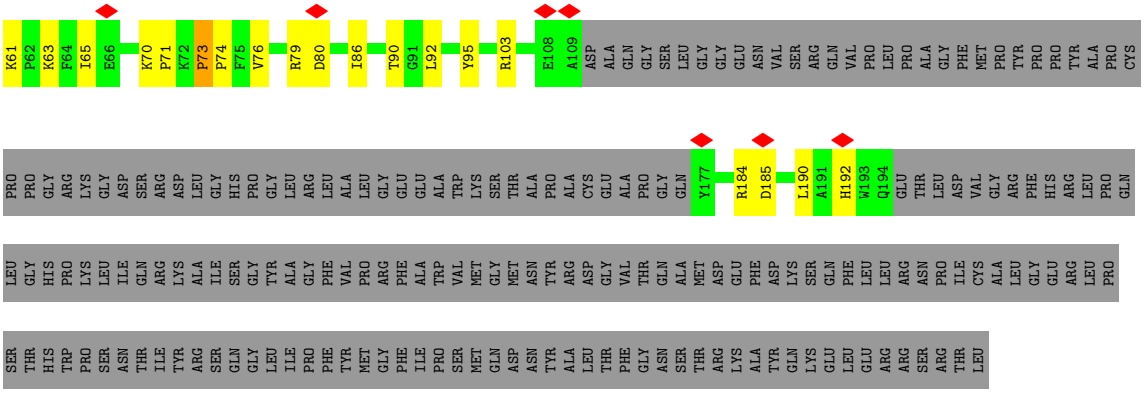


• Molecule 14: Family with sequence similarity 166 member A

Chain Ao:



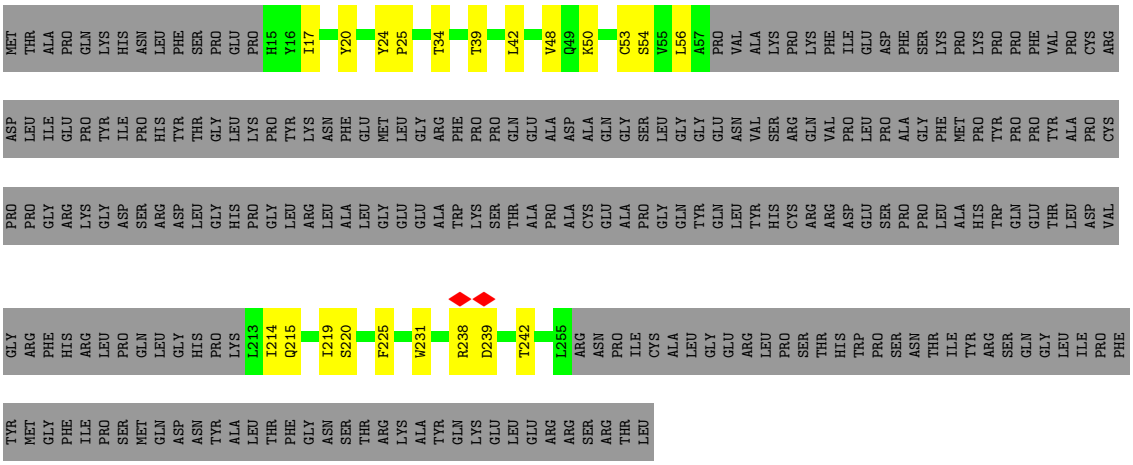




• Molecule 14: Family with sequence similarity 166 member A

Chain B7:

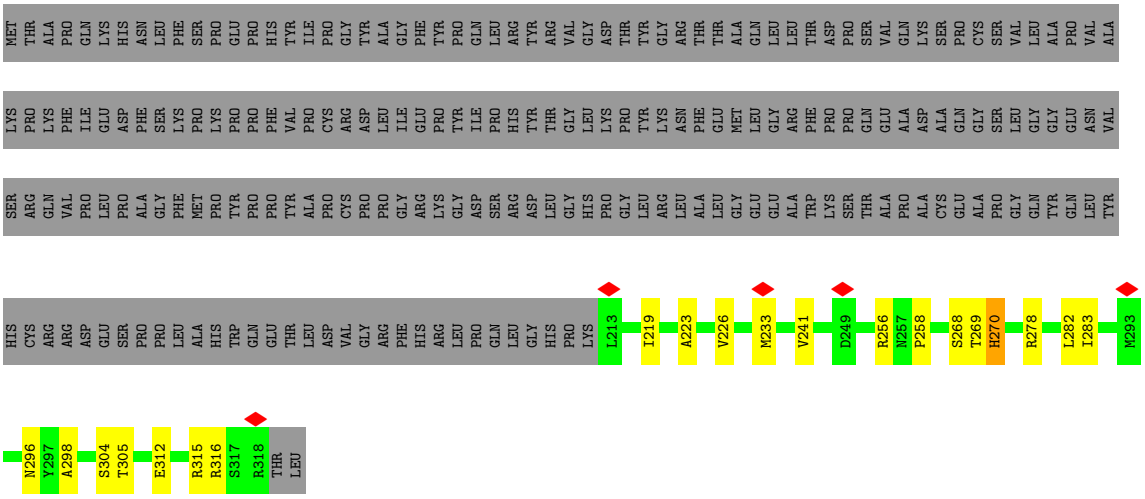




• Molecule 14: Family with sequence similarity 166 member A

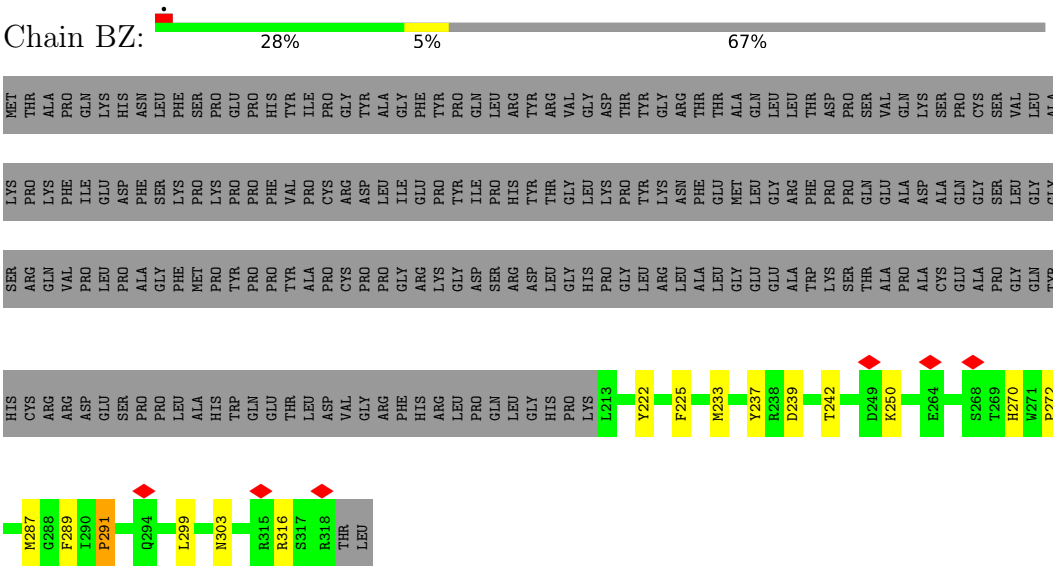
Chain BY:





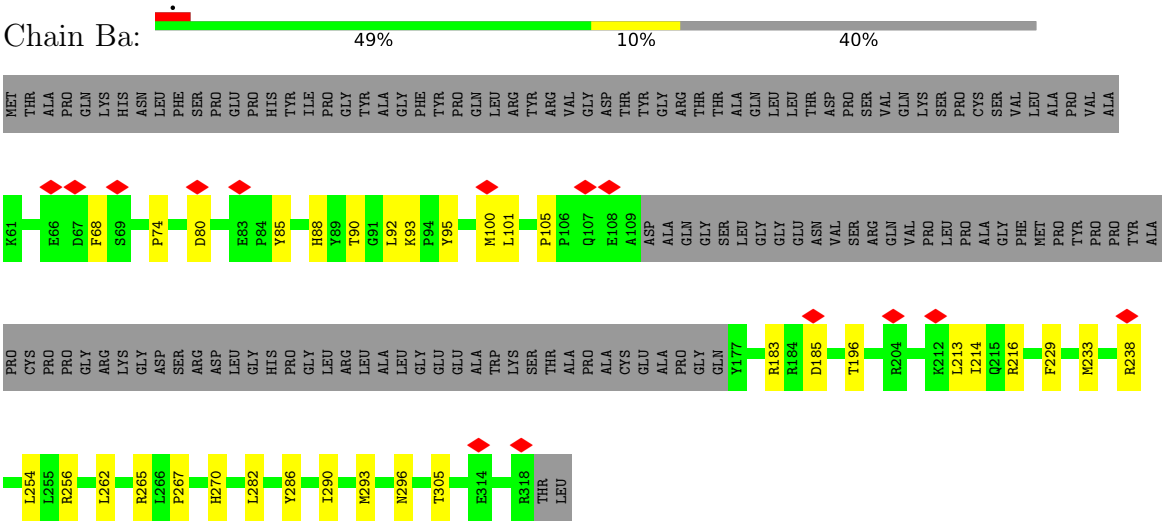
• Molecule 14: Family with sequence similarity 166 member A

Chain BZ:



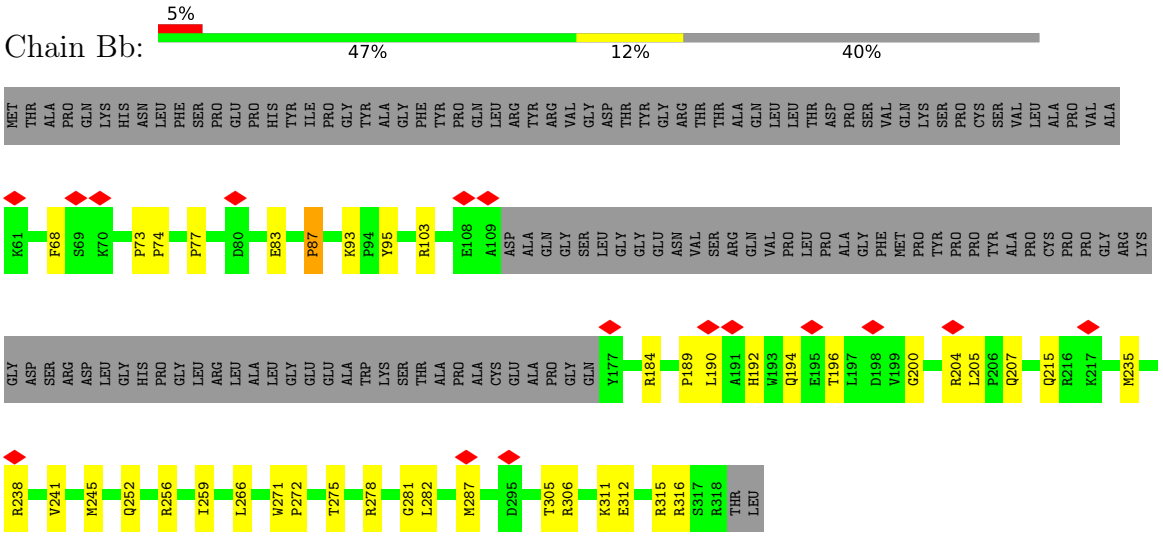
• Molecule 14: Family with sequence similarity 166 member A

Chain Ba:



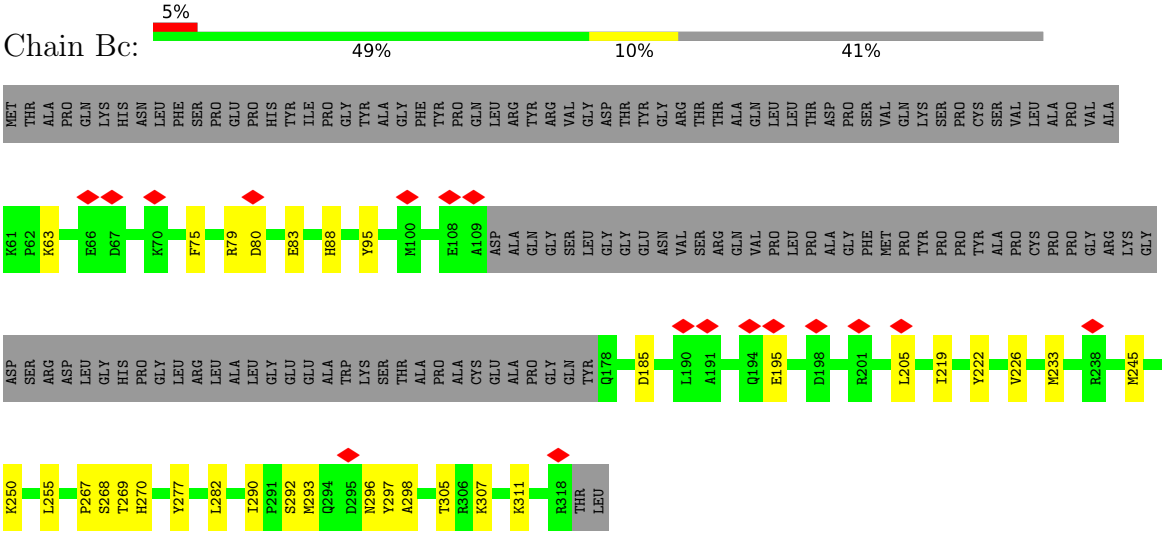
• Molecule 14: Family with sequence similarity 166 member A

Chain Bb:



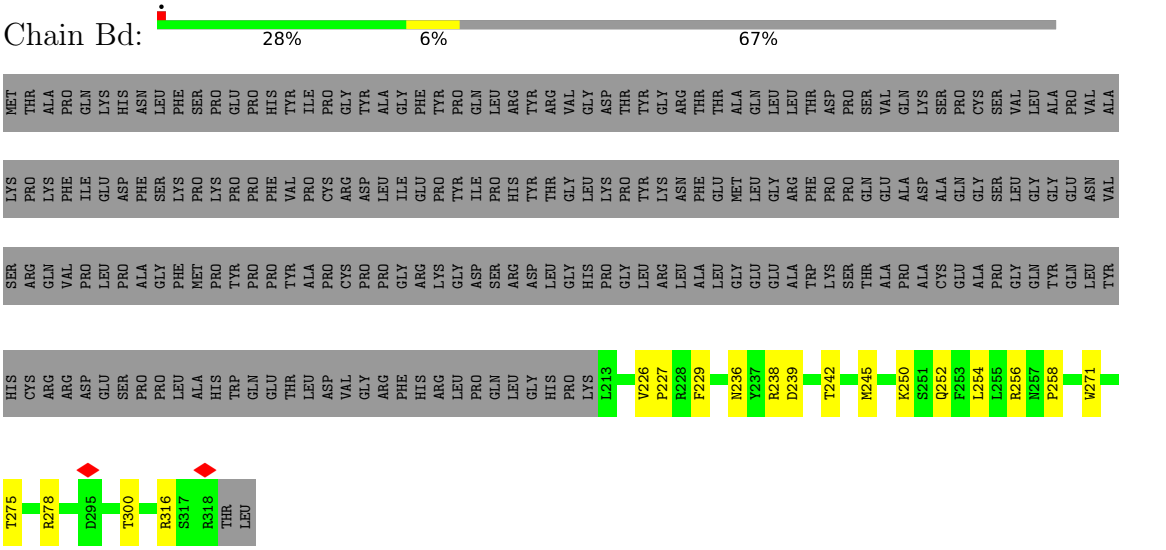
• Molecule 14: Family with sequence similarity 166 member A

Chain Bc:



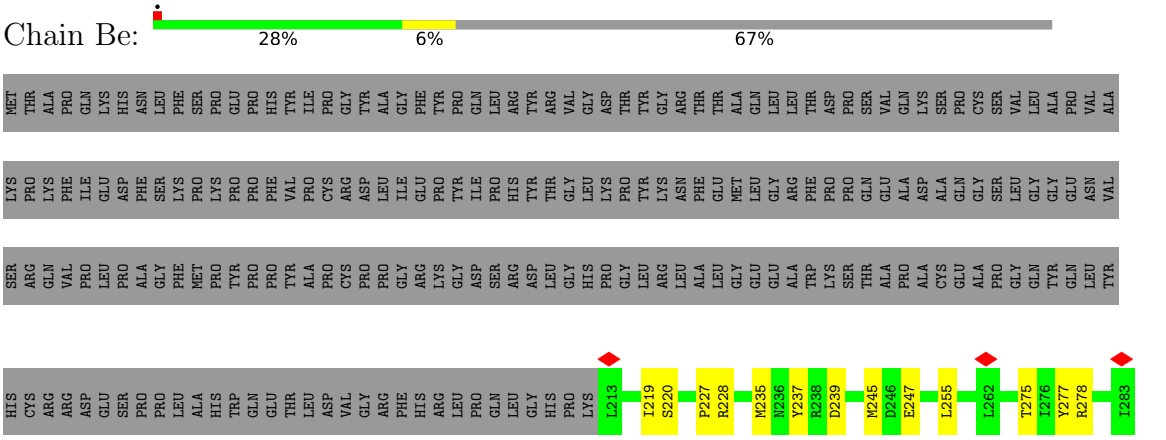
• Molecule 14: Family with sequence similarity 166 member A

Chain Bd:



• Molecule 14: Family with sequence similarity 166 member A

Chain Be:

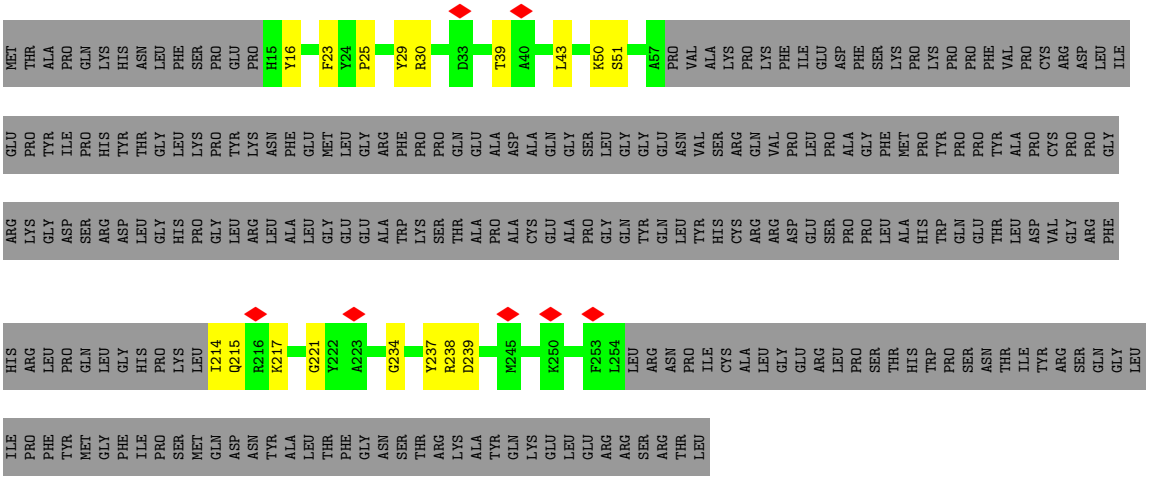




• Molecule 14: Family with sequence similarity 166 member A

Chain CN:

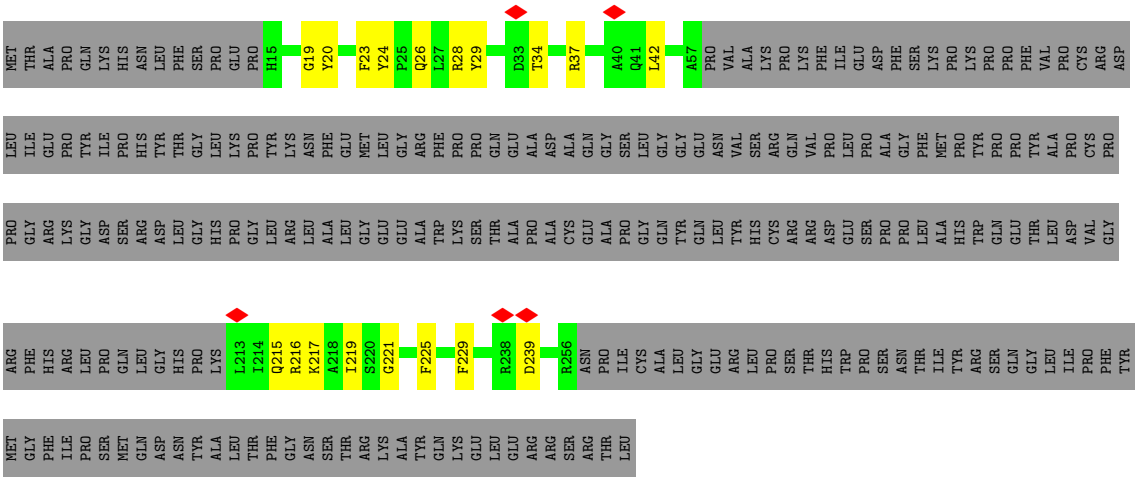




• Molecule 14: Family with sequence similarity 166 member A

Chain CO:

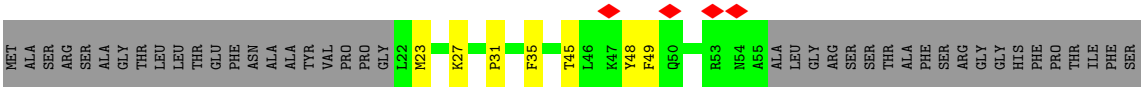


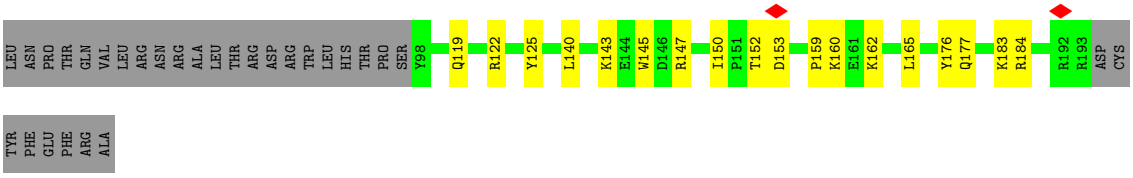


• Molecule 15: Protein FAM166C

Chain Ap:







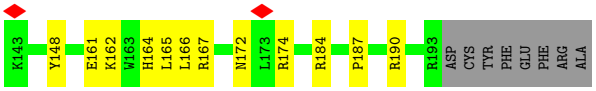
• Molecule 15: Protein FAM166C

Chain Aq:





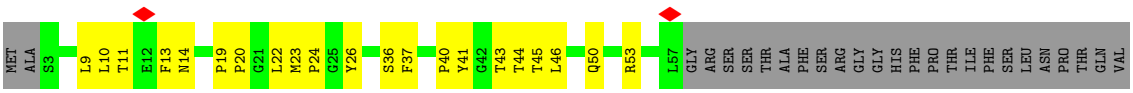




• Molecule 15: Protein FAM166C

Chain Ar:



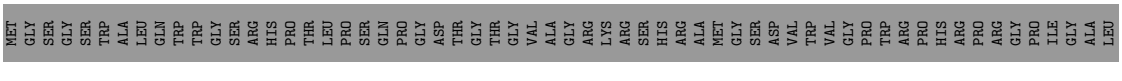


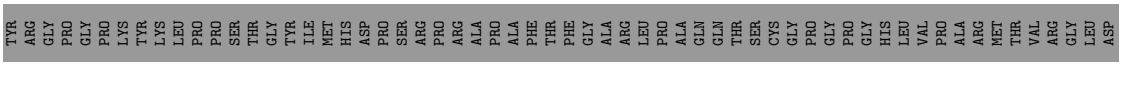


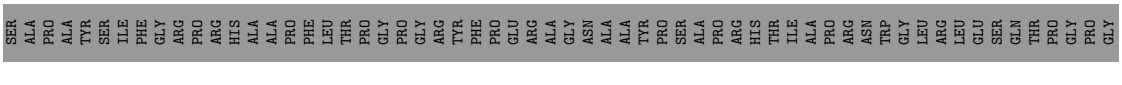
• Molecule 16: Outer dense fiber of sperm tails 3B

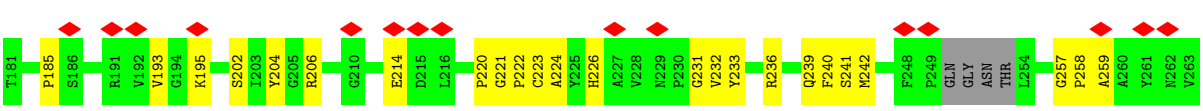
Chain At:





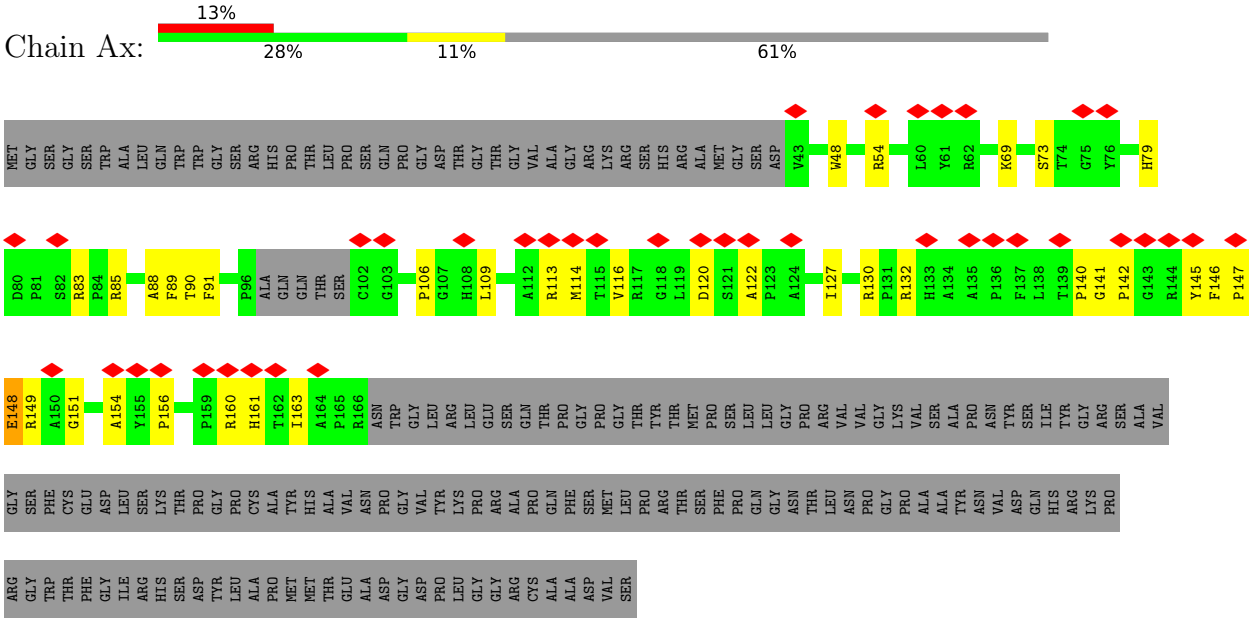






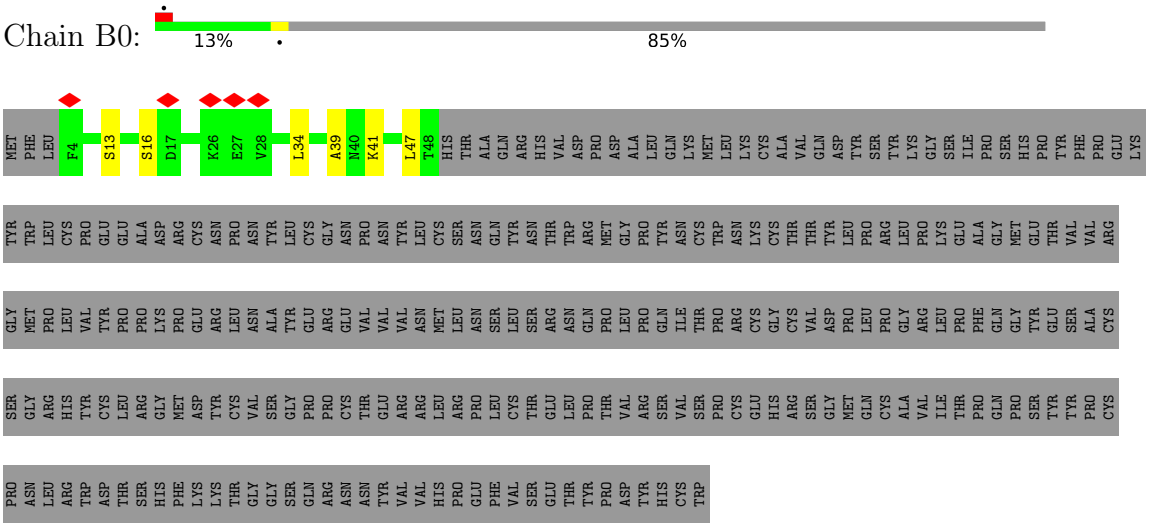
• Molecule 16: Outer dense fiber of sperm tails 3B

Chain Ax:



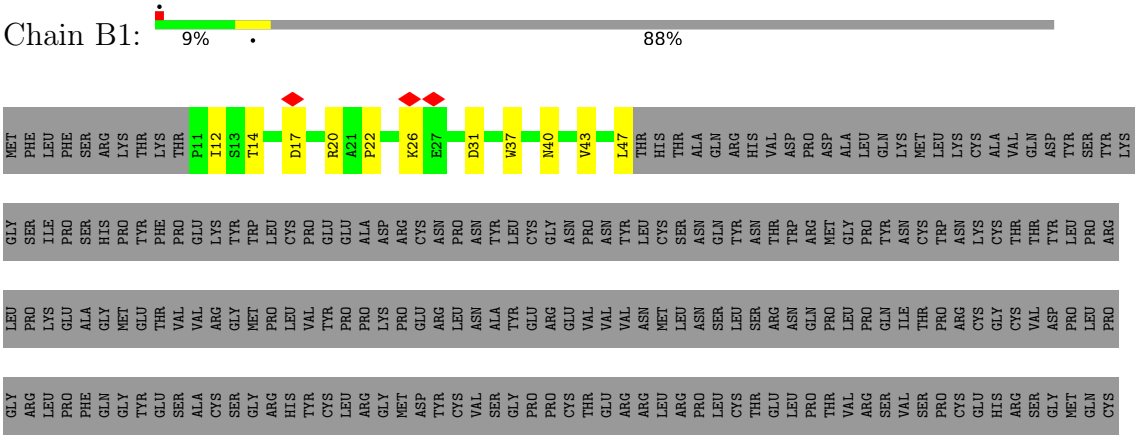
• Molecule 17: Spermatid-specific manchette-related protein 1

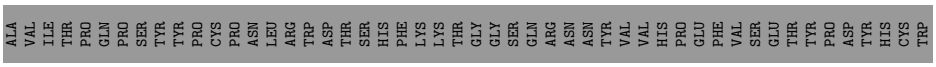
Chain B0:



• Molecule 17: Spermatid-specific manchette-related protein 1

Chain B1:

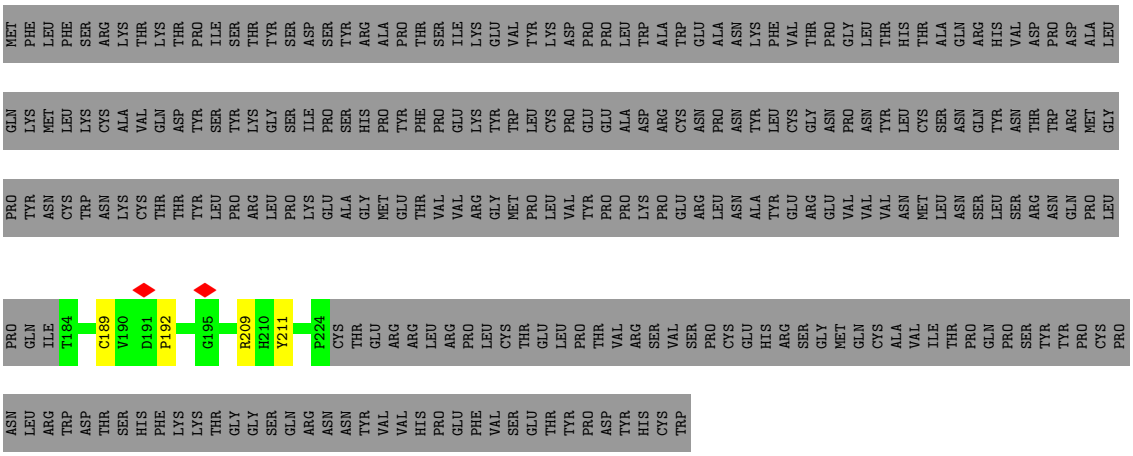




• Molecule 17: Spermatid-specific manchette-related protein 1

Chain B2:

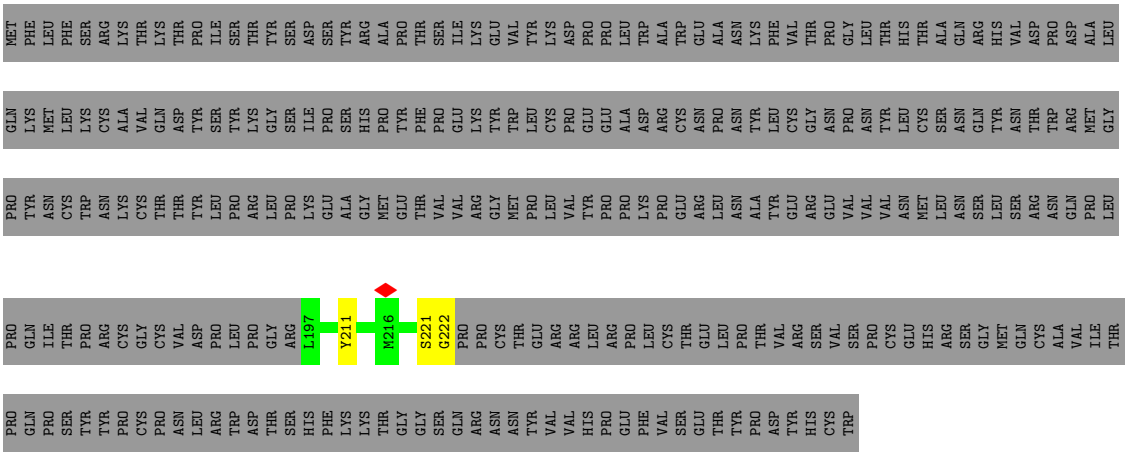




• Molecule 17: Spermatid-specific manchette-related protein 1

Chain B3:

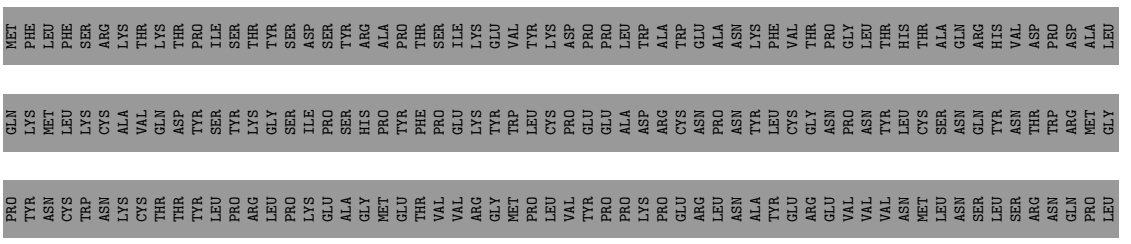


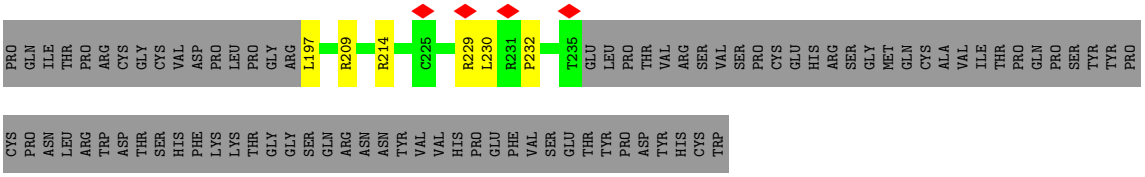


• Molecule 17: Spermatid-specific manchette-related protein 1

Chain B4:



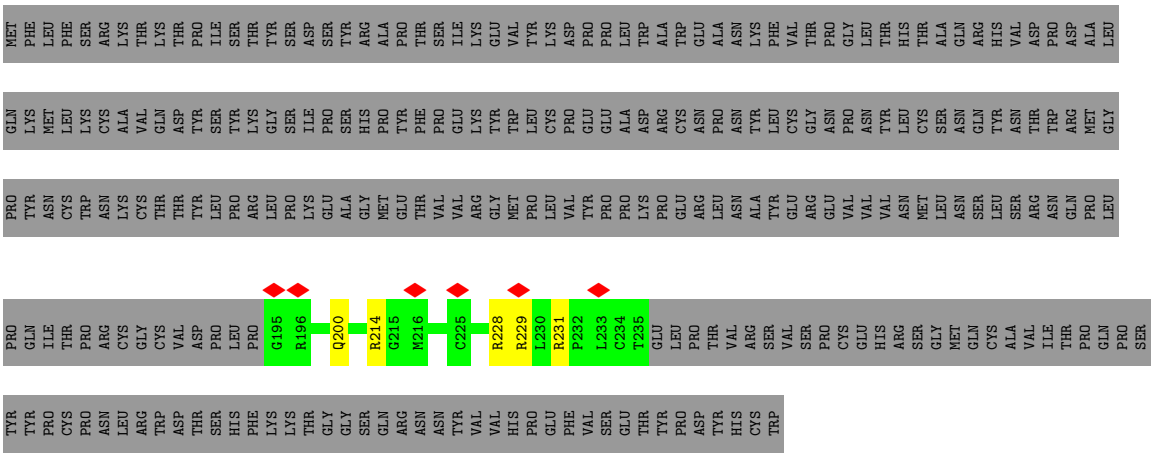




• Molecule 17: Spermatid-specific manchette-related protein 1

Chain B8:

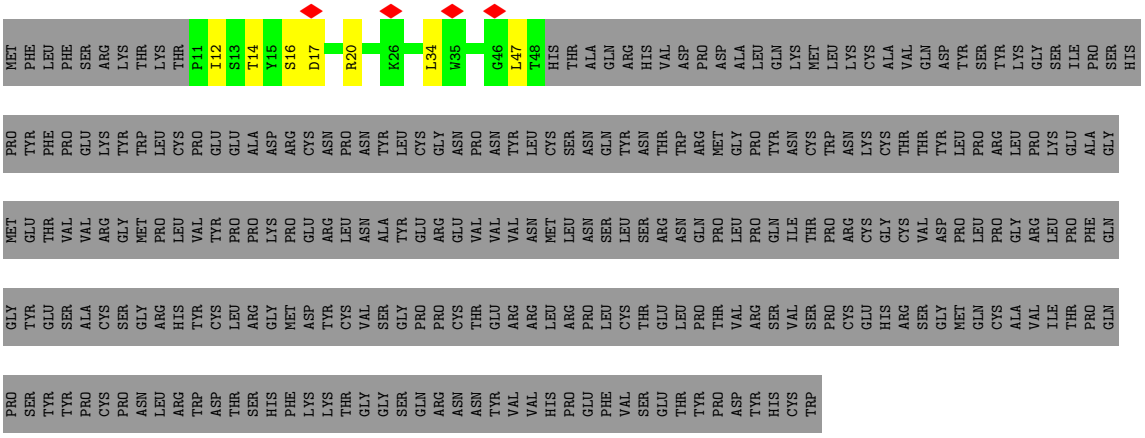




• Molecule 17: Spermatid-specific manchette-related protein 1

Chain B9:

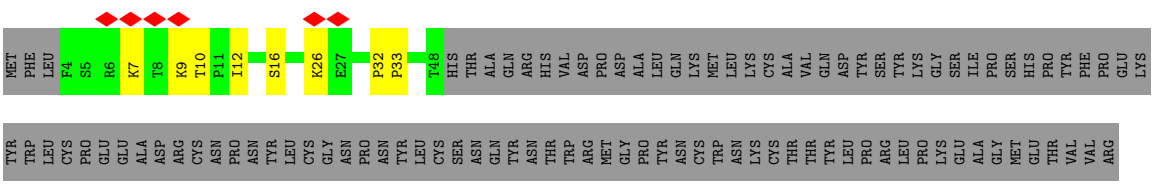


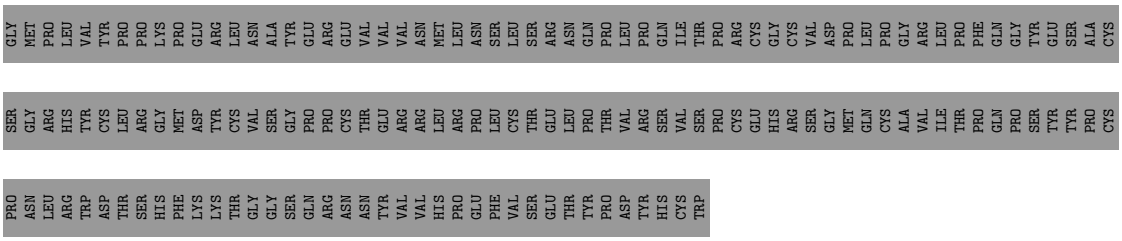


• Molecule 17: Spermatid-specific manchette-related protein 1

Chain CQ:



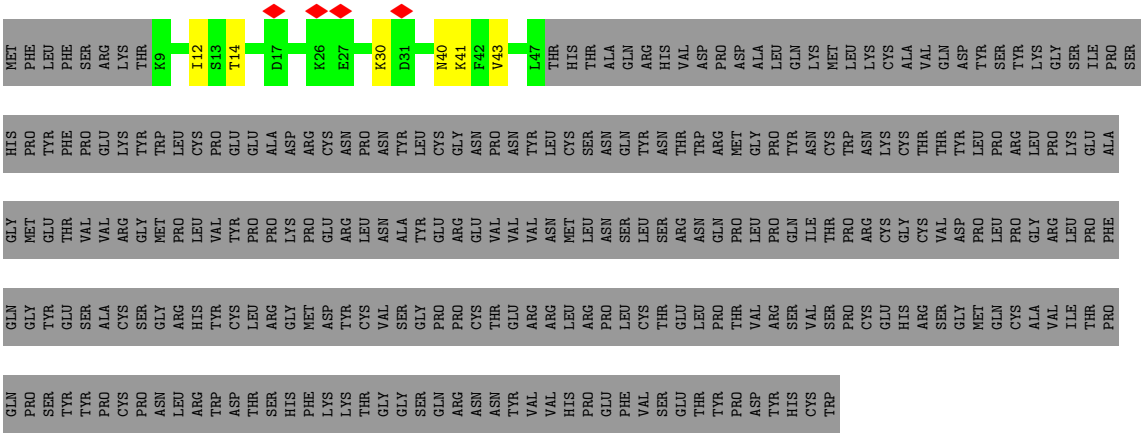




• Molecule 17: Spermatid-specific manchette-related protein 1

Chain CR:

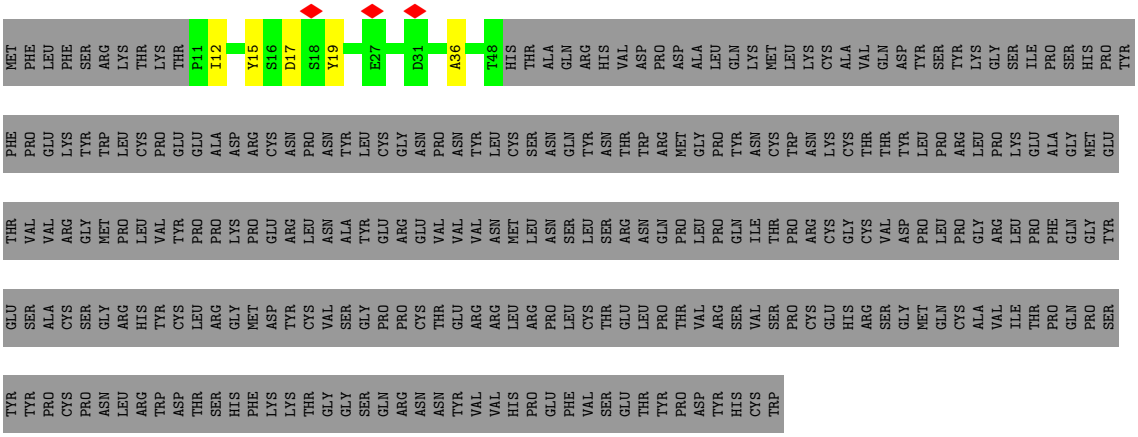




• Molecule 17: Spermatid-specific manchette-related protein 1

Chain CS:

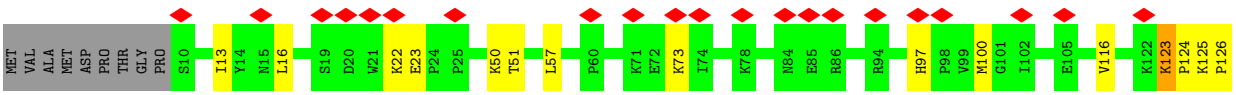


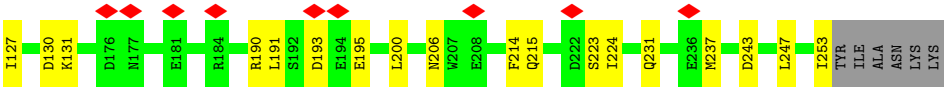


• Molecule 18: Enkurin

Chain B5:



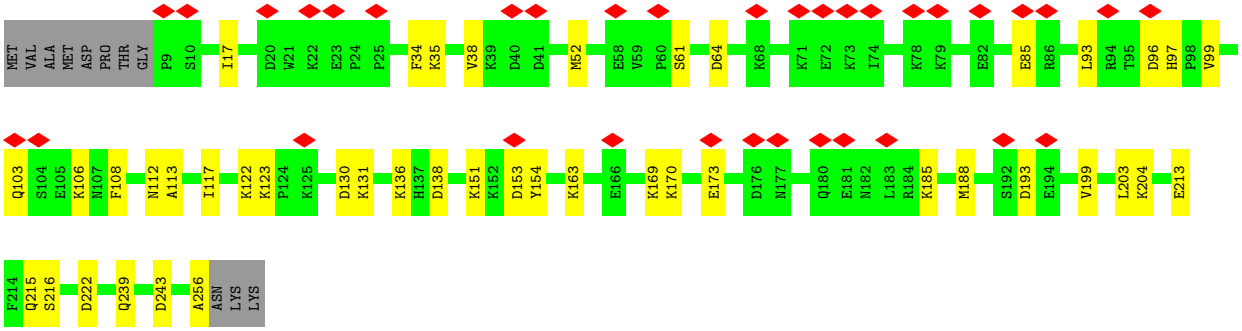




• Molecule 18: Enkurin

Chain B6:

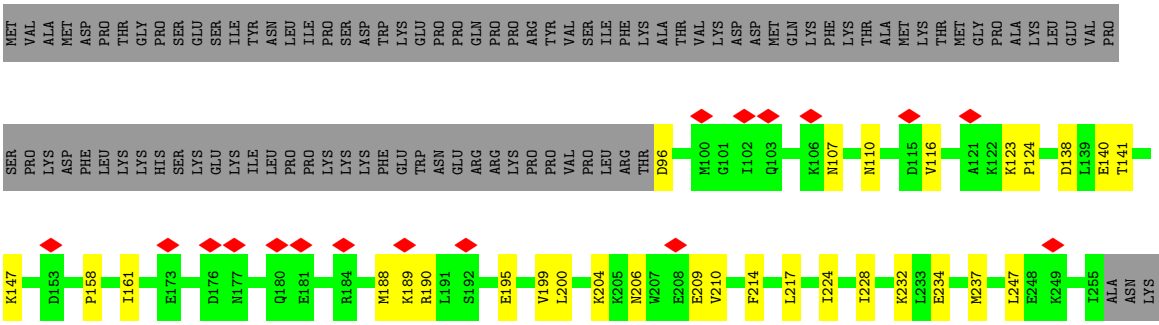




• Molecule 18: Enkurin

Chain By:

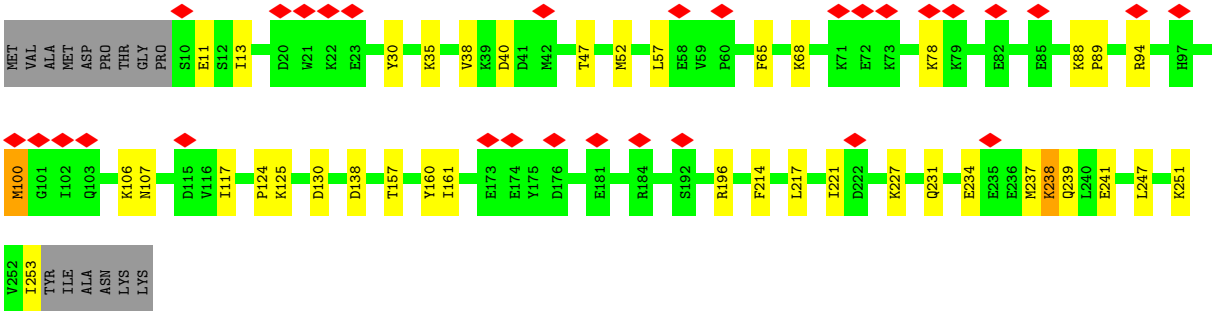




• Molecule 18: Enkurin

Chain Bz:

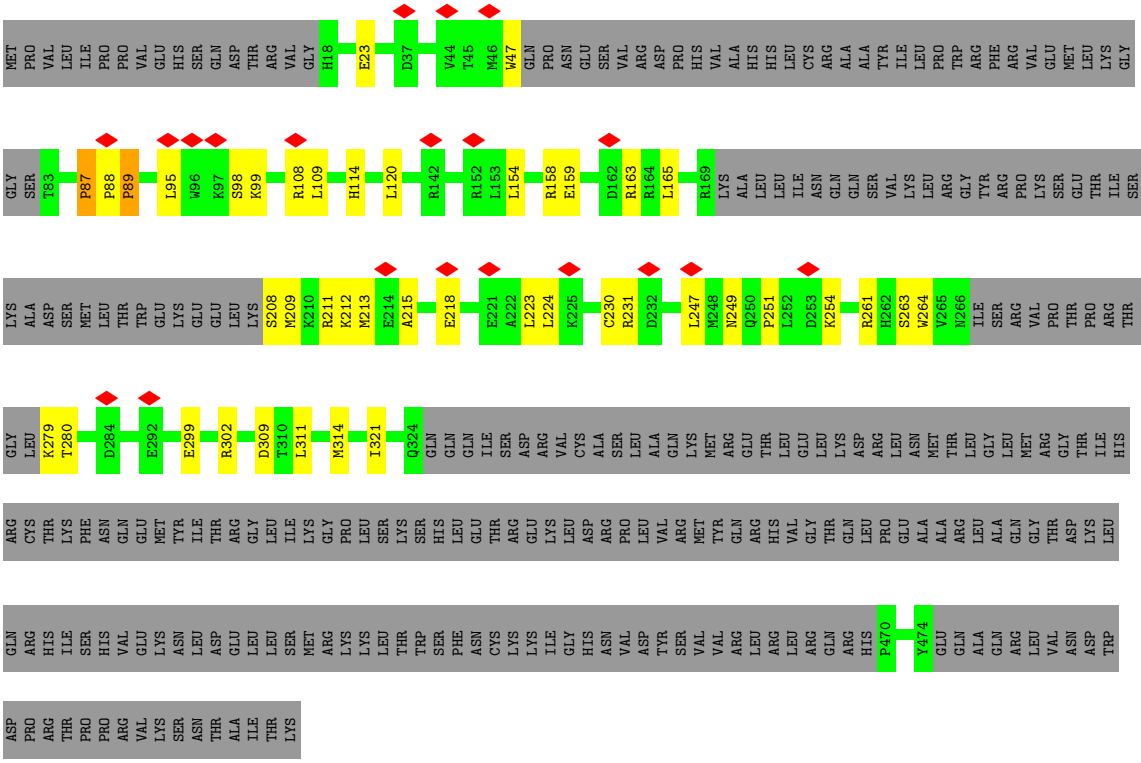




• Molecule 19: Coiled-coil domain-containing protein 105

Chain BO:

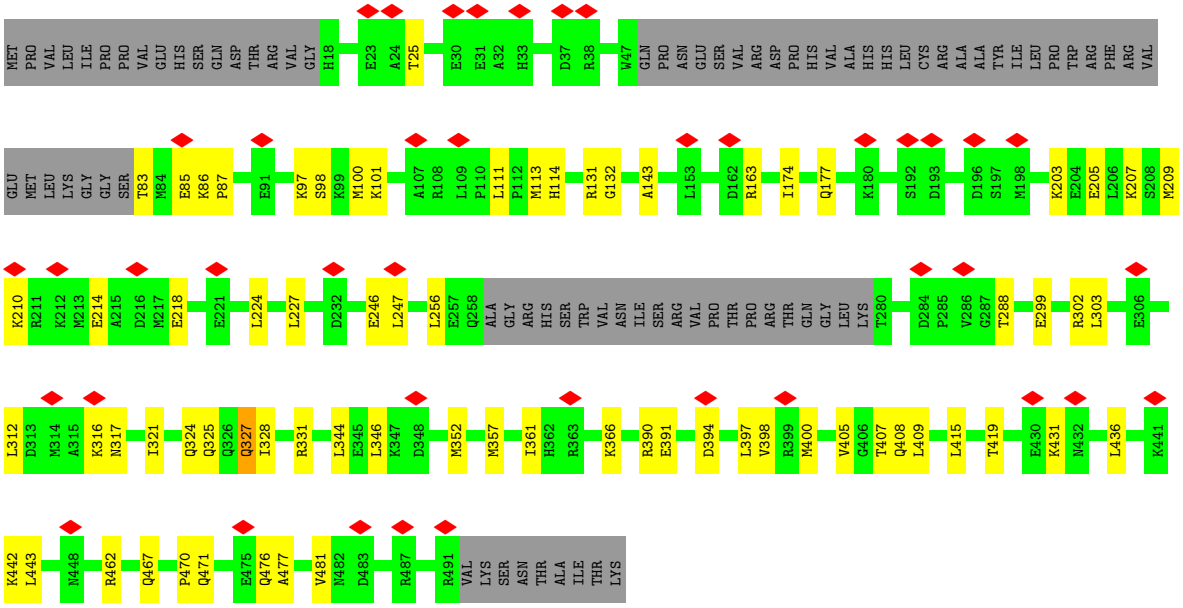




• Molecule 19: Coiled-coil domain-containing protein 105

Chain BP:



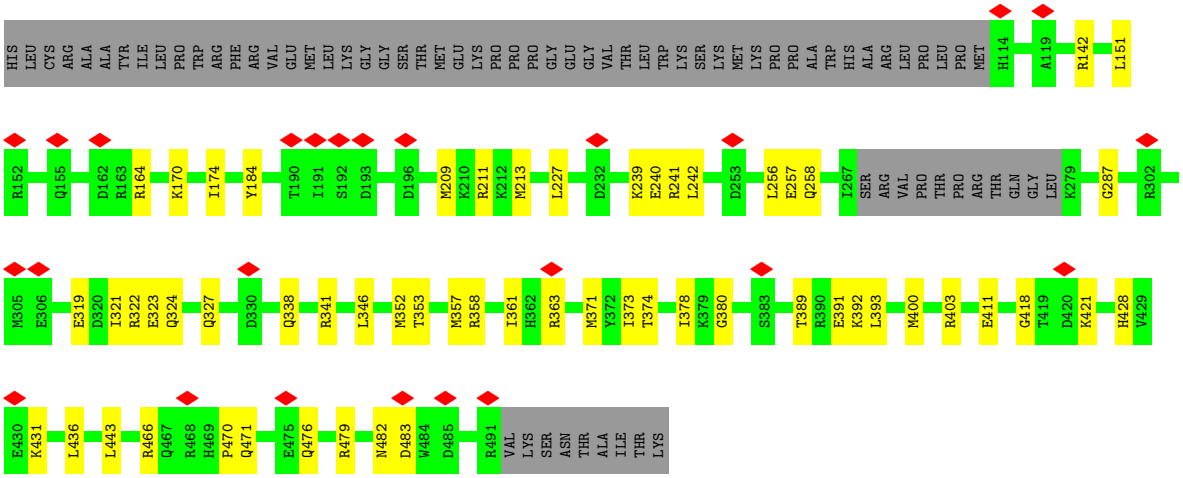


• Molecule 19: Coiled-coil domain-containing protein 105

Chain BQ:



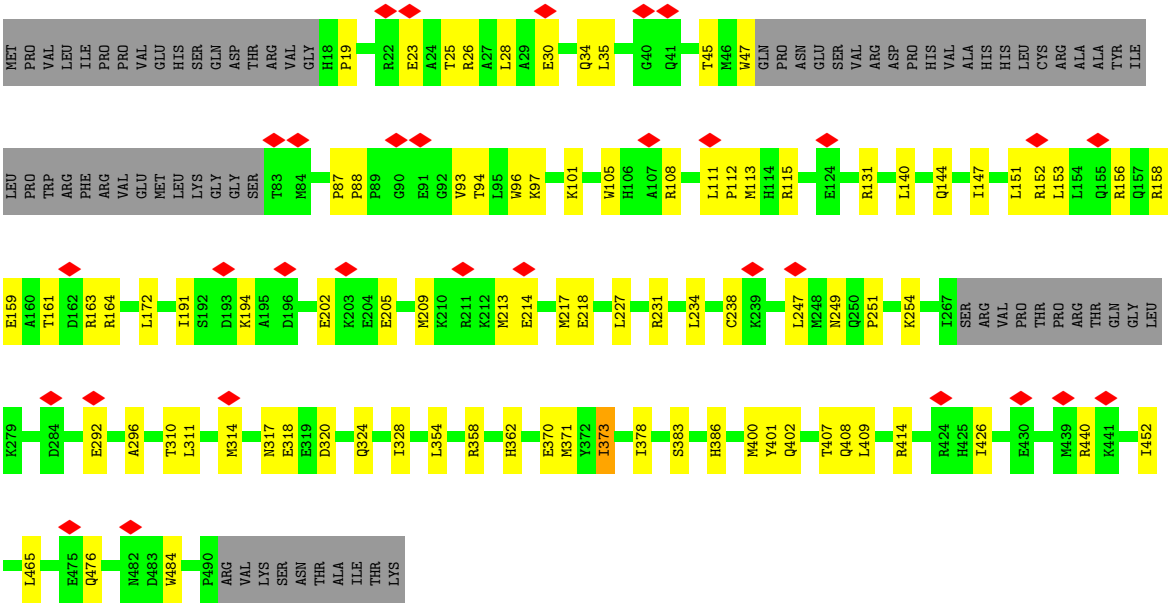




• Molecule 19: Coiled-coil domain-containing protein 105

Chain BR:

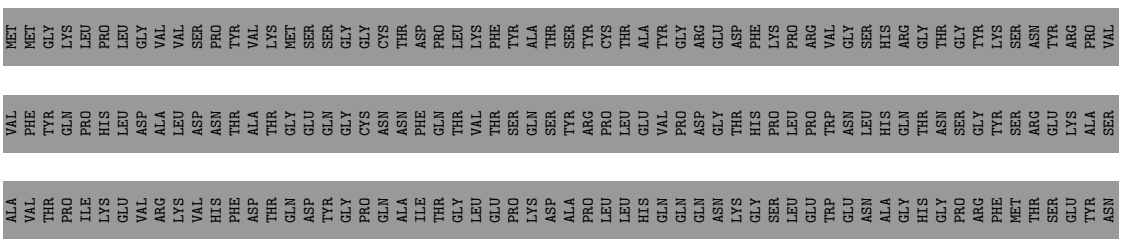


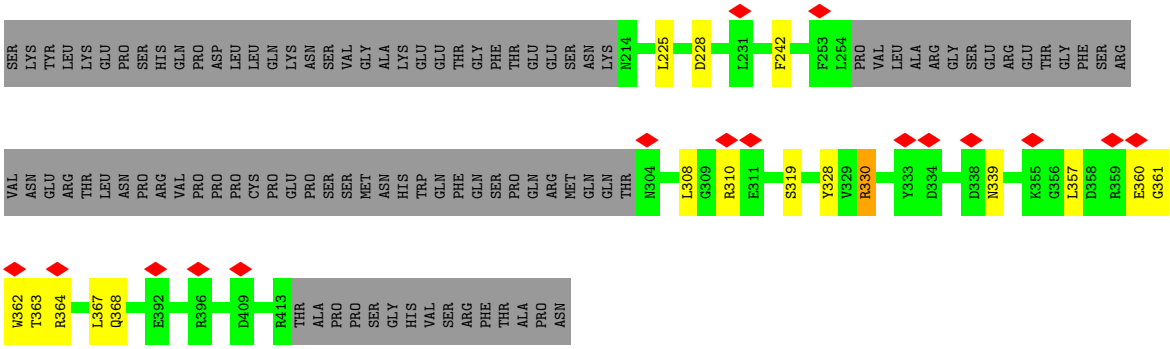


• Molecule 20: Protein phosphatase 1 regulatory subunit 32

Chain BS:

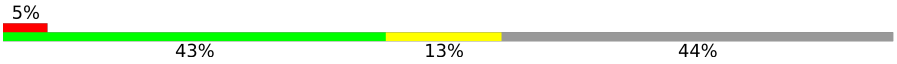


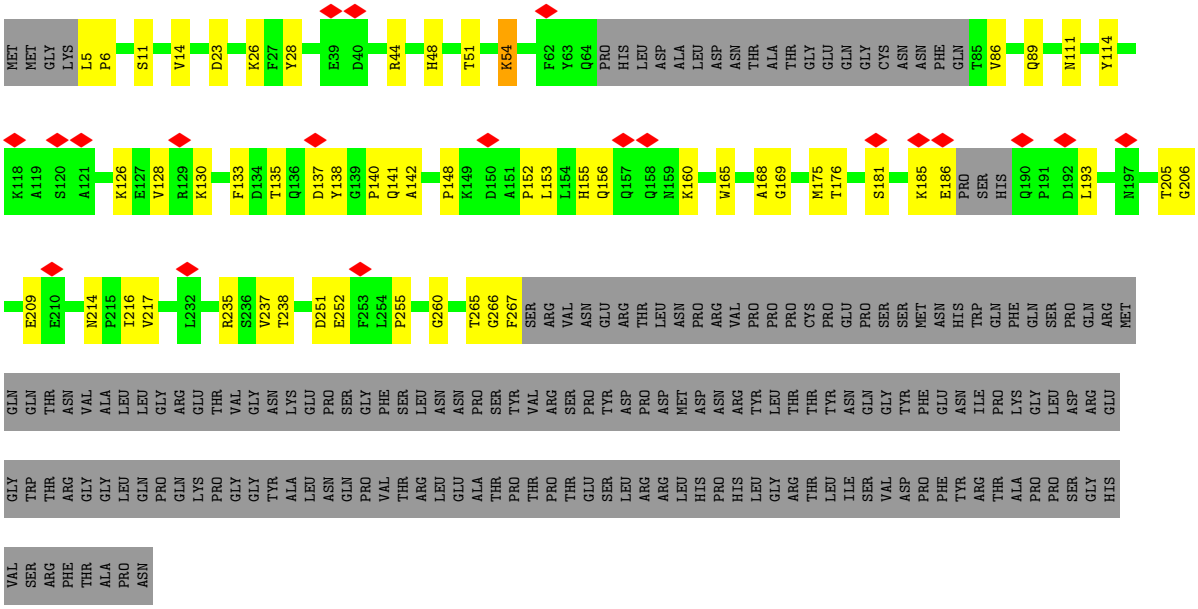




• Molecule 20: Protein phosphatase 1 regulatory subunit 32

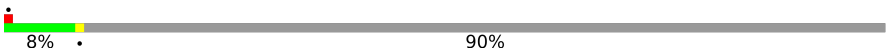
Chain BT:

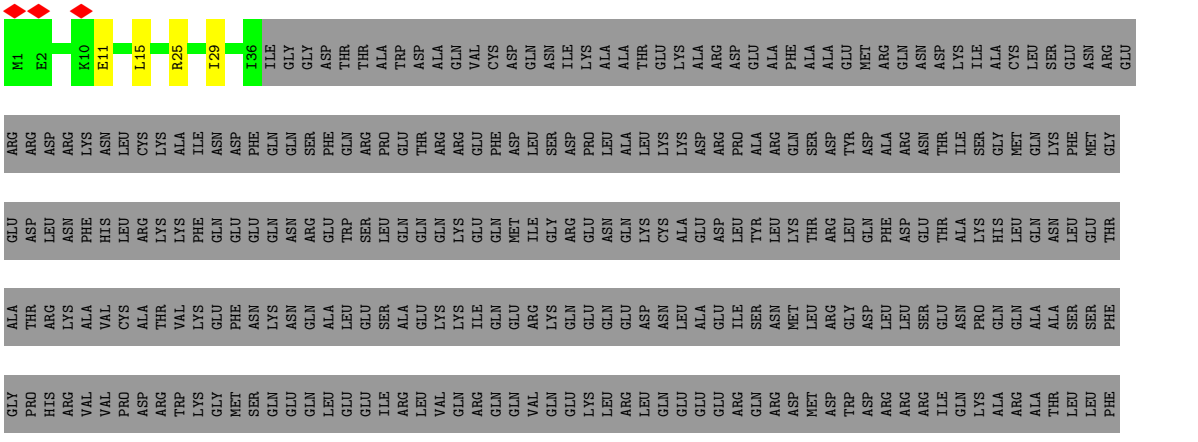




• Molecule 21: RIB43A-like with coiled-coils protein 2

Chain BU:

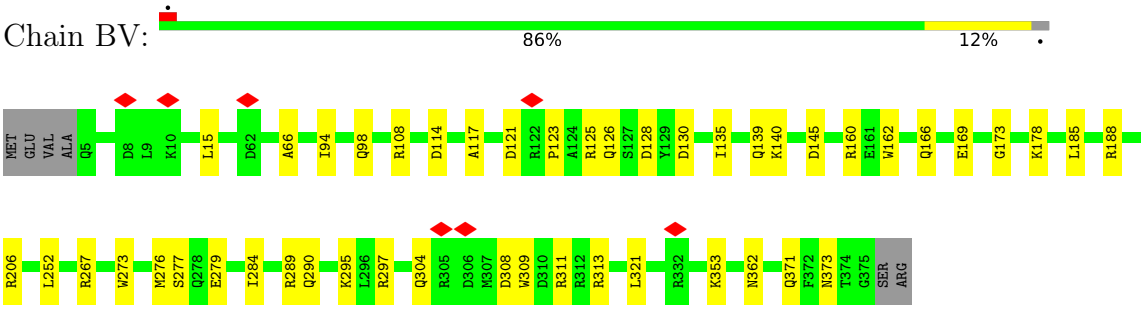






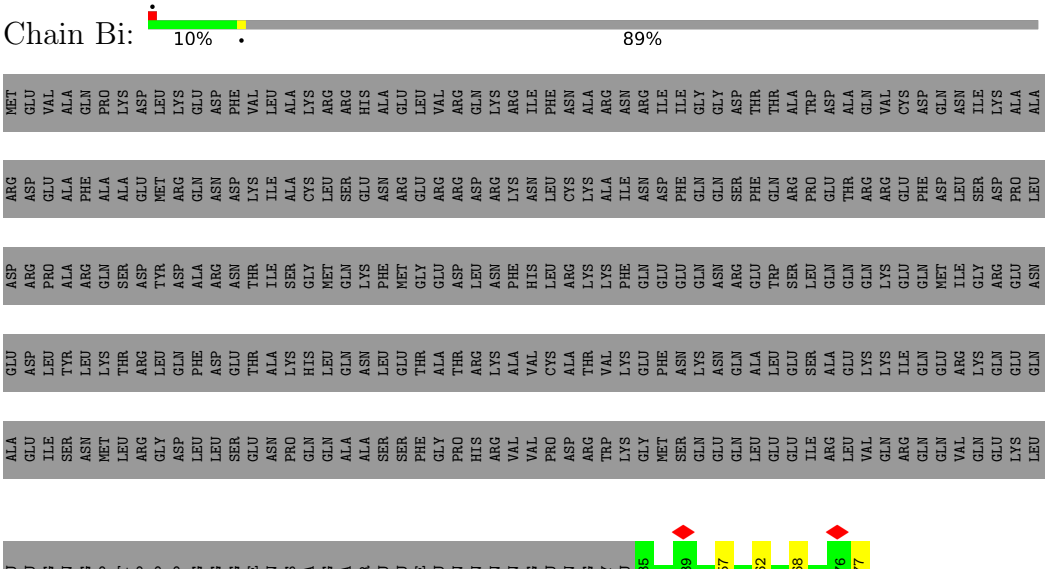
• Molecule 21: RIB43A-like with coiled-coils protein 2

Chain BV:



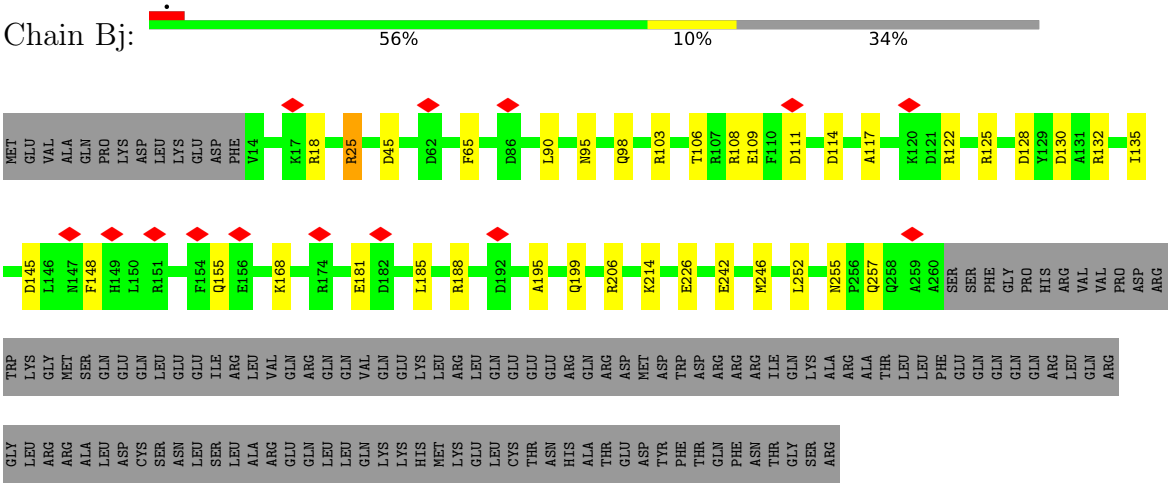
• Molecule 21: RIB43A-like with coiled-coils protein 2

Chain Bi:



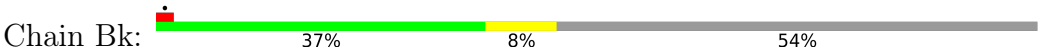
• Molecule 21: RIB43A-like with coiled-coils protein 2

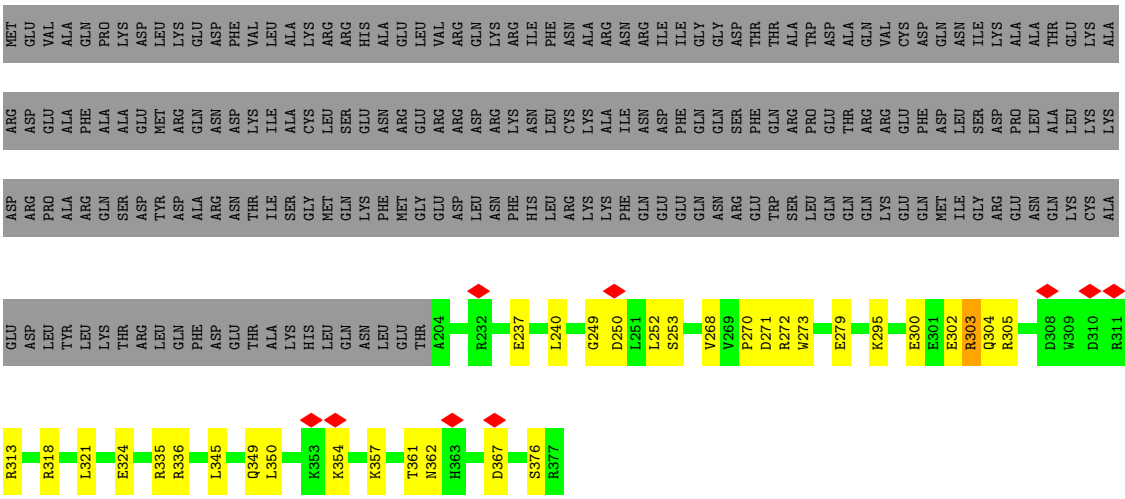
Chain Bj:



• Molecule 21: RIB43A-like with coiled-coils protein 2

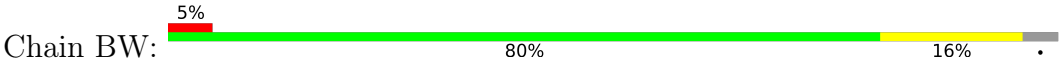
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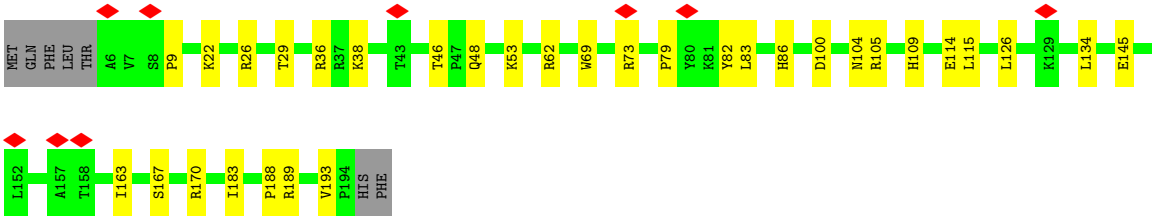




• Molecule 22: Cilia- and flagella-associated protein 107

Chain BW:

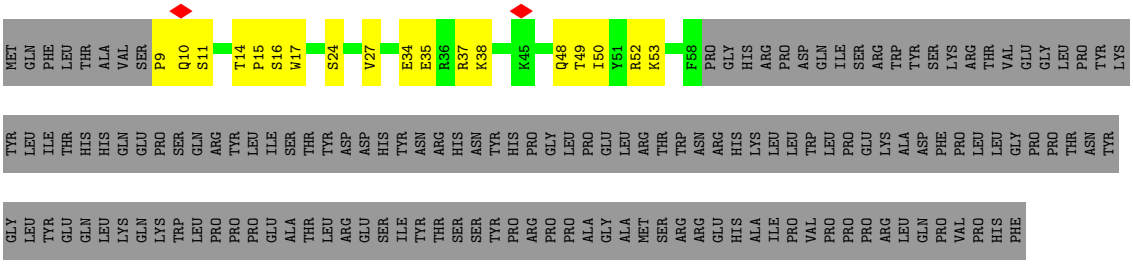




• Molecule 22: Cilia- and flagella-associated protein 107

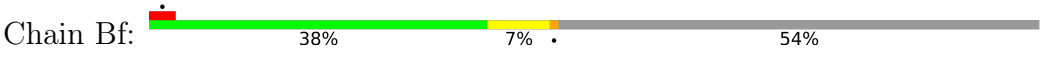
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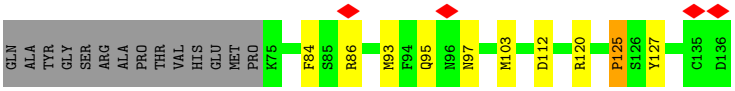


• Molecule 23: Piercer of microtubule wall 1 protein

Chain Bf:



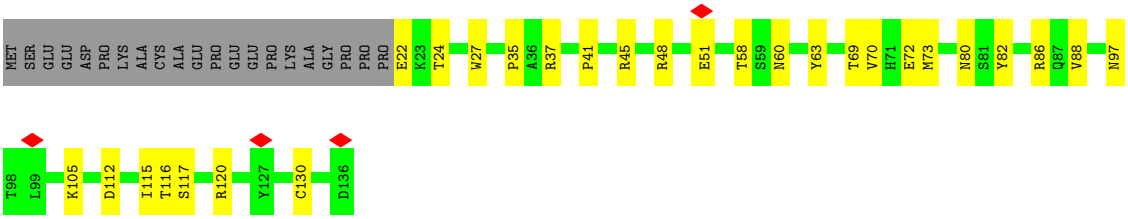




• Molecule 23: Piercer of microtubule wall 1 protein

Chain Bg:

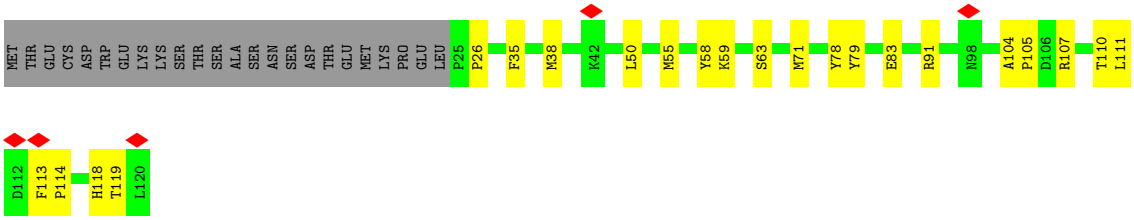




• Molecule 24: Piercer of microtubule wall 2 protein

Chain Bh:

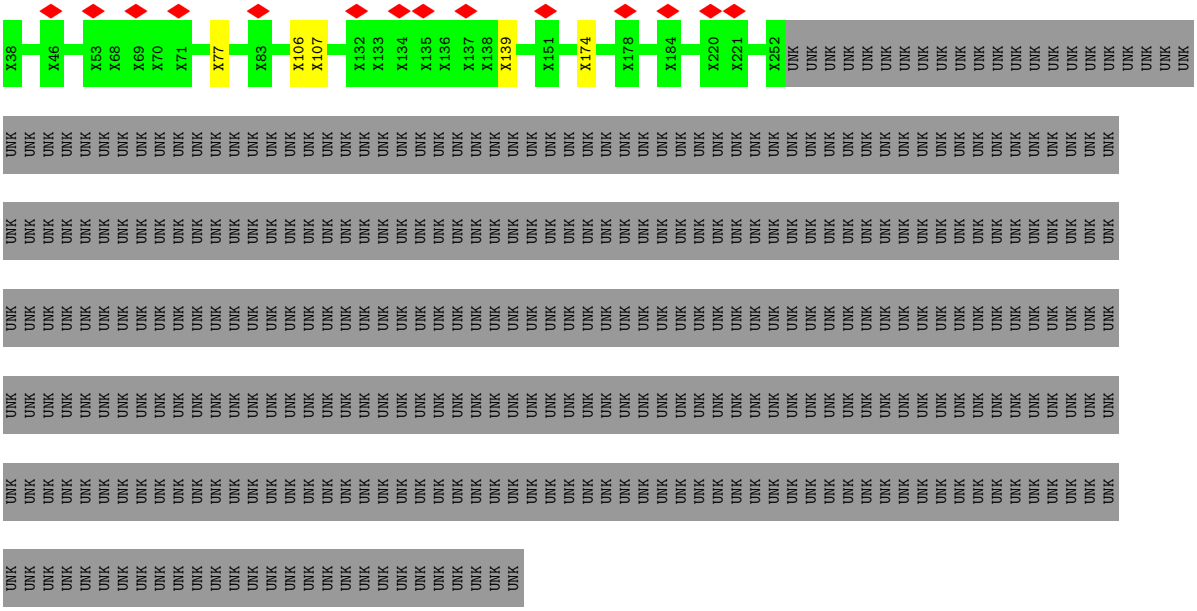




• Molecule 25: Stabilizer of axonemal microtubules 1

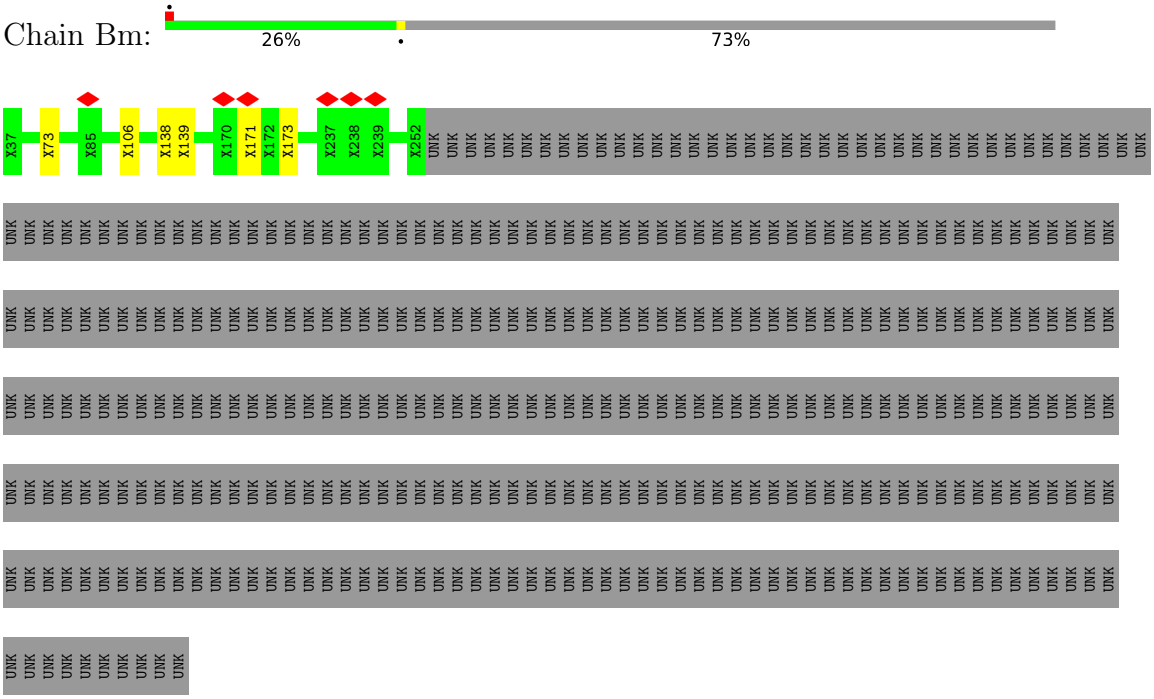
Chain Bl:





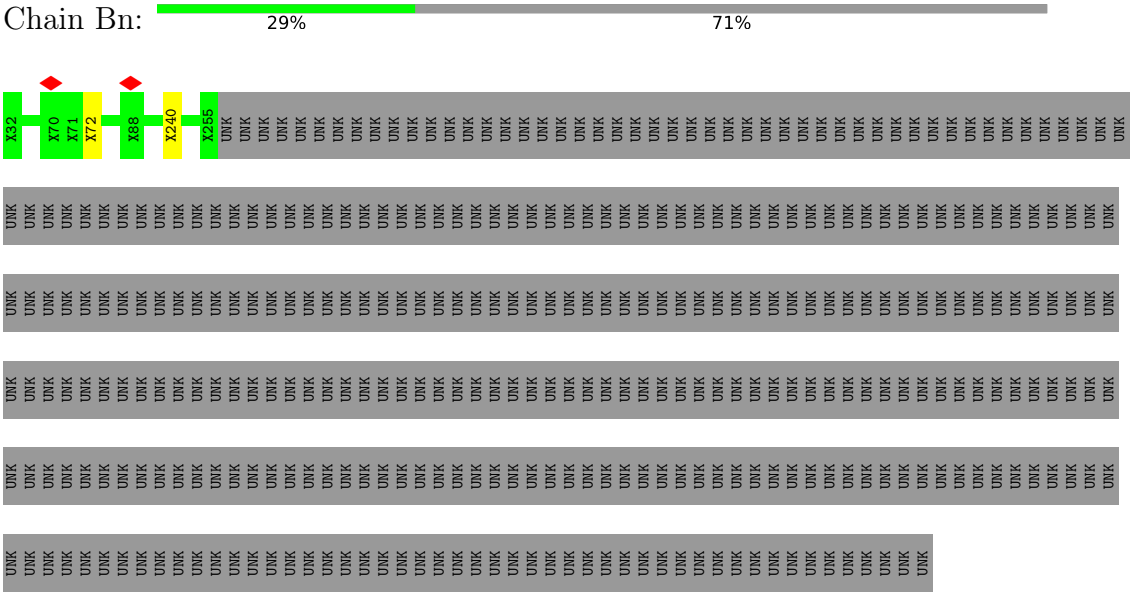
• Molecule 25: Stabilizer of axonemal microtubules 1

Chain Bm:



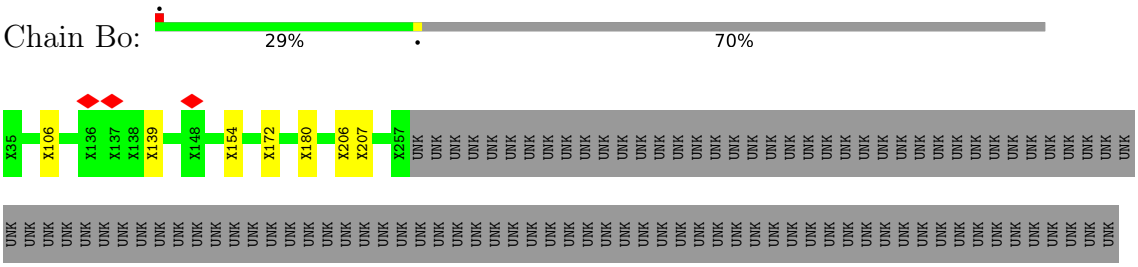
• Molecule 25: Stabilizer of axonemal microtubules 1

Chain Bn:



• Molecule 25: Stabilizer of axonemal microtubules 1

Chain Bo:

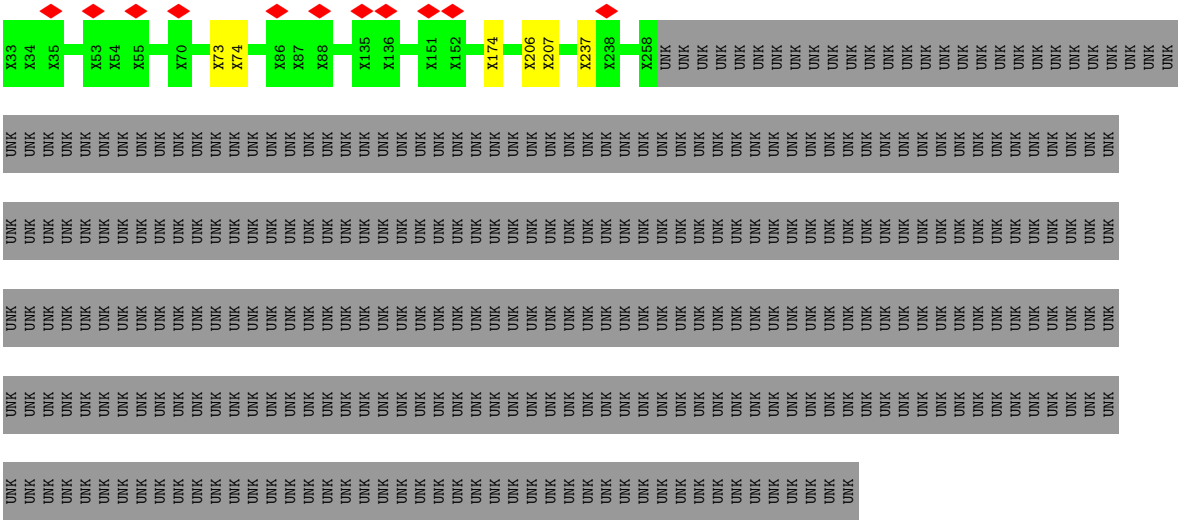




• Molecule 25: Stabilizer of axonemal microtubules 1

Chain Bp:

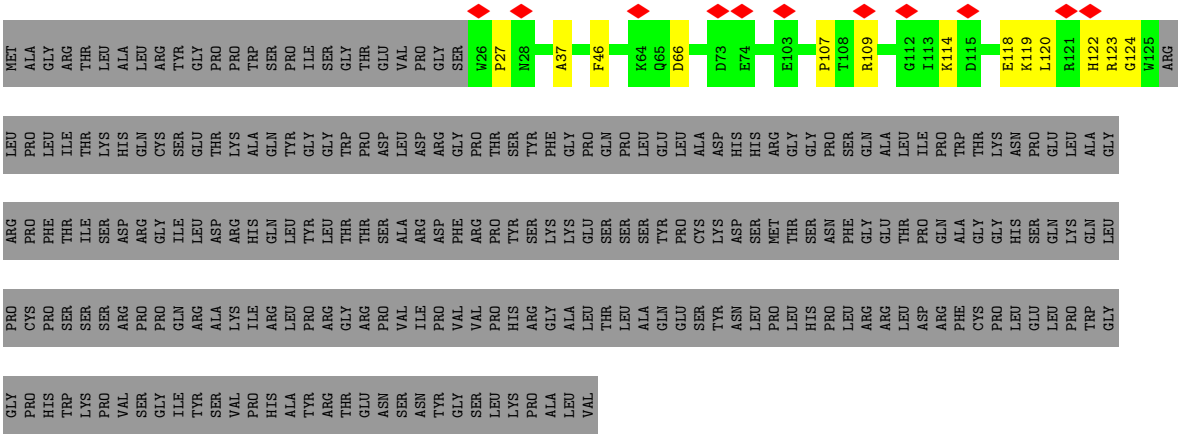




• Molecule 26: Stabilizer of axonemal microtubules 3

Chain Bq:

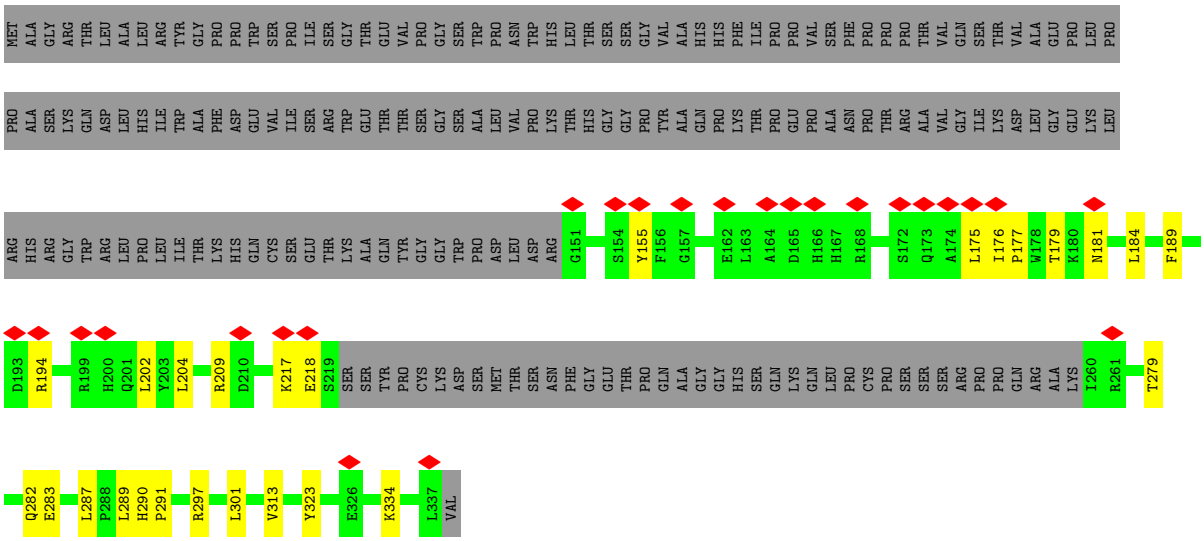




• Molecule 26: Stabilizer of axonemal microtubules 3

Chain Bu:

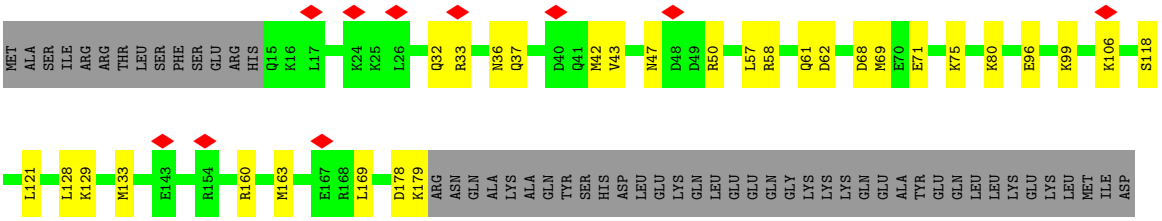


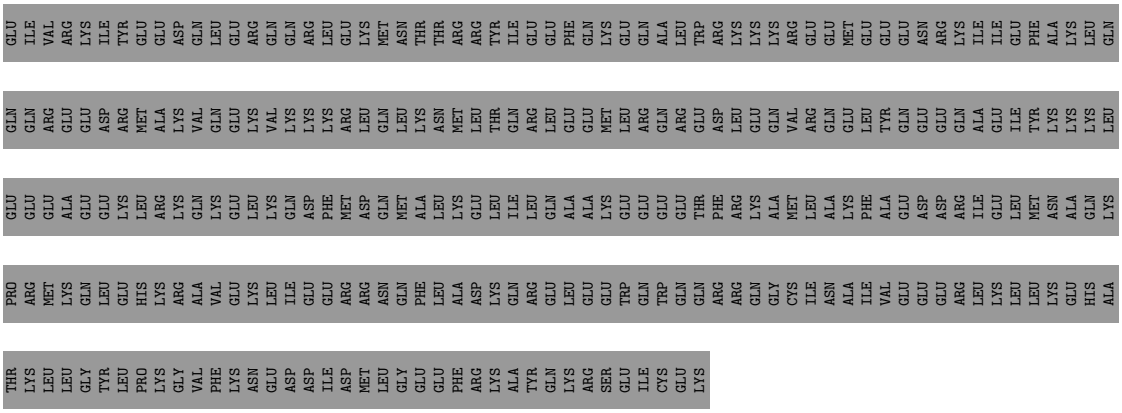


• Molecule 27: Meiosis-specific nuclear structural protein 1

Chain Br:



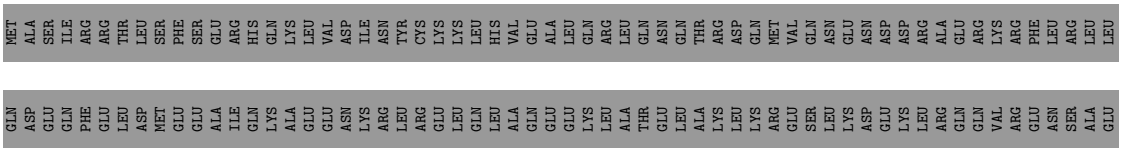


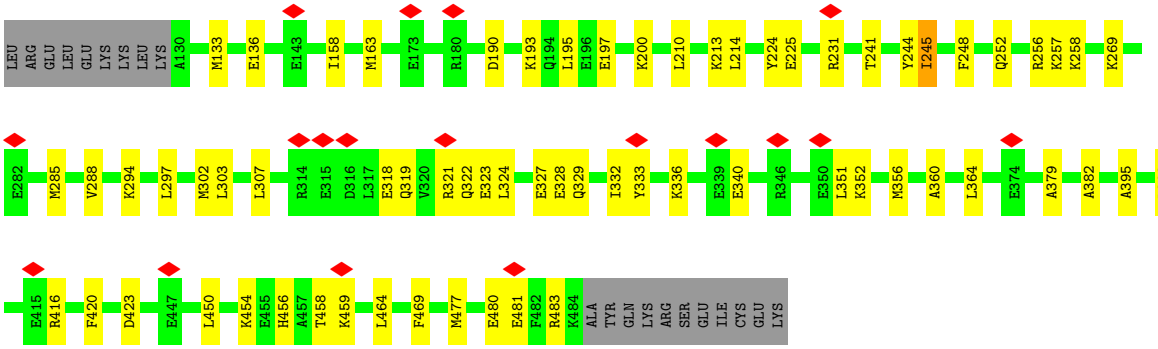


• Molecule 27: Meiosis-specific nuclear structural protein 1

Chain Bs:



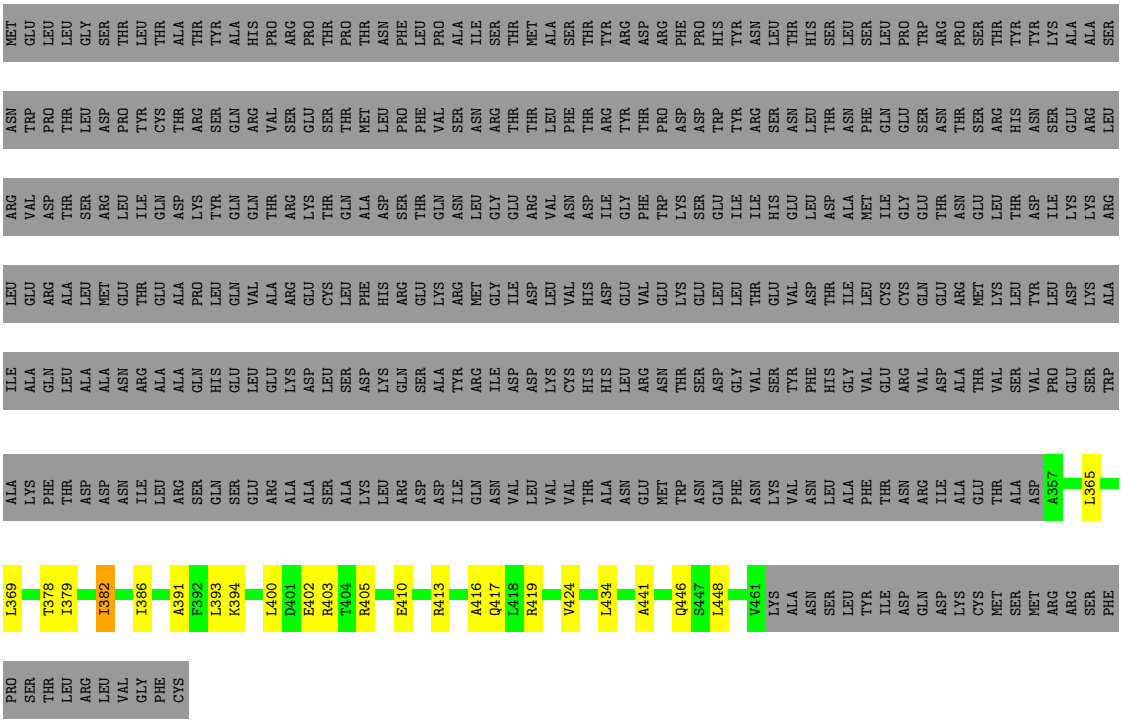




• Molecule 28: Tektin-3

Chain C0:

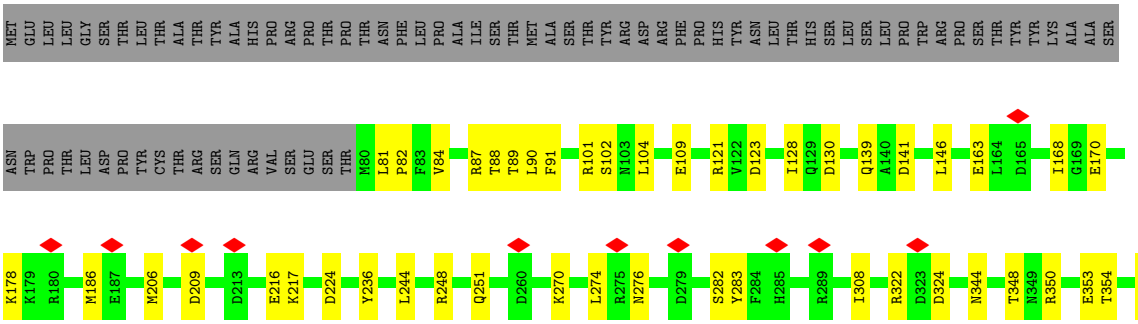




• Molecule 28: Tektin-3

Chain C2:



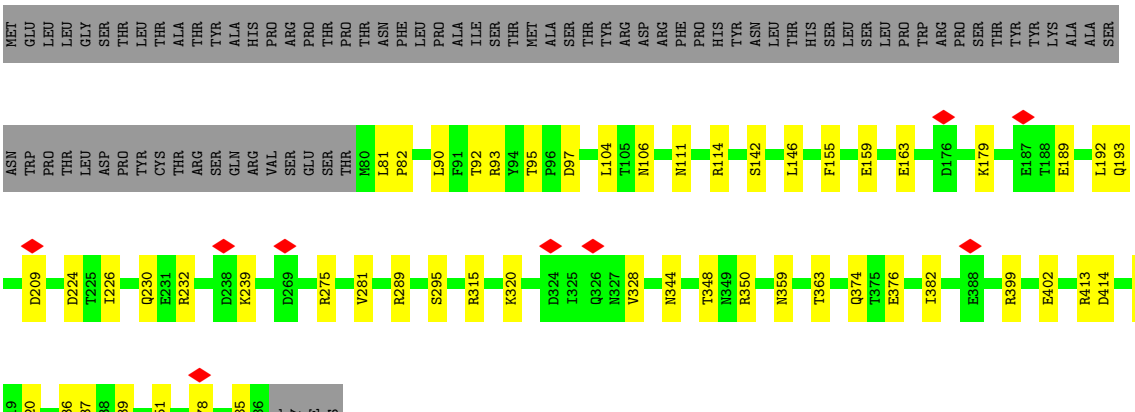




• Molecule 28: Tektin-3

Chain C3:

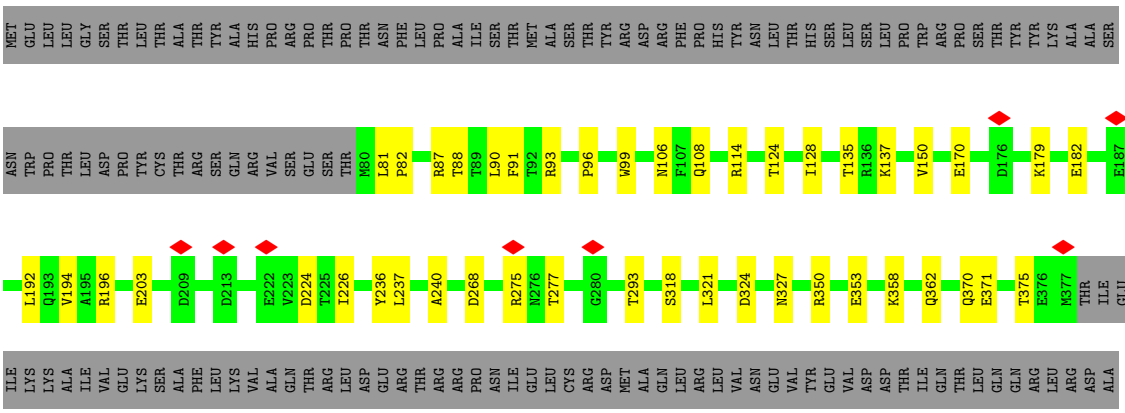




• Molecule 28: Tektin-3

Chain C4:

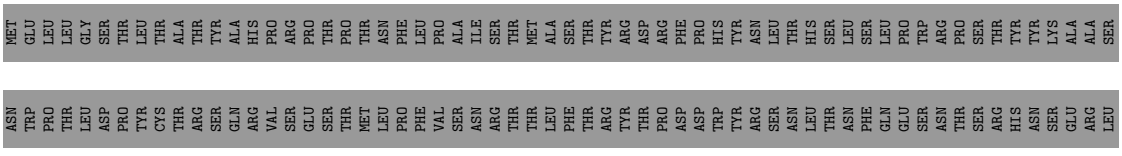


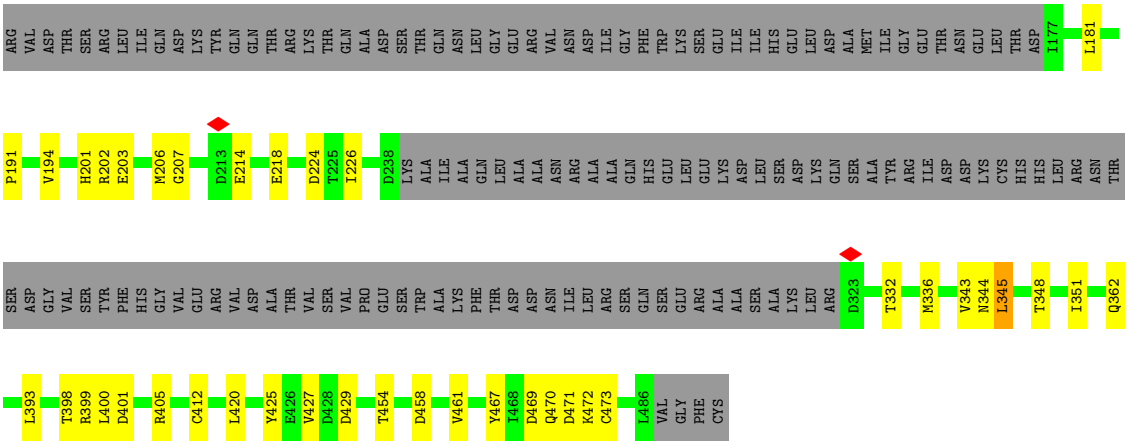


• Molecule 28: Tektin-3

Chain C5:



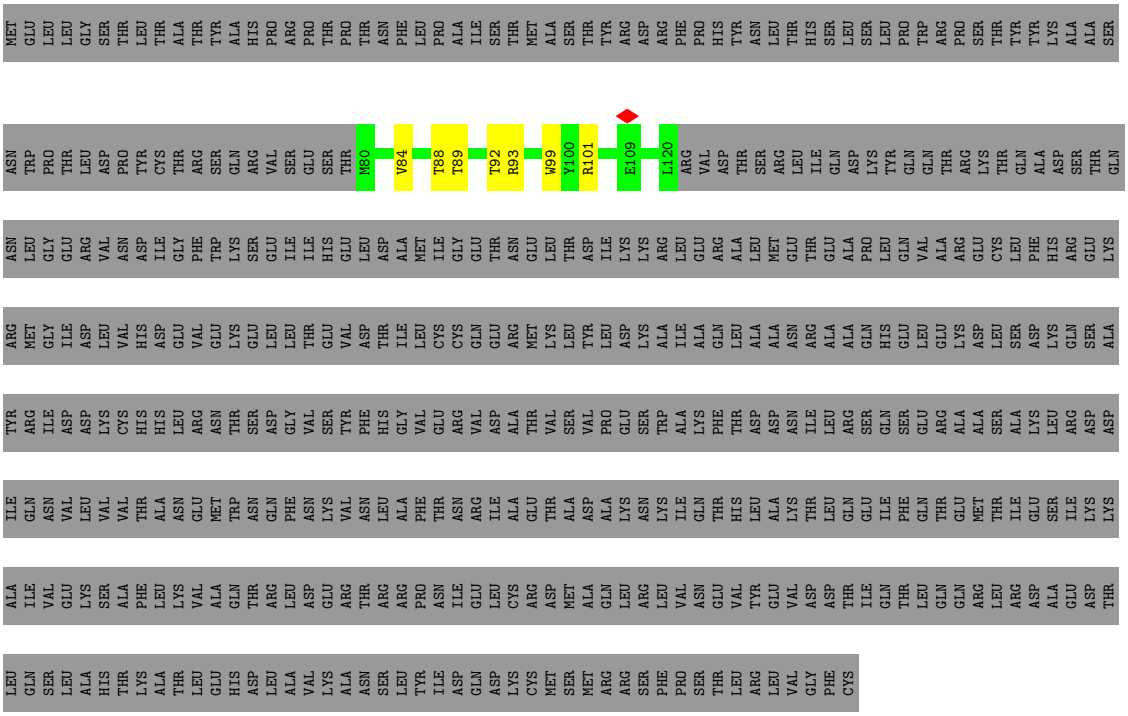




• Molecule 28: Tektin-3

Chain C6:

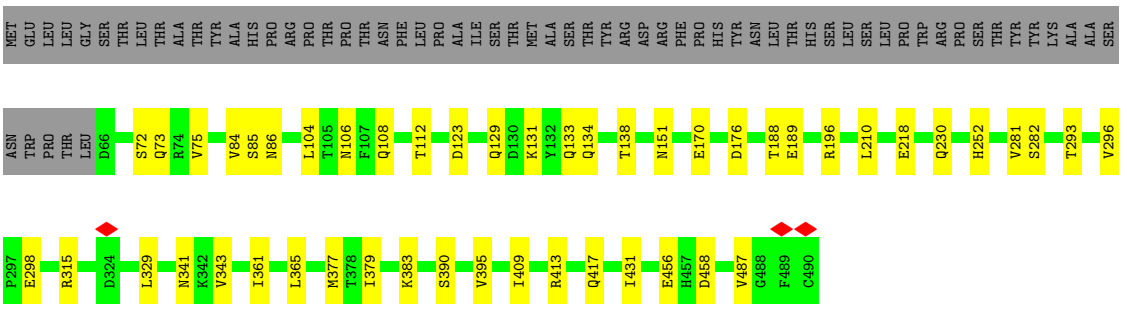




• Molecule 28: Tektin-3

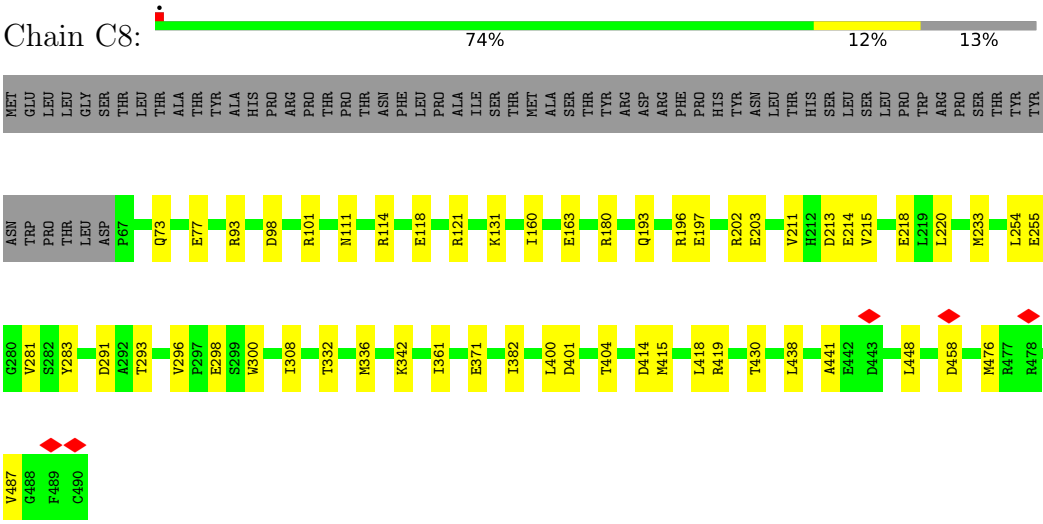
Chain C7:





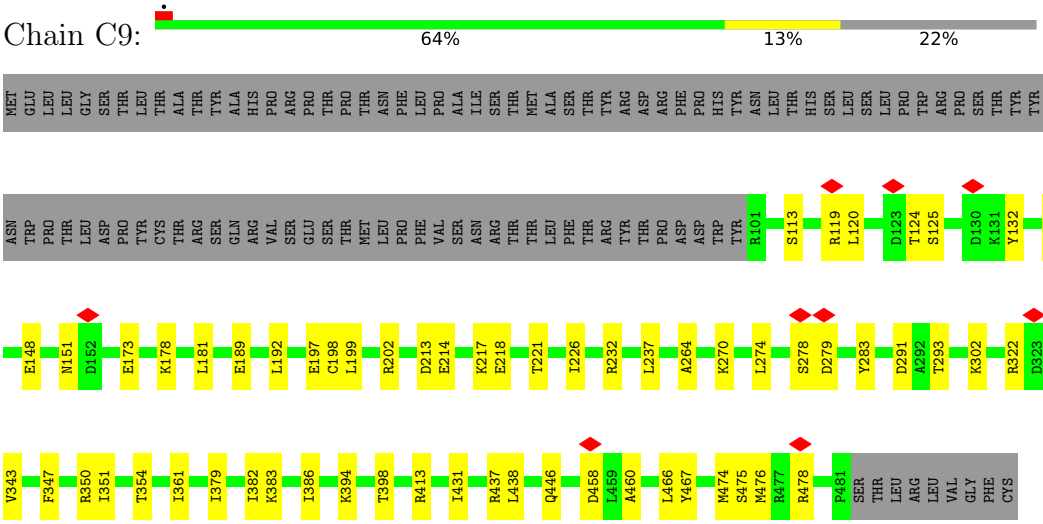
• Molecule 28: Tektin-3

Chain C8:



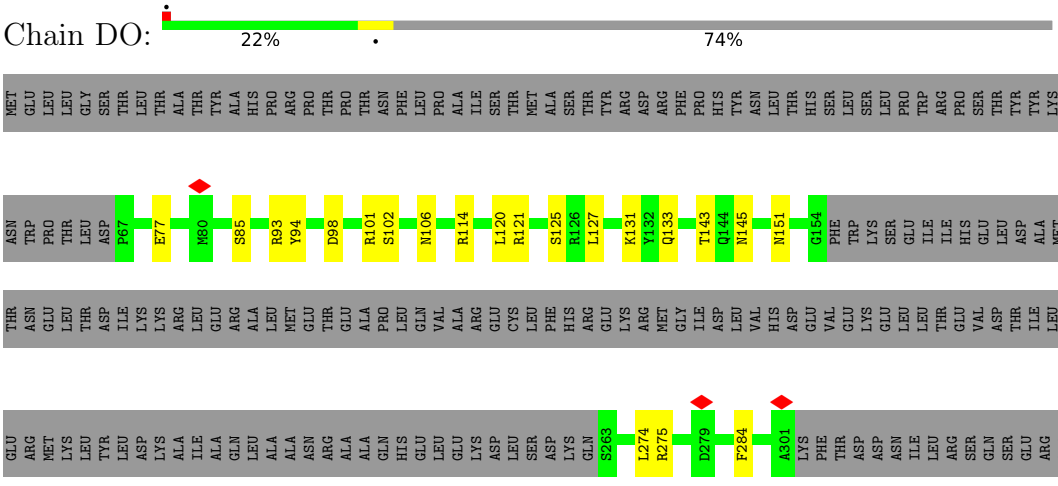
• Molecule 28: Tektin-3

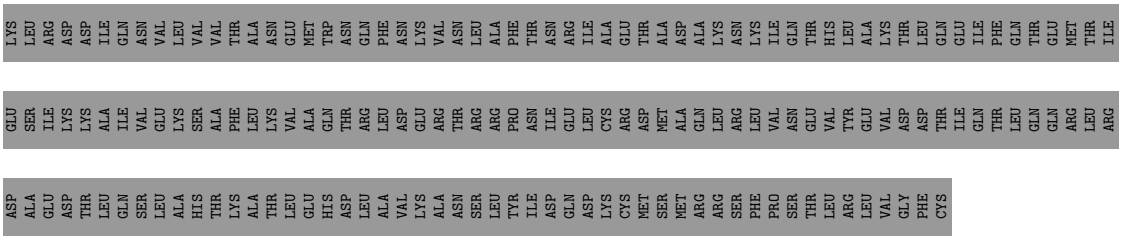
Chain C9:



• Molecule 28: Tektin-3

Chain DO:

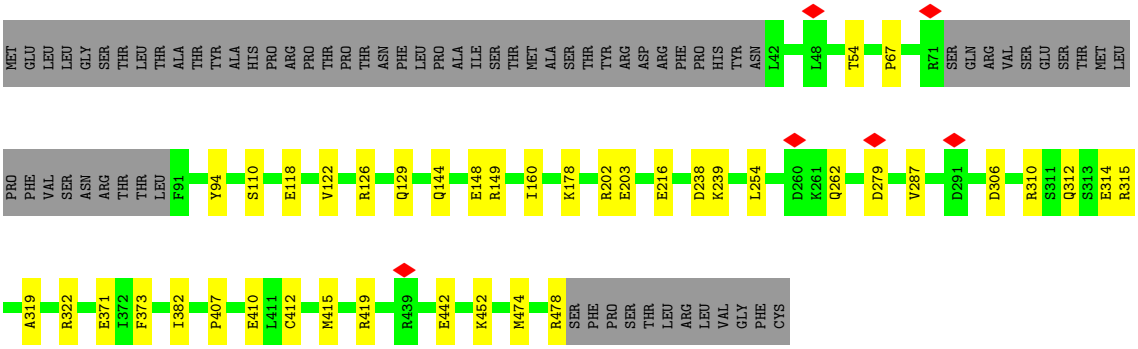




• Molecule 28: Tektin-3

Chain F2:

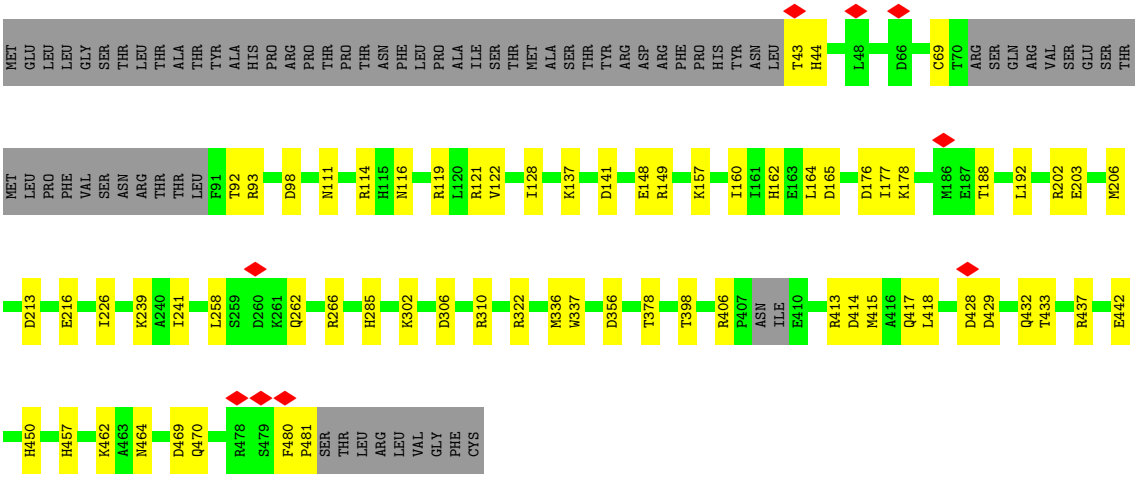




• Molecule 28: Tektin-3

Chain F3:

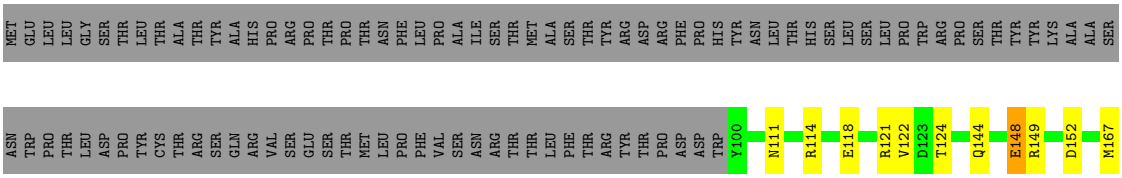


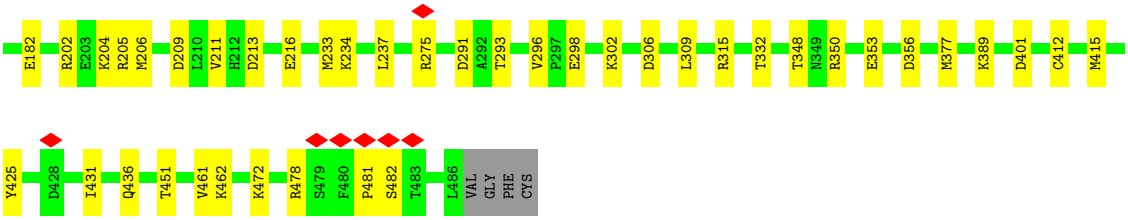


• Molecule 28: Tektin-3

Chain F4:



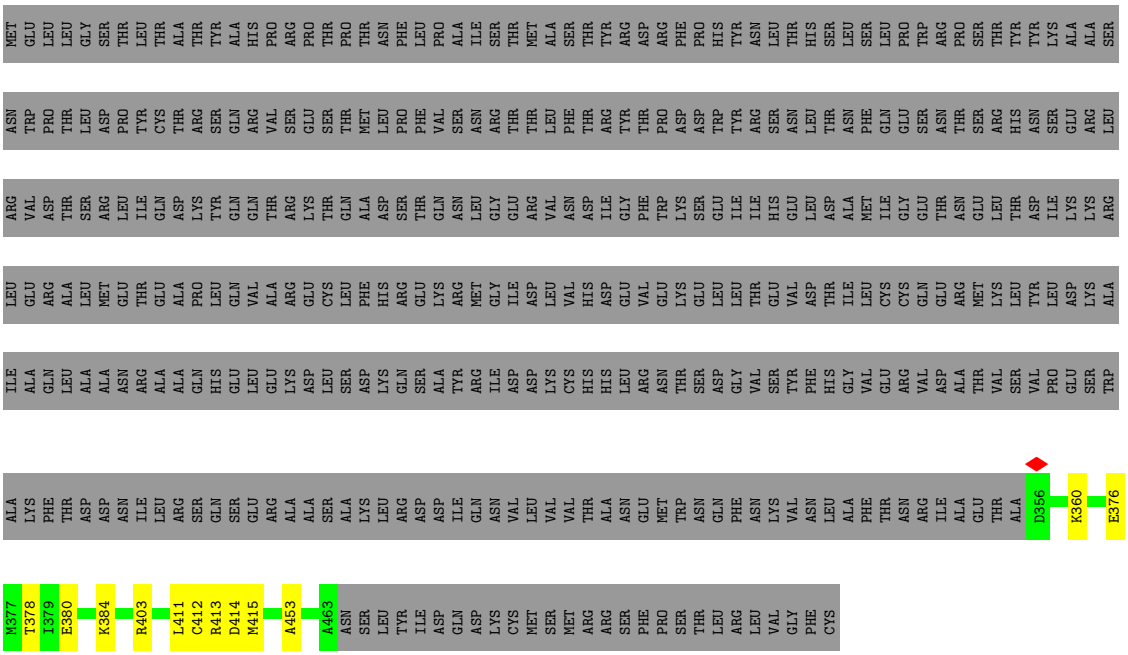




• Molecule 28: Tektin-3

Chain F5:

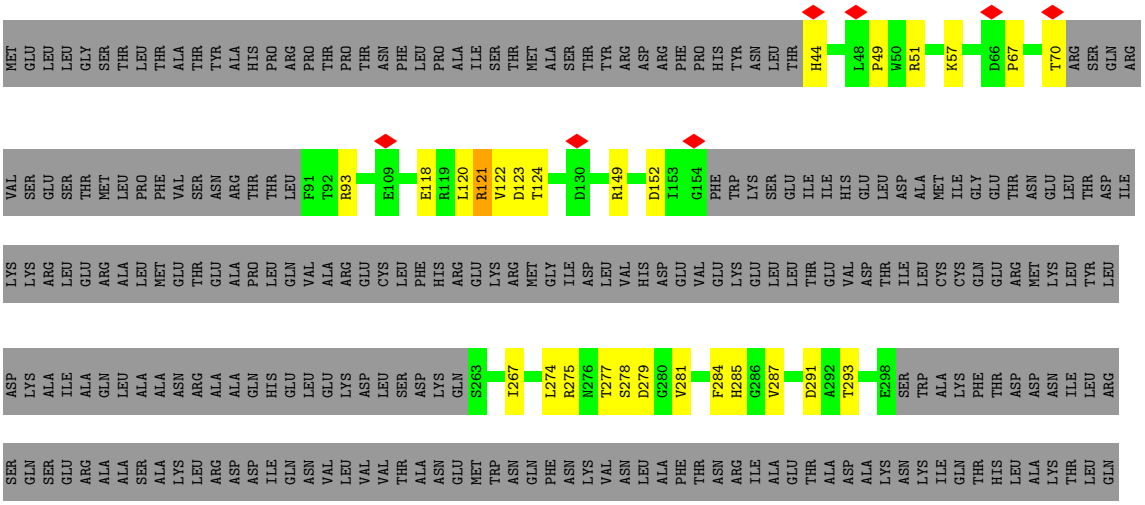


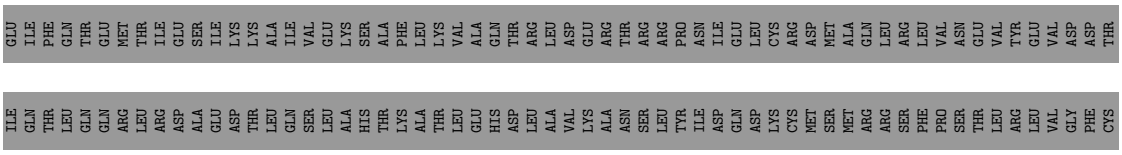


• Molecule 28: Tektin-3

Chain F6:



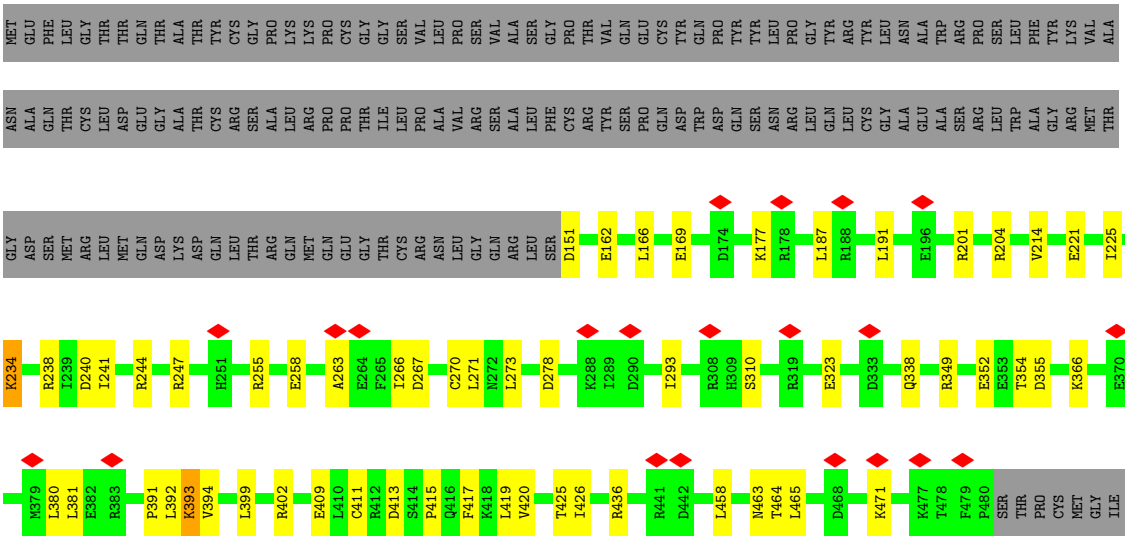




• Molecule 29: Tektin-5

Chain C1:

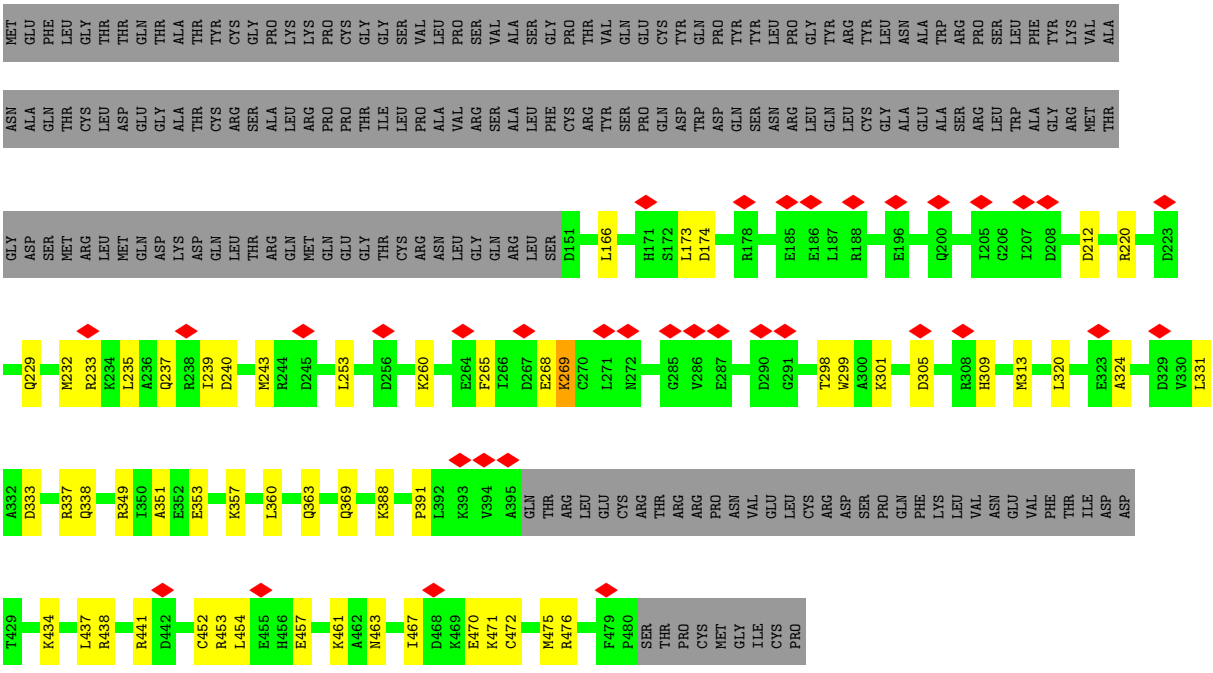




• Molecule 29: Tektin-5

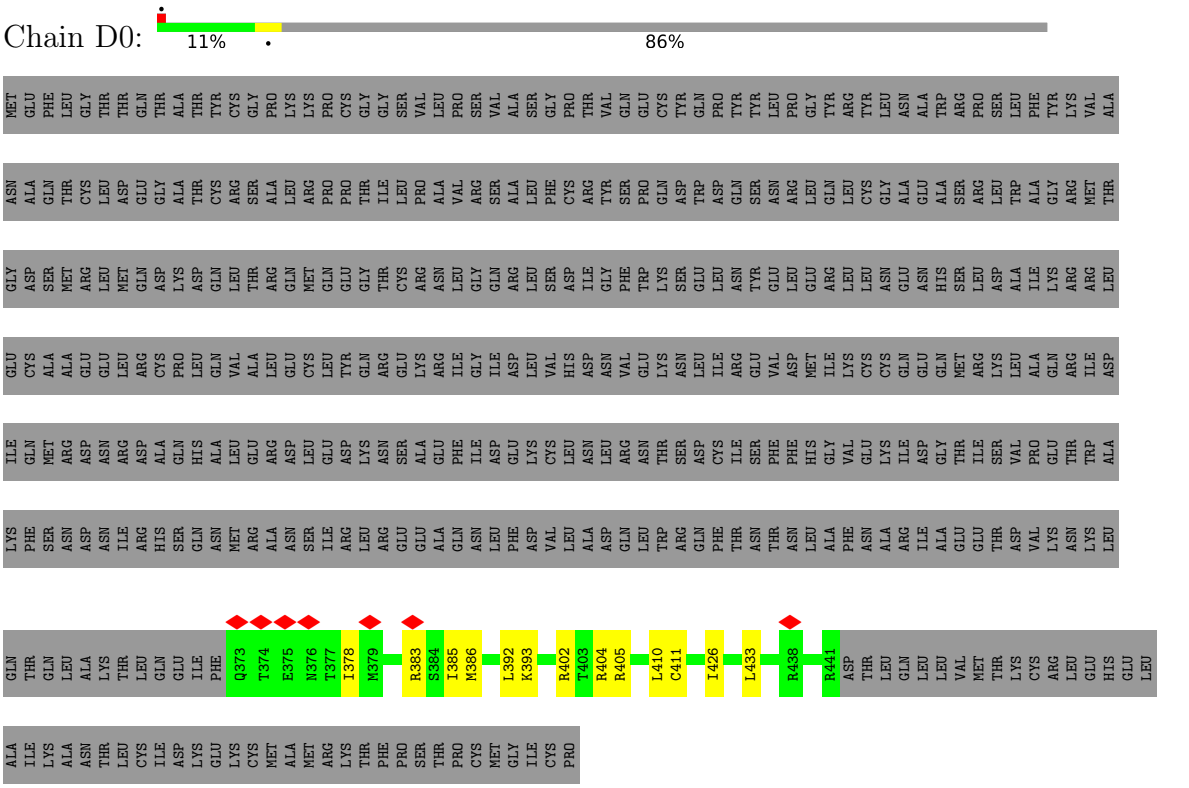
Chain Cz:





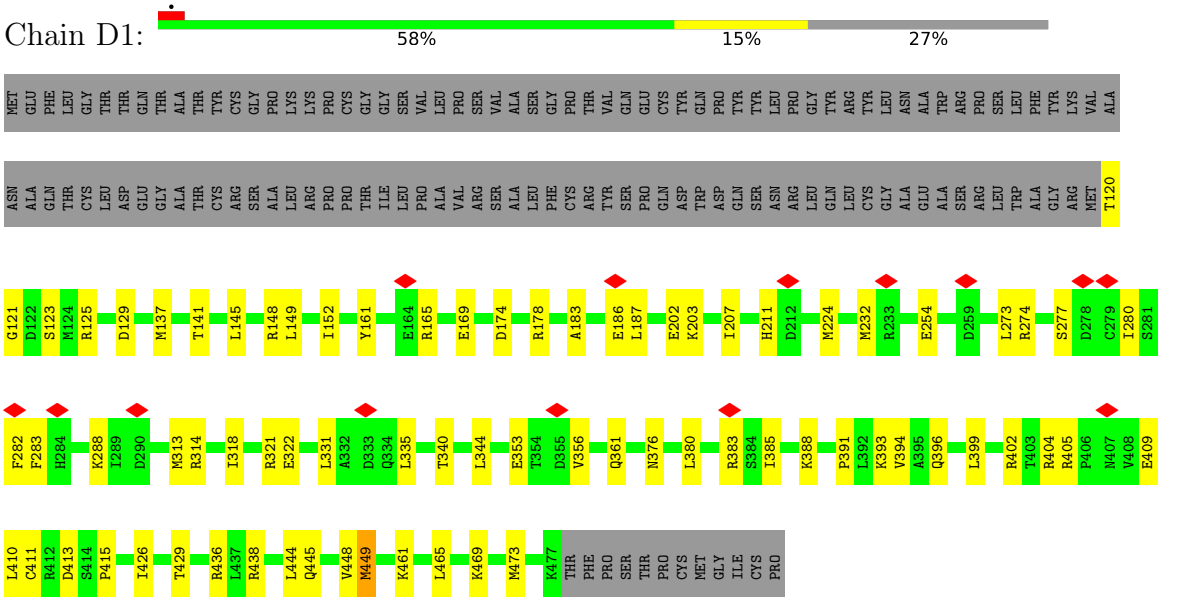
• Molecule 29: Tektin-5

Chain D0:



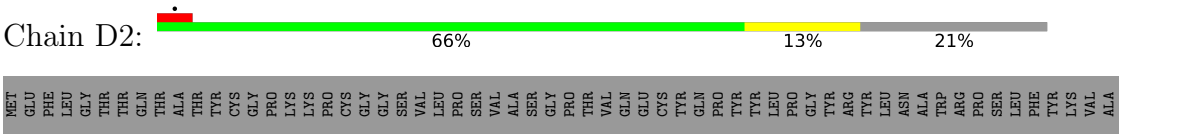
• Molecule 29: Tektin-5

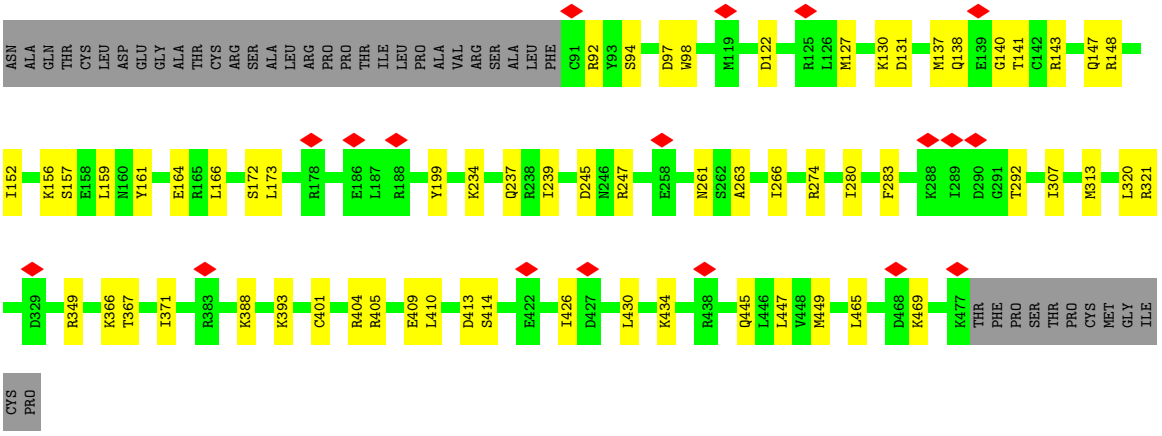
Chain D1:



• Molecule 29: Tektin-5

Chain D2:

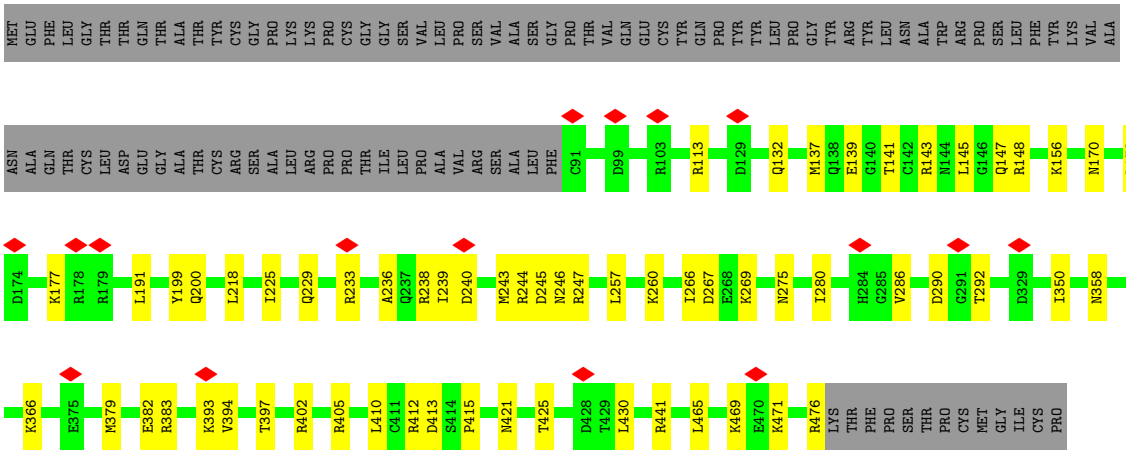




• Molecule 29: Tektin-5

Chain D3:

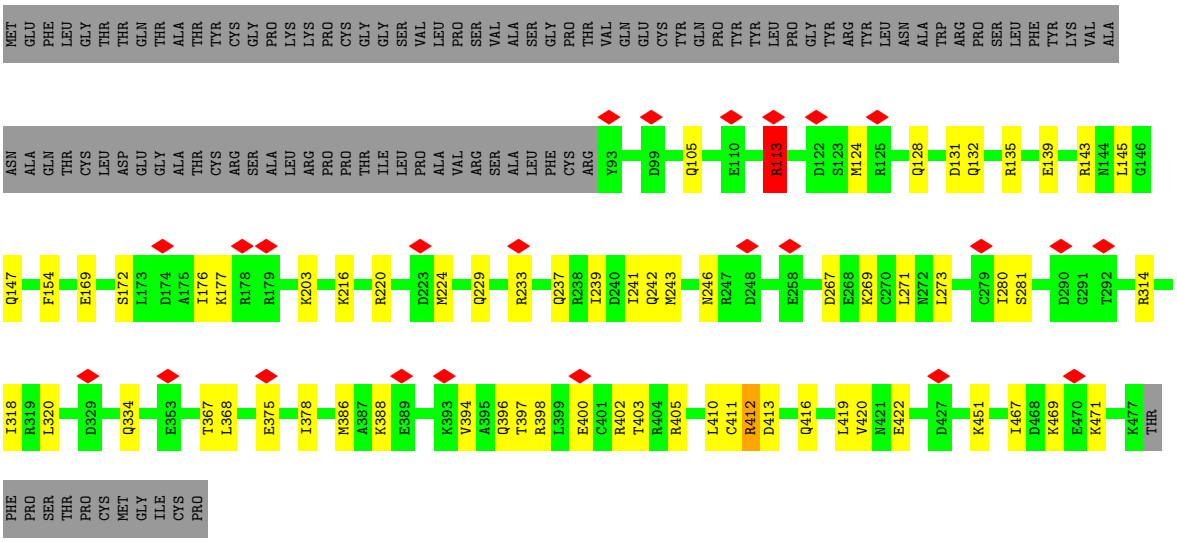




• Molecule 29: Tektin-5

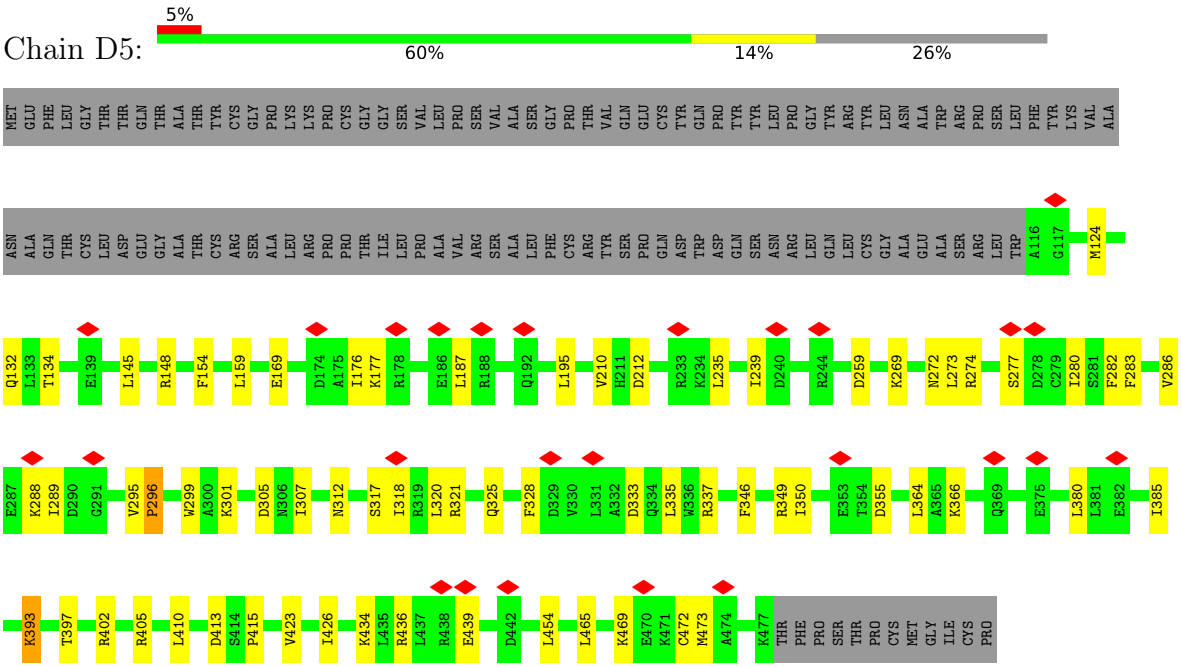
Chain D4:





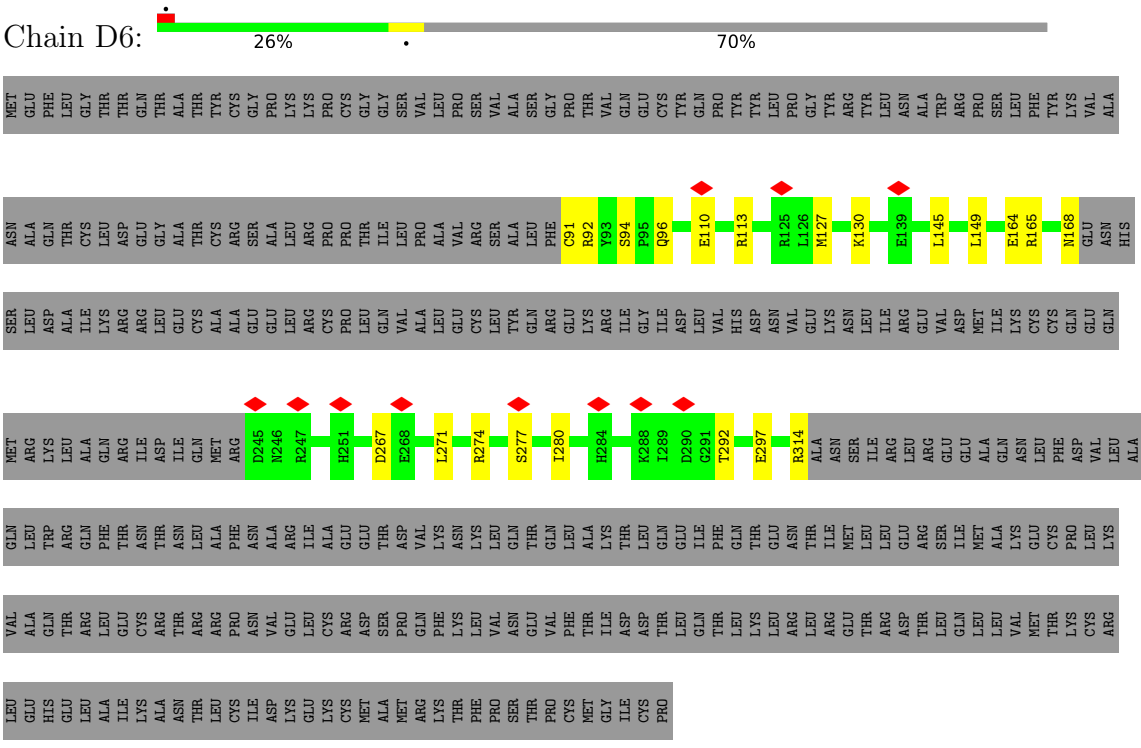
• Molecule 29: Tektin-5

Chain D5:



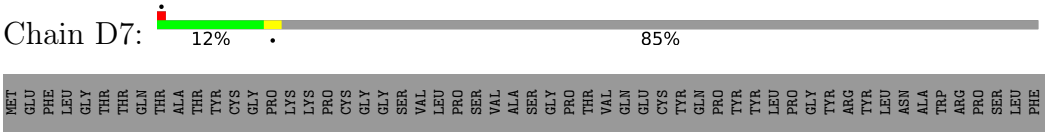
• Molecule 29: Tektin-5

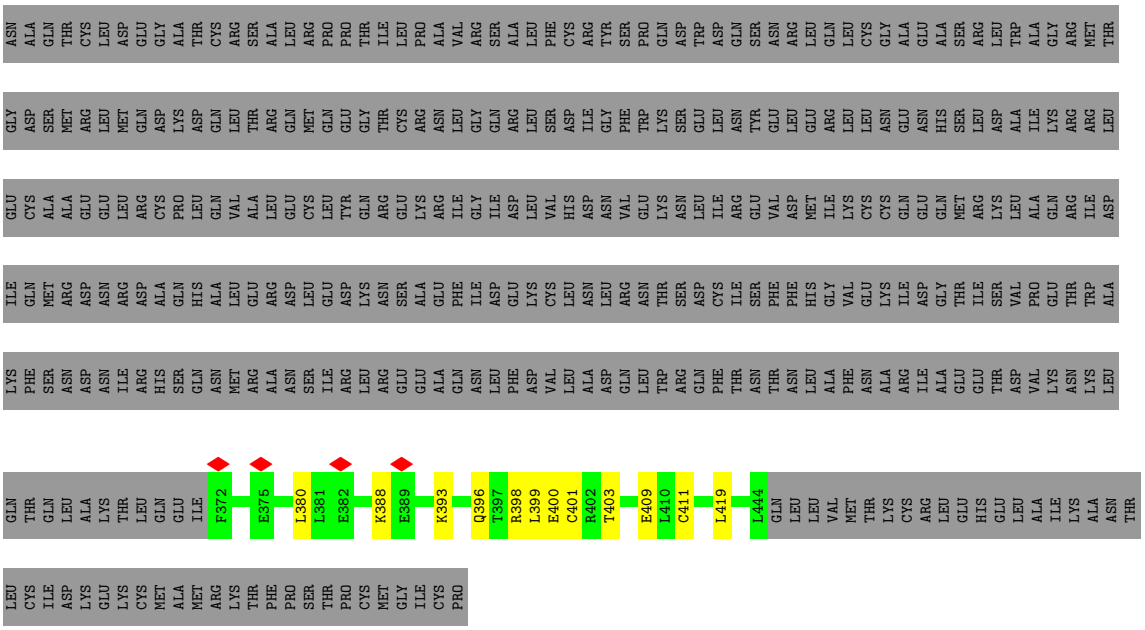
Chain D6:



• Molecule 29: Tektin-5

Chain D7:

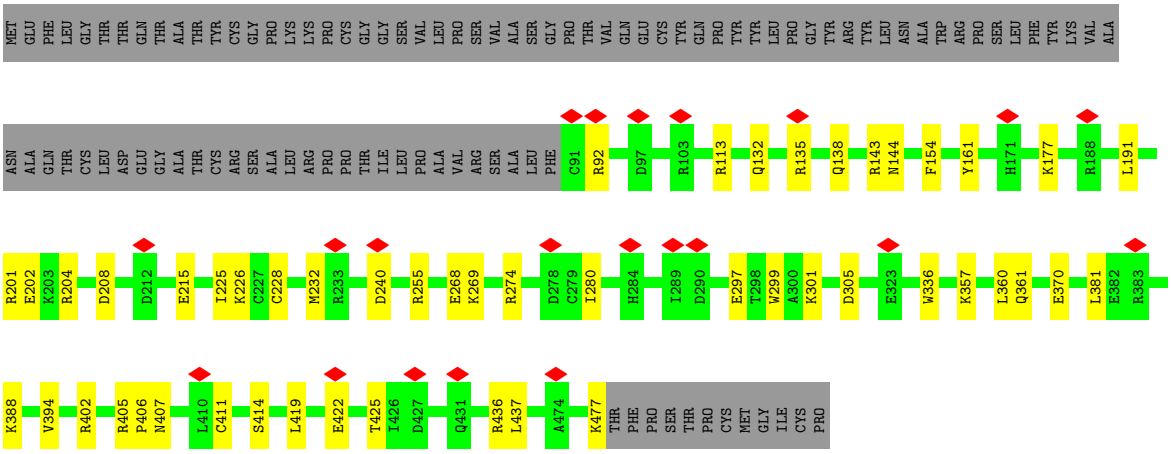




• Molecule 29: Tektin-5

Chain D8:

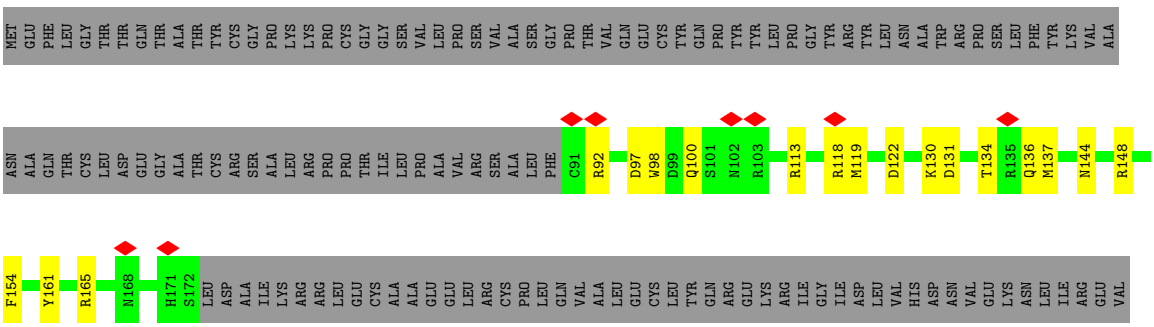


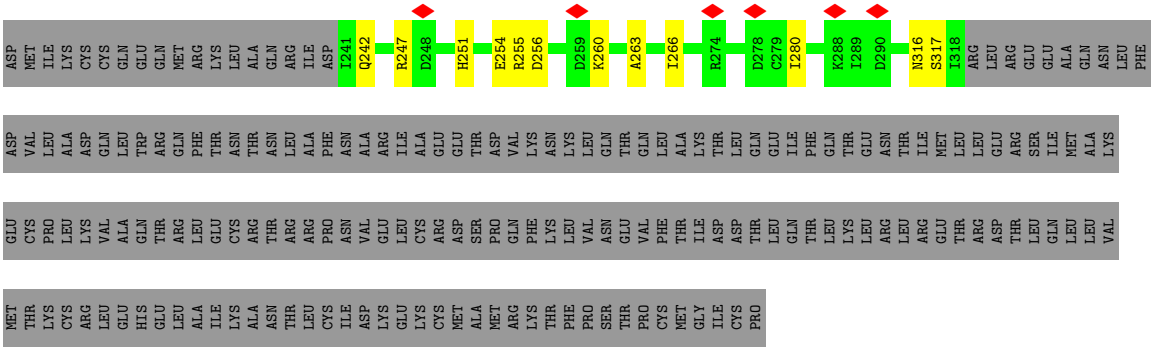


• Molecule 29: Tektin-5

Chain D9:



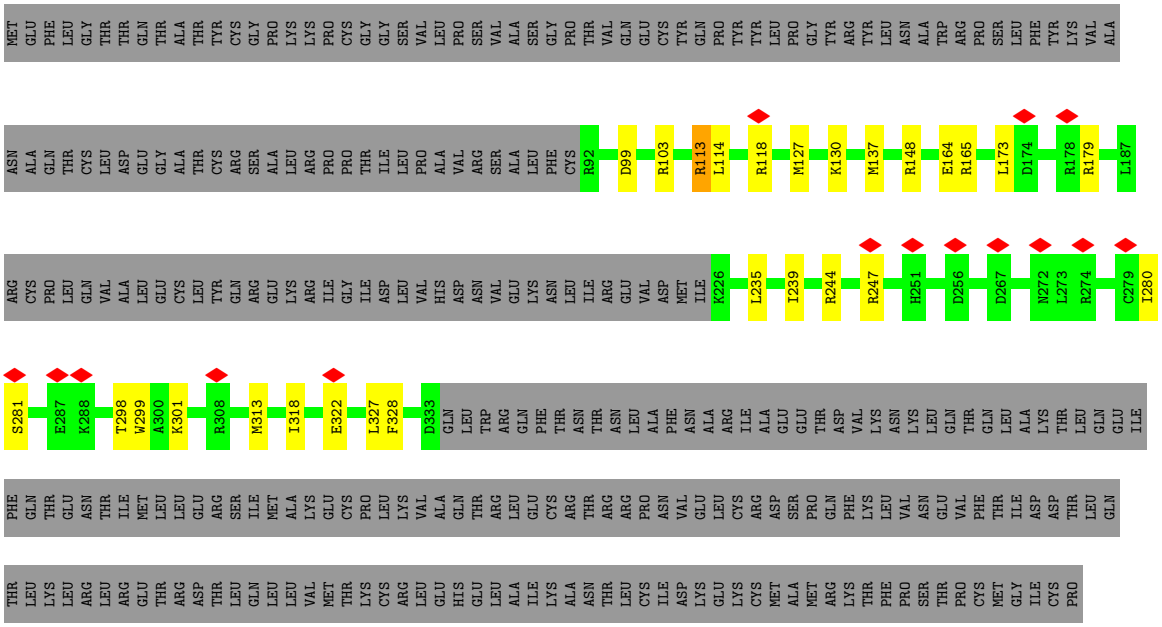




• Molecule 29: Tektin-5

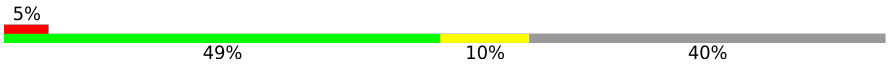
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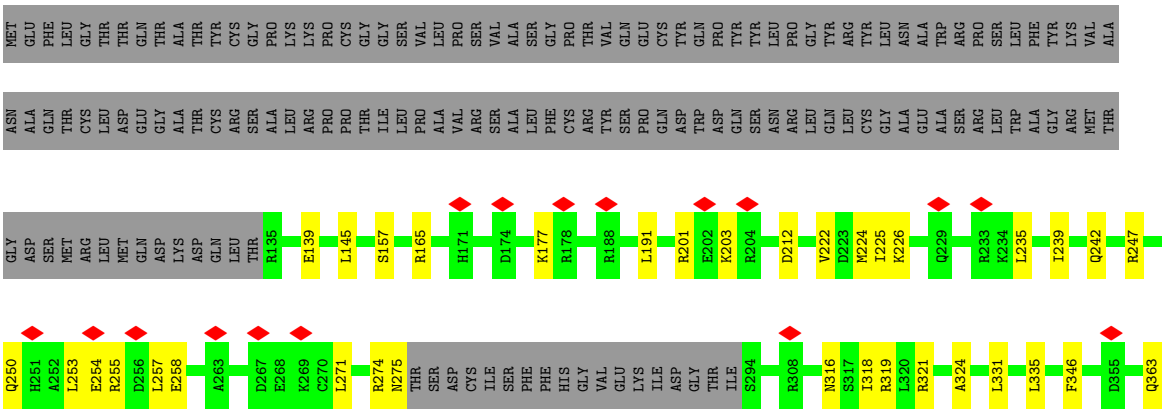


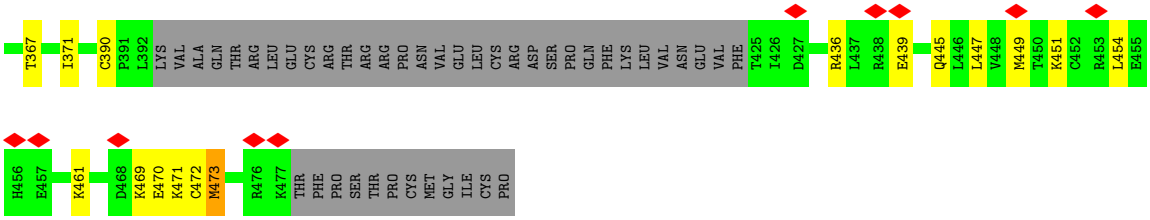


• Molecule 29: Tektin-5

Chain DQ:

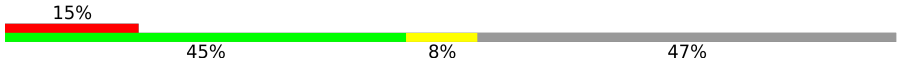


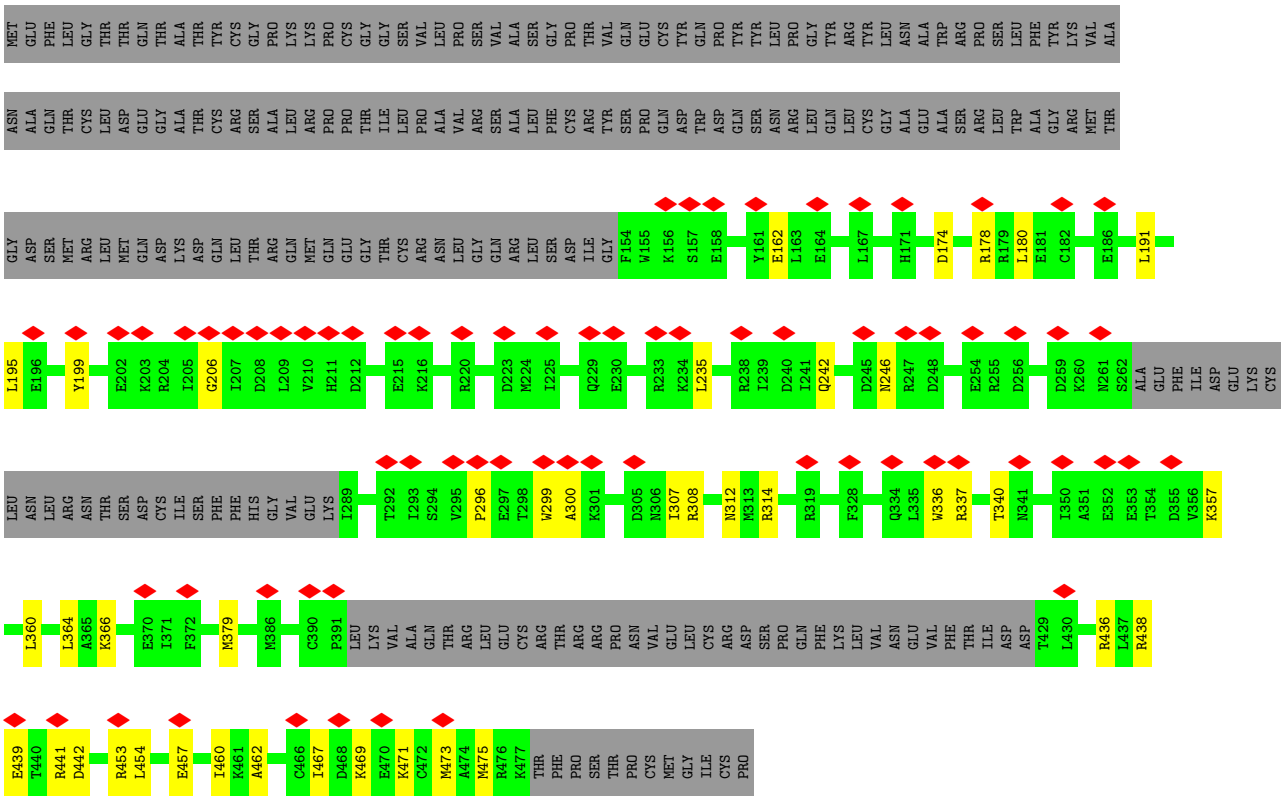




• Molecule 29: Tektin-5

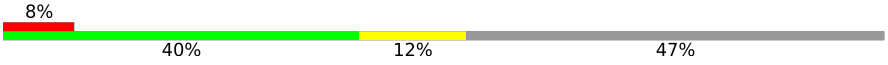
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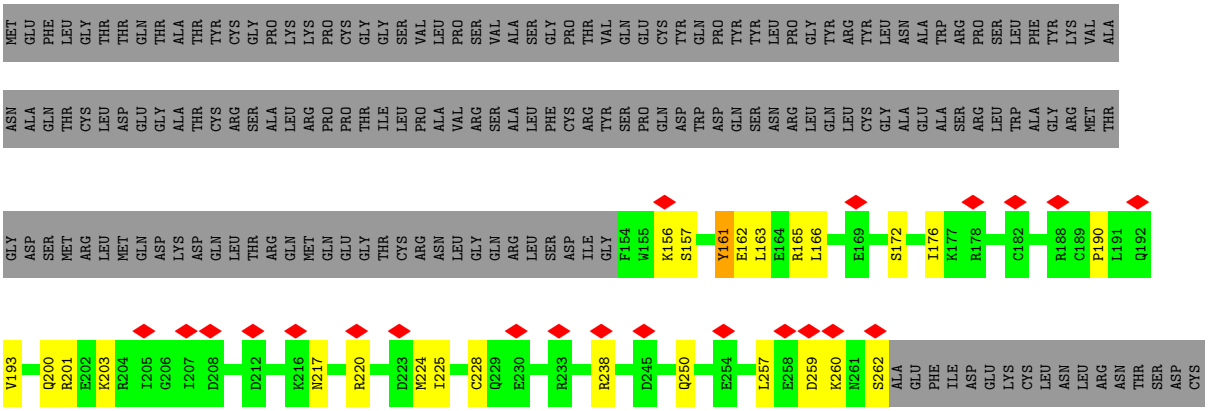


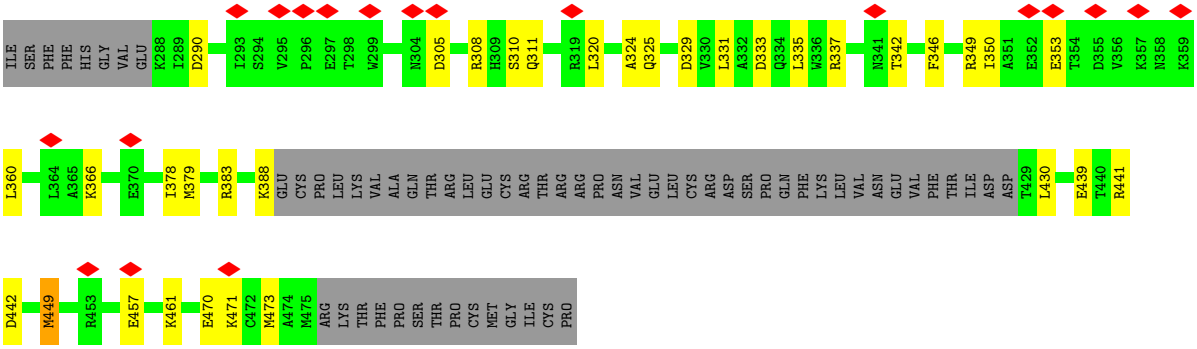


• Molecule 29: Tektin-5

Chain DS:



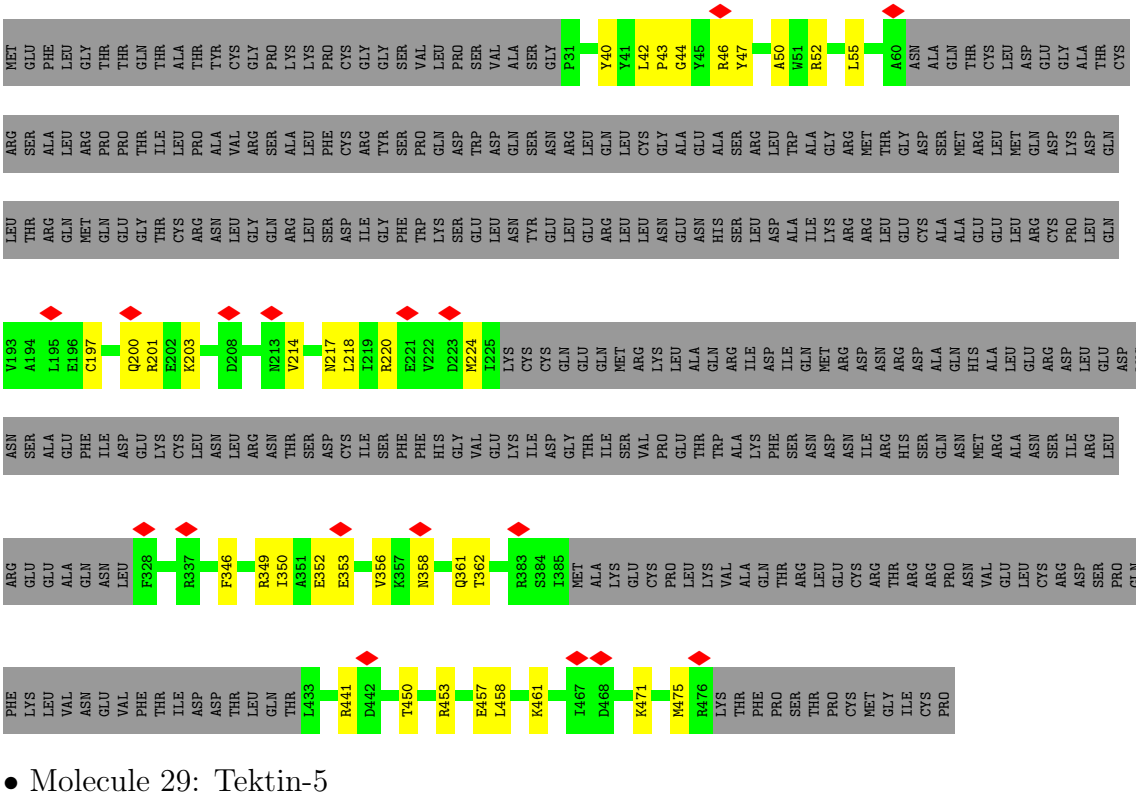




• Molecule 29: Tektin-5

Chain DT:

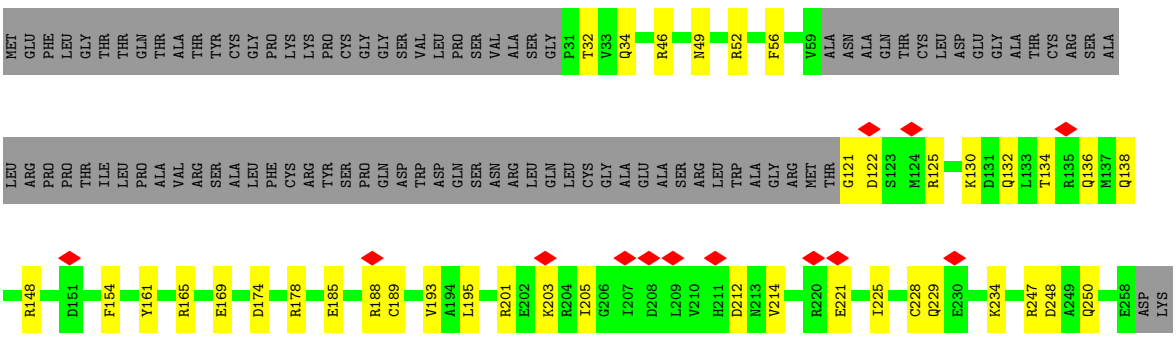


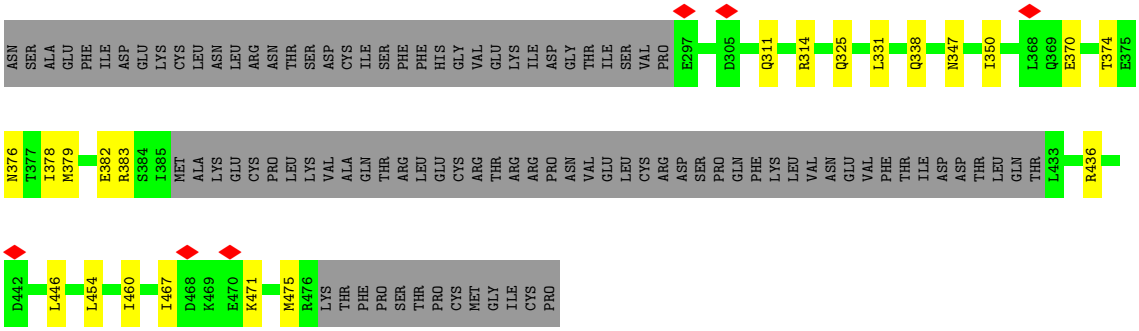


• Molecule 29: Tektin-5

Chain DU:

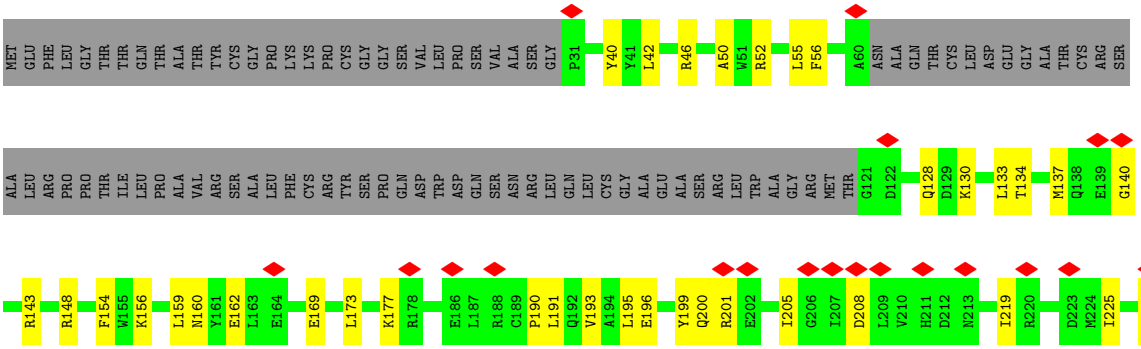






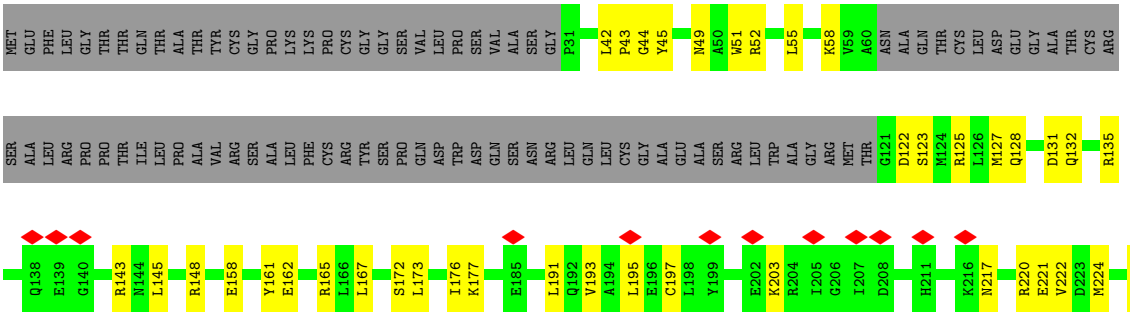
• Molecule 29: Tektin-5

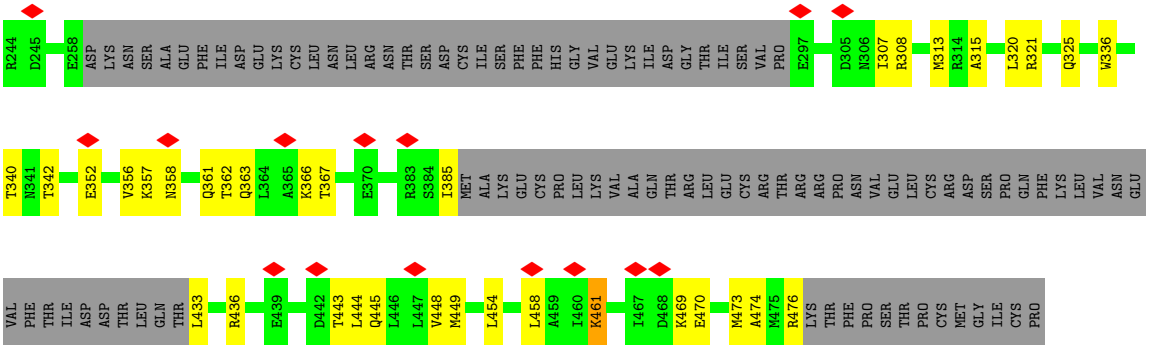




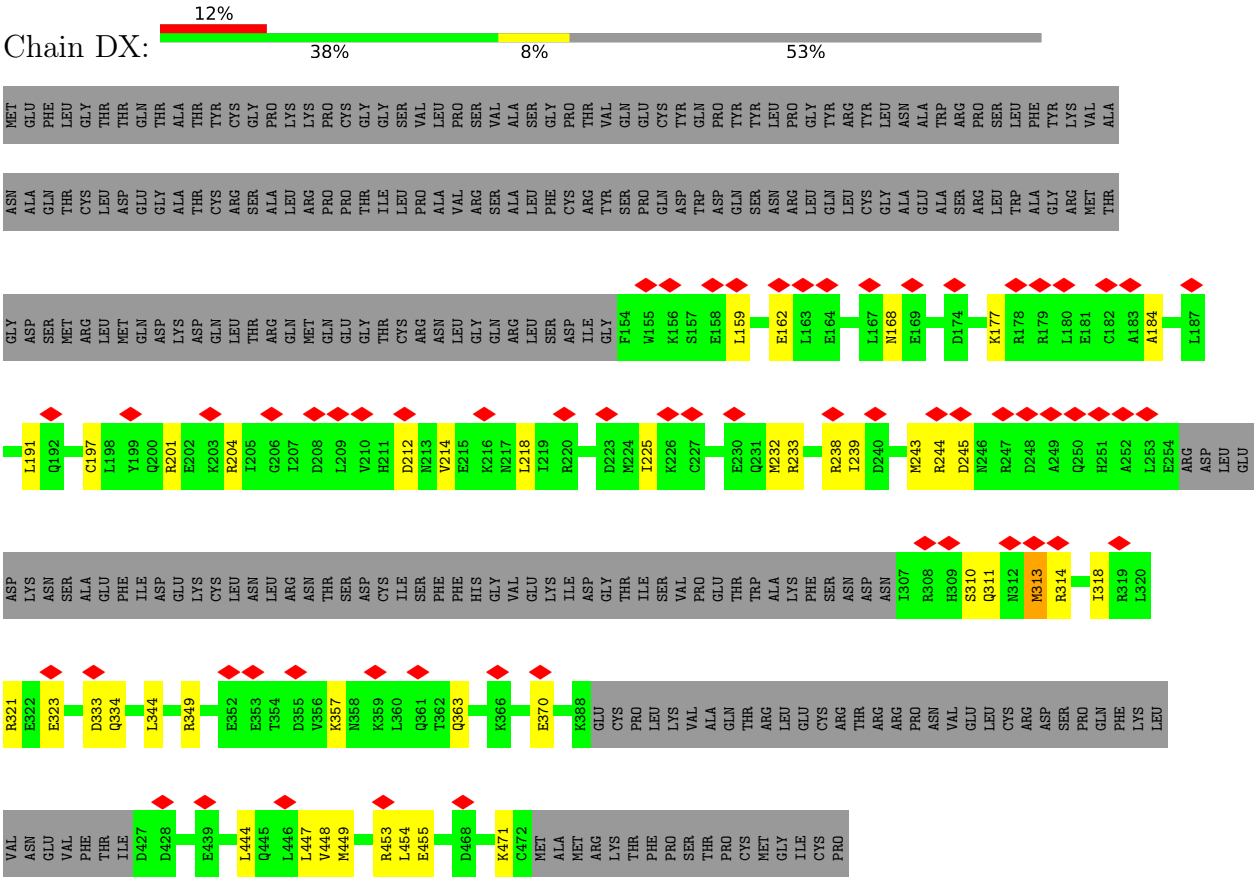
• Molecule 29: Tektin-5



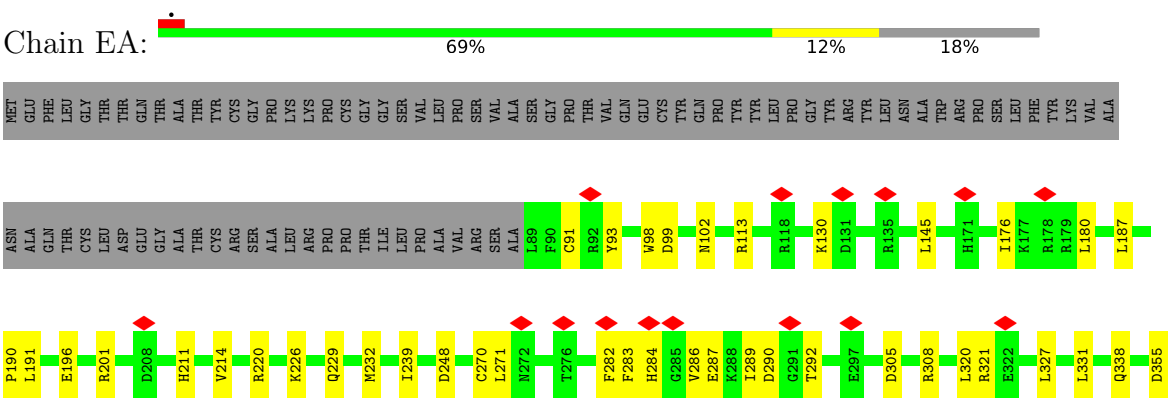




• Molecule 29: Tektin-5



• Molecule 29: Tektin-5

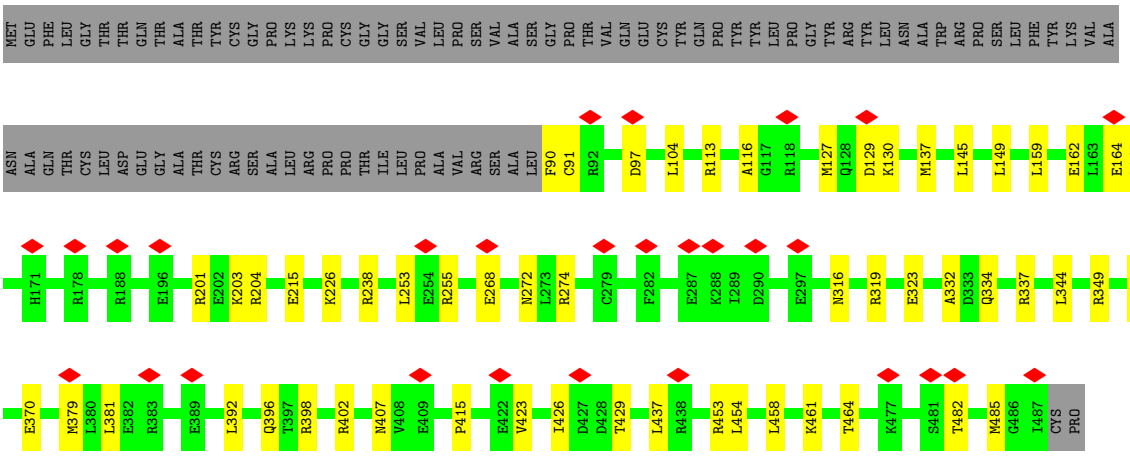




• Molecule 29: Tektin-5

Chain EO:

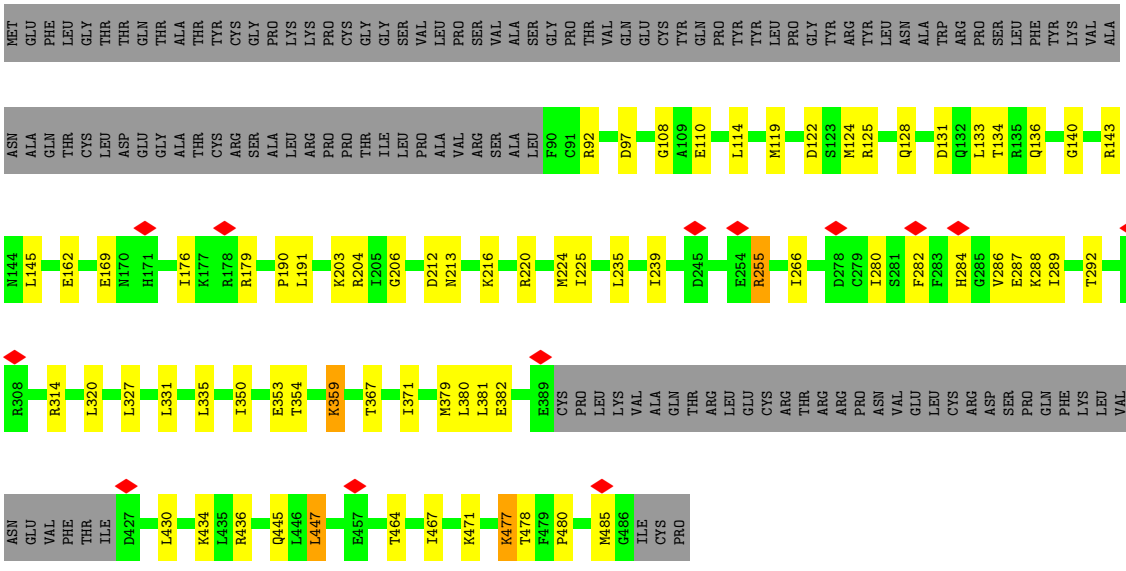




• Molecule 29: Tektin-5

Chain EP:

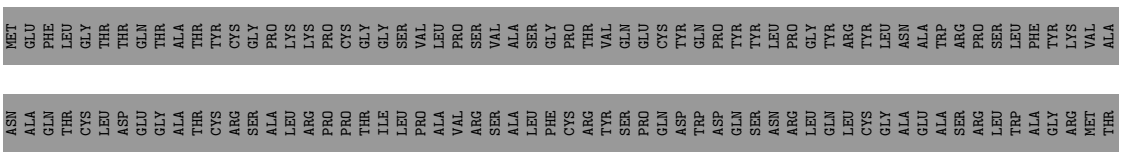


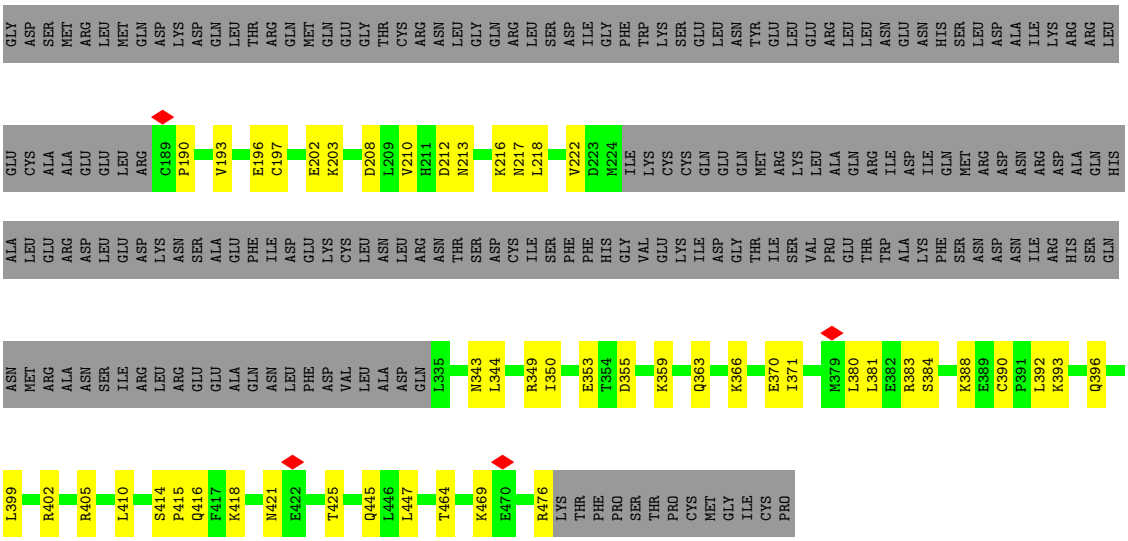


• Molecule 29: Tektin-5

Chain EQ:



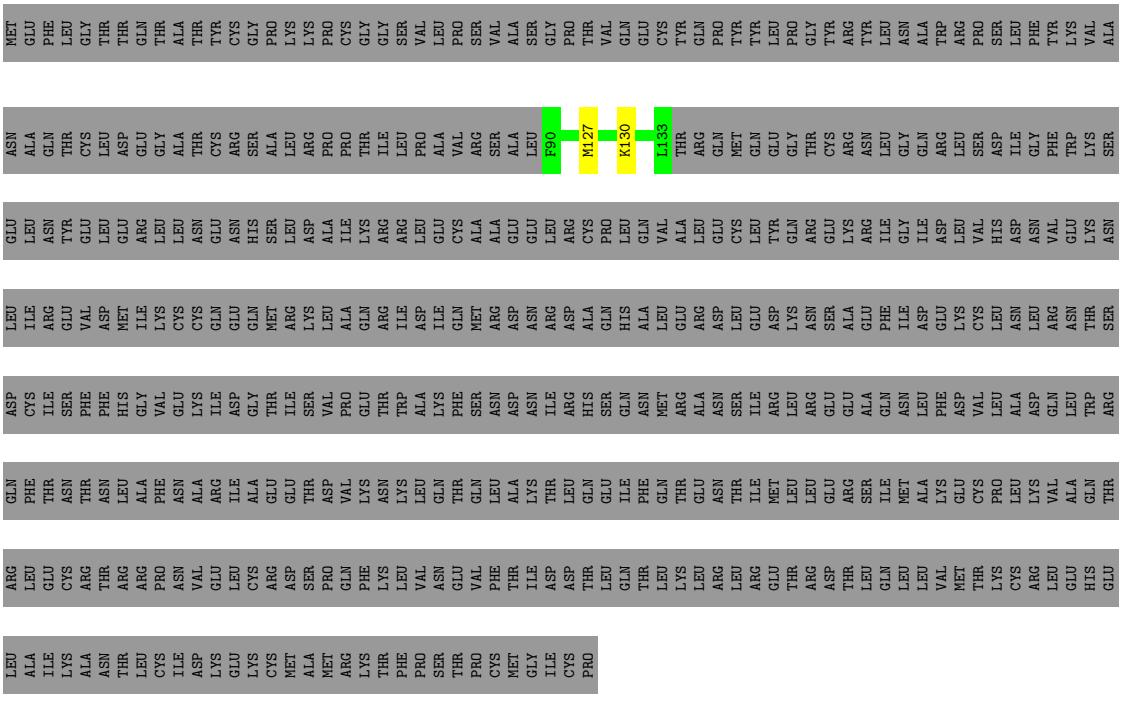




• Molecule 29: Tektin-5

Chain ER:

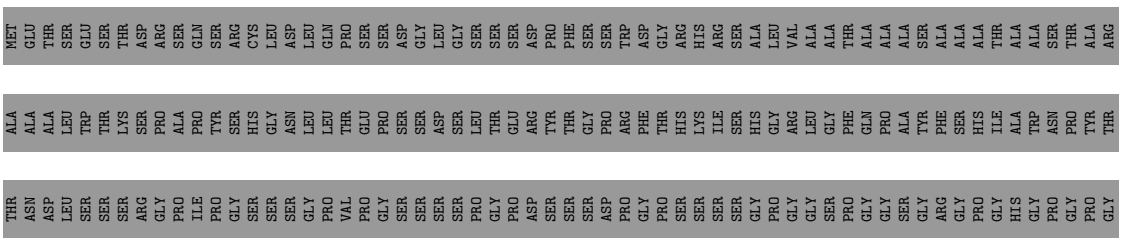


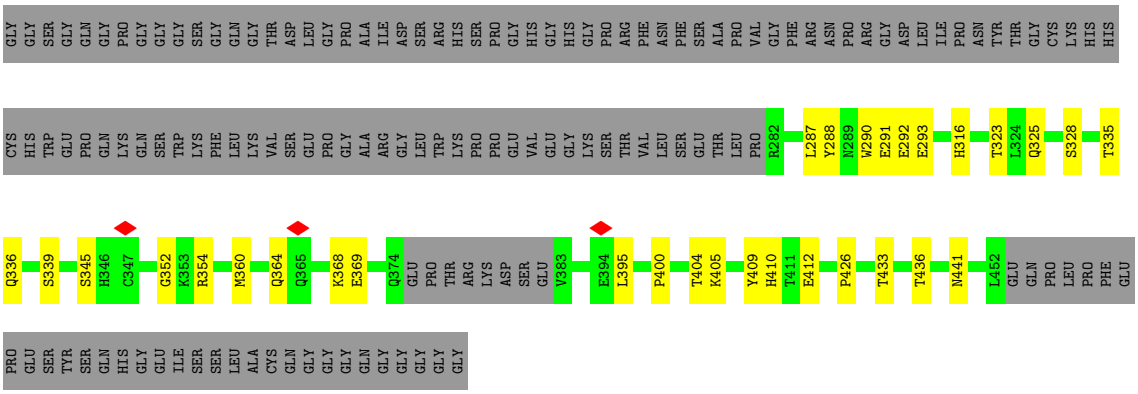


• Molecule 30: Sperm-associated antigen 8

Chain CW:



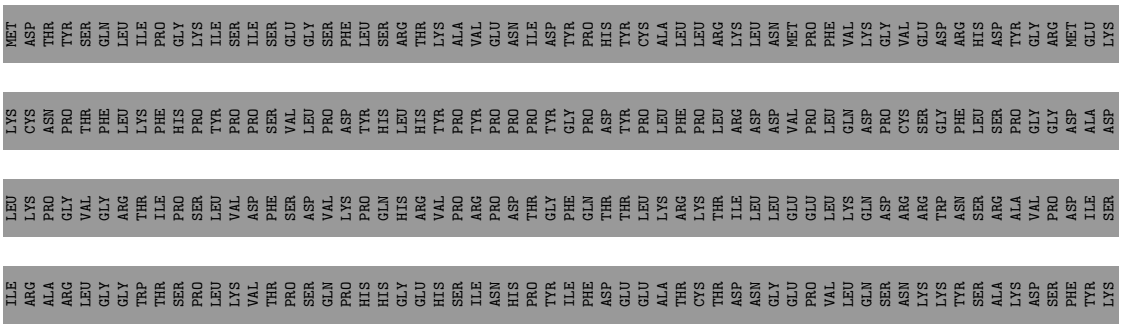




• Molecule 31: Spermatogenesis-associated protein 48

Chain Cl:

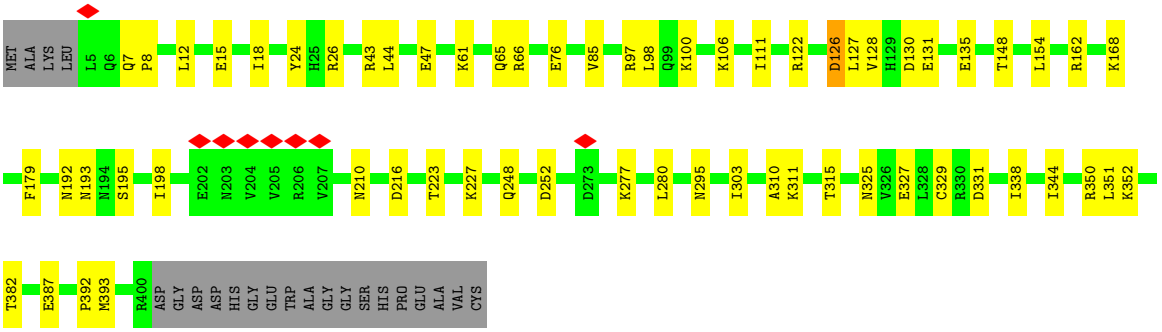




• Molecule 32: Tektin-1

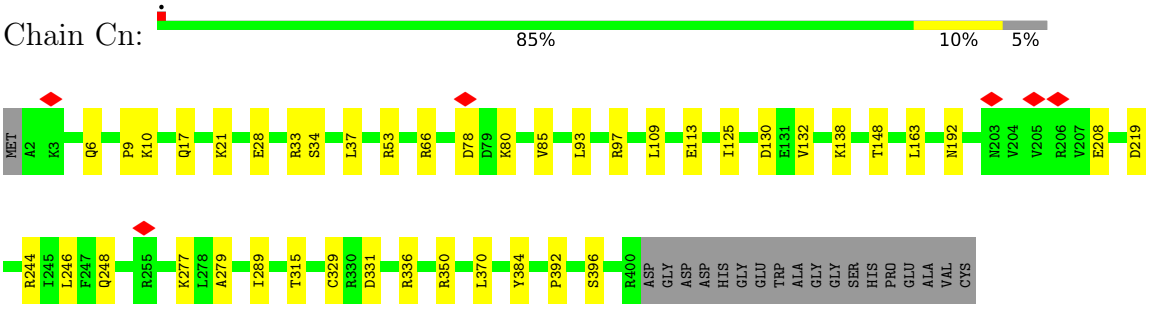
Chain Cm:





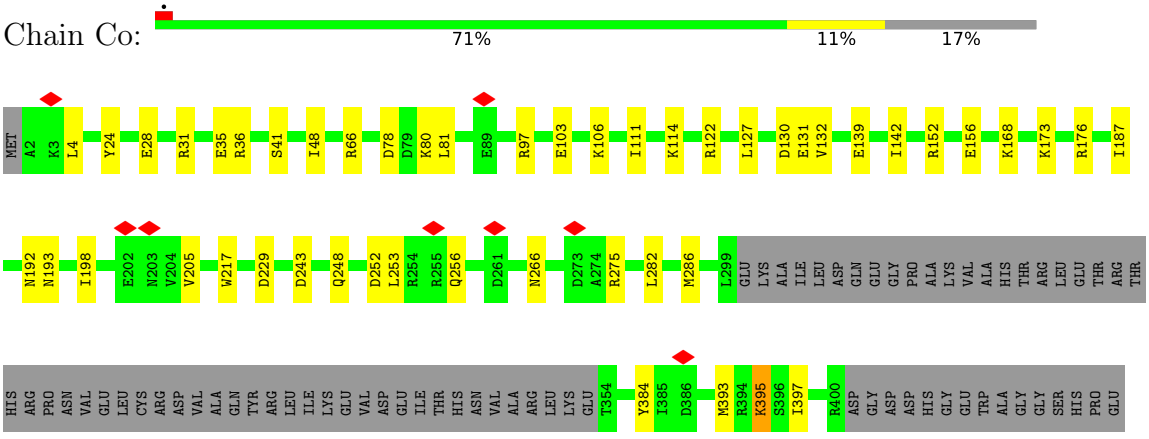
• Molecule 32: Tektin-1

Chain Cn:



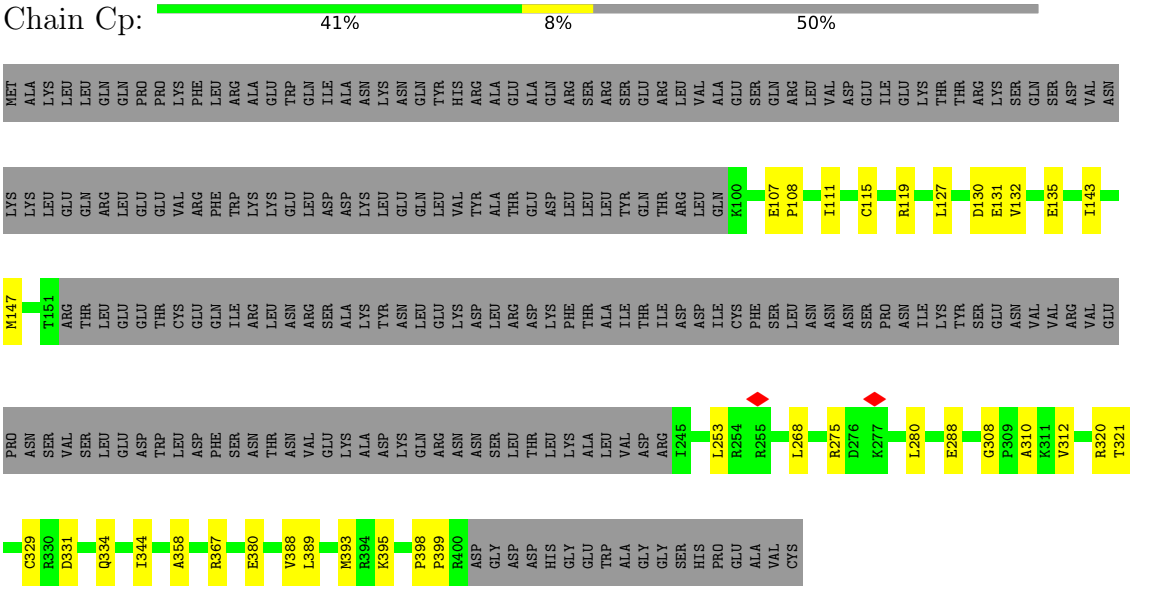
• Molecule 32: Tektin-1

Chain Co:



• Molecule 32: Tektin-1

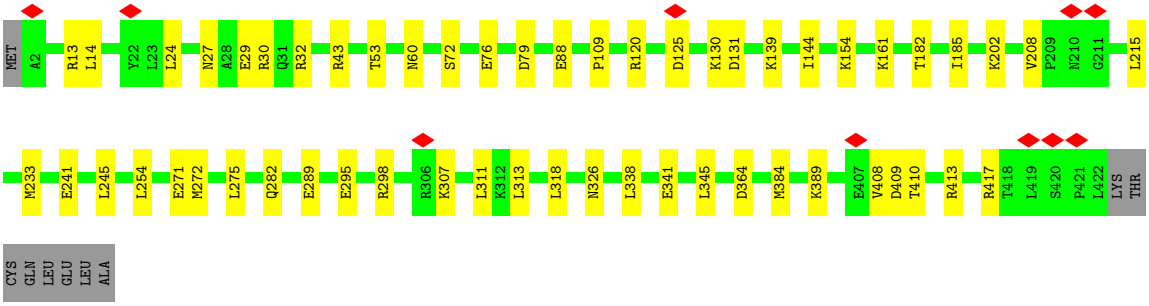
Chain Cp:



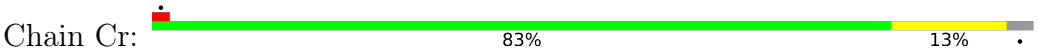
• Molecule 33: Tektin-2

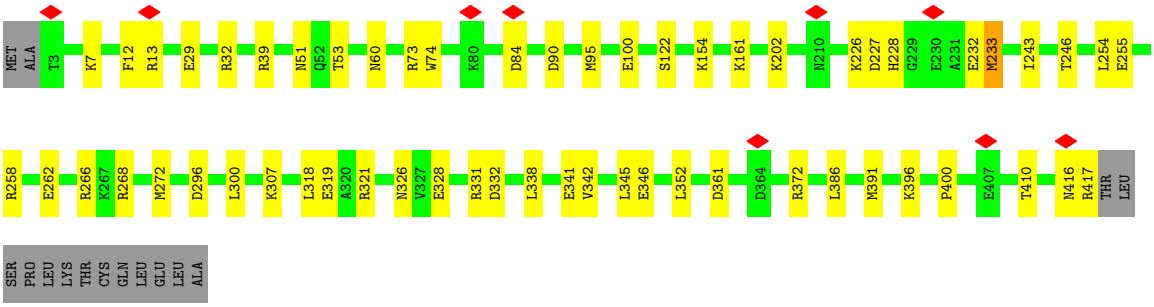
Chain Cq:



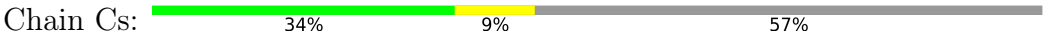


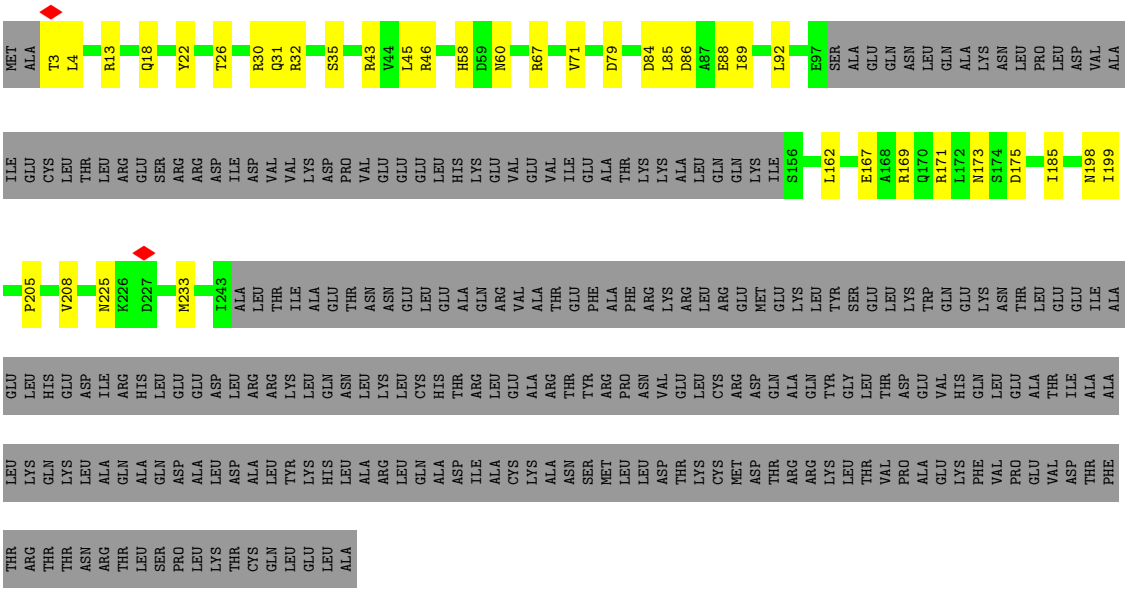
• Molecule 33: Tektin-2



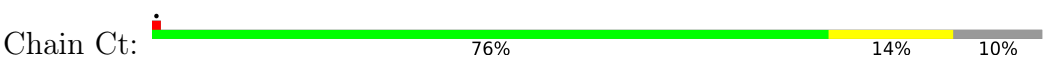


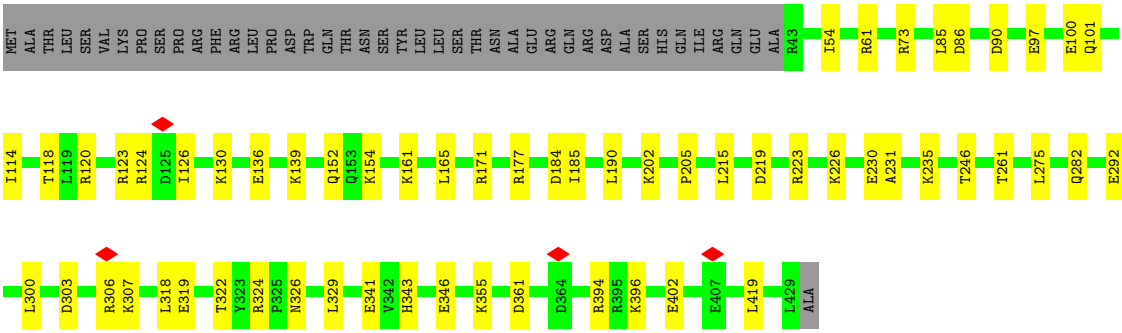
• Molecule 33: Tektin-2





• Molecule 33: Tektin-2

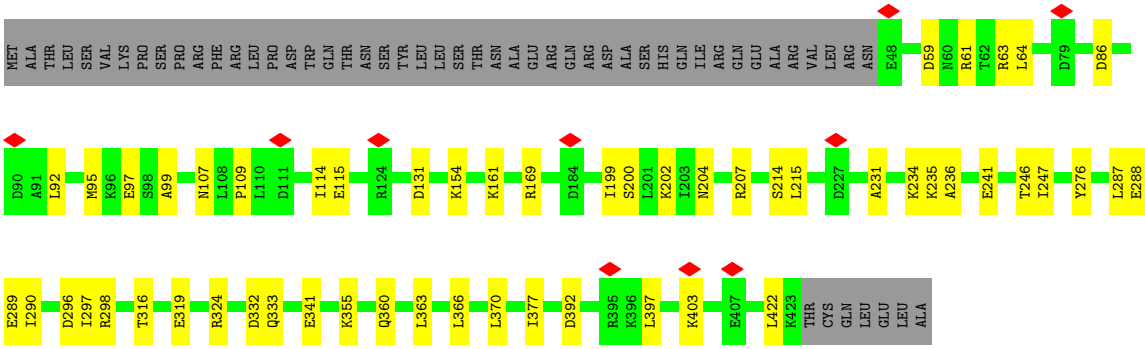




• Molecule 33: Tektin-2

Chain Cu:

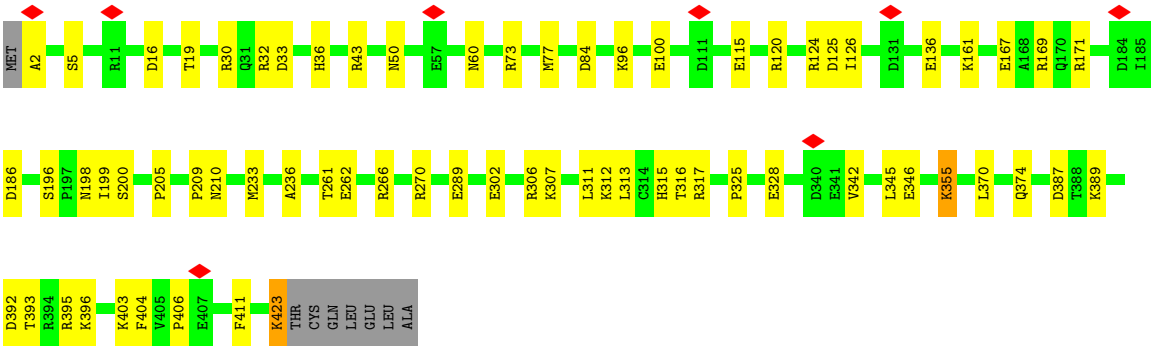




• Molecule 33: Tektin-2

Chain Cv:

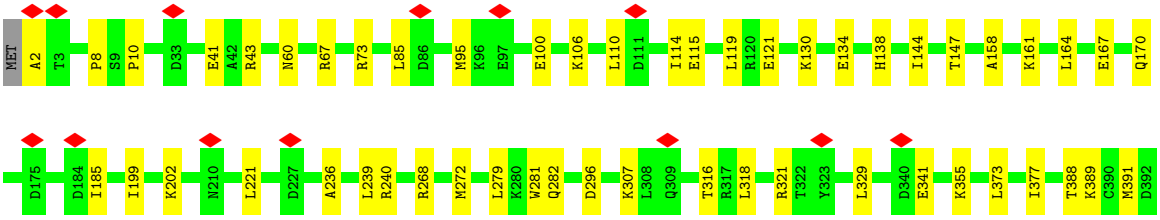


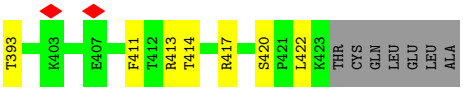


• Molecule 33: Tektin-2

Chain Cw:



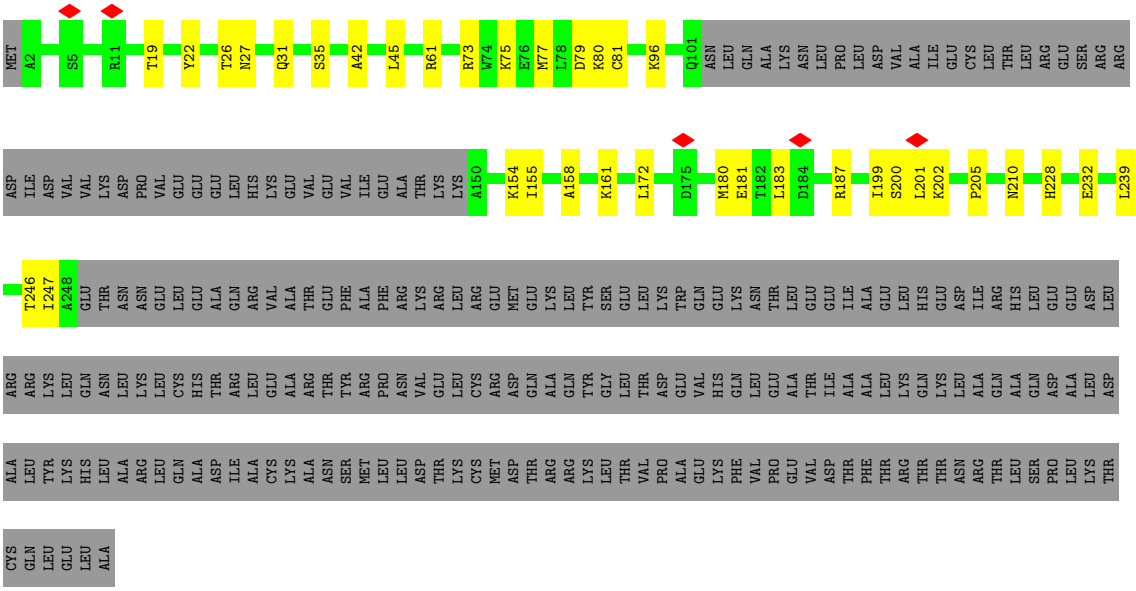




• Molecule 33: Tektin-2

Chain Cx:

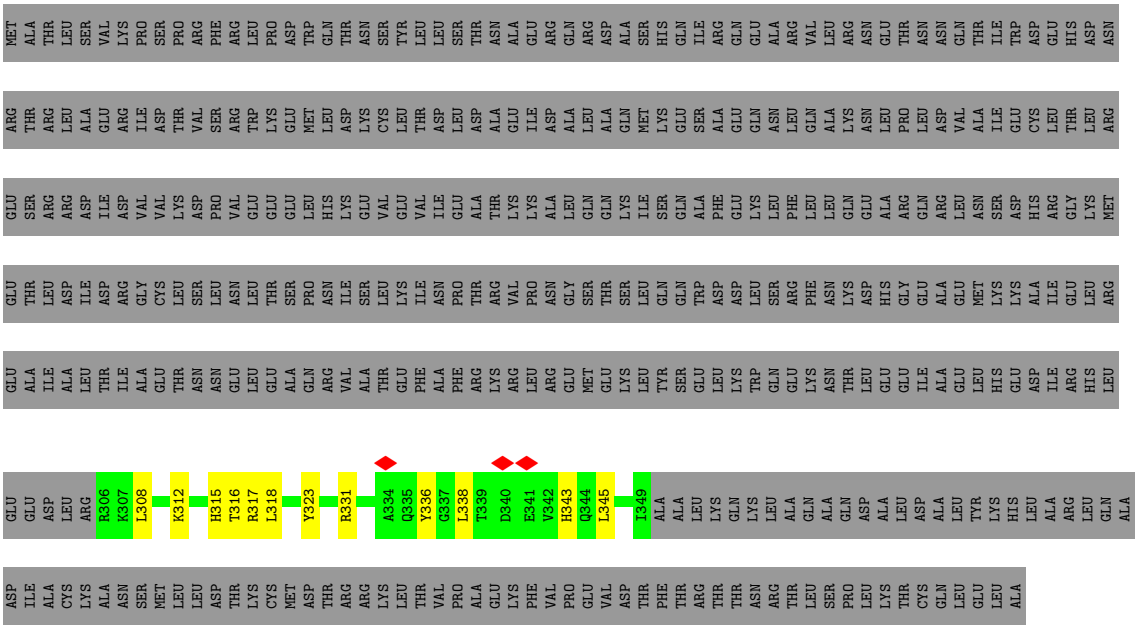




• Molecule 33: Tektin-2

Chain Cy:

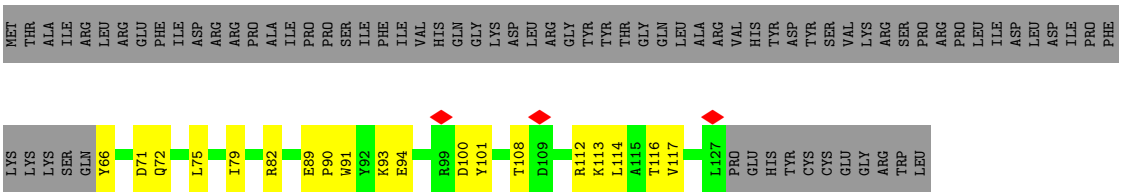




• Molecule 34: Uncharacterized protein C1orf100 homolog

Chain D:

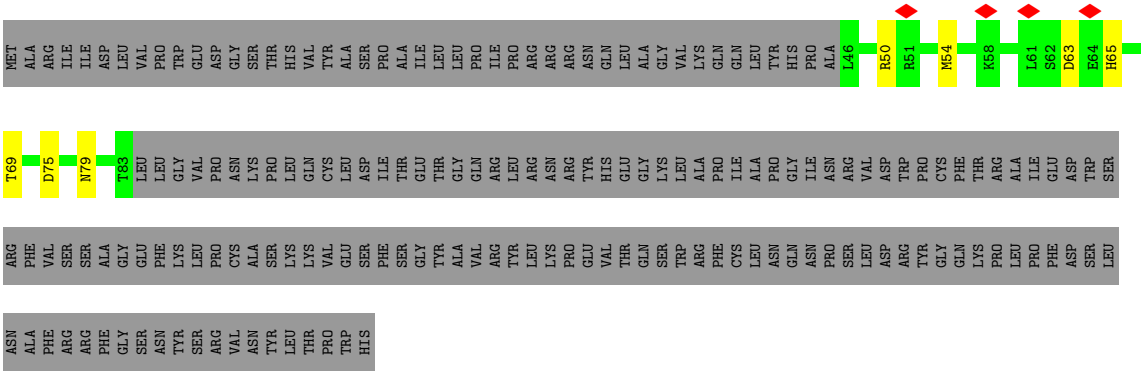




• Molecule 35: TEPP protein

Chain DY:

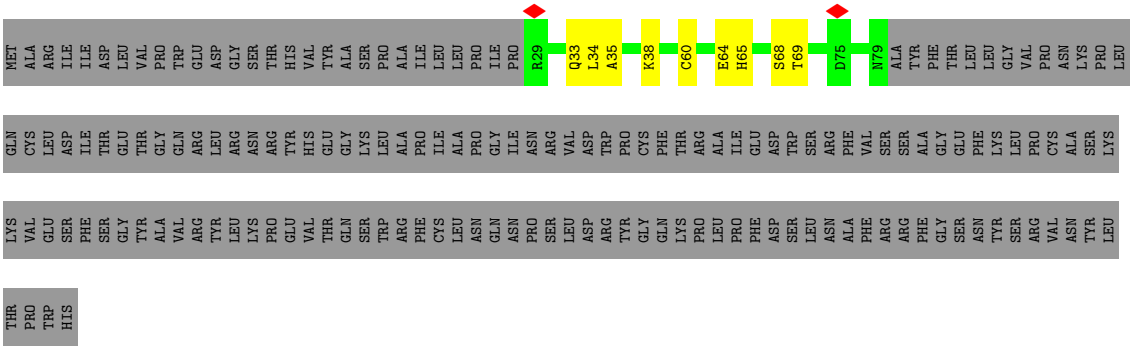




• Molecule 35: TEPP protein

Chain DZ:

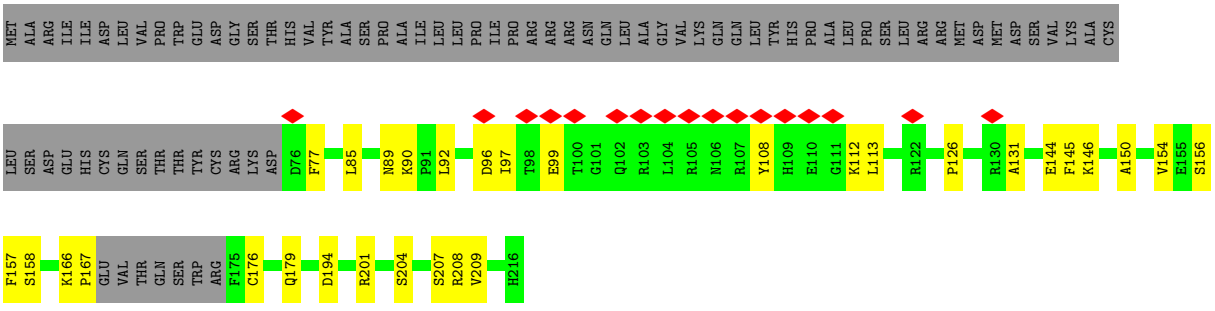




• Molecule 35: TEPP protein

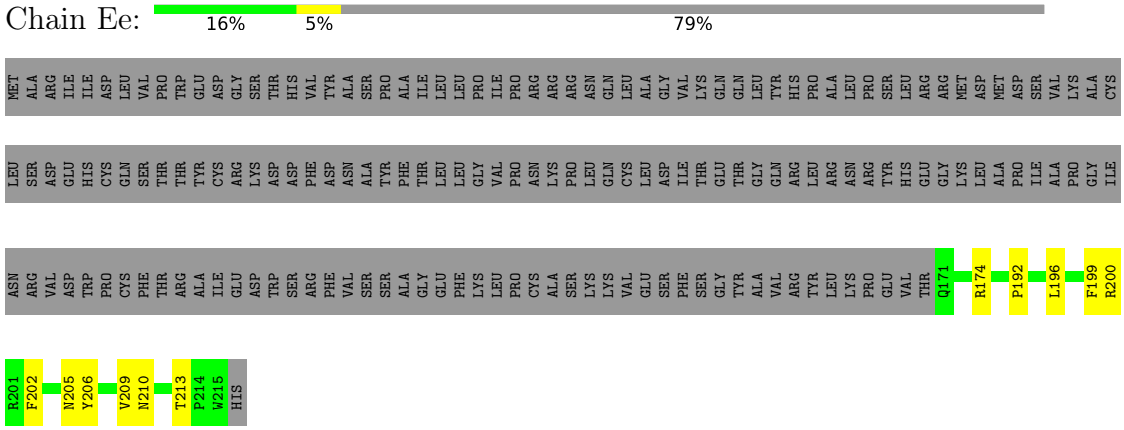
Chain Da:





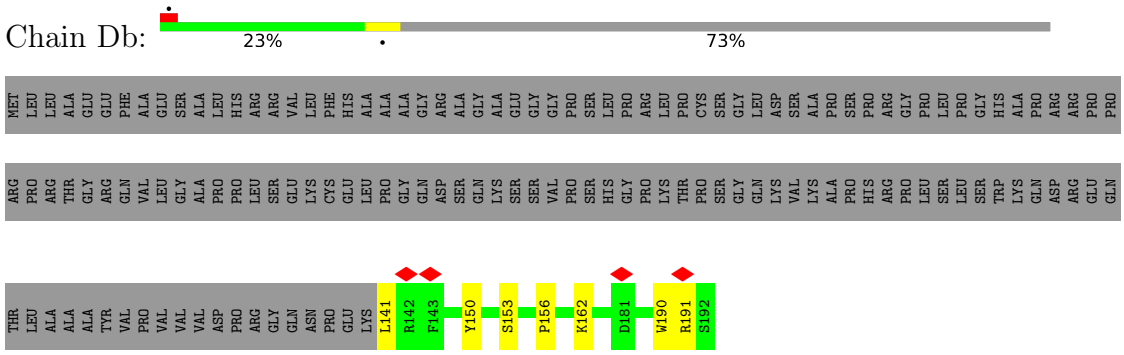
• Molecule 35: TEPP protein

Chain Ee:



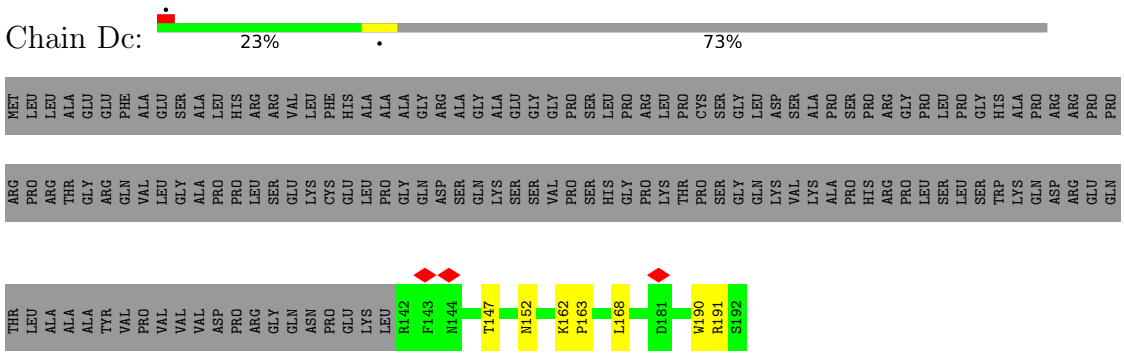
• Molecule 36: Uncharacterized protein MGC137036

Chain Db:



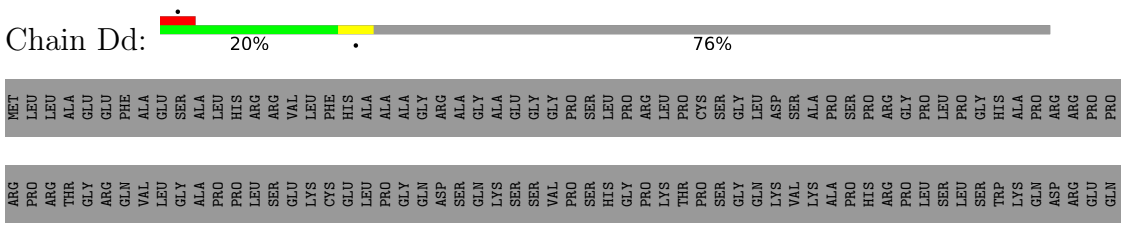
• Molecule 36: Uncharacterized protein MGC137036

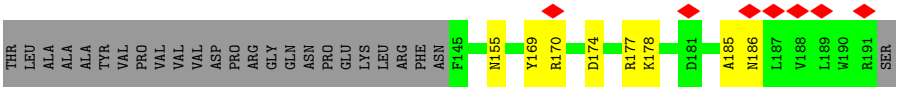
Chain Dc:



• Molecule 36: Uncharacterized protein MGC137036

Chain Dd:

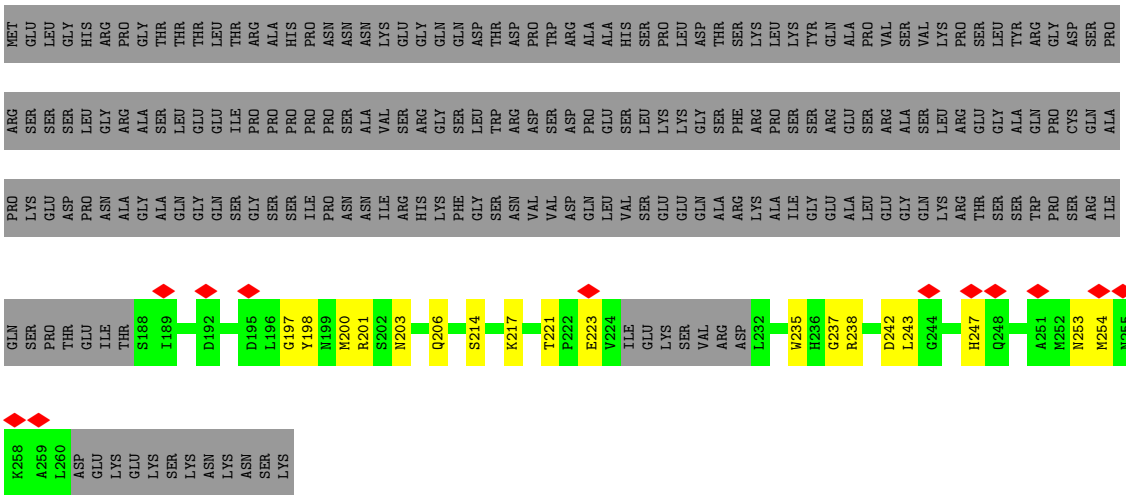




• Molecule 37: Testis expressed 33

Chain De:

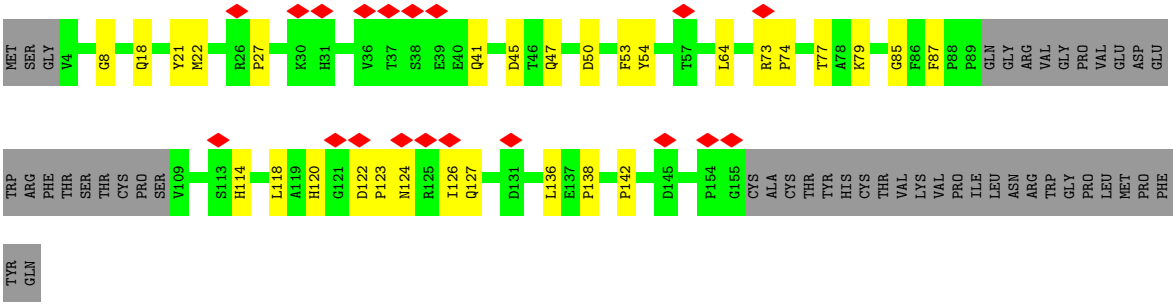




• Molecule 38: Testis-expressed sequence 37 protein

Chain Df:

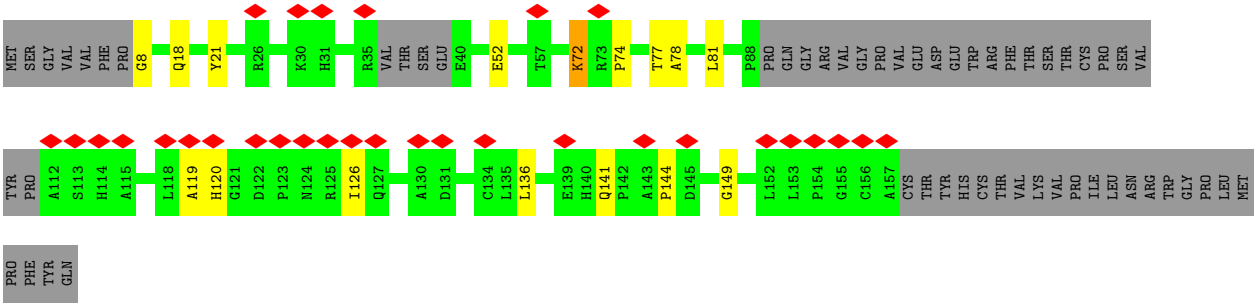




• Molecule 38: Testis-expressed sequence 37 protein

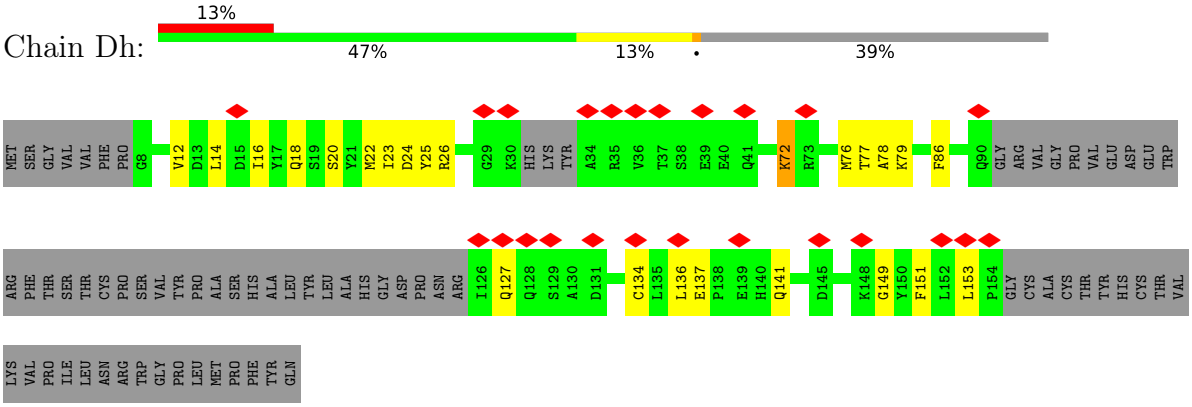
Chain Dg:





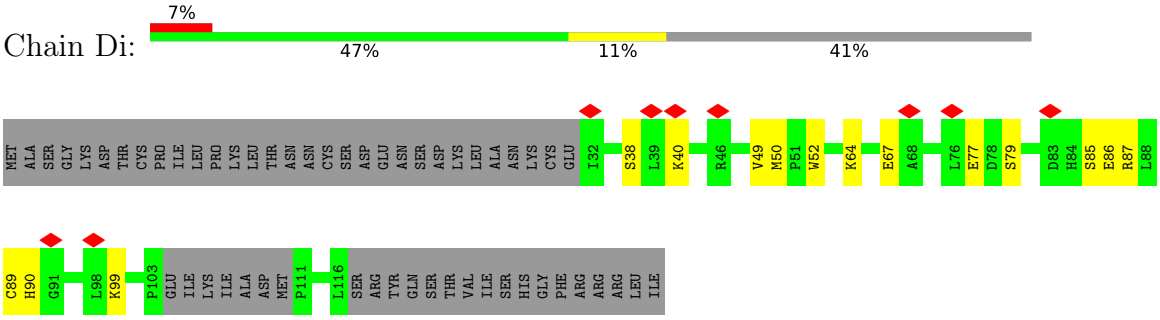
• Molecule 38: Testis-expressed sequence 37 protein

Chain Dh:



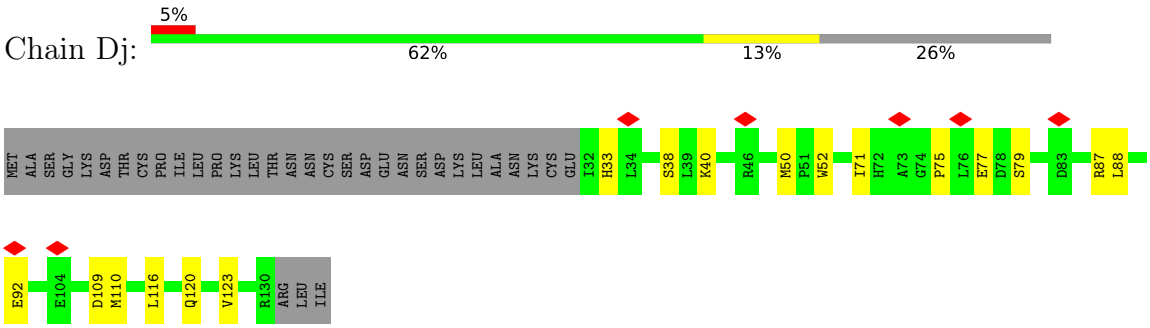
• Molecule 39: Testis-expressed protein 43

Chain Di:



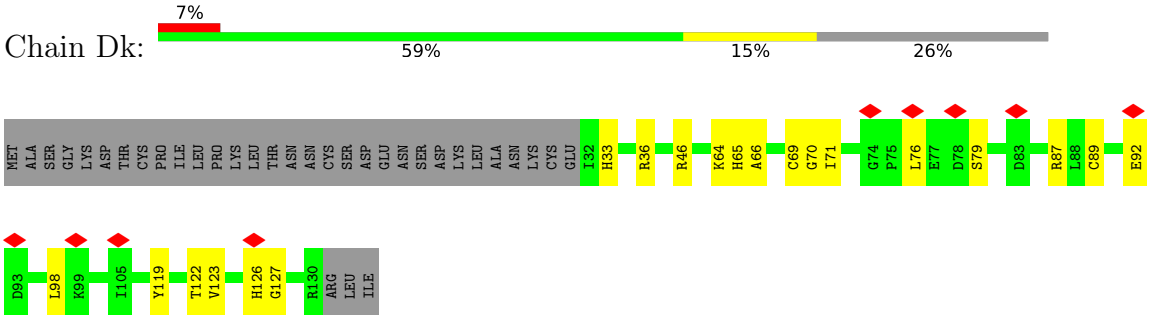
• Molecule 39: Testis-expressed protein 43

Chain Dj:



• Molecule 39: Testis-expressed protein 43

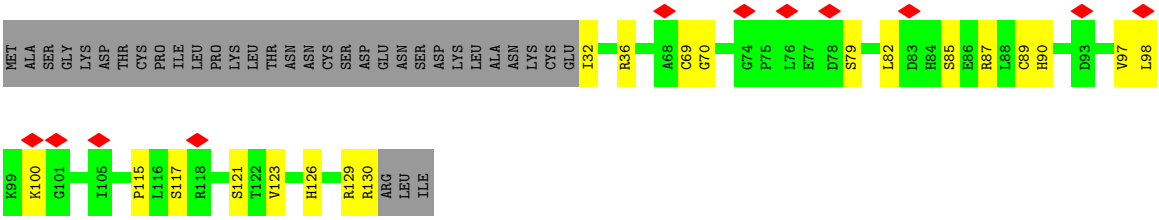
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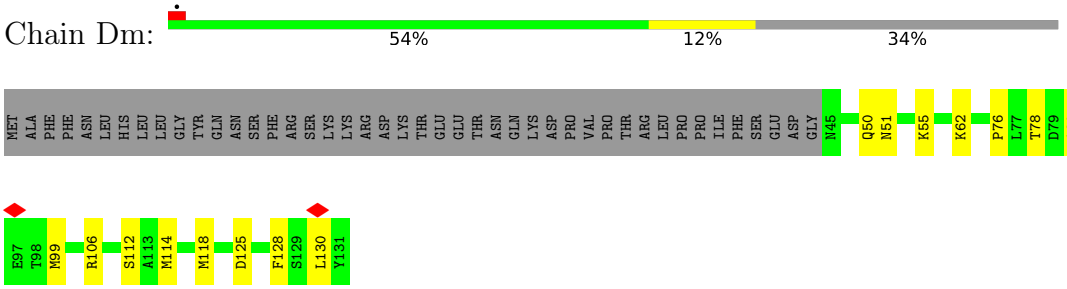
• Molecule 39: Testis-expressed protein 43

Chain Dl:

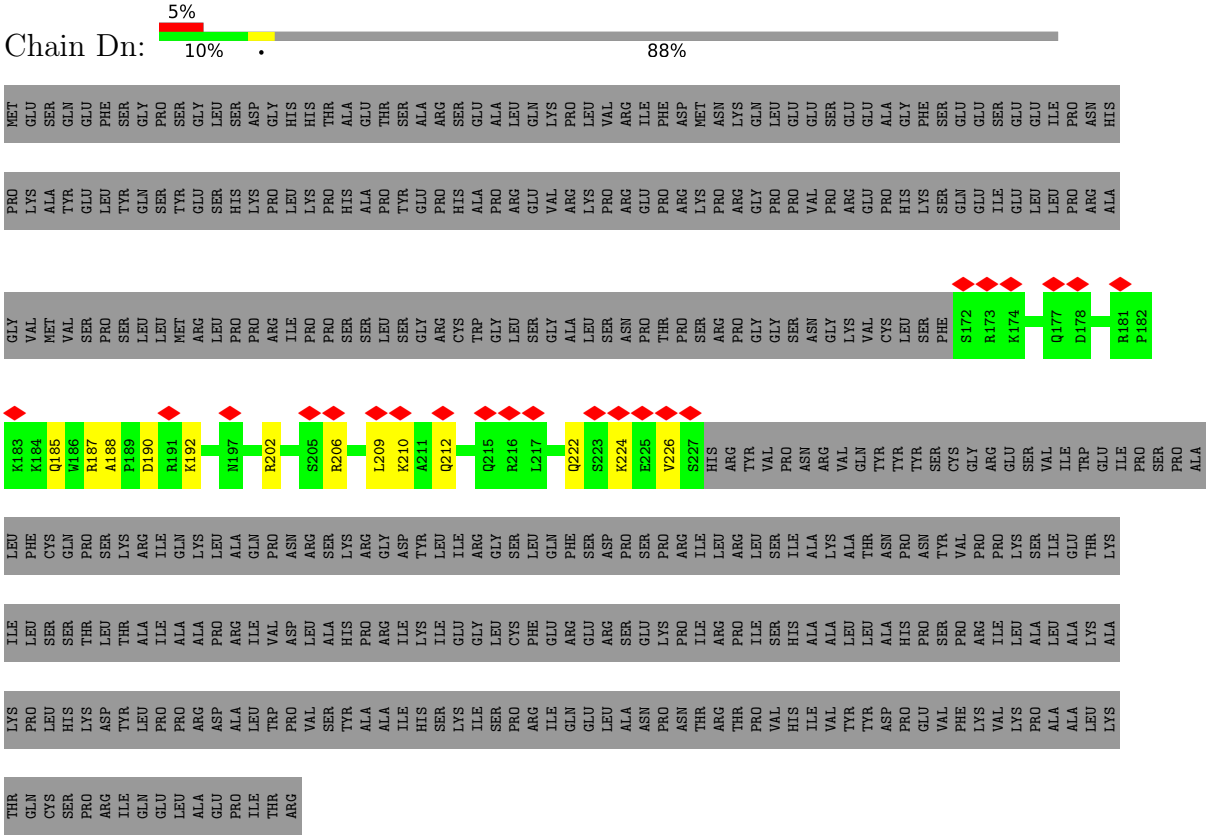




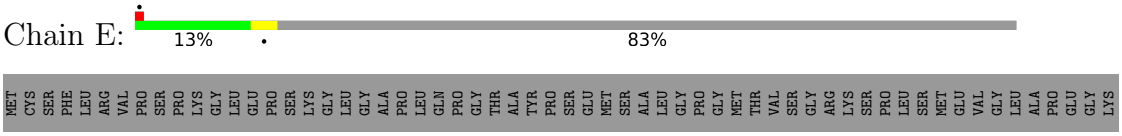
• Molecule 40: Testis expressed 49

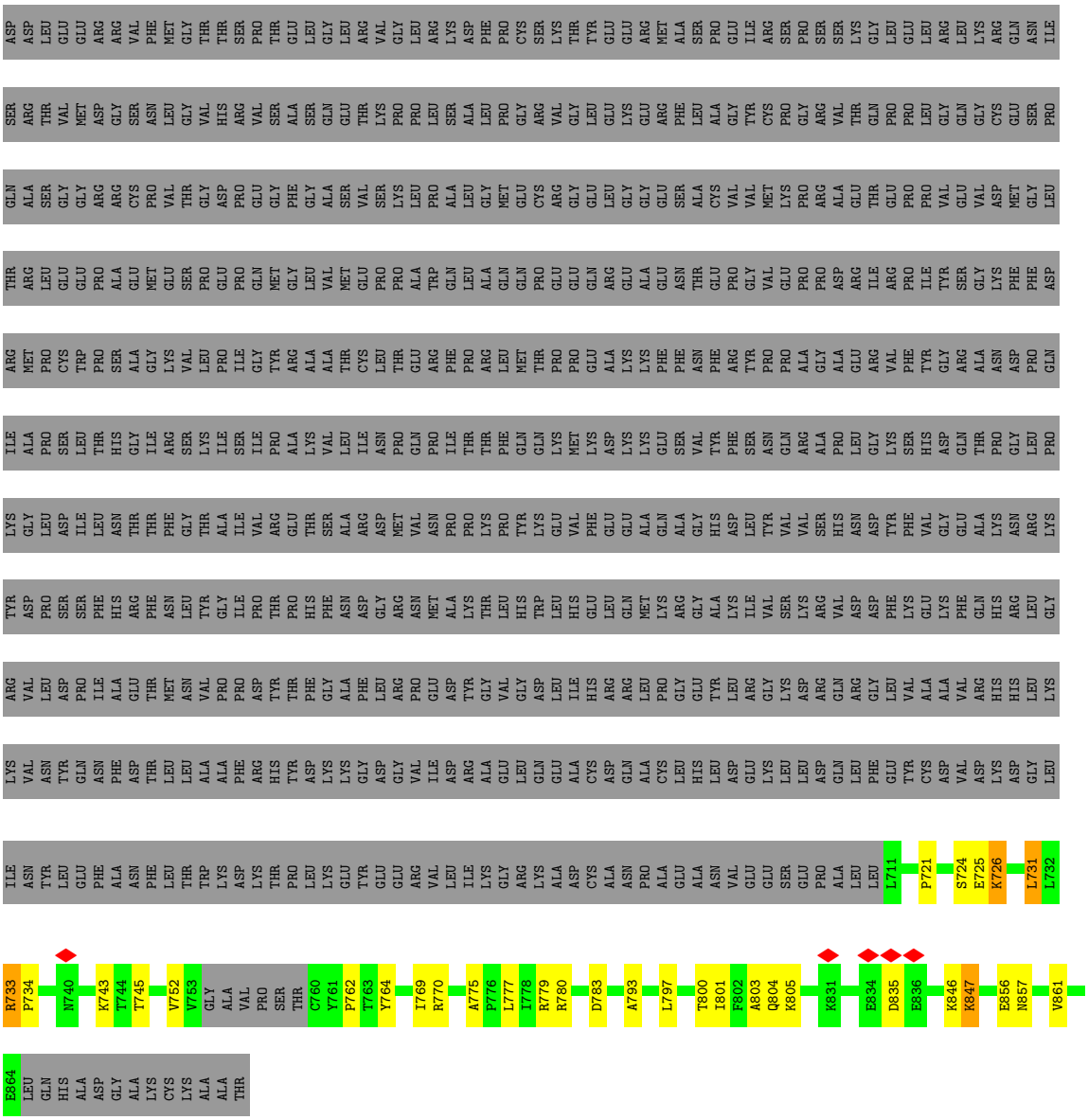


• Molecule 41: Theg spermatid protein like



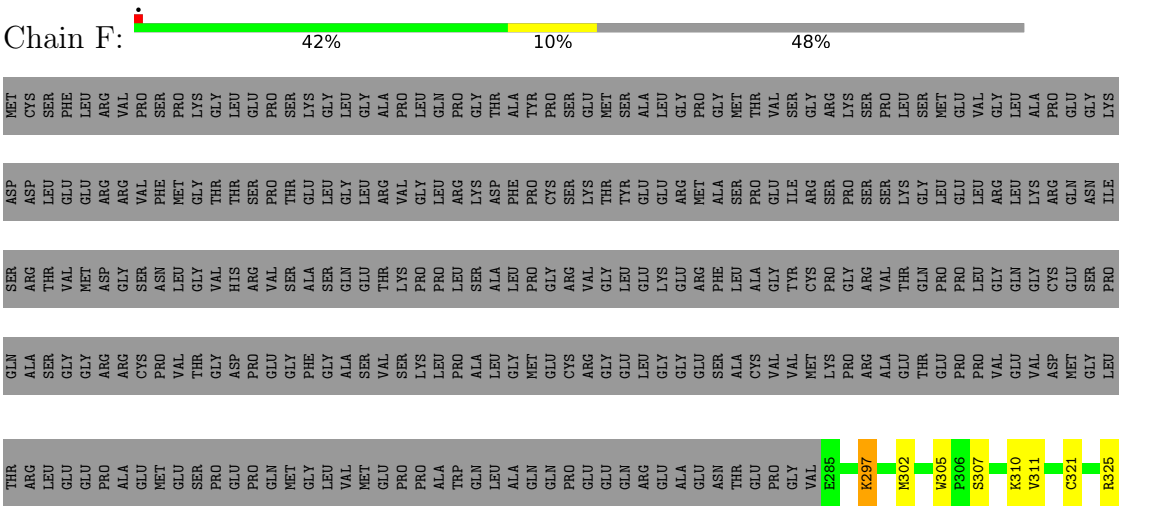
• Molecule 42: EF-hand domain-containing family member B

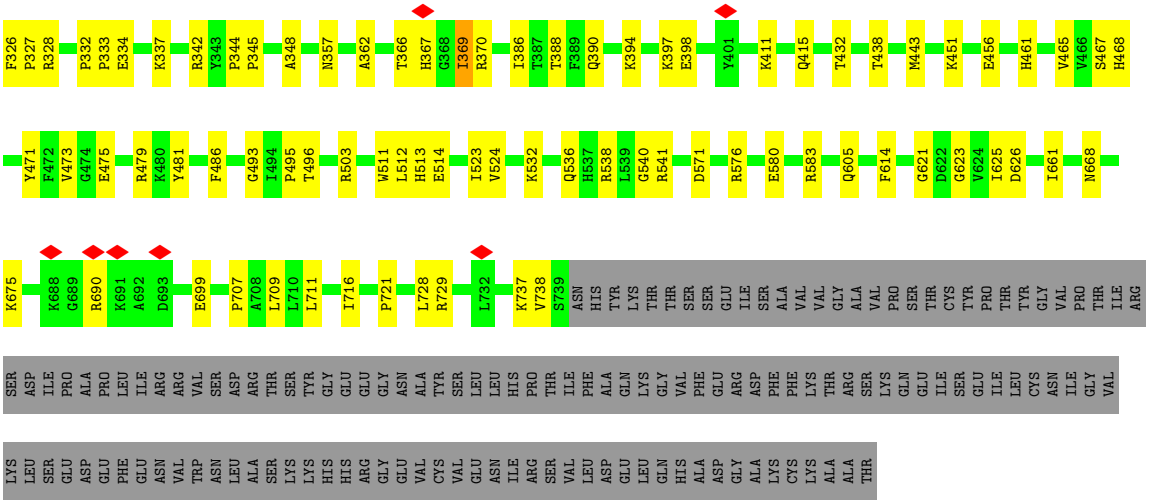




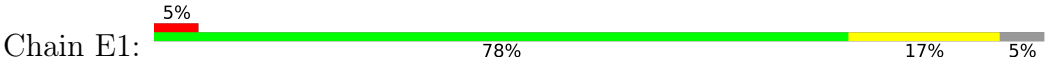
• Molecule 42: EF-hand domain-containing family member B

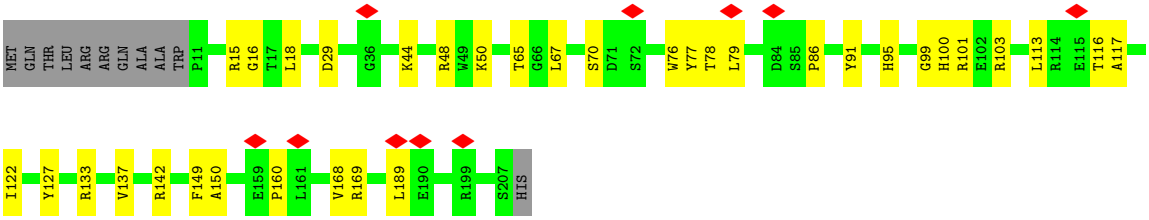
Chain F:



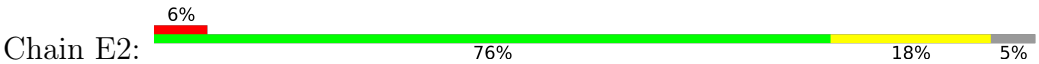


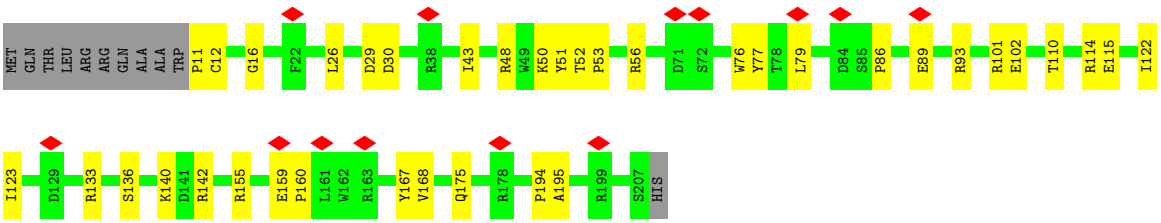
• Molecule 43: Tektin bundle interacting protein 1



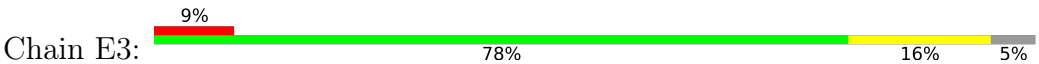


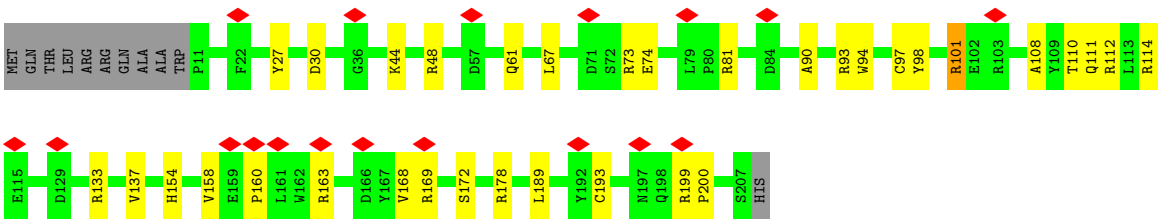
• Molecule 43: Tektin bundle interacting protein 1





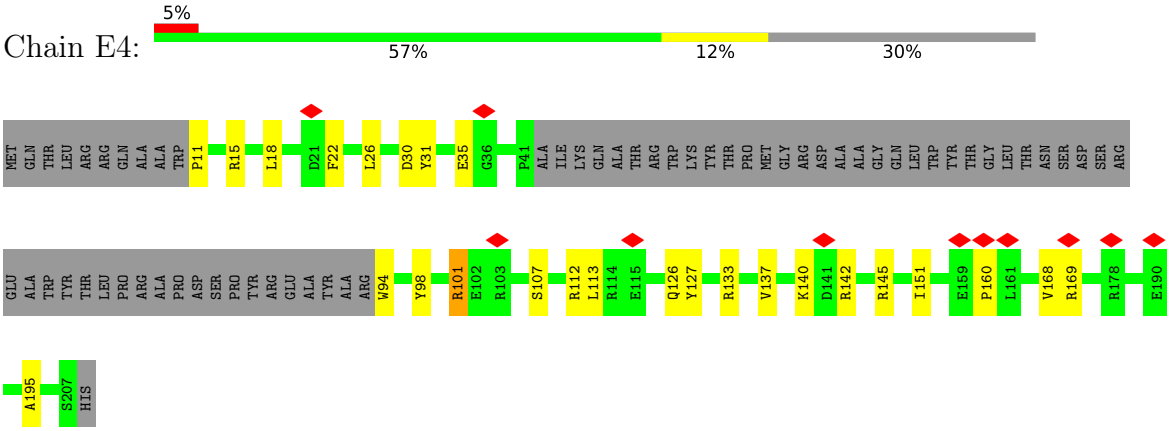
• Molecule 43: Tektin bundle interacting protein 1





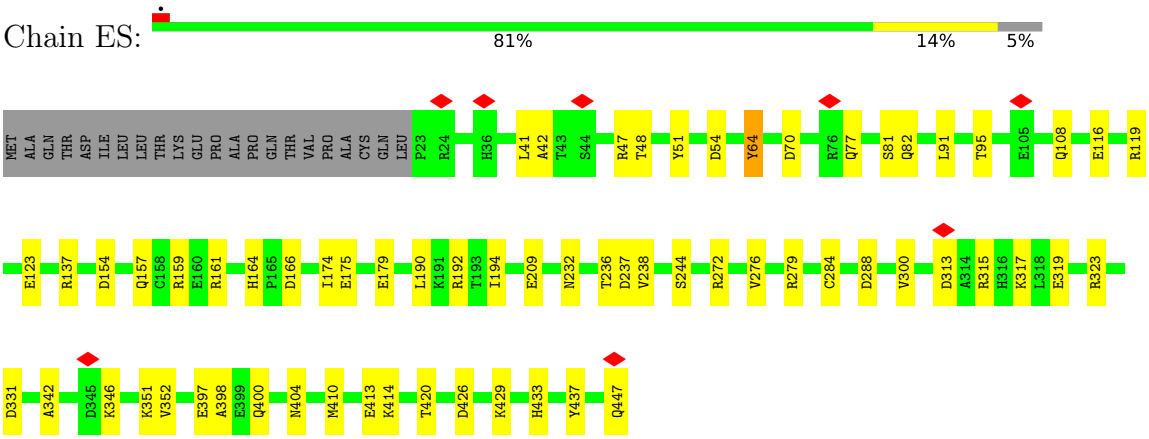
• Molecule 43: Tektin bundle interacting protein 1

Chain E4:



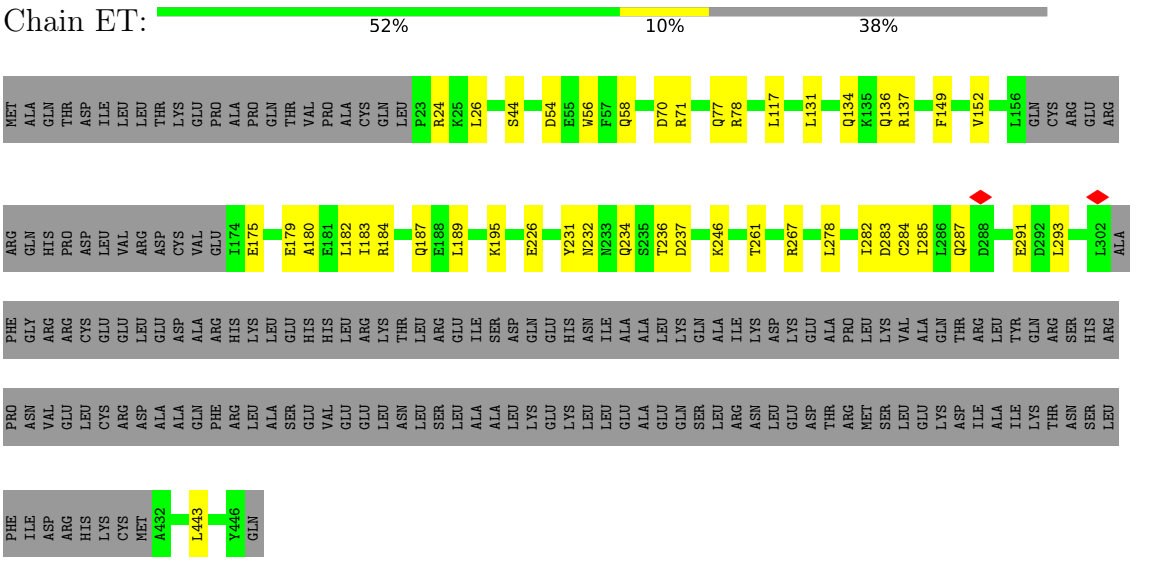
• Molecule 44: Tektin-4

Chain ES:



• Molecule 44: Tektin-4

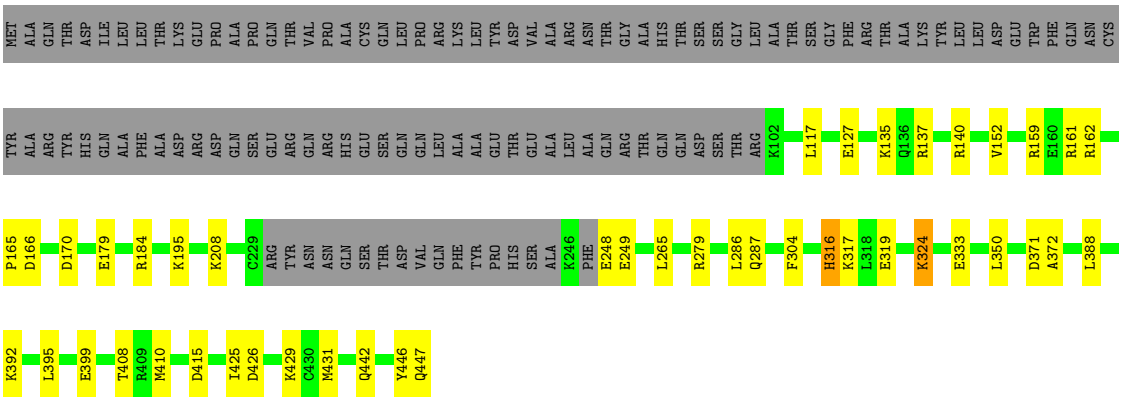
Chain ET:



• Molecule 44: Tektin-4

Chain EU:

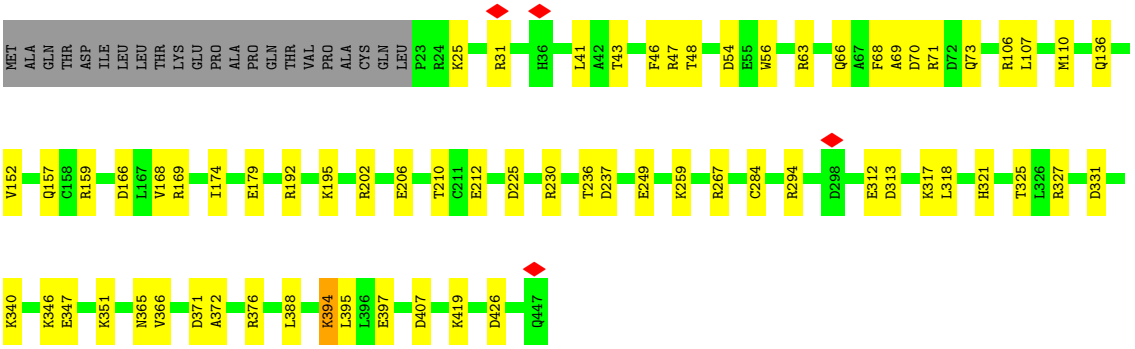




• Molecule 44: Tektin-4

Chain EV:

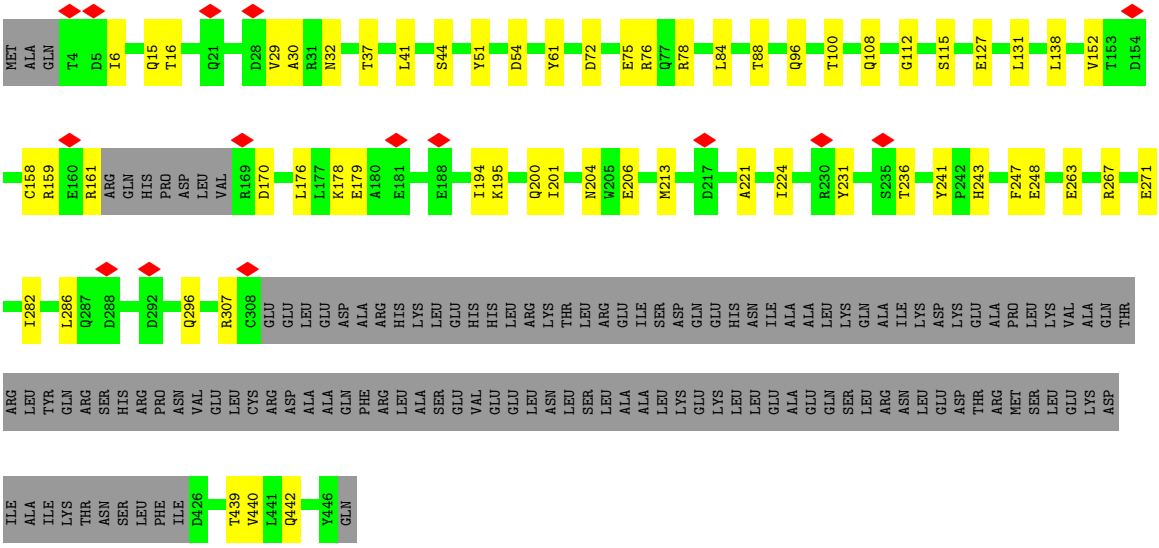




• Molecule 44: Tektin-4

Chain EW:

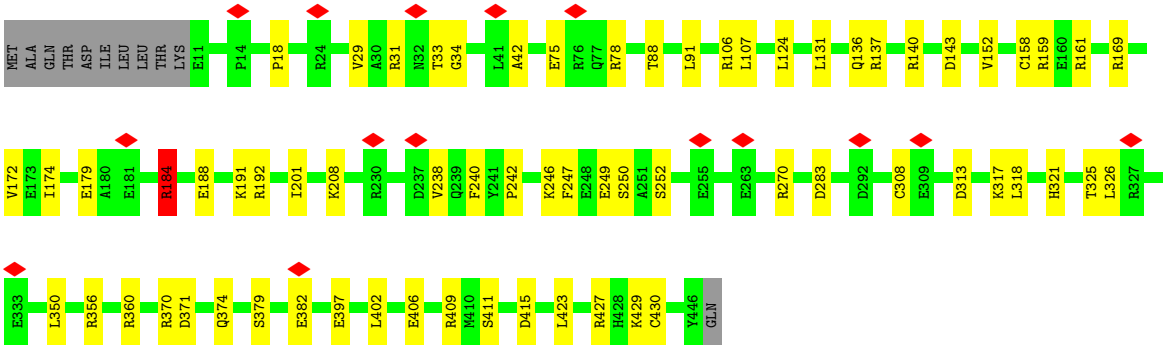




• Molecule 44: Tektin-4

Chain EX:

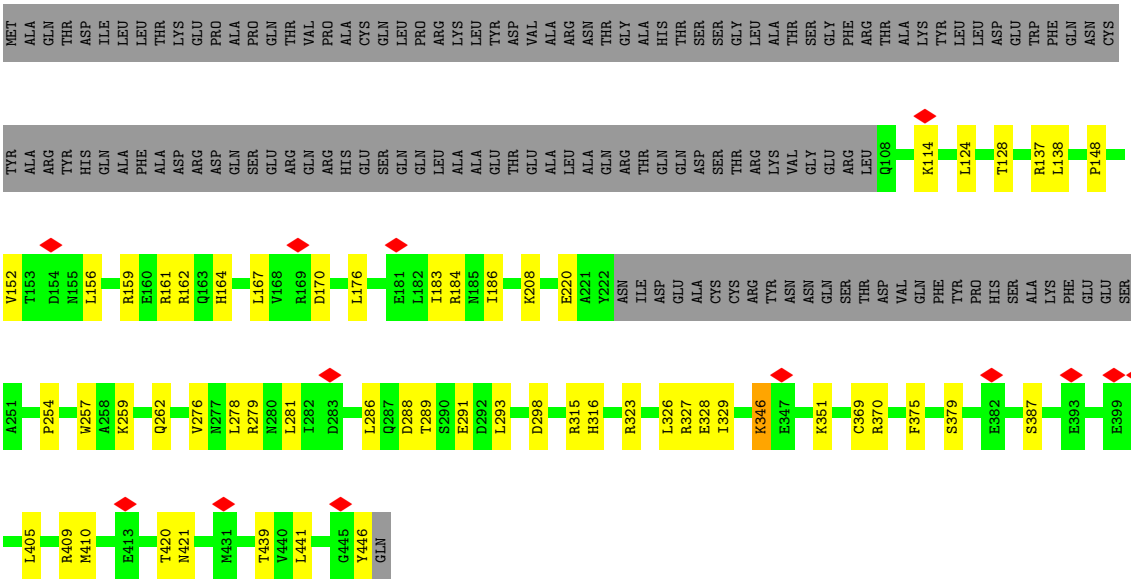




• Molecule 44: Tektin-4

Chain EY:

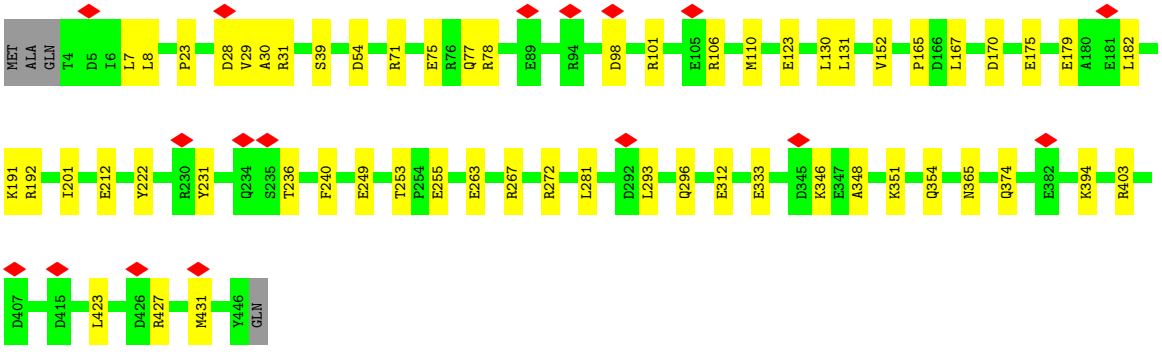




• Molecule 44: Tektin-4

Chain EZ:

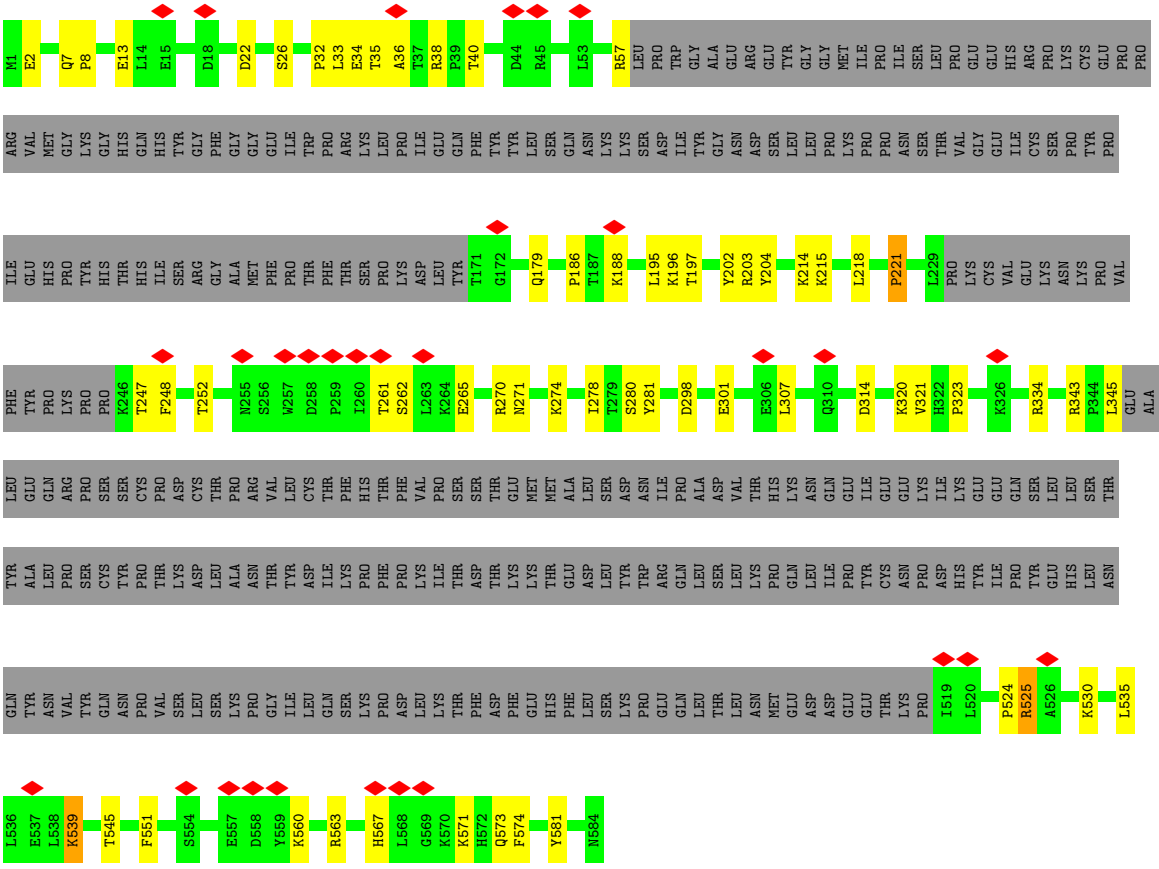




• Molecule 45: Chromosome 7 open reading frame 31

Chain G:

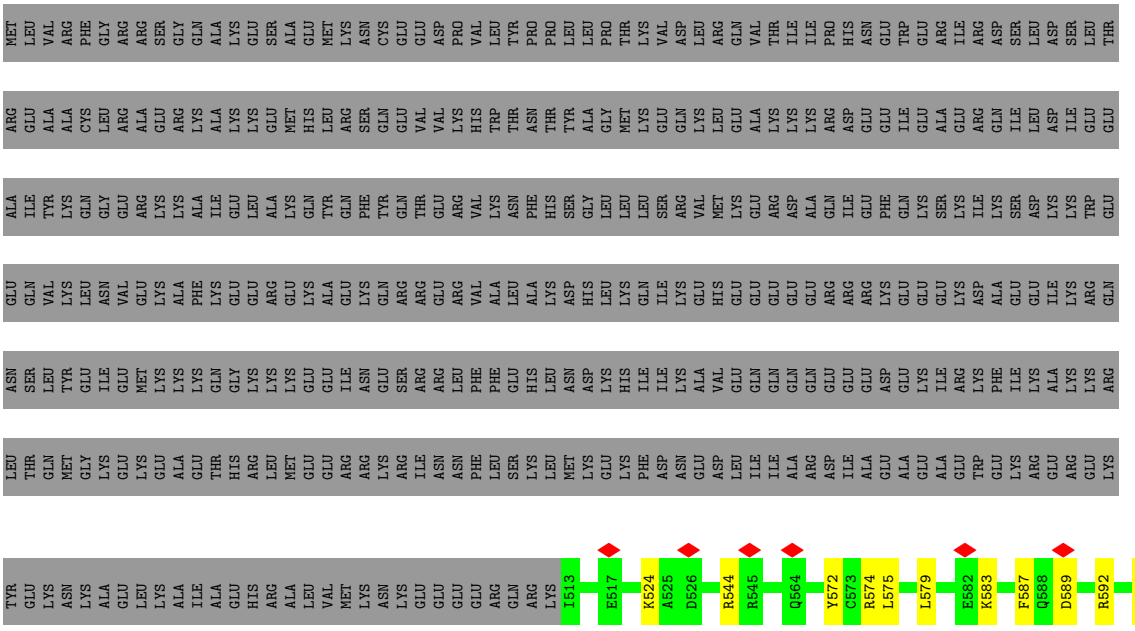


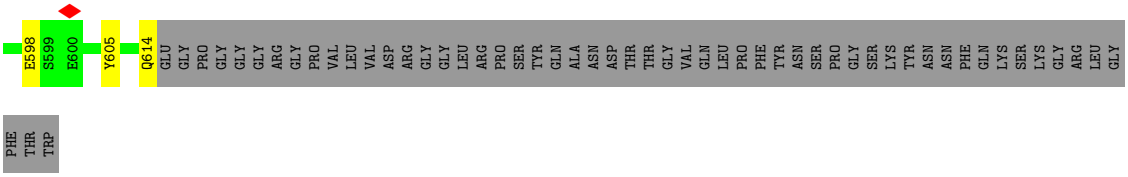


• Molecule 46: Cilia- and flagella- associated protein 210

Chain H:



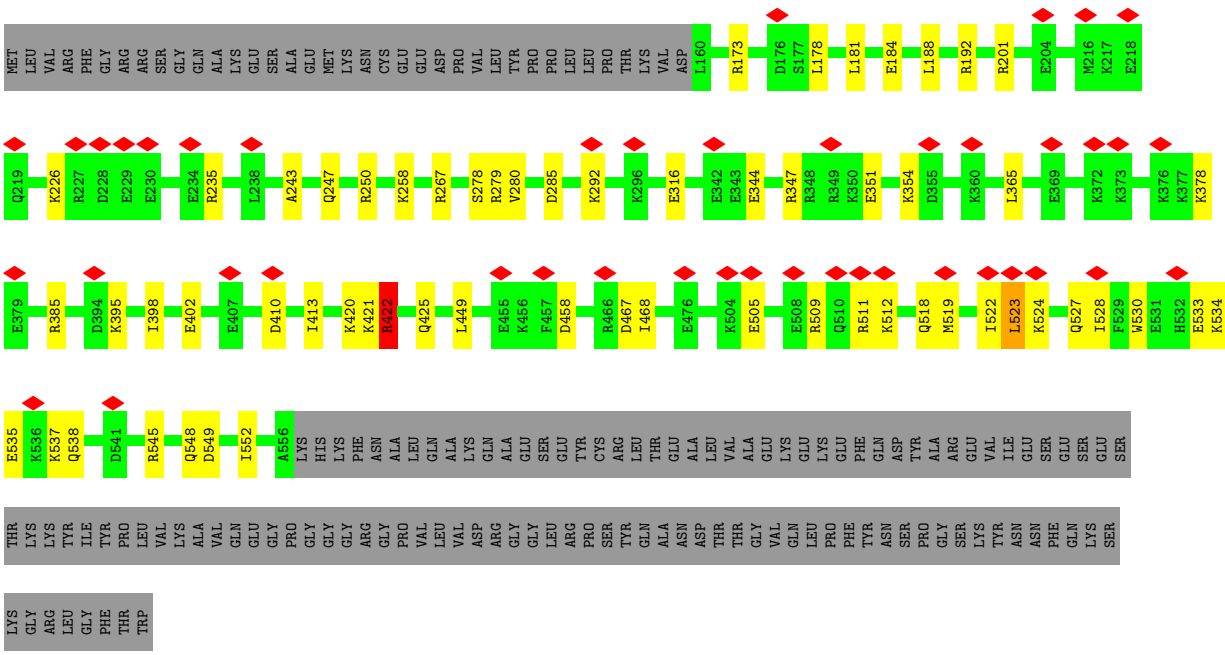




• Molecule 46: Cilia- and flagella- associated protein 210

Chain o:

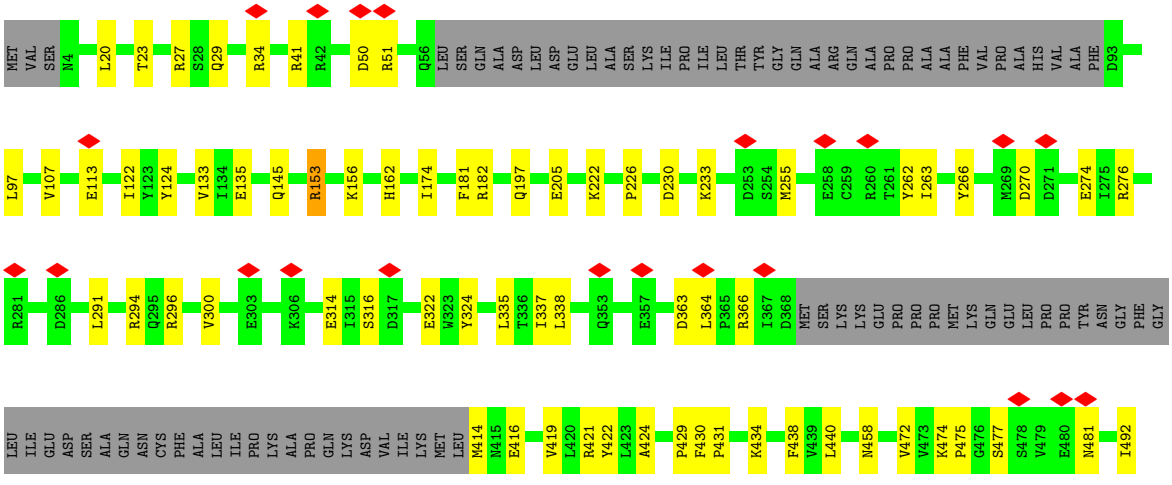


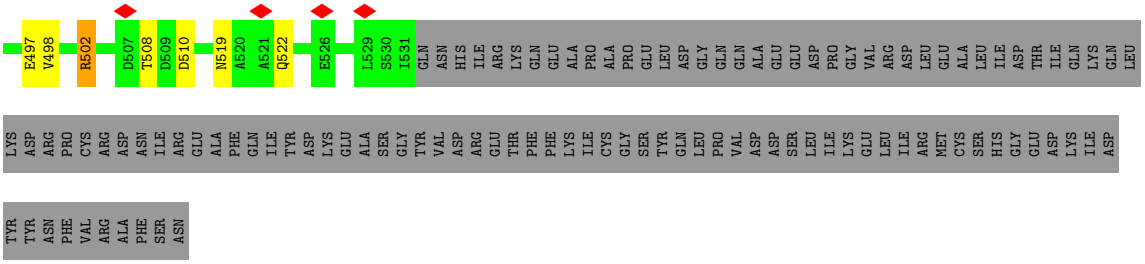


• Molecule 47: EF-hand domain-containing protein 1

Chain I:



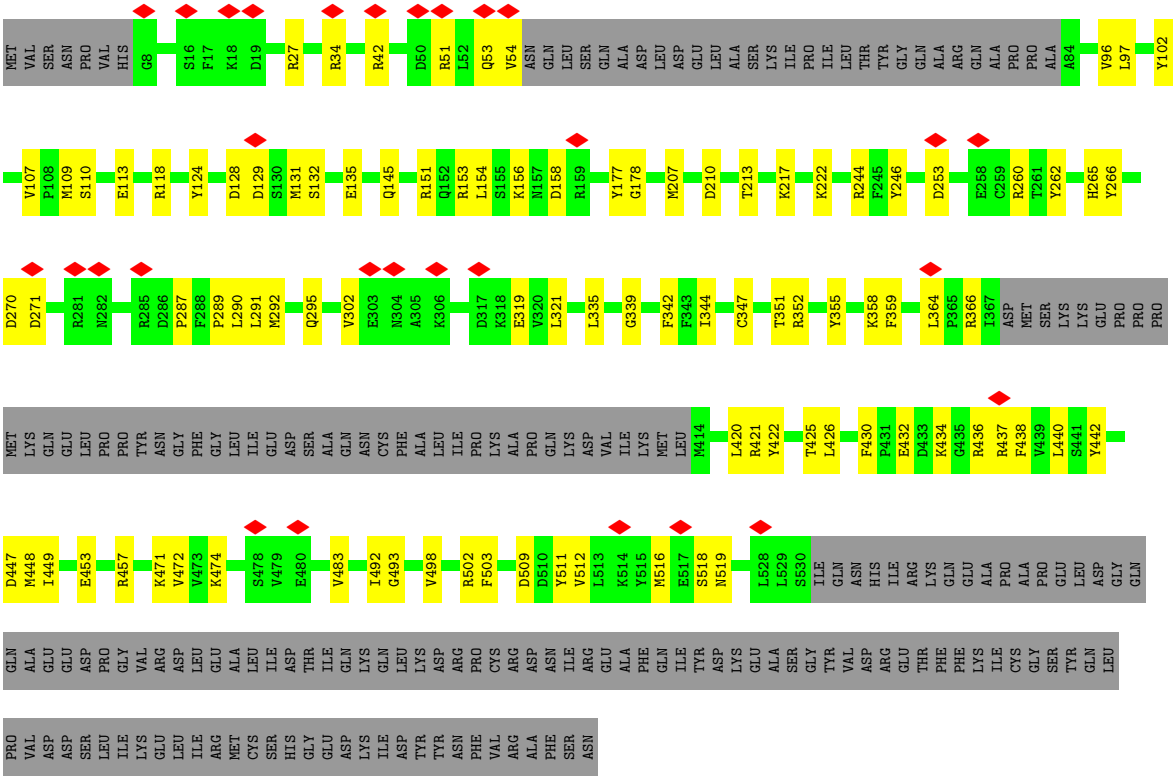




• Molecule 47: EF-hand domain-containing protein 1

Chain X:

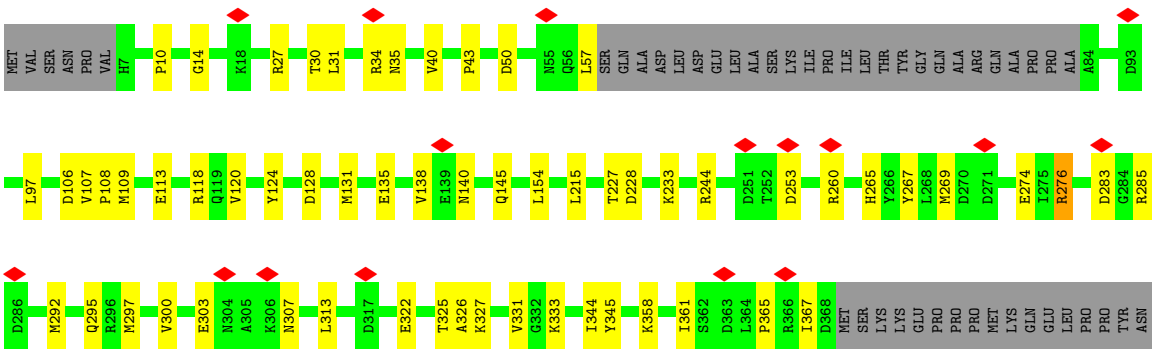


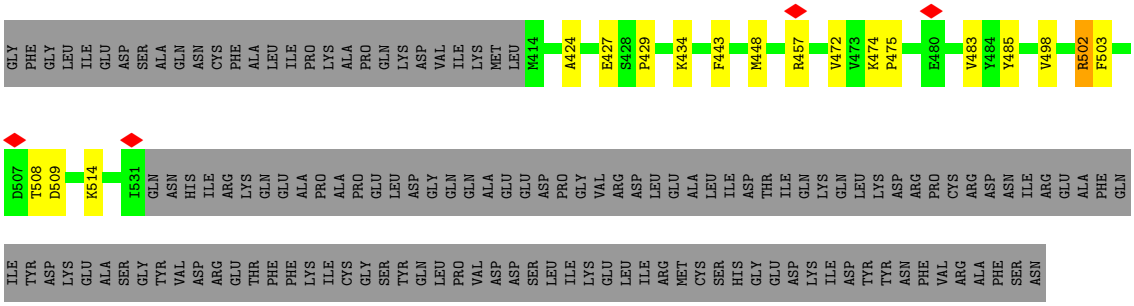


• Molecule 47: EF-hand domain-containing protein 1

Chain Y:



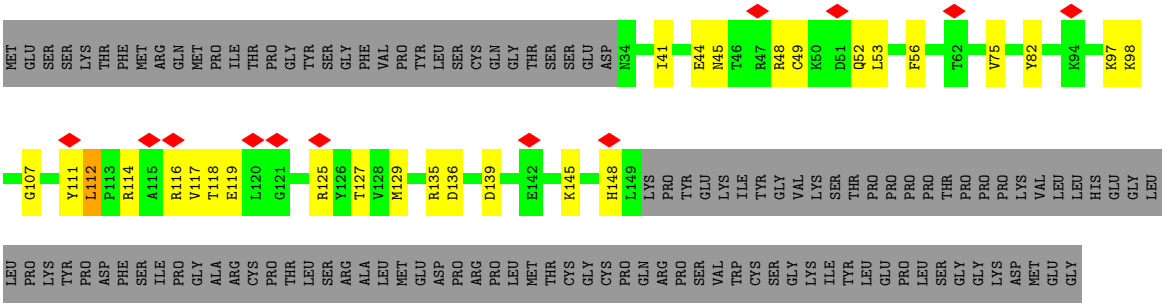




• Molecule 48: Uncharacterized protein C10orf82 homolog

Chain J:

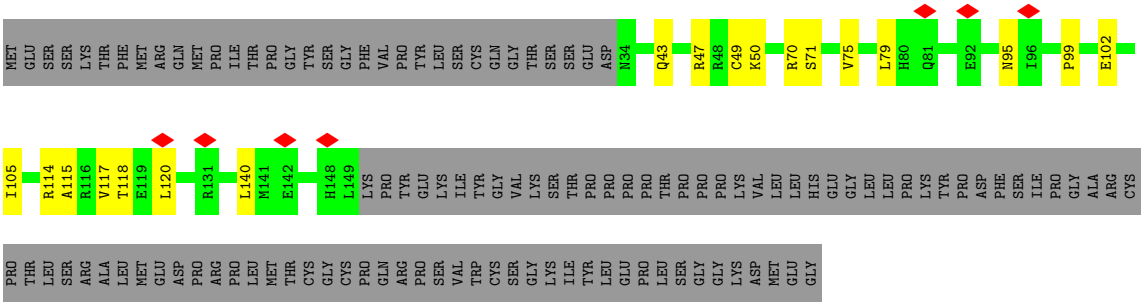




• Molecule 48: Uncharacterized protein C10orf82 homolog

Chain K:

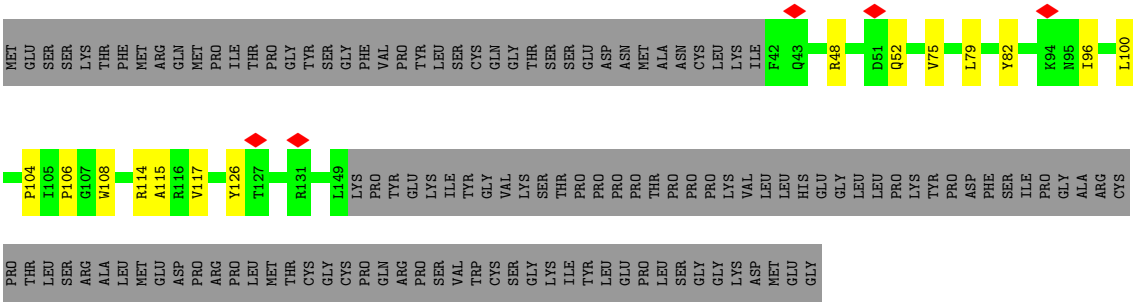




• Molecule 48: Uncharacterized protein C10orf82 homolog

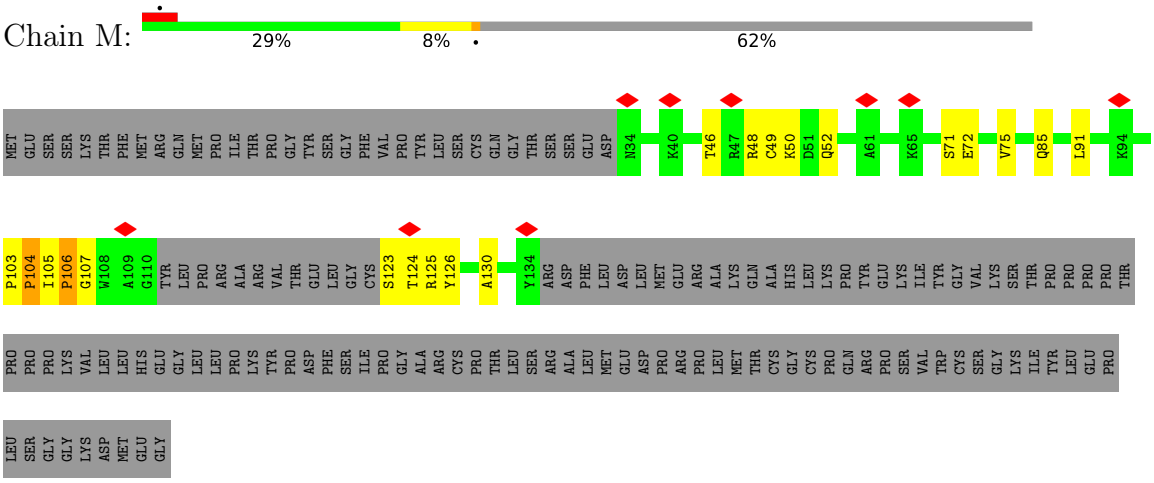
Chain L:





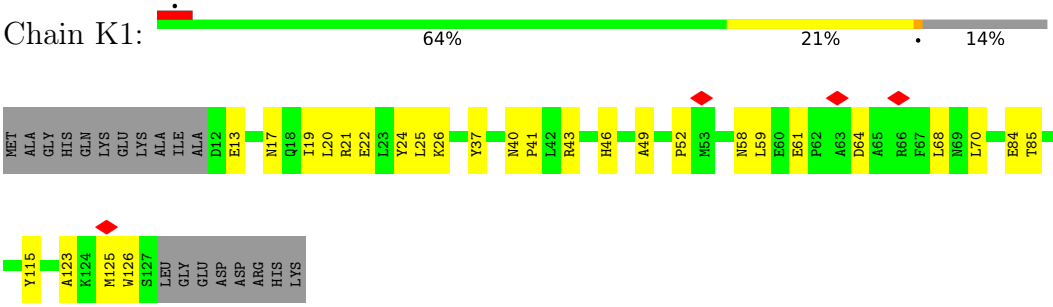
• Molecule 48: Uncharacterized protein C10orf82 homolog

Chain M:



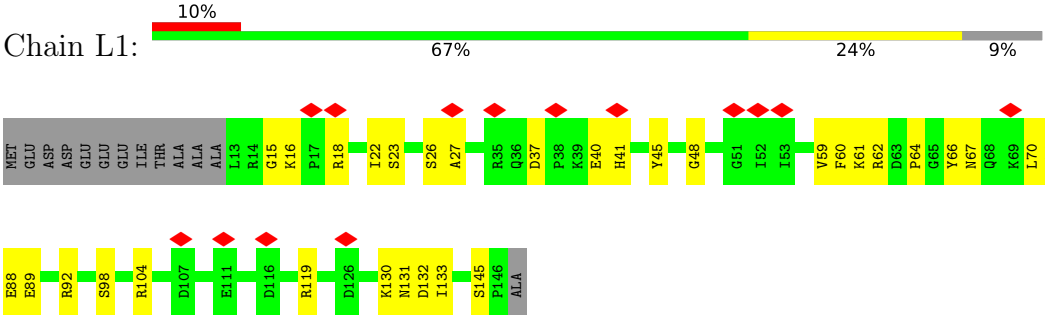
• Molecule 49: Cilia- and flagella-associated protein 144

Chain K1:



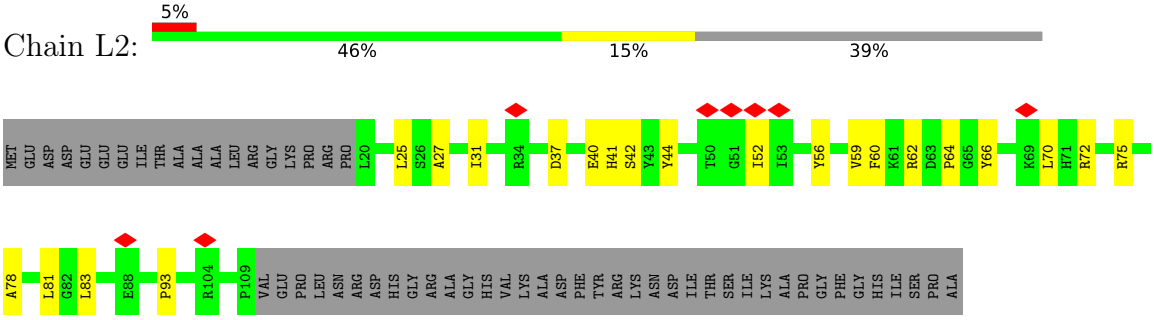
• Molecule 50: Chromosome 20 C5orf49 homolog

Chain L1:



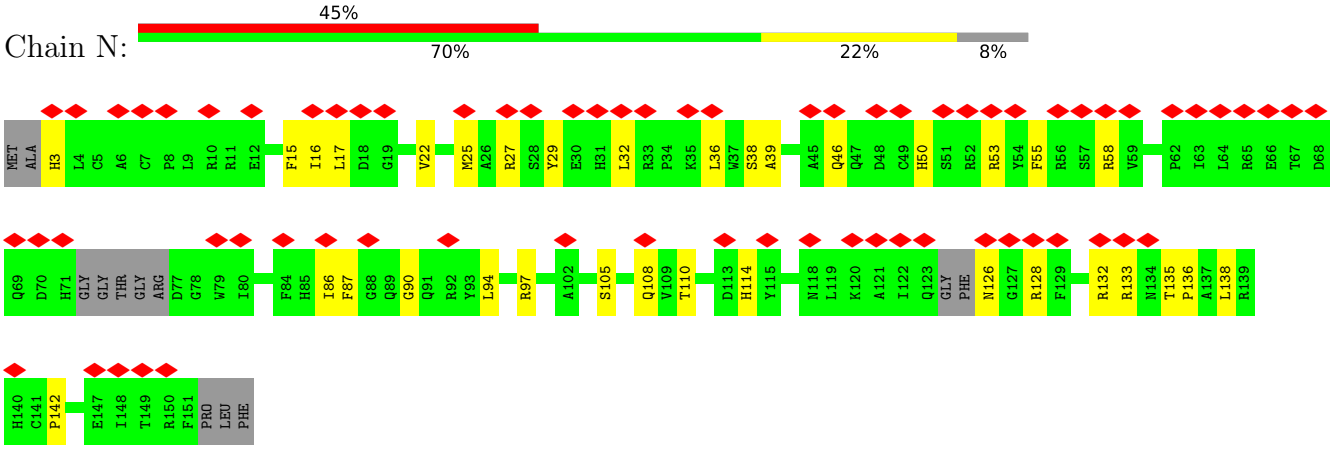
• Molecule 50: Chromosome 20 C5orf49 homolog

Chain L2:



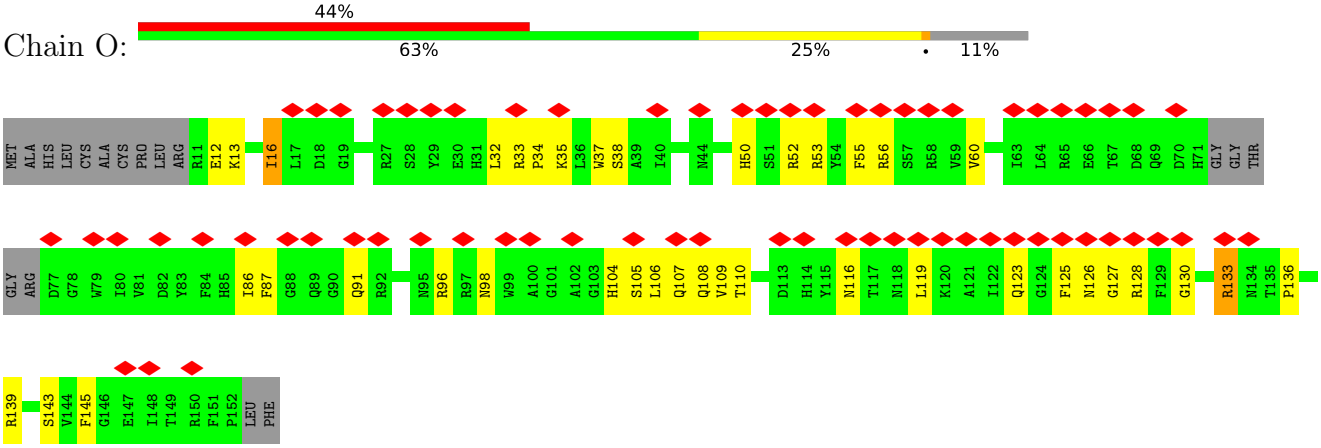
• Molecule 51: Chromosome 19 C17orf98 homolog

Chain N:



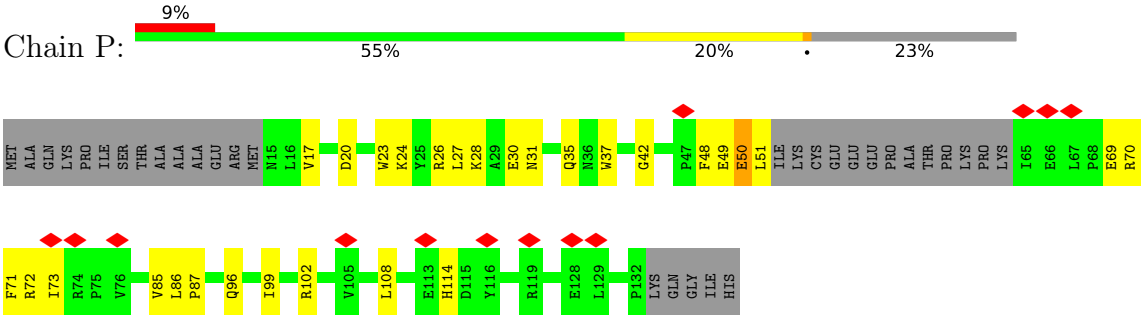
• Molecule 51: Chromosome 19 C17orf98 homolog

Chain O:



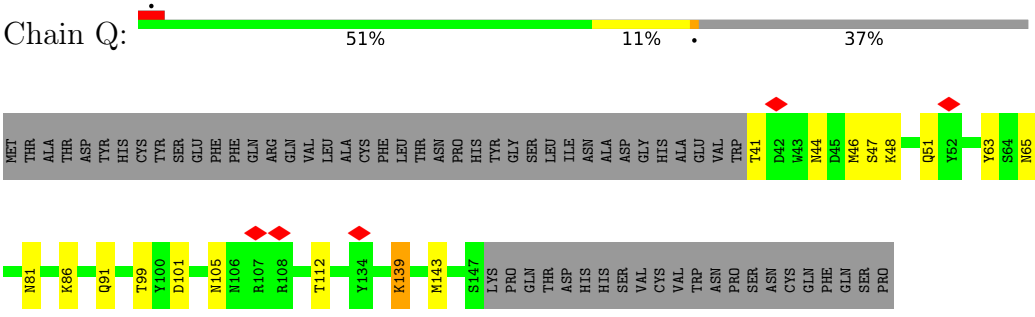
• Molecule 52: Chromosome 13 C20orf85 homolog

Chain P:



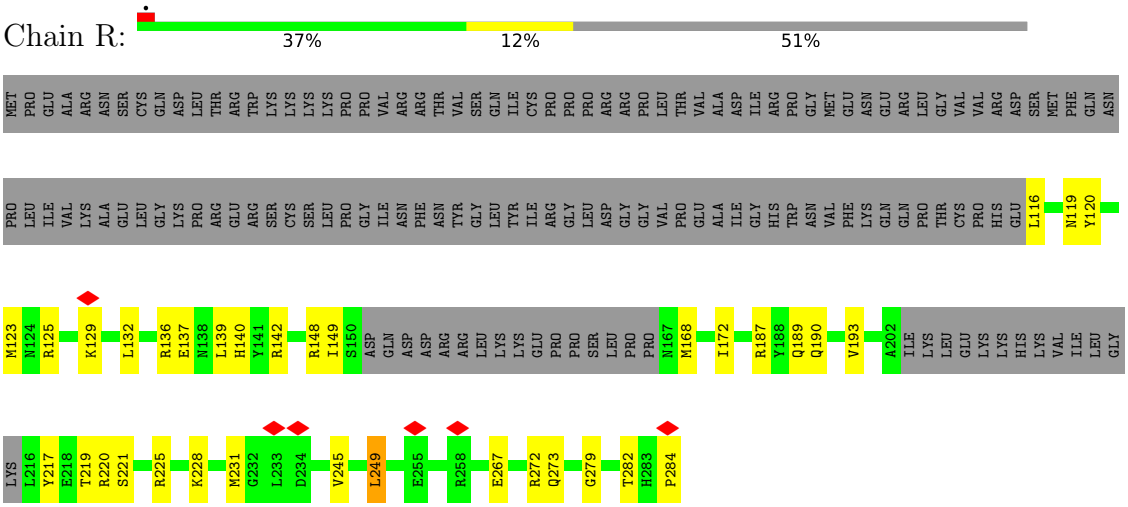
• Molecule 53: Cilia- and flagella-associated protein 68

Chain Q:



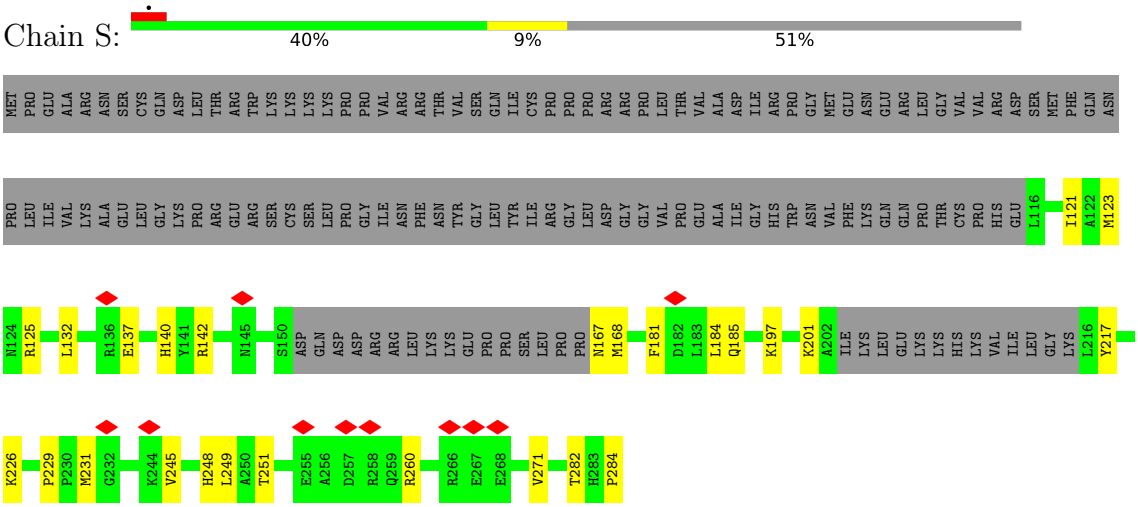
• Molecule 54: Cilia and flagella associated protein 77

Chain R:



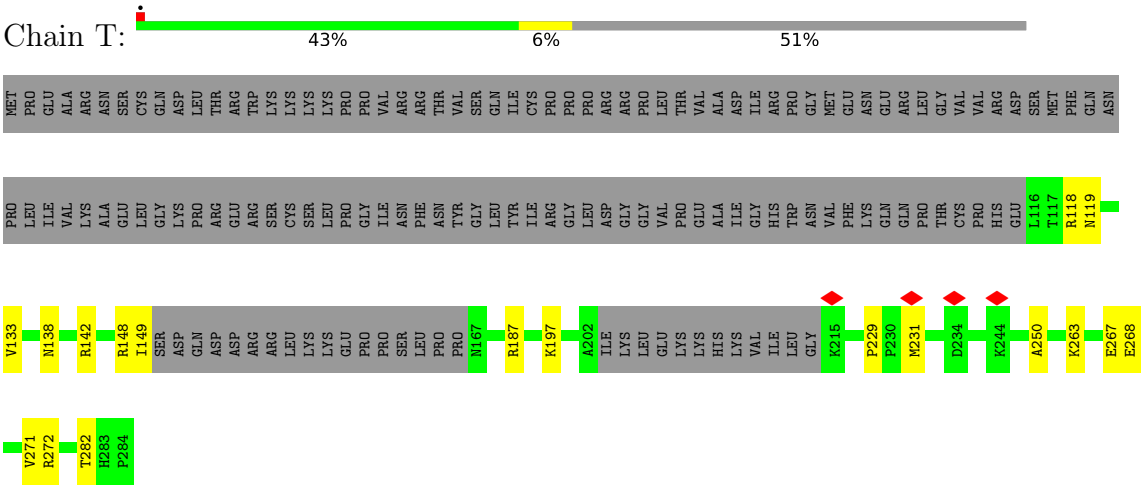
• Molecule 54: Cilia and flagella associated protein 77

Chain S:



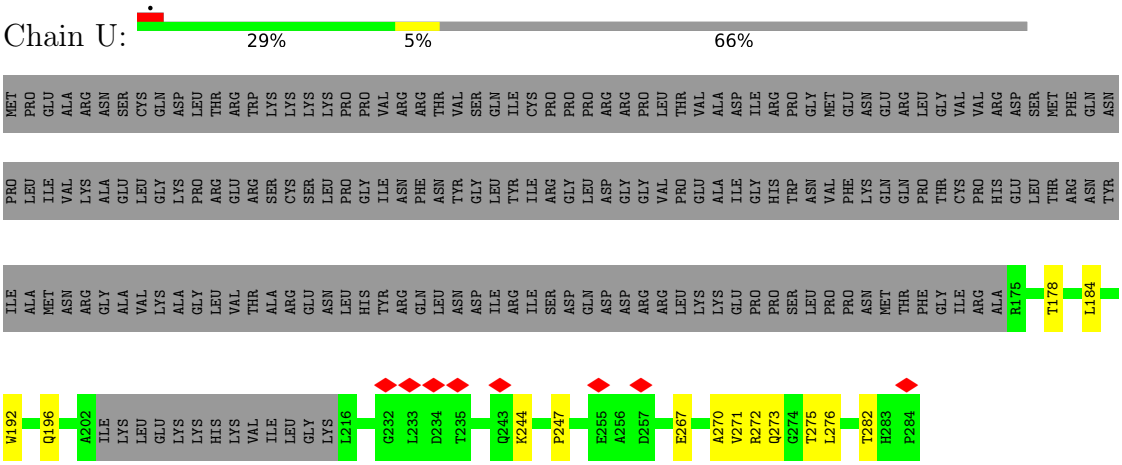
• Molecule 54: Cilia and flagella associated protein 77

Chain T:



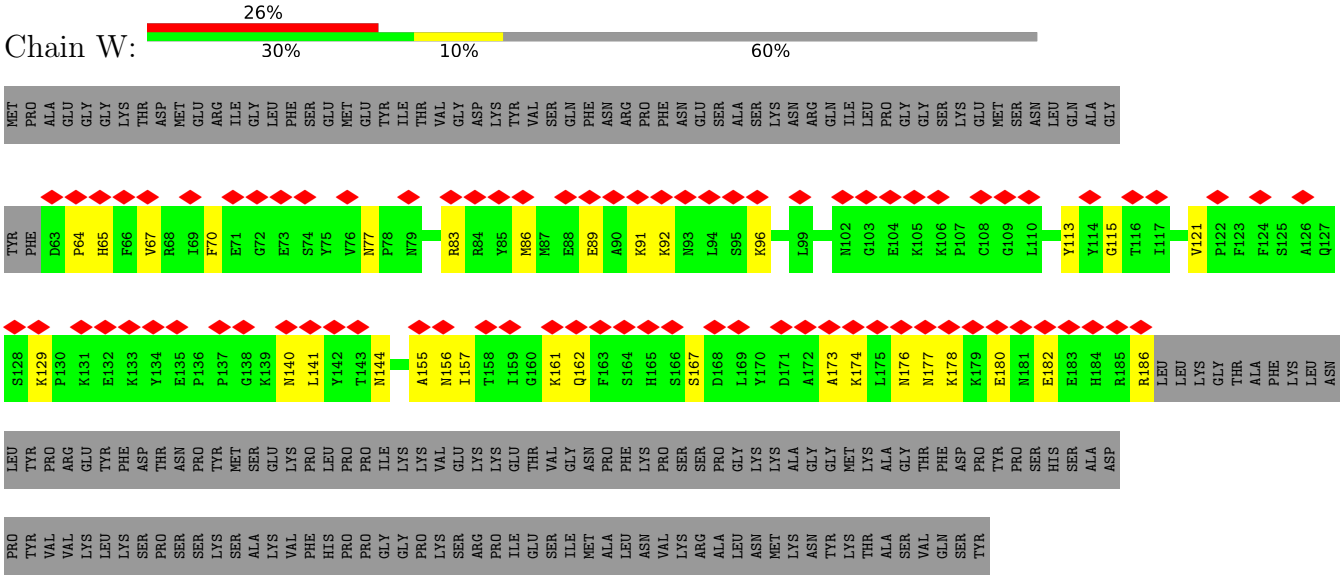
• Molecule 54: Cilia and flagella associated protein 77

Chain U:



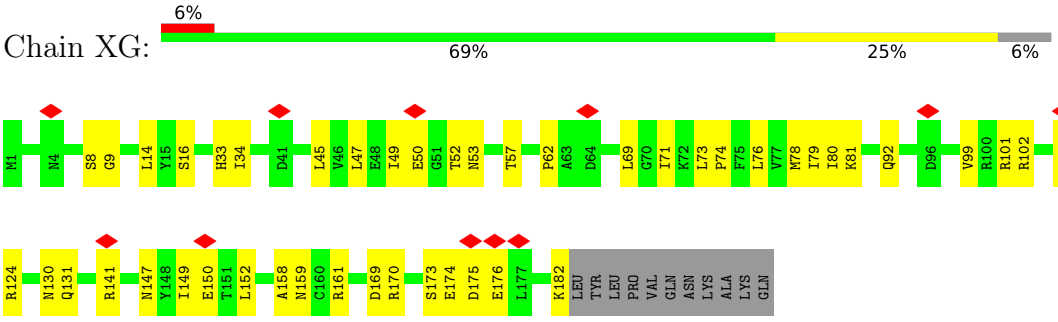
• Molecule 55: UPF0602 protein C4orf47 homolog

Chain W:



• Molecule 56: Cilia- and flagella-associated protein 20

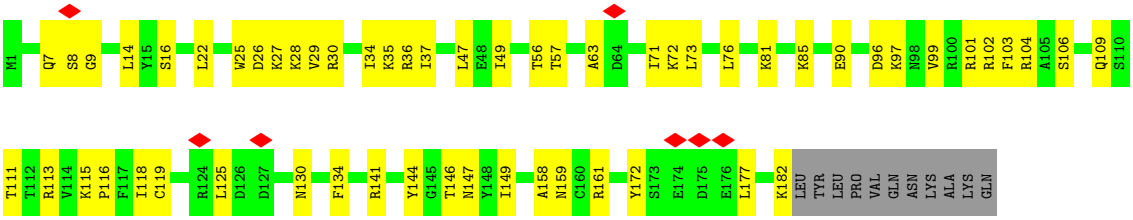
Chain XG:



• Molecule 56: Cilia- and flagella-associated protein 20

Chain XH:

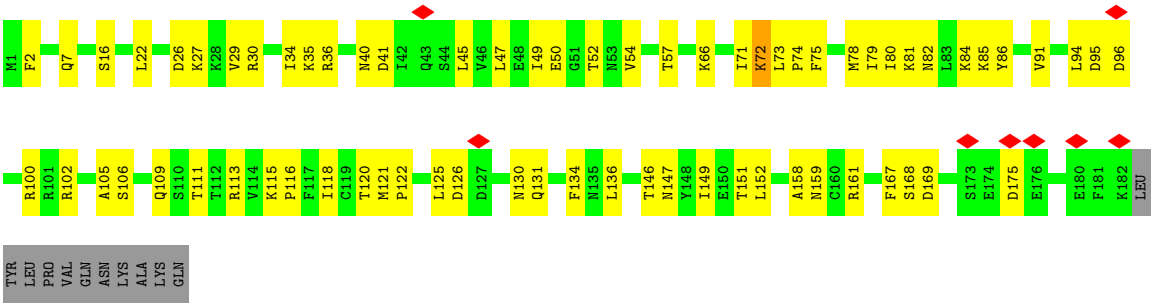




• Molecule 56: Cilia- and flagella-associated protein 20

Chain XI:

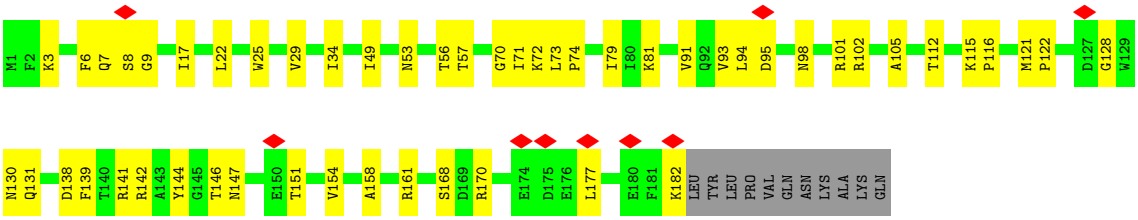




• Molecule 56: Cilia- and flagella-associated protein 20

Chain XJ:

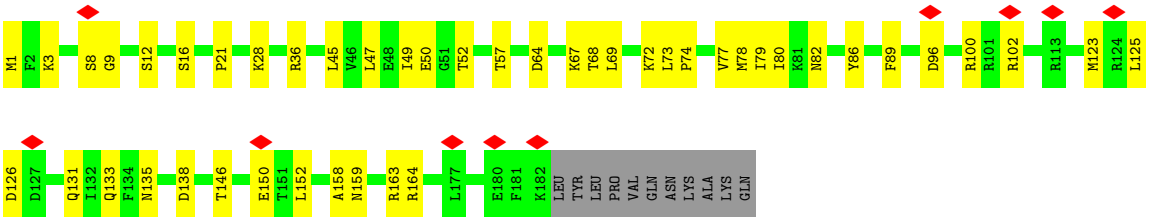




• Molecule 56: Cilia- and flagella-associated protein 20

Chain XK:

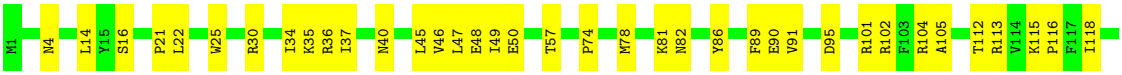


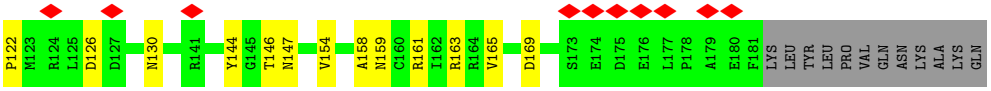


• Molecule 56: Cilia- and flagella-associated protein 20

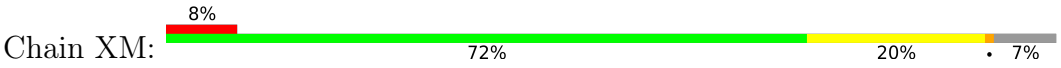
Chain XL:

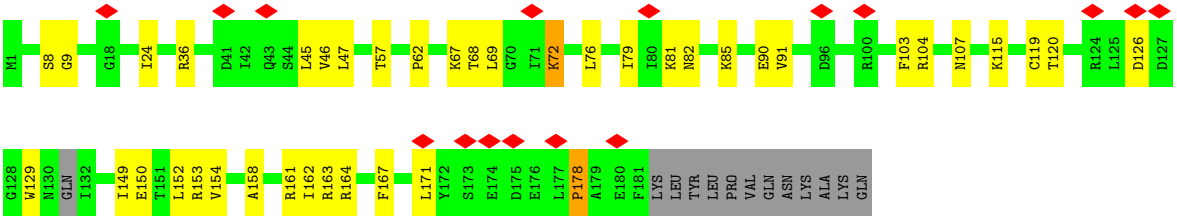






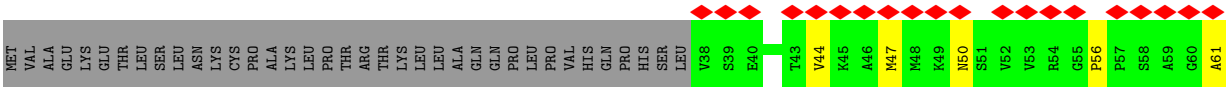
• Molecule 56: Cilia- and flagella-associated protein 20

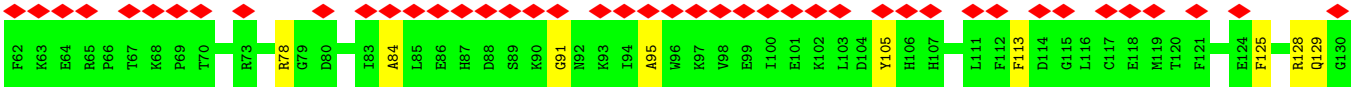




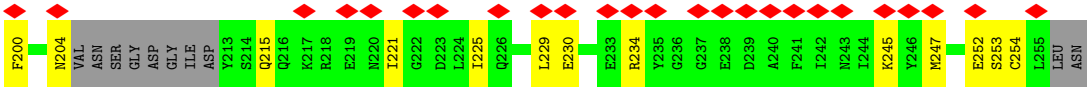
• Molecule 57: Parkin coregulated gene protein





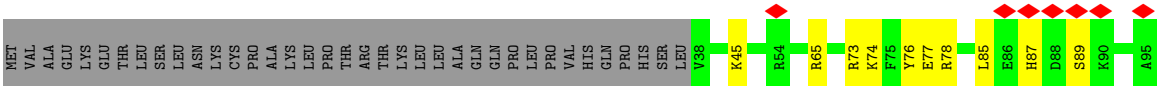


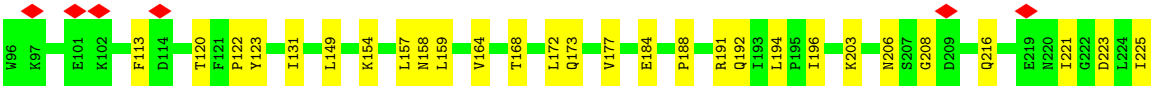


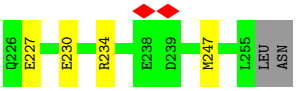


• Molecule 57: Parkin coregulated gene protein



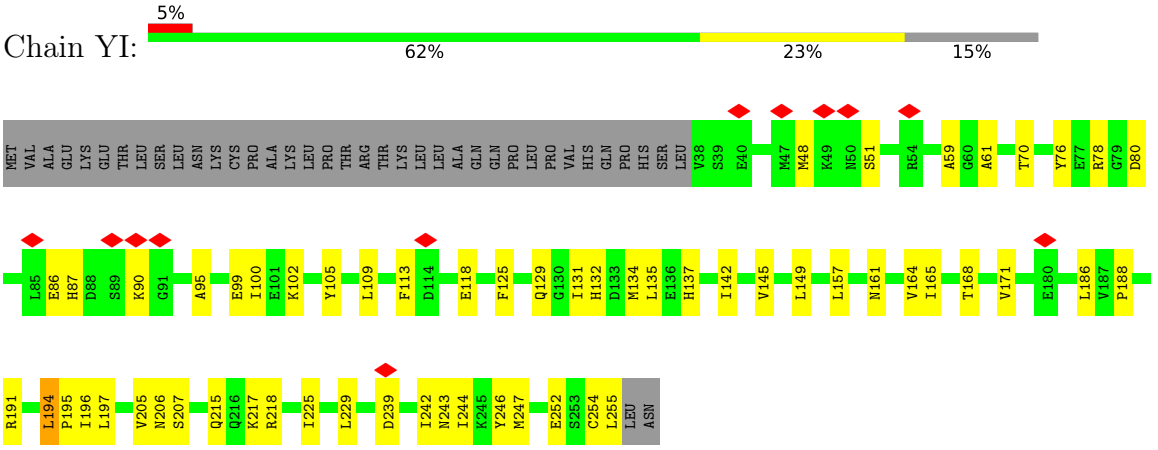






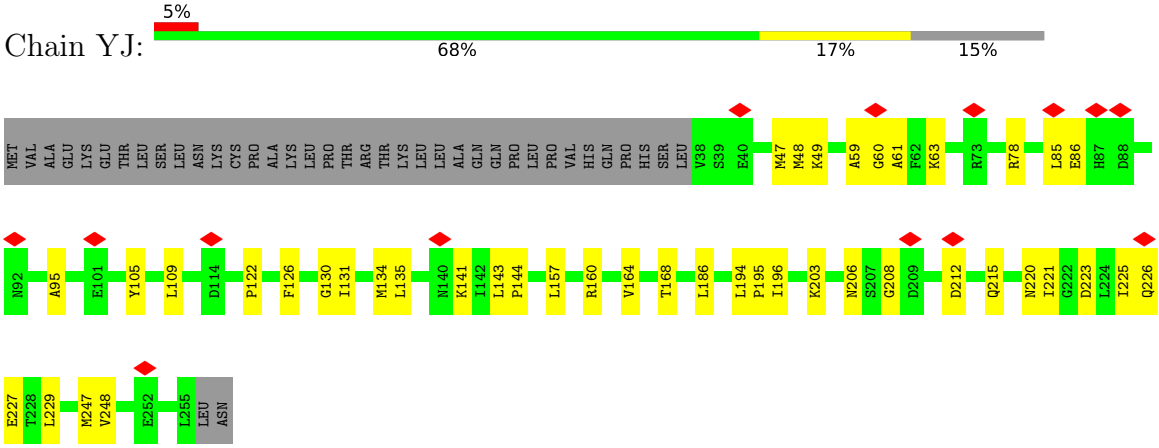
• Molecule 57: Parkin coregulated gene protein

Chain YI:



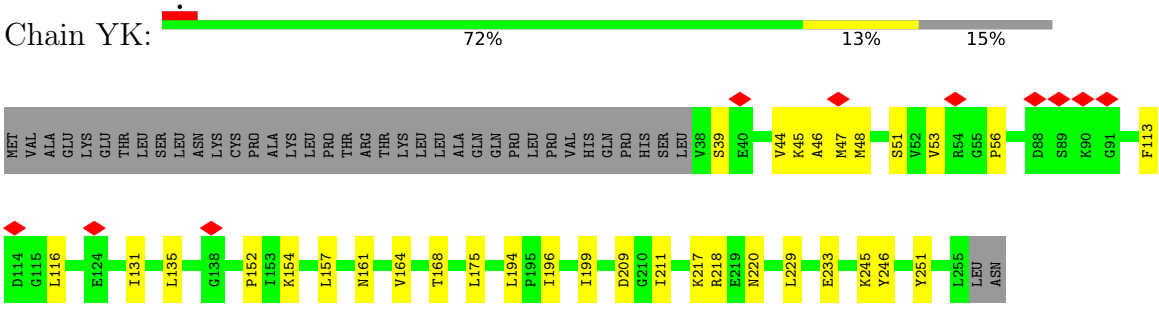
• Molecule 57: Parkin coregulated gene protein

Chain YJ:



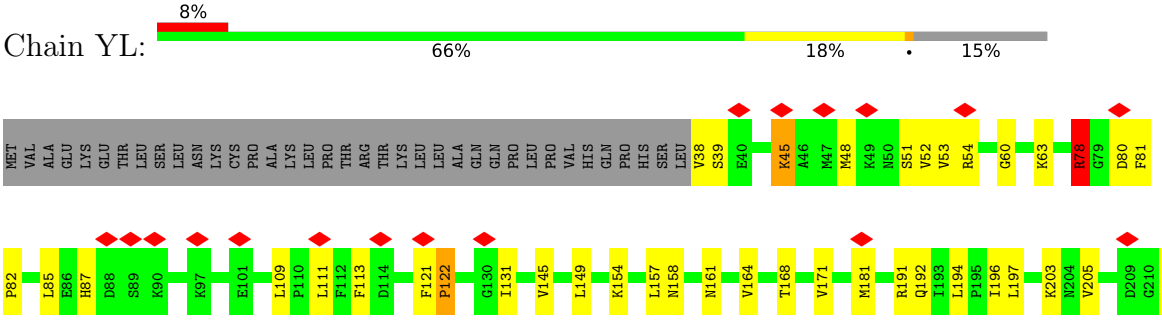
• Molecule 57: Parkin coregulated gene protein

Chain YK:



• Molecule 57: Parkin coregulated gene protein

Chain YL:

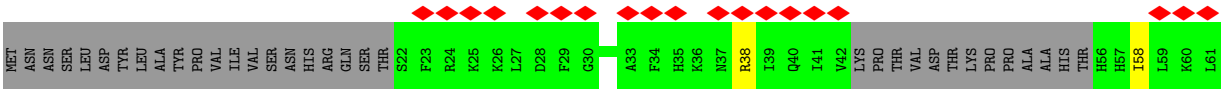


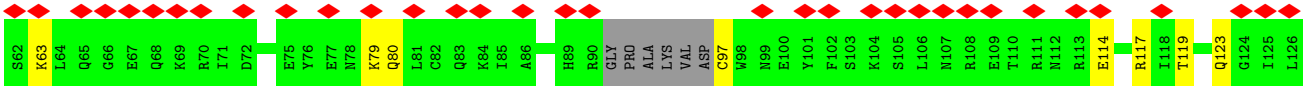


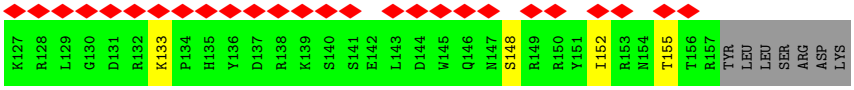
• Molecule 58: CFAP97 domain containing 1

Chain Z:





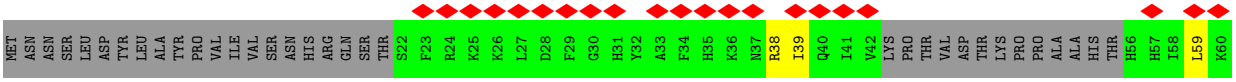


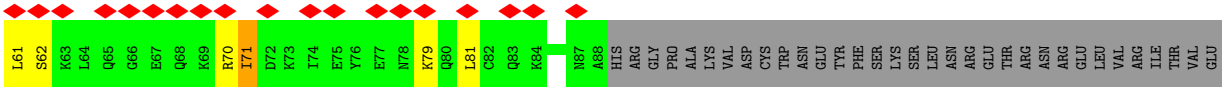


• Molecule 58: CFAP97 domain containing 1

Chain p:



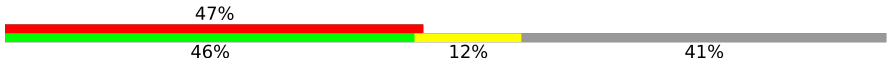


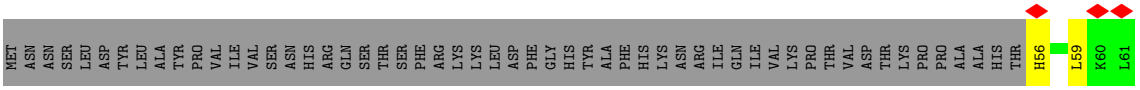


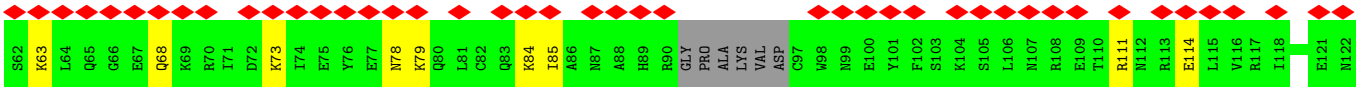


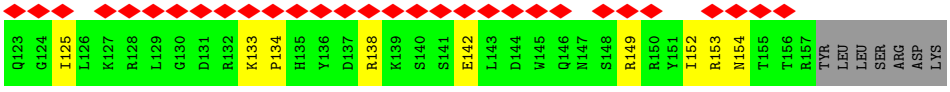
• Molecule 58: CFAP97 domain containing 1

Chain q:





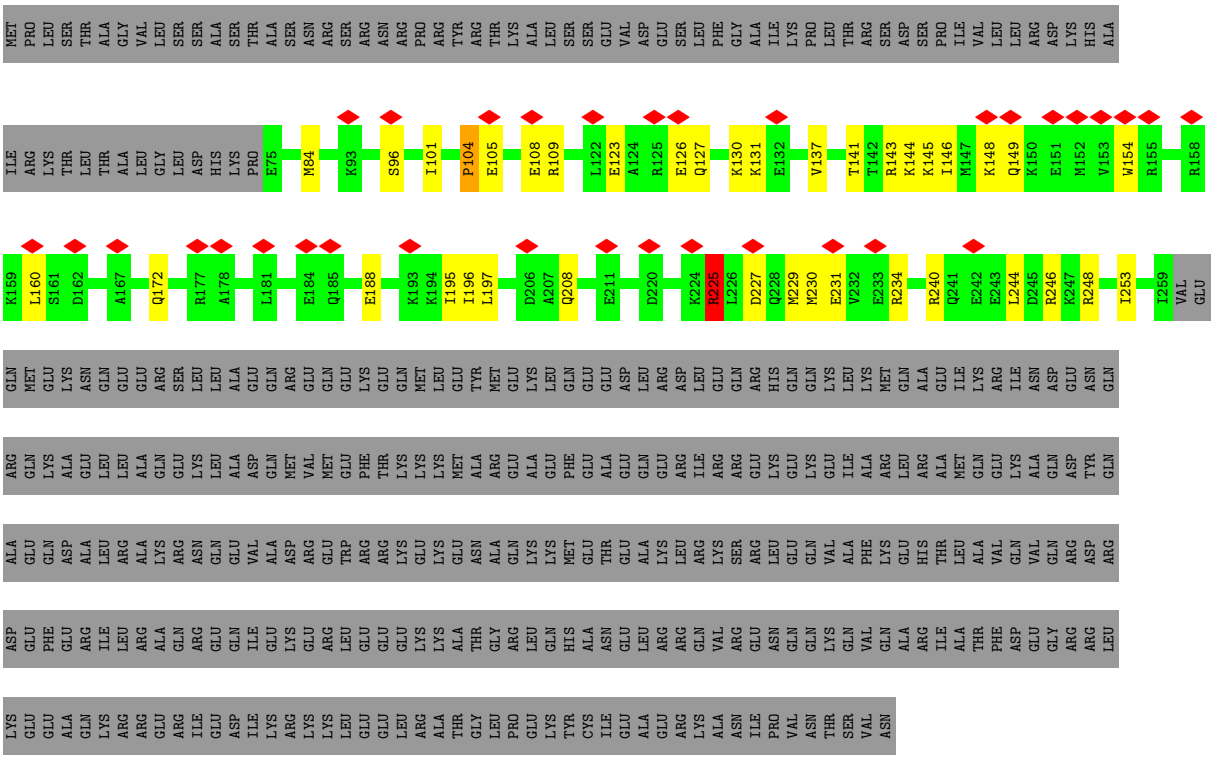




• Molecule 59: Cilia- and flagella-associated protein 45

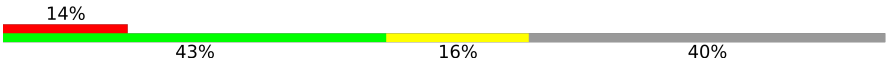
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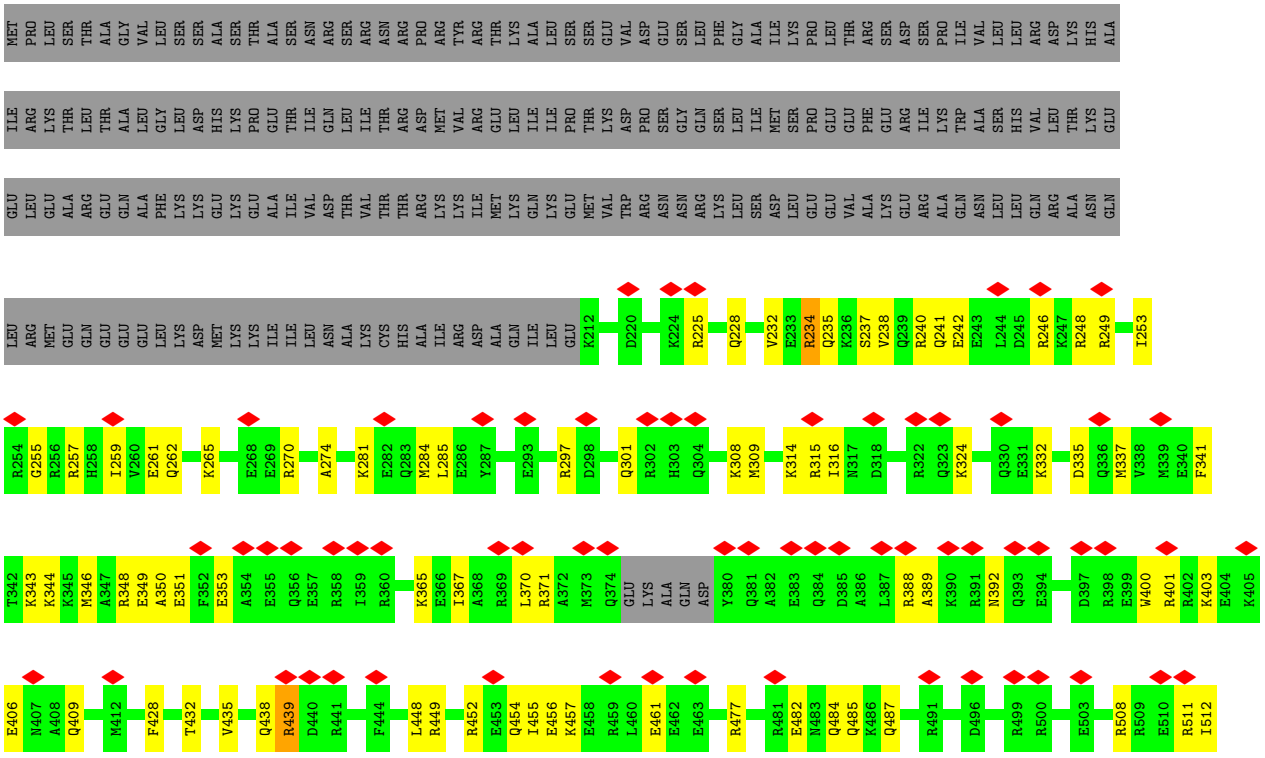


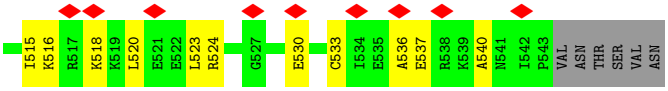


• Molecule 59: Cilia- and flagella-associated protein 45

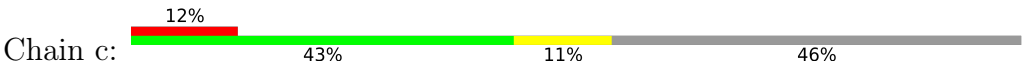
Chain b:

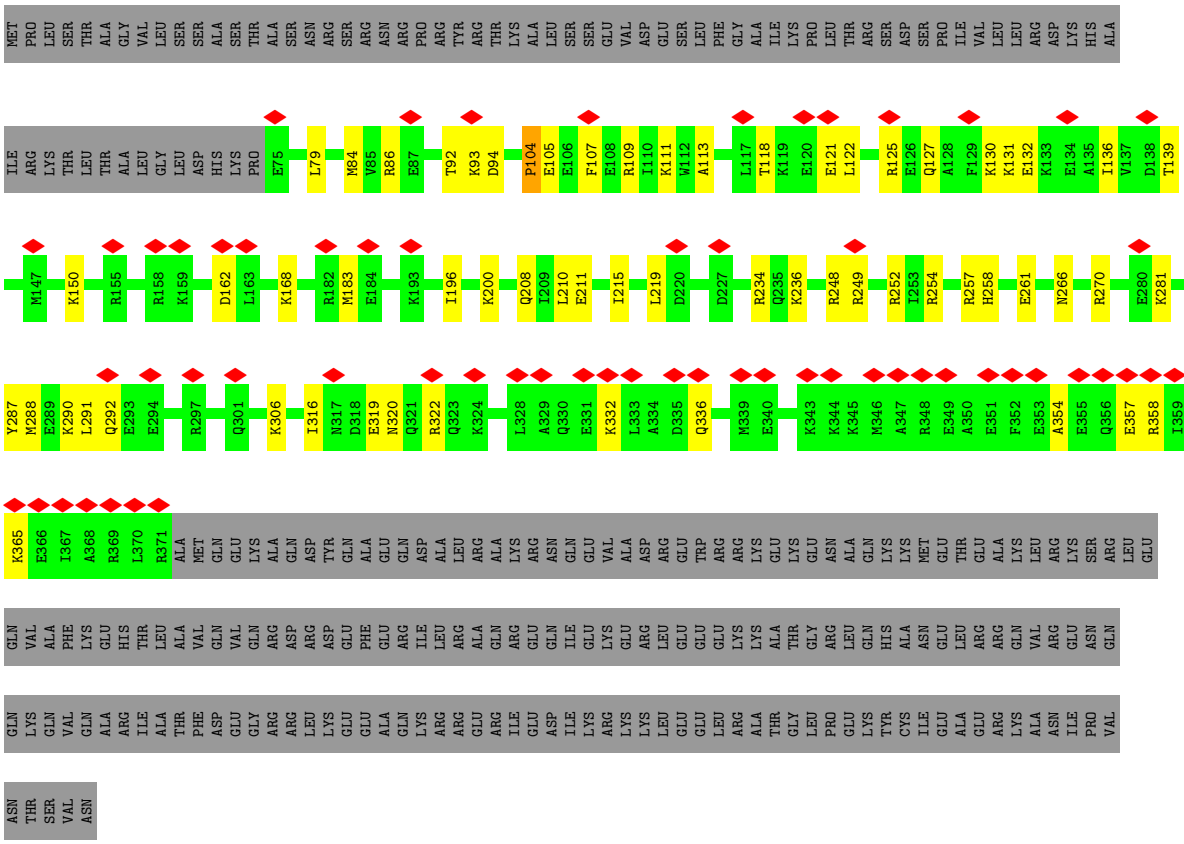






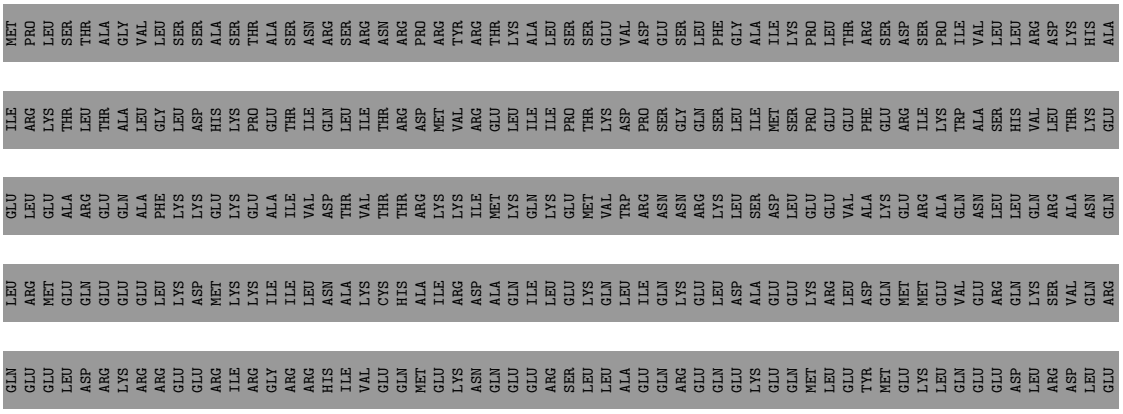
• Molecule 59: Cilia- and flagella-associated protein 45

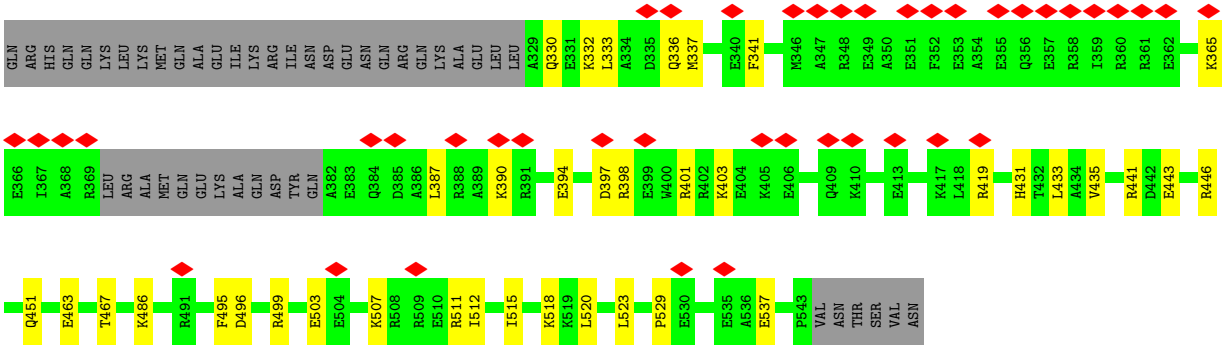




• Molecule 59: Cilia- and flagella-associated protein 45



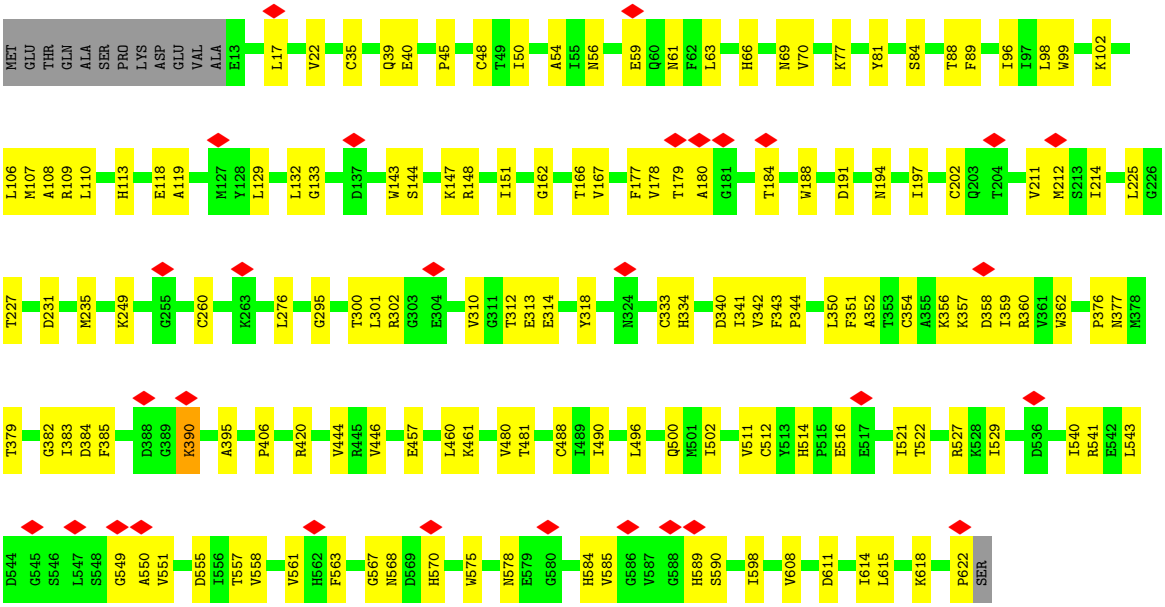




• Molecule 60: Cilia- and flagella-associated protein 52

Chain e:

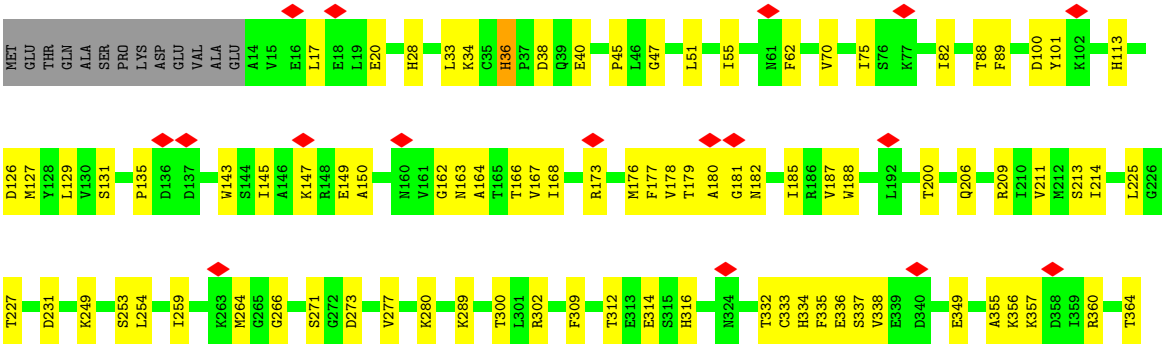


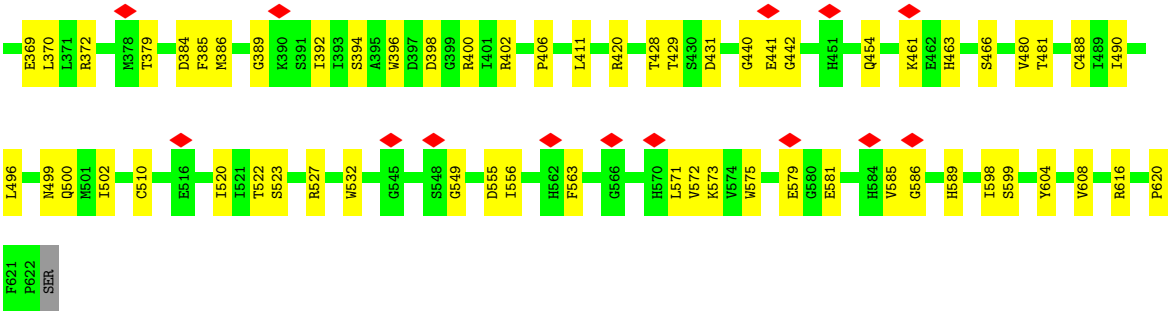


• Molecule 60: Cilia- and flagella-associated protein 52

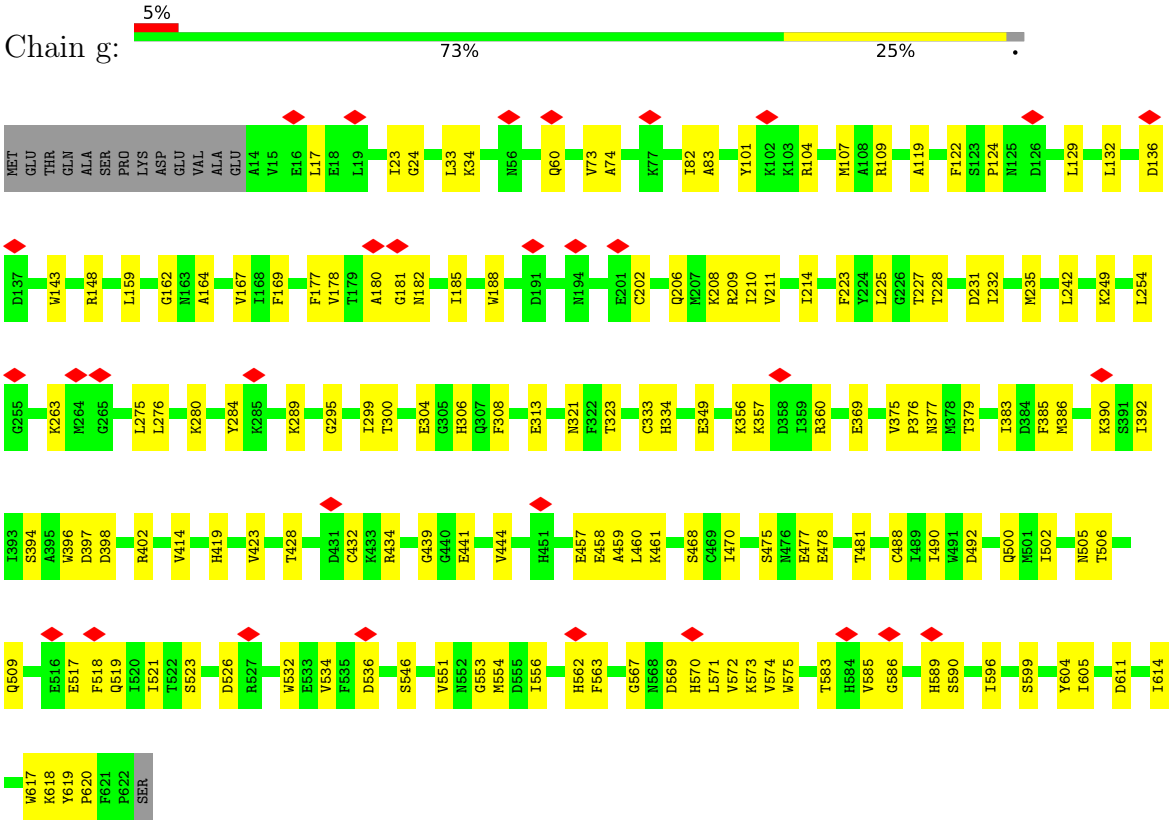
Chain f:



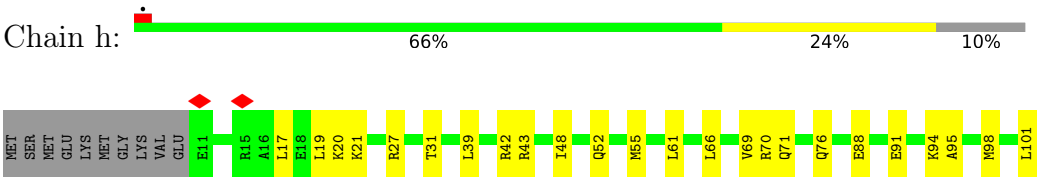




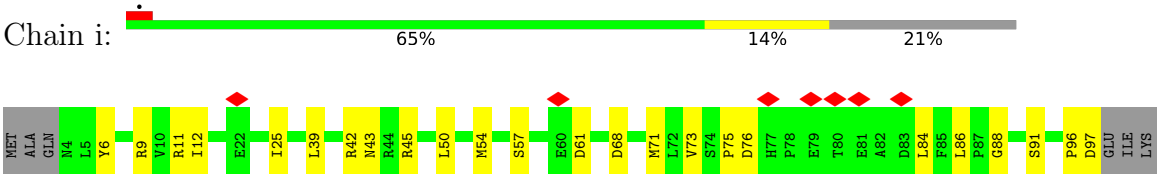
• Molecule 60: Cilia- and flagella-associated protein 52

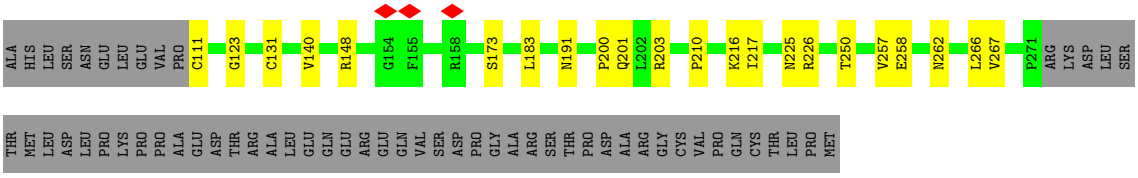


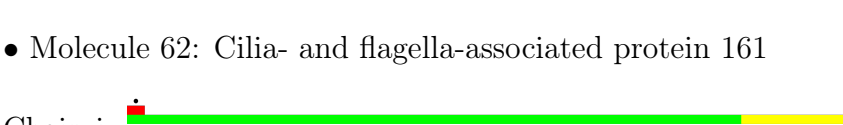
• Molecule 61: Cilia- and flagella-associated protein 141



• Molecule 62: Cilia- and flagella-associated protein 161



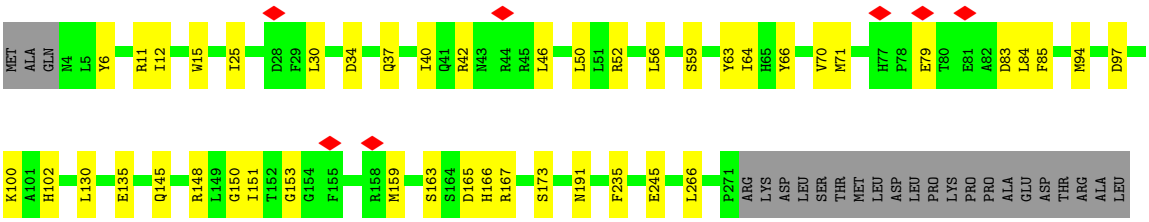


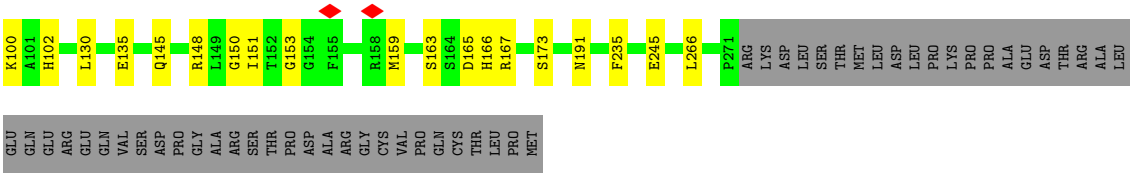


• Molecule 62: Cilia- and flagella-associated protein 161

Chain j:



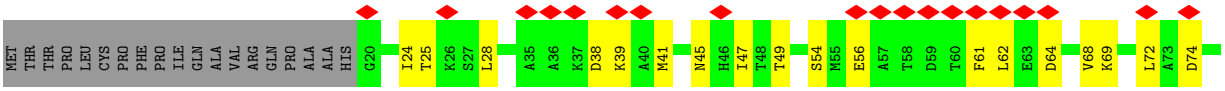


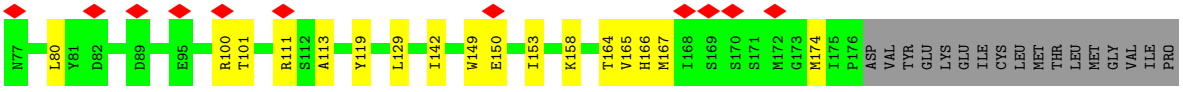


• Molecule 63: Dual specificity phosphatase 21

Chain k:





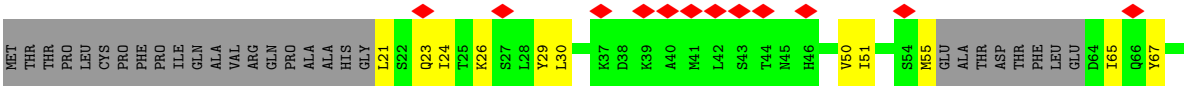


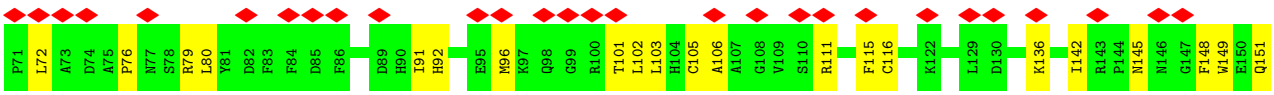


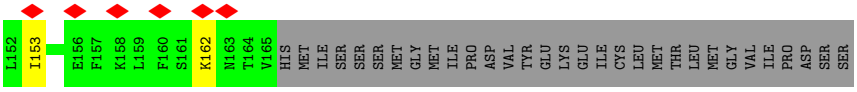
• Molecule 63: Dual specificity phosphatase 21

Chain l:



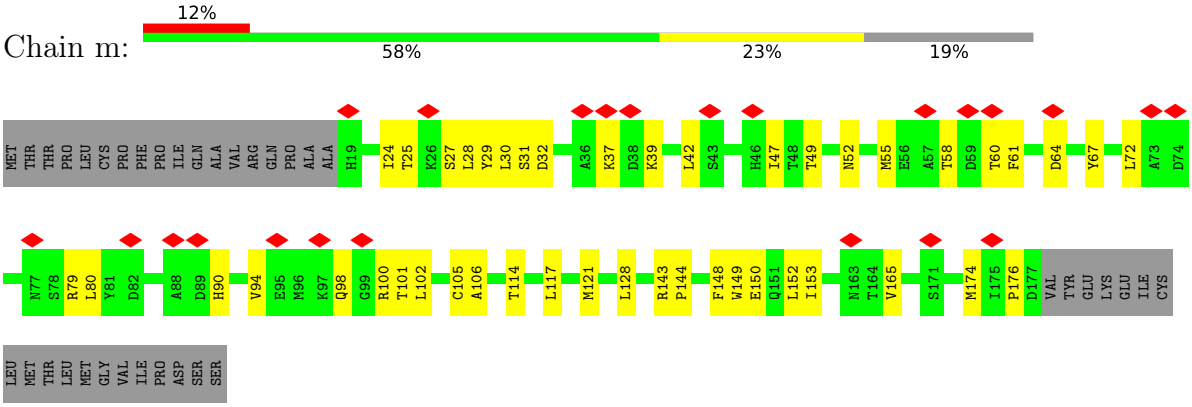






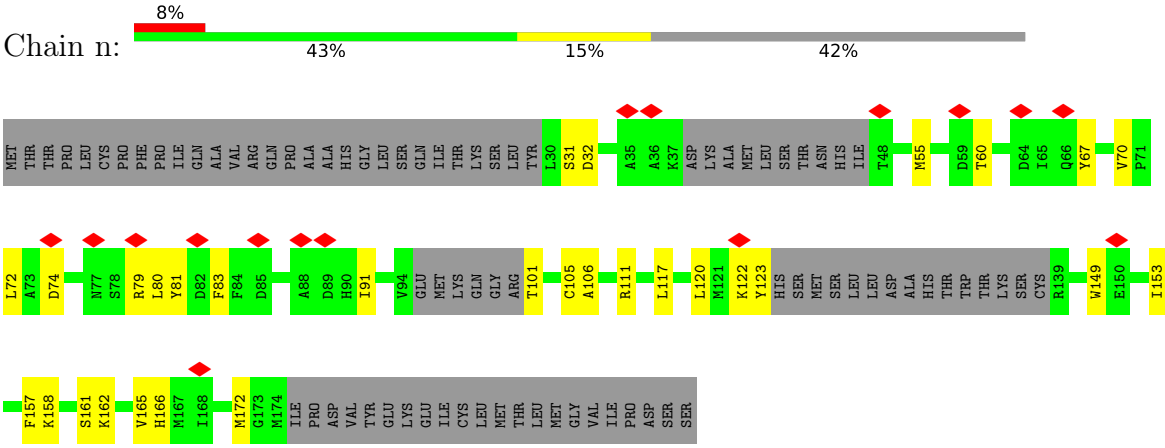
• Molecule 63: Dual specificity phosphatase 21

Chain m:



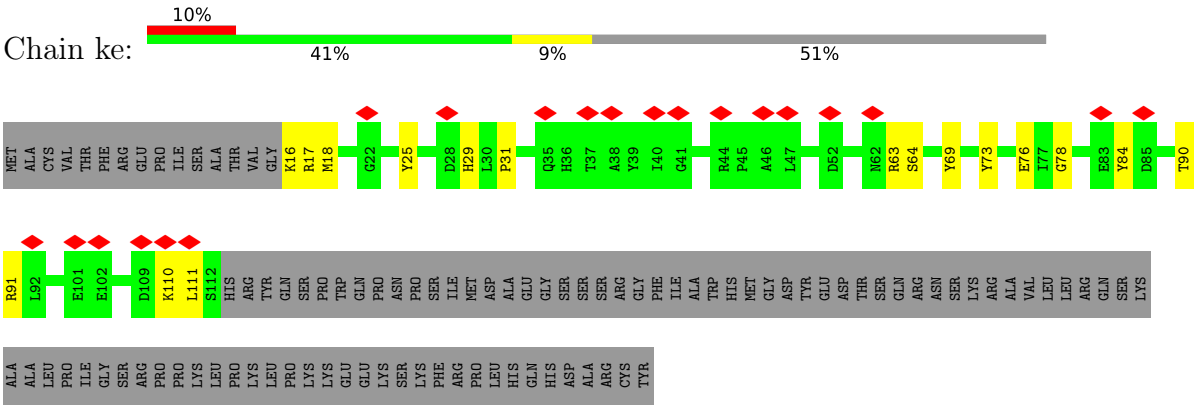
• Molecule 63: Dual specificity phosphatase 21

Chain n:



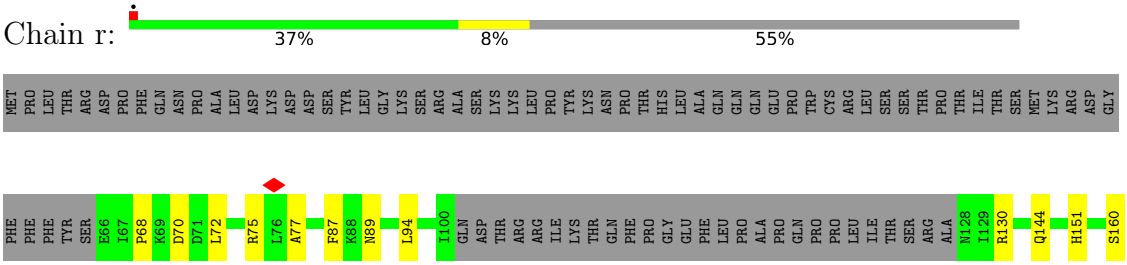
• Molecule 64: Uncharacterized protein C4orf45 homolog

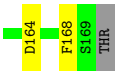
Chain ke:



• Molecule 65: Cilia- and flagella-associated protein 276

Chain r:

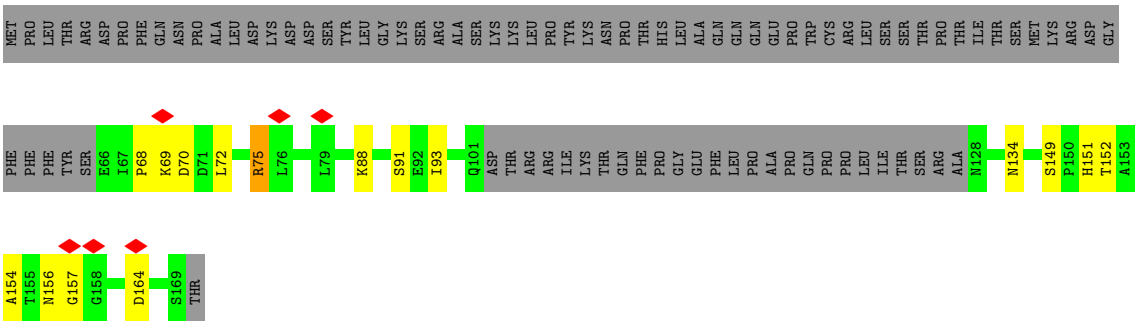




• Molecule 65: Cilia- and flagella-associated protein 276

Chain s:

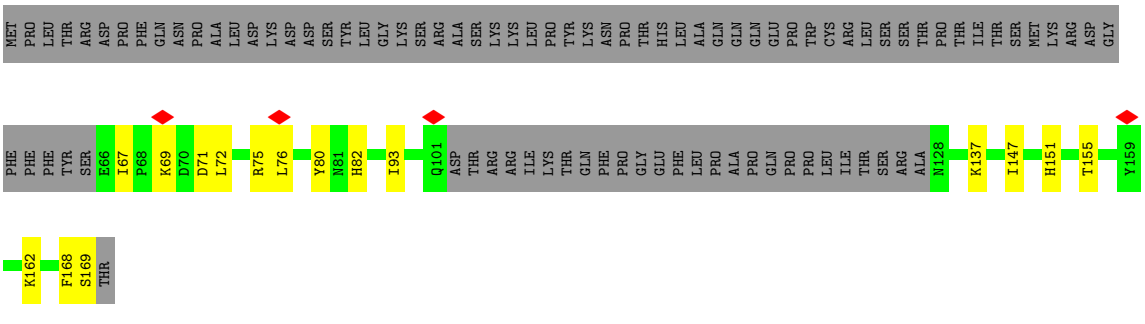




• Molecule 65: Cilia- and flagella-associated protein 276

Chain t:

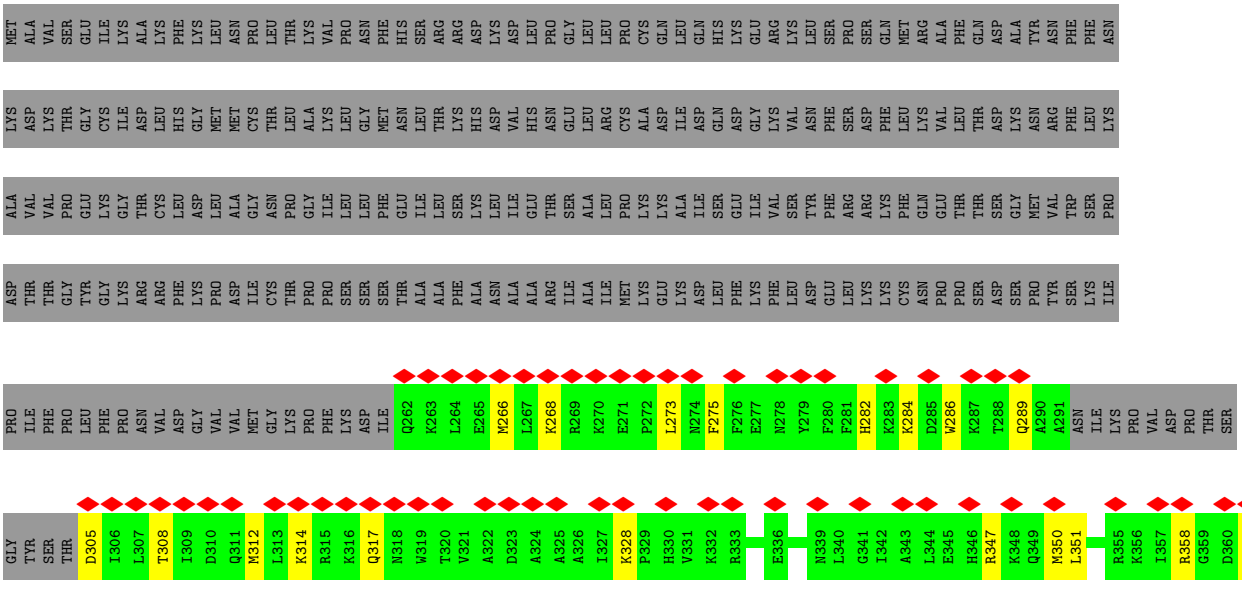


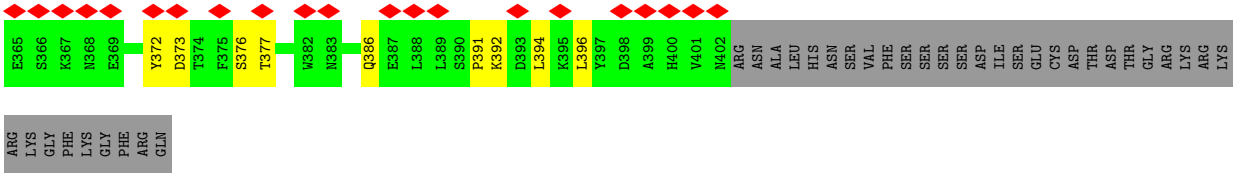


• Molecule 66: EF-hand calcium-binding domain-containing protein 3

Chain u:

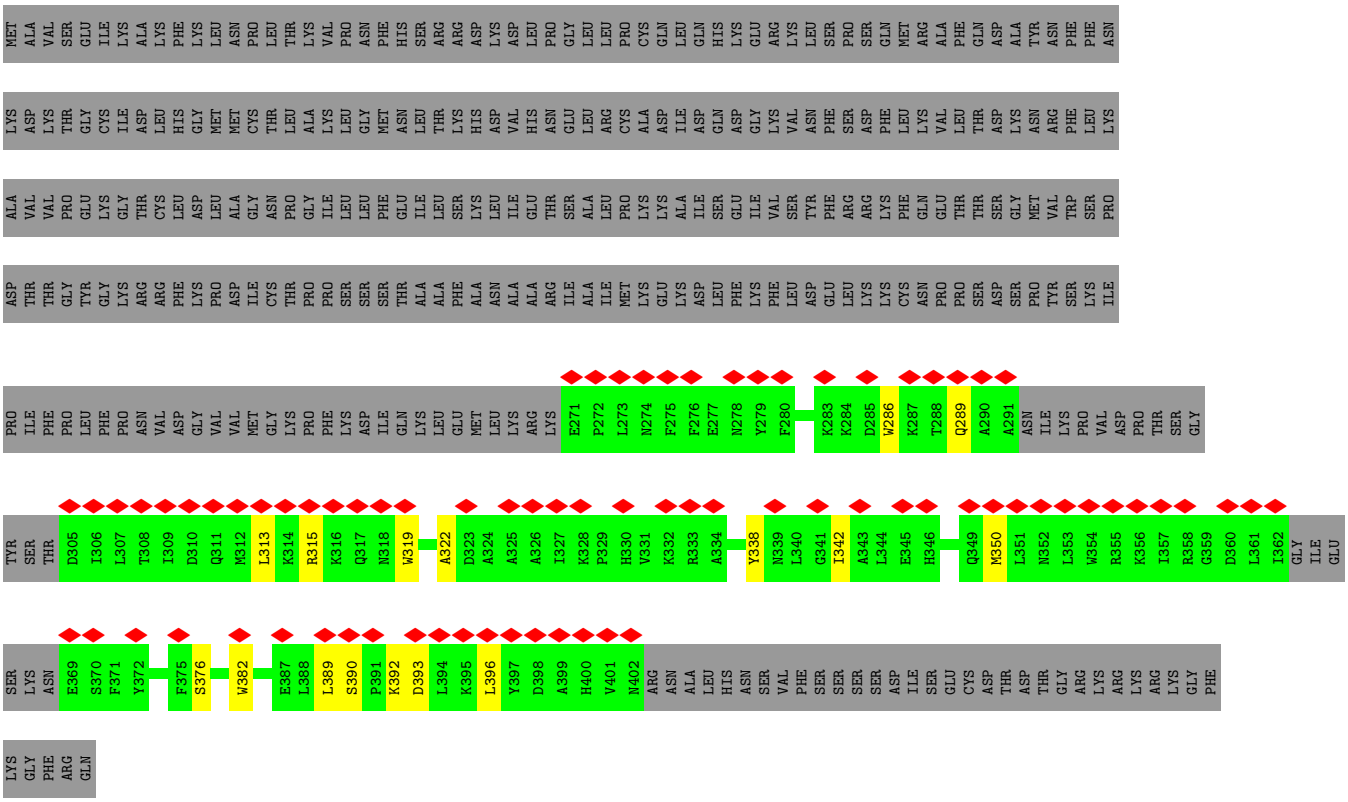






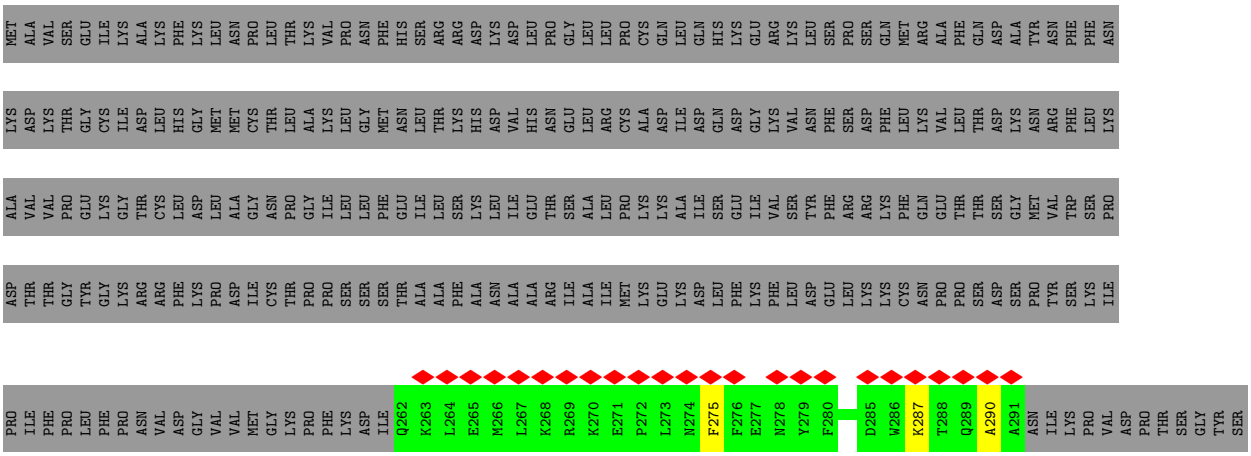
• Molecule 66: EF-hand calcium-binding domain-containing protein 3

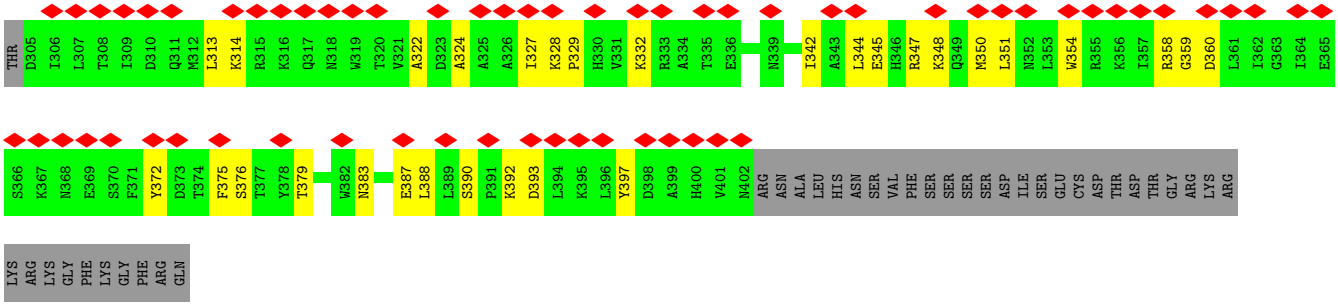




• Molecule 66: EF-hand calcium-binding domain-containing protein 3






THR D305 I306 L307 T308 I309 D310 Q311 M312 L313 K314 R315 K316 Q317 N318 W319 T320 V321 A322 D323 A324 A325 A326 I327 K328 P329 H330 V331 K332 R333 A334 T335 E336 N339 I342 A343 L344 E345 H346 R347 K348 Q349 M350 L351 N352 L353 W354 R355 K356 I357 R358 G359 D360 L361 I362 G363 I364 E365
S366 K367 N368 E369 S370 F371 Y372 D373 T374 F375 S376 T377 Y378 T379 W382 N383 E387 L388 L389 S390 P391 K392 D393 L394 K395 L396 Y397 D398 A399 H400 V401 N402 ARG ASN ALA LEU HIS ASN SER VAL PHE SER SER SER SER ASP ILE SER GLU CYS ASP THR ASP THR GLY ARG LYS ARG
LYS ARG LYS GLY PHE LYS GLY PHE ARG GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34083	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.294	Depositor
Minimum map value	0.000	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	699.552, 699.552, 699.552	wwPDB
Map dimensions	672, 672, 672	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.22	0/337	0.41	0/452
1	V	0.33	0/1525	0.64	1/2064 (0.0%)
2	0A	0.33	0/1276	0.68	2/1721 (0.1%)
2	0C	0.29	0/1276	0.74	4/1721 (0.2%)
2	0E	0.34	0/1284	0.67	0/1731
2	0G	0.24	0/1276	0.46	0/1721
2	0W	0.23	0/1276	0.50	0/1721
2	0Y	0.31	0/1276	0.67	0/1721
2	0a	0.34	0/1276	0.73	0/1721
2	0c	0.42	0/1276	0.87	2/1721 (0.1%)
2	0e	0.21	0/1268	0.48	0/1711
2	0g	0.30	0/1276	0.78	2/1721 (0.1%)
2	0i	0.51	2/1276 (0.2%)	1.00	7/1721 (0.4%)
2	0k	0.38	1/1276 (0.1%)	0.77	0/1721
2	CT	0.39	0/1284	0.77	2/1731 (0.1%)
2	CU	0.35	0/1268	0.74	6/1711 (0.4%)
2	CV	0.36	0/1276	0.75	1/1721 (0.1%)
2	CX	0.32	0/1276	0.78	2/1721 (0.1%)
2	CY	0.35	0/1276	0.67	1/1721 (0.1%)
2	CZ	0.27	0/1276	0.58	0/1721
2	Ca	0.35	0/1276	0.78	4/1721 (0.2%)
2	Cb	0.34	0/1276	0.79	3/1721 (0.2%)
2	Cc	0.29	0/1276	0.66	2/1721 (0.1%)
2	Cd	0.58	1/1276 (0.1%)	0.97	6/1721 (0.3%)
2	Ce	0.23	0/1268	0.50	1/1711 (0.1%)
2	Cf	0.27	0/1268	0.59	0/1711
2	Cg	0.24	0/1276	0.63	3/1721 (0.2%)
2	Ch	0.31	0/1276	0.64	0/1721
2	Ci	0.32	0/1276	0.62	0/1721
2	Cj	0.29	0/1268	0.67	0/1711
2	Ck	0.33	0/1276	0.76	4/1721 (0.2%)
3	1	0.32	1/1740 (0.1%)	0.72	6/2356 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	2	0.23	0/2074	0.54	0/2806
3	x	0.28	0/2074	0.58	1/2806 (0.0%)
4	3	0.27	0/1498	0.58	0/2007
4	y	0.25	0/1498	0.58	2/2007 (0.1%)
4	z	0.23	0/1498	0.60	0/2007
5	A	0.31	0/346	0.62	0/460
5	B	0.34	0/773	0.71	1/1046 (0.1%)
5	C	0.24	0/773	0.55	0/1046
6	A0	0.36	0/1054	0.79	3/1436 (0.2%)
6	BN	0.29	0/638	0.81	1/871 (0.1%)
7	A1	0.62	2/1891 (0.1%)	0.92	7/2580 (0.3%)
7	A2	0.31	0/402	0.85	0/549
7	A3	0.19	0/1199	0.63	0/1665
7	A4	0.21	0/542	0.67	0/747
7	A5	0.24	0/761	0.72	1/1056 (0.1%)
7	A6	0.32	0/380	0.85	1/518 (0.2%)
7	A7	0.40	0/1786	0.89	0/2434
7	A8	0.39	0/1322	0.91	7/1799 (0.4%)
7	A9	0.27	0/914	0.56	0/1249
7	Au	0.30	0/555	0.85	4/757 (0.5%)
7	Av	0.35	0/1161	0.81	6/1578 (0.4%)
7	Aw	0.25	0/1047	0.60	1/1429 (0.1%)
7	Ay	0.57	2/1462 (0.1%)	0.93	7/1986 (0.4%)
7	Az	0.40	0/322	0.71	0/439
8	AA	0.26	0/3490	0.52	0/4740
8	AC	0.24	0/3505	0.55	2/4760 (0.0%)
8	AE	0.22	0/3505	0.48	0/4760
8	AG	0.24	0/3505	0.51	0/4760
8	AI	0.23	0/3505	0.48	0/4760
8	AK	0.26	0/3505	0.50	1/4760 (0.0%)
8	AM	0.25	0/3498	0.53	3/4750 (0.1%)
8	BA	0.23	0/3431	0.54	2/4660 (0.0%)
8	BC	0.26	0/3492	0.55	2/4742 (0.0%)
8	BE	0.26	0/3439	0.53	1/4670 (0.0%)
8	BG	0.29	1/3498 (0.0%)	0.55	3/4750 (0.1%)
8	BI	0.28	0/3433	0.59	2/4662 (0.0%)
8	BK	0.37	2/3484 (0.1%)	0.62	4/4731 (0.1%)
8	BM	0.27	0/3439	0.54	1/4670 (0.0%)
8	CA	0.23	0/3484	0.51	0/4732
8	CC	0.23	0/3492	0.51	2/4742 (0.0%)
8	CE	0.21	0/3492	0.46	0/4742
8	CG	0.72	8/3477 (0.2%)	0.80	10/4721 (0.2%)
8	CI	0.39	2/3492 (0.1%)	0.65	5/4742 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	CK	0.25	0/3492	0.50	0/4742
8	CM	0.22	0/3492	0.50	1/4742 (0.0%)
8	DA	0.26	0/3025	0.58	1/4100 (0.0%)
8	DC	0.26	0/3425	0.54	1/4651 (0.0%)
8	DE	0.49	3/3425 (0.1%)	0.76	5/4651 (0.1%)
8	DG	0.24	0/3446	0.55	2/4680 (0.0%)
8	DI	0.60	3/3424 (0.1%)	0.85	6/4649 (0.1%)
8	DK	0.25	0/3418	0.57	3/4641 (0.1%)
8	DM	0.24	0/3418	0.54	2/4641 (0.0%)
8	EC	0.29	0/3468	0.58	1/4708 (0.0%)
8	EE	0.23	0/3498	0.51	1/4750 (0.0%)
8	EG	0.24	0/3484	0.55	0/4731
8	EI	0.24	0/3477	0.52	0/4721
8	EK	0.22	0/3489	0.52	0/4737
8	EM	0.24	0/3425	0.52	0/4651
8	FC	0.26	0/3433	0.55	0/4662
8	FE	0.29	1/3398 (0.0%)	0.55	2/4613 (0.0%)
8	FG	0.26	0/3439	0.56	1/4670 (0.0%)
8	FI	0.27	0/3399	0.61	2/4615 (0.0%)
8	FK	0.24	0/3425	0.52	1/4650 (0.0%)
8	FM	0.25	0/3431	0.58	2/4658 (0.0%)
8	GC	0.26	0/3498	0.56	1/4750 (0.0%)
8	GE	0.29	2/3446 (0.1%)	0.58	5/4680 (0.1%)
8	GG	0.28	0/3460	0.56	2/4699 (0.0%)
8	GI	0.24	0/3474	0.53	1/4717 (0.0%)
8	GK	0.24	0/3439	0.52	0/4669
8	GM	0.27	0/3498	0.55	3/4750 (0.1%)
8	HC	0.23	0/3433	0.51	1/4662 (0.0%)
8	HE	0.25	0/3433	0.54	3/4662 (0.1%)
8	HG	0.25	0/3446	0.52	0/4680
8	HI	0.22	0/3438	0.51	0/4669
8	HK	0.29	0/3446	0.56	1/4680 (0.0%)
8	HM	0.21	0/3469	0.48	0/4710
8	HO	0.27	0/3101	0.54	1/4203 (0.0%)
8	IC	0.25	0/3460	0.53	1/4699 (0.0%)
8	IE	0.23	0/3439	0.50	0/4670
8	IG	0.22	0/3498	0.53	1/4750 (0.0%)
8	II	0.26	0/3447	0.55	0/4681
8	IK	0.32	0/3477	0.60	8/4721 (0.2%)
8	IM	0.23	0/3484	0.52	0/4731
8	IO	0.28	2/3424 (0.1%)	0.55	0/4649
8	JC	0.22	0/3458	0.48	1/4696 (0.0%)
8	JE	0.23	0/3439	0.51	1/4670 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	JG	0.21	0/3425	0.46	0/4651
8	JI	0.24	0/3433	0.50	0/4662
8	JK	0.22	0/3492	0.48	1/4742 (0.0%)
8	JM	0.22	0/3439	0.48	0/4670
8	KC	0.22	0/3465	0.48	0/4705
8	KE	0.23	0/3447	0.49	0/4681
8	KG	0.25	0/3437	0.48	0/4667
8	KI	0.21	0/3425	0.46	2/4651 (0.0%)
8	KK	0.23	0/3447	0.50	1/4681 (0.0%)
8	KM	0.21	0/3459	0.48	0/4696
8	KO	0.20	0/3302	0.49	0/4480
8	LC	0.23	0/3505	0.48	0/4760
8	LE	0.23	0/3542	0.47	1/4810 (0.0%)
8	LG	0.24	0/3505	0.50	1/4760 (0.0%)
8	LI	0.21	0/3542	0.46	0/4810
8	LK	0.22	0/3505	0.48	1/4760 (0.0%)
8	LM	0.20	0/3480	0.45	0/4726
8	MC	0.22	0/3498	0.47	0/4750
8	ME	0.24	0/3433	0.51	2/4662 (0.0%)
8	MG	0.22	0/3453	0.50	0/4689
8	MI	0.24	0/3445	0.53	1/4678 (0.0%)
8	MK	0.26	0/3505	0.52	0/4760
8	MM	0.27	0/3484	0.53	2/4732 (0.0%)
8	NA	0.28	0/3409	0.59	4/4630 (0.1%)
8	NC	0.24	0/3419	0.51	0/4643
8	NE	0.27	0/3439	0.54	0/4670
8	NG	0.21	0/3439	0.46	0/4670
8	NI	0.26	0/3433	0.54	2/4662 (0.0%)
8	NK	0.27	0/3433	0.59	2/4662 (0.0%)
8	OA	0.23	0/3425	0.51	0/4652
8	OC	0.23	0/3433	0.51	0/4662
8	OE	0.24	0/3454	0.53	0/4691
8	OG	0.29	0/3451	0.57	1/4686 (0.0%)
8	OI	0.24	0/3454	0.56	0/4691
8	OK	0.24	0/3441	0.55	1/4673 (0.0%)
8	PA	0.27	0/3439	0.59	3/4671 (0.1%)
8	PC	0.25	0/3461	0.59	0/4699
8	PE	0.58	2/3447 (0.1%)	0.86	9/4681 (0.2%)
8	PG	0.23	0/3460	0.57	1/4699 (0.0%)
8	PI	0.26	0/3417	0.56	0/4641
8	PK	0.23	0/3431	0.53	1/4659 (0.0%)
8	PM	0.27	0/3445	0.60	2/4678 (0.0%)
8	QA	0.46	2/3423 (0.1%)	0.71	5/4649 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	QC	0.60	5/3425 (0.1%)	0.74	8/4651 (0.2%)
8	QE	0.26	0/3439	0.57	1/4670 (0.0%)
8	QG	0.27	0/3447	0.59	3/4681 (0.1%)
8	QI	0.30	1/3425 (0.0%)	0.60	2/4651 (0.0%)
8	QK	0.36	2/3439 (0.1%)	0.69	7/4670 (0.1%)
8	QM	0.25	0/3445	0.58	0/4678
8	RA	0.26	0/3431	0.60	1/4660 (0.0%)
8	RC	0.27	1/3454 (0.0%)	0.54	0/4691
8	RE	0.30	0/3433	0.59	2/4662 (0.0%)
8	RG	0.26	0/3452	0.57	1/4688 (0.0%)
8	RI	0.30	0/3452	0.65	3/4688 (0.1%)
8	RK	0.48	2/3460 (0.1%)	0.70	5/4699 (0.1%)
8	RM	0.50	2/3424 (0.1%)	0.74	7/4649 (0.2%)
8	SA	0.24	0/3425	0.57	2/4652 (0.0%)
8	SC	0.30	0/3438	0.58	1/4668 (0.0%)
8	SE	0.32	0/3447	0.63	0/4680
8	SG	0.30	0/3446	0.58	0/4680
8	SI	0.32	0/3416	0.66	2/4639 (0.0%)
8	SK	0.27	0/3454	0.55	0/4691
8	SM	0.26	1/3439 (0.0%)	0.57	1/4670 (0.0%)
8	TC	0.26	0/3433	0.55	1/4662 (0.0%)
8	TE	0.27	0/3454	0.58	0/4691
8	TG	0.25	0/3431	0.54	0/4659
8	TI	0.30	0/3439	0.59	2/4670 (0.0%)
8	TK	0.28	0/3447	0.57	0/4681
8	TM	0.26	0/3439	0.57	2/4670 (0.0%)
8	UC	0.26	0/3447	0.56	1/4681 (0.0%)
8	UE	0.25	0/3447	0.53	2/4681 (0.0%)
8	UG	0.32	2/3451 (0.1%)	0.55	0/4686
8	UI	0.26	0/3447	0.54	0/4681
8	UK	0.25	1/3439 (0.0%)	0.55	1/4670 (0.0%)
8	UM	0.23	0/3433	0.52	1/4662 (0.0%)
8	VC	0.27	0/3477	0.58	1/4721 (0.0%)
8	VE	0.22	0/3441	0.53	1/4671 (0.0%)
8	VG	0.28	1/3498 (0.0%)	0.55	2/4750 (0.0%)
8	VI	0.22	0/3426	0.48	0/4652
8	VK	0.28	0/3484	0.55	0/4731
8	VM	0.25	0/3453	0.51	1/4689 (0.0%)
8	WC	0.59	2/3484 (0.1%)	0.81	6/4731 (0.1%)
8	WE	0.50	4/3437 (0.1%)	0.78	8/4667 (0.2%)
8	WG	0.24	0/3477	0.54	0/4721
8	WI	0.26	0/3433	0.55	1/4662 (0.0%)
8	WK	0.25	0/3484	0.56	5/4731 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	WM	0.27	0/3439	0.58	1/4670 (0.0%)
9	AB	0.23	0/3500	0.48	0/4742
9	AD	0.24	0/3500	0.50	1/4742 (0.0%)
9	AF	0.26	0/3500	0.52	1/4742 (0.0%)
9	AH	0.25	0/3500	0.53	1/4742 (0.0%)
9	AJ	0.23	0/3500	0.49	1/4742 (0.0%)
9	AL	0.25	0/3458	0.52	1/4687 (0.0%)
9	BB	0.29	0/3423	0.61	5/4638 (0.1%)
9	BD	0.24	0/3423	0.52	3/4638 (0.1%)
9	BF	0.32	2/3436 (0.1%)	0.60	5/4656 (0.1%)
9	BH	0.31	2/3431 (0.1%)	0.59	4/4649 (0.1%)
9	BJ	0.26	0/3431	0.53	0/4649
9	BL	0.29	0/3415	0.60	2/4628 (0.0%)
9	CB	0.25	0/3423	0.53	0/4638
9	CD	0.27	0/3414	0.53	1/4626 (0.0%)
9	CF	0.24	0/3423	0.52	0/4638
9	CH	0.25	0/3423	0.55	4/4638 (0.1%)
9	CJ	0.24	0/3423	0.55	2/4638 (0.0%)
9	CL	0.22	0/3415	0.49	0/4628
9	DB	0.25	0/3423	0.55	1/4638 (0.0%)
9	DD	0.27	1/3423 (0.0%)	0.59	2/4638 (0.0%)
9	DF	0.24	0/3423	0.53	1/4638 (0.0%)
9	DH	0.27	0/3423	0.56	0/4638
9	DJ	0.26	0/3423	0.60	0/4638
9	DL	0.22	0/3415	0.51	0/4628
9	DN	0.28	1/3102 (0.0%)	0.57	1/4201 (0.0%)
9	EB	0.31	2/3423 (0.1%)	0.60	3/4638 (0.1%)
9	ED	0.28	0/3423	0.59	4/4638 (0.1%)
9	EF	0.25	0/3423	0.54	1/4638 (0.0%)
9	EH	0.64	3/3431 (0.1%)	0.74	7/4649 (0.2%)
9	EJ	0.30	1/3423 (0.0%)	0.56	2/4638 (0.0%)
9	EL	0.24	0/3415	0.51	2/4628 (0.0%)
9	EN	0.22	0/3423	0.52	1/4638 (0.0%)
9	FB	0.32	2/3423 (0.1%)	0.61	3/4638 (0.1%)
9	FD	0.24	0/3431	0.58	3/4649 (0.1%)
9	FF	0.24	0/3423	0.51	1/4638 (0.0%)
9	FH	0.28	0/3436	0.59	1/4656 (0.0%)
9	FJ	0.30	0/3423	0.61	7/4638 (0.2%)
9	FL	0.21	0/3415	0.49	0/4628
9	FN	0.25	0/3436	0.55	3/4656 (0.1%)
9	GB	0.23	0/3436	0.51	1/4656 (0.0%)
9	GD	0.24	0/3431	0.52	0/4649
9	GF	0.24	0/3436	0.53	0/4656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	GH	0.25	0/3436	0.50	0/4656
9	GJ	0.24	0/3436	0.54	1/4656 (0.0%)
9	GL	0.27	0/3415	0.57	1/4628 (0.0%)
9	GN	0.24	0/3431	0.52	1/4649 (0.0%)
9	HB	0.24	0/3423	0.53	1/4638 (0.0%)
9	HD	0.28	0/3431	0.56	3/4649 (0.1%)
9	HF	0.27	0/3423	0.55	1/4638 (0.0%)
9	HH	0.22	0/3431	0.46	0/4649
9	HJ	0.27	0/3436	0.57	3/4656 (0.1%)
9	HL	0.22	0/3415	0.50	0/4628
9	HN	0.25	0/3431	0.51	0/4649
9	IB	0.35	0/2949	0.69	2/3989 (0.1%)
9	ID	0.24	0/3431	0.52	2/4649 (0.0%)
9	IF	0.24	0/3431	0.51	1/4649 (0.0%)
9	IH	0.22	0/3423	0.49	0/4638
9	IJ	0.26	0/3431	0.55	1/4649 (0.0%)
9	IL	0.24	0/3423	0.52	1/4638 (0.0%)
9	IN	0.25	0/3423	0.57	1/4638 (0.0%)
9	JB	0.25	0/3423	0.52	0/4638
9	JD	0.23	0/3431	0.47	0/4649
9	JF	0.22	0/3423	0.49	0/4638
9	JH	0.23	0/3423	0.49	0/4638
9	JJ	0.24	0/3423	0.49	0/4638
9	JL	0.26	0/3423	0.55	2/4638 (0.0%)
9	JN	0.20	0/3423	0.43	0/4638
9	KB	0.25	0/3232	0.49	0/4380
9	KD	0.23	0/3443	0.48	1/4666 (0.0%)
9	KF	0.23	0/3431	0.49	0/4649
9	KH	0.25	0/3443	0.51	0/4666
9	KJ	0.22	0/3423	0.48	1/4638 (0.0%)
9	KL	0.46	3/3443 (0.1%)	0.80	6/4666 (0.1%)
9	KN	0.22	0/3436	0.47	0/4656
9	LB	0.21	0/3509	0.47	1/4754 (0.0%)
9	LD	0.23	0/3431	0.52	2/4649 (0.0%)
9	LF	0.24	0/3500	0.46	0/4742
9	LH	0.19	0/3436	0.44	0/4656
9	LJ	0.23	0/3509	0.47	1/4754 (0.0%)
9	LL	0.21	0/3423	0.40	0/4638
9	LN	0.19	0/3509	0.44	0/4754
9	MB	0.22	0/3423	0.45	0/4638
9	MD	0.23	0/3443	0.46	0/4666
9	MF	0.22	0/3443	0.47	0/4666
9	MH	0.21	0/3443	0.43	0/4666

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	MJ	0.26	0/3423	0.53	5/4638 (0.1%)
9	ML	0.24	1/3443 (0.0%)	0.49	1/4666 (0.0%)
9	MN	0.20	0/3443	0.44	1/4666 (0.0%)
9	N0	0.23	0/3414	0.53	2/4626 (0.0%)
9	NB	0.30	1/3423 (0.0%)	0.61	6/4638 (0.1%)
9	ND	0.24	0/3431	0.55	2/4649 (0.0%)
9	NF	0.25	0/3423	0.54	2/4638 (0.0%)
9	NH	0.35	2/3436 (0.1%)	0.63	4/4656 (0.1%)
9	NJ	0.25	0/3436	0.55	1/4656 (0.0%)
9	NL	0.26	0/3414	0.59	7/4626 (0.2%)
9	O0	0.28	0/3142	0.59	2/4253 (0.0%)
9	OB	0.25	0/3431	0.54	1/4649 (0.0%)
9	OD	0.25	0/3401	0.54	1/4608 (0.0%)
9	OF	0.27	0/3414	0.53	0/4626
9	OH	0.25	0/3436	0.57	1/4656 (0.0%)
9	OJ	0.29	0/3431	0.58	3/4649 (0.1%)
9	OL	0.27	0/3401	0.57	1/4608 (0.0%)
9	PB	0.25	0/3431	0.58	2/4649 (0.0%)
9	PD	0.29	0/3431	0.58	0/4649
9	PF	0.65	4/3431 (0.1%)	0.81	5/4649 (0.1%)
9	PH	0.26	0/3431	0.52	0/4649
9	PJ	0.23	0/3436	0.53	0/4656
9	PL	0.30	0/3415	0.64	6/4628 (0.1%)
9	QB	0.24	0/3436	0.56	2/4656 (0.0%)
9	QD	0.28	0/3431	0.64	7/4649 (0.2%)
9	QF	0.59	4/3431 (0.1%)	0.91	12/4649 (0.3%)
9	QH	0.25	1/3423 (0.0%)	0.54	1/4638 (0.0%)
9	QJ	0.26	0/3423	0.60	3/4638 (0.1%)
9	QL	0.31	0/3423	0.64	3/4638 (0.1%)
9	RB	0.32	0/3436	0.64	3/4656 (0.1%)
9	RD	0.52	3/3431 (0.1%)	0.78	10/4649 (0.2%)
9	RF	0.51	4/3431 (0.1%)	0.80	7/4649 (0.2%)
9	RH	0.64	6/3436 (0.2%)	0.73	6/4656 (0.1%)
9	RJ	0.63	5/3436 (0.1%)	0.80	9/4656 (0.2%)
9	RL	0.52	4/3423 (0.1%)	0.77	12/4638 (0.3%)
9	SB	0.38	2/3436 (0.1%)	0.63	1/4656 (0.0%)
9	SD	0.28	0/3431	0.60	1/4649 (0.0%)
9	SF	0.27	0/3436	0.59	0/4656
9	SH	0.40	2/3436 (0.1%)	0.65	7/4656 (0.2%)
9	SJ	0.31	1/3436 (0.0%)	0.63	5/4656 (0.1%)
9	SL	0.24	0/3423	0.55	2/4638 (0.0%)
9	TB	0.31	0/3431	0.65	4/4649 (0.1%)
9	TD	0.26	0/3431	0.56	1/4649 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	TF	0.27	0/3436	0.58	1/4656 (0.0%)
9	TH	0.30	0/3436	0.60	3/4656 (0.1%)
9	TJ	0.31	0/3436	0.59	0/4656
9	TL	0.27	0/3423	0.58	2/4638 (0.0%)
9	UB	0.30	0/3423	0.65	2/4638 (0.0%)
9	UD	0.30	0/3431	0.65	4/4649 (0.1%)
9	UF	0.25	0/3431	0.54	1/4649 (0.0%)
9	UH	0.24	0/3431	0.55	1/4649 (0.0%)
9	UJ	0.33	2/3431 (0.1%)	0.63	3/4649 (0.1%)
9	UL	0.24	0/3423	0.55	0/4638
9	UN	0.27	0/3431	0.54	0/4649
9	VB	0.28	0/3423	0.59	0/4638
9	VD	0.28	0/3423	0.57	0/4638
9	VF	0.66	5/3423 (0.1%)	0.85	9/4638 (0.2%)
9	VH	0.28	0/3436	0.60	4/4656 (0.1%)
9	VJ	0.29	0/3423	0.59	0/4638
9	VL	0.28	1/3423 (0.0%)	0.57	2/4638 (0.0%)
9	VN	0.29	0/3423	0.60	2/4638 (0.0%)
9	WB	0.24	0/3423	0.55	1/4638 (0.0%)
9	WD	0.24	0/3423	0.53	1/4638 (0.0%)
9	WF	0.29	2/3423 (0.1%)	0.58	4/4638 (0.1%)
9	WH	0.28	0/3423	0.55	2/4638 (0.0%)
9	WJ	0.26	0/3423	0.55	3/4638 (0.1%)
9	WL	0.27	0/3423	0.57	2/4638 (0.0%)
9	WN	0.27	0/3423	0.61	5/4638 (0.1%)
10	AP	0.22	0/949	0.46	0/1291
10	AQ	0.25	0/949	0.50	0/1291
10	AR	0.21	0/756	0.51	1/1027 (0.1%)
10	AS	0.19	0/949	0.48	0/1291
11	AT	0.37	0/2539	0.61	2/3368 (0.1%)
11	AU	0.37	0/1868	0.63	0/2471
12	AV	0.26	0/2964	0.55	2/4002 (0.0%)
12	AW	0.29	0/3011	0.58	3/4065 (0.1%)
13	Aa	0.27	0/4935	0.58	1/6639 (0.0%)
13	Ab	0.33	2/5047 (0.0%)	0.66	7/6797 (0.1%)
13	Ac	0.24	0/5061	0.57	0/6815
13	Ad	0.25	0/4337	0.63	5/5847 (0.1%)
14	Al	0.32	0/348	0.66	0/475
14	Am	0.23	0/348	0.61	0/475
14	An	0.24	0/348	0.56	0/475
14	Ao	0.33	0/598	0.77	2/812 (0.2%)
14	B7	0.26	0/704	0.60	0/952
14	BY	0.25	0/889	0.66	1/1198 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
14	BZ	0.27	0/889	0.64	2/1198 (0.2%)
14	Ba	0.27	0/1641	0.58	0/2220
14	Bb	0.28	0/1641	0.67	2/2220 (0.1%)
14	Bc	0.27	0/1628	0.55	0/2202
14	Bd	0.18	0/889	0.43	0/1198
14	Be	0.22	0/889	0.50	0/1198
14	CN	0.34	0/688	0.61	0/930
14	CO	0.26	0/715	0.72	0/966
15	Ap	0.26	0/1140	0.58	0/1547
15	Aq	0.25	0/794	0.50	0/1079
15	Ar	0.25	0/1300	0.57	1/1767 (0.1%)
16	At	0.30	0/800	0.65	0/1092
16	Ax	0.34	1/956 (0.1%)	0.70	1/1309 (0.1%)
17	B0	0.29	0/380	0.72	0/519
17	B1	0.30	0/312	0.58	0/428
17	B2	0.28	0/317	0.60	0/430
17	B3	0.14	0/205	0.36	0/274
17	B4	0.17	0/313	0.50	0/422
17	B8	0.19	0/328	0.48	0/441
17	B9	0.19	0/319	0.48	0/438
17	CQ	0.19	0/380	0.48	0/519
17	CR	0.18	0/328	0.44	0/450
17	CS	0.24	0/319	0.64	0/438
18	B5	0.27	0/2053	0.59	1/2757 (0.0%)
18	B6	0.23	0/2087	0.49	0/2804
18	By	0.28	0/1338	0.63	0/1792
18	Bz	0.34	2/2053 (0.1%)	0.60	1/2757 (0.0%)
19	BO	0.47	3/1848 (0.2%)	0.80	5/2489 (0.2%)
19	BP	0.33	0/3450	0.62	1/4641 (0.0%)
19	BQ	0.29	0/3030	0.57	0/4067
19	BR	0.34	0/3524	0.65	2/4742 (0.0%)
20	BS	0.25	0/1229	0.63	1/1679 (0.1%)
20	BT	0.29	0/1941	0.66	1/2637 (0.0%)
21	BU	0.22	0/310	0.59	0/411
21	BV	0.24	0/3125	0.39	0/4176
21	Bi	0.15	0/356	0.26	0/475
21	Bj	0.33	0/2051	0.55	1/2740 (0.0%)
21	Bk	0.31	0/1459	0.52	1/1949 (0.1%)
22	BW	0.27	0/1648	0.58	0/2254
22	BX	0.32	0/436	0.78	1/589 (0.2%)
23	Bf	0.30	0/522	0.60	2/707 (0.3%)
23	Bg	0.28	0/981	0.63	0/1334
24	Bh	0.23	0/802	0.50	0/1094

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
26	Bq	0.29	0/816	0.64	2/1125 (0.2%)
26	Bu	0.20	0/1219	0.53	2/1664 (0.1%)
27	Br	0.39	0/1386	0.64	0/1839
27	Bs	0.37	1/3070 (0.0%)	0.64	2/4068 (0.0%)
28	C0	0.28	0/857	0.51	1/1154 (0.1%)
28	C2	0.26	0/3358	0.49	1/4529 (0.0%)
28	C3	0.27	0/3358	0.47	0/4529
28	C4	0.27	0/2819	0.49	0/3802
28	C5	0.33	0/1860	0.52	1/2502 (0.0%)
28	C6	0.23	0/361	0.47	0/490
28	C7	0.25	0/3501	0.47	0/4723
28	C8	0.26	0/3493	0.48	0/4711
28	C9	0.30	0/3125	0.47	0/4209
28	DO	0.26	0/1061	0.49	0/1436
28	F2	0.26	0/3462	0.44	2/4675 (0.0%)
28	F3	0.29	0/3452	0.49	0/4661
28	F4	0.31	0/3178	0.51	4/4281 (0.1%)
28	F5	0.24	0/879	0.41	0/1183
28	F6	0.32	0/1072	0.51	0/1456
29	C1	0.35	2/2741 (0.1%)	0.59	1/3684 (0.0%)
29	Cz	0.46	1/2461 (0.0%)	0.72	6/3304 (0.2%)
29	D0	0.34	0/573	0.74	1/770 (0.1%)
29	D1	0.32	0/2962	0.59	2/3975 (0.1%)
29	D2	0.30	0/3204	0.49	0/4302
29	D3	0.33	0/3195	0.59	3/4291 (0.1%)
29	D4	0.33	0/3187	0.61	1/4280 (0.0%)
29	D5	0.38	1/2990 (0.0%)	0.68	3/4011 (0.1%)
29	D6	0.31	0/1227	0.57	0/1646
29	D7	0.30	0/608	0.59	0/818
29	D8	0.29	0/3204	0.52	1/4302 (0.0%)
29	D9	0.33	0/1324	0.62	0/1776
29	DP	0.35	0/1688	0.61	0/2261
29	DQ	0.31	0/2431	0.60	1/3258 (0.0%)
29	DR	0.33	0/2170	0.57	1/2910 (0.0%)
29	DS	0.33	0/2136	0.61	3/2864 (0.1%)
29	DT	0.34	1/1391 (0.1%)	0.71	3/1872 (0.2%)
29	DU	0.28	0/2526	0.53	0/3388
29	DV	0.31	0/2531	0.58	0/3395
29	DW	0.35	0/2531	0.69	4/3395 (0.1%)
29	DX	0.35	0/1911	0.61	2/2561 (0.1%)
29	EA	0.30	0/3298	0.54	1/4431 (0.0%)
29	EO	0.29	0/3290	0.52	0/4420
29	EP	0.41	1/2973 (0.0%)	0.69	6/3989 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	EQ	0.37	0/1470	0.73	1/1976 (0.1%)
29	ER	0.23	0/364	0.41	0/487
30	CW	0.23	0/1354	0.53	0/1838
31	Cl	0.26	0/1003	0.56	0/1368
32	Cm	0.31	0/3304	0.54	2/4451 (0.0%)
32	Cn	0.30	0/3326	0.51	1/4480 (0.0%)
32	Co	0.35	0/2878	0.51	1/3873 (0.0%)
32	Cp	0.34	0/1708	0.61	0/2298
33	Cq	0.28	0/3471	0.47	0/4682
33	Cr	0.32	1/3429 (0.0%)	0.48	1/4623 (0.0%)
33	Cs	0.31	0/1517	0.53	0/2044
33	Ct	0.29	0/3183	0.49	0/4289
33	Cu	0.29	0/3091	0.53	0/4165
33	Cv	0.32	1/3480 (0.0%)	0.51	2/4693 (0.0%)
33	Cw	0.32	0/3480	0.58	1/4693 (0.0%)
33	Cx	0.31	0/1632	0.54	0/2200
33	Cy	0.34	0/369	0.53	0/497
34	D	0.35	0/554	0.72	0/753
35	DY	0.31	0/313	0.53	0/420
35	DZ	0.20	0/422	0.50	0/565
35	Da	0.26	0/1129	0.44	1/1531 (0.1%)
35	Ee	0.19	0/400	0.39	0/543
36	Db	0.22	0/465	0.64	0/632
36	Dc	0.28	0/457	0.67	0/621
36	Dd	0.21	0/420	0.55	0/572
37	De	0.34	0/558	0.62	0/749
38	Df	0.22	0/1099	0.56	0/1500
38	Dg	0.26	0/1014	0.51	1/1376 (0.1%)
38	Dh	0.28	0/901	0.61	1/1224 (0.1%)
39	Di	0.22	0/651	0.55	0/875
39	Dj	0.19	0/829	0.48	0/1115
39	Dk	0.22	0/829	0.55	0/1115
39	Dl	0.23	0/829	0.59	0/1115
40	Dm	0.30	0/747	0.54	0/1012
41	Dn	0.27	0/476	0.61	0/637
42	E	0.85	4/1203 (0.3%)	1.19	10/1625 (0.6%)
42	F	0.29	0/3776	0.71	3/5106 (0.1%)
43	E1	0.23	0/1714	0.55	1/2351 (0.0%)
43	E2	0.21	0/1714	0.53	1/2351 (0.0%)
43	E3	0.28	0/1707	0.59	2/2340 (0.1%)
43	E4	0.28	0/1271	0.59	1/1744 (0.1%)
44	ES	0.29	0/3537	0.48	0/4765
44	ET	0.26	0/2311	0.44	0/3120

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
44	EU	0.29	0/2725	0.54	4/3664 (0.1%)
44	EV	0.33	0/3537	0.52	2/4765 (0.0%)
44	EW	0.32	0/2644	0.57	0/3569
44	EX	0.31	0/3617	0.54	2/4879 (0.0%)
44	EY	0.32	0/2586	0.55	1/3481 (0.0%)
44	EZ	0.28	0/3672	0.52	2/4954 (0.0%)
45	G	0.30	0/2380	0.69	2/3223 (0.1%)
46	H	0.37	0/860	0.60	0/1149
46	o	0.35	0/3439	0.70	5/4555 (0.1%)
47	I	0.20	0/3783	0.46	0/5118
47	X	0.29	2/3788 (0.1%)	0.59	5/5125 (0.1%)
47	Y	0.52	3/3840 (0.1%)	0.65	6/5196 (0.1%)
48	J	0.27	0/974	0.63	0/1315
48	K	0.23	0/974	0.52	0/1315
48	L	0.84	2/914 (0.2%)	1.05	4/1235 (0.3%)
48	M	0.39	0/746	0.82	4/1007 (0.4%)
49	K1	0.33	0/1019	0.73	0/1379
50	L1	0.33	0/1121	0.73	0/1514
50	L2	0.24	0/763	0.66	0/1031
51	N	0.27	0/1207	0.64	0/1631
51	O	0.27	0/1169	0.62	1/1581 (0.1%)
52	P	0.37	0/897	0.85	3/1219 (0.2%)
53	Q	0.25	0/955	0.56	1/1300 (0.1%)
54	R	0.22	0/1190	0.60	1/1603 (0.1%)
54	S	0.23	0/1190	0.55	1/1603 (0.1%)
54	T	0.27	0/1193	0.65	0/1606
54	U	0.25	0/843	0.64	0/1138
55	W	0.24	0/1017	0.61	2/1365 (0.1%)
56	XG	0.21	0/1544	0.51	1/2082 (0.0%)
56	XH	0.24	0/1544	0.53	0/2082
56	XI	0.24	0/1544	0.54	1/2082 (0.0%)
56	XJ	0.19	0/1544	0.49	0/2082
56	XK	0.29	0/1544	0.59	0/2082
56	XL	0.19	0/1535	0.46	0/2071
56	XM	0.31	0/1525	0.77	7/2056 (0.3%)
57	YG	0.27	0/1748	0.59	0/2360
57	YH	0.25	0/1802	0.51	0/2435
57	YI	0.25	0/1802	0.52	1/2435 (0.0%)
57	YJ	0.30	1/1802 (0.1%)	0.57	1/2435 (0.0%)
57	YK	0.26	0/1802	0.58	1/2435 (0.0%)
57	YL	0.39	0/1802	0.73	5/2435 (0.2%)
58	Z	0.20	0/1031	0.44	0/1372
58	p	0.35	0/466	0.53	1/616 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
58	q	0.20	0/841	0.48	0/1121
59	a	0.47	1/1570 (0.1%)	0.81	4/2088 (0.2%)
59	b	0.34	0/2828	0.70	1/3738 (0.0%)
59	c	0.33	0/2540	0.68	2/3369 (0.1%)
59	d	0.37	0/1738	0.66	1/2298 (0.0%)
60	e	0.25	0/4821	0.61	3/6527 (0.0%)
60	f	0.24	0/4812	0.56	0/6515
60	g	0.25	0/4812	0.59	4/6515 (0.1%)
61	h	0.25	0/801	0.49	0/1073
62	i	0.26	0/2105	0.50	0/2851
62	j	0.25	0/2211	0.50	0/2997
63	k	0.23	0/1275	0.55	1/1727 (0.1%)
63	l	0.22	0/1124	0.57	1/1522 (0.1%)
63	m	0.19	0/1294	0.50	0/1753
63	n	0.29	0/928	0.66	1/1255 (0.1%)
64	ke	0.23	0/820	0.52	0/1109
65	r	0.25	0/630	0.57	0/849
65	s	0.30	0/639	0.50	0/861
65	t	0.23	0/639	0.44	0/861
66	u	0.23	0/1107	0.46	0/1491
66	v	0.23	0/982	0.50	0/1327
66	w	0.23	0/1107	0.48	0/1491
All	All	0.30	158/1475221 (0.0%)	0.58	847/1997530 (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	V	0	1
2	0C	0	3
2	0E	0	2
2	0Y	0	1
2	0a	0	1
2	0c	0	1
2	0g	0	2
2	0i	0	3
2	CT	0	2
2	CY	0	1
2	Cb	0	3
2	Ci	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	A0	0	2
7	A5	0	1
7	A7	0	3
7	A8	0	4
7	A9	0	1
7	Aw	0	1
7	Ay	0	2
8	AG	0	1
8	AI	0	1
8	BE	0	1
8	BM	0	1
8	CK	0	1
8	EI	0	1
8	EK	0	1
8	FE	0	1
8	FK	0	1
8	GG	0	1
8	GK	0	2
8	HO	0	1
8	IC	0	1
8	IE	0	1
8	IG	0	1
8	IK	0	2
8	KE	0	1
8	KI	0	1
8	LC	0	1
8	LK	0	1
8	ME	0	1
8	MK	0	1
8	NC	0	1
8	NI	0	1
8	NK	0	1
8	OE	0	1
8	OG	0	1
8	PA	0	1
8	PC	0	1
8	PI	0	1
8	QA	0	1
8	RA	0	1
8	RI	0	2
8	RK	0	1
8	SG	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	SK	0	1
8	TI	0	2
8	UE	0	1
8	WI	0	1
9	DH	0	1
9	ED	0	1
9	EJ	0	1
9	EL	0	2
9	FB	0	2
9	FH	0	1
9	FJ	0	1
9	GD	0	1
9	GF	0	2
9	GH	0	1
9	GJ	0	1
9	GL	0	1
9	HB	0	1
9	HD	0	1
9	HJ	0	1
9	IN	0	1
9	MD	0	1
9	MF	0	1
9	NF	0	1
9	NL	0	1
9	O0	0	1
9	OL	0	1
9	PH	0	1
9	PJ	0	2
9	RF	0	1
9	RH	0	3
9	RL	0	1
9	SD	0	1
9	TL	0	1
9	UJ	0	1
9	UL	0	1
9	VB	0	1
9	WJ	0	1
11	AT	0	1
13	Aa	0	1
13	Ab	0	1
13	Ac	0	2
13	Ad	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	Al	0	1
14	BY	0	1
14	Bb	0	1
15	Ap	0	1
15	Ar	0	1
18	Bz	0	1
19	BR	0	1
21	Bj	0	1
28	F2	0	1
28	F6	0	1
29	D4	0	2
29	DP	0	1
29	EP	0	1
32	Co	0	1
33	Ct	0	1
42	E	0	1
42	F	0	2
43	E2	0	1
43	E4	0	1
44	ES	0	1
44	EX	0	2
45	G	0	2
46	H	0	1
46	o	0	1
47	I	0	2
47	Y	0	1
48	J	0	1
49	K1	0	1
50	L1	0	3
51	O	0	1
56	XI	0	1
57	YL	0	1
59	a	0	2
59	b	0	3
59	d	0	2
60	f	0	1
65	s	0	1
All	All	0	172

The worst 5 of 158 bond length outliers are listed below:

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	PF	80	PRO	CG-CD	-30.41	0.47	1.50
8	WC	268	PRO	CG-CD	-28.60	0.53	1.50
9	EH	268	PRO	CG-CD	-27.70	0.56	1.50
9	RJ	268	PRO	CG-CD	-26.93	0.59	1.50
9	VF	261	PRO	CB-CG	26.51	2.82	1.49

The worst 5 of 847 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	KL	220	PRO	N-CD-CG	-34.16	51.96	103.20
9	PF	80	PRO	N-CD-CG	-32.94	53.79	103.20
9	QF	272	PRO	N-CD-CG	-32.79	54.01	103.20
8	WC	268	PRO	N-CD-CG	-32.30	54.76	103.20
8	DE	268	PRO	N-CD-CG	-28.57	60.35	103.20

There are no chirality outliers.

5 of 172 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	0C	118	TYR	Peptide
2	0C	33	CYS	Peptide
2	0C	55	GLU	Peptide
2	0E	118	TYR	Peptide
2	0E	58	CYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	330	0	317	2	0
1	V	1487	0	1428	46	0
2	0A	1252	0	1232	26	0
2	0C	1252	0	1232	27	0
2	0E	1260	0	1244	30	0
2	0G	1252	0	1232	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	0W	1252	0	1232	11	0
2	0Y	1252	0	1232	26	0
2	0a	1252	0	1232	27	0
2	0c	1252	0	1232	26	0
2	0e	1244	0	1223	21	0
2	0g	1252	0	1232	26	0
2	0i	1252	0	1232	38	0
2	0k	1252	0	1232	32	0
2	CT	1260	0	1244	31	0
2	CU	1244	0	1223	30	0
2	CV	1252	0	1232	33	0
2	CX	1252	0	1232	34	0
2	CY	1252	0	1232	24	0
2	CZ	1252	0	1232	19	0
2	Ca	1252	0	1232	23	0
2	Cb	1252	0	1232	32	0
2	Cc	1252	0	1232	24	0
2	Cd	1252	0	1232	26	0
2	Ce	1244	0	1223	19	0
2	Cf	1244	0	1223	27	0
2	Cg	1252	0	1232	25	0
2	Ch	1252	0	1232	14	0
2	Ci	1252	0	1232	30	0
2	Cj	1244	0	1223	28	0
2	Ck	1252	0	1232	39	0
3	1	1700	0	1698	32	0
3	2	2027	0	2056	38	0
3	x	2027	0	2056	48	0
4	3	1469	0	1476	26	0
4	y	1469	0	1476	16	0
4	z	1469	0	1476	24	0
5	A	338	0	340	8	0
5	B	751	0	746	28	0
5	C	751	0	746	21	0
6	A0	1017	0	1002	44	0
6	BN	614	0	605	18	0
7	A1	1828	0	1841	69	0
7	A2	385	0	393	13	0
7	A3	1200	0	524	21	0
7	A4	546	0	243	21	0
7	A5	762	0	329	14	0
7	A6	369	0	368	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A7	1726	0	1752	73	0
7	A8	1281	0	1280	56	0
7	A9	879	0	891	20	0
7	Au	540	0	547	14	0
7	Av	1126	0	1130	47	0
7	Aw	1009	0	1021	32	0
7	Ay	1412	0	1408	43	0
7	Az	313	0	324	10	0
8	AA	3413	0	3329	60	0
8	AC	3428	0	3350	55	0
8	AE	3428	0	3350	67	0
8	AG	3428	0	3350	47	0
8	AI	3428	0	3350	48	0
8	AK	3428	0	3350	60	0
8	AM	3421	0	3341	47	0
8	BA	3355	0	3275	80	0
8	BC	3415	0	3336	61	0
8	BE	3363	0	3287	59	0
8	BG	3421	0	3341	66	0
8	BI	3357	0	3282	72	0
8	BK	3407	0	3332	76	0
8	BM	3363	0	3287	61	0
8	CA	3407	0	3324	76	0
8	CC	3415	0	3336	78	0
8	CE	3415	0	3336	73	0
8	CG	3400	0	3323	67	0
8	CI	3415	0	3336	56	0
8	CK	3415	0	3336	74	0
8	CM	3415	0	3336	63	0
8	DA	2965	0	2916	79	0
8	DC	3349	0	3278	80	0
8	DE	3349	0	3278	78	0
8	DG	3370	0	3295	60	0
8	DI	3348	0	3274	83	0
8	DK	3342	0	3267	72	0
8	DM	3342	0	3269	81	0
8	EC	3392	0	3316	89	0
8	EE	3421	0	3341	75	0
8	EG	3407	0	3332	72	0
8	EI	3400	0	3323	68	0
8	EK	3413	0	3334	88	0
8	EM	3349	0	3277	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	FC	3357	0	3282	79	0
8	FE	3323	0	3254	78	0
8	FG	3363	0	3287	87	0
8	FI	3325	0	3257	97	0
8	FK	3350	0	3275	74	0
8	FM	3356	0	3280	49	0
8	GC	3421	0	3341	68	0
8	GE	3370	0	3296	53	0
8	GG	3384	0	3305	66	0
8	GI	3398	0	3320	71	0
8	GK	3364	0	3284	61	0
8	GM	3421	0	3341	65	0
8	HC	3357	0	3282	55	0
8	HE	3357	0	3282	72	0
8	HG	3370	0	3296	63	0
8	HI	3362	0	3292	59	0
8	HK	3370	0	3296	71	0
8	HM	3393	0	3316	43	0
8	HO	3035	0	2964	63	0
8	IC	3384	0	3305	57	0
8	IE	3363	0	3287	49	0
8	IG	3421	0	3341	61	0
8	II	3371	0	3291	60	0
8	IK	3400	0	3323	79	0
8	IM	3407	0	3332	46	0
8	IO	3348	0	3274	63	0
8	JC	3382	0	3303	54	0
8	JE	3363	0	3287	48	0
8	JG	3349	0	3278	50	0
8	JI	3357	0	3282	56	0
8	JK	3415	0	3336	68	0
8	JM	3363	0	3287	55	0
8	KC	3389	0	3303	56	0
8	KE	3371	0	3291	46	0
8	KG	3361	0	3285	65	0
8	KI	3349	0	3278	49	0
8	KK	3371	0	3291	33	0
8	KM	3383	0	3300	33	0
8	KO	3229	0	3135	49	0
8	LC	3428	0	3350	64	0
8	LE	3465	0	3378	28	0
8	LG	3428	0	3350	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	LI	3465	0	3378	42	0
8	LK	3428	0	3350	49	0
8	LM	3404	0	3323	45	0
8	MC	3421	0	3341	43	0
8	ME	3357	0	3282	62	0
8	MG	3377	0	3295	60	0
8	MI	3369	0	3292	62	0
8	MK	3428	0	3350	61	0
8	MM	3407	0	3324	62	0
8	NA	3333	0	3262	61	0
8	NC	3343	0	3273	81	0
8	NE	3363	0	3287	54	0
8	NG	3363	0	3287	64	0
8	NI	3357	0	3282	68	0
8	NK	3357	0	3282	67	0
8	OA	3349	0	3270	66	0
8	OC	3357	0	3282	90	0
8	OE	3378	0	3300	84	0
8	OG	3375	0	3294	73	0
8	OI	3378	0	3300	77	0
8	OK	3365	0	3286	69	0
8	PA	3363	0	3279	64	0
8	PC	3385	0	3302	92	0
8	PE	3371	0	3291	89	0
8	PG	3384	0	3305	80	0
8	PI	3341	0	3266	82	0
8	PK	3355	0	3283	65	0
8	PM	3369	0	3292	68	0
8	QA	3347	0	3271	65	0
8	QC	3349	0	3278	98	0
8	QE	3363	0	3287	87	0
8	QG	3371	0	3290	88	0
8	QI	3349	0	3278	101	0
8	QK	3363	0	3286	88	0
8	QM	3369	0	3292	93	0
8	RA	3355	0	3274	93	0
8	RC	3378	0	3299	86	0
8	RE	3357	0	3282	87	0
8	RG	3376	0	3301	81	0
8	RI	3376	0	3301	98	0
8	RK	3384	0	3305	83	0
8	RM	3348	0	3274	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	SA	3349	0	3269	77	0
8	SC	3363	0	3288	95	0
8	SE	3372	0	3295	106	0
8	SG	3370	0	3296	81	0
8	SI	3341	0	3263	93	0
8	SK	3378	0	3300	78	0
8	SM	3363	0	3286	84	0
8	TC	3357	0	3282	71	0
8	TE	3378	0	3300	89	0
8	TG	3355	0	3283	66	0
8	TI	3363	0	3287	66	0
8	TK	3371	0	3291	82	0
8	TM	3363	0	3287	75	0
8	UC	3371	0	3291	53	0
8	UE	3371	0	3291	63	0
8	UG	3375	0	3294	45	0
8	UI	3371	0	3291	55	0
8	UK	3363	0	3287	67	0
8	UM	3357	0	3282	59	0
8	VC	3400	0	3323	67	0
8	VE	3365	0	3291	77	0
8	VG	3421	0	3341	83	0
8	VI	3350	0	3273	74	0
8	VK	3407	0	3332	84	0
8	VM	3377	0	3296	59	0
8	WC	3407	0	3332	76	0
8	WE	3361	0	3285	68	0
8	WG	3400	0	3323	71	0
8	WI	3357	0	3282	77	0
8	WK	3407	0	3332	80	0
8	WM	3363	0	3287	65	0
9	AB	3424	0	3290	46	0
9	AD	3424	0	3291	76	0
9	AF	3424	0	3292	68	0
9	AH	3424	0	3290	71	0
9	AJ	3424	0	3291	61	0
9	AL	3383	0	3256	69	0
9	BB	3348	0	3235	75	0
9	BD	3348	0	3235	65	0
9	BF	3361	0	3244	70	0
9	BH	3356	0	3239	50	0
9	BJ	3356	0	3239	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	BL	3340	0	3223	80	0
9	CB	3348	0	3235	83	0
9	CD	3339	0	3226	68	0
9	CF	3348	0	3236	64	0
9	CH	3348	0	3234	76	0
9	CJ	3348	0	3234	84	0
9	CL	3340	0	3222	69	0
9	DB	3348	0	3236	97	0
9	DD	3348	0	3236	77	0
9	DF	3348	0	3233	77	0
9	DH	3348	0	3236	103	0
9	DJ	3348	0	3236	91	0
9	DL	3340	0	3224	69	0
9	DN	3035	0	2929	66	0
9	EB	3348	0	3235	87	0
9	ED	3348	0	3235	72	0
9	EF	3348	0	3235	73	0
9	EH	3356	0	3239	82	0
9	EJ	3348	0	3235	75	0
9	EL	3340	0	3223	62	0
9	EN	3348	0	3235	67	0
9	FB	3348	0	3236	83	0
9	FD	3356	0	3240	67	0
9	FF	3348	0	3236	69	0
9	FH	3361	0	3245	74	0
9	FJ	3348	0	3236	68	0
9	FL	3340	0	3224	70	0
9	FN	3361	0	3245	68	0
9	GB	3361	0	3245	53	0
9	GD	3356	0	3240	48	0
9	GF	3361	0	3245	64	0
9	GH	3361	0	3245	75	0
9	GJ	3361	0	3243	62	0
9	GL	3340	0	3224	73	0
9	GN	3356	0	3240	53	0
9	HB	3348	0	3236	58	0
9	HD	3356	0	3240	67	0
9	HF	3348	0	3236	77	0
9	HH	3356	0	3240	59	0
9	HJ	3361	0	3245	71	0
9	HL	3340	0	3223	62	0
9	HN	3356	0	3238	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	IB	2892	0	2820	54	0
9	ID	3356	0	3240	65	0
9	IF	3356	0	3240	61	0
9	IH	3348	0	3236	74	0
9	IJ	3356	0	3240	76	0
9	IL	3348	0	3236	73	0
9	IN	3348	0	3235	73	0
9	JB	3348	0	3236	62	0
9	JD	3356	0	3240	70	0
9	JF	3348	0	3236	66	0
9	JH	3348	0	3236	64	0
9	JJ	3348	0	3236	61	0
9	JL	3348	0	3236	77	0
9	JN	3348	0	3236	47	0
9	KB	3165	0	3063	53	0
9	KD	3368	0	3252	69	0
9	KF	3356	0	3240	58	0
9	KH	3368	0	3252	64	0
9	KJ	3348	0	3236	52	0
9	KL	3368	0	3252	54	0
9	KN	3361	0	3245	51	0
9	LB	3433	0	3299	52	0
9	LD	3356	0	3240	66	0
9	LF	3424	0	3293	47	0
9	LH	3361	0	3245	50	0
9	LJ	3433	0	3299	44	0
9	LL	3348	0	3236	59	0
9	LN	3433	0	3299	66	0
9	MB	3348	0	3236	56	0
9	MD	3368	0	3252	62	0
9	MF	3368	0	3252	74	0
9	MH	3368	0	3252	56	0
9	MJ	3348	0	3236	61	0
9	ML	3368	0	3252	56	0
9	MN	3368	0	3252	58	0
9	N0	3339	0	3228	86	0
9	NB	3348	0	3235	54	0
9	ND	3356	0	3240	66	0
9	NF	3348	0	3234	72	0
9	NH	3361	0	3245	79	0
9	NJ	3361	0	3245	62	0
9	NL	3339	0	3228	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	O0	3078	0	2980	68	0
9	OB	3356	0	3240	70	0
9	OD	3327	0	3219	71	0
9	OF	3339	0	3225	82	0
9	OH	3361	0	3244	80	0
9	OJ	3356	0	3240	74	0
9	OL	3327	0	3219	79	0
9	PB	3356	0	3240	81	0
9	PD	3356	0	3238	103	0
9	PF	3356	0	3240	83	0
9	PH	3356	0	3240	83	0
9	PJ	3361	0	3245	105	0
9	PL	3340	0	3224	69	0
9	QB	3361	0	3244	94	0
9	QD	3356	0	3238	91	0
9	QF	3356	0	3239	100	0
9	QH	3348	0	3235	103	0
9	QJ	3348	0	3235	105	0
9	QL	3348	0	3235	113	0
9	RB	3361	0	3243	111	0
9	RD	3356	0	3240	97	0
9	RF	3356	0	3240	76	0
9	RH	3361	0	3245	92	0
9	RJ	3361	0	3245	111	0
9	RL	3348	0	3236	109	0
9	SB	3361	0	3245	83	0
9	SD	3356	0	3240	82	0
9	SF	3361	0	3243	85	0
9	SH	3361	0	3245	76	0
9	SJ	3361	0	3245	87	0
9	SL	3348	0	3236	67	0
9	TB	3356	0	3240	75	0
9	TD	3356	0	3240	68	0
9	TF	3361	0	3245	75	0
9	TH	3361	0	3245	82	0
9	TJ	3361	0	3245	83	0
9	TL	3348	0	3236	91	0
9	UB	3348	0	3234	75	0
9	UD	3356	0	3238	73	0
9	UF	3356	0	3238	75	0
9	UH	3356	0	3240	67	0
9	UJ	3356	0	3238	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	UL	3348	0	3234	74	0
9	UN	3356	0	3238	78	0
9	VB	3348	0	3236	66	0
9	VD	3348	0	3236	82	0
9	VF	3348	0	3236	81	0
9	VH	3361	0	3245	75	0
9	VJ	3348	0	3236	96	0
9	VL	3348	0	3234	86	0
9	VN	3348	0	3236	88	0
9	WB	3348	0	3236	82	0
9	WD	3348	0	3236	92	0
9	WF	3348	0	3236	64	0
9	WH	3348	0	3236	61	0
9	WJ	3348	0	3236	78	0
9	WL	3348	0	3236	70	0
9	WN	3348	0	3236	62	0
10	AP	920	0	921	21	0
10	AQ	920	0	921	14	0
10	AR	735	0	753	8	0
10	AS	920	0	921	10	0
11	AT	2521	0	2557	53	0
11	AU	1855	0	1862	31	0
12	AV	2901	0	2864	50	0
12	AW	2947	0	2925	63	0
13	Aa	4829	0	4760	83	0
13	Ab	4935	0	4869	111	0
13	Ac	4948	0	4885	92	0
13	Ad	4235	0	4149	98	0
14	Al	338	0	329	15	0
14	Am	338	0	329	11	0
14	An	338	0	329	7	0
14	Ao	573	0	554	15	0
14	B7	686	0	670	17	0
14	BY	866	0	850	17	0
14	BZ	866	0	850	14	0
14	Ba	1587	0	1554	28	0
14	Bb	1587	0	1554	36	0
14	Bc	1575	0	1545	32	0
14	Bd	866	0	850	13	0
14	Be	866	0	850	14	0
14	CN	670	0	648	15	0
14	CO	697	0	683	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Ap	1101	0	1073	26	0
15	Aq	766	0	758	21	0
15	Ar	1257	0	1227	33	0
16	At	772	0	753	38	0
16	Ax	914	0	905	42	0
17	B0	367	0	363	5	0
17	B1	300	0	290	11	0
17	B2	307	0	287	5	0
17	B3	200	0	180	3	0
17	B4	305	0	291	7	0
17	B8	320	0	308	5	0
17	B9	307	0	297	8	0
17	CQ	367	0	363	7	0
17	CR	316	0	309	6	0
17	CS	307	0	297	4	0
18	B5	2008	0	2070	27	0
18	B6	2040	0	2103	38	0
18	By	1316	0	1340	20	0
18	Bz	2008	0	2070	33	0
19	BO	1817	0	1832	37	0
19	BP	3394	0	3477	59	0
19	BQ	2989	0	3080	44	0
19	BR	3465	0	3546	74	0
20	BS	1192	0	1158	17	0
20	BT	1886	0	1816	53	0
21	BU	307	0	329	3	0
21	BV	3087	0	3058	46	0
21	Bi	352	0	345	5	0
21	Bj	2029	0	2007	33	0
21	Bk	1444	0	1441	28	0
22	BW	1586	0	1560	25	0
22	BX	424	0	426	12	0
23	Bf	508	0	487	9	0
23	Bg	950	0	898	23	0
24	Bh	775	0	745	21	0
25	Bl	635	0	150	5	0
25	Bm	640	0	148	6	0
25	Bn	690	0	159	2	0
25	Bo	715	0	166	8	0
25	Bp	815	0	187	8	0
26	Bq	782	0	757	14	0
26	Bu	1177	0	1169	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	Br	1380	0	1406	25	0
27	Bs	3042	0	3095	66	0
28	C0	851	0	879	20	0
28	C2	3314	0	3295	58	0
28	C3	3314	0	3295	44	0
28	C4	2779	0	2738	46	0
28	C5	1843	0	1883	34	0
28	C6	352	0	327	6	0
28	C7	3454	0	3424	40	0
28	C8	3446	0	3421	50	0
28	C9	3089	0	3075	53	0
28	DO	1041	0	981	21	0
28	F2	3411	0	3370	34	0
28	F3	3400	0	3349	66	0
28	F4	3141	0	3131	47	0
28	F5	873	0	901	11	0
28	F6	1047	0	973	25	0
29	C1	2710	0	2737	42	0
29	Cz	2435	0	2466	39	0
29	D0	569	0	599	12	0
29	D1	2933	0	2964	65	0
29	D2	3169	0	3184	54	0
29	D3	3160	0	3171	52	0
29	D4	3152	0	3164	58	0
29	D5	2961	0	2994	68	0
29	D6	1209	0	1144	18	0
29	D7	603	0	630	15	0
29	D8	3169	0	3184	48	0
29	D9	1305	0	1236	26	0
29	DP	1668	0	1609	20	0
29	DQ	2411	0	2441	33	0
29	DR	2151	0	2187	26	0
29	DS	2118	0	2156	44	0
29	DT	1373	0	1409	22	0
29	DU	2497	0	2511	45	0
29	DV	2502	0	2516	45	0
29	DW	2502	0	2516	55	0
29	DX	1897	0	1938	30	0
29	EA	3259	0	3271	51	0
29	EO	3251	0	3261	46	0
29	EP	2940	0	2934	64	0
29	EQ	1458	0	1522	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	ER	358	0	337	3	0
30	CW	1319	0	1281	27	0
31	Cl	977	0	957	21	0
32	Cm	3264	0	3327	58	0
32	Cn	3286	0	3356	46	0
32	Co	2845	0	2905	45	0
32	Cp	1690	0	1752	28	0
33	Cq	3427	0	3450	49	0
33	Cr	3386	0	3404	48	0
33	Cs	1496	0	1476	36	0
33	Ct	3147	0	3183	46	0
33	Cu	3055	0	3083	49	0
33	Cv	3436	0	3463	58	0
33	Cw	3436	0	3463	49	0
33	Cx	1611	0	1600	28	0
33	Cy	365	0	367	15	0
34	D	537	0	521	17	0
35	DY	308	0	284	6	0
35	DZ	416	0	403	7	0
35	Da	1095	0	1059	27	0
35	Ee	386	0	362	10	0
36	Db	450	0	433	6	0
36	Dc	442	0	422	8	0
36	Dd	406	0	389	9	0
37	De	545	0	518	19	0
38	Df	1060	0	1003	22	0
38	Dg	981	0	930	13	0
38	Dh	873	0	832	21	0
39	Di	632	0	642	9	0
39	Dj	806	0	818	11	0
39	Dk	806	0	818	20	0
39	Dl	806	0	818	16	0
40	Dm	725	0	696	15	0
41	Dn	468	0	487	15	0
42	E	1181	0	1179	30	0
42	F	3679	0	3659	75	0
43	E1	1648	0	1556	30	0
43	E2	1648	0	1556	31	0
43	E3	1641	0	1547	36	0
43	E4	1221	0	1150	26	0
44	ES	3483	0	3423	51	0
44	ET	2273	0	2194	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	EU	2692	0	2693	35	0
44	EV	3483	0	3423	56	0
44	EW	2601	0	2524	49	0
44	EX	3560	0	3499	52	0
44	EY	2552	0	2559	49	0
44	EZ	3615	0	3562	46	0
45	G	2317	0	2275	50	0
46	H	848	0	844	12	0
46	o	3401	0	3468	57	0
47	I	3689	0	3637	58	0
47	X	3692	0	3644	75	0
47	Y	3743	0	3691	68	0
48	J	951	0	957	28	0
48	K	951	0	957	17	0
48	L	891	0	891	10	0
48	M	728	0	728	21	0
49	K1	992	0	974	23	0
50	L1	1090	0	1070	35	0
50	L2	743	0	720	22	0
51	N	1173	0	1124	28	0
51	O	1134	0	1080	36	0
52	P	870	0	859	28	0
53	Q	919	0	839	16	0
54	R	1162	0	1151	29	0
54	S	1162	0	1151	23	0
54	T	1165	0	1159	17	0
54	U	818	0	795	13	0
55	W	990	0	965	27	0
56	XG	1512	0	1539	30	0
56	XH	1512	0	1539	39	0
56	XI	1512	0	1539	52	0
56	XJ	1512	0	1539	35	0
56	XK	1512	0	1539	31	0
56	XL	1503	0	1526	38	0
56	XM	1494	0	1515	30	0
57	YG	1706	0	1720	32	0
57	YH	1759	0	1766	33	0
57	YI	1759	0	1766	48	0
57	YJ	1759	0	1766	35	0
57	YK	1759	0	1766	25	0
57	YL	1759	0	1766	39	0
58	Z	1014	0	1025	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	p	459	0	477	10	0
58	q	829	0	838	21	0
59	a	1559	0	1626	38	0
59	b	2814	0	2869	79	0
59	c	2525	0	2598	56	0
59	d	1728	0	1771	30	0
60	e	4722	0	4705	101	0
60	f	4713	0	4699	101	0
60	g	4713	0	4699	107	0
61	h	785	0	787	26	0
62	i	2055	0	2024	36	0
62	j	2158	0	2128	32	0
63	k	1245	0	1232	23	0
63	l	1098	0	1092	21	0
63	m	1263	0	1243	30	0
63	n	908	0	887	23	0
64	ke	796	0	789	23	0
65	r	615	0	590	12	0
65	s	624	0	598	14	0
65	t	624	0	598	18	0
66	u	1081	0	1079	19	0
66	v	957	0	937	12	0
66	w	1081	0	1079	23	0
67	AA	32	0	11	1	0
67	AC	32	0	11	1	0
67	AD	32	0	11	0	0
67	AG	32	0	11	2	0
67	AH	32	0	11	0	0
67	AK	32	0	11	1	0
67	AM	32	0	11	0	0
67	BA	32	0	12	1	0
67	BC	32	0	12	3	0
67	BE	32	0	12	0	0
67	BG	32	0	12	1	0
67	BI	32	0	12	1	0
67	BK	32	0	12	2	0
67	BM	32	0	12	0	0
67	CA	32	0	12	2	0
67	CB	32	0	12	1	0
67	CD	32	0	12	1	0
67	CG	32	0	12	1	0
67	CH	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	CJ	32	0	12	1	0
67	CL	32	0	12	1	0
67	DA	32	0	12	1	0
67	DC	32	0	12	2	0
67	DE	32	0	12	1	0
67	DF	32	0	12	1	0
67	DI	32	0	12	1	0
67	DK	32	0	12	3	0
67	DM	32	0	12	2	0
67	EC	32	0	12	2	0
67	EE	32	0	12	0	0
67	EG	32	0	12	1	0
67	EI	32	0	12	1	0
67	EK	32	0	12	2	0
67	EM	32	0	12	2	0
67	FC	32	0	12	2	0
67	FE	32	0	12	0	0
67	FG	32	0	12	2	0
67	FI	32	0	12	0	0
67	FK	32	0	12	0	0
67	FM	32	0	12	0	0
67	GC	32	0	12	1	0
67	GE	32	0	12	0	0
67	GG	32	0	12	0	0
67	GI	32	0	12	1	0
67	GJ	32	0	12	1	0
67	GM	32	0	12	1	0
67	HC	32	0	12	2	0
67	HE	32	0	12	2	0
67	HG	32	0	12	1	0
67	HI	32	0	12	4	0
67	HK	32	0	12	2	0
67	HL	32	0	12	0	0
67	HN	32	0	12	0	0
67	IC	32	0	12	3	0
67	IE	32	0	12	1	0
67	IG	32	0	12	2	0
67	II	32	0	12	1	0
67	IK	32	0	12	1	0
67	IM	32	0	12	2	0
67	IN	32	0	12	1	0
67	JC	32	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	JE	32	0	12	0	0
67	JG	32	0	12	1	0
67	JI	32	0	12	3	0
67	JK	32	0	12	2	0
67	JM	32	0	12	1	0
67	KC	32	0	12	2	0
67	KE	32	0	12	0	0
67	KG	32	0	11	0	0
67	KI	32	0	12	0	0
67	KK	32	0	12	0	0
67	KM	32	0	12	0	0
67	KO	32	0	12	1	0
67	LC	32	0	12	0	0
67	LE	32	0	12	2	0
67	LG	32	0	12	0	0
67	LI	32	0	12	0	0
67	LK	32	0	12	1	0
67	LM	32	0	12	0	0
67	MC	32	0	12	3	0
67	ME	32	0	12	1	0
67	MG	32	0	12	3	0
67	MI	32	0	11	1	0
67	MK	32	0	12	1	0
67	MM	32	0	12	1	0
67	NA	32	0	12	2	0
67	NB	32	0	12	1	0
67	NE	32	0	12	1	0
67	NF	32	0	12	1	0
67	NI	32	0	12	1	0
67	NK	32	0	12	1	0
67	O0	32	0	12	2	0
67	OC	32	0	12	1	0
67	OE	32	0	12	5	0
67	OF	32	0	12	1	0
67	OH	32	0	12	2	0
67	OK	32	0	12	1	0
67	PA	32	0	12	1	0
67	PC	32	0	12	1	0
67	PD	32	0	12	4	0
67	PG	32	0	10	0	0
67	PI	32	0	12	3	0
67	PK	32	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	PM	32	0	12	1	0
67	QA	32	0	12	0	0
67	QC	32	0	12	1	0
67	QE	32	0	12	2	0
67	QG	32	0	12	1	0
67	QI	32	0	12	2	0
67	QK	32	0	12	3	0
67	QM	32	0	12	2	0
67	RA	32	0	12	0	0
67	RB	32	0	12	0	0
67	RE	32	0	12	0	0
67	RG	32	0	12	1	0
67	RI	32	0	11	4	0
67	RK	32	0	12	1	0
67	RM	32	0	12	2	0
67	SA	32	0	12	0	0
67	SC	32	0	12	1	0
67	SE	32	0	12	3	0
67	SF	32	0	12	2	0
67	SI	32	0	12	2	0
67	SK	32	0	12	2	0
67	SM	32	0	12	1	0
67	TC	32	0	12	2	0
67	TE	32	0	12	1	0
67	TG	32	0	12	3	0
67	TI	32	0	12	4	0
67	TK	32	0	12	2	0
67	TM	32	0	12	1	0
67	UC	32	0	12	3	0
67	UE	32	0	12	4	0
67	UG	32	0	12	2	0
67	UI	32	0	12	0	0
67	UK	32	0	12	1	0
67	UM	32	0	12	1	0
67	VC	32	0	12	3	0
67	VE	32	0	12	3	0
67	VG	32	0	12	1	0
67	VI	32	0	12	3	0
67	VK	32	0	12	1	0
67	VL	32	0	12	6	0
67	WC	32	0	12	1	0
67	WE	32	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	WG	32	0	12	2	0
67	WI	32	0	12	1	0
67	WK	32	0	12	0	0
67	WM	32	0	12	1	0
68	AA	1	0	0	0	0
68	AC	1	0	0	0	0
68	AE	1	0	0	0	0
68	AG	1	0	0	0	0
68	AI	1	0	0	0	0
68	AK	1	0	0	0	0
68	AM	1	0	0	0	0
68	BA	1	0	0	0	0
68	BC	1	0	0	0	0
68	BE	1	0	0	0	0
68	BG	1	0	0	0	0
68	BI	1	0	0	0	0
68	BK	1	0	0	0	0
68	BM	1	0	0	0	0
68	CA	1	0	0	0	0
68	CC	1	0	0	0	0
68	CE	1	0	0	0	0
68	CG	1	0	0	0	0
68	CI	1	0	0	0	0
68	CK	1	0	0	0	0
68	CM	1	0	0	0	0
68	DA	1	0	0	0	0
68	DC	1	0	0	0	0
68	DE	1	0	0	0	0
68	DG	1	0	0	0	0
68	DI	1	0	0	0	0
68	DK	1	0	0	0	0
68	DM	1	0	0	0	0
68	EC	1	0	0	0	0
68	EE	1	0	0	0	0
68	EG	1	0	0	0	0
68	EI	1	0	0	0	0
68	EJ	1	0	0	0	0
68	EM	1	0	0	0	0
68	FC	1	0	0	0	0
68	FE	1	0	0	0	0
68	FG	1	0	0	0	0
68	FI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	FK	1	0	0	0	0
68	FM	1	0	0	0	0
68	GC	1	0	0	0	0
68	GE	1	0	0	0	0
68	GG	1	0	0	0	0
68	GI	1	0	0	0	0
68	GK	1	0	0	0	0
68	GM	1	0	0	0	0
68	HC	1	0	0	0	0
68	HE	1	0	0	0	0
68	HG	1	0	0	0	0
68	HI	1	0	0	0	0
68	HK	1	0	0	0	0
68	HM	1	0	0	0	0
68	HO	1	0	0	0	0
68	IC	1	0	0	0	0
68	IE	1	0	0	0	0
68	IG	1	0	0	0	0
68	II	1	0	0	0	0
68	IK	1	0	0	0	0
68	IM	1	0	0	0	0
68	IO	1	0	0	0	0
68	JC	1	0	0	0	0
68	JE	1	0	0	0	0
68	JG	1	0	0	0	0
68	JI	1	0	0	0	0
68	JK	1	0	0	0	0
68	JM	1	0	0	0	0
68	KC	1	0	0	0	0
68	KE	1	0	0	0	0
68	KG	1	0	0	0	0
68	KI	1	0	0	0	0
68	KK	1	0	0	0	0
68	KM	1	0	0	0	0
68	KN	1	0	0	0	0
68	LC	1	0	0	0	0
68	LE	1	0	0	0	0
68	LG	1	0	0	0	0
68	LI	1	0	0	0	0
68	LK	1	0	0	0	0
68	LL	1	0	0	0	0
68	MC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	ME	1	0	0	0	0
68	MG	1	0	0	0	0
68	MI	1	0	0	0	0
68	MK	1	0	0	0	0
68	MM	1	0	0	0	0
68	NA	1	0	0	0	0
68	NC	1	0	0	0	0
68	NE	1	0	0	0	0
68	NG	1	0	0	0	0
68	NI	1	0	0	0	0
68	NK	1	0	0	0	0
68	OA	1	0	0	0	0
68	OC	1	0	0	0	0
68	OE	1	0	0	0	0
68	OG	1	0	0	0	0
68	OI	1	0	0	0	0
68	OK	1	0	0	0	0
68	PA	1	0	0	0	0
68	PC	1	0	0	0	0
68	PE	1	0	0	0	0
68	PG	1	0	0	0	0
68	PH	1	0	0	0	0
68	PK	1	0	0	0	0
68	PM	1	0	0	0	0
68	QA	1	0	0	0	0
68	QC	1	0	0	0	0
68	QE	1	0	0	0	0
68	QG	1	0	0	0	0
68	QI	1	0	0	0	0
68	QK	1	0	0	0	0
68	QM	1	0	0	0	0
68	RA	1	0	0	0	0
68	RC	1	0	0	0	0
68	RE	1	0	0	0	0
68	RG	1	0	0	0	0
68	RI	1	0	0	0	0
68	RK	1	0	0	0	0
68	RM	1	0	0	0	0
68	SA	1	0	0	0	0
68	SC	1	0	0	0	0
68	SE	1	0	0	0	0
68	SG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	SI	1	0	0	0	0
68	SK	1	0	0	0	0
68	SM	1	0	0	0	0
68	TC	1	0	0	0	0
68	TE	1	0	0	0	0
68	TG	1	0	0	0	0
68	TH	1	0	0	0	0
68	TK	1	0	0	0	0
68	TM	1	0	0	0	0
68	UC	1	0	0	0	0
68	UE	1	0	0	0	0
68	UG	1	0	0	0	0
68	UI	1	0	0	0	0
68	UK	1	0	0	0	0
68	UM	1	0	0	0	0
68	VC	1	0	0	0	0
68	VE	1	0	0	0	0
68	VG	1	0	0	0	0
68	VI	1	0	0	0	0
68	VK	1	0	0	0	0
68	VM	1	0	0	0	0
68	WC	1	0	0	0	0
68	WE	1	0	0	0	0
68	WG	1	0	0	0	0
68	WI	1	0	0	0	0
68	WK	1	0	0	0	0
68	WM	1	0	0	0	0
69	AB	28	0	12	1	0
69	AD	28	0	12	0	0
69	AF	28	0	12	0	0
69	AH	28	0	12	0	0
69	AJ	28	0	12	0	0
69	AL	28	0	12	1	0
69	BB	28	0	12	1	0
69	BD	28	0	12	2	0
69	BF	28	0	12	2	0
69	BH	28	0	12	1	0
69	BJ	28	0	12	1	0
69	BL	28	0	12	1	0
69	CB	28	0	12	1	0
69	CD	28	0	12	3	0
69	CF	28	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	CH	28	0	12	2	0
69	CJ	28	0	12	1	0
69	CL	28	0	12	3	0
69	DB	28	0	12	3	0
69	DD	28	0	12	0	0
69	DF	28	0	12	2	0
69	DH	28	0	12	3	0
69	DJ	28	0	12	1	0
69	DL	28	0	12	1	0
69	DN	28	0	12	1	0
69	EB	28	0	12	0	0
69	ED	28	0	12	2	0
69	EF	28	0	12	0	0
69	EH	28	0	12	1	0
69	EJ	28	0	12	0	0
69	EL	28	0	12	0	0
69	EN	28	0	12	2	0
69	FB	28	0	12	0	0
69	FD	28	0	12	1	0
69	FF	28	0	12	1	0
69	FH	28	0	12	1	0
69	FJ	28	0	12	0	0
69	FL	28	0	12	0	0
69	FN	28	0	12	3	0
69	GB	28	0	12	1	0
69	GD	28	0	12	0	0
69	GF	28	0	12	1	0
69	GH	28	0	12	0	0
69	GJ	28	0	12	0	0
69	GL	28	0	12	2	0
69	GN	28	0	12	0	0
69	HB	28	0	12	2	0
69	HD	28	0	12	0	0
69	HF	28	0	12	1	0
69	HH	28	0	12	0	0
69	HJ	28	0	12	5	0
69	HL	28	0	12	0	0
69	HN	28	0	12	0	0
69	IB	28	0	11	1	0
69	ID	28	0	12	1	0
69	IF	28	0	12	1	0
69	IH	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	IJ	28	0	12	1	0
69	IL	28	0	12	2	0
69	IN	28	0	12	1	0
69	JB	28	0	12	0	0
69	JD	28	0	12	0	0
69	JF	28	0	12	3	0
69	JH	28	0	12	2	0
69	JJ	28	0	12	1	0
69	JL	28	0	12	1	0
69	JN	28	0	12	1	0
69	KB	28	0	12	1	0
69	KD	28	0	12	1	0
69	KF	28	0	12	0	0
69	KH	28	0	12	0	0
69	KJ	28	0	12	0	0
69	KL	28	0	12	0	0
69	KN	28	0	12	0	0
69	LB	28	0	11	0	0
69	LD	28	0	11	0	0
69	LF	28	0	11	0	0
69	LH	28	0	11	0	0
69	LJ	28	0	11	0	0
69	LL	28	0	11	1	0
69	LN	28	0	12	0	0
69	MB	28	0	11	1	0
69	MD	28	0	11	0	0
69	MF	28	0	11	0	0
69	MH	28	0	11	0	0
69	MJ	28	0	11	1	0
69	ML	28	0	11	1	0
69	MN	28	0	11	1	0
69	N0	28	0	11	1	0
69	NB	28	0	11	1	0
69	ND	28	0	11	0	0
69	NF	28	0	11	2	0
69	NH	28	0	10	0	0
69	NJ	28	0	11	2	0
69	NL	28	0	12	1	0
69	O0	28	0	12	1	0
69	OB	28	0	12	1	0
69	OD	28	0	12	2	0
69	OF	28	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	OH	28	0	12	2	0
69	OJ	28	0	12	1	0
69	OL	28	0	12	1	0
69	PB	28	0	11	3	0
69	PD	28	0	11	4	0
69	PF	28	0	11	2	0
69	PH	28	0	10	5	0
69	PJ	28	0	11	1	0
69	PL	28	0	11	1	0
69	QB	28	0	12	1	0
69	QD	28	0	12	3	0
69	QF	28	0	12	3	0
69	QH	28	0	12	2	0
69	QJ	28	0	12	1	0
69	QL	28	0	12	2	0
69	RB	28	0	12	0	0
69	RD	28	0	12	1	0
69	RF	28	0	12	0	0
69	RH	28	0	12	0	0
69	RJ	28	0	12	2	0
69	RL	28	0	12	1	0
69	SB	28	0	12	1	0
69	SD	28	0	12	0	0
69	SF	28	0	12	1	0
69	SH	28	0	12	0	0
69	SJ	28	0	12	0	0
69	SL	28	0	12	0	0
69	TB	28	0	12	0	0
69	TD	28	0	12	0	0
69	TF	28	0	12	2	0
69	TH	28	0	12	1	0
69	TJ	28	0	12	3	0
69	TL	28	0	12	0	0
69	UB	28	0	11	1	0
69	UD	28	0	11	0	0
69	UF	28	0	11	0	0
69	UH	28	0	12	4	0
69	UJ	28	0	11	1	0
69	UL	28	0	11	2	0
69	UN	28	0	11	0	0
69	VB	28	0	12	0	0
69	VD	28	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	VF	28	0	12	0	0
69	VH	28	0	12	2	0
69	VJ	28	0	12	2	0
69	VL	28	0	12	3	0
69	VN	28	0	12	4	0
69	WB	28	0	12	0	0
69	WD	28	0	12	1	0
69	WF	28	0	12	1	0
69	WH	28	0	12	1	0
69	WJ	28	0	12	0	0
69	WL	28	0	12	0	0
69	WN	28	0	12	1	0
All	All	1456841	0	1416075	25938	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 25938 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:253:LEU:O	9:UL:257:MET:HB2	1.56	1.03
9:CF:37:HIS:HE2	48:J:49:CYS:HG	1.04	1.01
13:Ac:316:GLN:N	13:Ac:316:GLN:HE21	1.58	1.00
9:PF:253:LEU:O	9:PF:257:MET:HB2	1.62	0.99
9:NL:186:THR:HG21	9:NL:385:PHE:HE2	1.29	0.95

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 451 ligands modelled in this entry, 149 are monoatomic - leaving 302 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	$\#\|Z\| > 2$
69	GDP	ML	501	-	29,30,30	1.13	3 (10%)	45,47,47	2.41	16 (35%)
67	GTP	DF	502	68	33,34,34	0.93	1 (3%)	50,54,54	1.61	9 (18%)
69	GDP	LJ	501	-	29,30,30	1.08	4 (13%)	45,47,47	1.77	6 (13%)
69	GDP	GJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
67	GTP	QI	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.55	9 (18%)
69	GDP	GH	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	7 (15%)
67	GTP	WM	501	68	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
69	GDP	UB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.71	6 (13%)
67	GTP	FM	501	68	33,34,34	0.88	1 (3%)	50,54,54	1.59	9 (18%)
67	GTP	LG	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.60	8 (16%)
67	GTP	GC	501	68	33,34,34	0.89	1 (3%)	50,54,54	1.60	9 (18%)
69	GDP	QL	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.80	6 (13%)
67	GTP	IM	501	68	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
67	GTP	DI	501	68	33,34,34	0.98	1 (3%)	50,54,54	1.64	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
67	GTP	O0	502	68	33,34,34	1.02	2 (6%)	50,54,54	1.62	9 (18%)
69	GDP	SB	501	-	29,30,30	1.13	4 (13%)	45,47,47	1.80	9 (20%)
67	GTP	WI	501	68	33,34,34	0.97	1 (3%)	50,54,54	1.58	9 (18%)
69	GDP	VF	501	-	29,30,30	1.12	2 (6%)	45,47,47	1.74	6 (13%)
67	GTP	MG	501	68	33,34,34	0.90	0	50,54,54	1.46	7 (14%)
67	GTP	KM	501	68	33,34,34	0.90	1 (3%)	50,54,54	1.56	9 (18%)
67	GTP	GI	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.66	9 (18%)
69	GDP	SF	501	-	29,30,30	1.14	4 (13%)	45,47,47	1.71	7 (15%)
69	GDP	UN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
69	GDP	QH	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.72	6 (13%)
69	GDP	NF	501	-	29,30,30	1.12	2 (6%)	45,47,47	1.77	6 (13%)
69	GDP	DF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	7 (15%)
67	GTP	CB	502	68	33,34,34	0.97	2 (6%)	50,54,54	1.64	11 (22%)
69	GDP	VH	501	-	29,30,30	1.20	3 (10%)	45,47,47	1.78	7 (15%)
69	GDP	OH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	7 (15%)
67	GTP	RI	501	68	33,34,34	0.89	0	50,54,54	1.64	12 (24%)
69	GDP	VN	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.97	8 (17%)
69	GDP	MF	501	-	29,30,30	1.07	2 (6%)	45,47,47	2.11	15 (33%)
69	GDP	CF	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.76	7 (15%)
67	GTP	RG	501	68	33,34,34	0.92	1 (3%)	50,54,54	1.56	9 (18%)
69	GDP	OJ	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.72	7 (15%)
67	GTP	KE	501	68	33,34,34	0.95	1 (3%)	50,54,54	1.61	8 (16%)
67	GTP	BE	501	68	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
69	GDP	FD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
69	GDP	SL	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	7 (15%)
69	GDP	UH	501	-	29,30,30	1.13	2 (6%)	45,47,47	1.77	5 (11%)
67	GTP	EG	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.54	9 (18%)
69	GDP	FN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
67	GTP	BA	501	68	33,34,34	0.96	1 (3%)	50,54,54	1.63	9 (18%)
67	GTP	MC	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.61	9 (18%)
67	GTP	SA	501	68	33,34,34	0.90	1 (3%)	50,54,54	1.62	9 (18%)
67	GTP	HE	501	68	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
67	GTP	VI	502	68	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
69	GDP	BJ	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.78	7 (15%)
69	GDP	DN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	GDP	ED	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
67	GTP	EI	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.62	9 (18%)
67	GTP	JE	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.65	9 (18%)
69	GDP	CH	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.80	8 (17%)
67	GTP	WK	501	68	33,34,34	0.97	1 (3%)	50,54,54	1.63	9 (18%)
69	GDP	PF	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.86	8 (17%)
67	GTP	UM	501	68	33,34,34	0.88	0	50,54,54	1.55	8 (16%)
67	GTP	LE	501	68	33,34,34	0.87	1 (3%)	50,54,54	1.63	9 (18%)
67	GTP	RE	501	-	33,34,34	0.85	1 (3%)	50,54,54	1.63	8 (16%)
69	GDP	LD	501	-	29,30,30	1.09	4 (13%)	45,47,47	1.81	8 (17%)
69	GDP	WH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
67	GTP	QK	501	68	33,34,34	0.97	1 (3%)	50,54,54	1.60	9 (18%)
69	GDP	HN	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
67	GTP	LC	501	68	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
69	GDP	UL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
69	GDP	RF	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.74	6 (13%)
67	GTP	BC	501	-	33,34,34	0.88	1 (3%)	50,54,54	1.63	9 (18%)
67	GTP	AA	501	68	33,34,34	0.87	1 (3%)	50,54,54	1.60	10 (20%)
67	GTP	QE	501	68	33,34,34	0.92	1 (3%)	50,54,54	1.71	9 (18%)
67	GTP	TK	501	68	33,34,34	0.96	1 (3%)	50,54,54	1.56	8 (16%)
67	GTP	UC	501	68	33,34,34	0.96	2 (6%)	50,54,54	1.59	10 (20%)
69	GDP	SH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
67	GTP	RA	501	68	33,34,34	0.92	1 (3%)	50,54,54	1.55	8 (16%)
67	GTP	KK	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
67	GTP	SC	501	68	33,34,34	0.87	1 (3%)	50,54,54	1.58	9 (18%)
67	GTP	UI	501	68	33,34,34	0.88	1 (3%)	50,54,54	1.58	9 (18%)
69	GDP	EL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
67	GTP	GE	501	68	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
69	GDP	CJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
69	GDP	DB	501	-	29,30,30	1.13	2 (6%)	45,47,47	1.77	7 (15%)
69	GDP	DH	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.75	7 (15%)
69	GDP	EB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
69	GDP	LB	501	-	29,30,30	1.10	2 (6%)	45,47,47	1.84	7 (15%)
69	GDP	MD	501	-	29,30,30	1.09	2 (6%)	45,47,47	2.10	11 (24%)
69	GDP	OD	501	-	29,30,30	1.14	2 (6%)	45,47,47	1.72	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	GDP	RD	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	6 (13%)
69	GDP	IN	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
69	GDP	WN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.69	7 (15%)
67	GTP	BI	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
67	GTP	CH	502	68	33,34,34	0.84	1 (3%)	50,54,54	1.66	11 (22%)
67	GTP	PD	502	68	33,34,34	1.12	4 (12%)	50,54,54	1.64	8 (16%)
67	GTP	RM	501	-	33,34,34	0.83	1 (3%)	50,54,54	1.56	9 (18%)
67	GTP	WC	501	68	33,34,34	0.94	1 (3%)	50,54,54	1.60	9 (18%)
67	GTP	JC	501	68	33,34,34	0.90	1 (3%)	50,54,54	1.58	10 (20%)
69	GDP	GD	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.72	6 (13%)
69	GDP	KN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	8 (17%)
69	GDP	LL	501	-	29,30,30	1.11	4 (13%)	45,47,47	1.77	6 (13%)
69	GDP	HF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
69	GDP	IB	501	-	29,30,30	1.23	3 (10%)	45,47,47	1.92	8 (17%)
69	GDP	IL	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.75	6 (13%)
67	GTP	TG	501	68	33,34,34	0.96	1 (3%)	50,54,54	1.71	8 (16%)
69	GDP	DJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.69	6 (13%)
67	GTP	CG	501	68	33,34,34	0.90	1 (3%)	50,54,54	1.65	9 (18%)
69	GDP	IH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
67	GTP	AC	501	68	33,34,34	0.94	1 (3%)	50,54,54	1.61	12 (24%)
69	GDP	QJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	9 (20%)
69	GDP	UD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
67	GTP	PG	501	68	33,34,34	0.98	1 (3%)	50,54,54	1.58	8 (16%)
69	GDP	KL	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.75	6 (13%)
69	GDP	CD	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.73	6 (13%)
69	GDP	IJ	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	6 (13%)
67	GTP	AM	501	68	33,34,34	0.84	1 (3%)	50,54,54	1.57	10 (20%)
67	GTP	SK	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.60	10 (20%)
69	GDP	DD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.70	6 (13%)
67	GTP	MK	501	68	33,34,34	0.94	1 (3%)	50,54,54	1.62	10 (20%)
69	GDP	WB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
67	GTP	AD	502	68	33,34,34	0.95	1 (3%)	50,54,54	1.64	13 (26%)
69	GDP	HL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
69	GDP	TB	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.78	7 (15%)
67	GTP	GG	501	68	33,34,34	0.91	1 (3%)	50,54,54	1.57	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	GDP	TF	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	6 (13%)
69	GDP	UF	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	7 (15%)
67	GTP	FE	501	68	33,34,34	0.89	1 (3%)	50,54,54	1.57	9 (18%)
69	GDP	AL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
69	GDP	JL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
69	GDP	RJ	501	-	29,30,30	1.27	5 (17%)	45,47,47	1.74	7 (15%)
67	GTP	IE	501	68	33,34,34	0.98	1 (3%)	50,54,54	1.64	10 (20%)
69	GDP	GB	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.73	7 (15%)
69	GDP	QD	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.80	9 (20%)
67	GTP	RB	502	-	33,34,34	0.89	1 (3%)	50,54,54	1.57	8 (16%)
67	GTP	EE	501	-	33,34,34	1.03	3 (9%)	50,54,54	1.70	8 (16%)
67	GTP	MI	501	68	33,34,34	0.92	0	50,54,54	1.85	13 (26%)
69	GDP	RH	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	7 (15%)
67	GTP	HK	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
67	GTP	WG	501	-	33,34,34	1.00	2 (6%)	50,54,54	1.74	12 (24%)
67	GTP	DC	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
67	GTP	PI	501	68	33,34,34	0.86	1 (3%)	50,54,54	1.54	9 (18%)
69	GDP	VL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.72	6 (13%)
67	GTP	BM	501	68	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
67	GTP	SF	502	68	33,34,34	1.05	3 (9%)	50,54,54	1.68	11 (22%)
69	GDP	BH	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.75	7 (15%)
69	GDP	FF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.84	6 (13%)
69	GDP	GF	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	7 (15%)
69	GDP	EH	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.75	7 (15%)
67	GTP	QA	501	68	33,34,34	0.99	3 (9%)	50,54,54	1.56	9 (18%)
69	GDP	FB	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	7 (15%)
67	GTP	NF	502	68	33,34,34	1.04	4 (12%)	50,54,54	1.61	9 (18%)
67	GTP	EC	501	68	33,34,34	0.90	1 (3%)	50,54,54	1.67	9 (18%)
69	GDP	LF	501	-	29,30,30	1.09	4 (13%)	45,47,47	1.78	6 (13%)
69	GDP	TH	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.72	6 (13%)
67	GTP	NE	501	68	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
69	GDP	SJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
67	GTP	KC	501	68	33,34,34	0.88	1 (3%)	50,54,54	1.58	9 (18%)
67	GTP	DK	501	68	33,34,34	1.27	3 (9%)	50,54,54	1.76	12 (24%)
69	GDP	AF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
67	GTP	HI	501	68	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
69	GDP	BF	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.71	7 (15%)
67	GTP	OE	501	68	33,34,34	0.84	1 (3%)	50,54,54	1.55	9 (18%)
67	GTP	AK	501	68	33,34,34	1.00	1 (3%)	50,54,54	1.66	11 (22%)
69	GDP	VJ	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	7 (15%)
67	GTP	BK	501	68	33,34,34	0.88	1 (3%)	50,54,54	1.58	9 (18%)
67	GTP	TC	501	68	33,34,34	0.96	1 (3%)	50,54,54	1.56	8 (16%)
67	GTP	NK	501	68	33,34,34	1.01	4 (12%)	50,54,54	1.59	9 (18%)
69	GDP	FH	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	7 (15%)
69	GDP	PB	501	-	29,30,30	1.10	2 (6%)	45,47,47	2.01	12 (26%)
69	GDP	OF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.93	12 (26%)
67	GTP	UK	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
69	GDP	TJ	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.82	8 (17%)
67	GTP	LK	501	68	33,34,34	0.92	1 (3%)	50,54,54	1.62	11 (22%)
67	GTP	UG	501	68	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
69	GDP	NJ	501	-	29,30,30	1.14	2 (6%)	45,47,47	1.80	7 (15%)
67	GTP	DA	501	68	33,34,34	1.04	2 (6%)	50,54,54	1.76	11 (22%)
67	GTP	FC	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.34	6 (12%)
69	GDP	NB	501	-	29,30,30	1.11	2 (6%)	45,47,47	2.14	13 (28%)
69	GDP	BB	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.76	6 (13%)
69	GDP	MJ	501	-	29,30,30	1.11	2 (6%)	45,47,47	1.79	7 (15%)
67	GTP	JG	501	68	33,34,34	0.94	1 (3%)	50,54,54	1.58	8 (16%)
69	GDP	RB	501	-	29,30,30	1.10	3 (10%)	45,47,47	1.77	7 (15%)
67	GTP	SM	501	68	33,34,34	0.91	1 (3%)	50,54,54	1.62	10 (20%)
67	GTP	OK	501	68	33,34,34	0.98	1 (3%)	50,54,54	1.63	8 (16%)
67	GTP	OC	501	68	33,34,34	0.92	1 (3%)	50,54,54	1.56	8 (16%)
67	GTP	HC	501	68	33,34,34	0.99	3 (9%)	50,54,54	1.70	11 (22%)
67	GTP	PK	501	68	33,34,34	0.94	1 (3%)	50,54,54	1.53	8 (16%)
69	GDP	HH	501	-	29,30,30	1.13	2 (6%)	45,47,47	1.74	6 (13%)
67	GTP	KO	501	68	33,34,34	0.89	1 (3%)	50,54,54	1.57	9 (18%)
69	GDP	OB	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.71	7 (15%)
67	GTP	LM	501	68	33,34,34	0.89	1 (3%)	50,54,54	1.58	9 (18%)
67	GTP	KI	501	68	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
69	GDP	PL	501	-	29,30,30	1.18	4 (13%)	45,47,47	1.77	6 (13%)
67	GTP	CJ	502	68	33,34,34	0.92	1 (3%)	50,54,54	1.61	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
67	GTP	EK	501	68	33,34,34	0.91	1 (3%)	50,54,54	1.66	9 (18%)
69	GDP	MB	501	-	29,30,30	1.09	3 (10%)	45,47,47	1.84	8 (17%)
69	GDP	SD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
69	GDP	DL	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.79	7 (15%)
67	GTP	AG	501	68	33,34,34	0.84	0	50,54,54	1.62	10 (20%)
67	GTP	CA	501	-	33,34,34	0.94	0	50,54,54	1.51	10 (20%)
67	GTP	IN	502	68	33,34,34	0.87	1 (3%)	50,54,54	1.76	13 (26%)
67	GTP	TI	501	68	33,34,34	1.00	2 (6%)	50,54,54	1.56	9 (18%)
67	GTP	VL	502	68	33,34,34	1.14	2 (6%)	50,54,54	1.71	11 (22%)
69	GDP	BD	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.79	8 (17%)
67	GTP	NB	502	68	33,34,34	0.97	1 (3%)	50,54,54	1.59	9 (18%)
69	GDP	EJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
67	GTP	QM	501	68	33,34,34	0.94	1 (3%)	50,54,54	1.65	9 (18%)
67	GTP	PM	501	68	33,34,34	0.89	1 (3%)	50,54,54	1.62	9 (18%)
67	GTP	SE	501	68	33,34,34	0.85	1 (3%)	50,54,54	1.66	8 (16%)
67	GTP	TM	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.59	8 (16%)
67	GTP	KG	501	68	33,34,34	0.96	1 (3%)	50,54,54	1.59	10 (20%)
67	GTP	WE	501	68	33,34,34	1.04	3 (9%)	50,54,54	1.63	10 (20%)
69	GDP	AB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
69	GDP	UJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	8 (17%)
69	GDP	WD	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.74	6 (13%)
69	GDP	FL	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	7 (15%)
67	GTP	DM	501	68	33,34,34	0.97	2 (6%)	50,54,54	1.65	8 (16%)
69	GDP	TL	501	-	29,30,30	1.11	3 (10%)	45,47,47	1.77	7 (15%)
67	GTP	NI	501	68	33,34,34	0.95	1 (3%)	50,54,54	1.63	9 (18%)
67	GTP	ME	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)
69	GDP	EN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
67	GTP	VK	501	68	33,34,34	0.99	1 (3%)	50,54,54	1.55	9 (18%)
69	GDP	KB	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.78	8 (17%)
69	GDP	ID	501	-	29,30,30	1.13	2 (6%)	45,47,47	1.73	6 (13%)
67	GTP	HL	502	68	33,34,34	1.03	3 (9%)	50,54,54	1.58	10 (20%)
69	GDP	KJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
67	GTP	FI	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.62	9 (18%)
69	GDP	KF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	8 (17%)
69	GDP	LH	501	-	29,30,30	1.08	3 (10%)	45,47,47	2.07	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	GDP	O0	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
69	GDP	JN	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	7 (15%)
67	GTP	TE	501	68	33,34,34	0.95	1 (3%)	50,54,54	1.62	8 (16%)
67	GTP	JK	501	-	33,34,34	0.89	1 (3%)	50,54,54	1.56	9 (18%)
69	GDP	WL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
67	GTP	BG	501	68	33,34,34	0.90	1 (3%)	50,54,54	1.60	9 (18%)
69	GDP	FJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
69	GDP	TD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
69	GDP	HJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	5 (11%)
67	GTP	CD	502	68	33,34,34	0.90	1 (3%)	50,54,54	1.65	11 (22%)
69	GDP	VB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
69	GDP	VD	501	-	29,30,30	1.17	2 (6%)	45,47,47	1.78	7 (15%)
69	GDP	WF	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.74	7 (15%)
69	GDP	WJ	501	-	29,30,30	1.21	3 (10%)	45,47,47	1.77	7 (15%)
69	GDP	PD	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.83	7 (15%)
69	GDP	JH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
67	GTP	CL	502	68	33,34,34	0.90	1 (3%)	50,54,54	1.55	9 (18%)
67	GTP	IC	501	68	33,34,34	0.92	1 (3%)	50,54,54	1.56	9 (18%)
67	GTP	LI	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
67	GTP	DE	501	68	33,34,34	0.88	1 (3%)	50,54,54	1.55	9 (18%)
67	GTP	SI	501	-	33,34,34	1.00	1 (3%)	50,54,54	1.74	10 (20%)
69	GDP	IF	501	-	29,30,30	1.12	2 (6%)	45,47,47	1.71	7 (15%)
69	GDP	OL	501	-	29,30,30	1.13	2 (6%)	45,47,47	1.73	6 (13%)
67	GTP	JI	501	68	33,34,34	0.87	1 (3%)	50,54,54	1.59	9 (18%)
69	GDP	JB	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
69	GDP	NH	501	-	29,30,30	1.08	2 (6%)	45,47,47	2.06	12 (26%)
67	GTP	FG	501	68	33,34,34	1.00	3 (9%)	50,54,54	1.72	8 (16%)
69	GDP	NL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
69	GDP	QF	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.77	8 (17%)
67	GTP	GM	501	68	33,34,34	0.87	1 (3%)	50,54,54	1.60	10 (20%)
69	GDP	JJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	7 (15%)
67	GTP	PA	501	68	33,34,34	0.87	1 (3%)	50,54,54	1.60	8 (16%)
67	GTP	PC	501	-	33,34,34	0.94	2 (6%)	50,54,54	1.65	9 (18%)
69	GDP	LN	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)
67	GTP	EM	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	GDP	JD	501	-	29,30,30	1.13	2 (6%)	45,47,47	1.73	6 (13%)
67	GTP	VE	501	-	33,34,34	0.87	0	50,54,54	1.59	11 (22%)
67	GTP	II	501	68	33,34,34	0.95	1 (3%)	50,54,54	1.56	9 (18%)
67	GTP	IK	501	68	33,34,34	0.91	1 (3%)	50,54,54	1.62	9 (18%)
67	GTP	HN	502	68	33,34,34	0.92	1 (3%)	50,54,54	1.62	12 (24%)
69	GDP	CL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
67	GTP	RK	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.50	9 (18%)
67	GTP	OH	502	68	33,34,34	0.90	1 (3%)	50,54,54	1.64	11 (22%)
69	GDP	AH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
69	GDP	CB	501	-	29,30,30	1.13	2 (6%)	45,47,47	1.79	7 (15%)
67	GTP	AH	502	68	33,34,34	0.88	0	50,54,54	1.68	11 (22%)
67	GTP	OF	502	68	33,34,34	0.97	2 (6%)	50,54,54	1.72	12 (24%)
69	GDP	QB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.81	7 (15%)
67	GTP	HG	502	68	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
69	GDP	MH	501	-	29,30,30	1.10	2 (6%)	45,47,47	1.78	6 (13%)
69	GDP	GL	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	6 (13%)
69	GDP	RL	501	-	29,30,30	1.11	3 (10%)	45,47,47	1.81	8 (17%)
67	GTP	FK	501	68	33,34,34	0.91	1 (3%)	50,54,54	1.62	9 (18%)
69	GDP	GN	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	6 (13%)
67	GTP	VG	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.60	8 (16%)
69	GDP	EF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
67	GTP	GJ	502	68	33,34,34	0.87	1 (3%)	50,54,54	1.63	9 (18%)
67	GTP	MM	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
67	GTP	IG	501	68	33,34,34	0.89	1 (3%)	50,54,54	1.60	10 (20%)
67	GTP	QG	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.65	9 (18%)
69	GDP	HD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
69	GDP	KH	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	6 (13%)
69	GDP	N0	501	-	29,30,30	1.14	4 (13%)	45,47,47	1.88	9 (20%)
67	GTP	JM	501	68	33,34,34	0.96	1 (3%)	50,54,54	1.55	8 (16%)
67	GTP	UE	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
67	GTP	QC	501	68	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
69	GDP	KD	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.73	6 (13%)
67	GTP	NA	502	68	33,34,34	0.93	1 (3%)	50,54,54	1.62	10 (20%)
69	GDP	ND	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	6 (13%)
69	GDP	HB	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	GDP	AJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
69	GDP	PH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
67	GTP	VC	501	68	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
69	GDP	BL	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.76	7 (15%)
69	GDP	MN	501	-	29,30,30	1.12	4 (13%)	45,47,47	1.75	6 (13%)
69	GDP	JF	501	-	29,30,30	1.14	2 (6%)	45,47,47	1.74	6 (13%)
69	GDP	PJ	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.90	11 (24%)
69	GDP	AD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	7 (15%)

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
69	GDP	ML	501	-	-	6/16/32/32	0/3/3/3
67	GTP	DF	502	68	-	6/22/38/38	0/3/3/3
69	GDP	LJ	501	-	-	3/16/32/32	0/3/3/3
69	GDP	GJ	501	-	-	4/16/32/32	0/3/3/3
67	GTP	QI	501	-	-	1/22/38/38	0/3/3/3
69	GDP	GH	501	-	-	3/16/32/32	0/3/3/3
67	GTP	WM	501	68	-	3/22/38/38	0/3/3/3
69	GDP	UB	501	-	-	2/16/32/32	0/3/3/3
67	GTP	FM	501	68	-	4/22/38/38	0/3/3/3
67	GTP	LG	501	68	-	9/22/38/38	0/3/3/3
67	GTP	GC	501	68	-	5/22/38/38	0/3/3/3
69	GDP	QL	501	-	-	0/16/32/32	0/3/3/3
67	GTP	IM	501	68	-	3/22/38/38	0/3/3/3
67	GTP	DI	501	68	-	4/22/38/38	0/3/3/3
67	GTP	O0	502	68	-	5/22/38/38	0/3/3/3
69	GDP	SB	501	-	-	5/16/32/32	0/3/3/3
67	GTP	WI	501	68	-	3/22/38/38	0/3/3/3
69	GDP	VF	501	-	-	5/16/32/32	0/3/3/3
67	GTP	MG	501	68	-	5/22/38/38	0/3/3/3
67	GTP	KM	501	68	-	5/22/38/38	0/3/3/3
67	GTP	GI	501	68	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	GDP	SF	501	-	-	3/16/32/32	0/3/3/3
69	GDP	UN	501	-	-	1/16/32/32	0/3/3/3
69	GDP	QH	501	-	-	1/16/32/32	0/3/3/3
69	GDP	NF	501	-	-	2/16/32/32	0/3/3/3
69	GDP	DF	501	-	-	3/16/32/32	0/3/3/3
67	GTP	CB	502	68	-	3/22/38/38	0/3/3/3
69	GDP	VH	501	-	-	2/16/32/32	0/3/3/3
69	GDP	OH	501	-	-	2/16/32/32	0/3/3/3
67	GTP	RI	501	68	-	6/22/38/38	0/3/3/3
69	GDP	VN	501	-	-	1/16/32/32	0/3/3/3
69	GDP	MF	501	-	-	4/16/32/32	0/3/3/3
69	GDP	CF	501	-	-	3/16/32/32	0/3/3/3
67	GTP	RG	501	68	-	2/22/38/38	0/3/3/3
69	GDP	OJ	501	-	-	3/16/32/32	0/3/3/3
67	GTP	KE	501	68	-	4/22/38/38	0/3/3/3
67	GTP	BE	501	68	-	4/22/38/38	0/3/3/3
69	GDP	FD	501	-	-	3/16/32/32	0/3/3/3
69	GDP	SL	501	-	-	2/16/32/32	0/3/3/3
69	GDP	UH	501	-	-	0/16/32/32	0/3/3/3
67	GTP	EG	501	68	-	11/22/38/38	0/3/3/3
69	GDP	FN	501	-	-	2/16/32/32	0/3/3/3
67	GTP	BA	501	68	-	3/22/38/38	0/3/3/3
67	GTP	MC	501	68	-	6/22/38/38	0/3/3/3
67	GTP	SA	501	68	-	5/22/38/38	0/3/3/3
67	GTP	HE	501	68	-	6/22/38/38	0/3/3/3
67	GTP	VI	502	68	-	6/22/38/38	0/3/3/3
69	GDP	BJ	501	-	-	6/16/32/32	0/3/3/3
69	GDP	DN	501	-	-	0/16/32/32	0/3/3/3
69	GDP	ED	501	-	-	4/16/32/32	0/3/3/3
67	GTP	EI	501	68	-	8/22/38/38	0/3/3/3
67	GTP	JE	501	68	-	2/22/38/38	0/3/3/3
69	GDP	CH	501	-	-	6/16/32/32	0/3/3/3
67	GTP	WK	501	68	-	6/22/38/38	0/3/3/3
69	GDP	PF	501	-	-	1/16/32/32	0/3/3/3
67	GTP	UM	501	68	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	GTP	LE	501	68	-	8/22/38/38	0/3/3/3
67	GTP	RE	501	-	-	4/22/38/38	0/3/3/3
69	GDP	LD	501	-	-	4/16/32/32	0/3/3/3
69	GDP	WH	501	-	-	5/16/32/32	0/3/3/3
67	GTP	QK	501	68	-	2/22/38/38	0/3/3/3
69	GDP	HN	501	-	-	3/16/32/32	0/3/3/3
67	GTP	LC	501	68	-	0/22/38/38	0/3/3/3
69	GDP	UL	501	-	-	3/16/32/32	0/3/3/3
69	GDP	RF	501	-	-	1/16/32/32	0/3/3/3
67	GTP	BC	501	-	-	7/22/38/38	0/3/3/3
67	GTP	AA	501	68	-	8/22/38/38	0/3/3/3
67	GTP	QE	501	68	-	3/22/38/38	0/3/3/3
67	GTP	TK	501	68	-	3/22/38/38	0/3/3/3
67	GTP	UC	501	68	-	6/22/38/38	0/3/3/3
69	GDP	SH	501	-	-	0/16/32/32	0/3/3/3
67	GTP	RA	501	68	-	8/22/38/38	0/3/3/3
67	GTP	KK	501	68	-	6/22/38/38	0/3/3/3
67	GTP	SC	501	68	-	6/22/38/38	0/3/3/3
67	GTP	UI	501	68	-	6/22/38/38	0/3/3/3
69	GDP	EL	501	-	-	4/16/32/32	0/3/3/3
67	GTP	GE	501	68	-	5/22/38/38	0/3/3/3
69	GDP	CJ	501	-	-	4/16/32/32	0/3/3/3
69	GDP	DB	501	-	-	4/16/32/32	0/3/3/3
69	GDP	DH	501	-	-	4/16/32/32	0/3/3/3
69	GDP	EB	501	-	-	3/16/32/32	0/3/3/3
69	GDP	LB	501	-	-	3/16/32/32	0/3/3/3
69	GDP	MD	501	-	-	6/16/32/32	0/3/3/3
69	GDP	OD	501	-	-	3/16/32/32	0/3/3/3
69	GDP	RD	501	-	-	3/16/32/32	0/3/3/3
69	GDP	IN	501	-	-	3/16/32/32	0/3/3/3
69	GDP	WN	501	-	-	2/16/32/32	0/3/3/3
67	GTP	BI	501	68	-	8/22/38/38	0/3/3/3
67	GTP	CH	502	68	-	3/22/38/38	0/3/3/3
67	GTP	PD	502	68	-	6/22/38/38	0/3/3/3
67	GTP	RM	501	-	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	GTP	WC	501	68	-	3/22/38/38	0/3/3/3
67	GTP	JC	501	68	-	2/22/38/38	0/3/3/3
69	GDP	GD	501	-	-	2/16/32/32	0/3/3/3
69	GDP	KN	501	-	-	7/16/32/32	0/3/3/3
69	GDP	LL	501	-	-	2/16/32/32	0/3/3/3
69	GDP	HF	501	-	-	4/16/32/32	0/3/3/3
69	GDP	IB	501	-	-	3/16/32/32	0/3/3/3
69	GDP	IL	501	-	-	2/16/32/32	0/3/3/3
67	GTP	TG	501	68	-	5/22/38/38	0/3/3/3
69	GDP	DJ	501	-	-	3/16/32/32	0/3/3/3
67	GTP	CG	501	68	-	5/22/38/38	0/3/3/3
69	GDP	IH	501	-	-	4/16/32/32	0/3/3/3
67	GTP	AC	501	68	-	4/22/38/38	0/3/3/3
69	GDP	QJ	501	-	-	0/16/32/32	0/3/3/3
69	GDP	UD	501	-	-	6/16/32/32	0/3/3/3
67	GTP	PG	501	68	-	2/22/38/38	0/3/3/3
69	GDP	KL	501	-	-	2/16/32/32	0/3/3/3
69	GDP	CD	501	-	-	5/16/32/32	0/3/3/3
69	GDP	IJ	501	-	-	2/16/32/32	0/3/3/3
67	GTP	AM	501	68	-	3/22/38/38	0/3/3/3
67	GTP	SK	501	68	-	4/22/38/38	0/3/3/3
69	GDP	DD	501	-	-	4/16/32/32	0/3/3/3
67	GTP	MK	501	68	-	6/22/38/38	0/3/3/3
69	GDP	WB	501	-	-	1/16/32/32	0/3/3/3
67	GTP	AD	502	68	-	4/22/38/38	0/3/3/3
69	GDP	HL	501	-	-	3/16/32/32	0/3/3/3
69	GDP	TB	501	-	-	4/16/32/32	0/3/3/3
67	GTP	GG	501	68	-	3/22/38/38	0/3/3/3
69	GDP	TF	501	-	-	5/16/32/32	0/3/3/3
69	GDP	UF	501	-	-	1/16/32/32	0/3/3/3
67	GTP	FE	501	68	-	6/22/38/38	0/3/3/3
69	GDP	AL	501	-	-	1/16/32/32	0/3/3/3
69	GDP	JL	501	-	-	4/16/32/32	0/3/3/3
69	GDP	RJ	501	-	-	2/16/32/32	0/3/3/3
67	GTP	IE	501	68	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	GDP	GB	501	-	-	3/16/32/32	0/3/3/3
69	GDP	QD	501	-	-	0/16/32/32	0/3/3/3
67	GTP	RB	502	-	-	3/22/38/38	0/3/3/3
67	GTP	EE	501	-	-	8/22/38/38	0/3/3/3
67	GTP	MI	501	68	-	5/22/38/38	0/3/3/3
69	GDP	RH	501	-	-	1/16/32/32	0/3/3/3
67	GTP	HK	501	68	-	6/22/38/38	0/3/3/3
67	GTP	WG	501	-	-	7/22/38/38	0/3/3/3
67	GTP	DC	501	-	-	8/22/38/38	0/3/3/3
67	GTP	PI	501	68	-	4/22/38/38	0/3/3/3
69	GDP	VL	501	-	-	4/16/32/32	0/3/3/3
67	GTP	BM	501	68	-	7/22/38/38	0/3/3/3
67	GTP	SF	502	68	-	6/22/38/38	0/3/3/3
69	GDP	BH	501	-	-	4/16/32/32	0/3/3/3
69	GDP	FF	501	-	-	4/16/32/32	0/3/3/3
69	GDP	GF	501	-	-	3/16/32/32	0/3/3/3
69	GDP	EH	501	-	-	3/16/32/32	0/3/3/3
67	GTP	QA	501	68	-	4/22/38/38	0/3/3/3
69	GDP	FB	501	-	-	2/16/32/32	0/3/3/3
67	GTP	NF	502	68	-	5/22/38/38	0/3/3/3
67	GTP	EC	501	68	-	8/22/38/38	0/3/3/3
69	GDP	LF	501	-	-	3/16/32/32	0/3/3/3
69	GDP	TH	501	-	-	2/16/32/32	0/3/3/3
67	GTP	NE	501	68	-	2/22/38/38	0/3/3/3
69	GDP	SJ	501	-	-	2/16/32/32	0/3/3/3
67	GTP	KC	501	68	-	5/22/38/38	0/3/3/3
67	GTP	DK	501	68	-	3/22/38/38	0/3/3/3
69	GDP	AF	501	-	-	1/16/32/32	0/3/3/3
67	GTP	HI	501	68	-	6/22/38/38	0/3/3/3
69	GDP	BF	501	-	-	4/16/32/32	0/3/3/3
67	GTP	OE	501	68	-	3/22/38/38	0/3/3/3
67	GTP	AK	501	68	-	4/22/38/38	0/3/3/3
69	GDP	VJ	501	-	-	2/16/32/32	0/3/3/3
67	GTP	BK	501	68	-	4/22/38/38	0/3/3/3
67	GTP	TC	501	68	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	GTP	NK	501	68	-	5/22/38/38	0/3/3/3
69	GDP	FH	501	-	-	3/16/32/32	0/3/3/3
69	GDP	PB	501	-	-	2/16/32/32	0/3/3/3
69	GDP	OF	501	-	-	3/16/32/32	0/3/3/3
67	GTP	UK	501	68	-	3/22/38/38	0/3/3/3
69	GDP	TJ	501	-	-	3/16/32/32	0/3/3/3
67	GTP	LK	501	68	-	6/22/38/38	0/3/3/3
67	GTP	UG	501	68	-	3/22/38/38	0/3/3/3
69	GDP	NJ	501	-	-	3/16/32/32	0/3/3/3
67	GTP	DA	501	68	-	1/22/38/38	0/3/3/3
67	GTP	FC	501	-	-	3/22/38/38	0/3/3/3
69	GDP	NB	501	-	-	2/16/32/32	0/3/3/3
69	GDP	BB	501	-	-	5/16/32/32	0/3/3/3
69	GDP	MJ	501	-	-	6/16/32/32	0/3/3/3
67	GTP	JG	501	68	-	2/22/38/38	0/3/3/3
69	GDP	RB	501	-	-	1/16/32/32	0/3/3/3
67	GTP	SM	501	68	-	7/22/38/38	0/3/3/3
67	GTP	OK	501	68	-	7/22/38/38	0/3/3/3
67	GTP	OC	501	68	-	8/22/38/38	0/3/3/3
67	GTP	HC	501	68	-	5/22/38/38	0/3/3/3
67	GTP	PK	501	68	-	3/22/38/38	0/3/3/3
69	GDP	HH	501	-	-	3/16/32/32	0/3/3/3
67	GTP	KO	501	68	-	6/22/38/38	0/3/3/3
69	GDP	OB	501	-	-	4/16/32/32	0/3/3/3
67	GTP	LM	501	68	-	6/22/38/38	0/3/3/3
67	GTP	KI	501	68	-	10/22/38/38	0/3/3/3
69	GDP	PL	501	-	-	3/16/32/32	0/3/3/3
67	GTP	CJ	502	68	-	6/22/38/38	0/3/3/3
67	GTP	EK	501	68	-	4/22/38/38	0/3/3/3
69	GDP	MB	501	-	-	6/16/32/32	0/3/3/3
69	GDP	SD	501	-	-	5/16/32/32	0/3/3/3
69	GDP	DL	501	-	-	2/16/32/32	0/3/3/3
67	GTP	AG	501	68	-	4/22/38/38	0/3/3/3
67	GTP	CA	501	-	-	2/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	GTP	IN	502	68	-	3/22/38/38	0/3/3/3
67	GTP	TI	501	68	-	5/22/38/38	0/3/3/3
67	GTP	VL	502	68	-	5/22/38/38	0/3/3/3
69	GDP	BD	501	-	-	0/16/32/32	0/3/3/3
67	GTP	NB	502	68	-	8/22/38/38	0/3/3/3
69	GDP	EJ	501	-	-	4/16/32/32	0/3/3/3
67	GTP	QM	501	68	-	3/22/38/38	0/3/3/3
67	GTP	PM	501	68	-	1/22/38/38	0/3/3/3
67	GTP	SE	501	68	-	3/22/38/38	0/3/3/3
67	GTP	TM	501	68	-	4/22/38/38	0/3/3/3
67	GTP	KG	501	68	-	5/22/38/38	0/3/3/3
67	GTP	WE	501	68	-	5/22/38/38	0/3/3/3
69	GDP	AB	501	-	-	1/16/32/32	0/3/3/3
69	GDP	UJ	501	-	-	1/16/32/32	0/3/3/3
69	GDP	WD	501	-	-	4/16/32/32	0/3/3/3
69	GDP	FL	501	-	-	3/16/32/32	0/3/3/3
67	GTP	DM	501	68	-	4/22/38/38	0/3/3/3
69	GDP	TL	501	-	-	2/16/32/32	0/3/3/3
67	GTP	NI	501	68	-	6/22/38/38	0/3/3/3
67	GTP	ME	501	68	-	3/22/38/38	0/3/3/3
69	GDP	EN	501	-	-	4/16/32/32	0/3/3/3
67	GTP	VK	501	68	-	8/22/38/38	0/3/3/3
69	GDP	KB	501	-	-	7/16/32/32	0/3/3/3
69	GDP	ID	501	-	-	3/16/32/32	0/3/3/3
67	GTP	HL	502	68	-	4/22/38/38	0/3/3/3
69	GDP	KJ	501	-	-	3/16/32/32	0/3/3/3
67	GTP	FI	501	68	-	4/22/38/38	0/3/3/3
69	GDP	KF	501	-	-	4/16/32/32	0/3/3/3
69	GDP	LH	501	-	-	3/16/32/32	0/3/3/3
69	GDP	O0	501	-	-	5/16/32/32	0/3/3/3
69	GDP	JN	501	-	-	3/16/32/32	0/3/3/3
67	GTP	TE	501	68	-	3/22/38/38	0/3/3/3
67	GTP	JK	501	-	-	3/22/38/38	0/3/3/3
69	GDP	WL	501	-	-	5/16/32/32	0/3/3/3
67	GTP	BG	501	68	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	GDP	FJ	501	-	-	2/16/32/32	0/3/3/3
69	GDP	TD	501	-	-	4/16/32/32	0/3/3/3
69	GDP	HJ	501	-	-	5/16/32/32	0/3/3/3
67	GTP	CD	502	68	-	3/22/38/38	0/3/3/3
69	GDP	VB	501	-	-	2/16/32/32	0/3/3/3
69	GDP	VD	501	-	-	0/16/32/32	0/3/3/3
69	GDP	WF	501	-	-	3/16/32/32	0/3/3/3
69	GDP	WJ	501	-	-	2/16/32/32	0/3/3/3
69	GDP	PD	501	-	-	3/16/32/32	0/3/3/3
69	GDP	JH	501	-	-	6/16/32/32	0/3/3/3
67	GTP	CL	502	68	-	1/22/38/38	0/3/3/3
67	GTP	IC	501	68	-	5/22/38/38	0/3/3/3
67	GTP	LI	501	68	-	8/22/38/38	0/3/3/3
67	GTP	DE	501	68	-	1/22/38/38	0/3/3/3
67	GTP	SI	501	-	-	4/22/38/38	0/3/3/3
69	GDP	IF	501	-	-	1/16/32/32	0/3/3/3
69	GDP	OL	501	-	-	3/16/32/32	0/3/3/3
67	GTP	JI	501	68	-	3/22/38/38	0/3/3/3
69	GDP	JB	501	-	-	5/16/32/32	0/3/3/3
69	GDP	NH	501	-	-	2/16/32/32	0/3/3/3
67	GTP	FG	501	68	-	3/22/38/38	0/3/3/3
69	GDP	NL	501	-	-	2/16/32/32	0/3/3/3
69	GDP	QF	501	-	-	1/16/32/32	0/3/3/3
67	GTP	GM	501	68	-	4/22/38/38	0/3/3/3
69	GDP	JJ	501	-	-	4/16/32/32	0/3/3/3
67	GTP	PA	501	68	-	3/22/38/38	0/3/3/3
67	GTP	PC	501	-	-	5/22/38/38	0/3/3/3
69	GDP	LN	501	-	-	3/16/32/32	0/3/3/3
67	GTP	EM	501	-	-	3/22/38/38	0/3/3/3
69	GDP	JD	501	-	-	4/16/32/32	0/3/3/3
67	GTP	VE	501	-	-	4/22/38/38	0/3/3/3
67	GTP	II	501	68	-	5/22/38/38	0/3/3/3
67	GTP	IK	501	68	-	8/22/38/38	0/3/3/3
67	GTP	HN	502	68	-	4/22/38/38	0/3/3/3
69	GDP	CL	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	GTP	RK	501	-	-	3/22/38/38	0/3/3/3
67	GTP	OH	502	68	-	5/22/38/38	0/3/3/3
69	GDP	AH	501	-	-	1/16/32/32	0/3/3/3
69	GDP	CB	501	-	-	2/16/32/32	0/3/3/3
67	GTP	AH	502	68	-	2/22/38/38	0/3/3/3
67	GTP	OF	502	68	-	10/22/38/38	0/3/3/3
69	GDP	QB	501	-	-	5/16/32/32	0/3/3/3
67	GTP	HG	502	68	-	2/22/38/38	0/3/3/3
69	GDP	MH	501	-	-	6/16/32/32	0/3/3/3
69	GDP	GL	501	-	-	2/16/32/32	0/3/3/3
69	GDP	RL	501	-	-	2/16/32/32	0/3/3/3
67	GTP	FK	501	68	-	1/22/38/38	0/3/3/3
69	GDP	GN	501	-	-	4/16/32/32	0/3/3/3
67	GTP	VG	501	68	-	6/22/38/38	0/3/3/3
69	GDP	EF	501	-	-	4/16/32/32	0/3/3/3
67	GTP	GJ	502	68	-	8/22/38/38	0/3/3/3
67	GTP	MM	501	68	-	7/22/38/38	0/3/3/3
67	GTP	IG	501	68	-	3/22/38/38	0/3/3/3
67	GTP	QG	501	-	-	2/22/38/38	0/3/3/3
69	GDP	HD	501	-	-	3/16/32/32	0/3/3/3
69	GDP	KH	501	-	-	4/16/32/32	0/3/3/3
69	GDP	N0	501	-	-	2/16/32/32	0/3/3/3
67	GTP	JM	501	68	-	4/22/38/38	0/3/3/3
67	GTP	UE	501	68	-	3/22/38/38	0/3/3/3
67	GTP	QC	501	68	-	5/22/38/38	0/3/3/3
69	GDP	KD	501	-	-	3/16/32/32	0/3/3/3
67	GTP	NA	502	68	-	6/22/38/38	0/3/3/3
69	GDP	ND	501	-	-	3/16/32/32	0/3/3/3
69	GDP	HB	501	-	-	3/16/32/32	0/3/3/3
69	GDP	AJ	501	-	-	2/16/32/32	0/3/3/3
69	GDP	PH	501	-	-	3/16/32/32	0/3/3/3
67	GTP	VC	501	68	-	4/22/38/38	0/3/3/3
69	GDP	BL	501	-	-	4/16/32/32	0/3/3/3
69	GDP	MN	501	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	GDP	JF	501	-	-	4/16/32/32	0/3/3/3
69	GDP	PJ	501	-	-	1/16/32/32	0/3/3/3
69	GDP	AD	501	-	-	1/16/32/32	0/3/3/3

The worst 5 of 628 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DK	501	GTP	PA-O3A	4.26	1.64	1.59
67	VL	502	GTP	PB-O3B	4.12	1.64	1.59
67	DK	501	GTP	PB-O3A	3.40	1.63	1.59
69	RJ	501	GDP	C5-C4	3.35	1.48	1.38
69	IB	501	GDP	C5-C4	3.27	1.47	1.38

The worst 5 of 2466 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	IB	501	GDP	C5-C4-N3	-6.64	117.82	128.39
69	FF	501	GDP	C5-C4-N3	-6.53	117.99	128.39
69	ML	501	GDP	N2-C2-N1	6.52	130.53	116.76
69	PJ	501	GDP	C5-C4-N3	-6.39	118.22	128.39
69	BJ	501	GDP	C5-C4-N3	-6.28	118.40	128.39

There are no chirality outliers.

5 of 1145 torsion outliers are listed below:

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

There are no ring outliers.

212 monomers are involved in 369 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	ML	501	GDP	1	0
67	DF	502	GTP	1	0
67	QI	501	GTP	2	0
67	WM	501	GTP	1	0
69	UB	501	GDP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	GC	501	GTP	1	0
69	QL	501	GDP	2	0
67	IM	501	GTP	2	0
67	DI	501	GTP	1	0
67	O0	502	GTP	2	0
69	SB	501	GDP	1	0
67	WI	501	GTP	1	0
67	MG	501	GTP	3	0
67	GI	501	GTP	1	0
69	SF	501	GDP	1	0
69	QH	501	GDP	2	0
69	NF	501	GDP	2	0
69	DF	501	GDP	2	0
67	CB	502	GTP	1	0
69	VH	501	GDP	2	0
69	OH	501	GDP	2	0
67	RI	501	GTP	4	0
69	VN	501	GDP	4	0
69	CF	501	GDP	4	0
67	RG	501	GTP	1	0
69	OJ	501	GDP	1	0
69	FD	501	GDP	1	0
69	UH	501	GDP	4	0
67	EG	501	GTP	1	0
69	FN	501	GDP	3	0
67	BA	501	GTP	1	0
67	MC	501	GTP	3	0
67	HE	501	GTP	2	0
67	VI	502	GTP	3	0
69	BJ	501	GDP	1	0
69	DN	501	GDP	1	0
69	ED	501	GDP	2	0
67	EI	501	GTP	1	0
69	CH	501	GDP	2	0
69	PF	501	GDP	2	0
67	UM	501	GTP	1	0
67	LE	501	GTP	2	0
69	WH	501	GDP	1	0
67	QK	501	GTP	3	0
69	UL	501	GDP	2	0
67	BC	501	GTP	3	0
67	AA	501	GTP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	QE	501	GTP	2	0
67	TK	501	GTP	2	0
67	UC	501	GTP	3	0
67	SC	501	GTP	1	0
69	CJ	501	GDP	1	0
69	DB	501	GDP	3	0
69	DH	501	GDP	3	0
69	OD	501	GDP	2	0
69	RD	501	GDP	1	0
69	IN	501	GDP	1	0
69	WN	501	GDP	1	0
67	BI	501	GTP	1	0
67	CH	502	GTP	1	0
67	PD	502	GTP	4	0
67	RM	501	GTP	2	0
67	WC	501	GTP	1	0
69	LL	501	GDP	1	0
69	HF	501	GDP	1	0
69	IB	501	GDP	1	0
69	IL	501	GDP	2	0
67	TG	501	GTP	3	0
69	DJ	501	GDP	1	0
67	CG	501	GTP	1	0
67	AC	501	GTP	1	0
69	QJ	501	GDP	1	0
69	CD	501	GDP	3	0
69	IJ	501	GDP	1	0
67	SK	501	GTP	2	0
67	MK	501	GTP	1	0
69	TF	501	GDP	2	0
69	AL	501	GDP	1	0
69	JL	501	GDP	1	0
69	RJ	501	GDP	2	0
67	IE	501	GTP	1	0
69	GB	501	GDP	1	0
69	QD	501	GDP	3	0
67	MI	501	GTP	1	0
67	HK	501	GTP	2	0
67	WG	501	GTP	2	0
67	DC	501	GTP	2	0
67	PI	501	GTP	3	0
69	VL	501	GDP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	SF	502	GTP	2	0
69	BH	501	GDP	1	0
69	FF	501	GDP	1	0
69	GF	501	GDP	1	0
69	EH	501	GDP	1	0
67	NF	502	GTP	1	0
67	EC	501	GTP	2	0
69	TH	501	GDP	1	0
67	NE	501	GTP	1	0
67	KC	501	GTP	2	0
67	DK	501	GTP	3	0
67	HI	501	GTP	4	0
69	BF	501	GDP	2	0
67	OE	501	GTP	5	0
67	AK	501	GTP	1	0
69	VJ	501	GDP	2	0
67	BK	501	GTP	2	0
67	TC	501	GTP	2	0
67	NK	501	GTP	1	0
69	FH	501	GDP	1	0
69	PB	501	GDP	3	0
69	OF	501	GDP	1	0
67	UK	501	GTP	1	0
69	TJ	501	GDP	3	0
67	LK	501	GTP	1	0
67	UG	501	GTP	2	0
69	NJ	501	GDP	2	0
67	DA	501	GTP	1	0
67	FC	501	GTP	2	0
69	NB	501	GDP	1	0
69	BB	501	GDP	1	0
69	MJ	501	GDP	1	0
67	JG	501	GTP	1	0
67	SM	501	GTP	1	0
67	OK	501	GTP	1	0
67	OC	501	GTP	1	0
67	HC	501	GTP	2	0
67	PK	501	GTP	5	0
67	KO	501	GTP	1	0
69	OB	501	GDP	1	0
69	PL	501	GDP	1	0
67	CJ	502	GTP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	EK	501	GTP	2	0
69	MB	501	GDP	1	0
69	DL	501	GDP	1	0
67	AG	501	GTP	2	0
67	CA	501	GTP	2	0
67	IN	502	GTP	1	0
67	TI	501	GTP	4	0
67	VL	502	GTP	6	0
69	BD	501	GDP	2	0
67	NB	502	GTP	1	0
67	QM	501	GTP	2	0
67	PM	501	GTP	1	0
67	SE	501	GTP	3	0
67	TM	501	GTP	1	0
67	WE	501	GTP	3	0
69	AB	501	GDP	1	0
69	UJ	501	GDP	1	0
69	WD	501	GDP	1	0
67	DM	501	GTP	2	0
67	NI	501	GTP	1	0
67	ME	501	GTP	1	0
69	EN	501	GDP	2	0
67	VK	501	GTP	1	0
69	KB	501	GDP	1	0
69	ID	501	GDP	1	0
69	O0	501	GDP	1	0
69	JN	501	GDP	1	0
67	TE	501	GTP	1	0
67	JK	501	GTP	2	0
67	BG	501	GTP	1	0
69	HJ	501	GDP	5	0
67	CD	502	GTP	1	0
69	VD	501	GDP	4	0
69	WF	501	GDP	1	0
69	PD	501	GDP	4	0
69	JH	501	GDP	2	0
67	CL	502	GTP	1	0
67	IC	501	GTP	3	0
67	DE	501	GTP	1	0
67	SI	501	GTP	2	0
69	IF	501	GDP	1	0
69	OL	501	GDP	1	0

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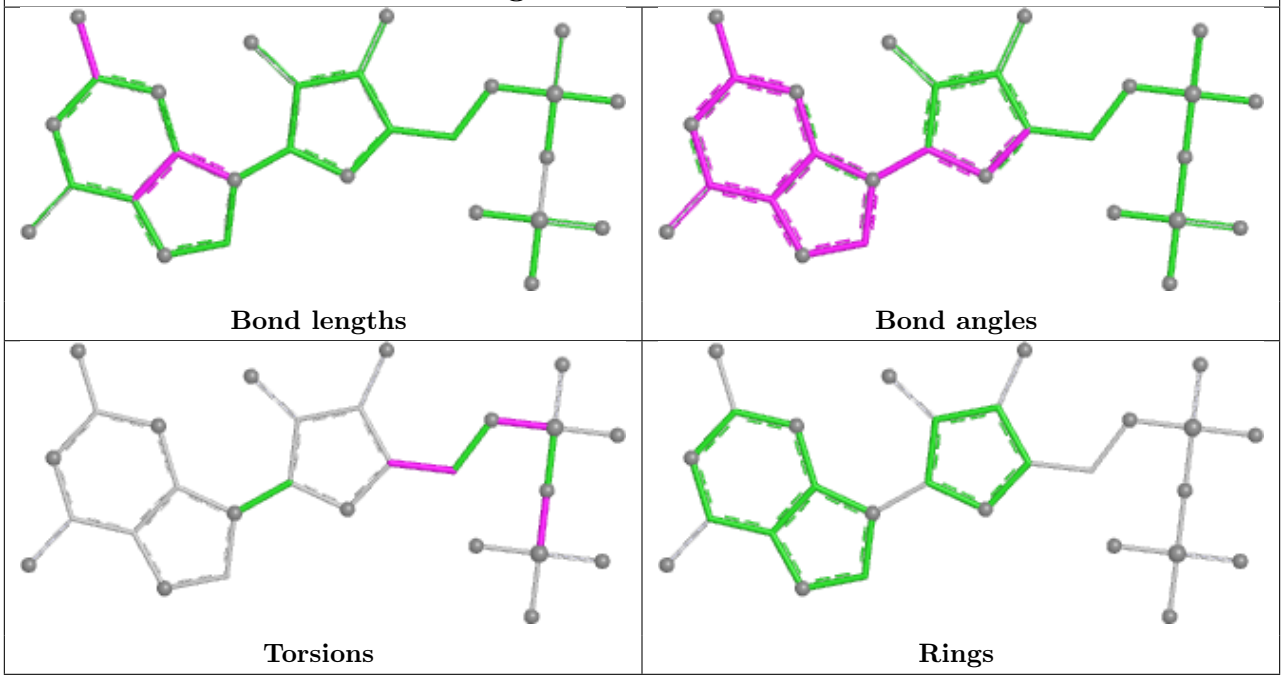
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	JI	501	GTP	3	0
67	FG	501	GTP	2	0
69	NL	501	GDP	1	0
69	QF	501	GDP	3	0
67	GM	501	GTP	1	0
69	JJ	501	GDP	1	0
67	PA	501	GTP	1	0
67	PC	501	GTP	1	0
67	EM	501	GTP	2	0
67	VE	501	GTP	3	0
67	II	501	GTP	1	0
67	IK	501	GTP	1	0
69	CL	501	GDP	3	0
67	RK	501	GTP	1	0
67	OH	502	GTP	2	0
69	CB	501	GDP	1	0
67	OF	502	GTP	1	0
69	QB	501	GDP	1	0
67	HG	502	GTP	1	0
69	GL	501	GDP	2	0
69	RL	501	GDP	1	0
67	VG	501	GTP	1	0
67	GJ	502	GTP	1	0
67	MM	501	GTP	1	0
67	IG	501	GTP	2	0
67	QG	501	GTP	1	0
69	N0	501	GDP	1	0
67	JM	501	GTP	1	0
67	UE	501	GTP	4	0
67	QC	501	GTP	1	0
69	KD	501	GDP	1	0
67	NA	502	GTP	2	0
69	HB	501	GDP	2	0
69	PH	501	GDP	5	0
67	VC	501	GTP	3	0
69	BL	501	GDP	1	0
69	MN	501	GDP	1	0
69	JF	501	GDP	3	0
69	PJ	501	GDP	1	0

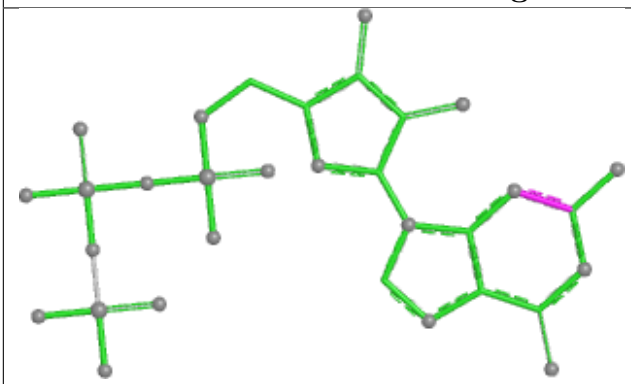
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

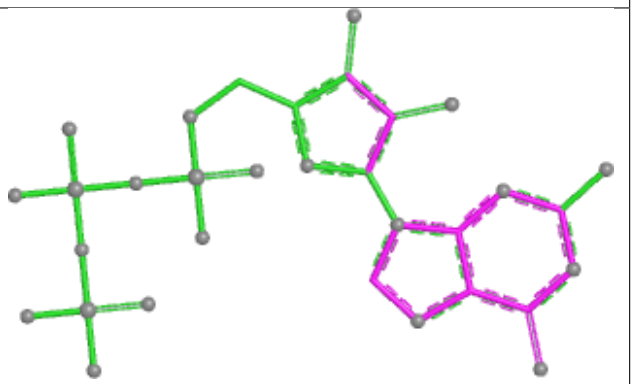
Ligand GDP ML 501



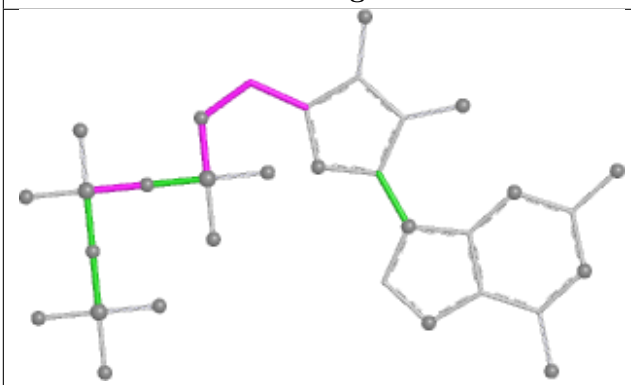
Ligand GTP DF 502



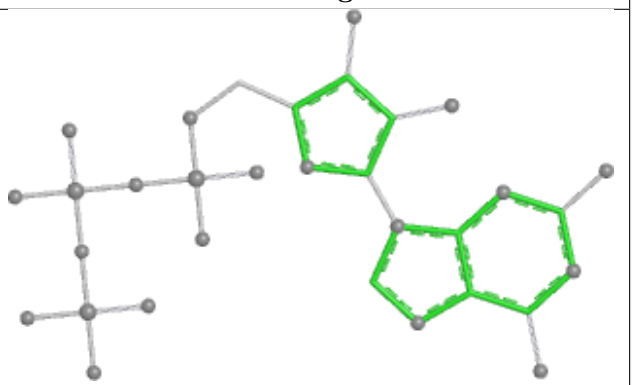
Bond lengths



Bond angles

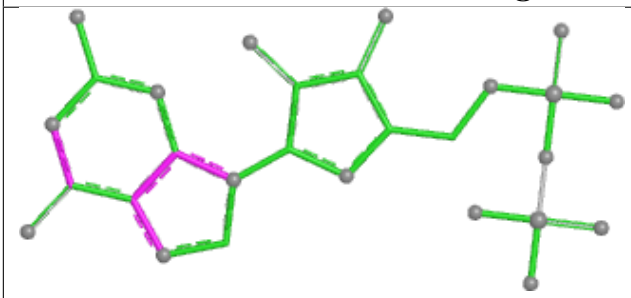


Torsions

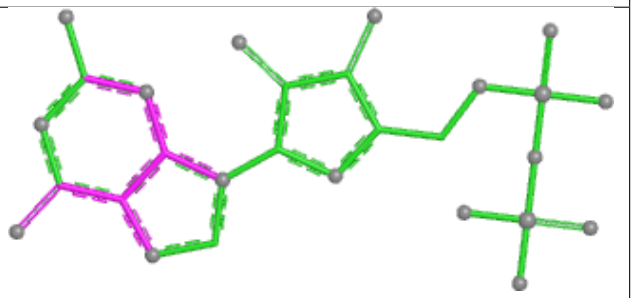


Rings

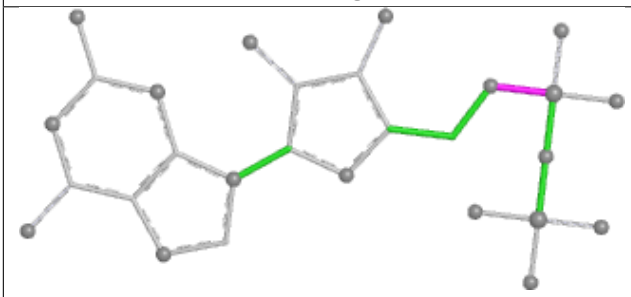
Ligand GDP LJ 501



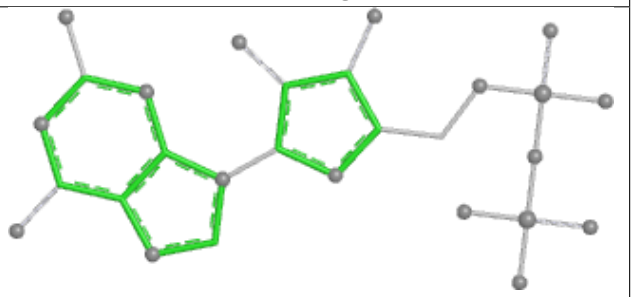
Bond lengths



Bond angles

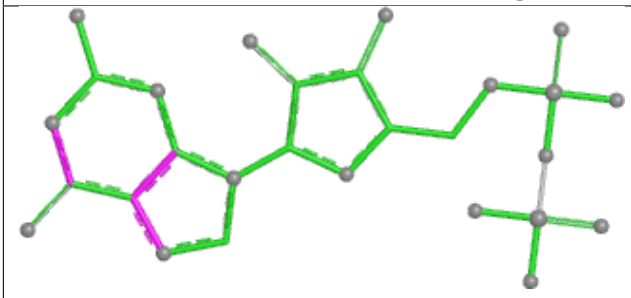


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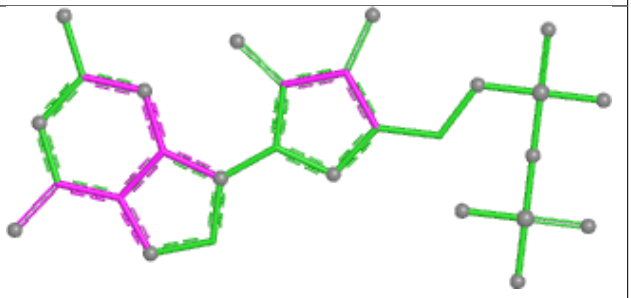


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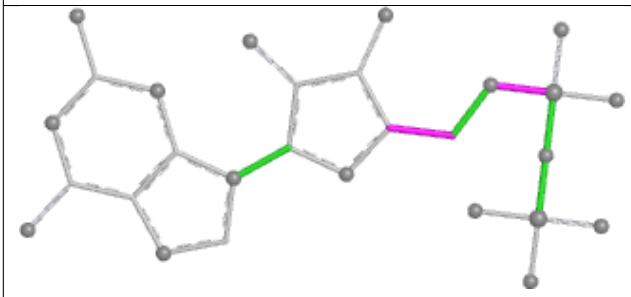
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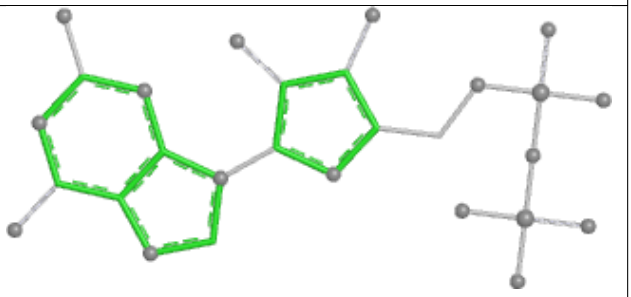
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Bond angles

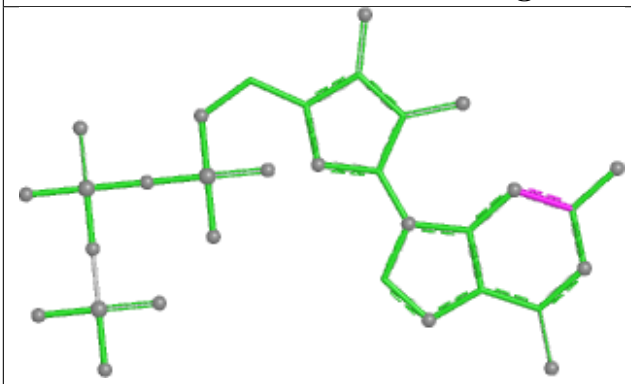


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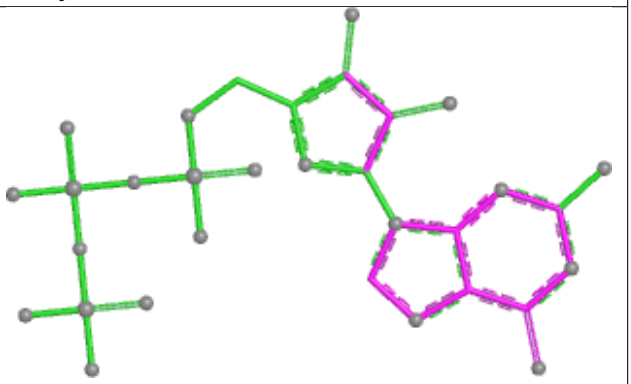


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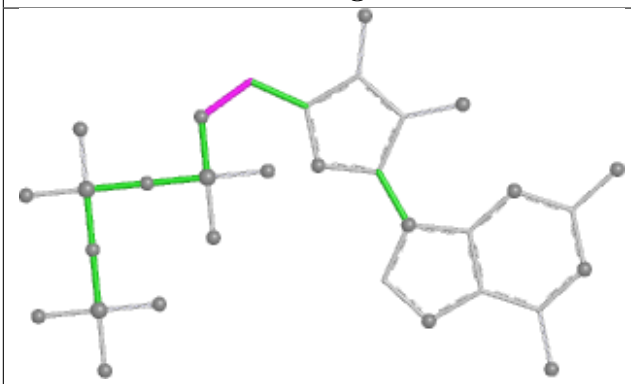
Ligand GTP QI 501



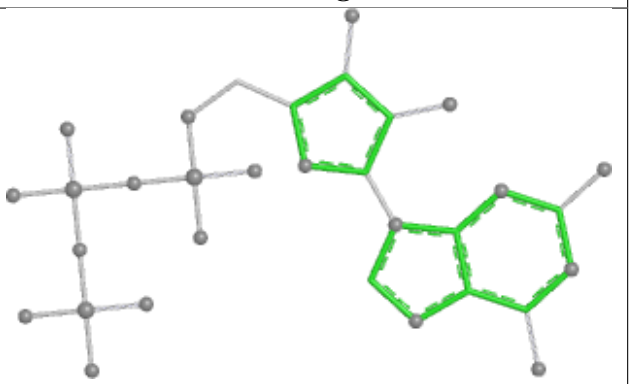
Bond lengths



Bond angles

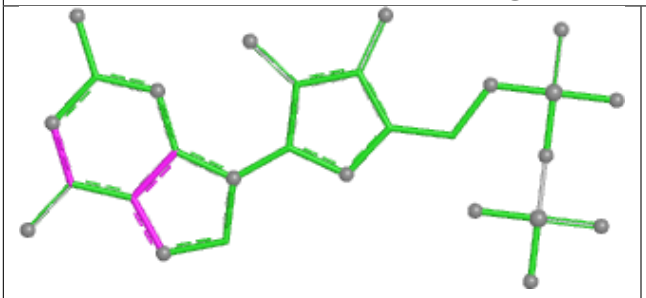


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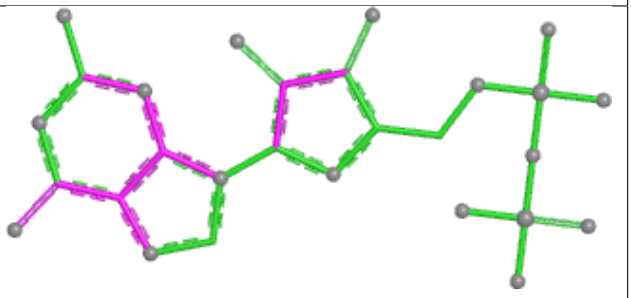


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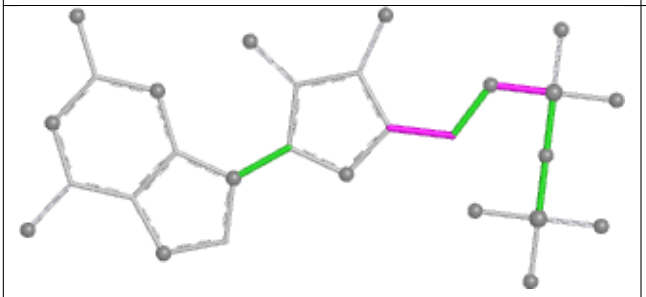
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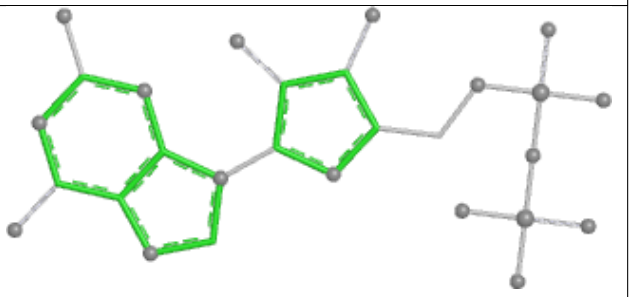
Bond lengths



Bond angles

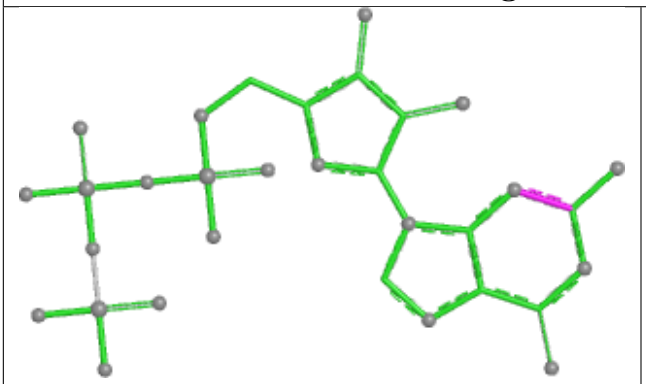


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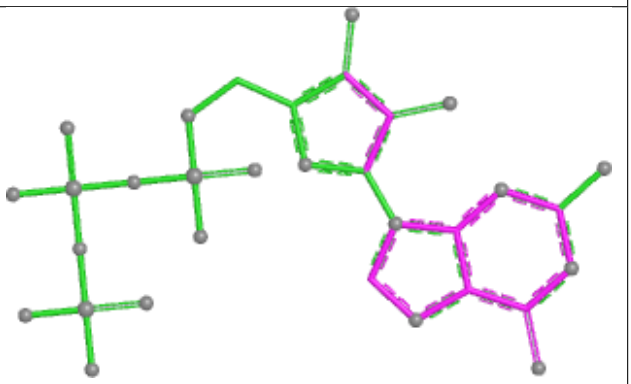


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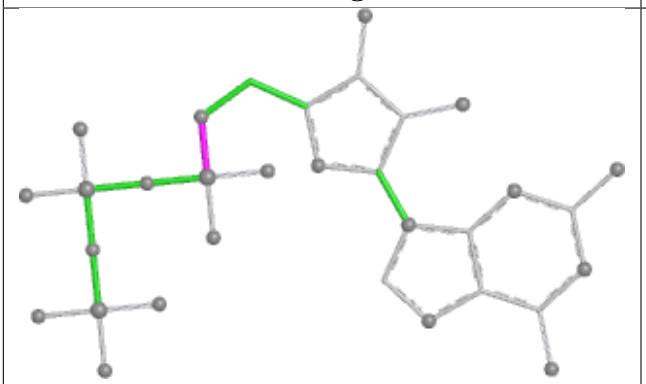
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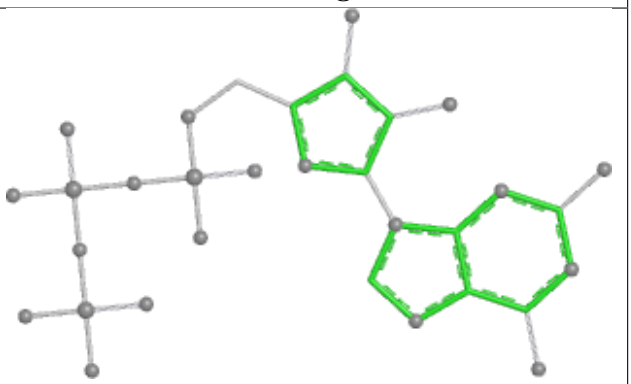
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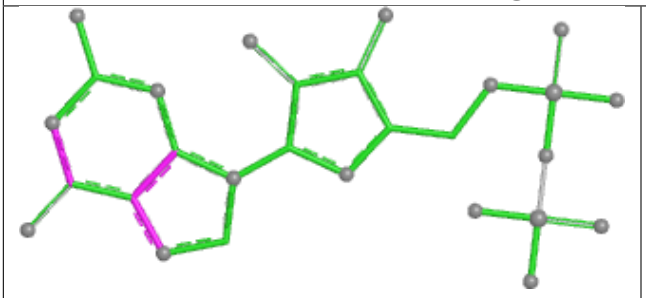


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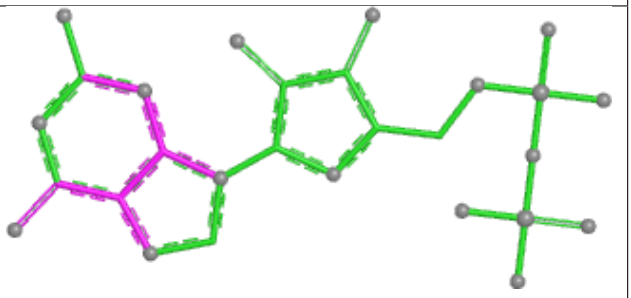


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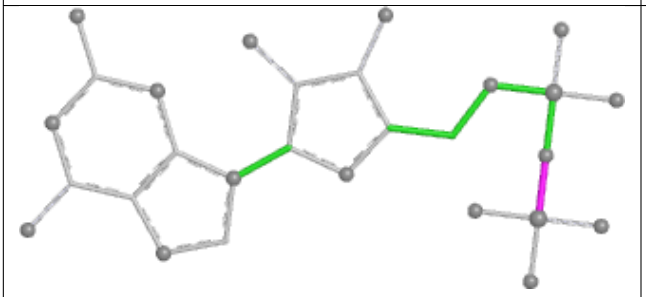
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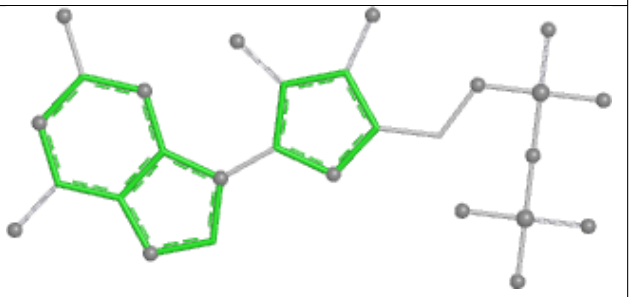
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Bond angles

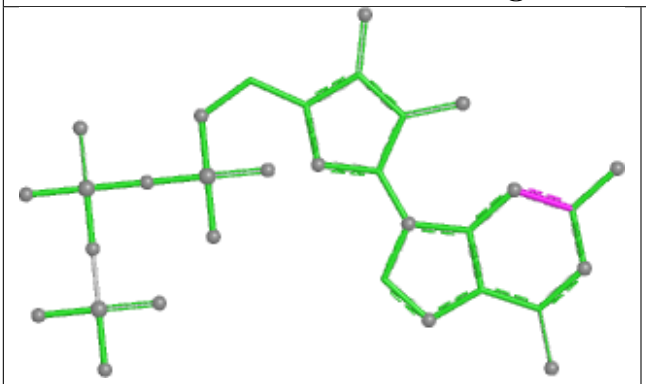


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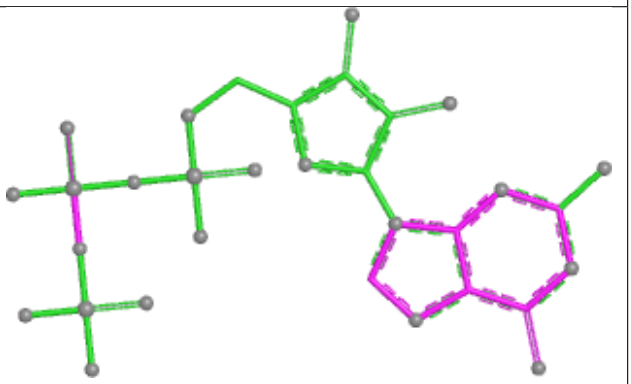


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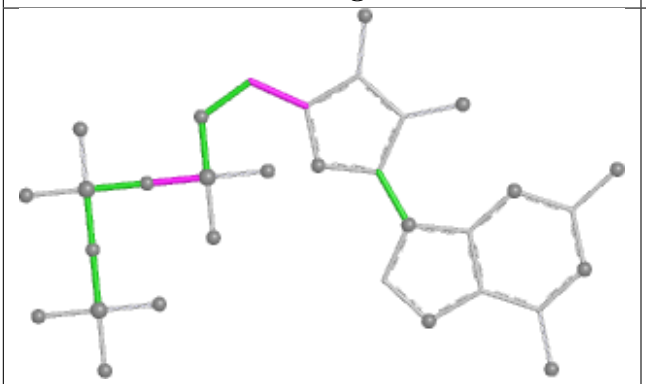
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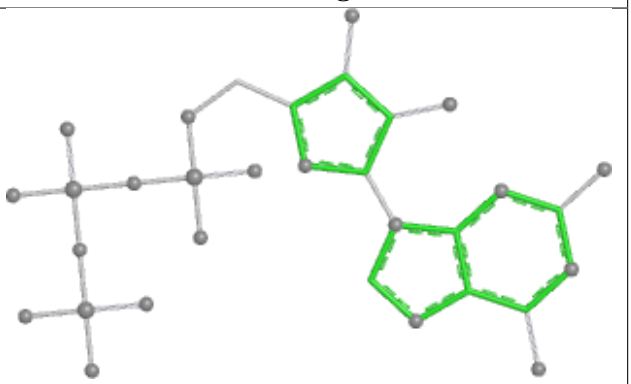
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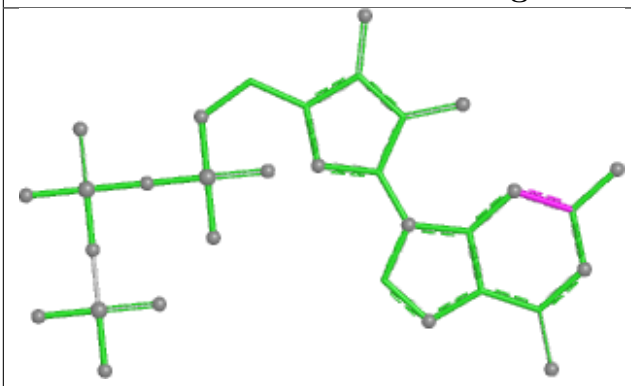


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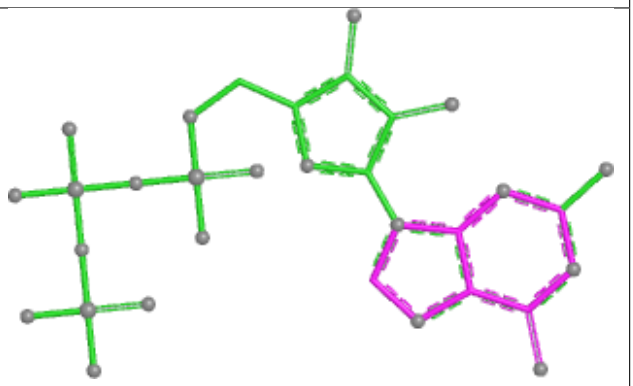


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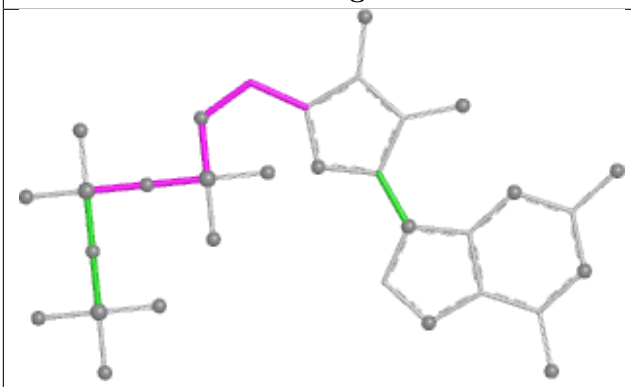
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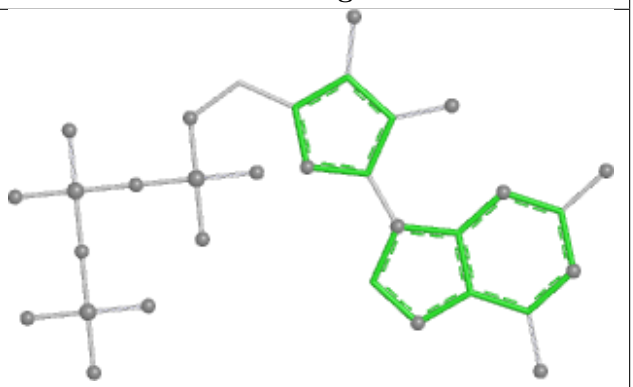
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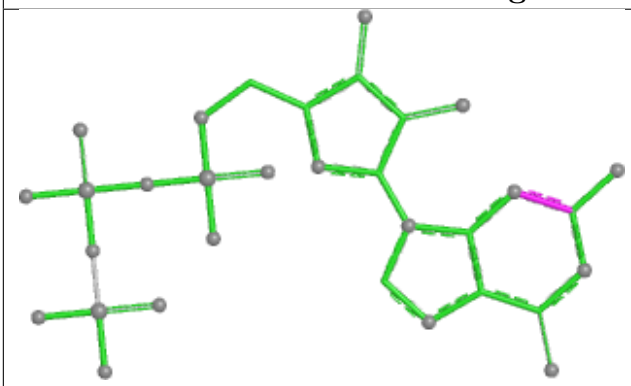


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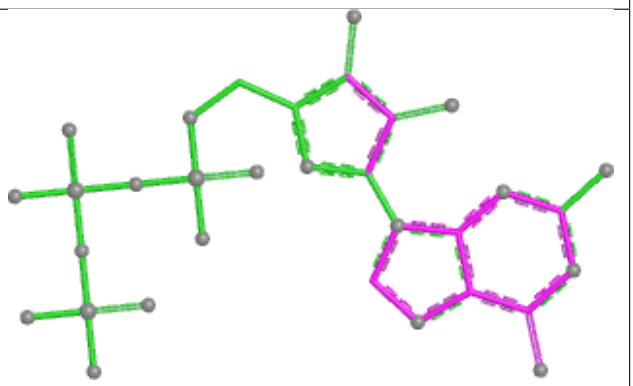


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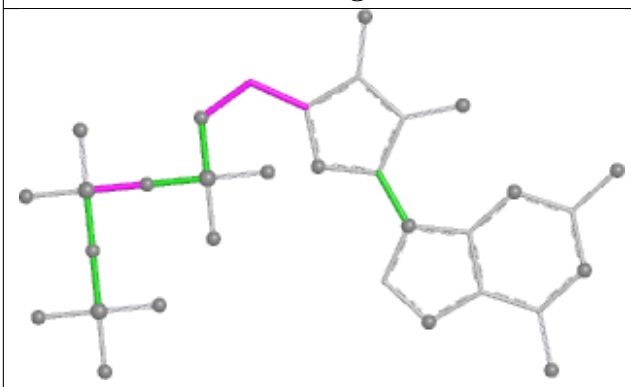
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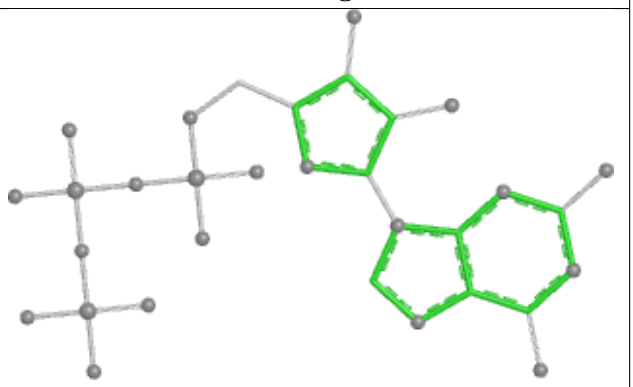
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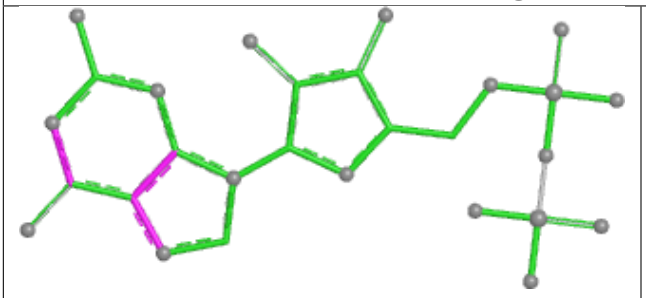


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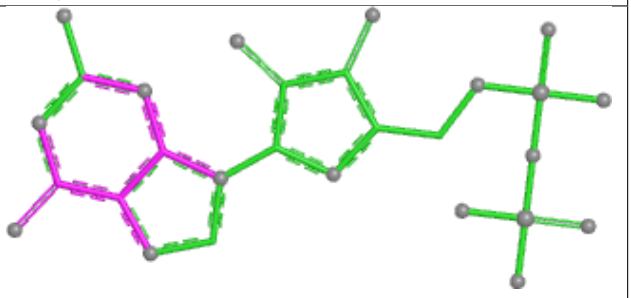


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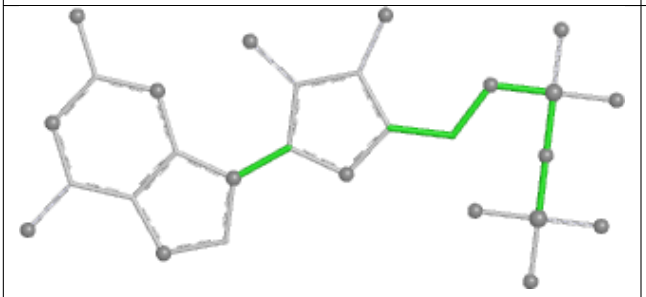
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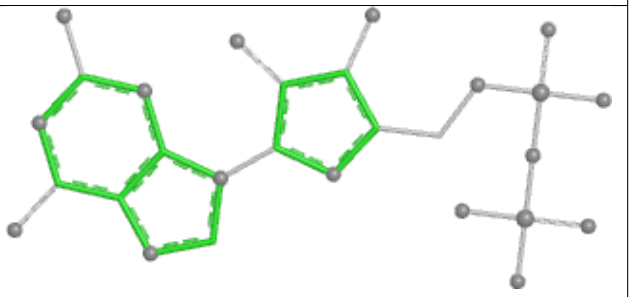
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Bond angles

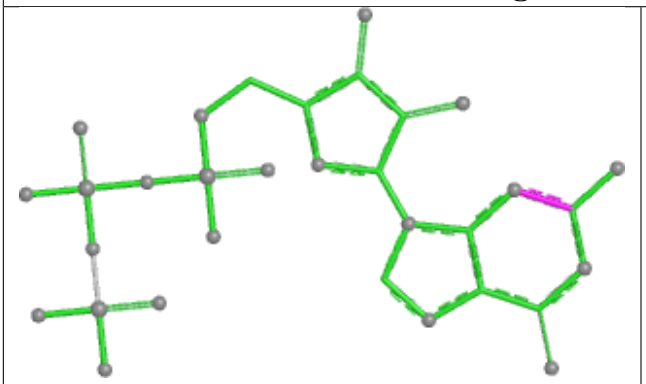


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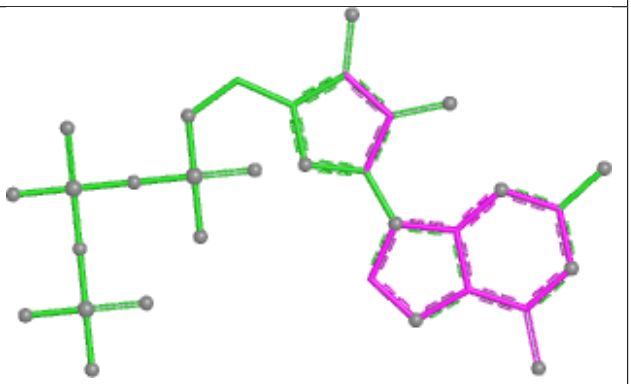


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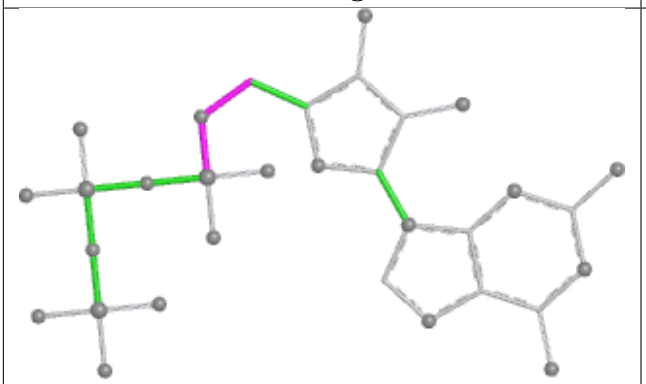
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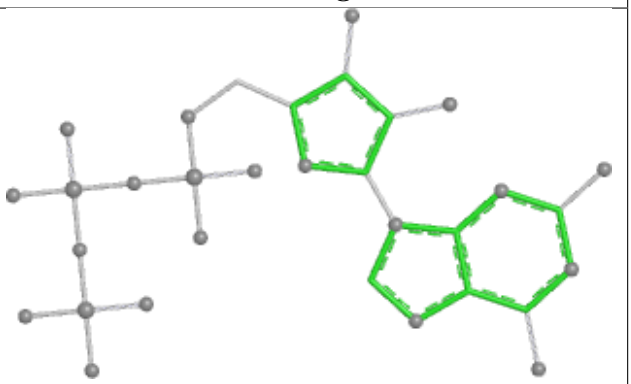
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Bond angles

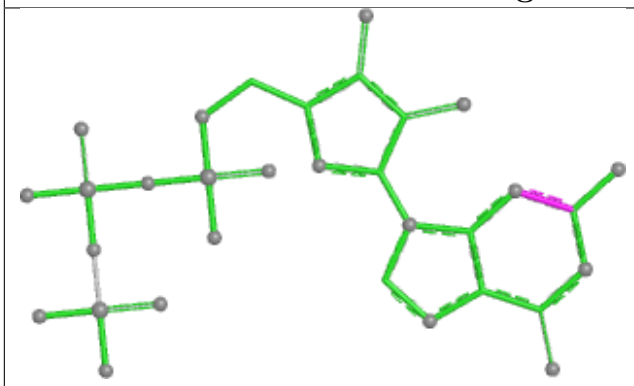


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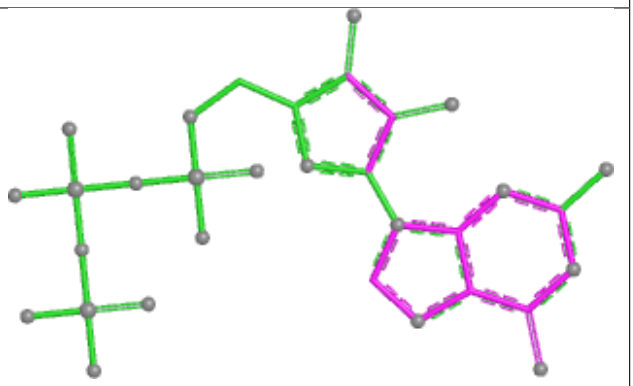


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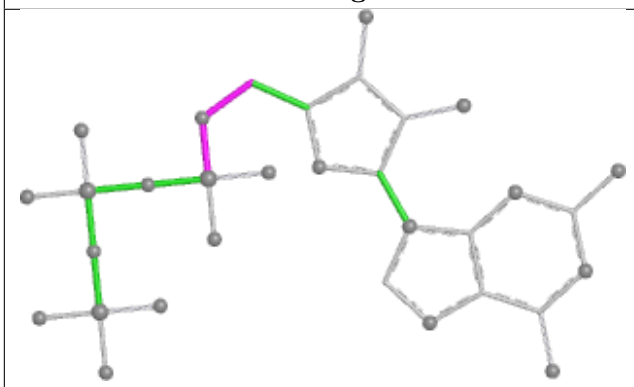
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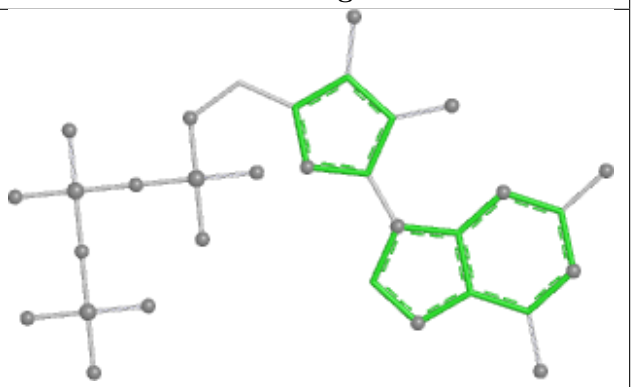
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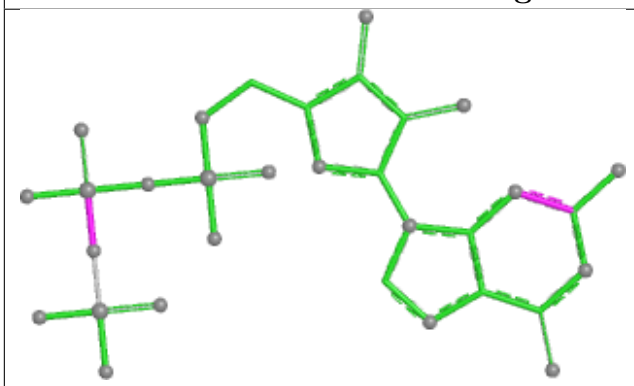


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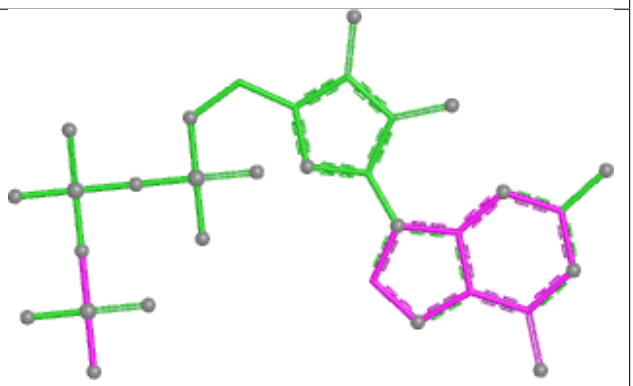


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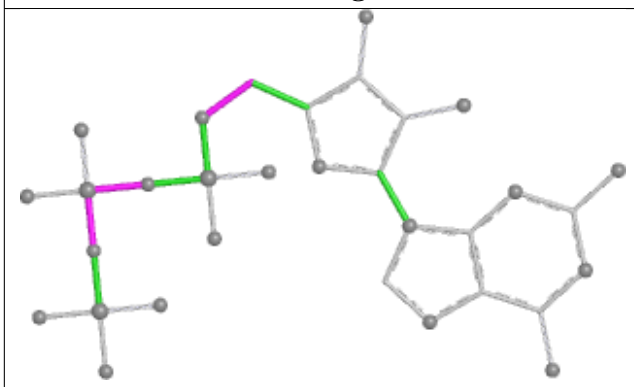
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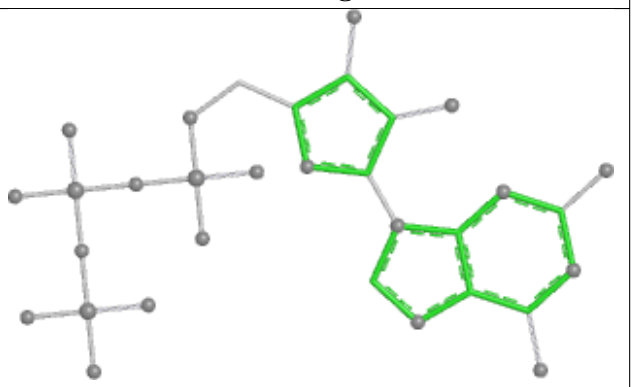
Bond lengths



Bond angles

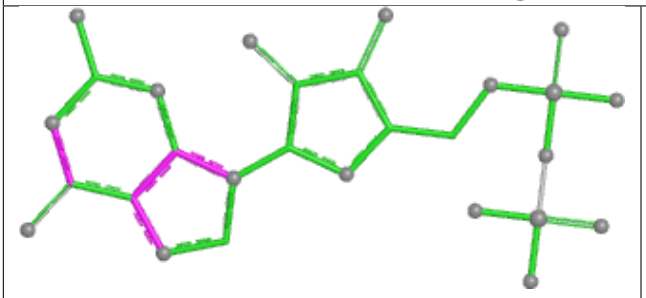


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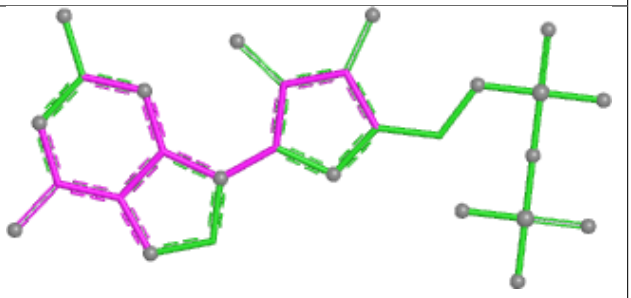


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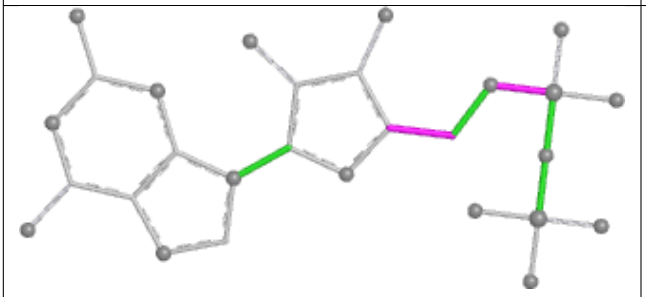
Ligand GDP SB 501



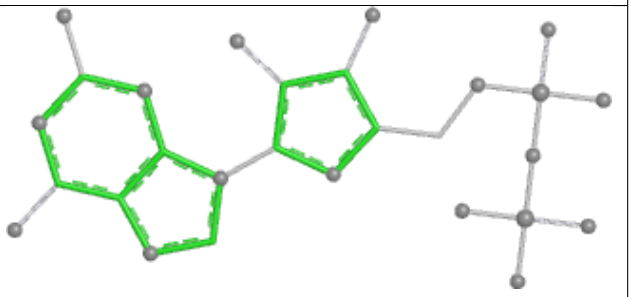
Bond lengths



Bond angles

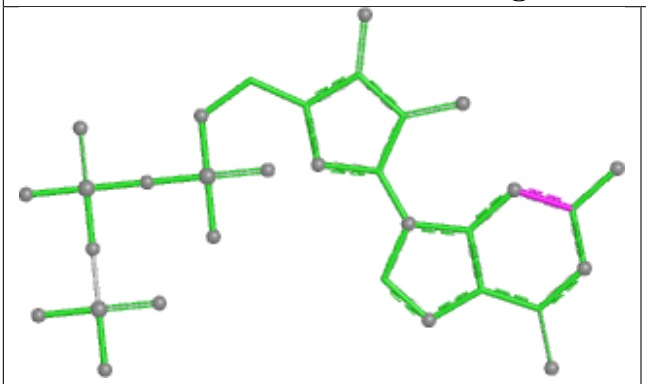


Torsions

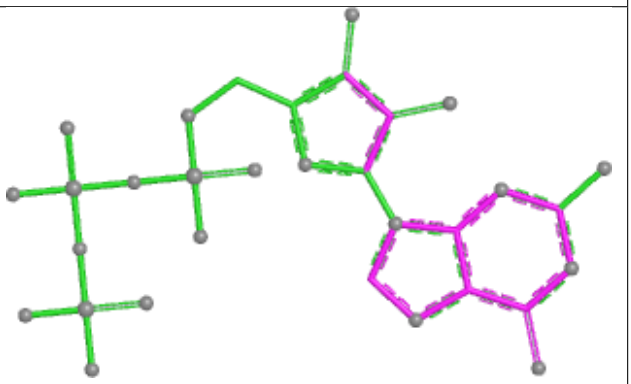


Rings

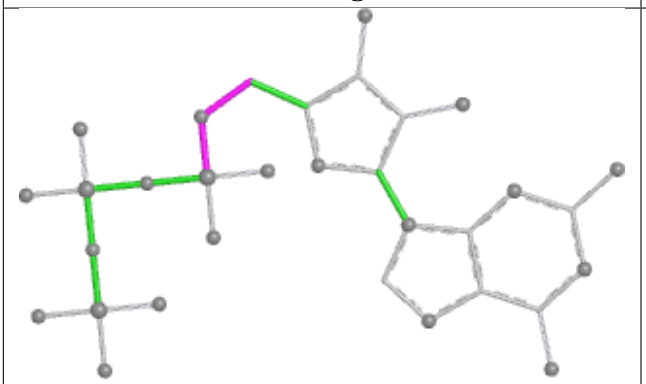
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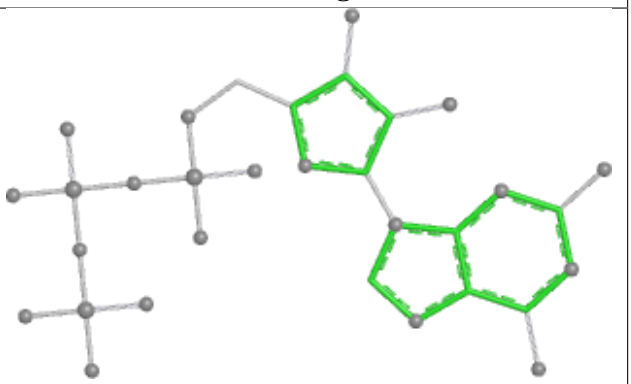
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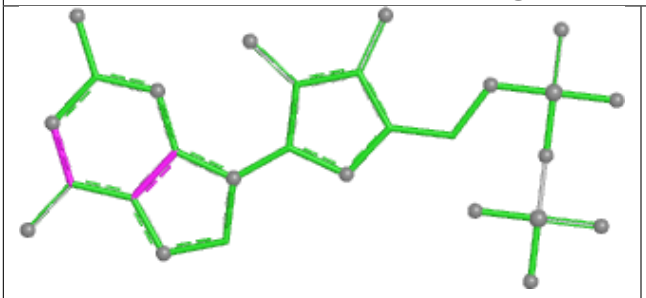


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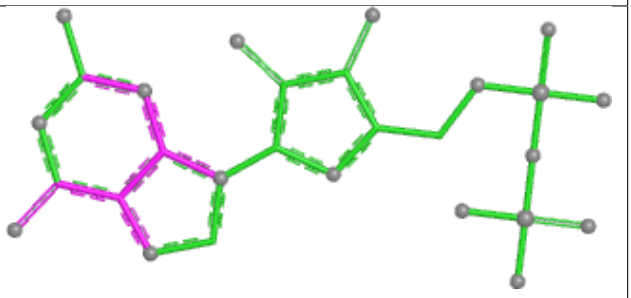


Rings

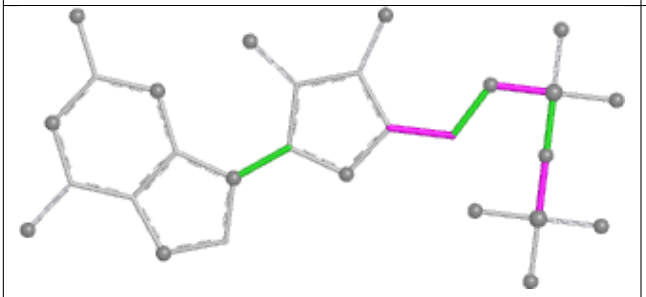
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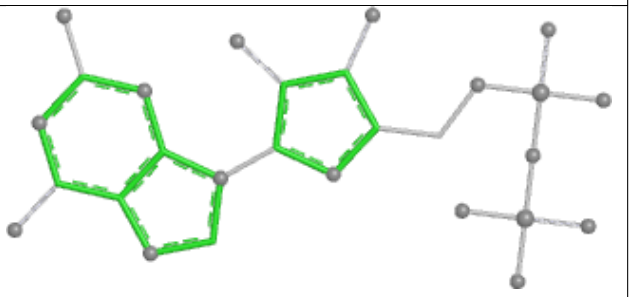
Bond lengths



Bond angles

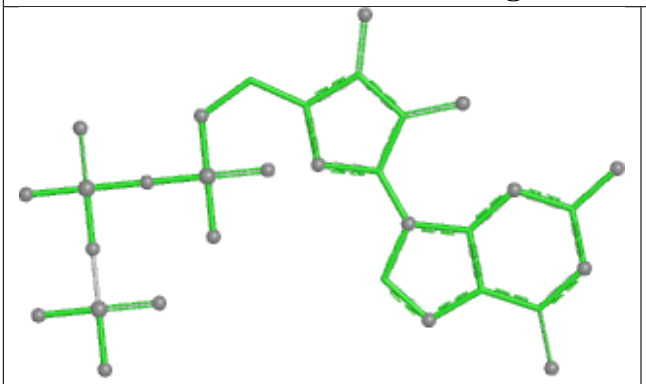


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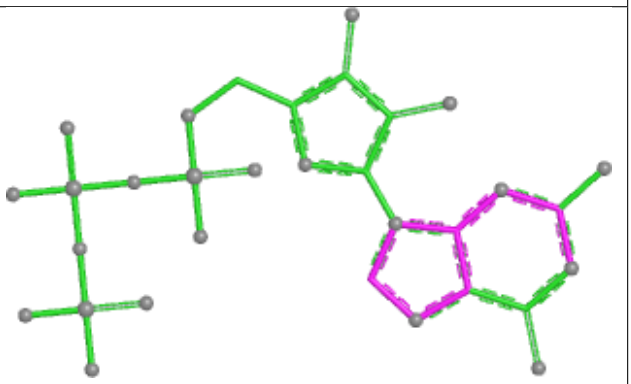


Rings

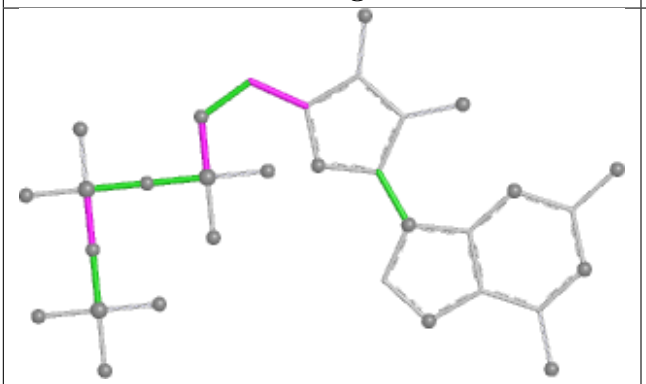
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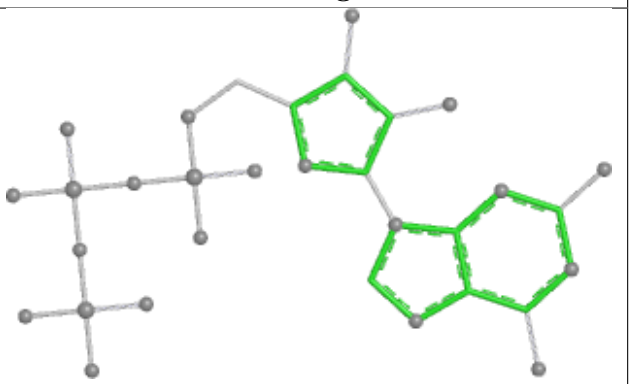
Bond lengths



Bond angles

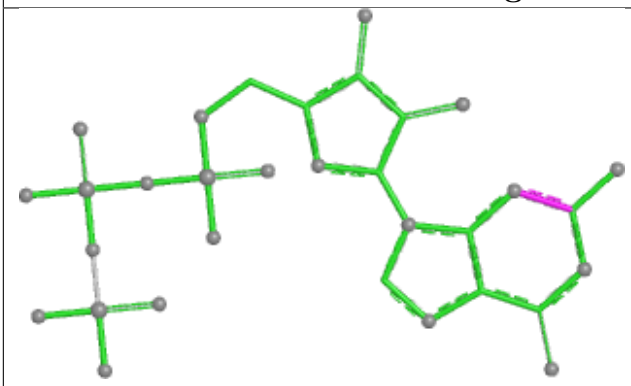


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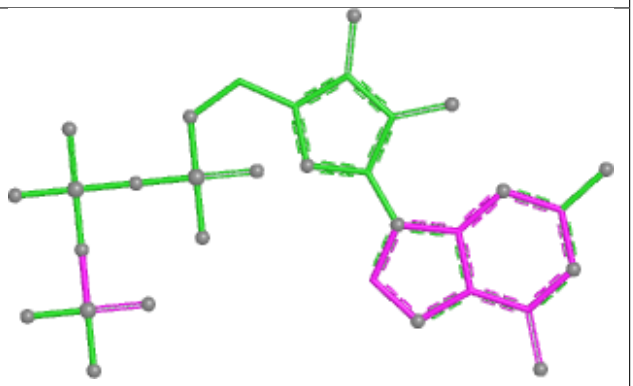


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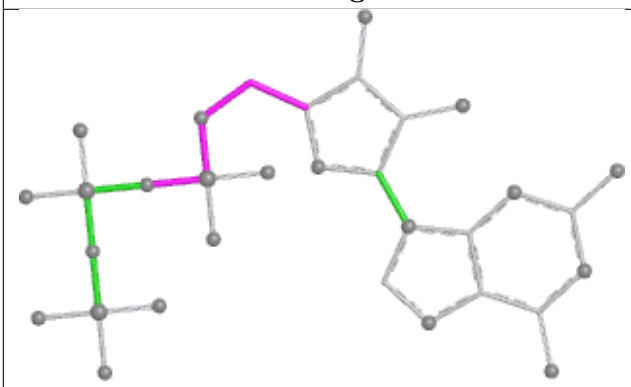
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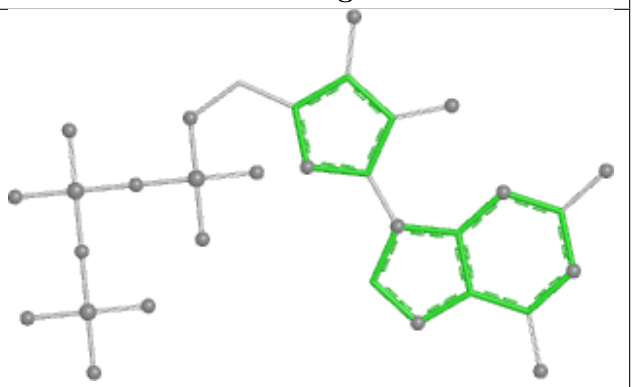
Bond lengths



Bond angles

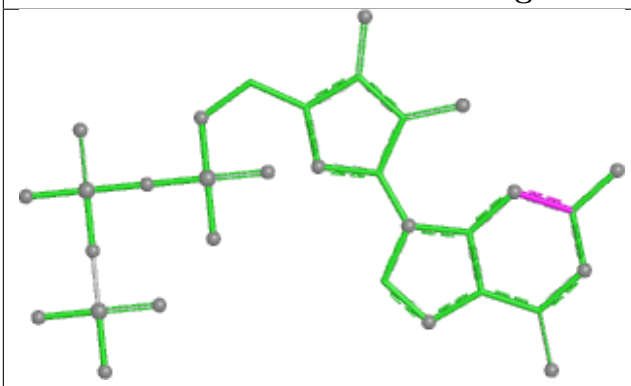


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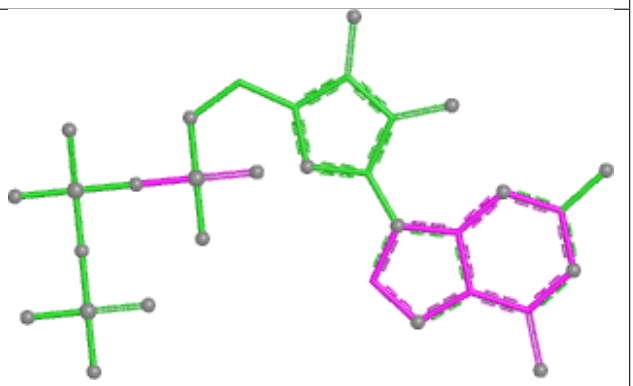


Rings

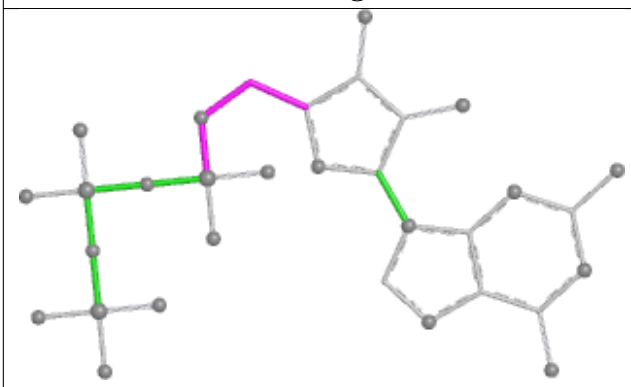
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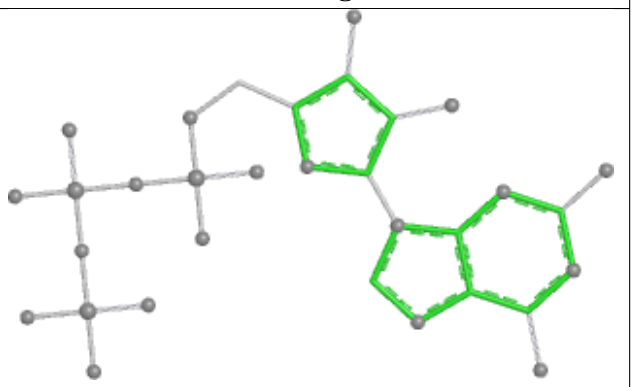
Bond lengths



Bond angles

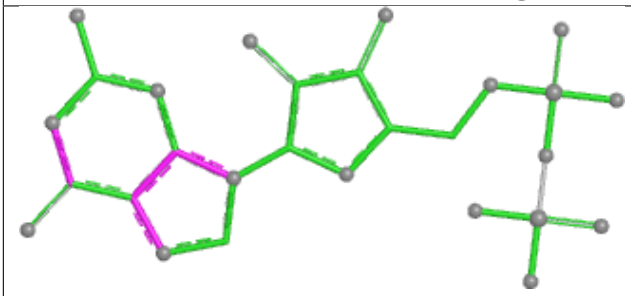


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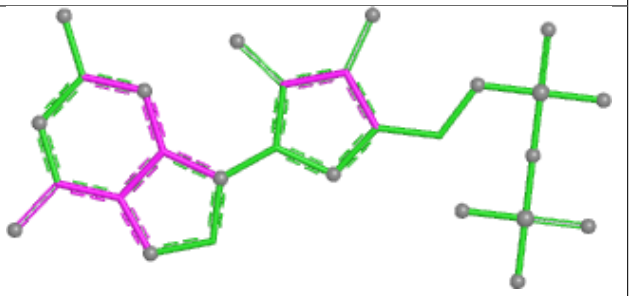


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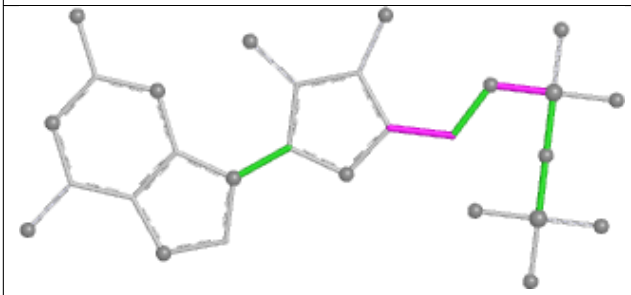
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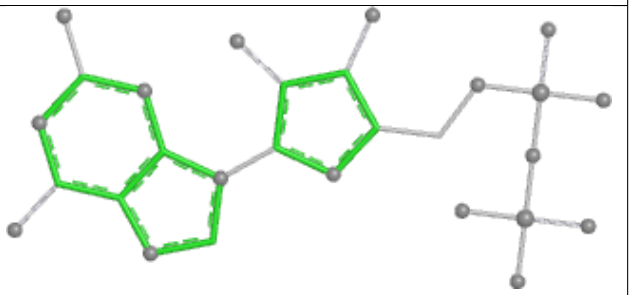
Bond lengths



Bond angles

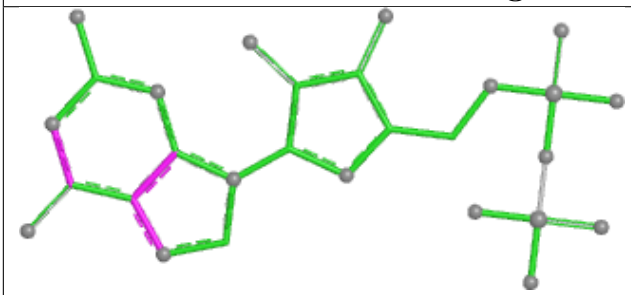


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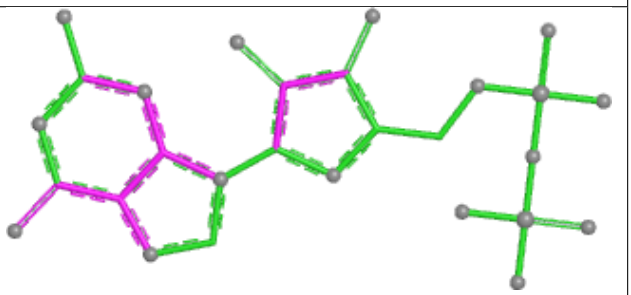


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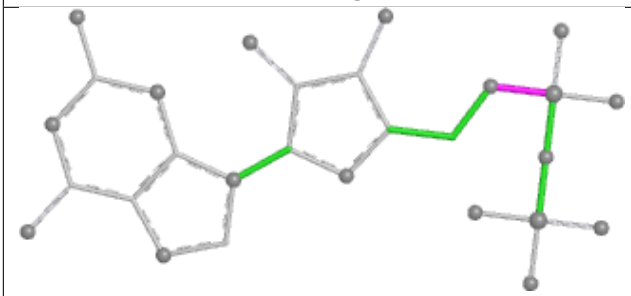
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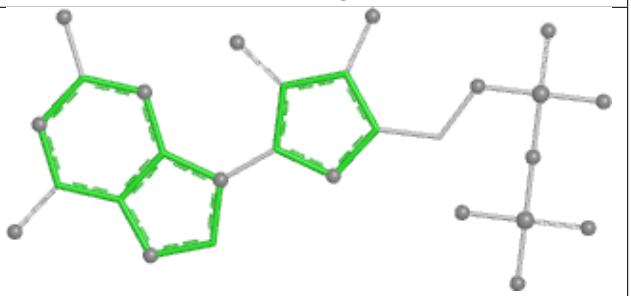
Bond lengths



Bond angles

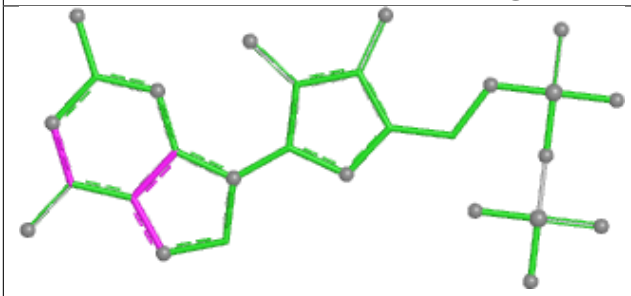


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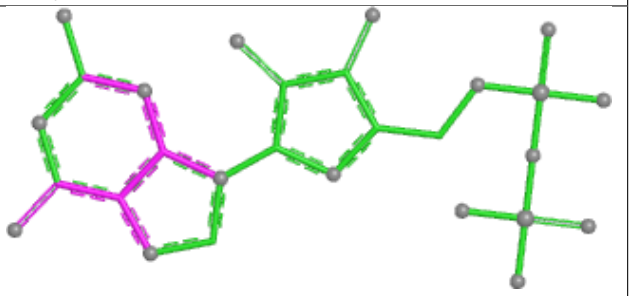


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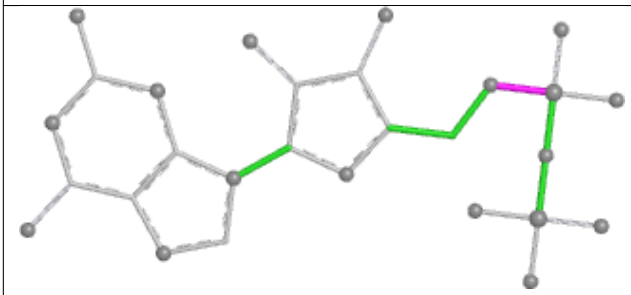
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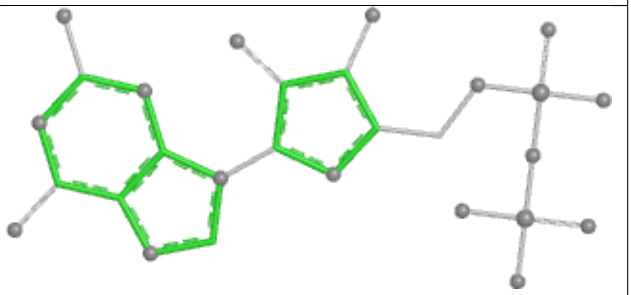
Bond lengths



Bond angles

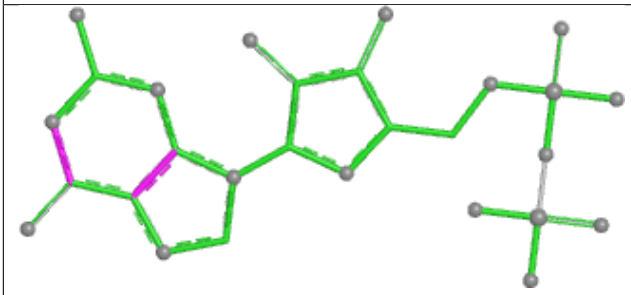


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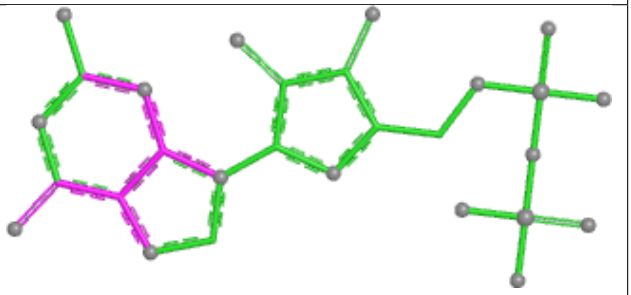


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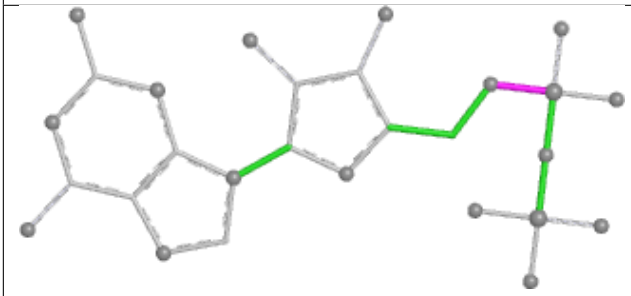
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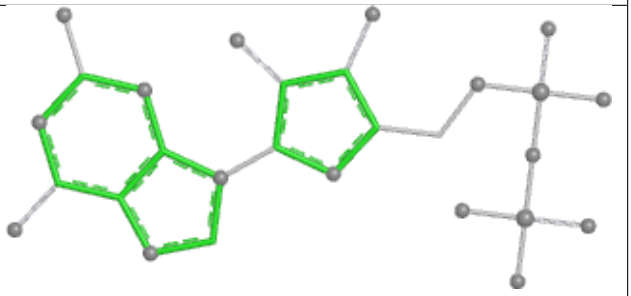
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Bond angles

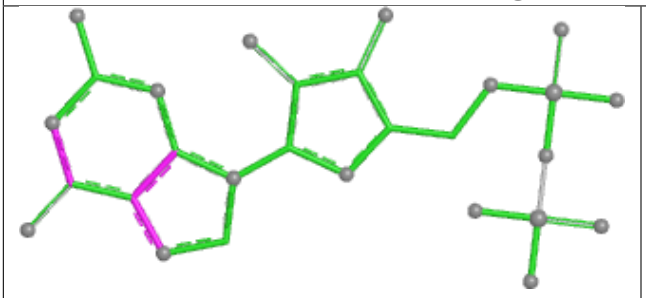


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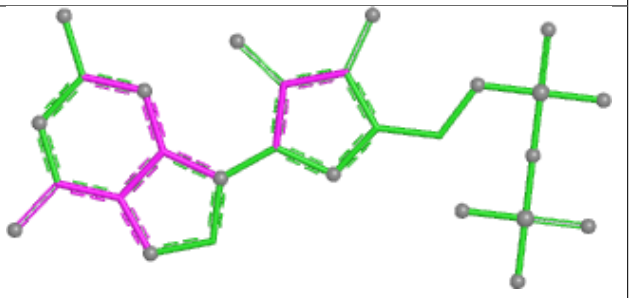


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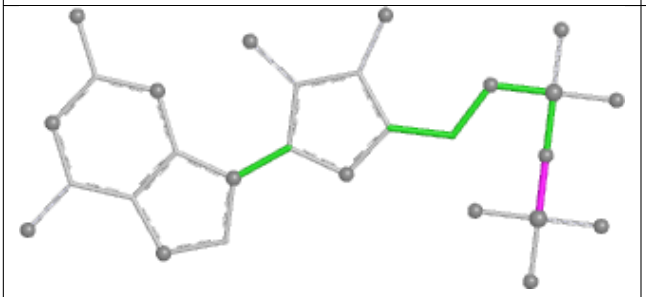
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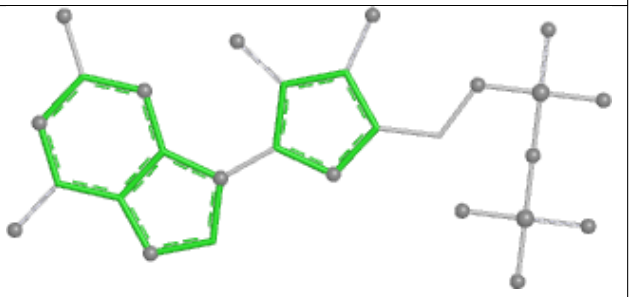
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Bond angles

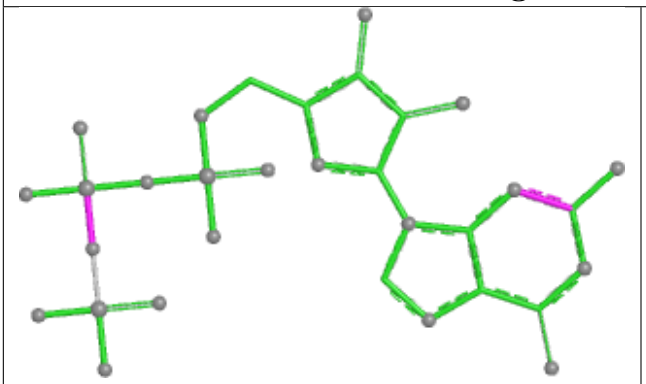


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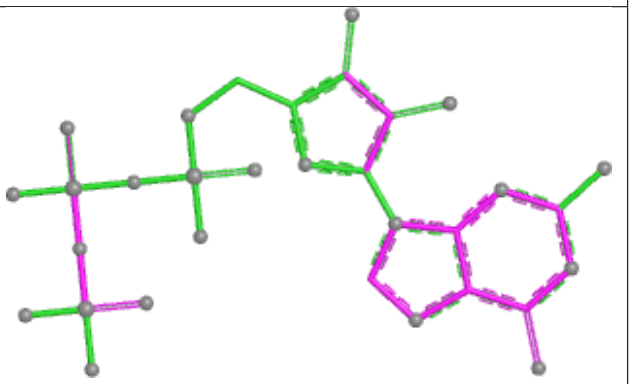


Rings

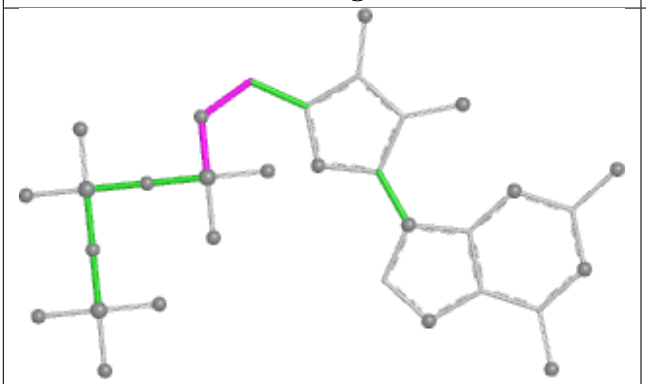
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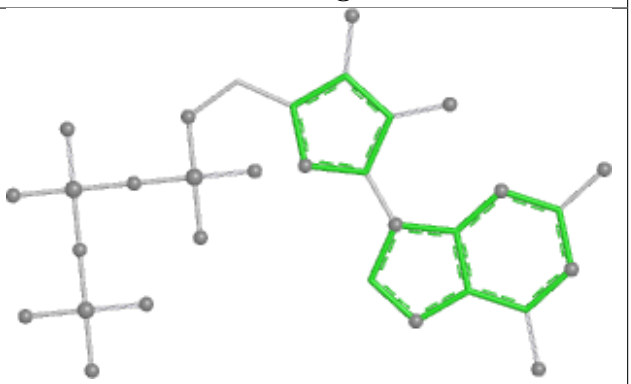
Bond lengths



Bond angles

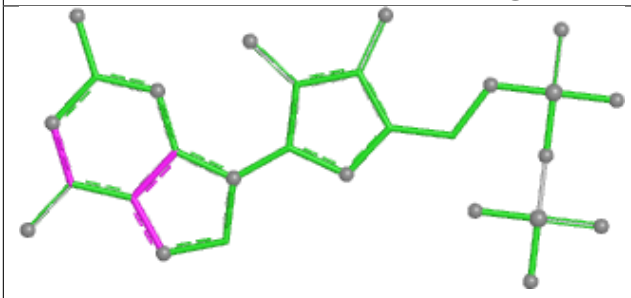


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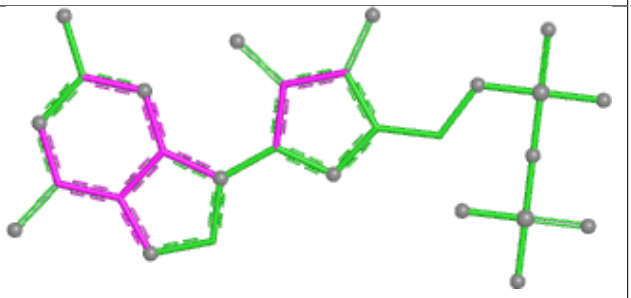


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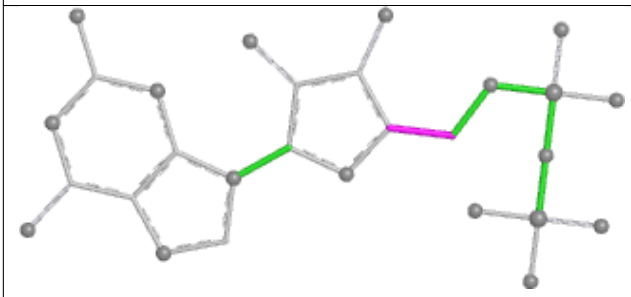
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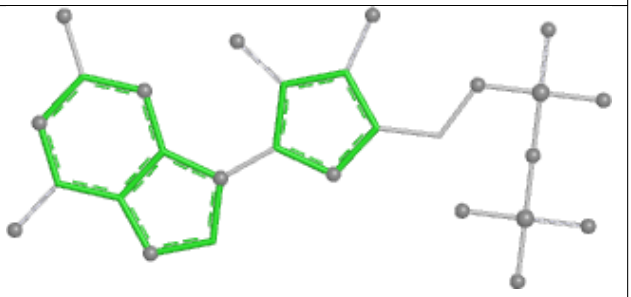
Bond lengths



Bond angles

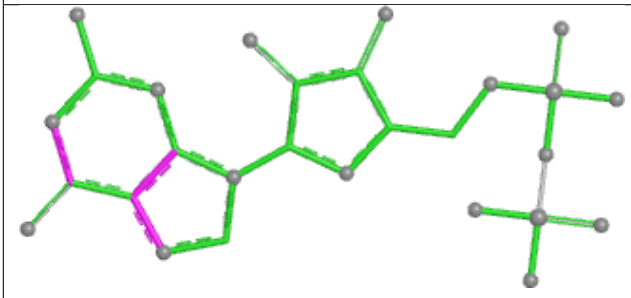


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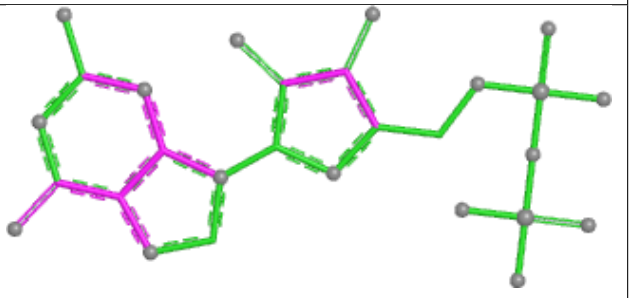


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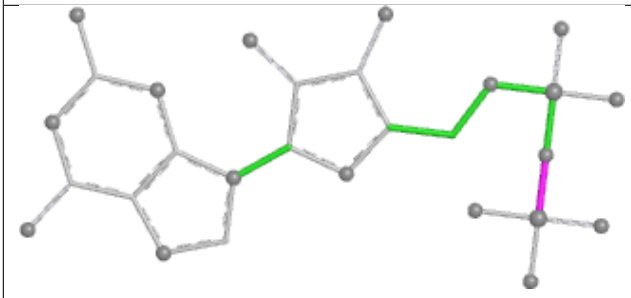
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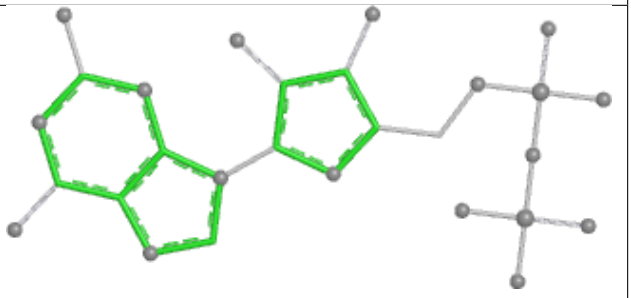
Bond lengths



Bond angles

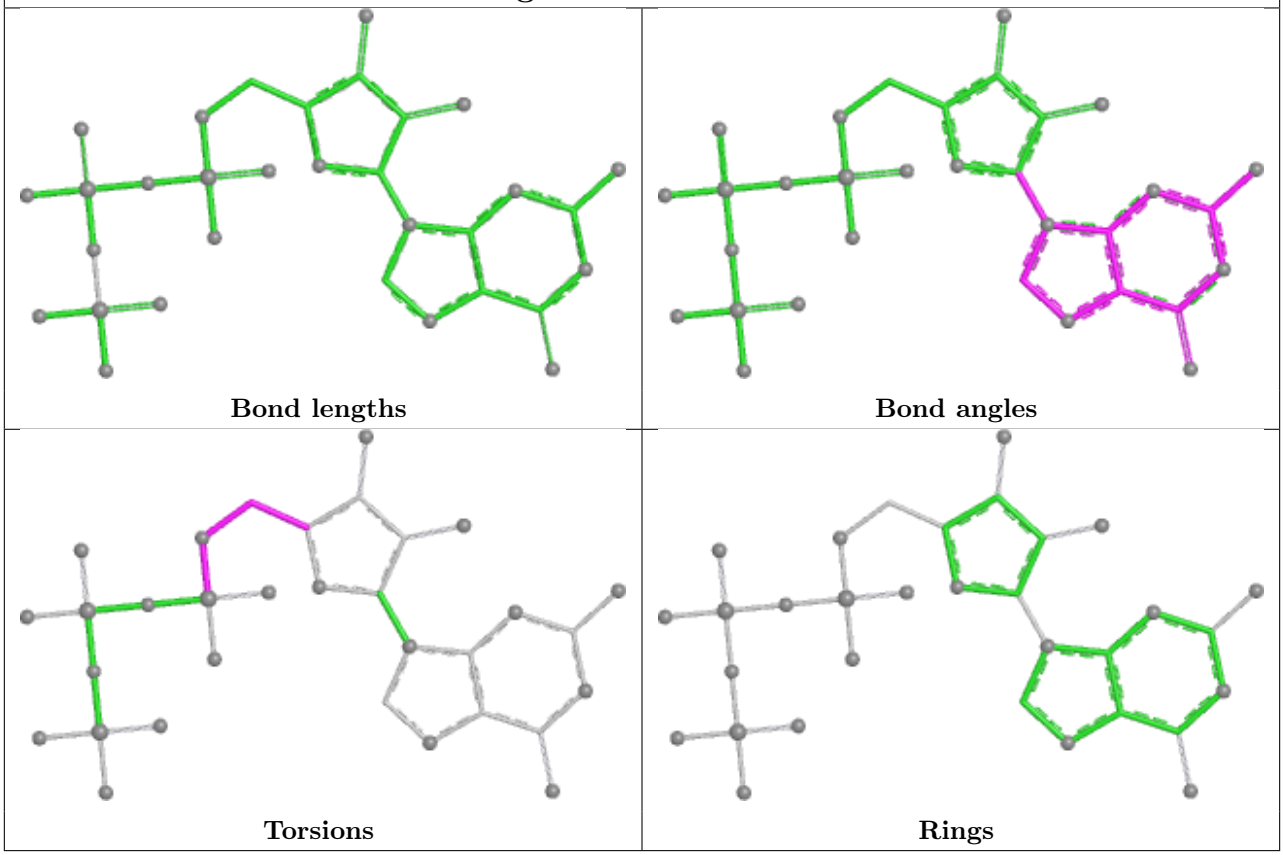


Torsions

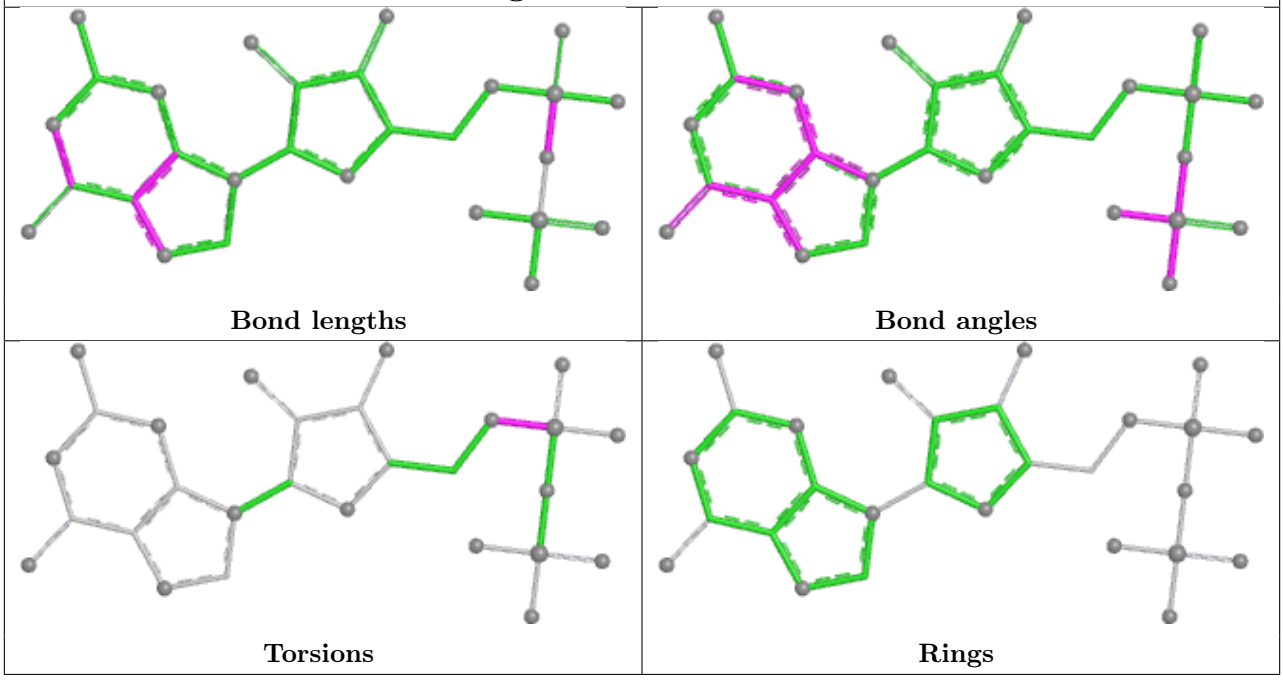


Rings

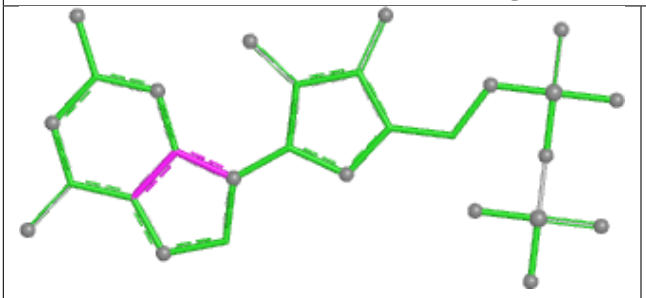
Ligand GTP RI 501



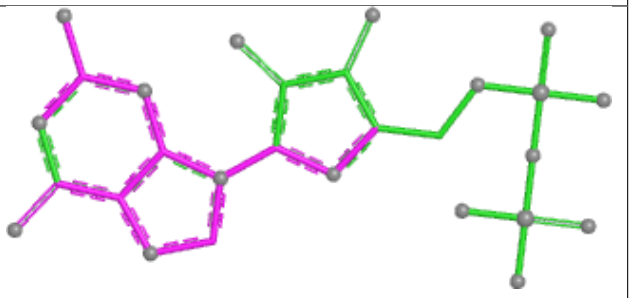
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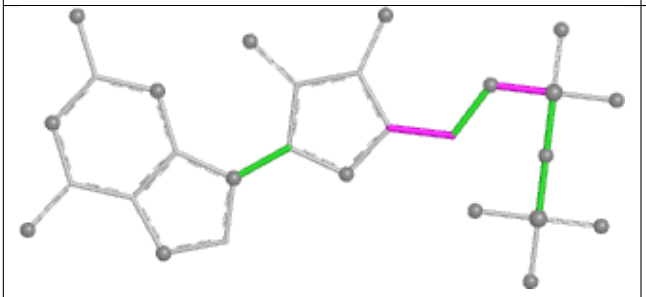
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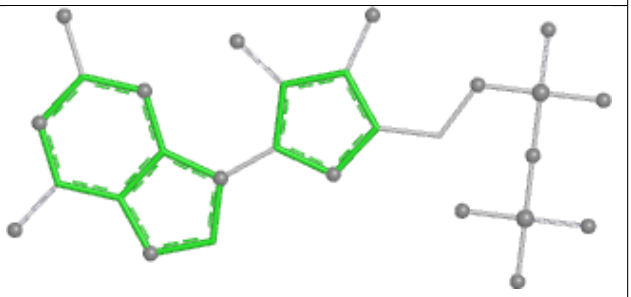
Bond lengths



Bond angles

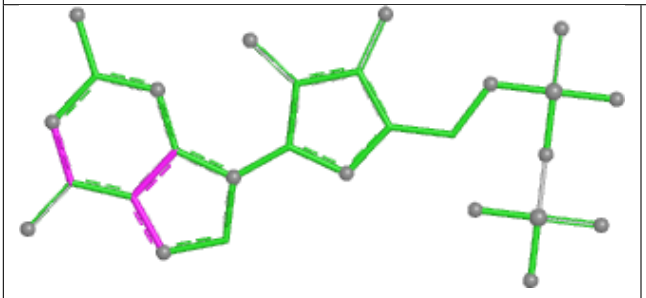


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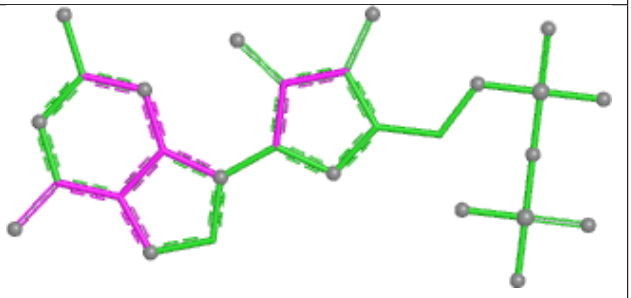


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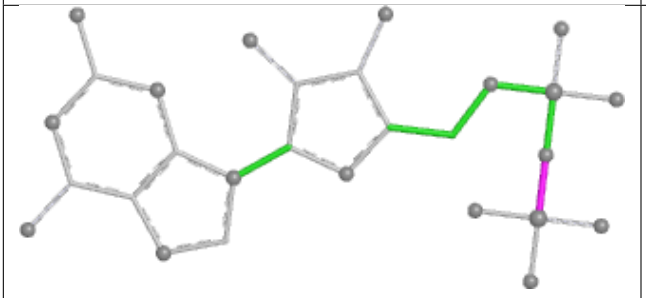
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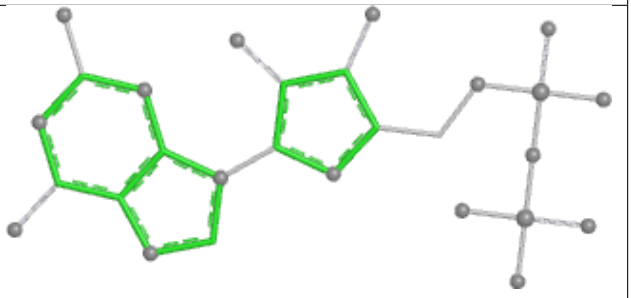
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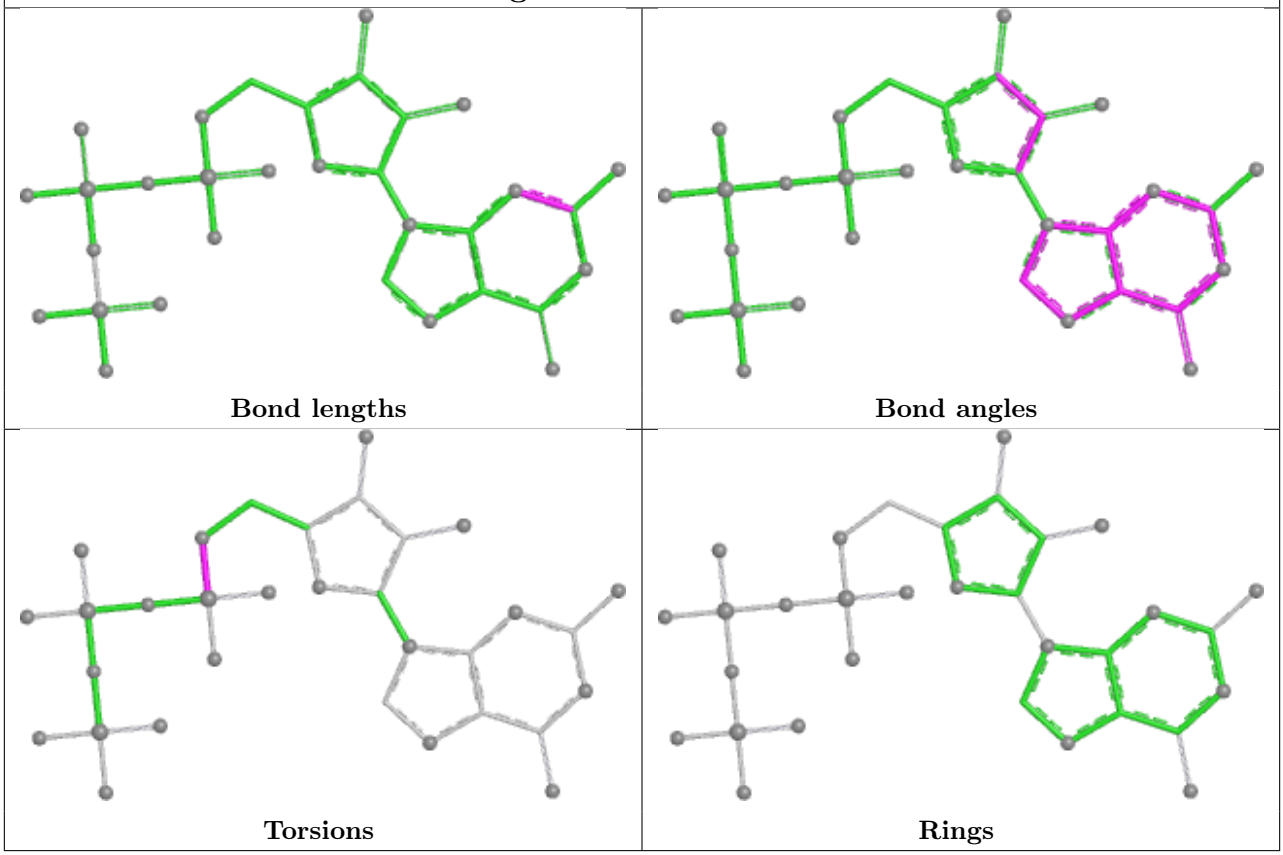


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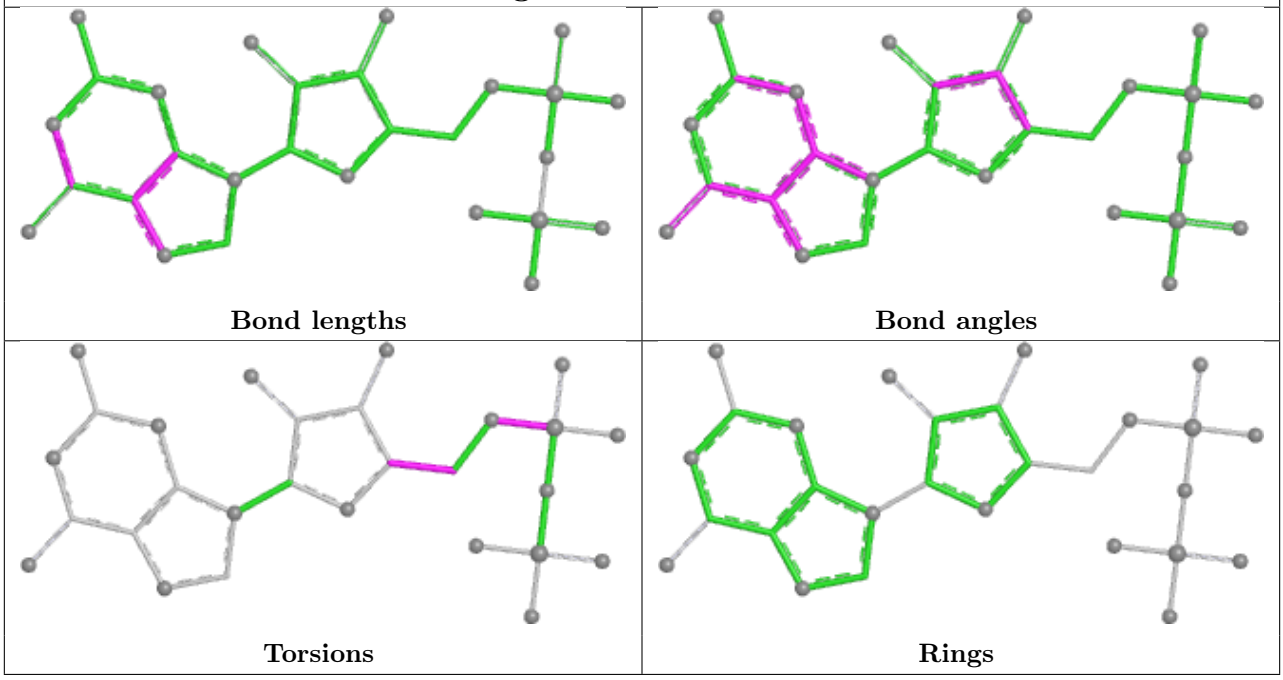


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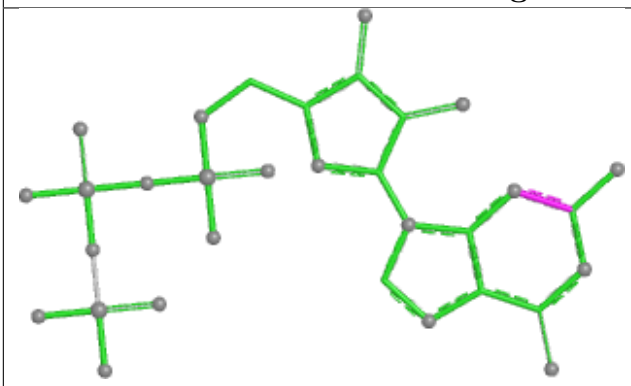
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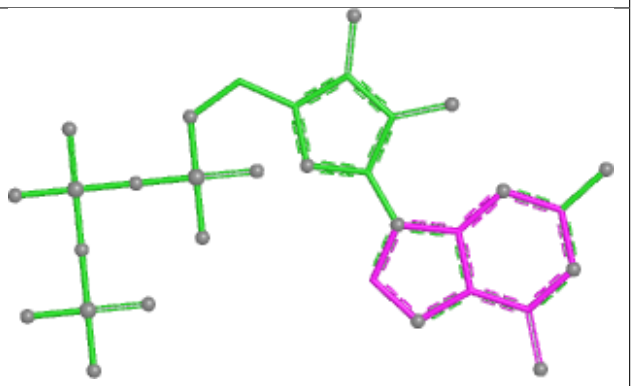
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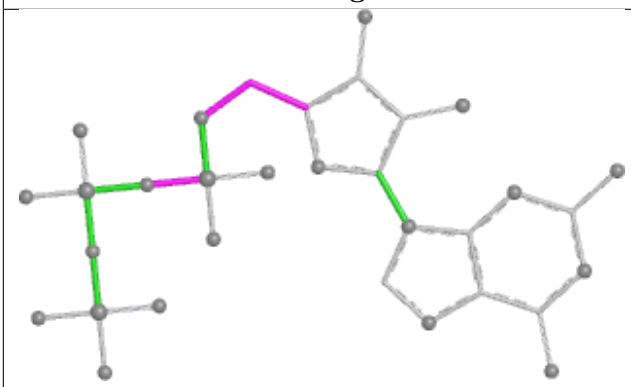
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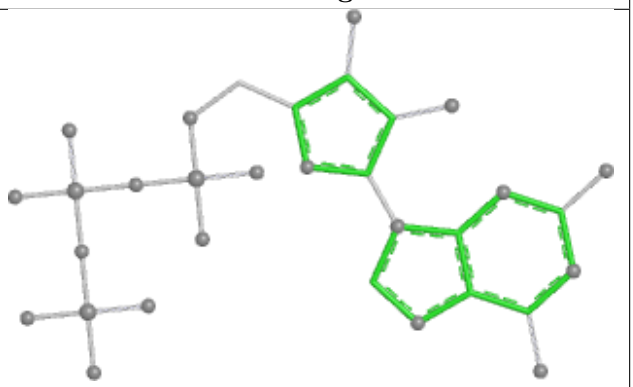
Bond lengths



Bond angles

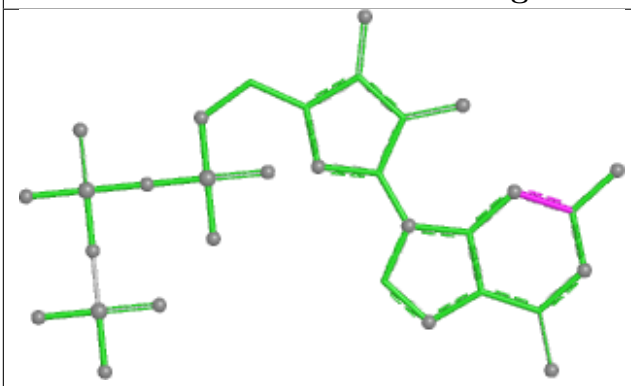


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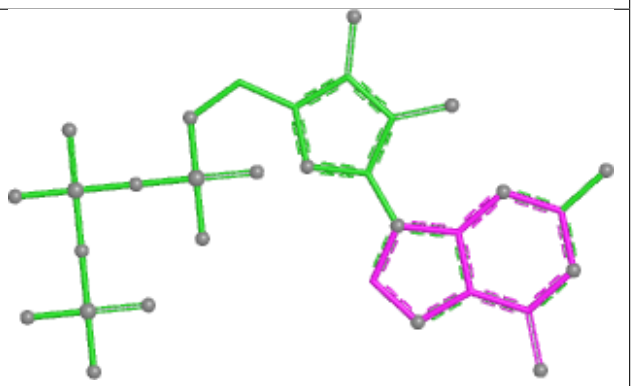


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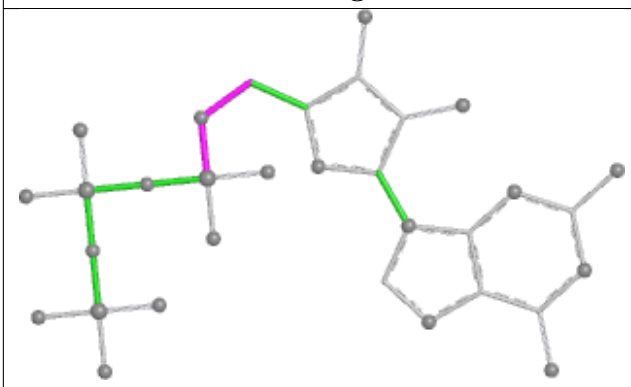
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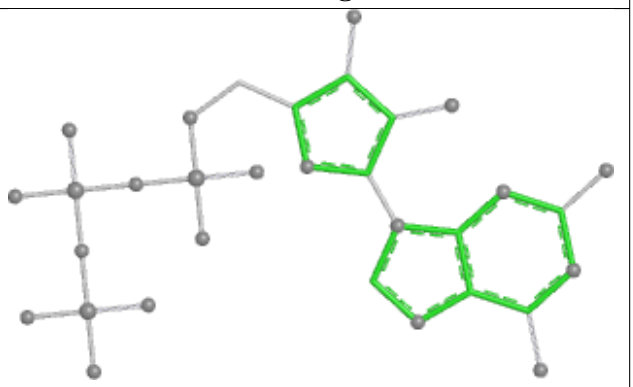
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Bond angles

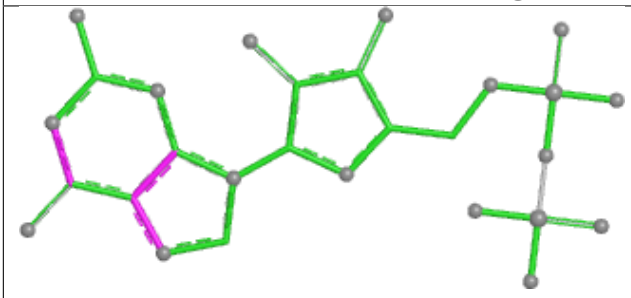


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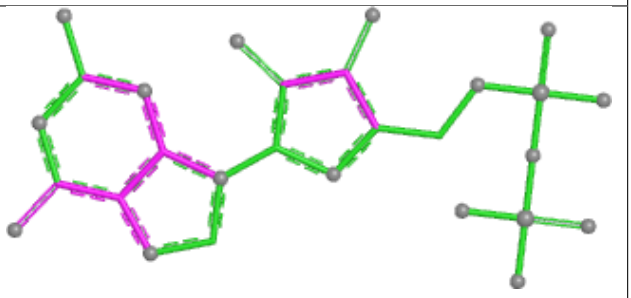


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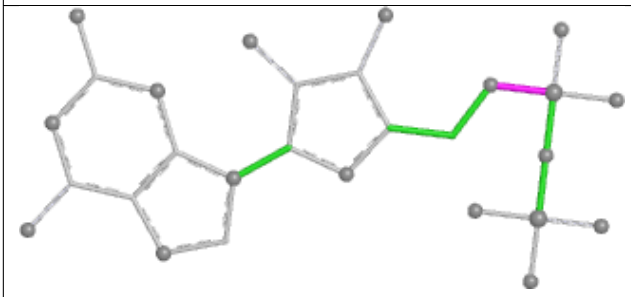
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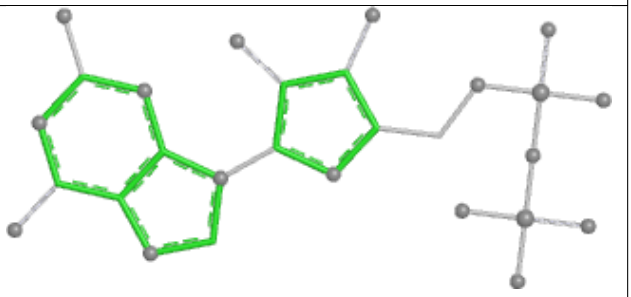
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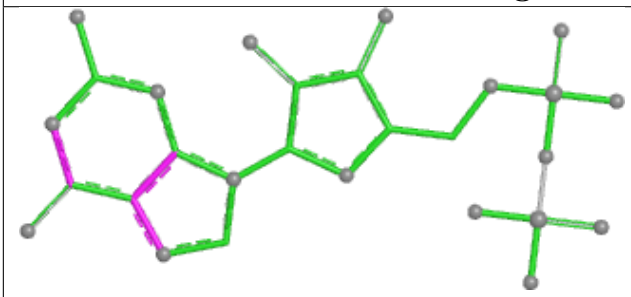


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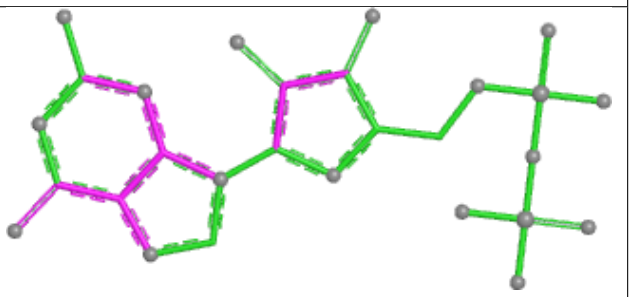


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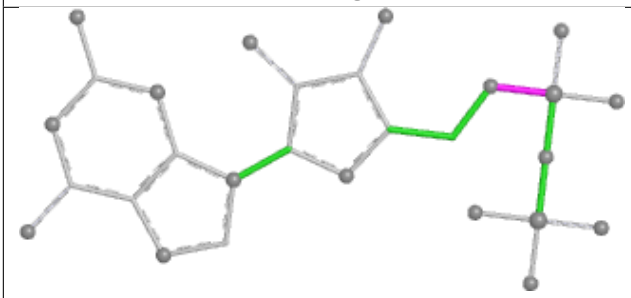
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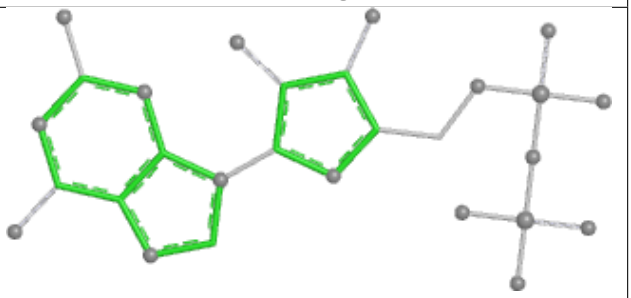
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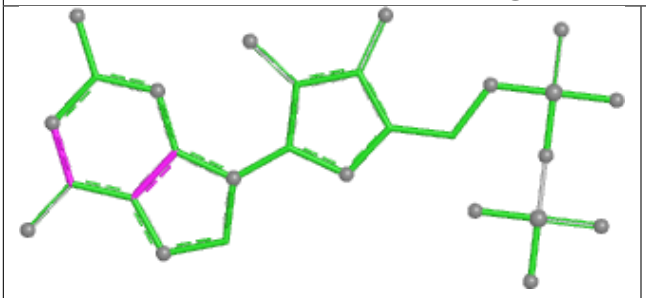


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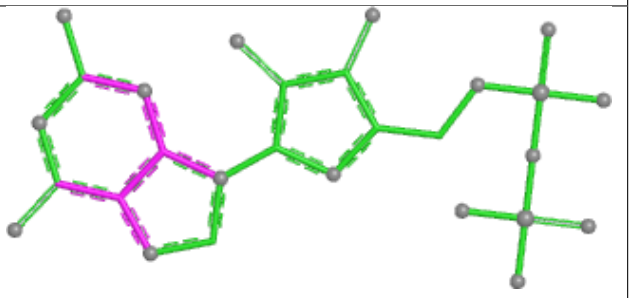


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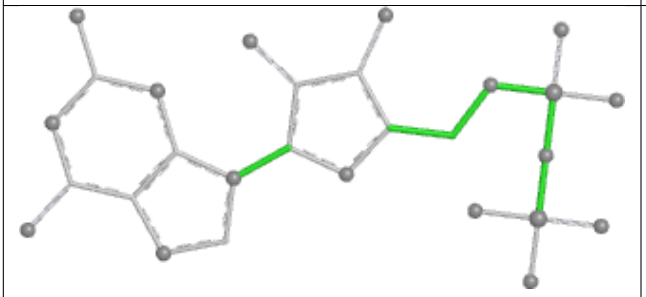
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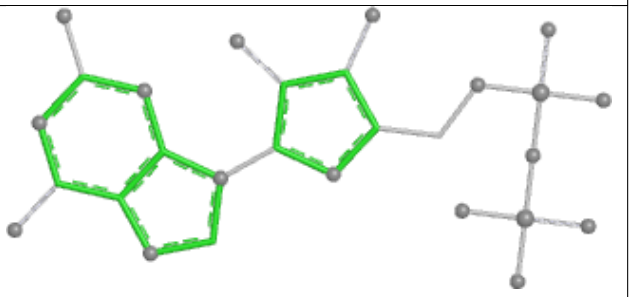
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Bond angles

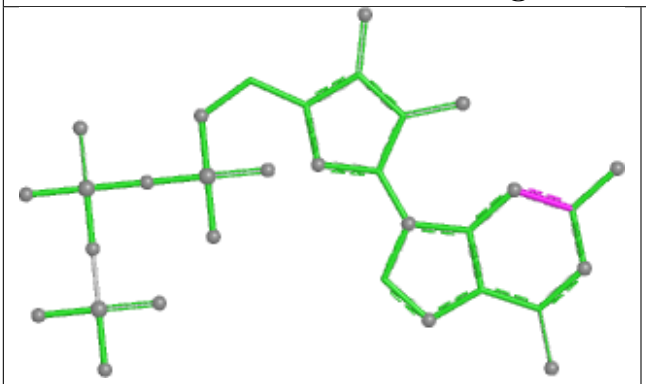


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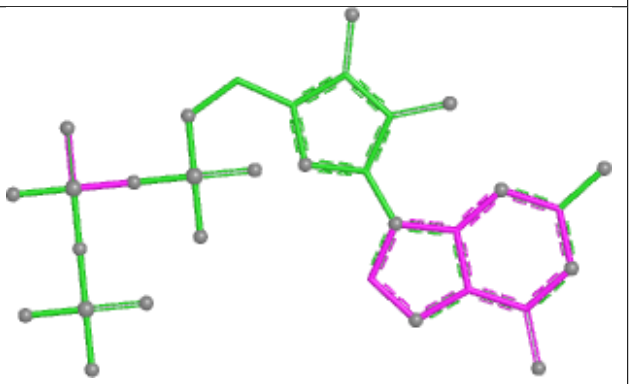


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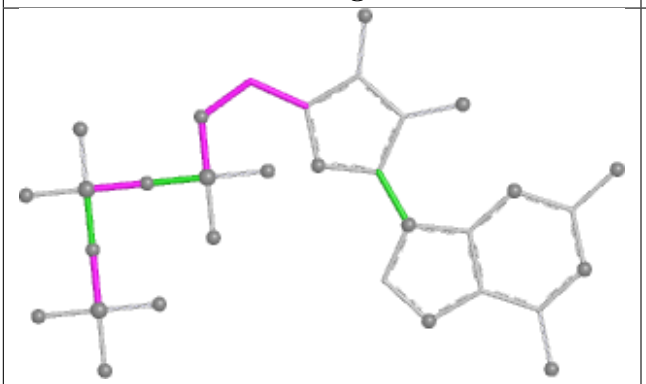
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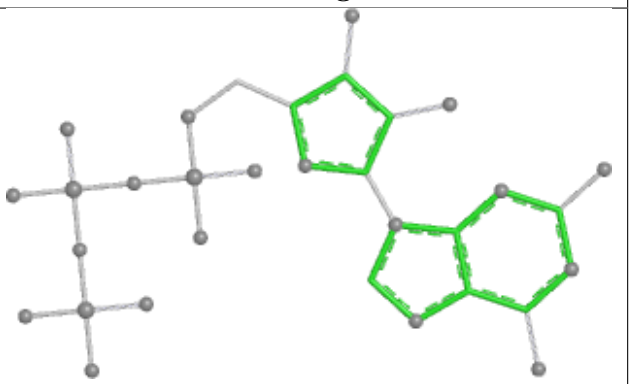
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Bond angles

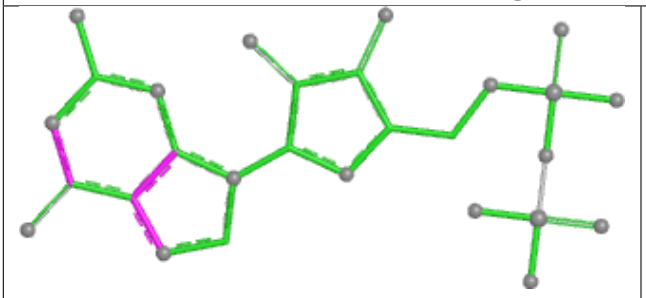


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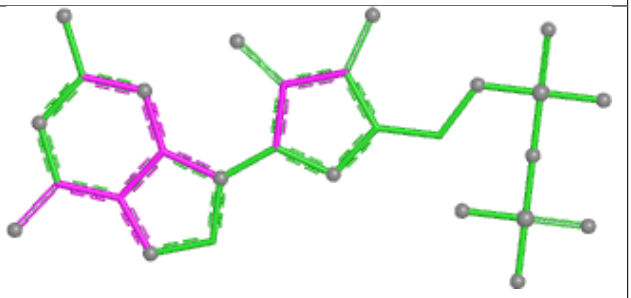


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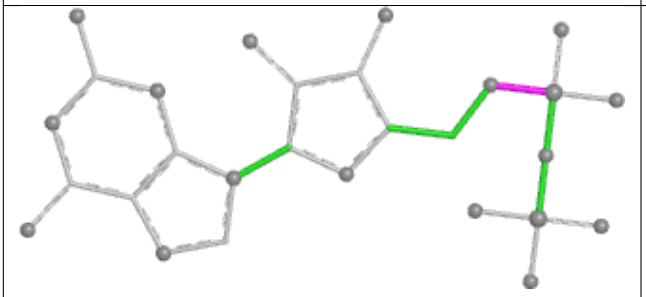
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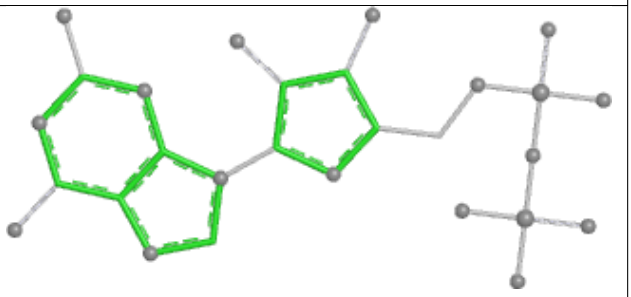
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Bond angles

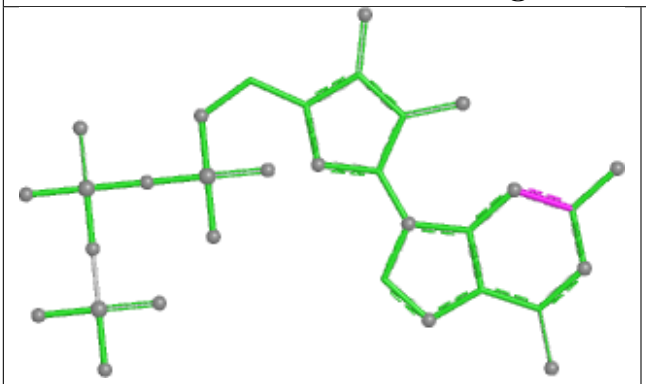


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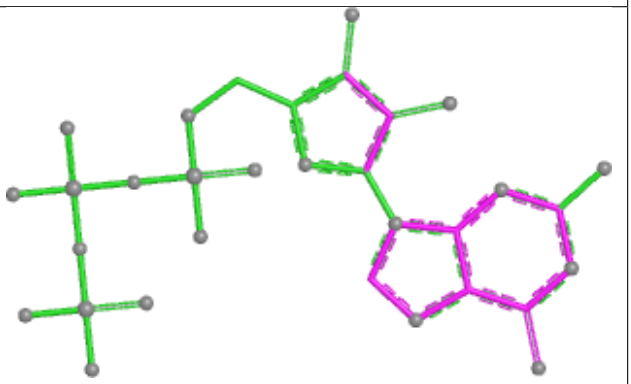


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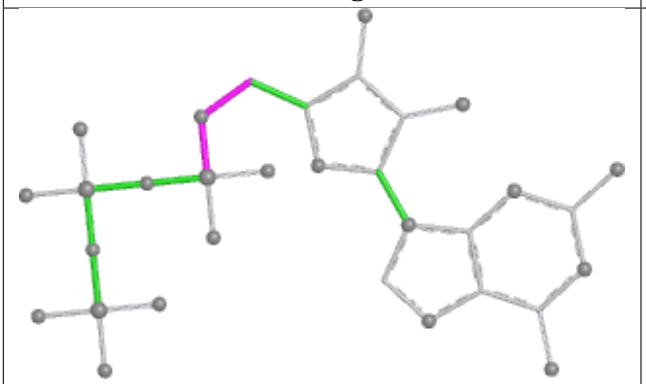
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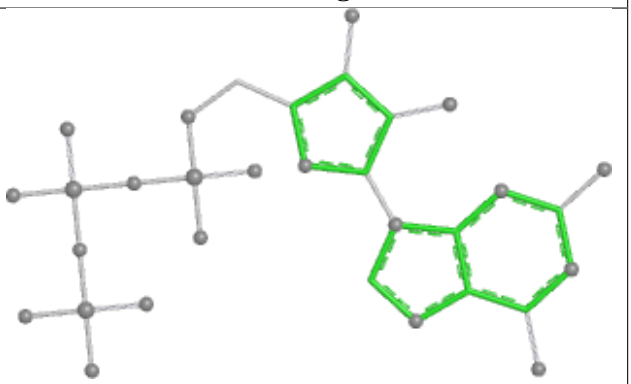
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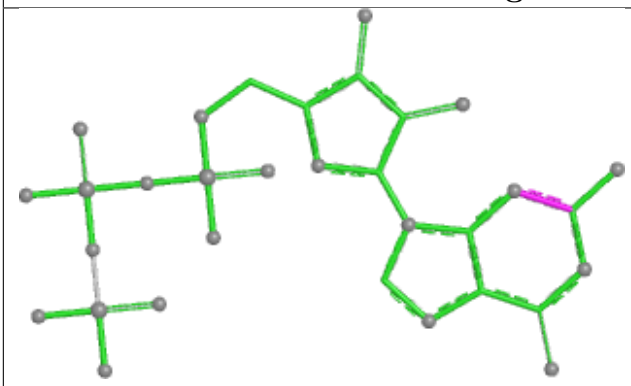


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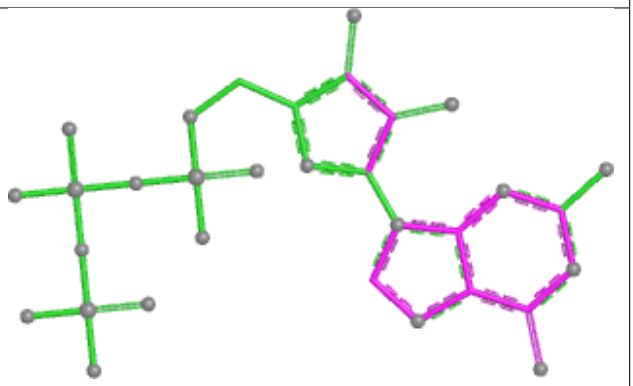


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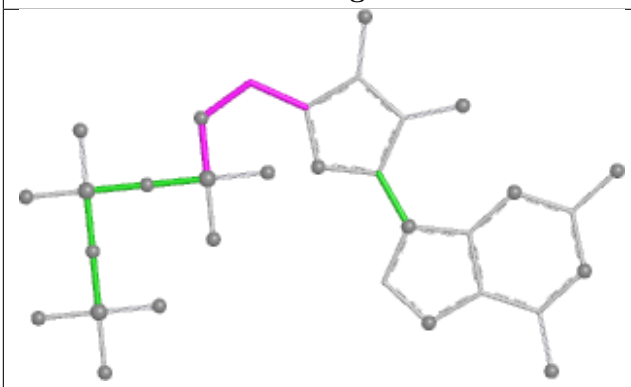
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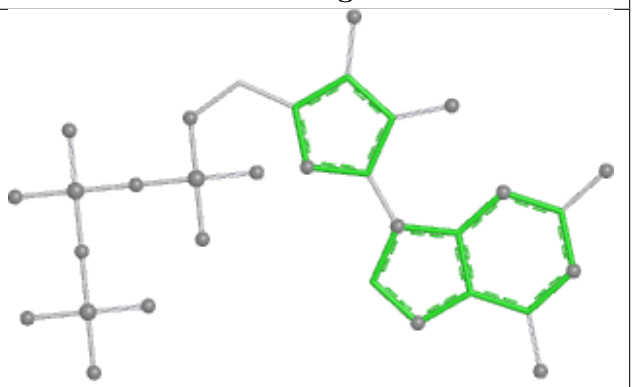
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Bond angles

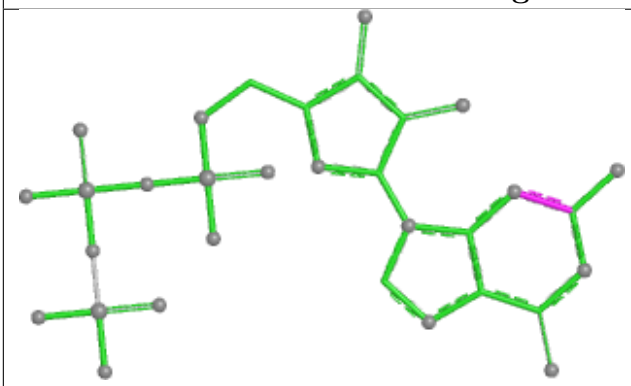


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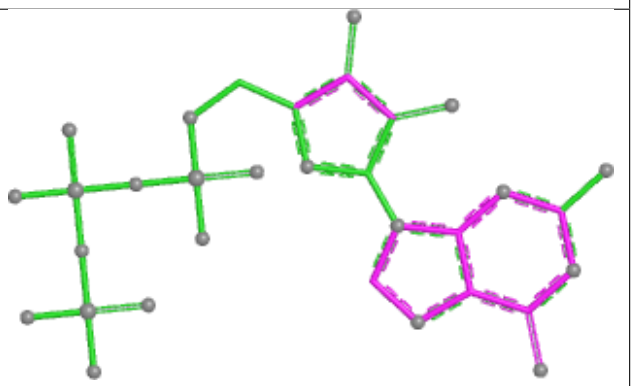


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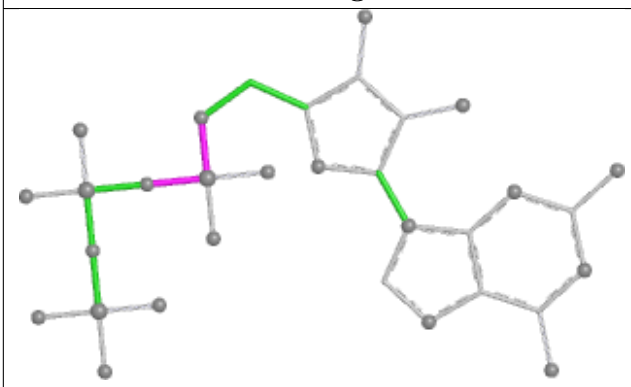
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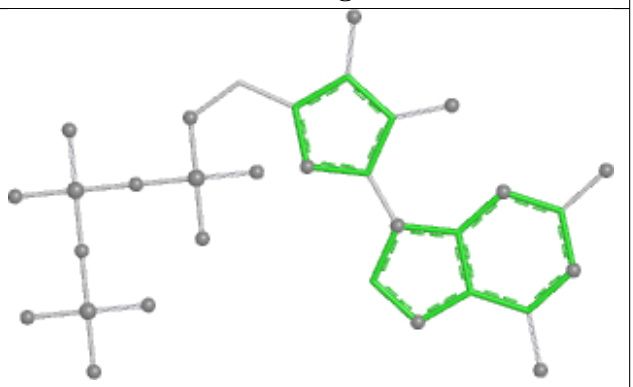
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Bond angles

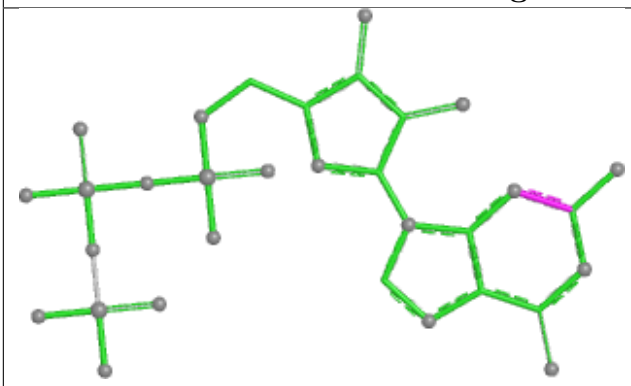


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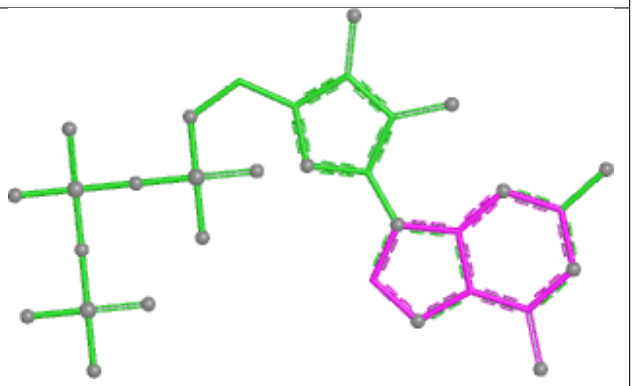


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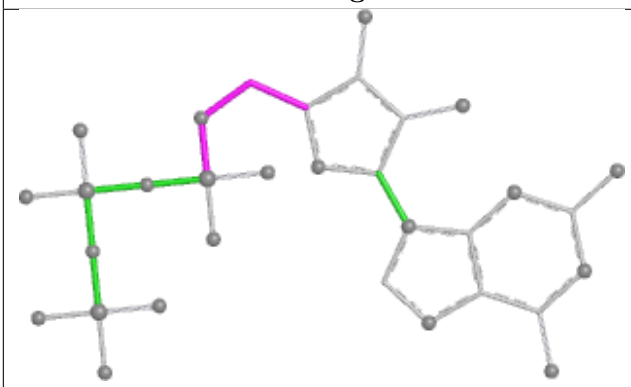
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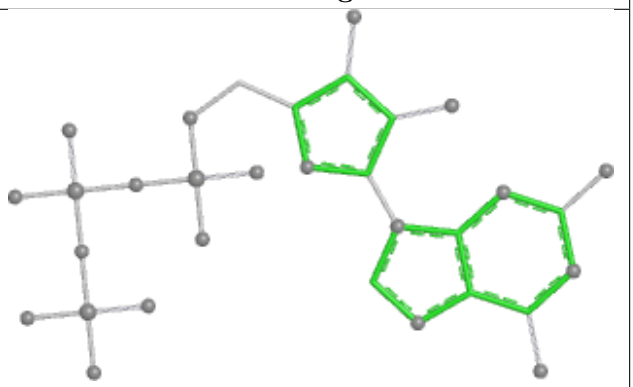
Bond lengths



Bond angles

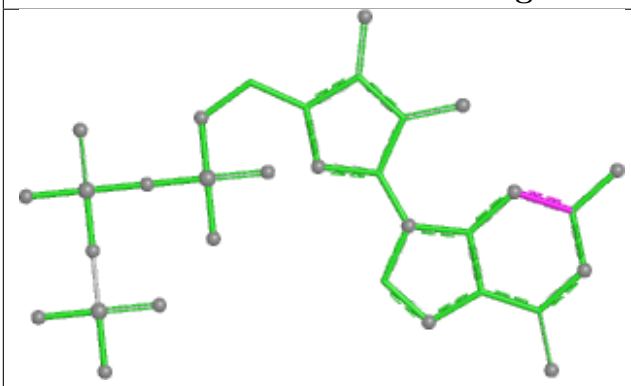


Torsions

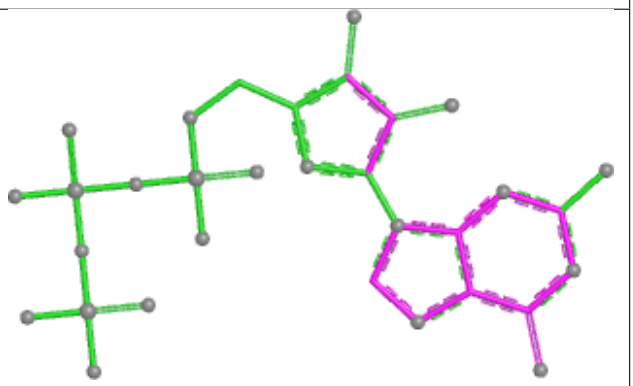


Rings

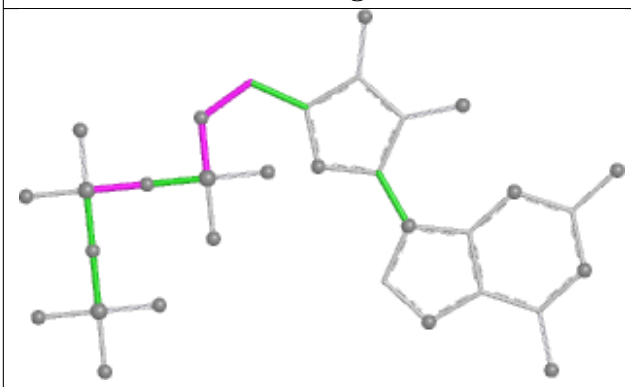
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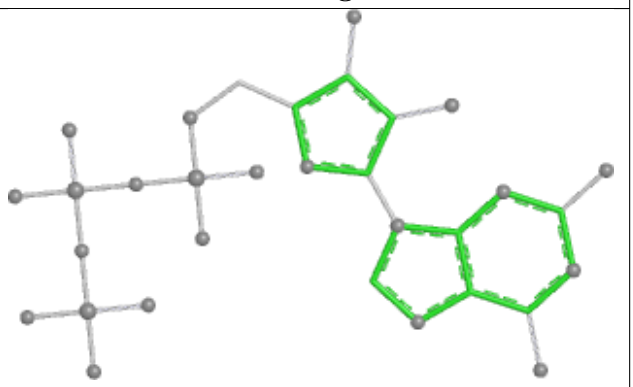
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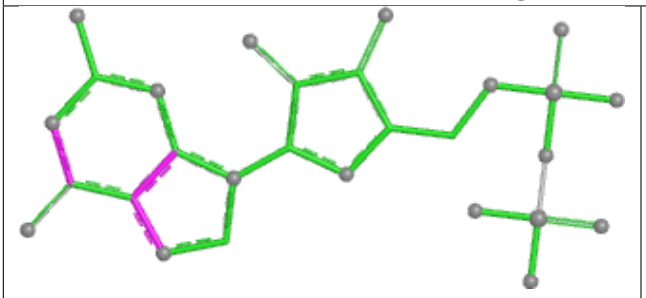


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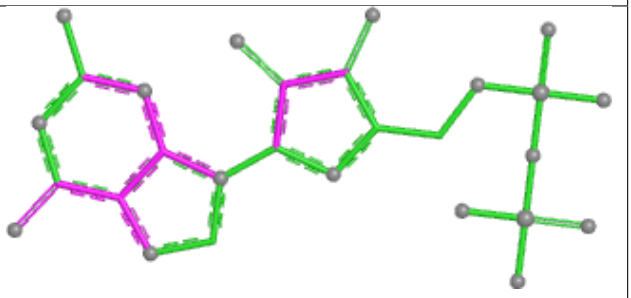


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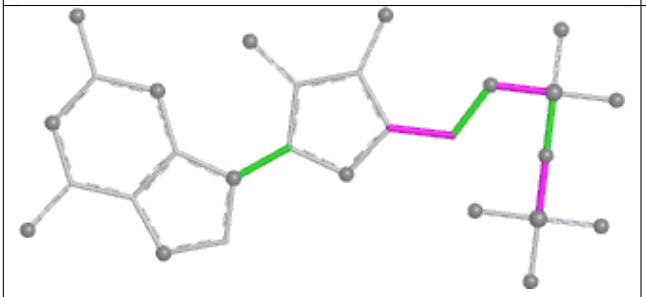
Ligand GDP BJ 501



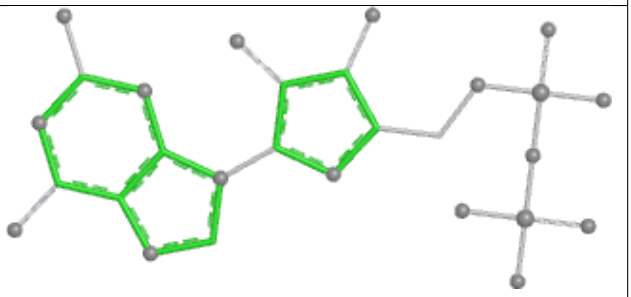
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Bond angles

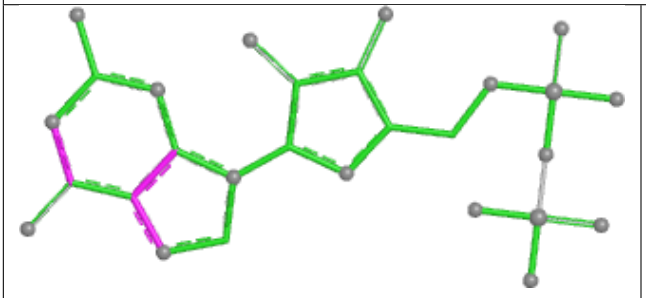


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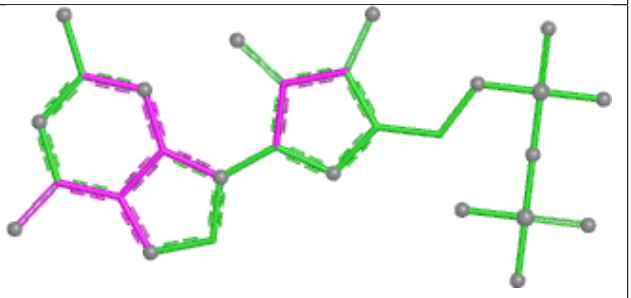


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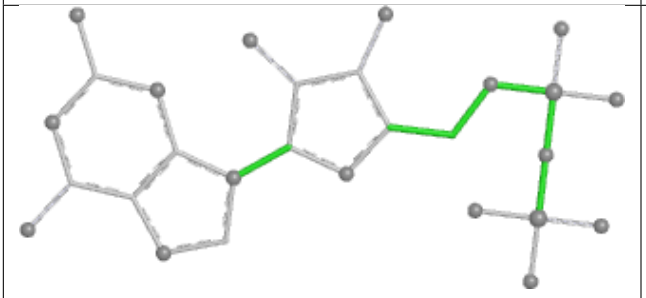
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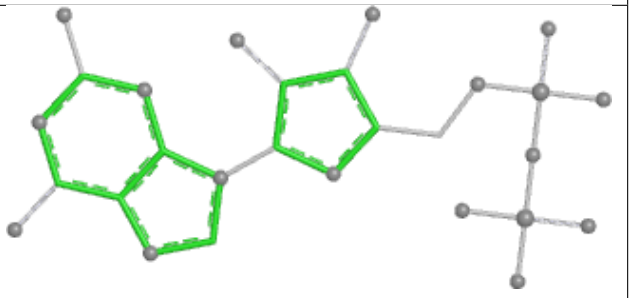
Bond lengths



Bond angles

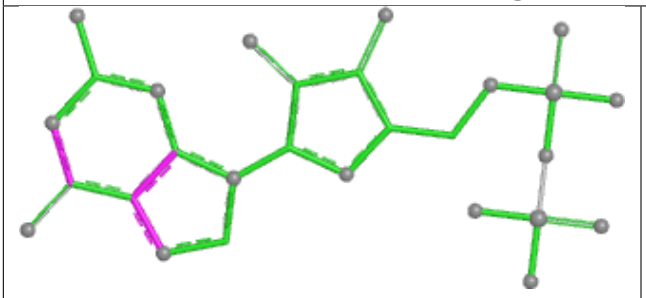


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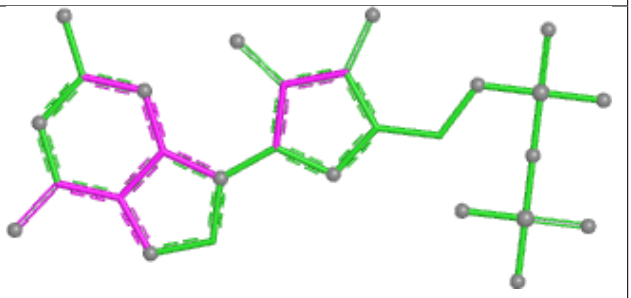


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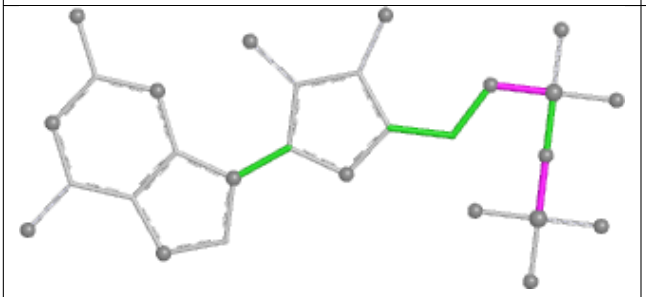
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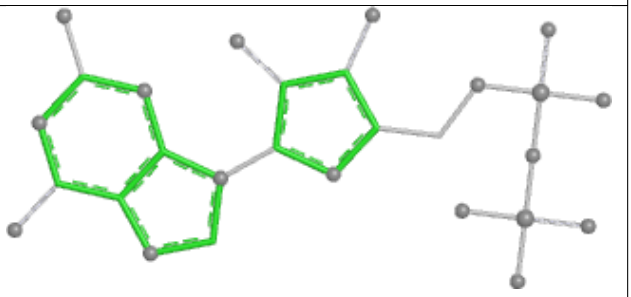
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Bond angles

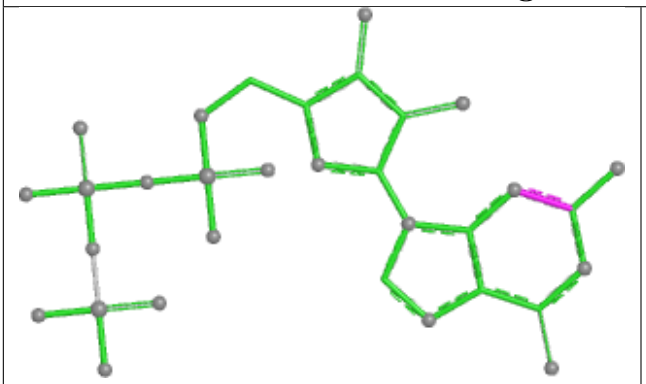


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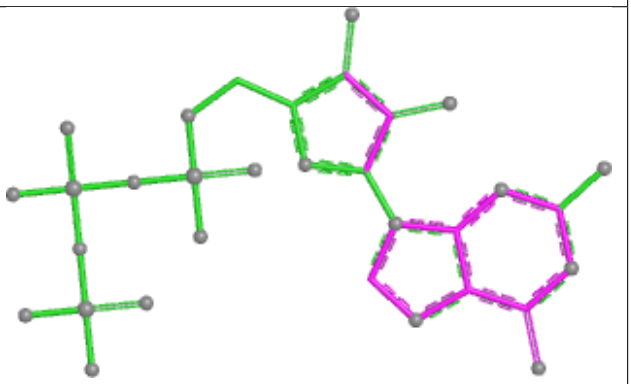


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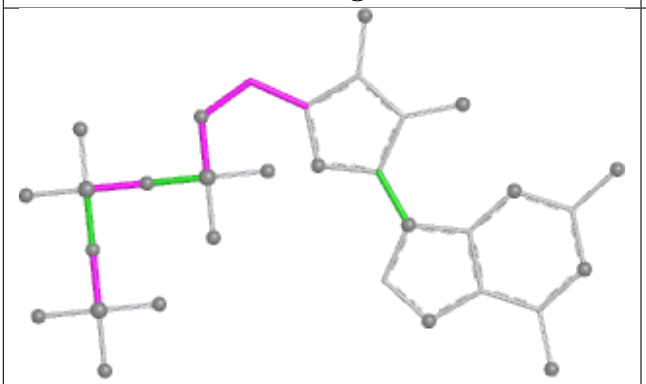
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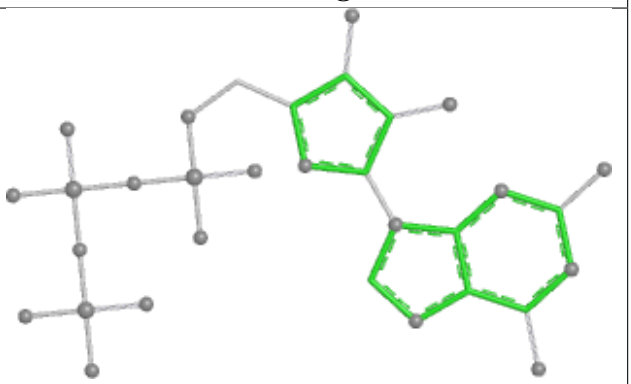
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Bond angles

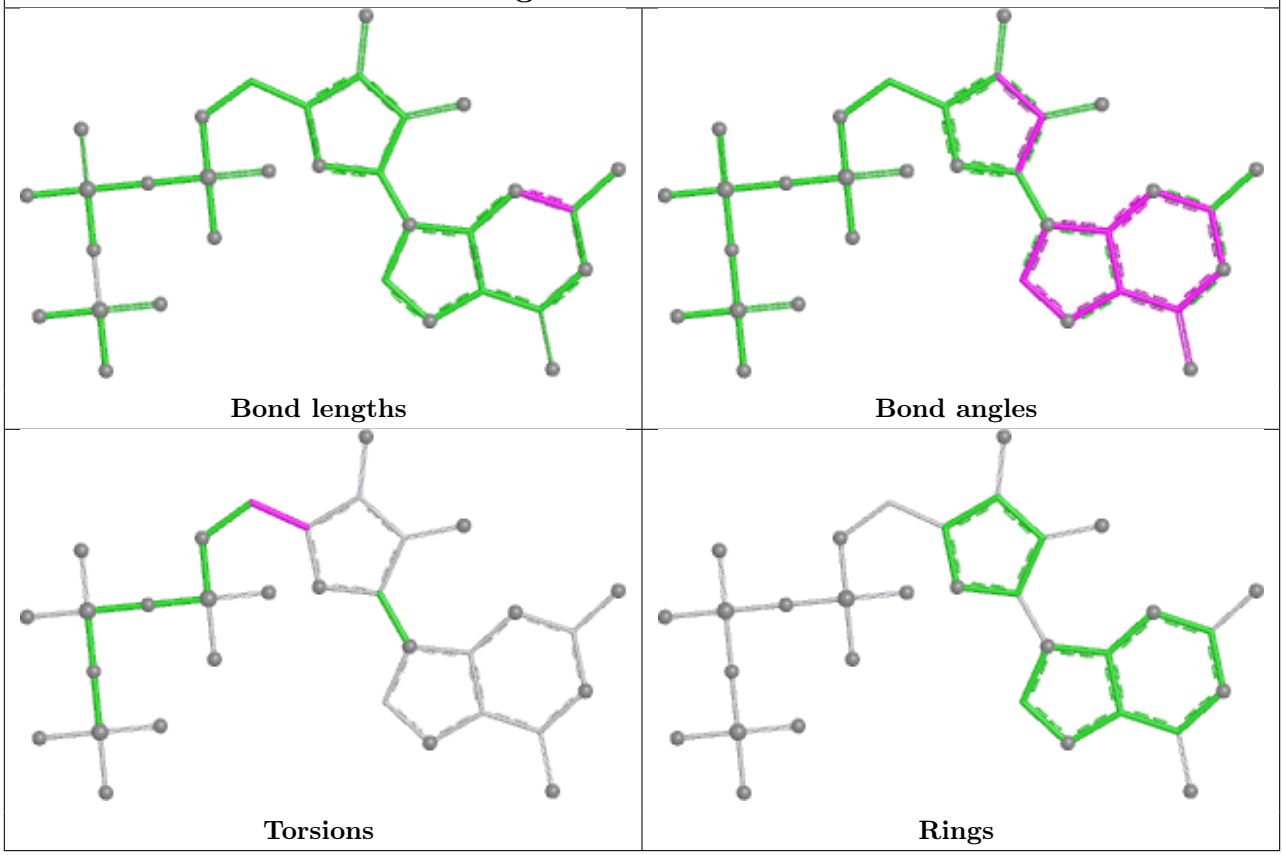


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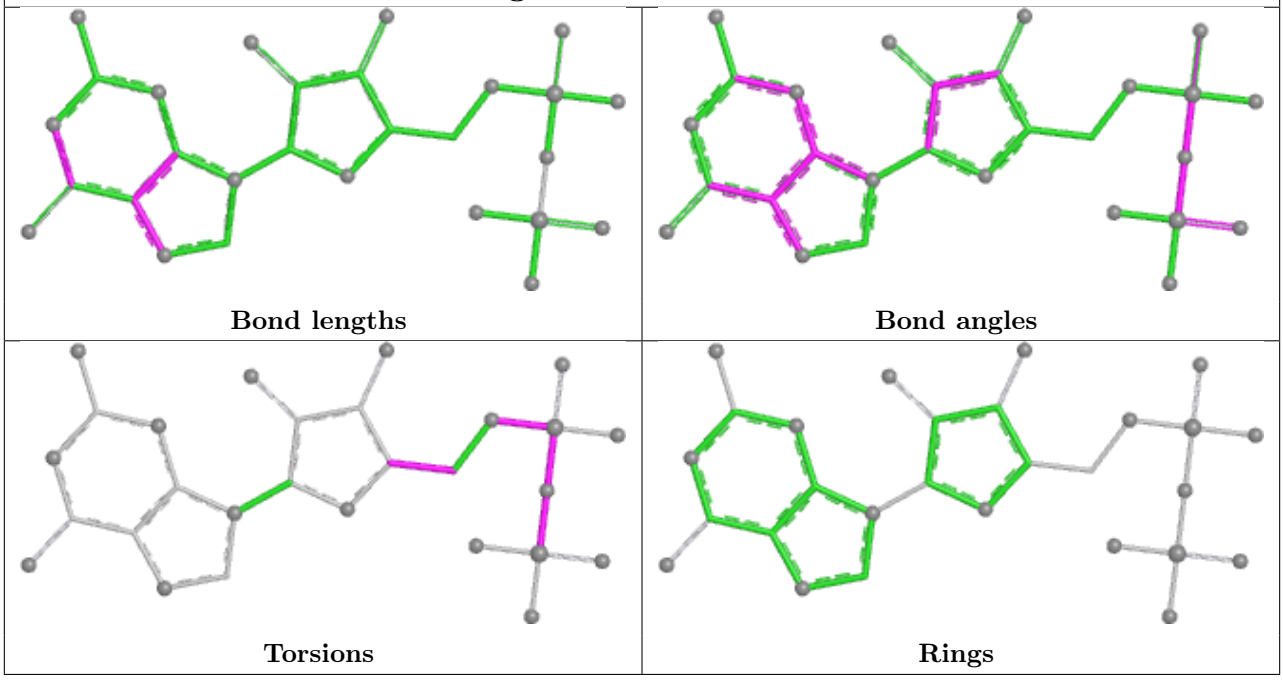


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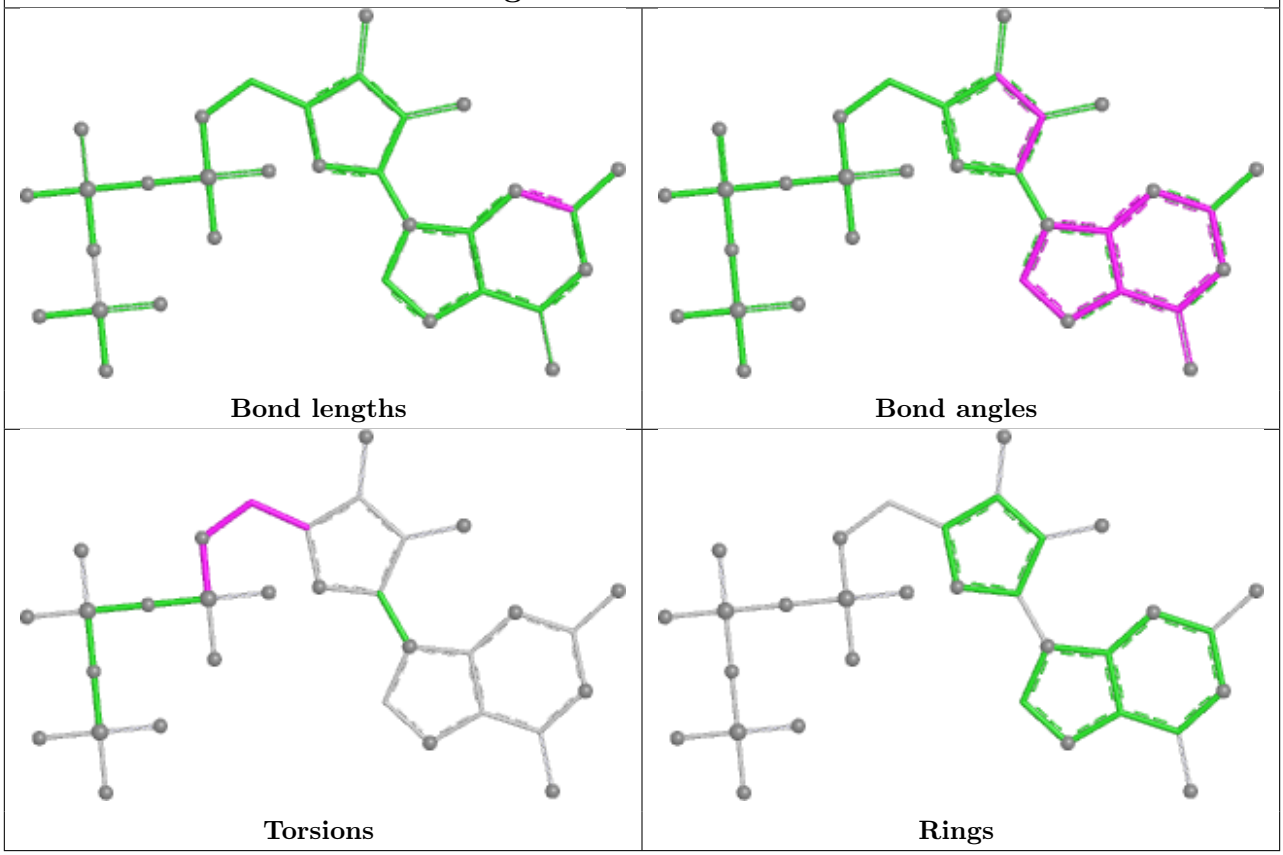
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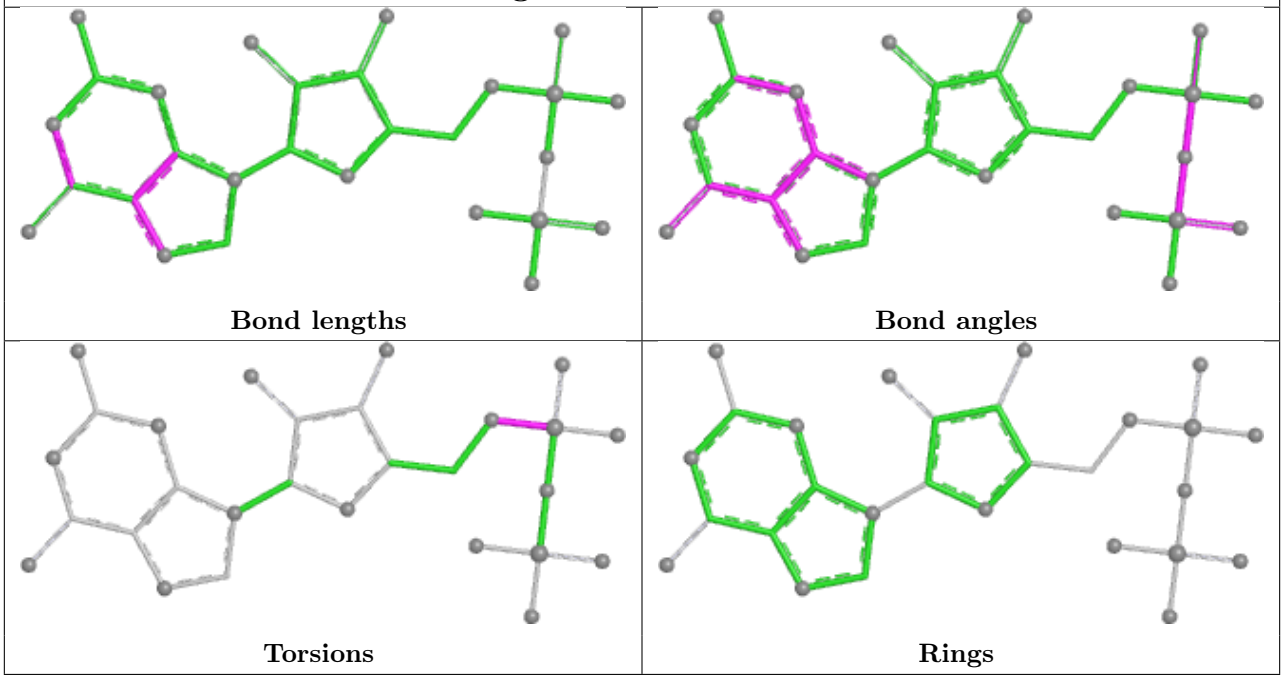
Ligand GDP CH 501



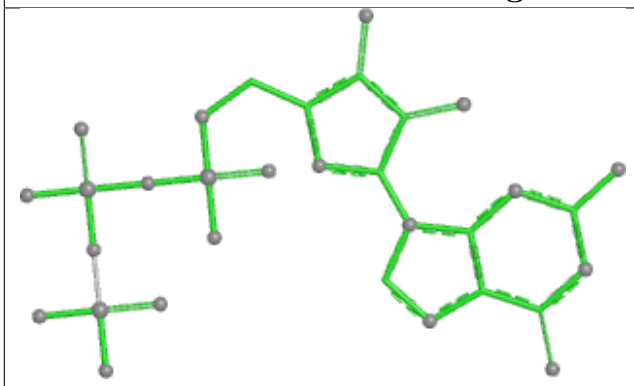
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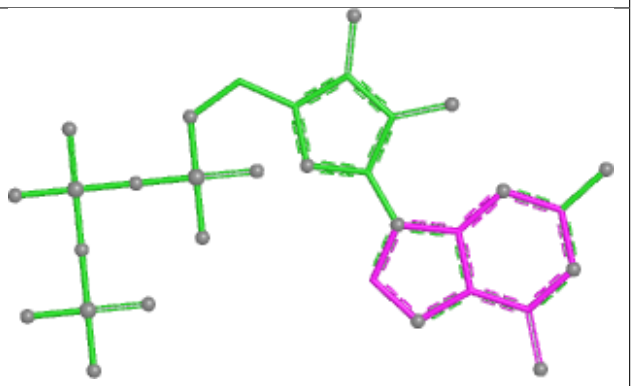
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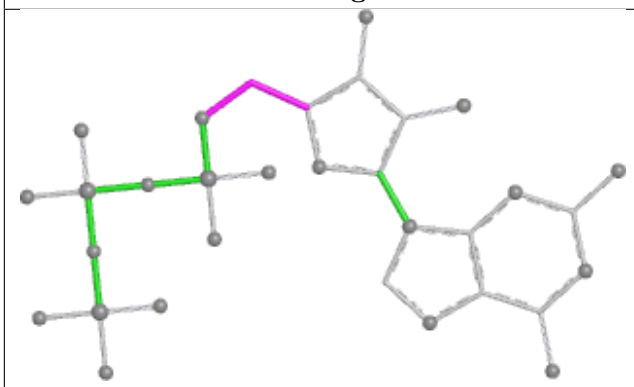
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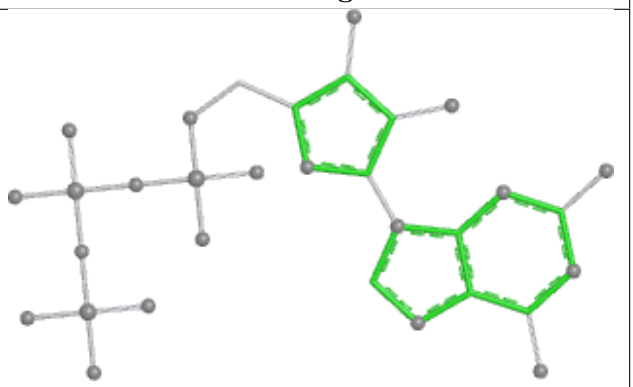
Bond lengths



Bond angles

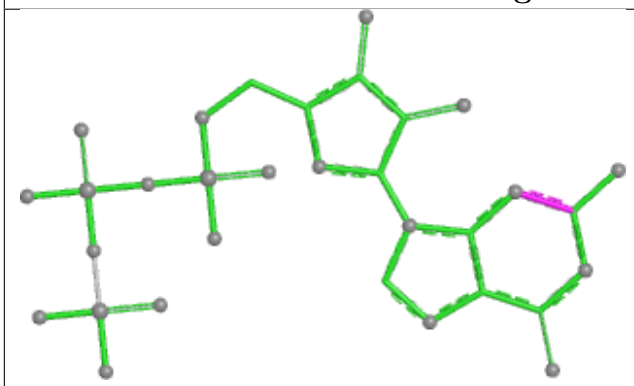


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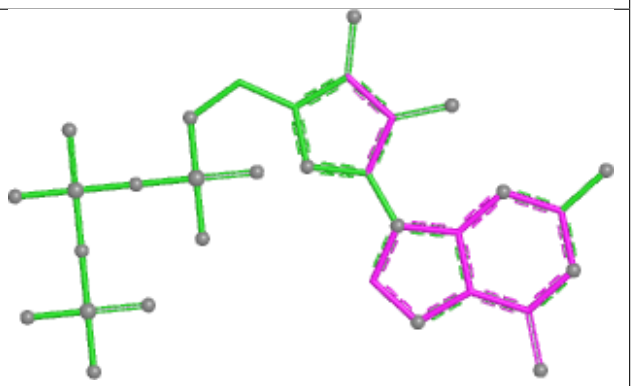


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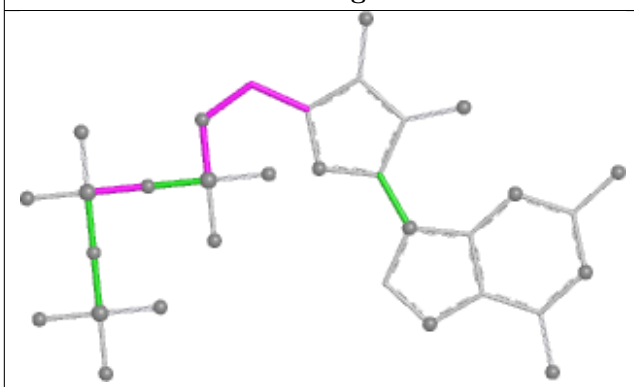
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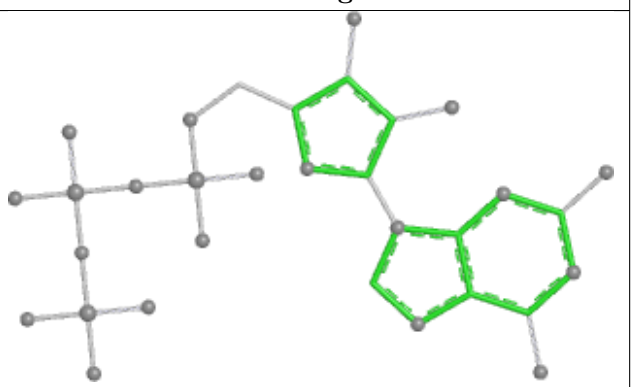
Bond lengths



Bond angles

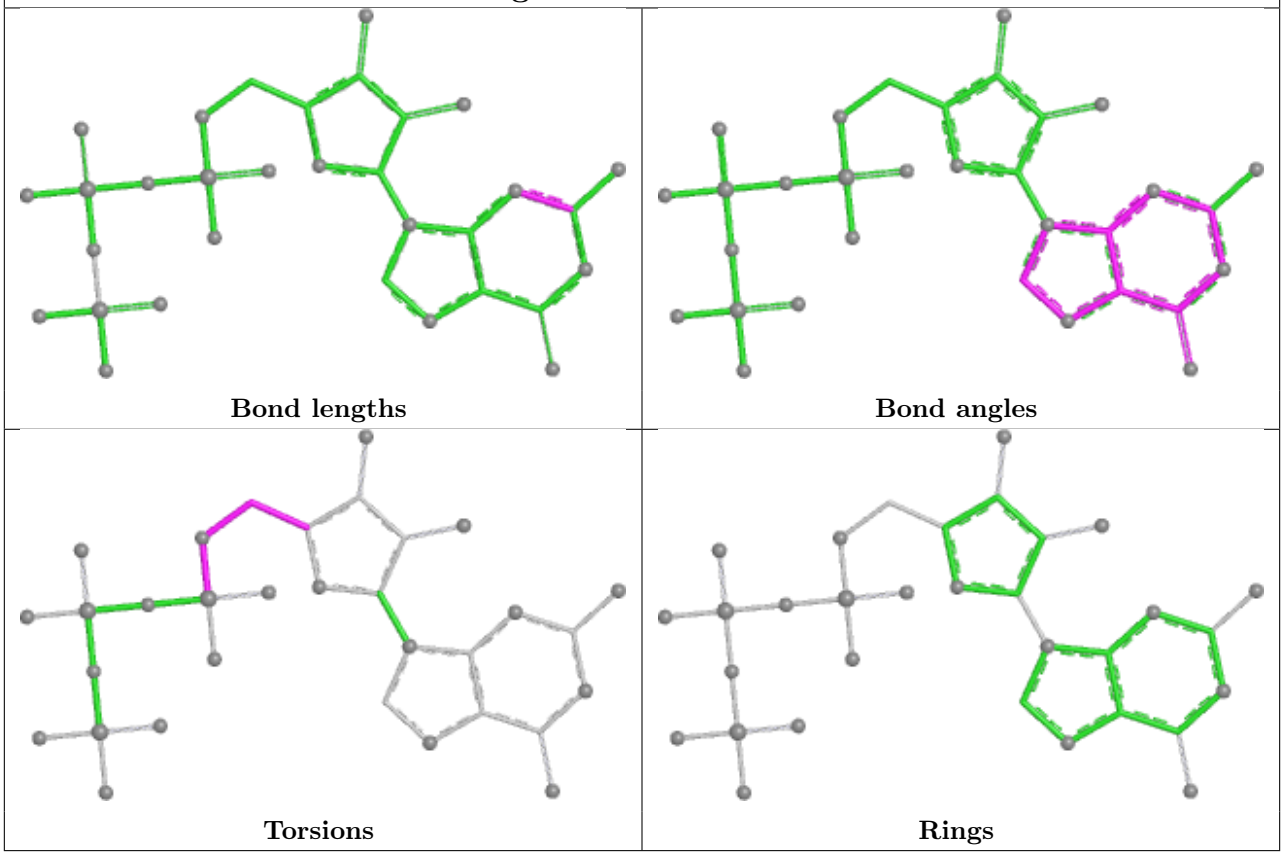


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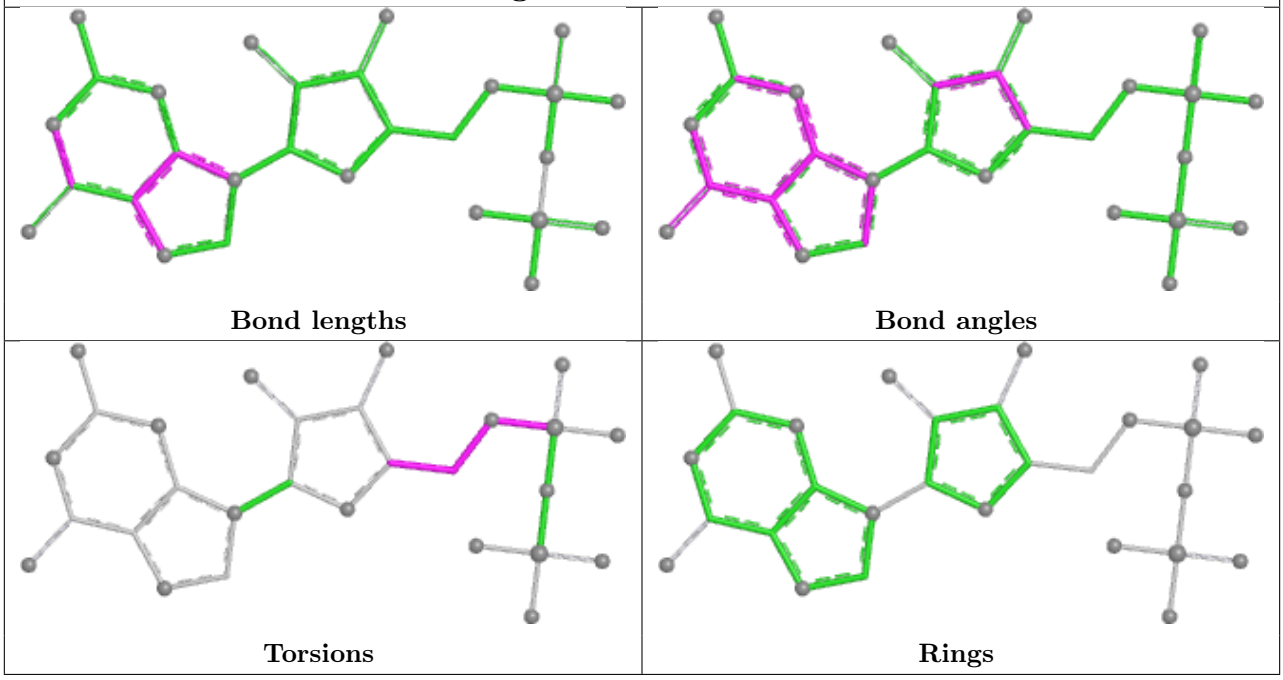


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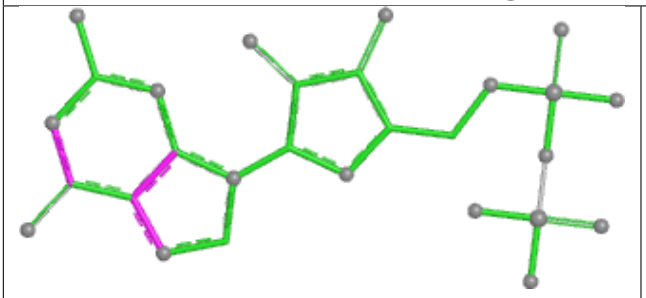
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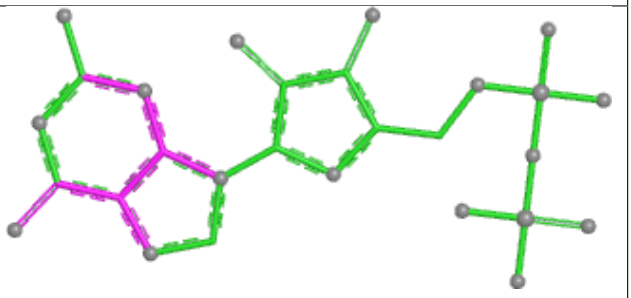
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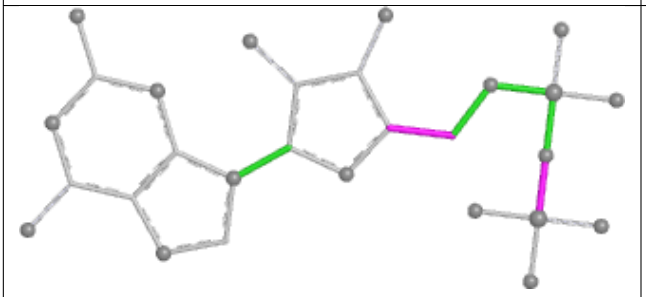
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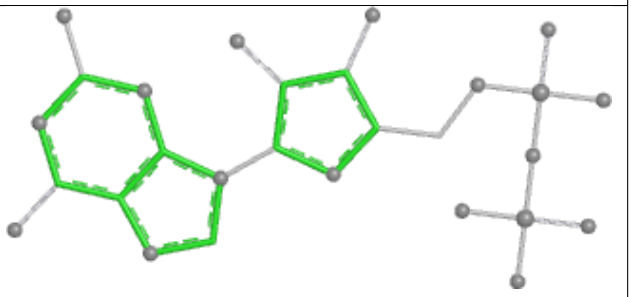
Bond lengths



Bond angles

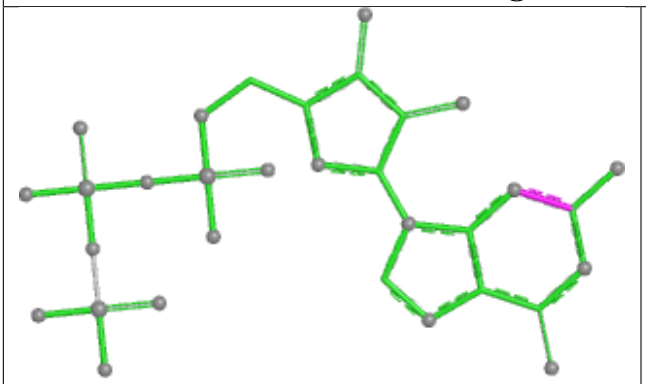


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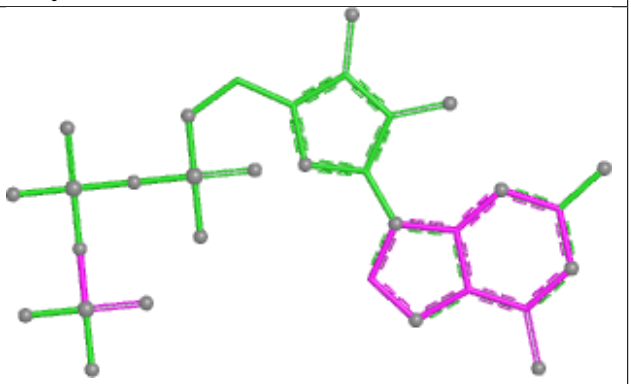


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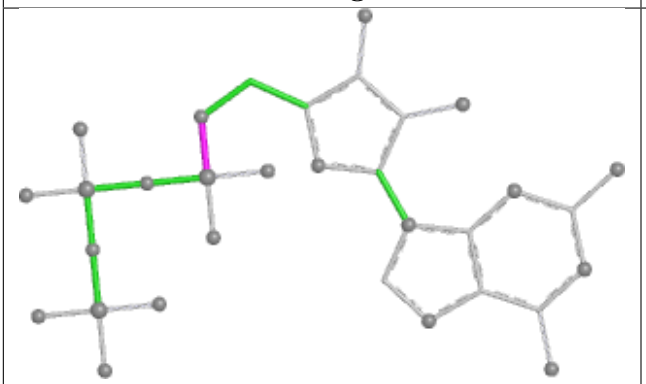
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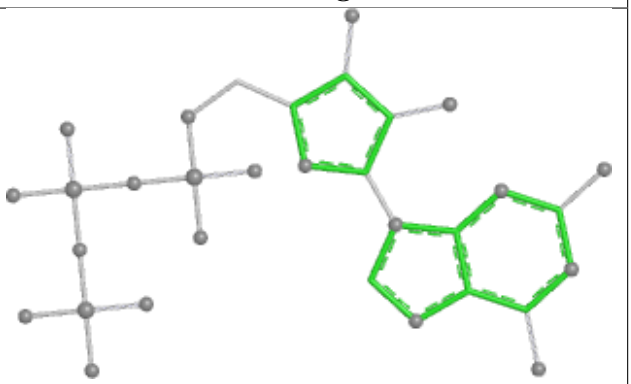
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Bond angles

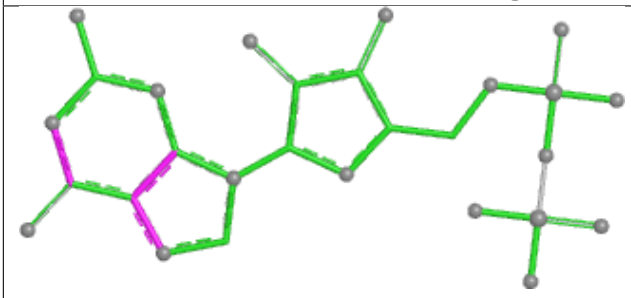


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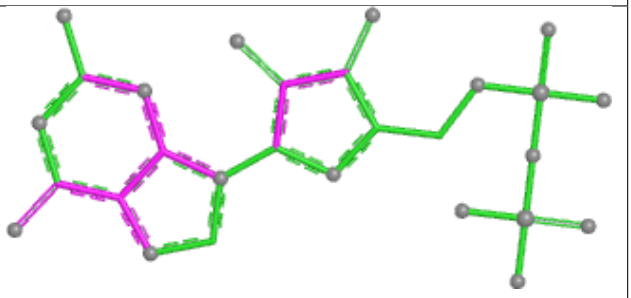


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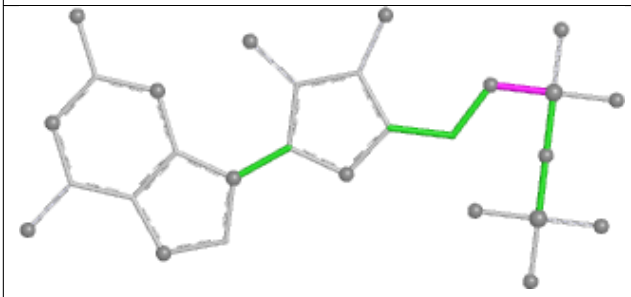
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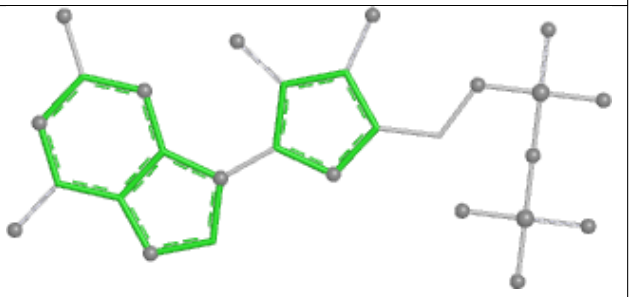
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Bond angles

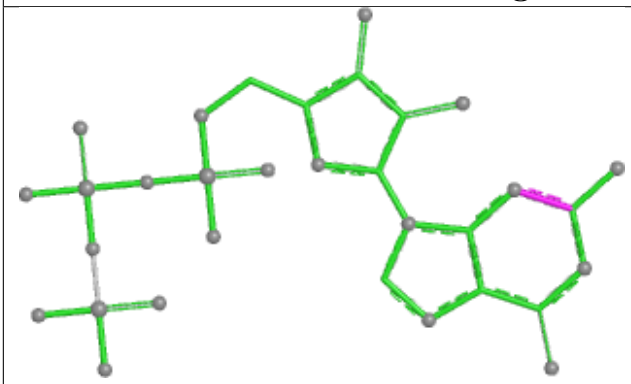


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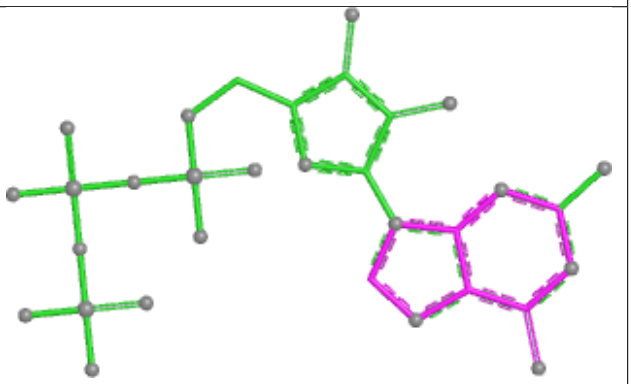


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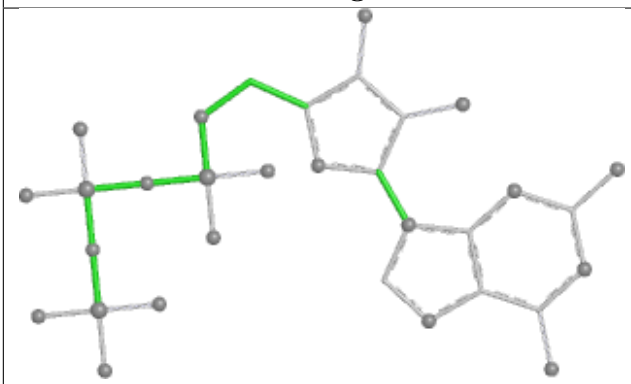
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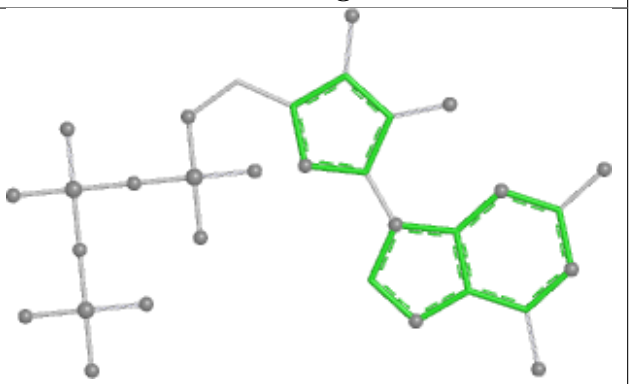
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Bond angles

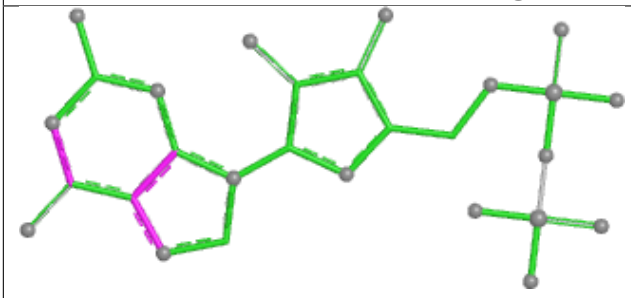


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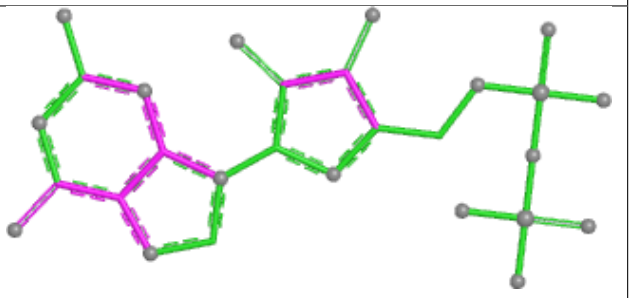


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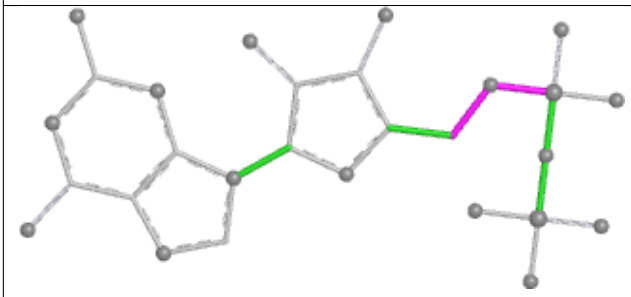
Ligand GDP UL 501



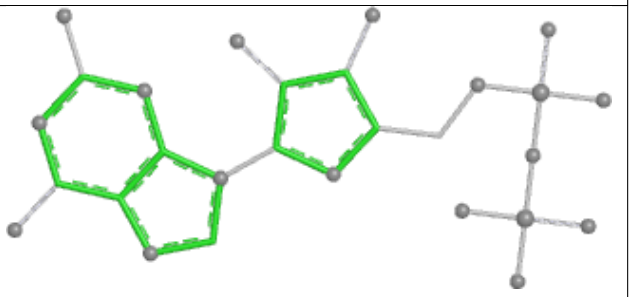
Bond lengths



Bond angles

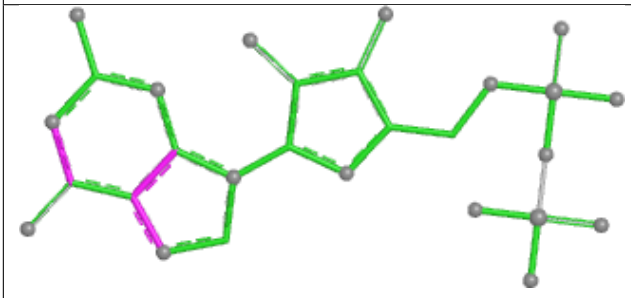


Torsions

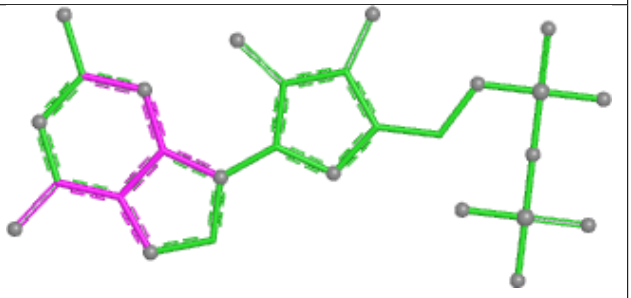


Rings

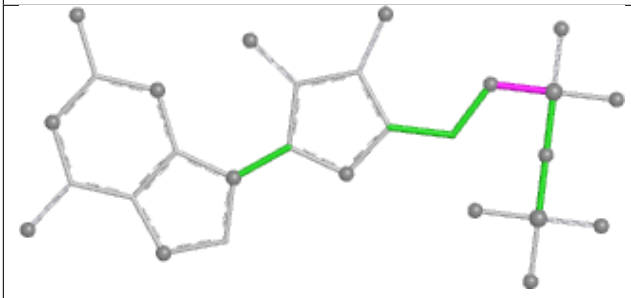
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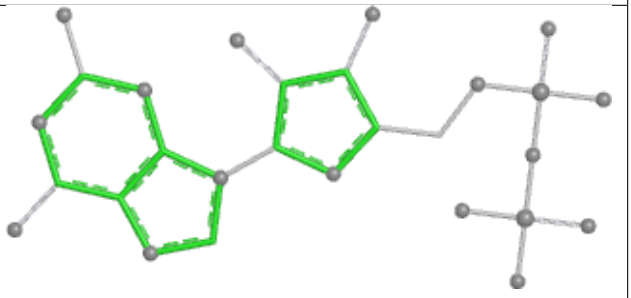
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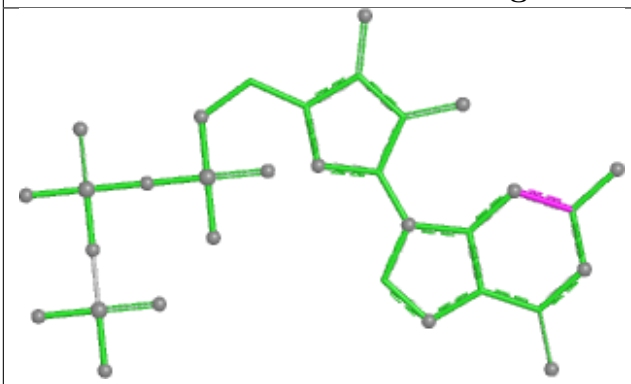


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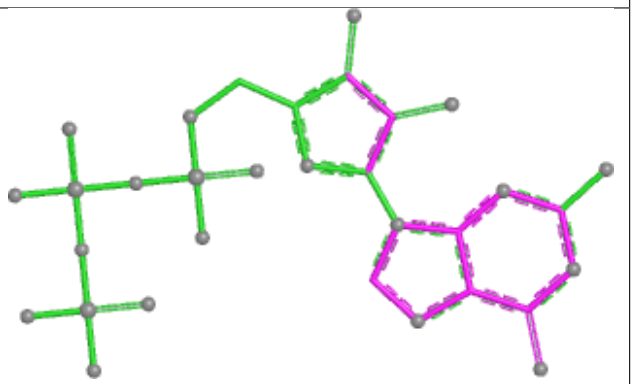


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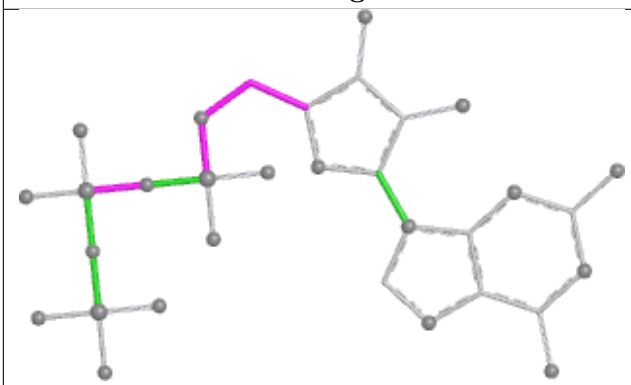
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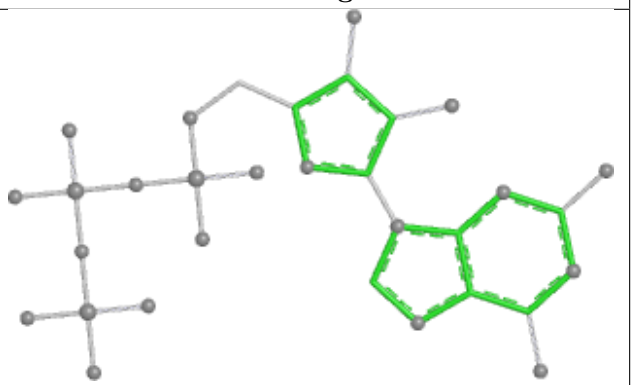
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Bond angles

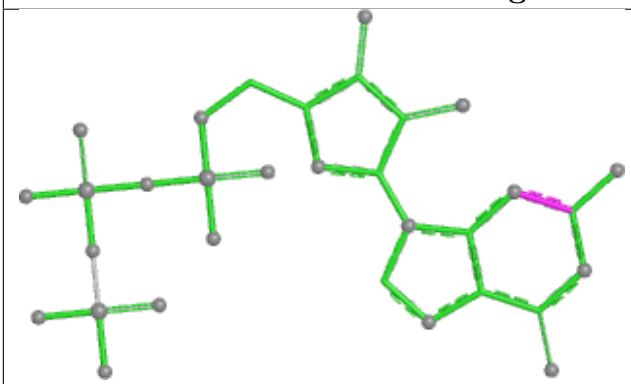


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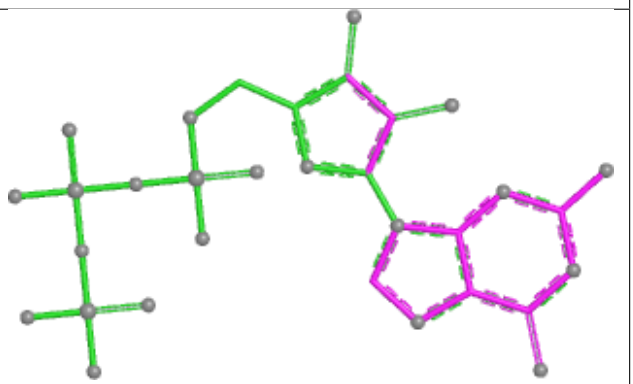


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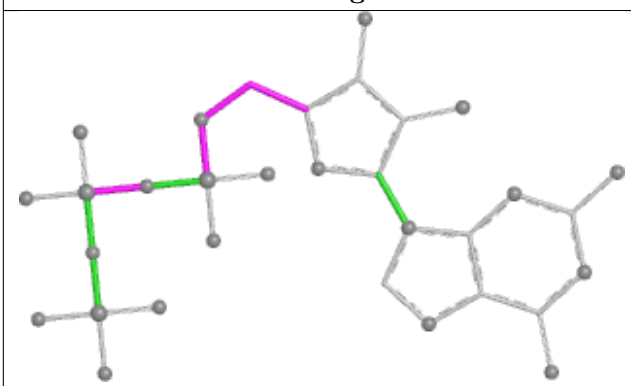
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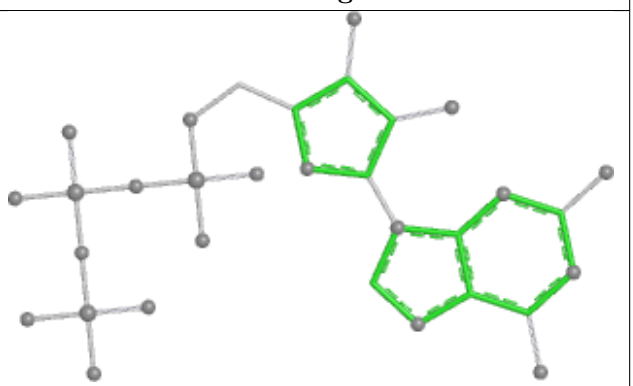
Bond lengths



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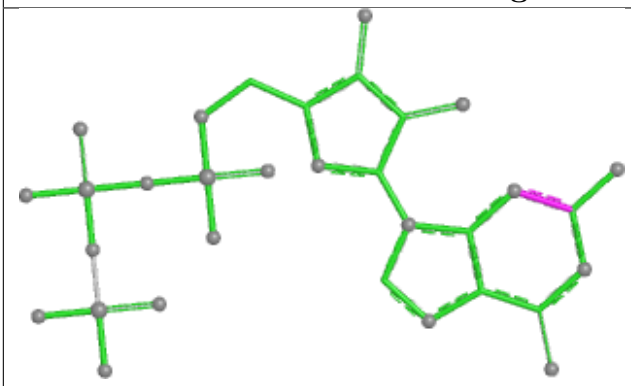


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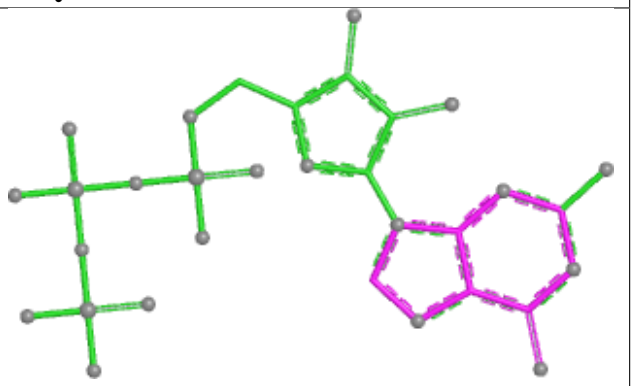


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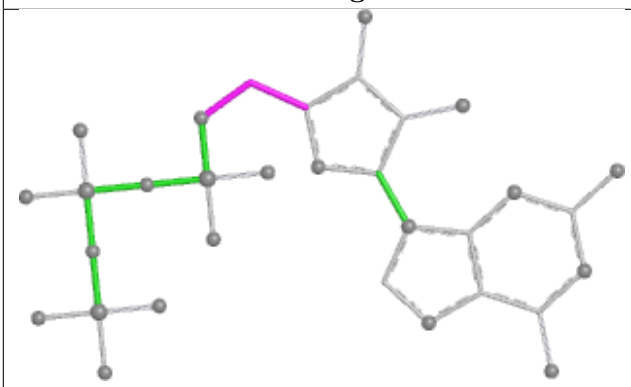
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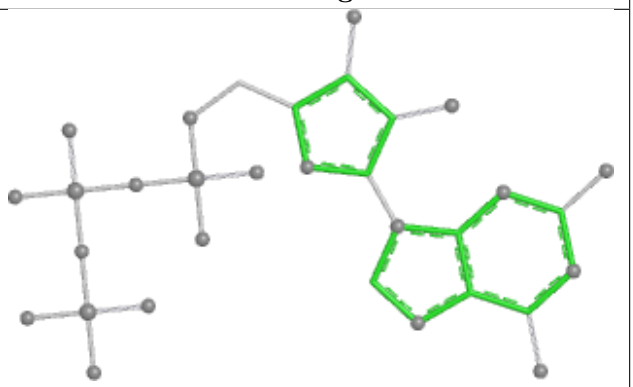
Bond lengths



Bond angles

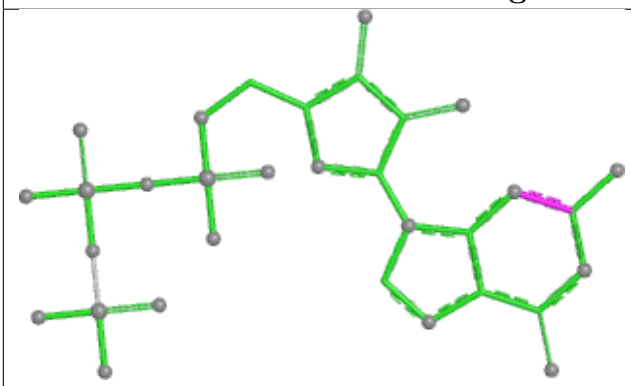


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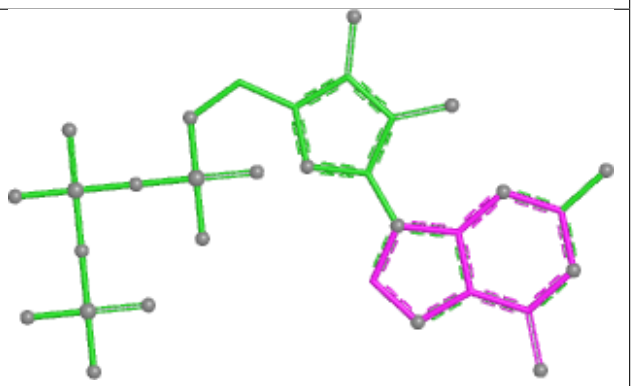


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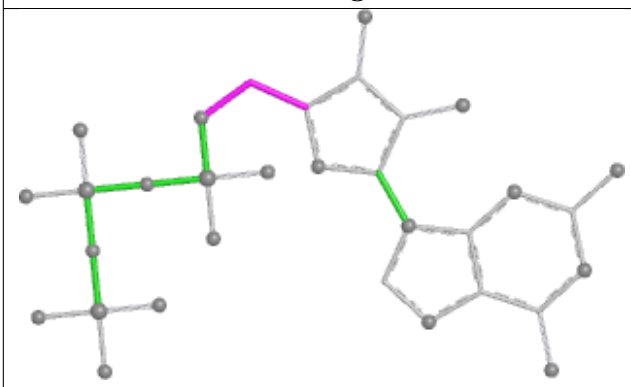
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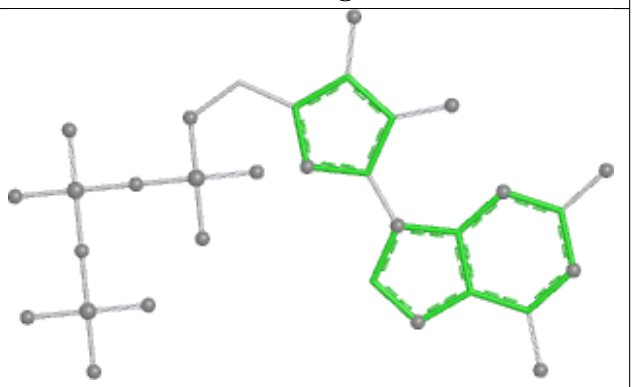
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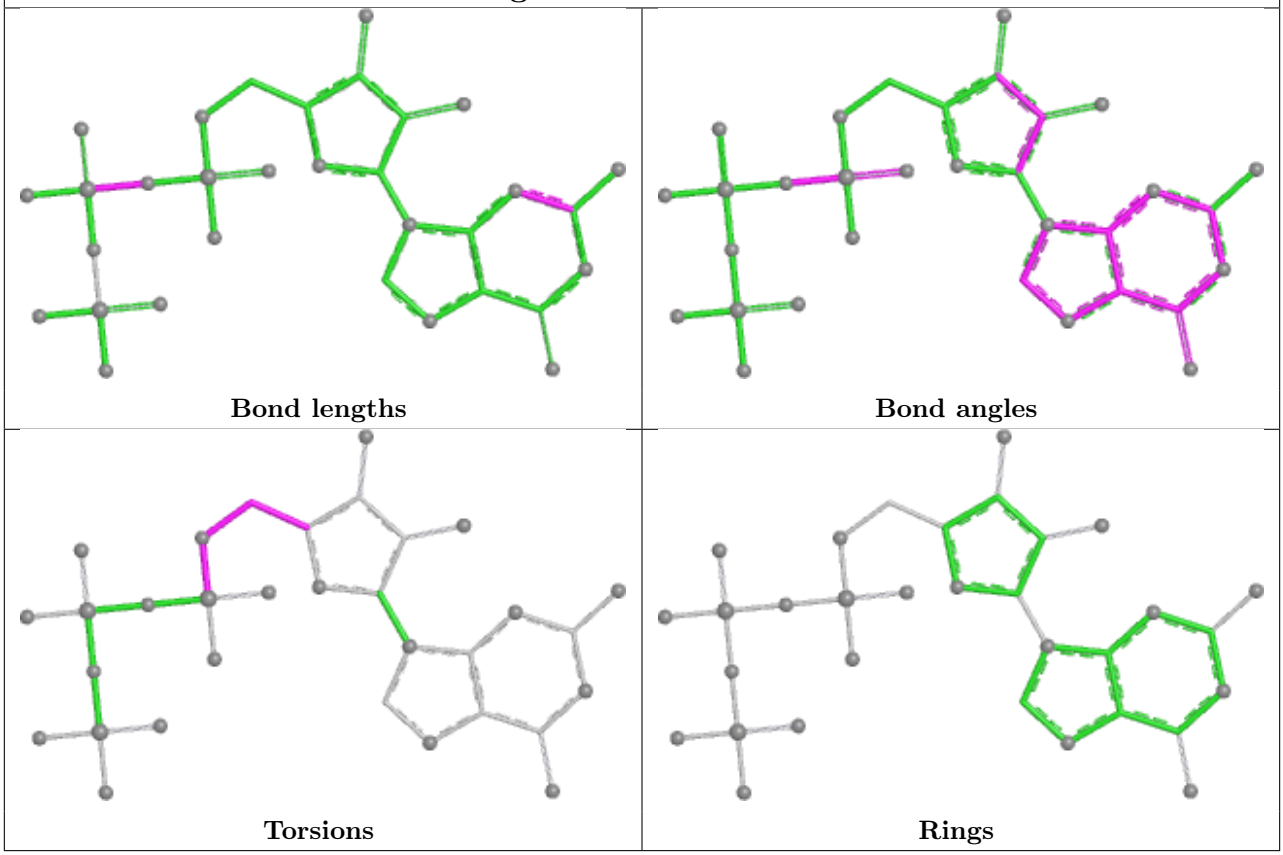


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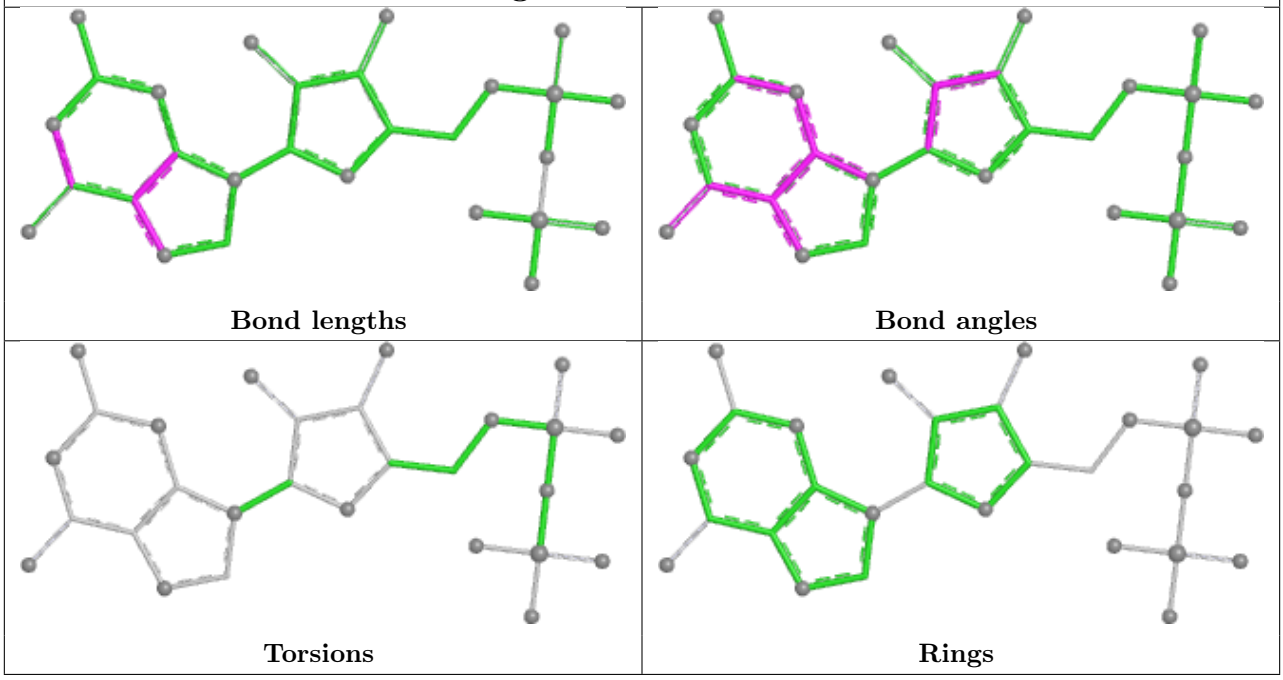


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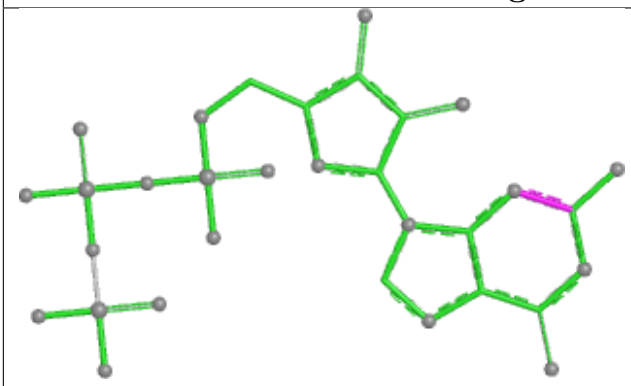
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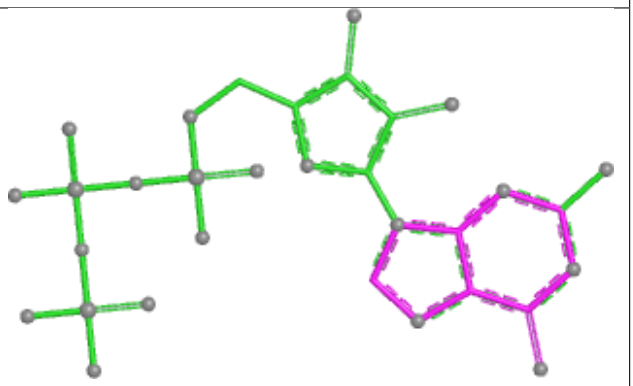
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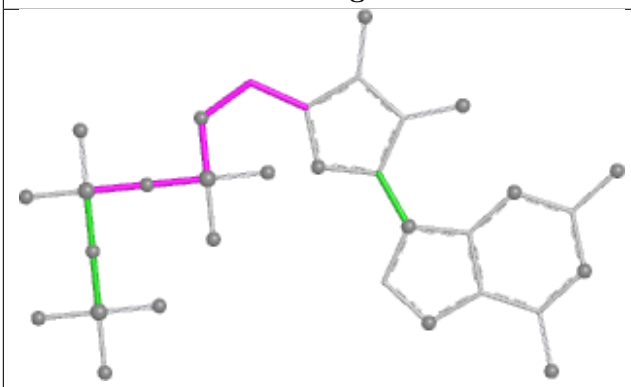
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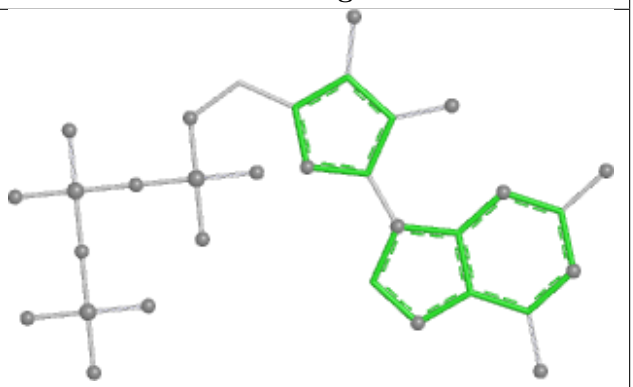
Bond lengths



Bond angles

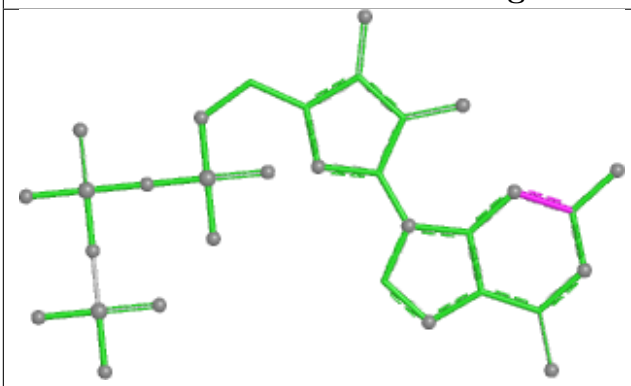


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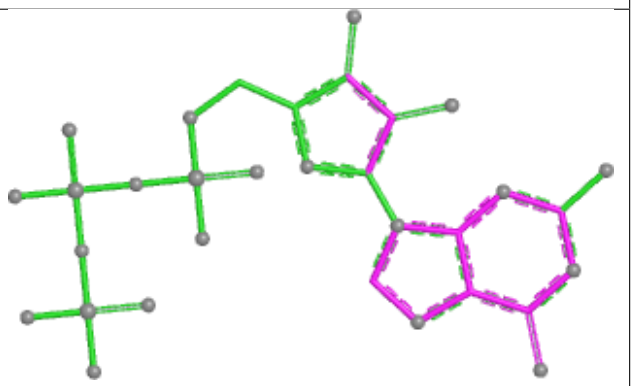


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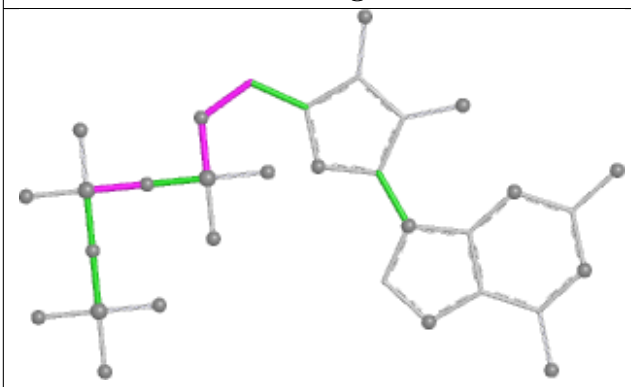
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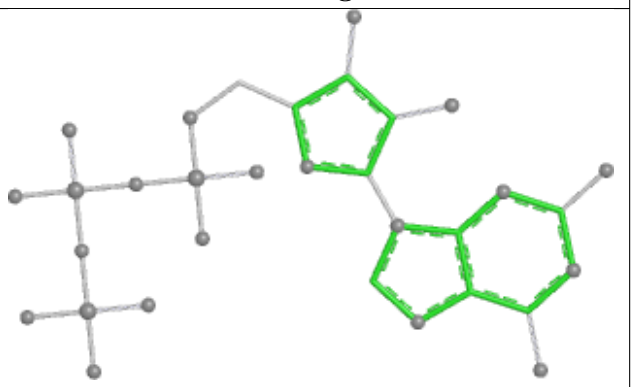
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Bond angles

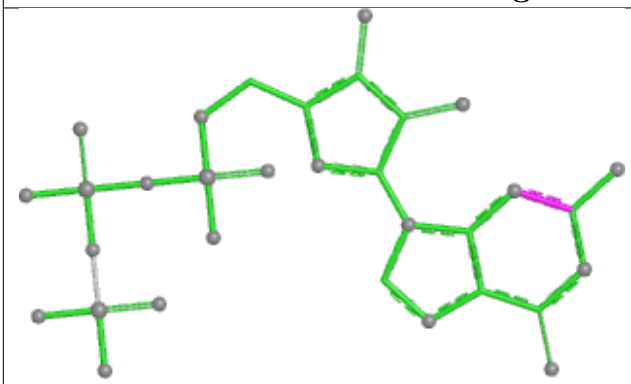


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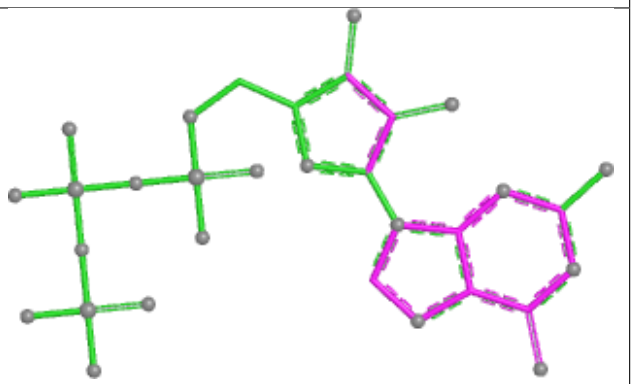


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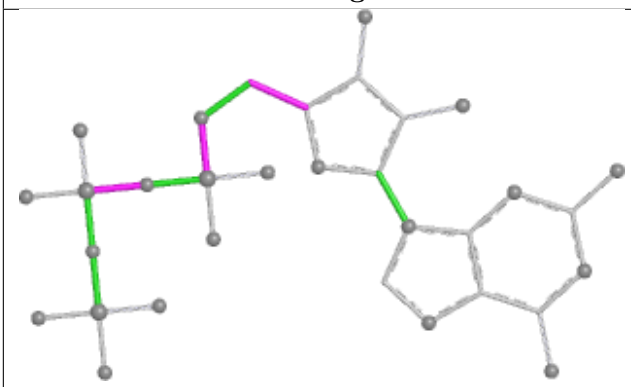
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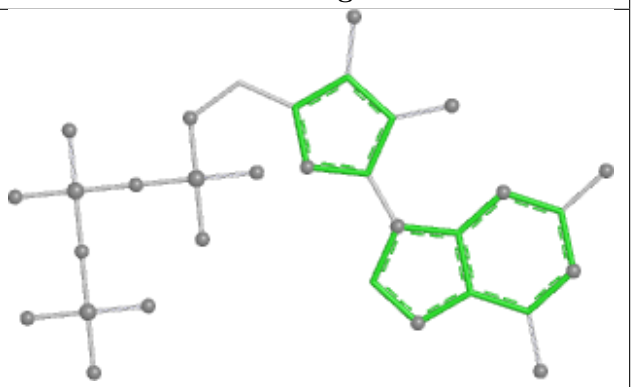
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Bond angles

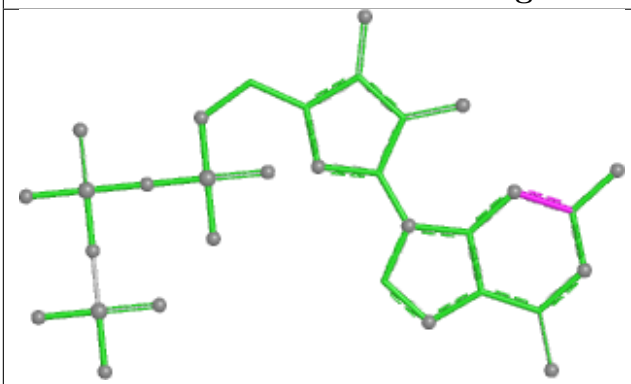


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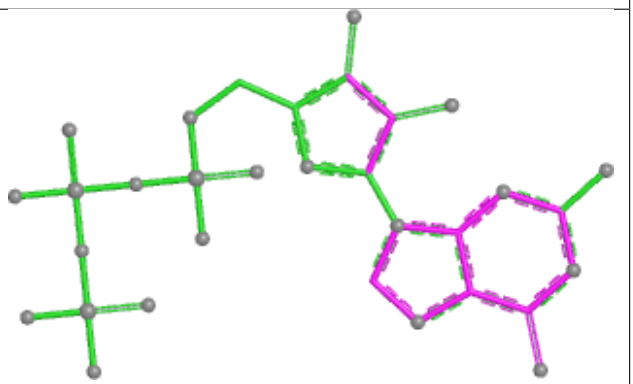


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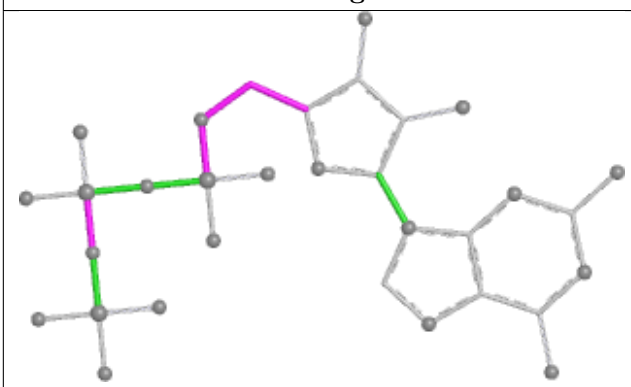
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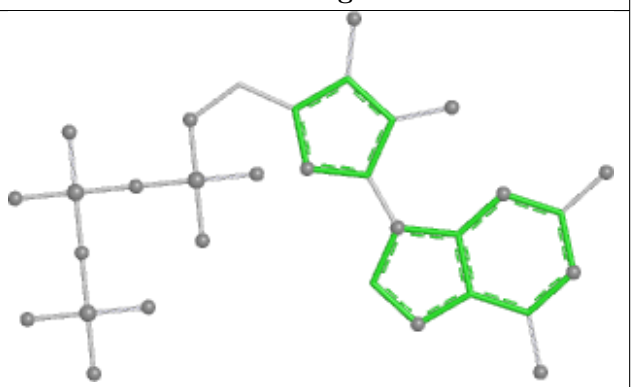
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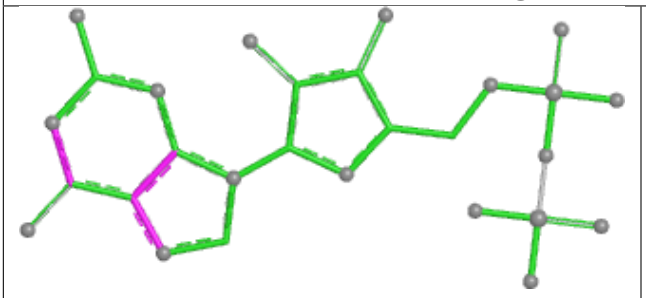


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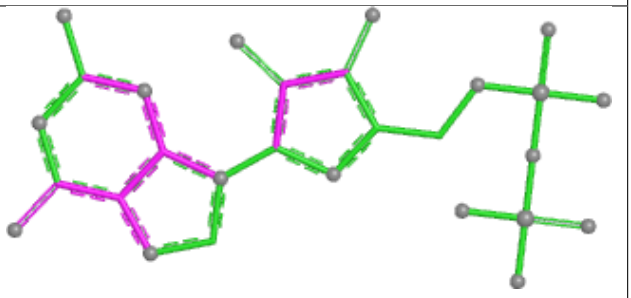


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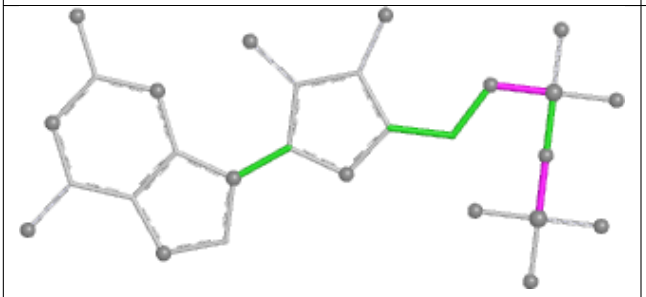
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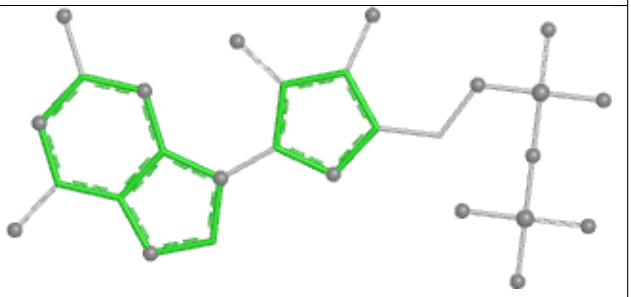
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Bond angles

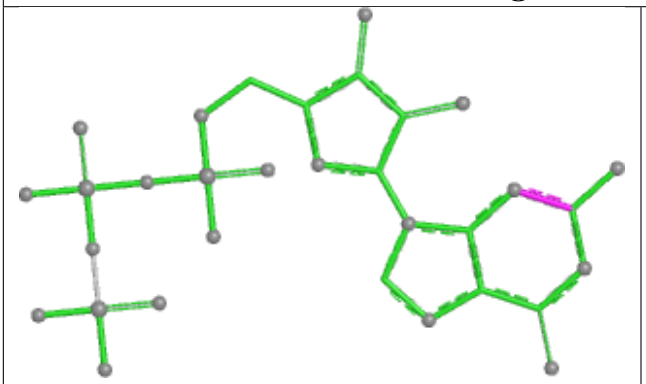


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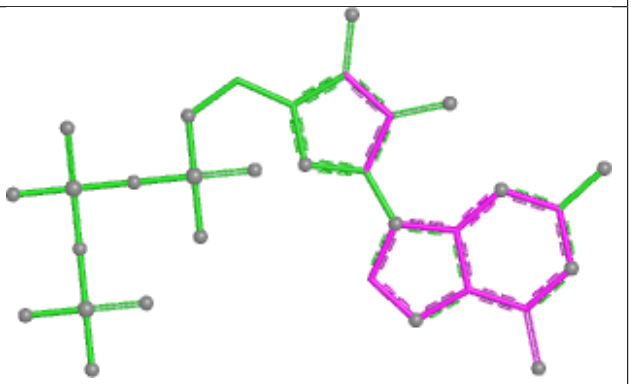


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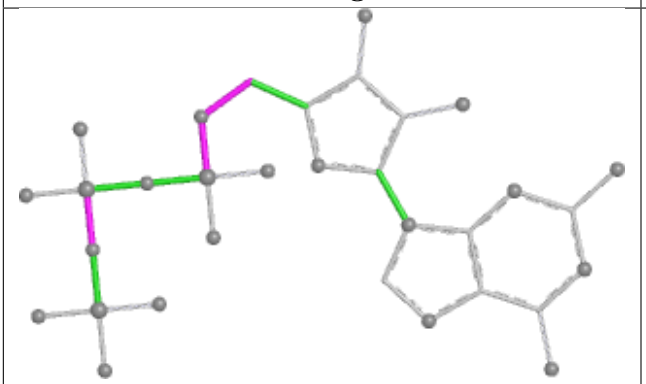
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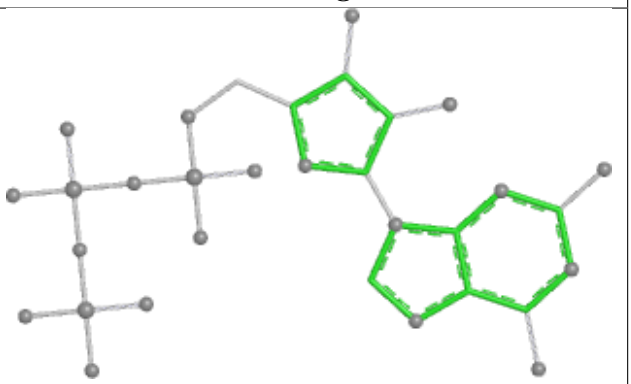
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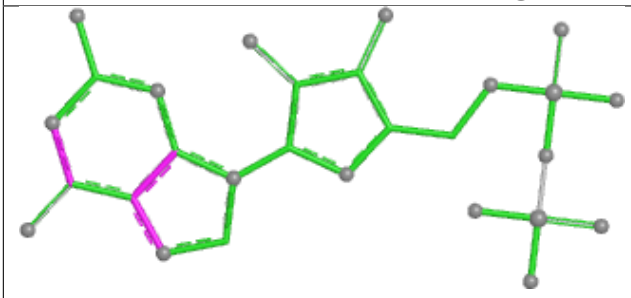


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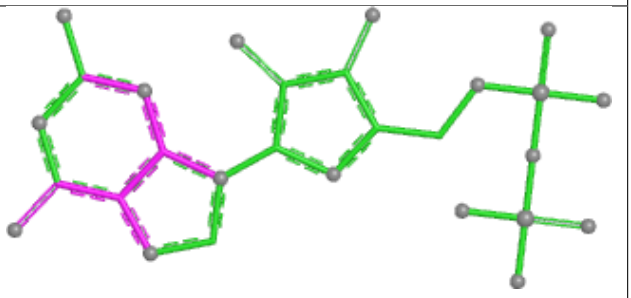


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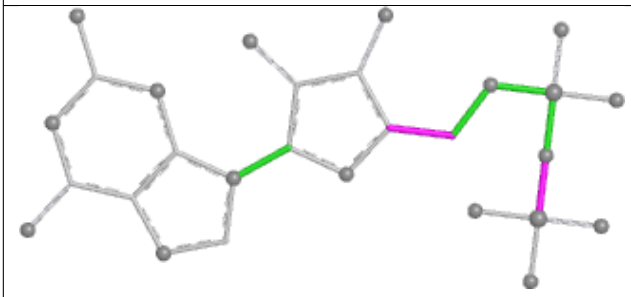
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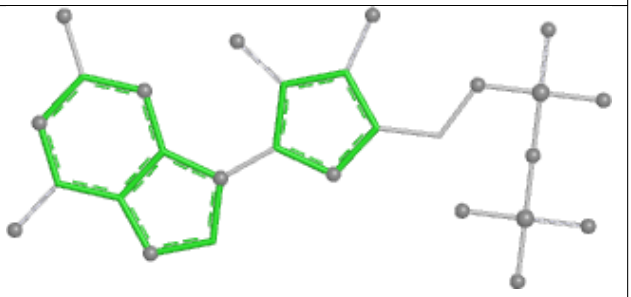
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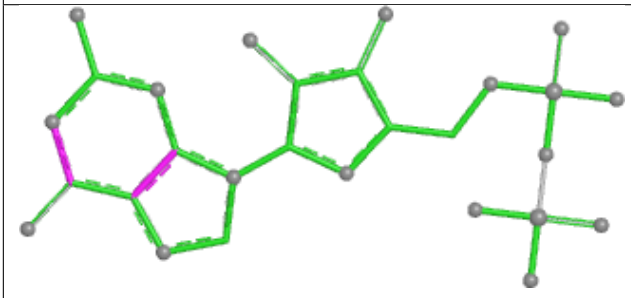


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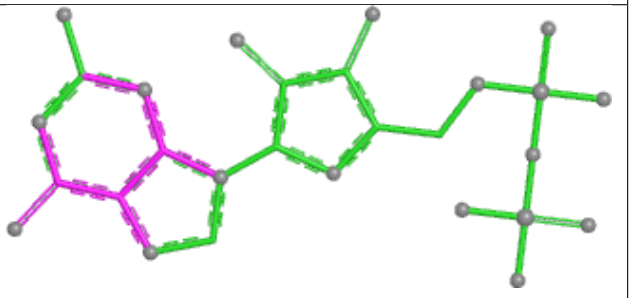


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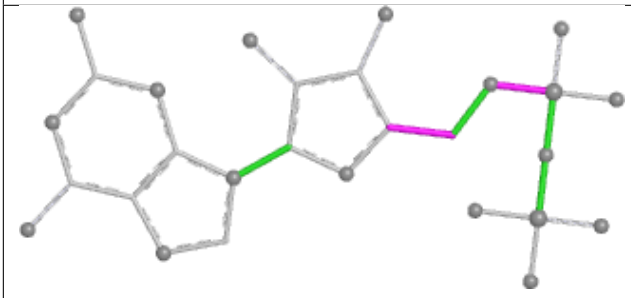
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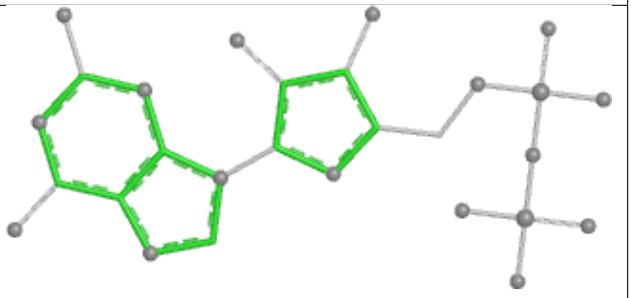
Bond lengths



Bond angles

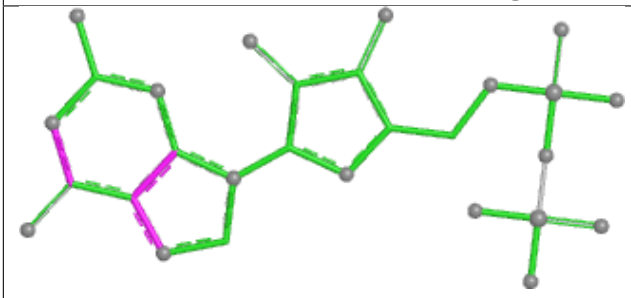


Torsions

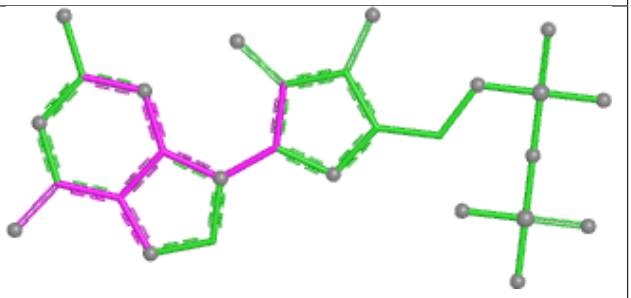


Rings

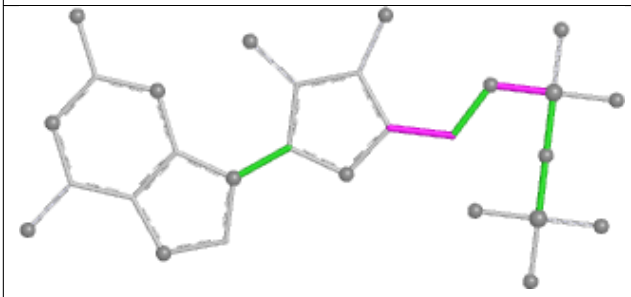
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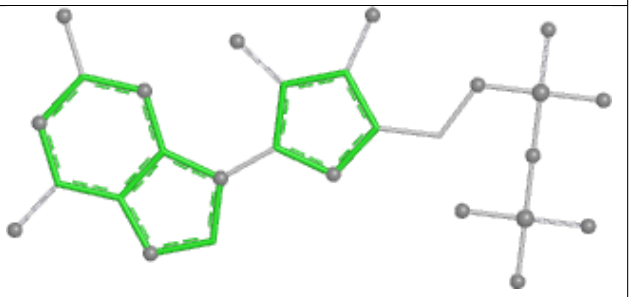
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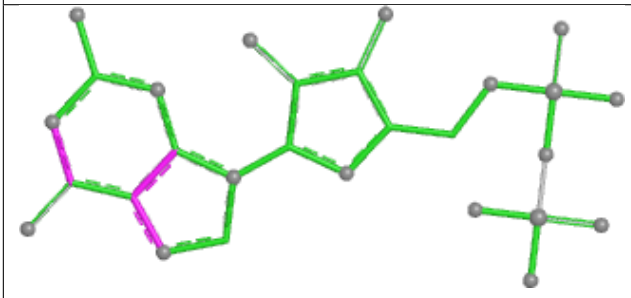


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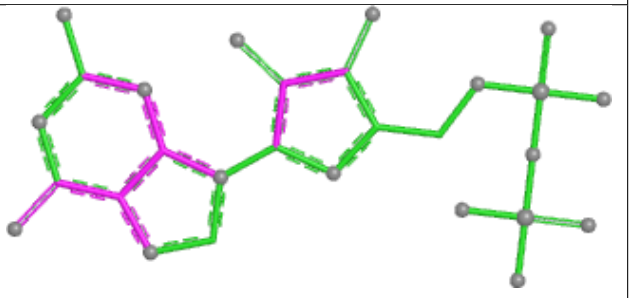


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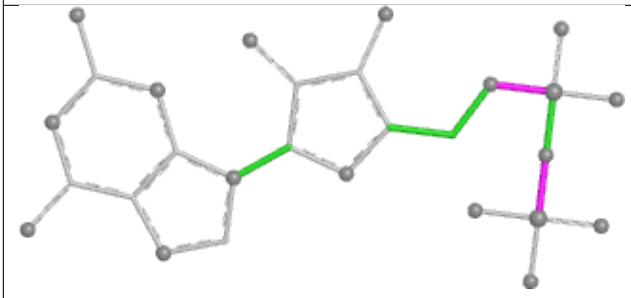
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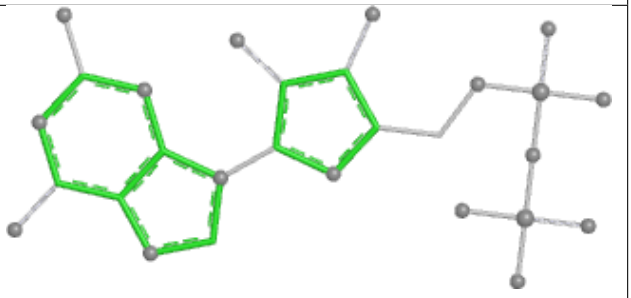
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Bond angles

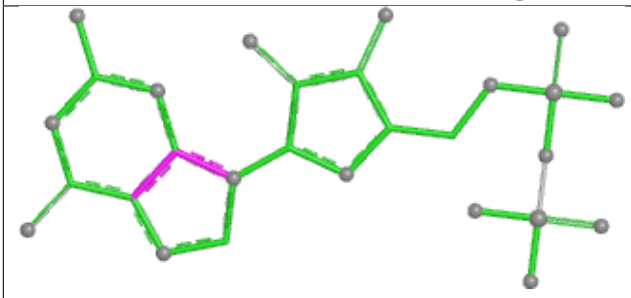


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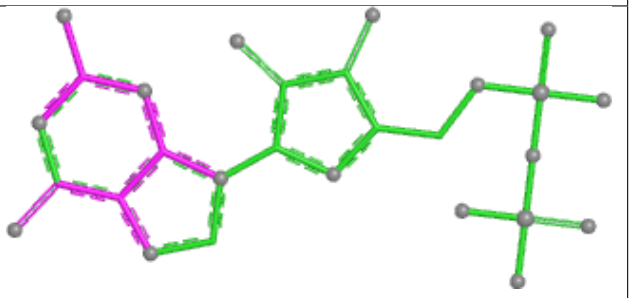


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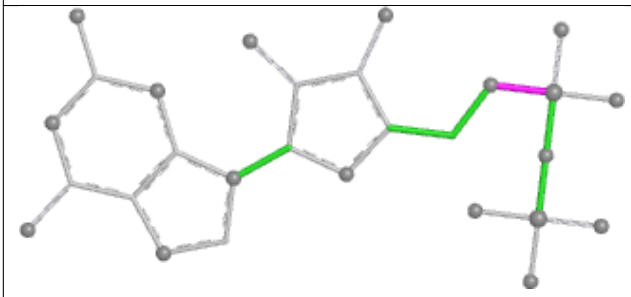
Ligand GDP LB 501



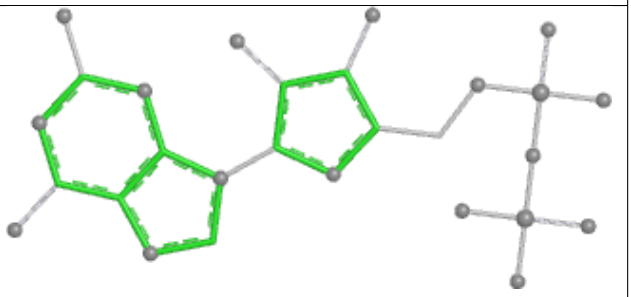
Bond lengths



Bond angles

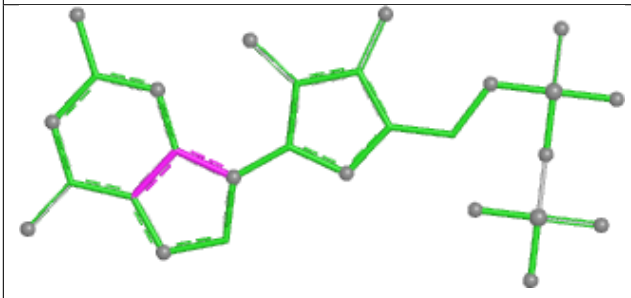


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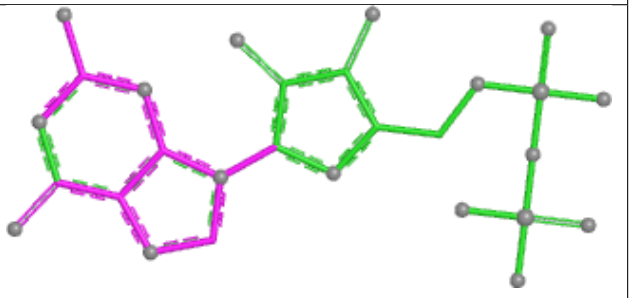


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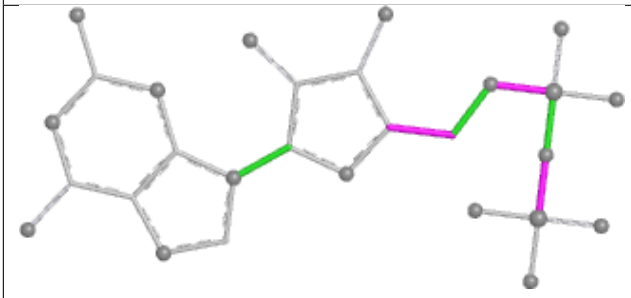
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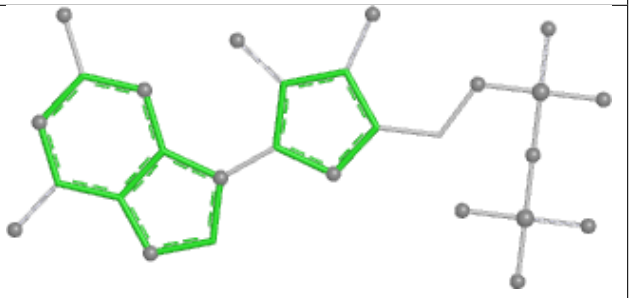
Bond lengths



Bond angles

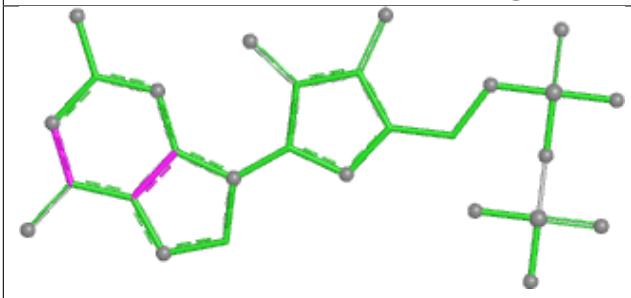


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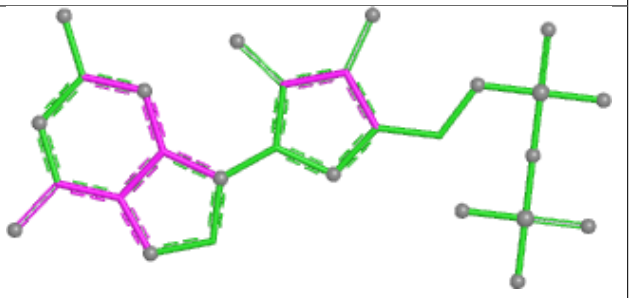


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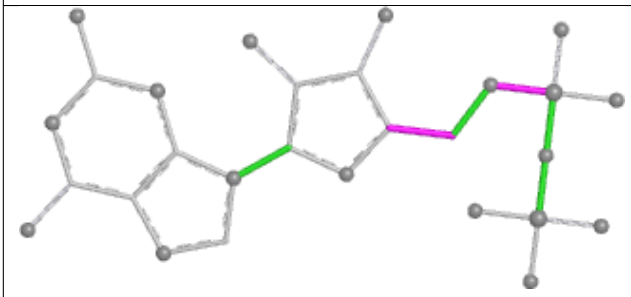
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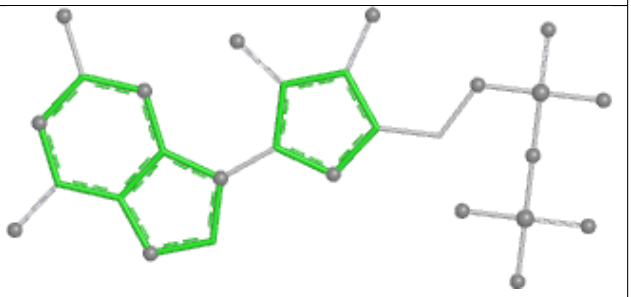
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Bond angles

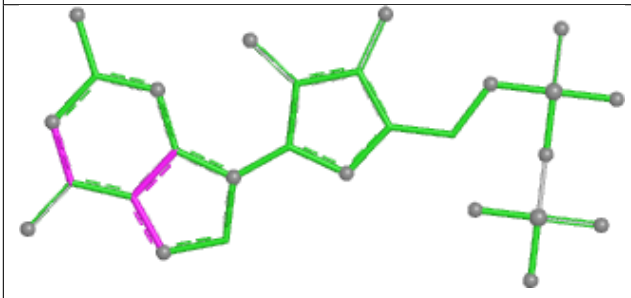


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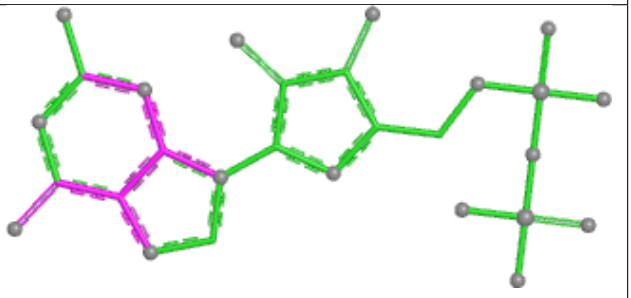


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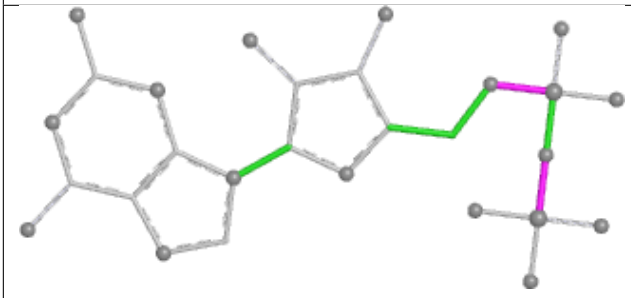
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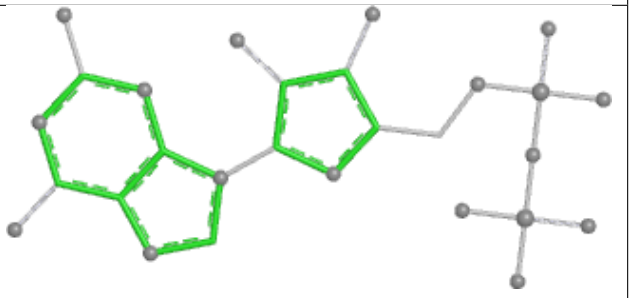
Bond lengths



Bond angles

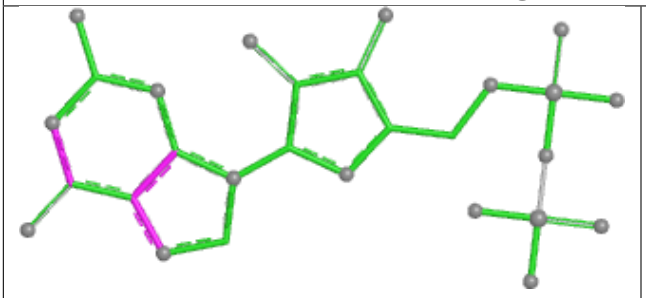


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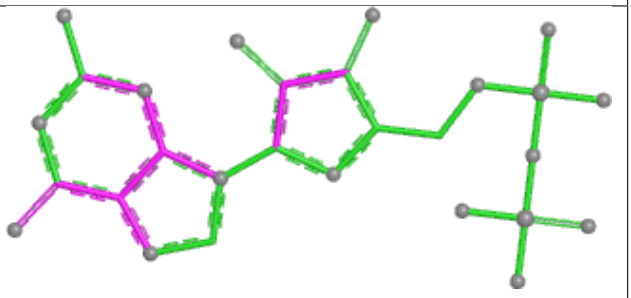


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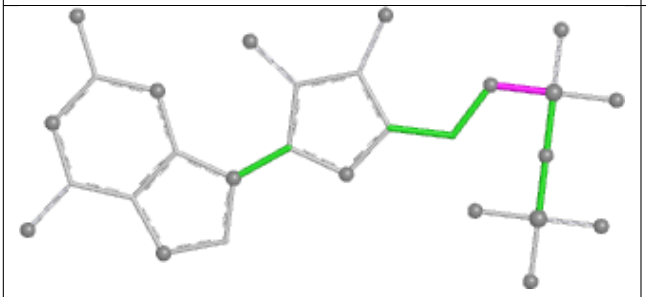
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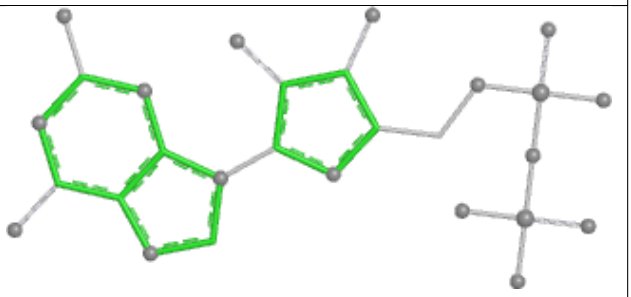
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Bond angles

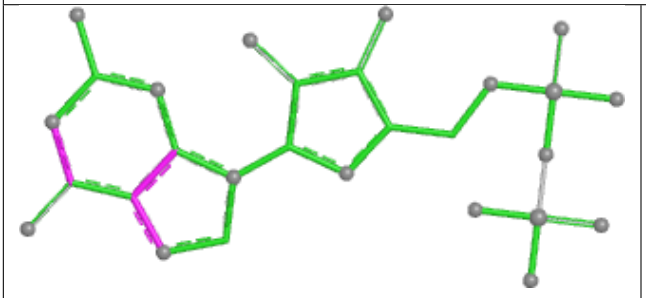


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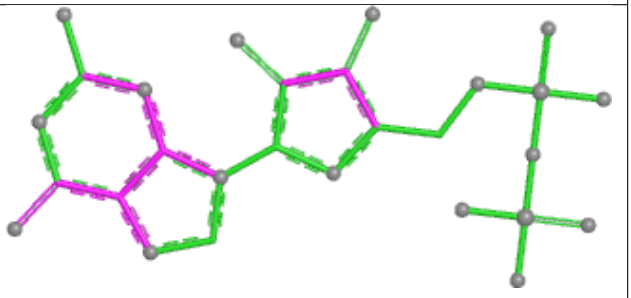


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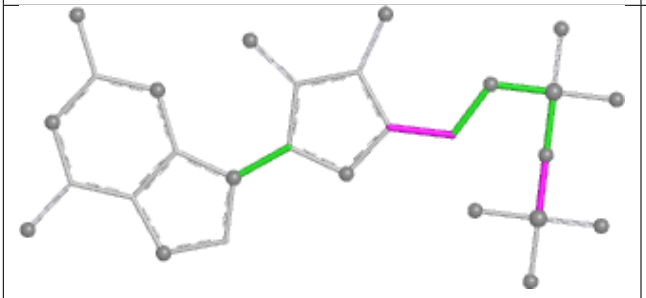
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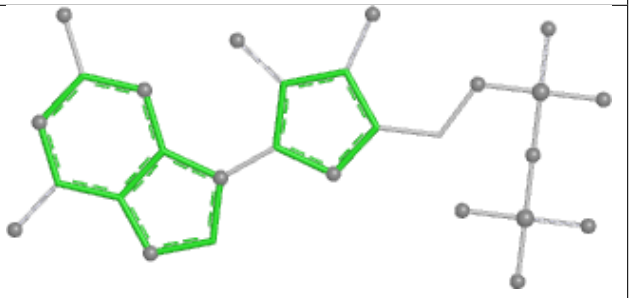
Bond lengths



Bond angles

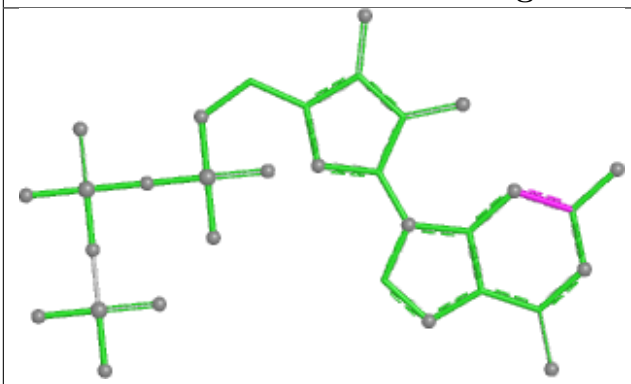


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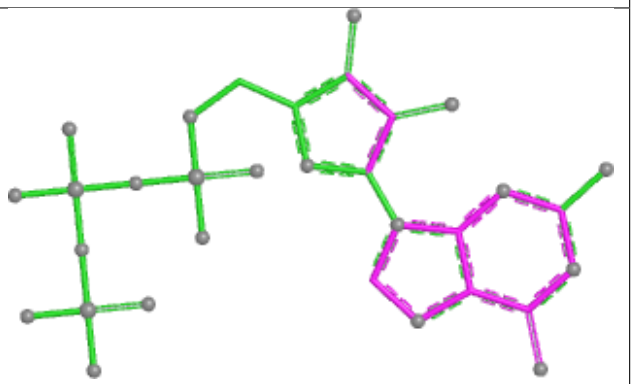


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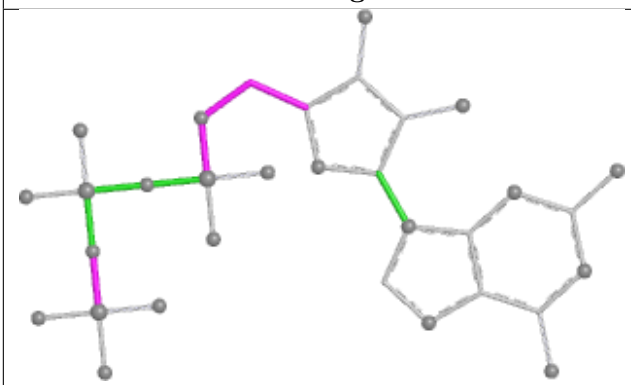
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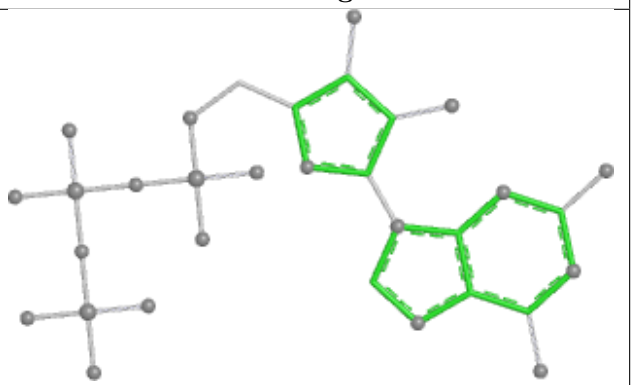
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Bond angles

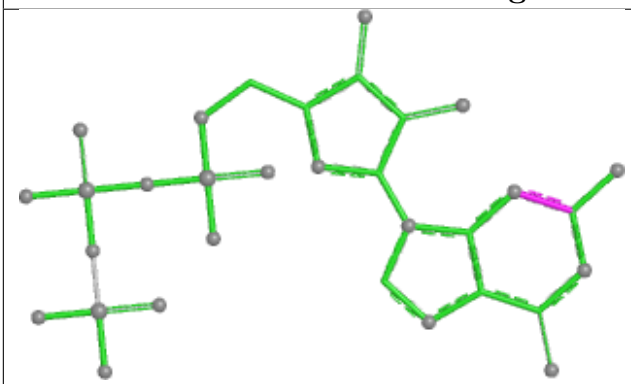


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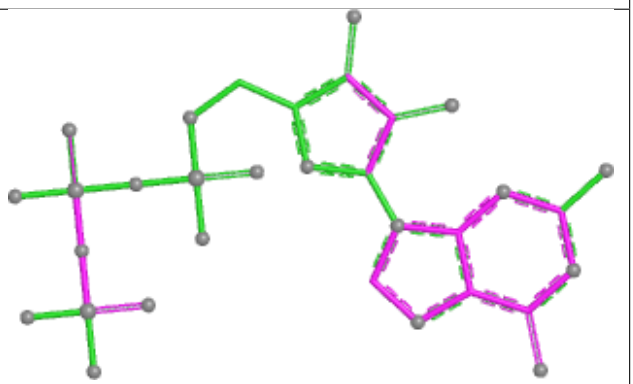


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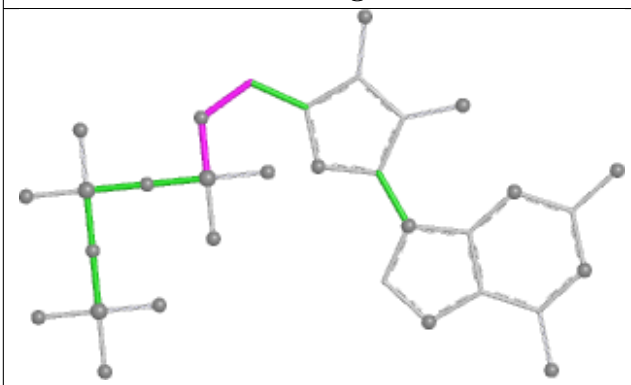
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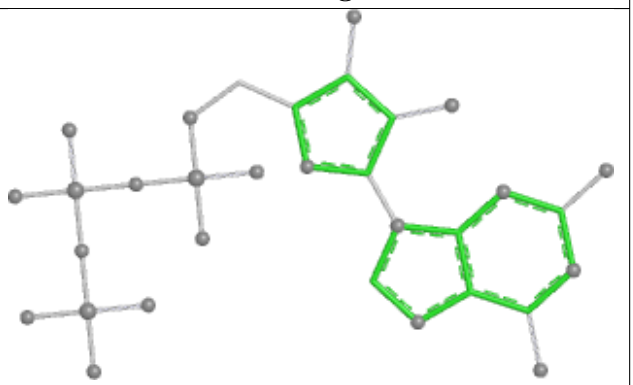
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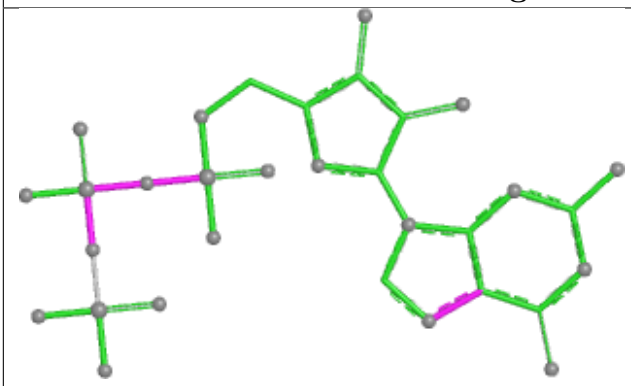


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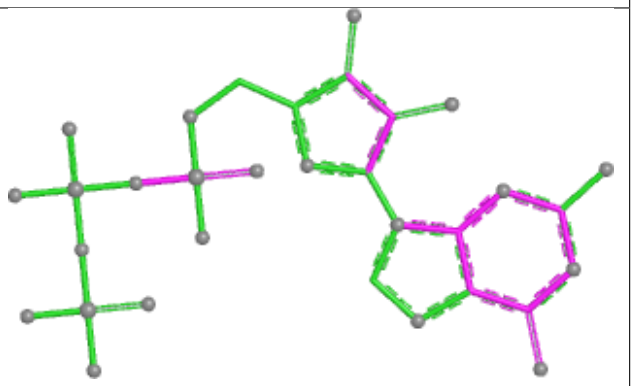


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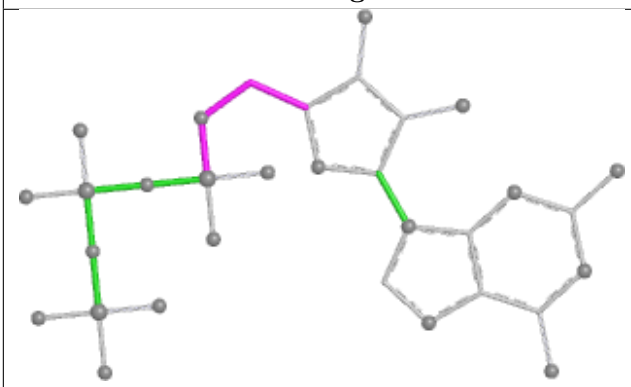
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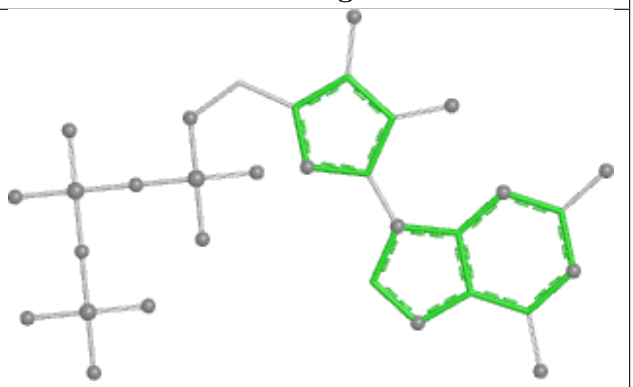
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Bond angles

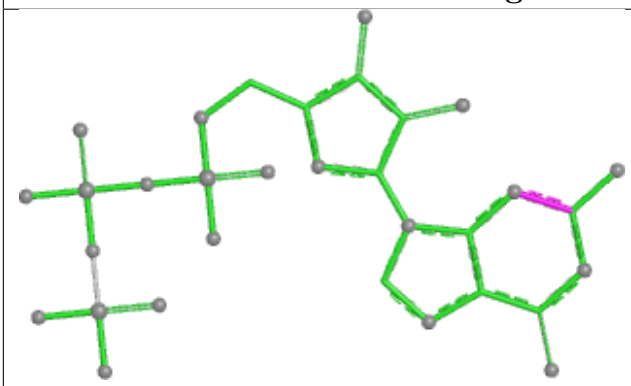


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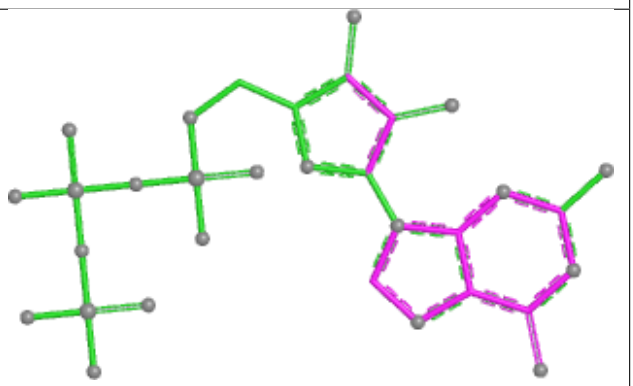


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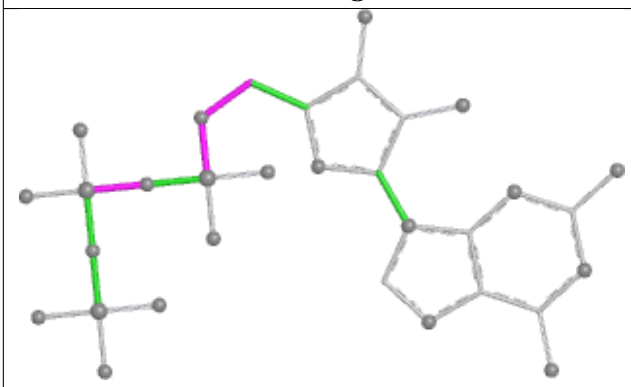
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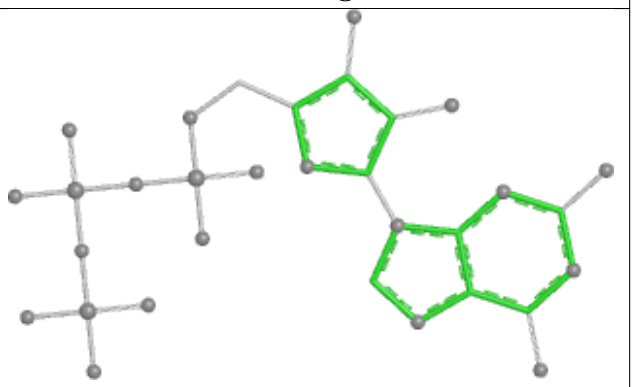
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Bond angles

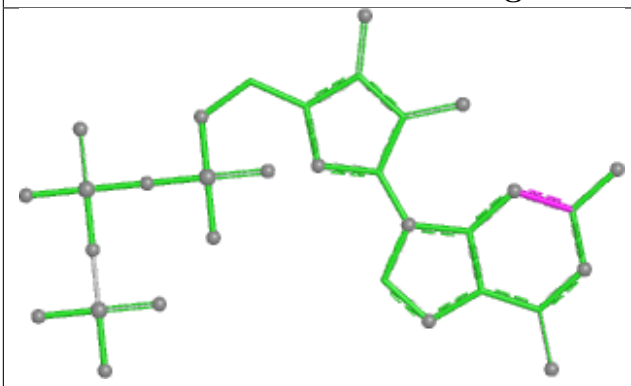


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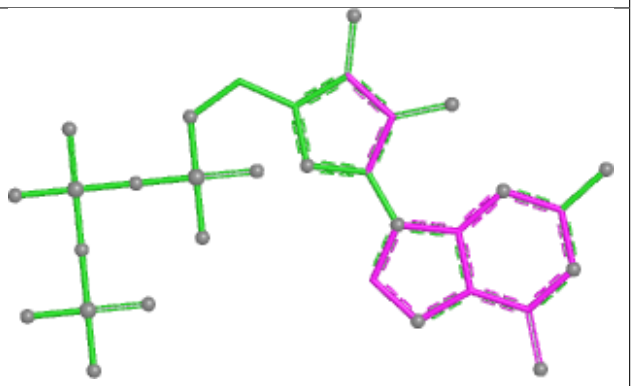


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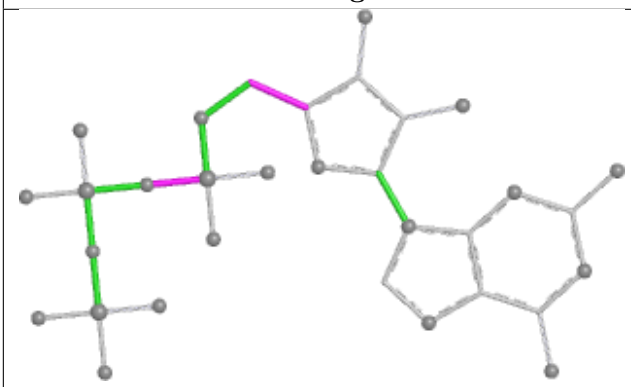
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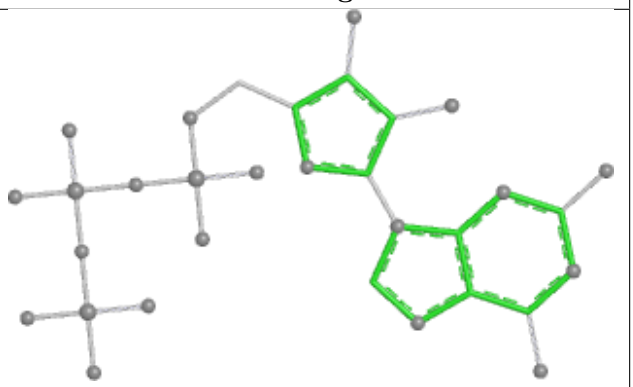
Bond lengths



Bond angles

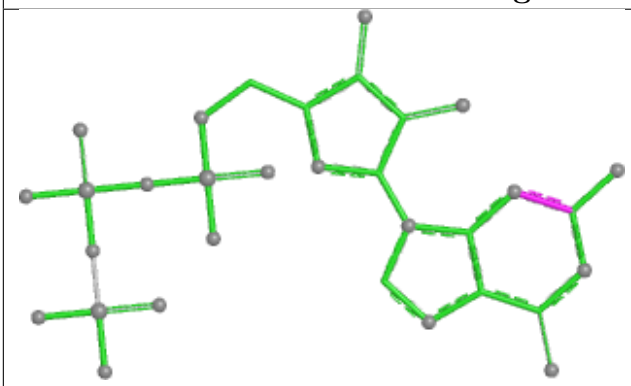


Torsions

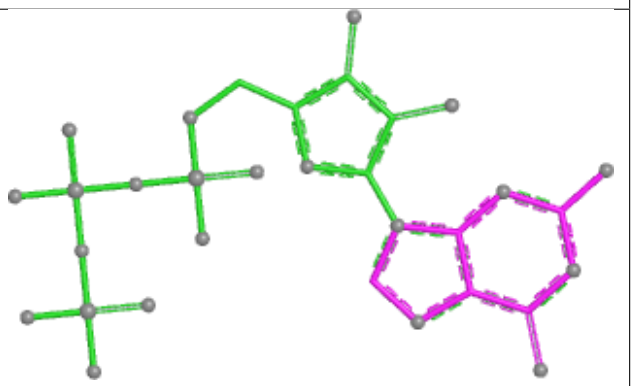


Rings

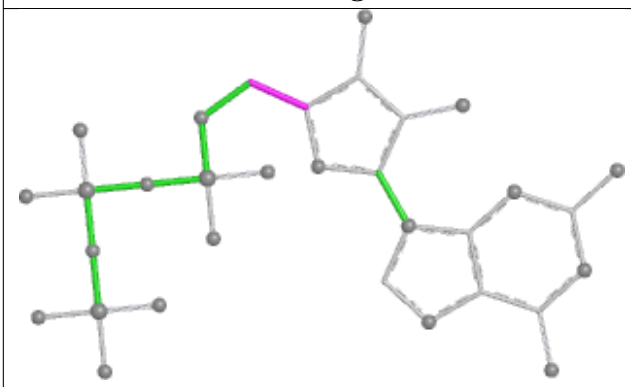
Ligand GTP JC 501



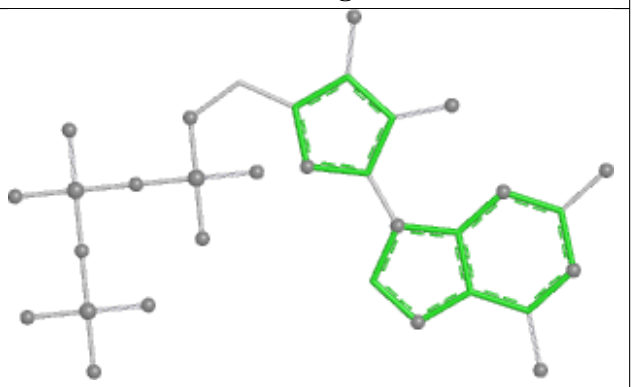
Bond lengths



Bond angles

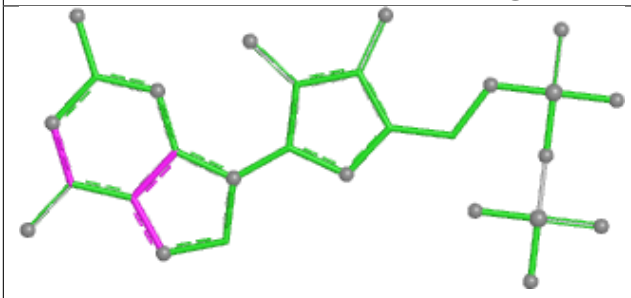


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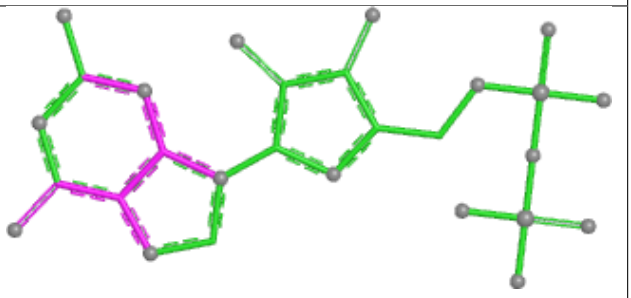


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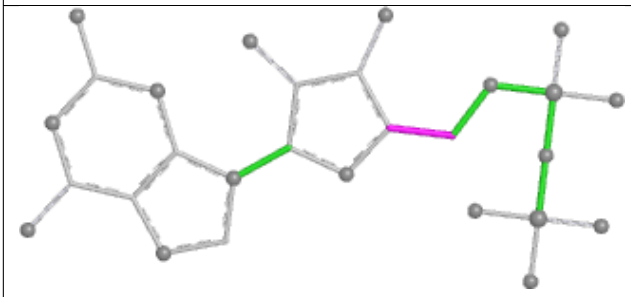
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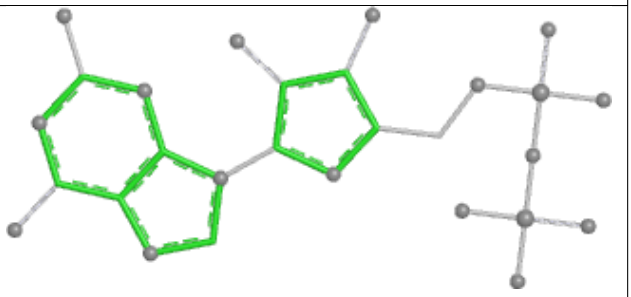
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Bond angles

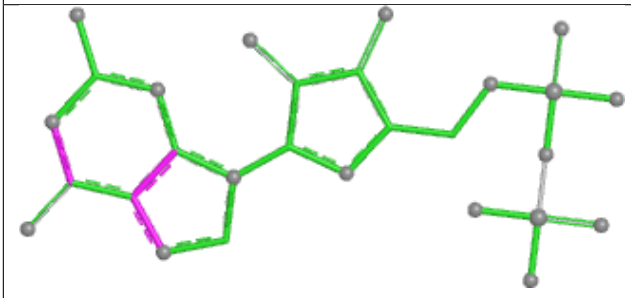


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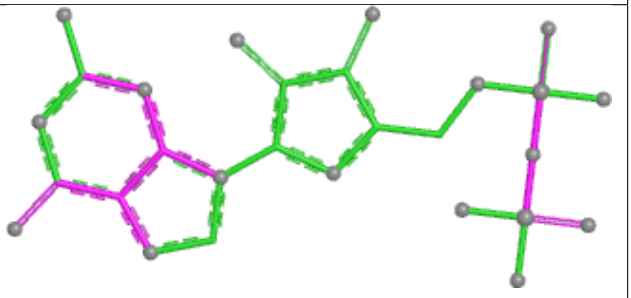


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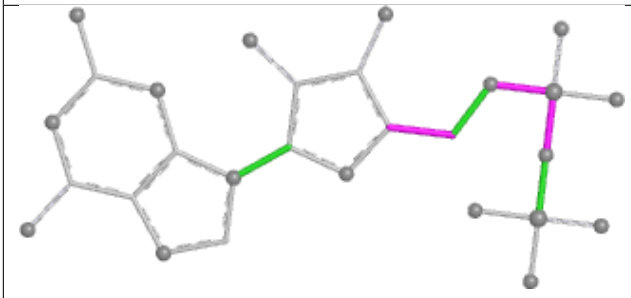
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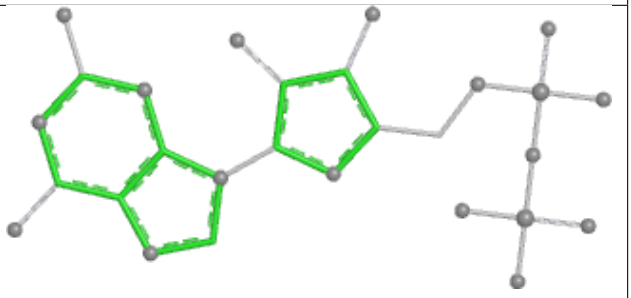
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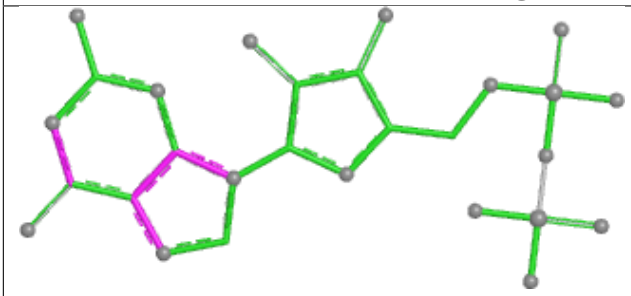


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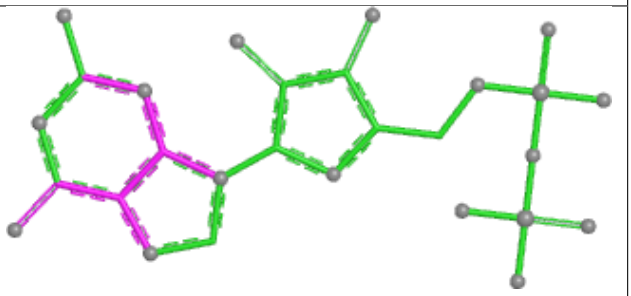


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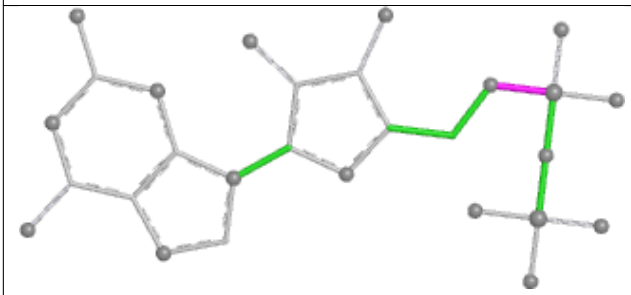
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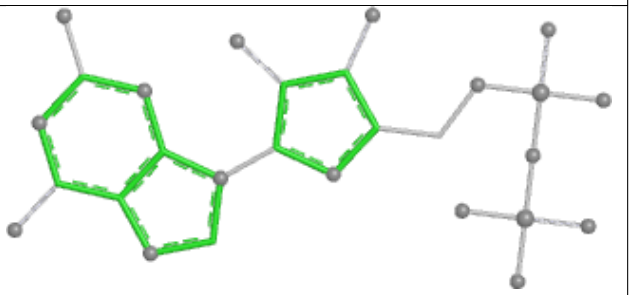
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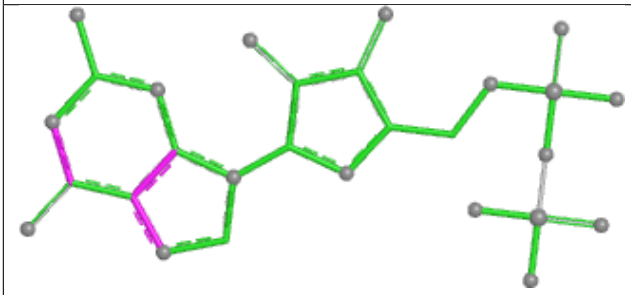


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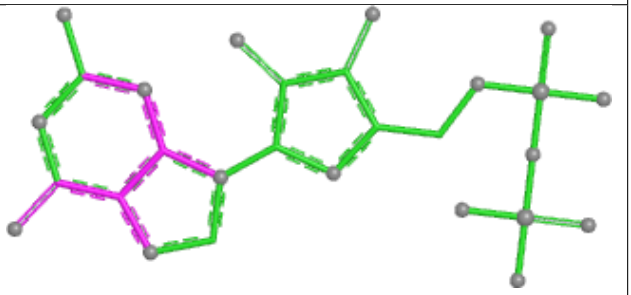


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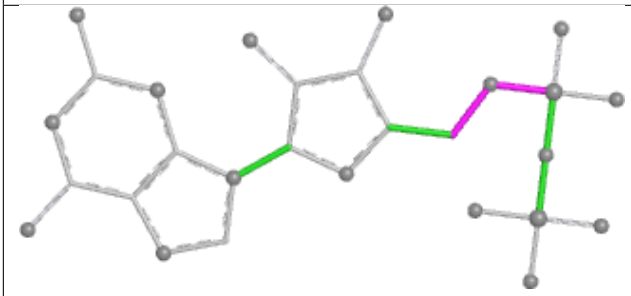
Ligand GDP HF 501



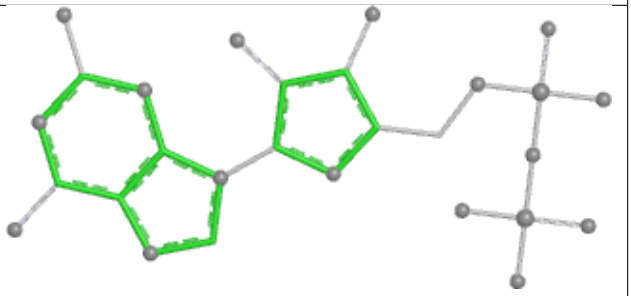
Bond lengths



Bond angles

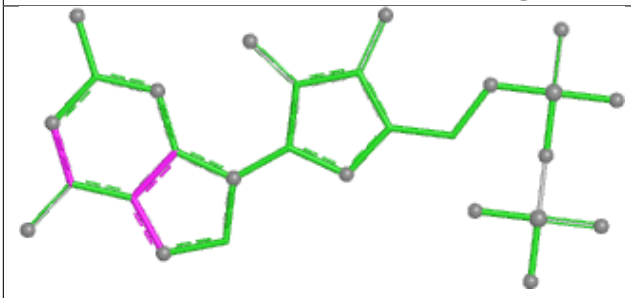


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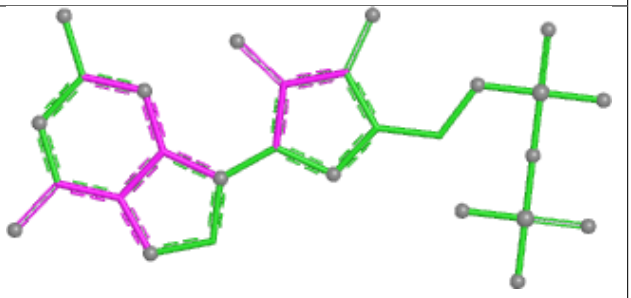


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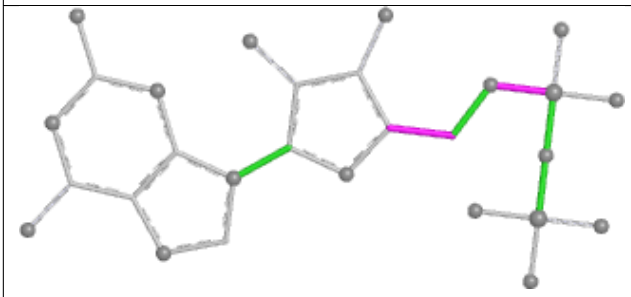
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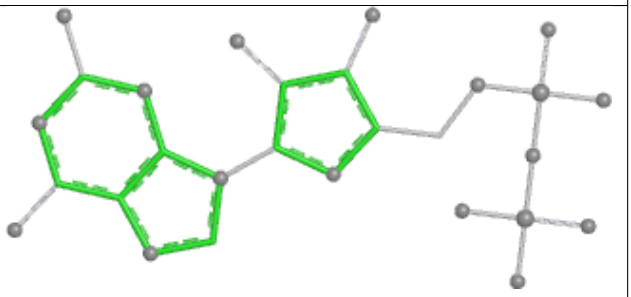
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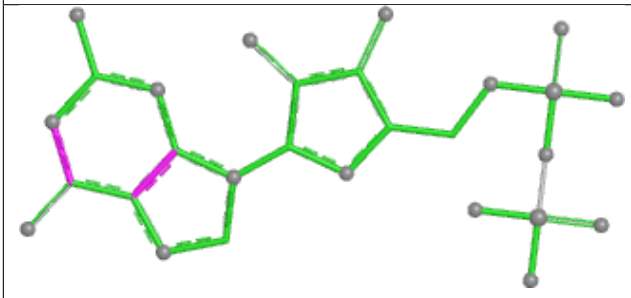


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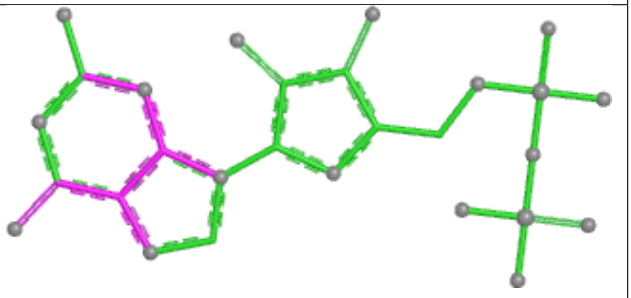


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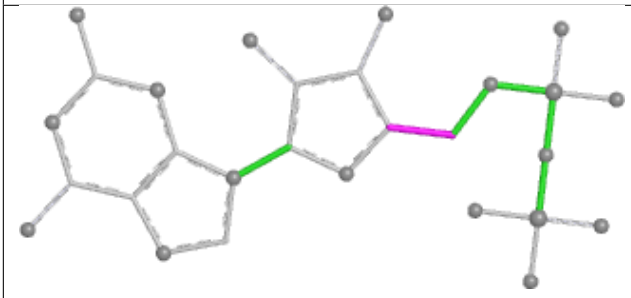
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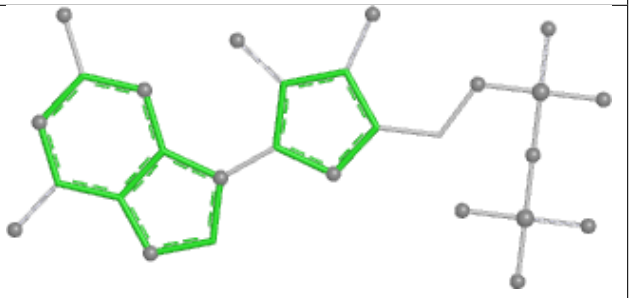
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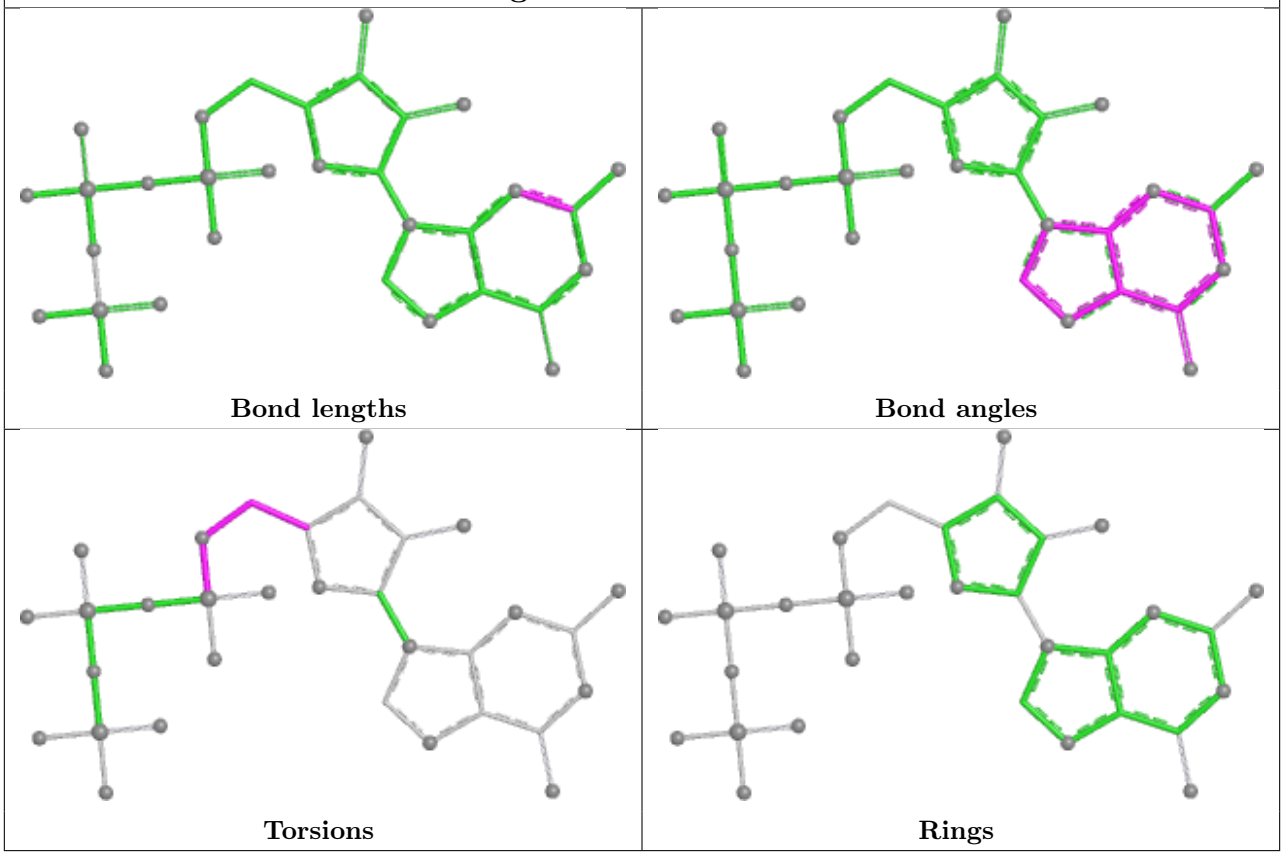


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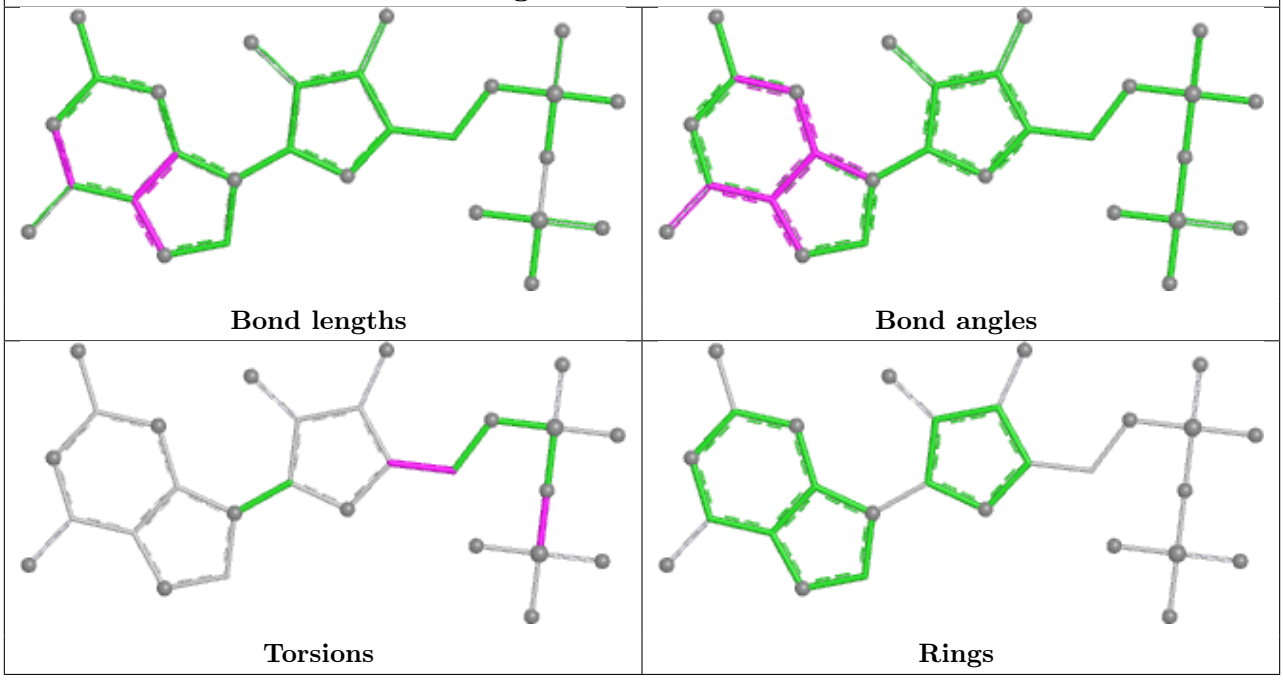


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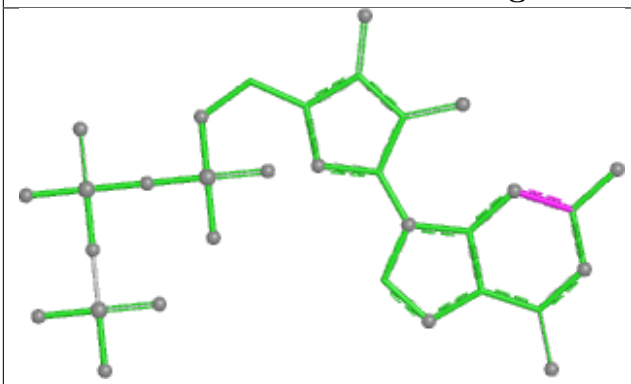
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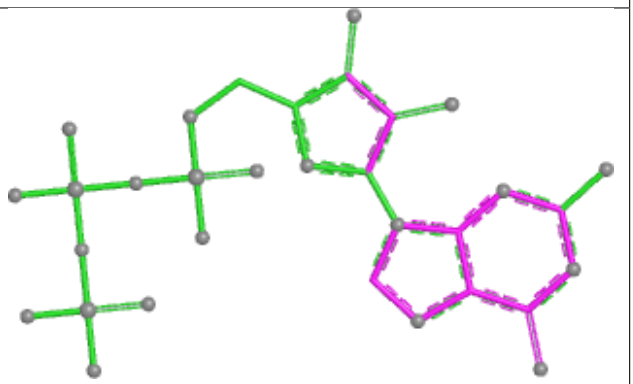
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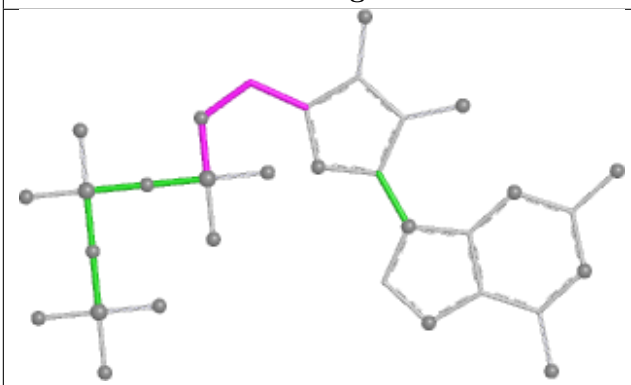
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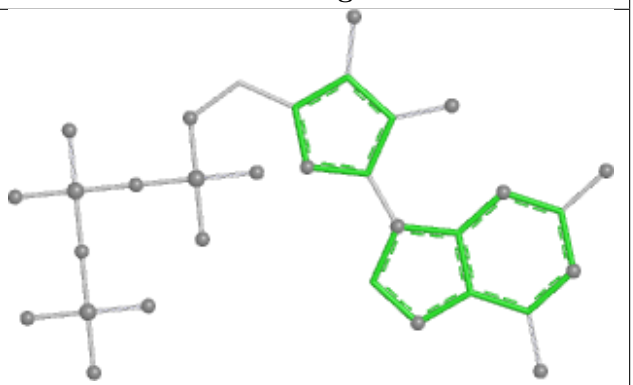
Bond lengths



Bond angles

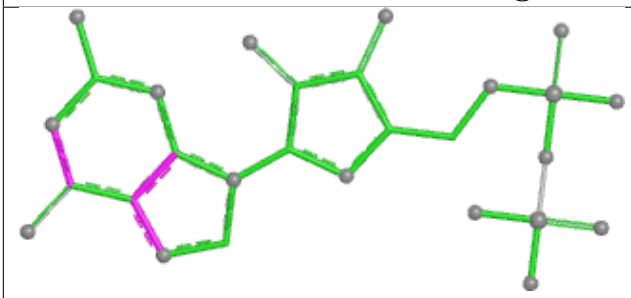


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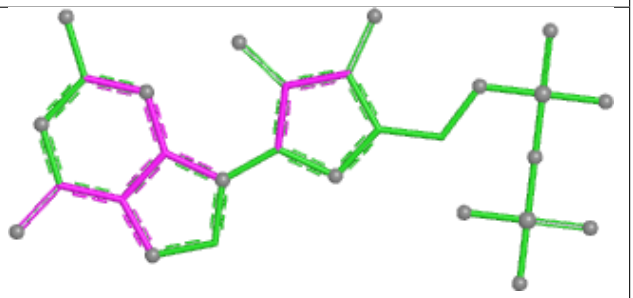


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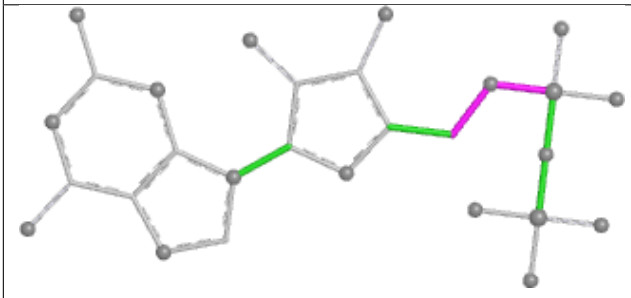
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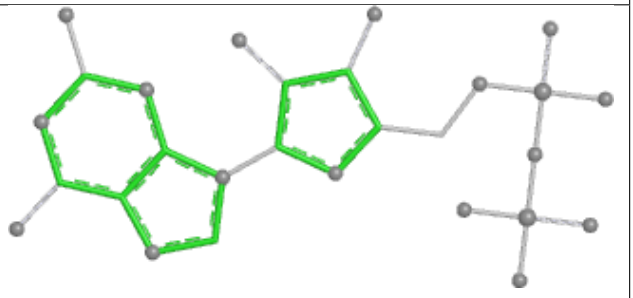
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Bond angles

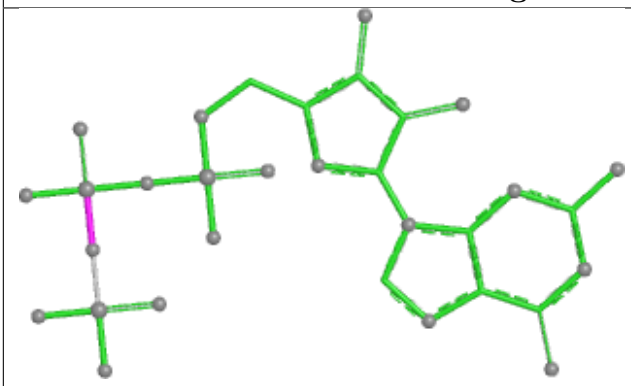


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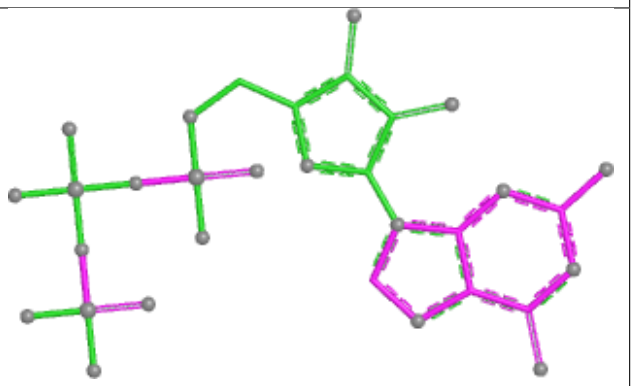


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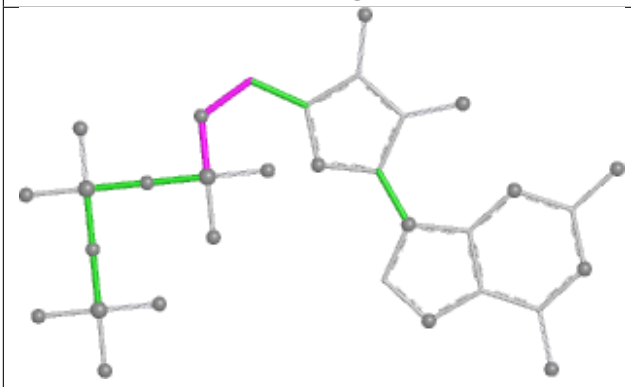
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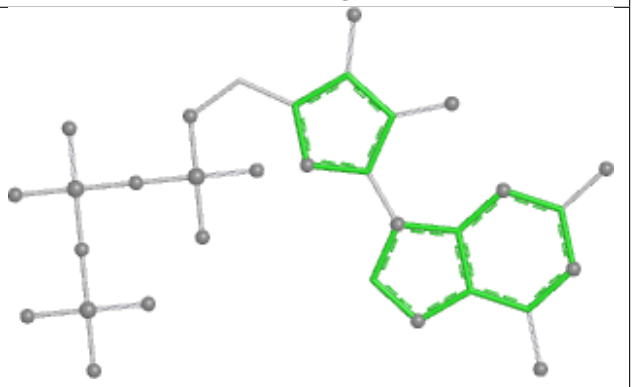
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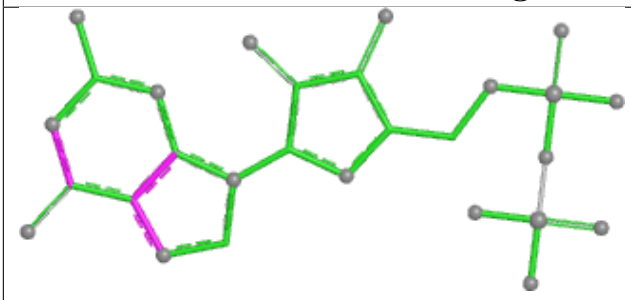


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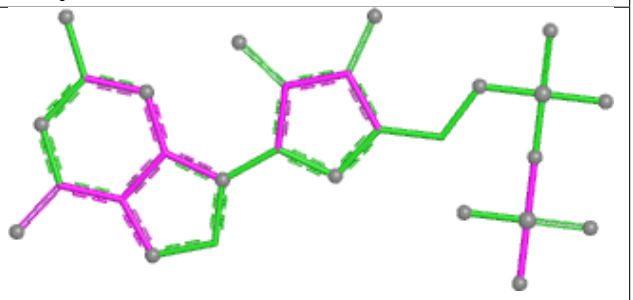


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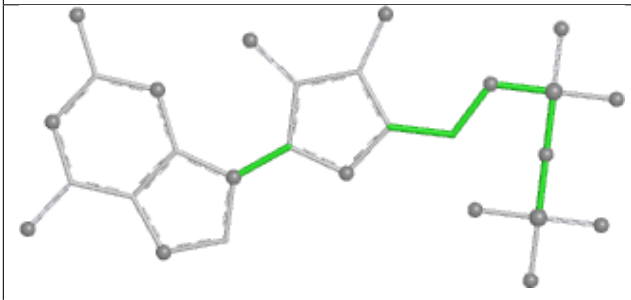
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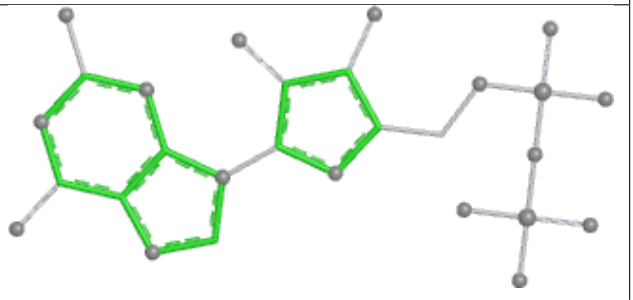
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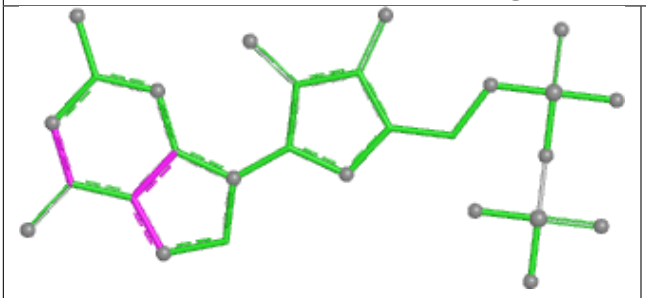


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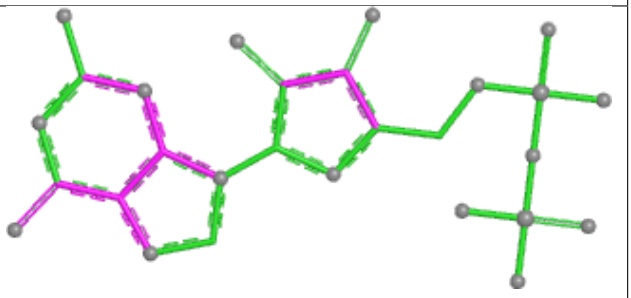


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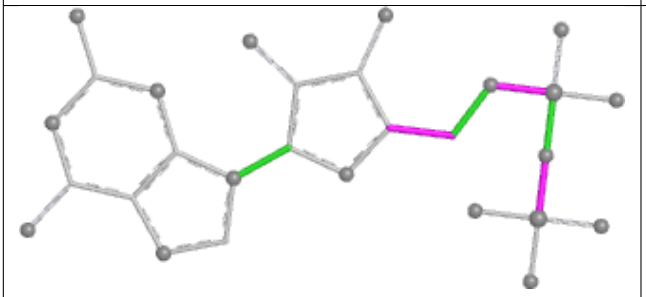
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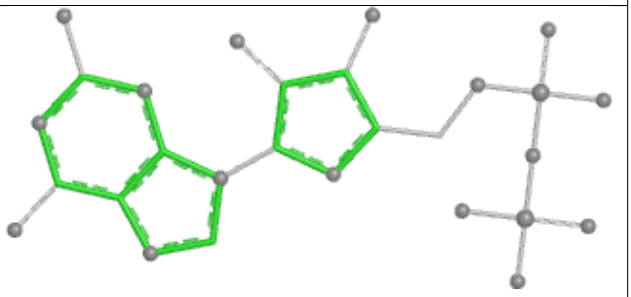
Bond lengths



Bond angles

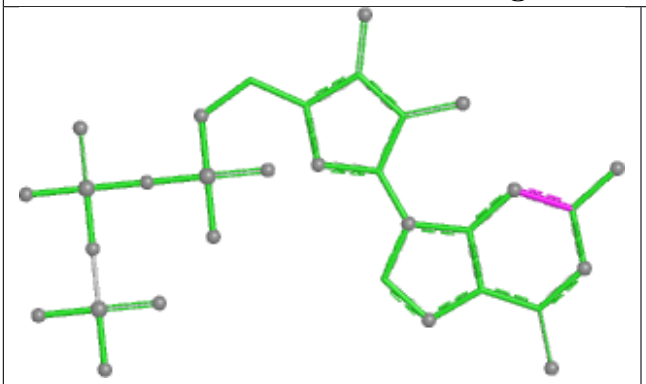


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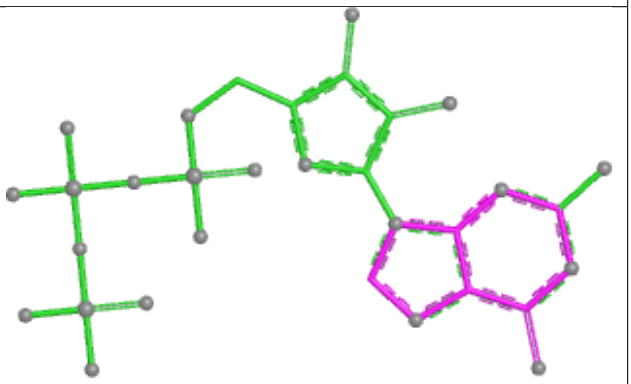


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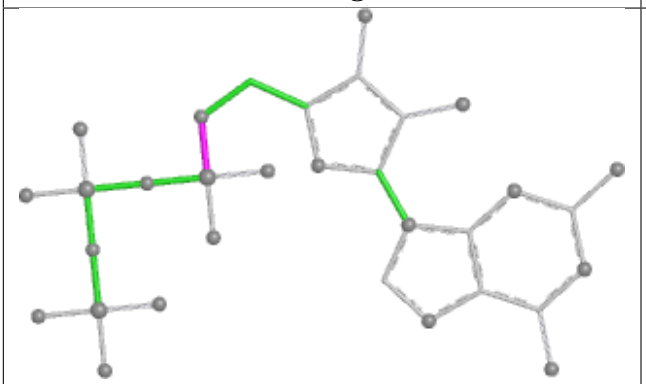
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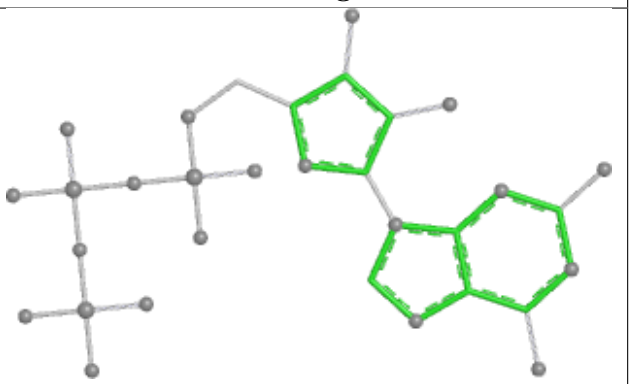
Bond lengths



Bond angles

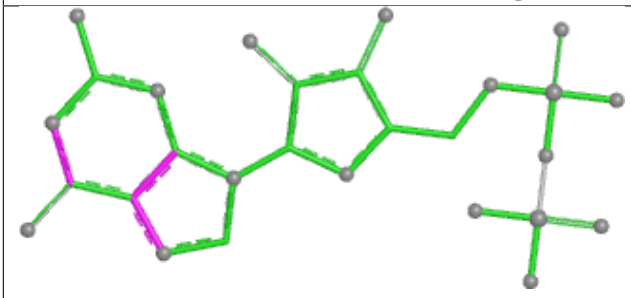


Torsions

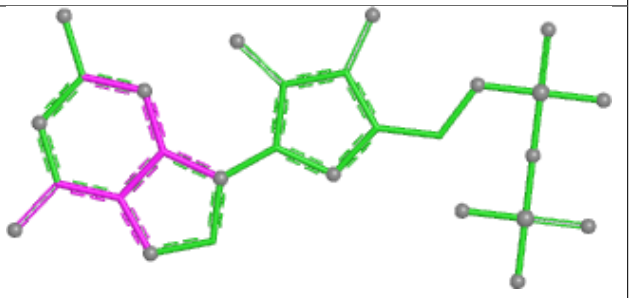


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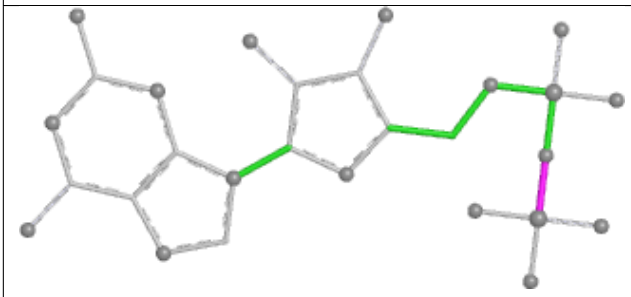
Ligand GDP KL 501



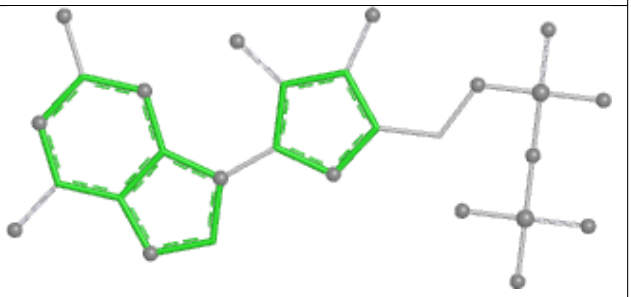
Bond lengths



Bond angles

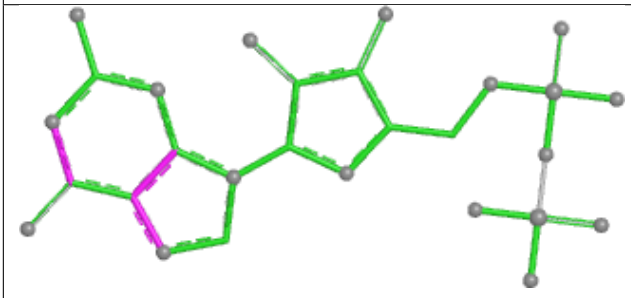


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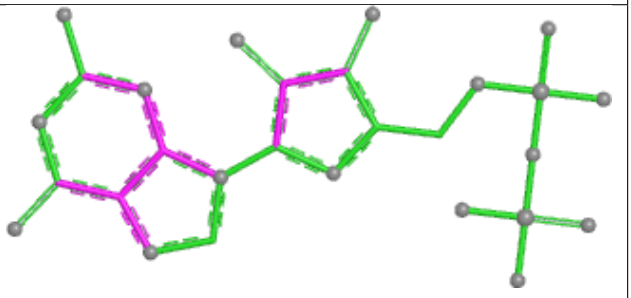


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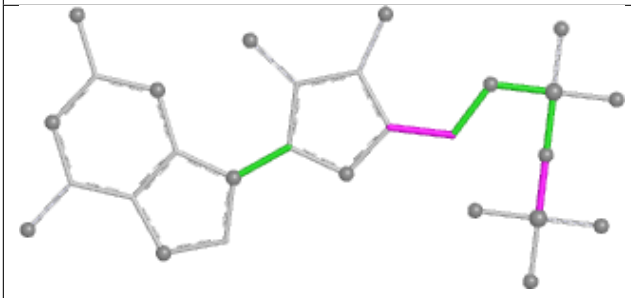
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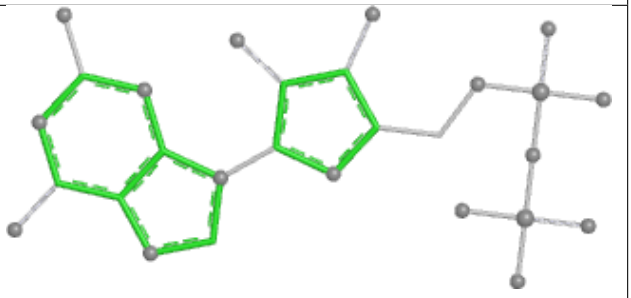
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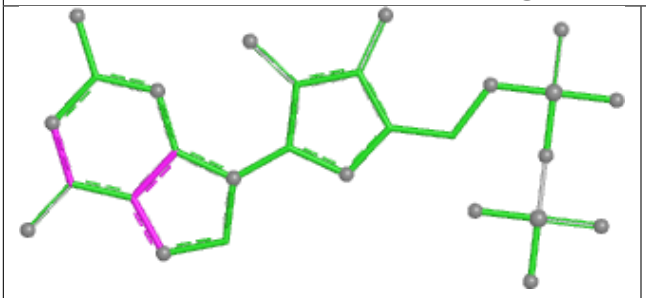


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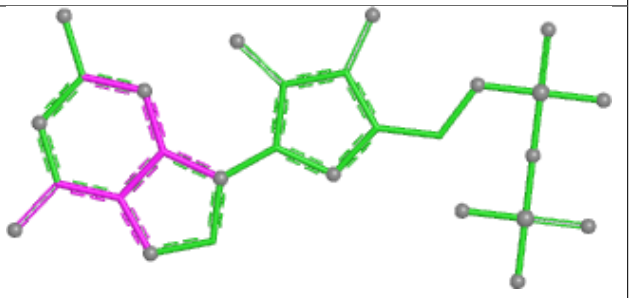


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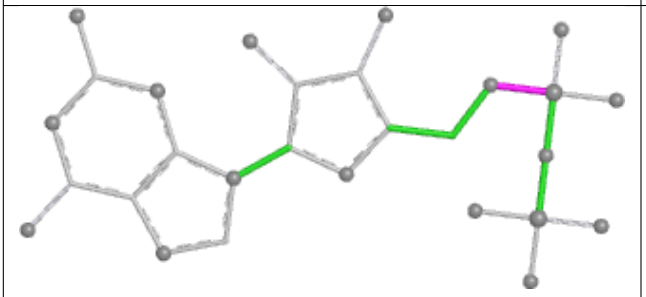
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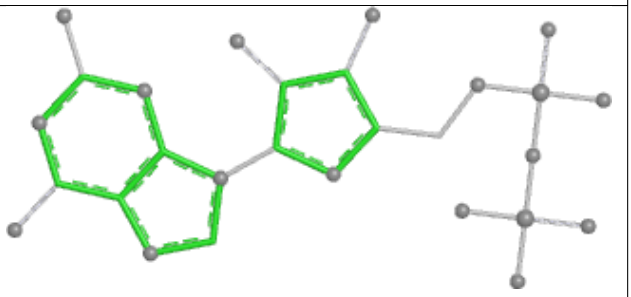
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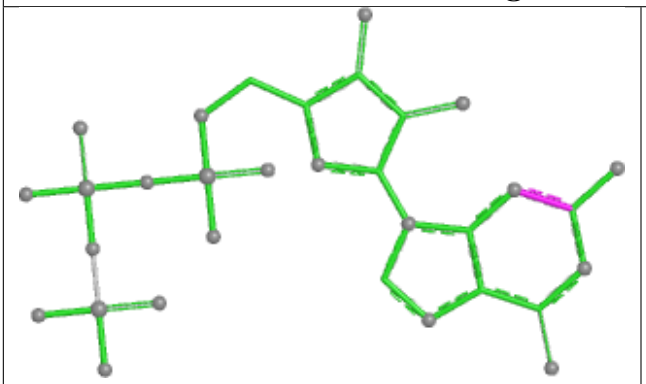


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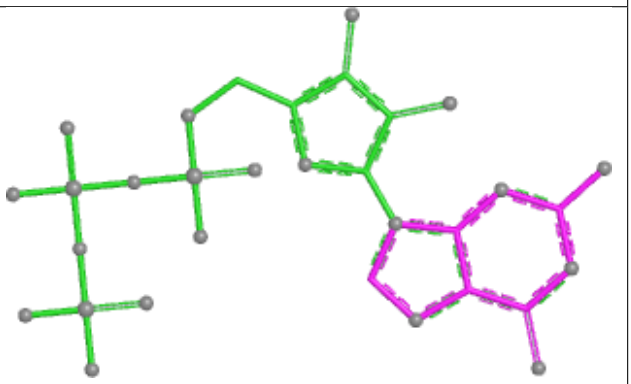


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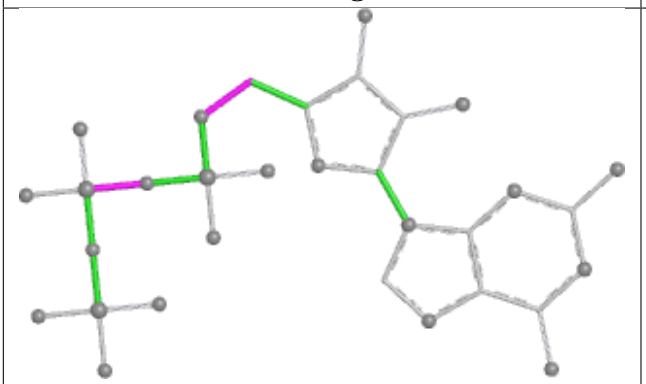
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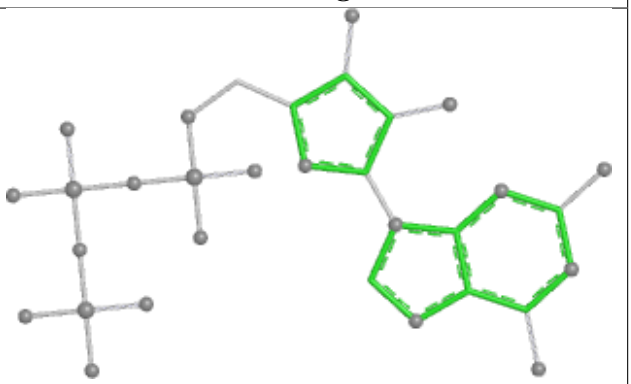
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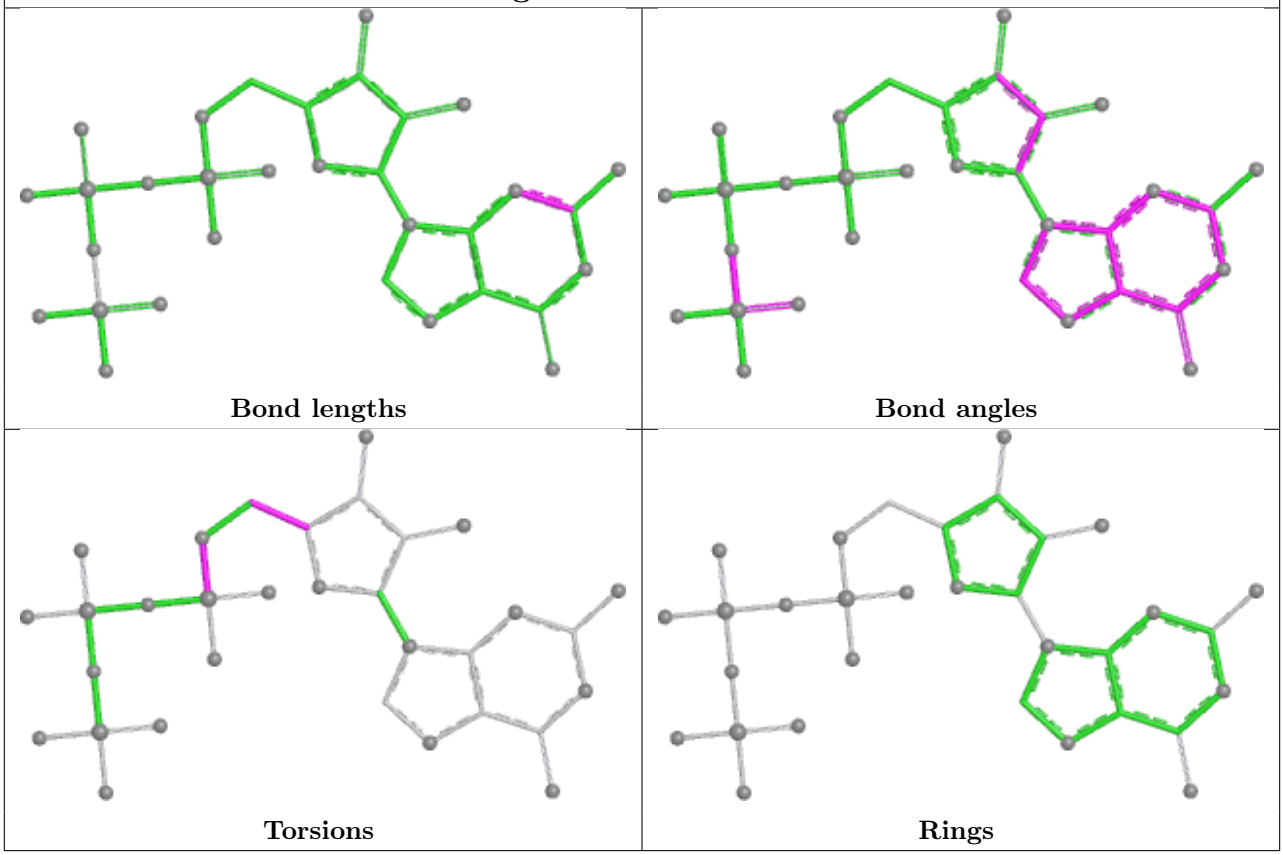


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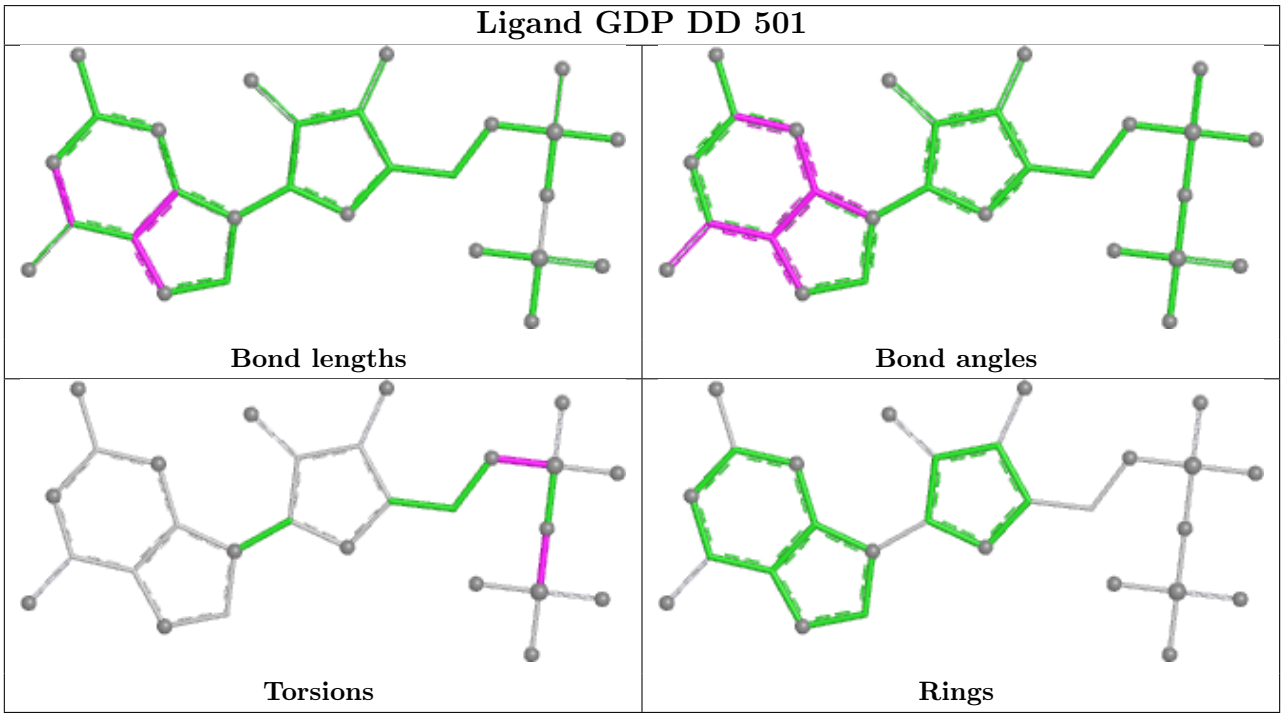


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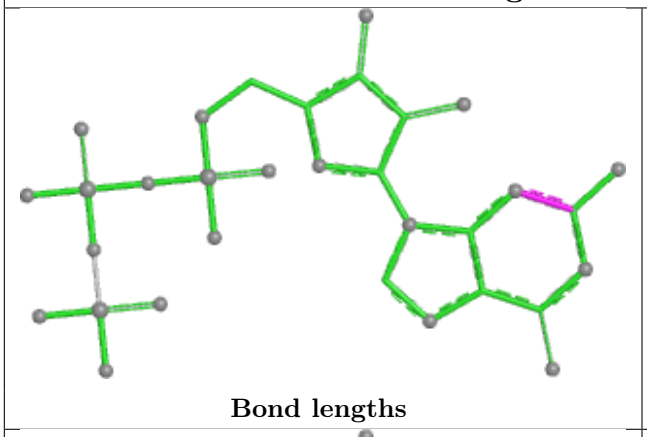
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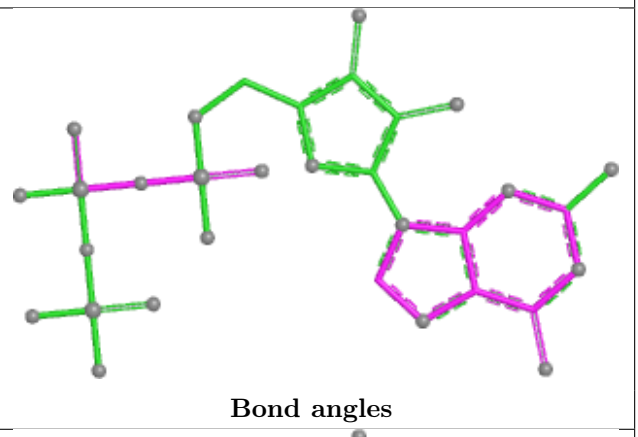
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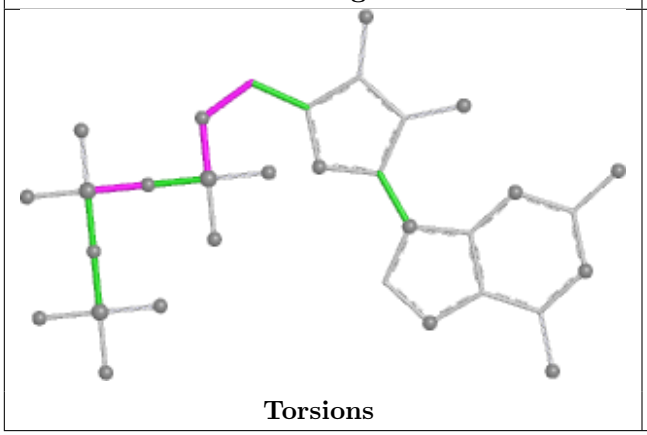
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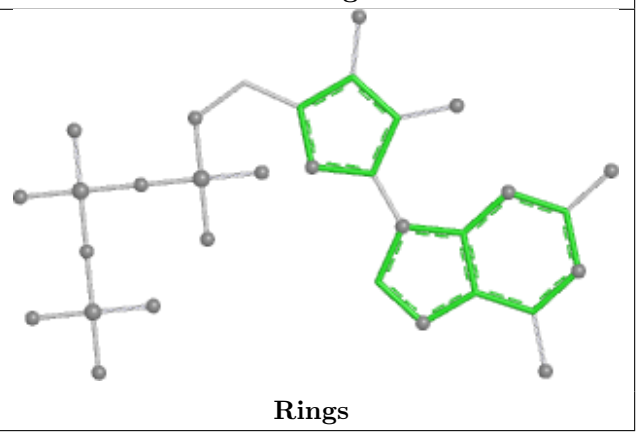
Bond lengths



Bond angles

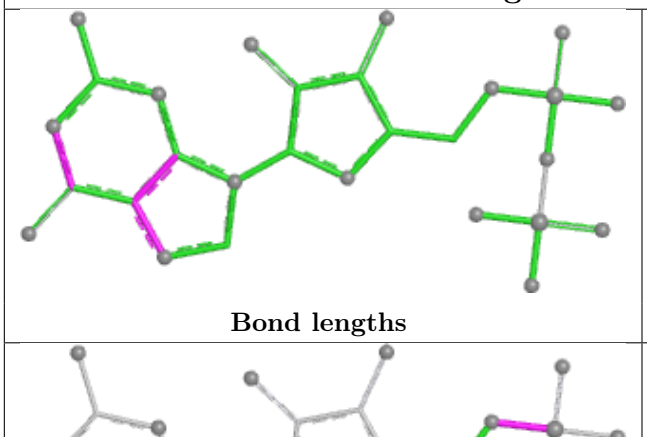


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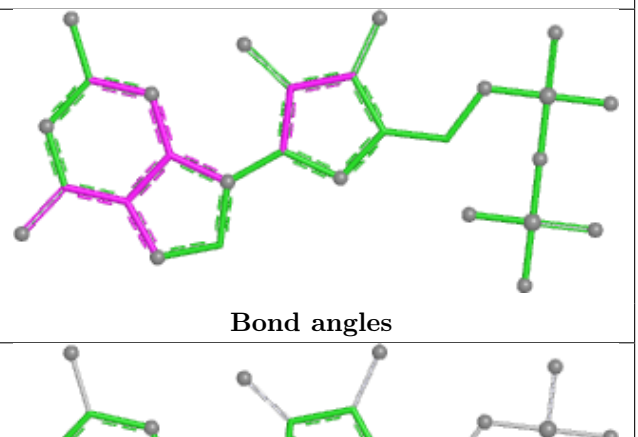


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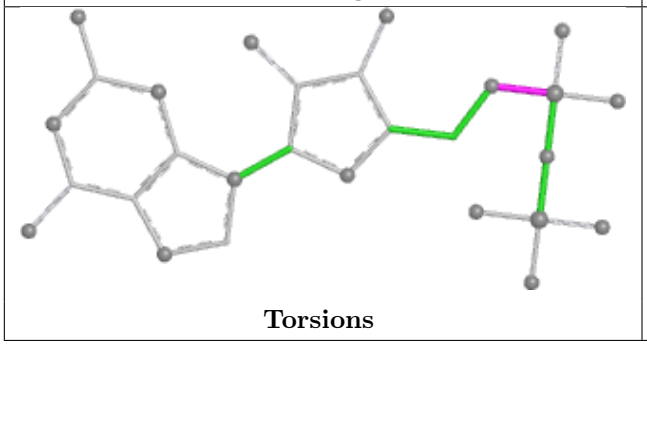
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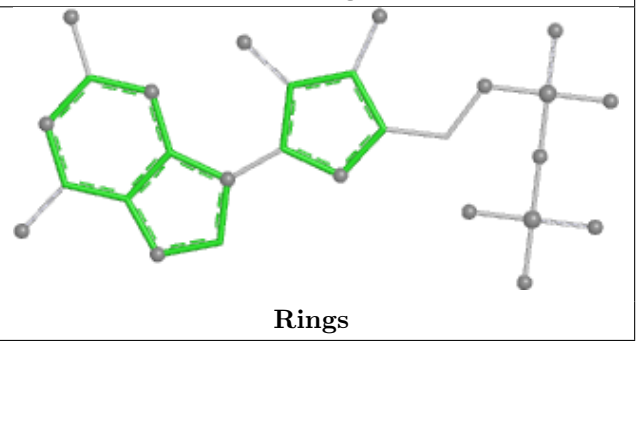
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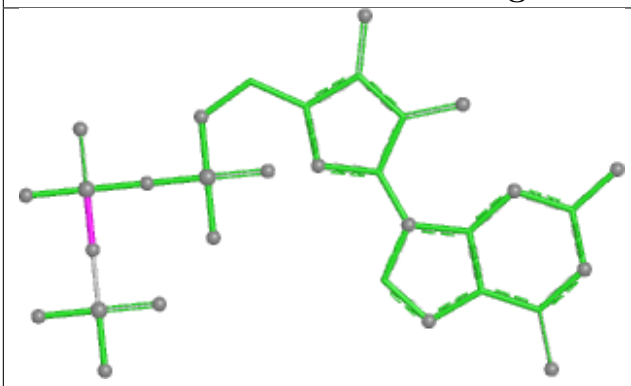


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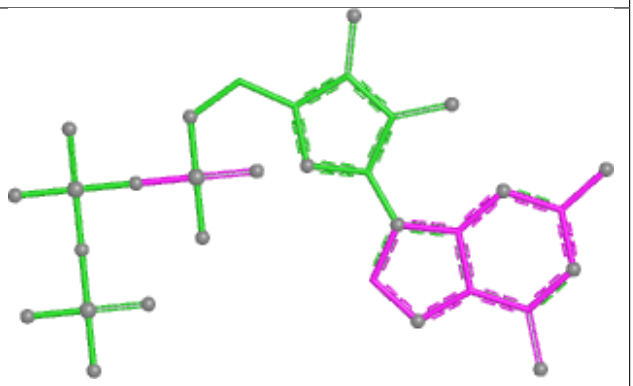


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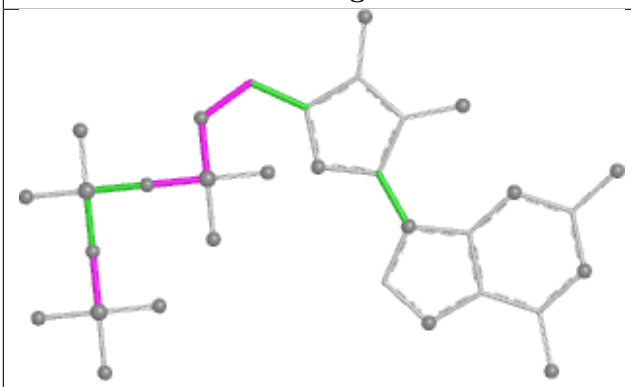
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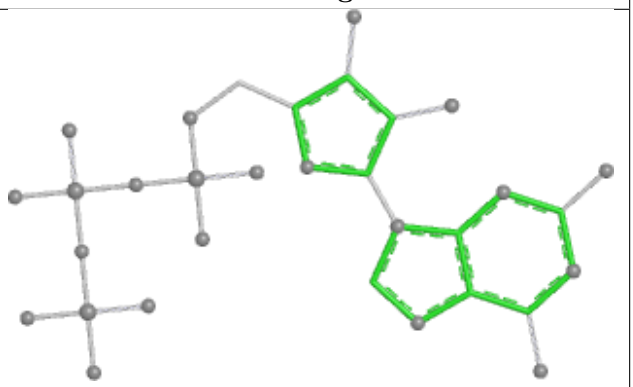
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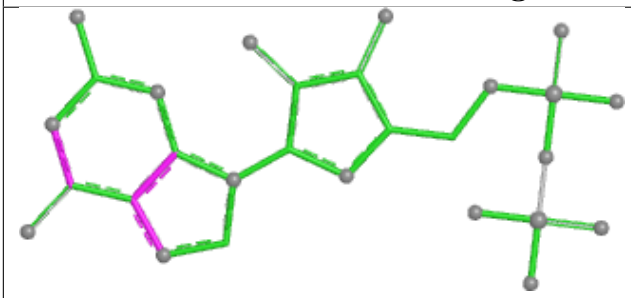


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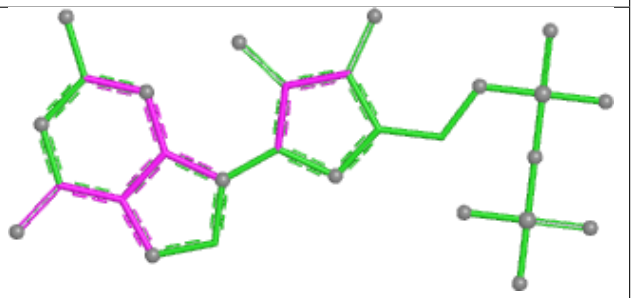


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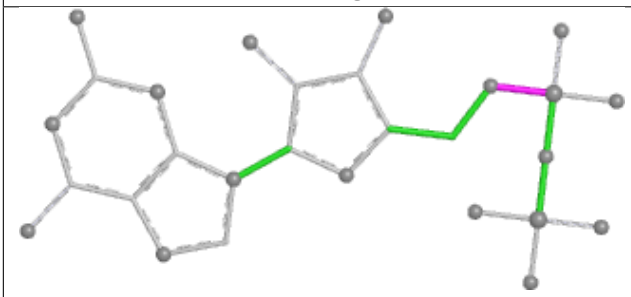
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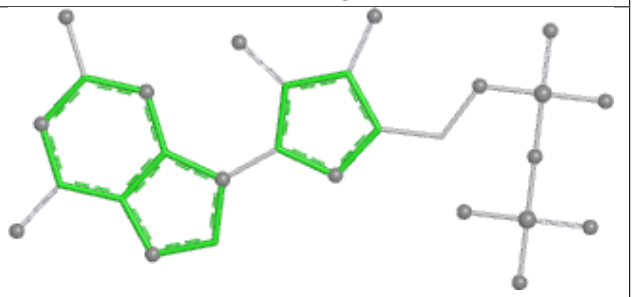
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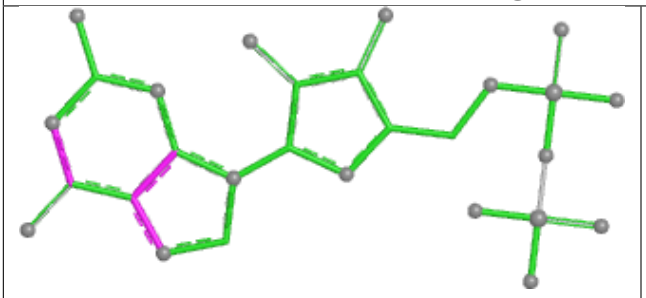


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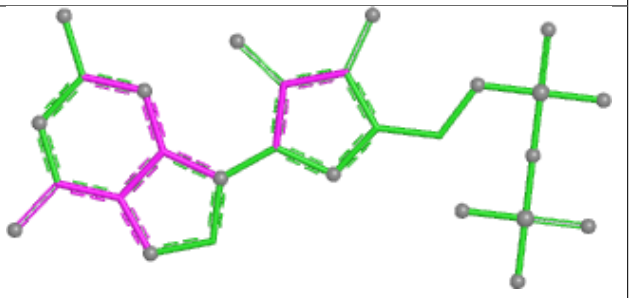


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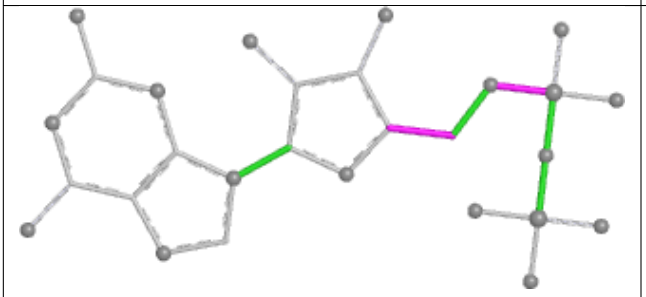
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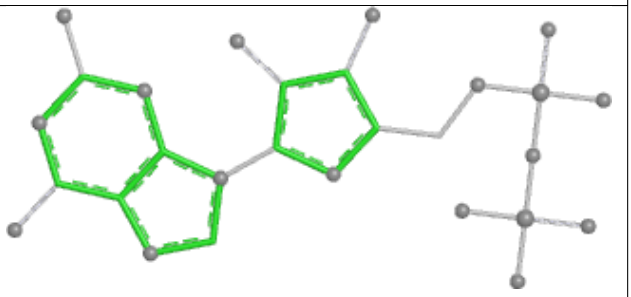
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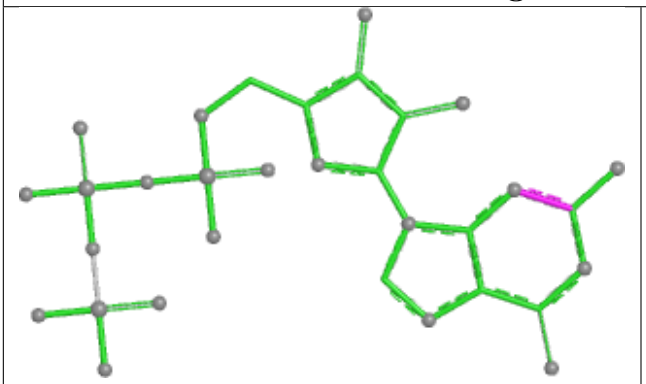


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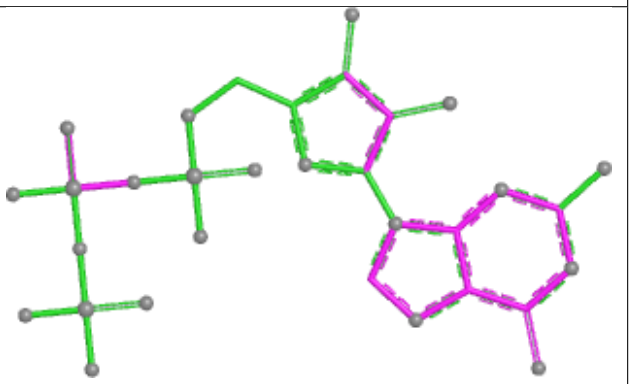


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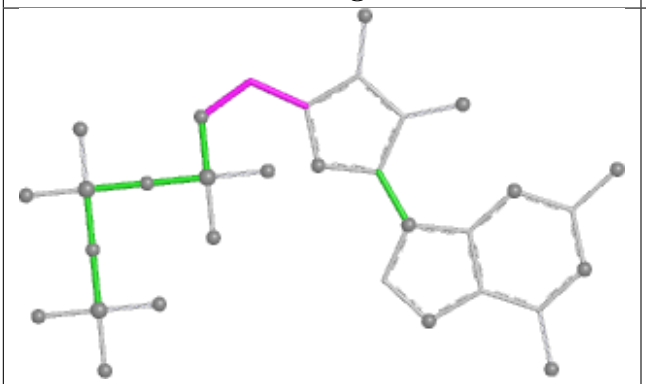
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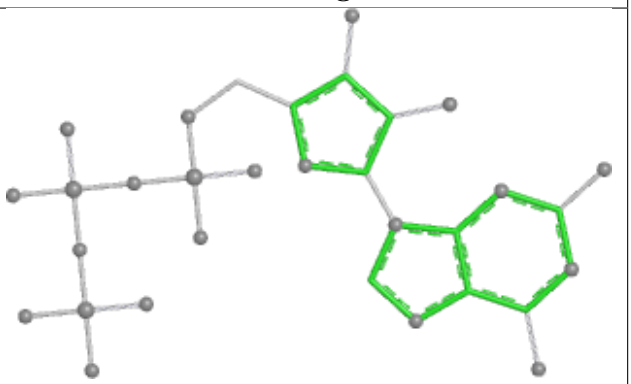
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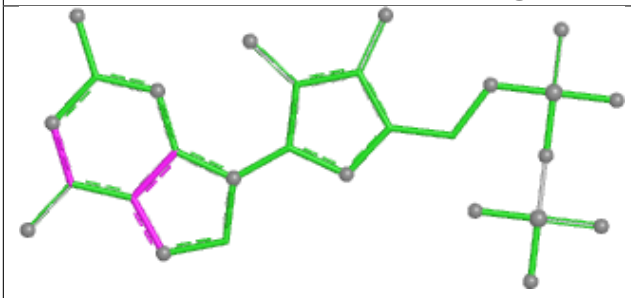


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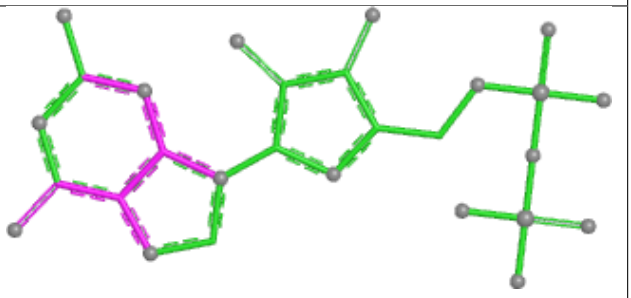


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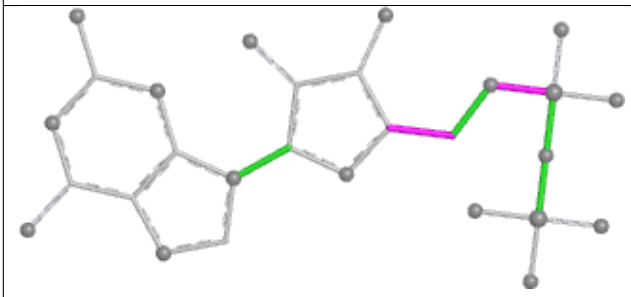
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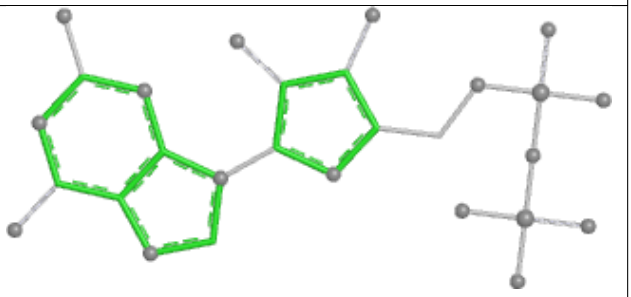
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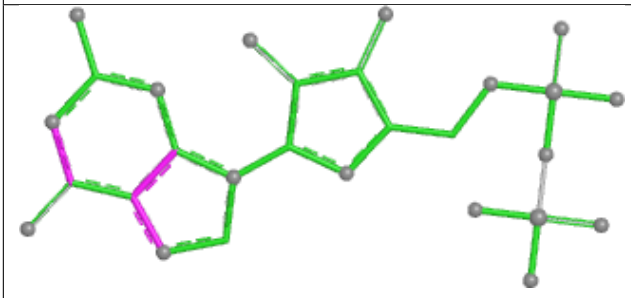


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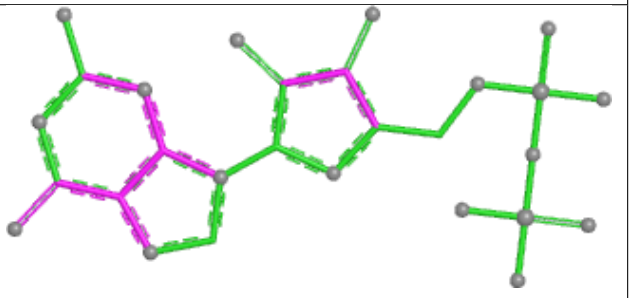


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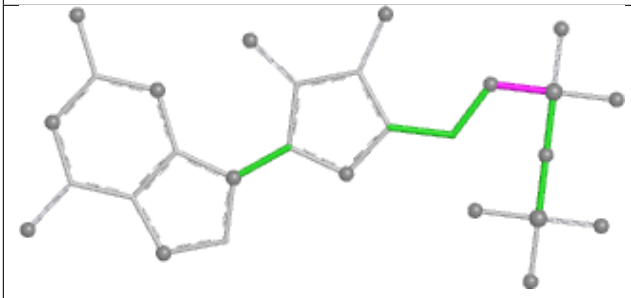
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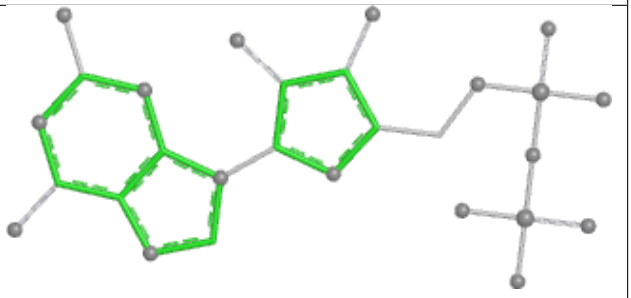
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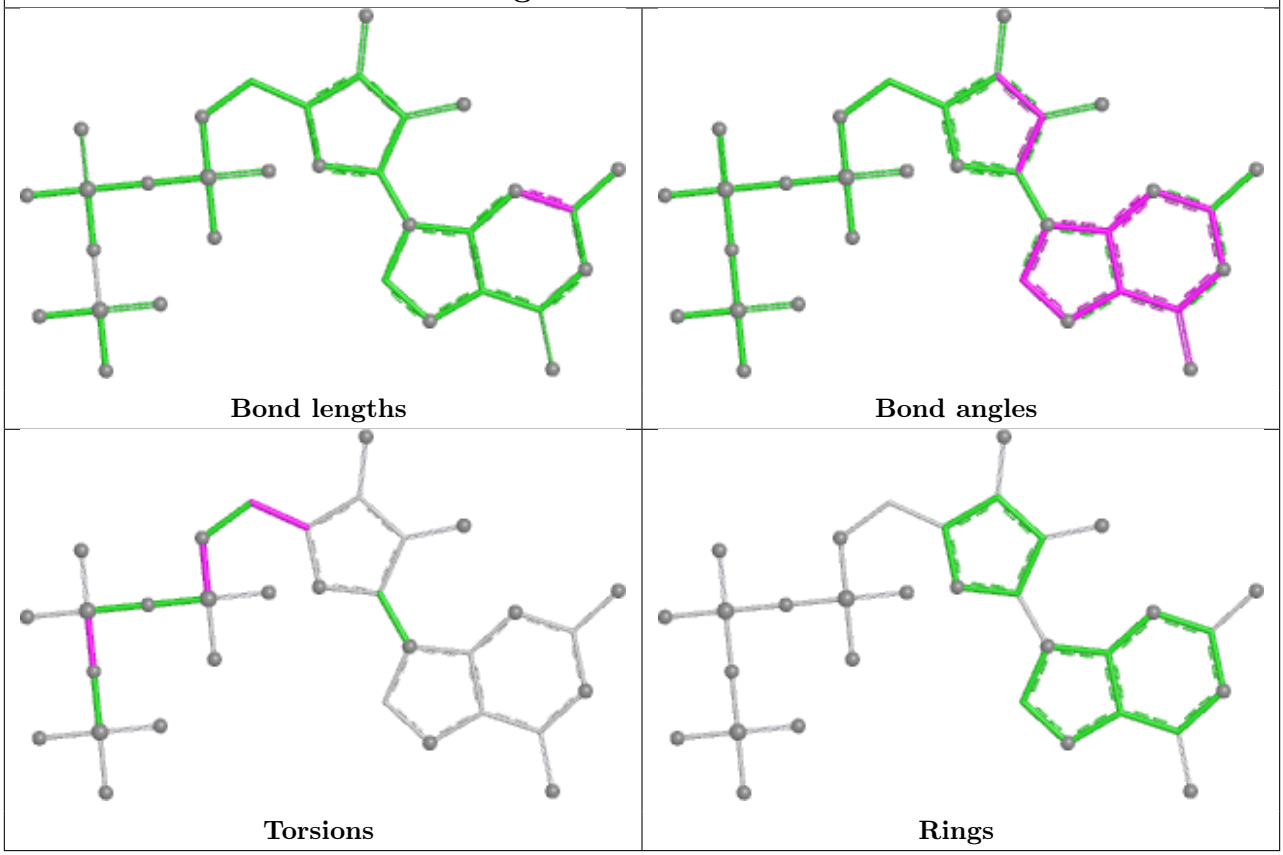


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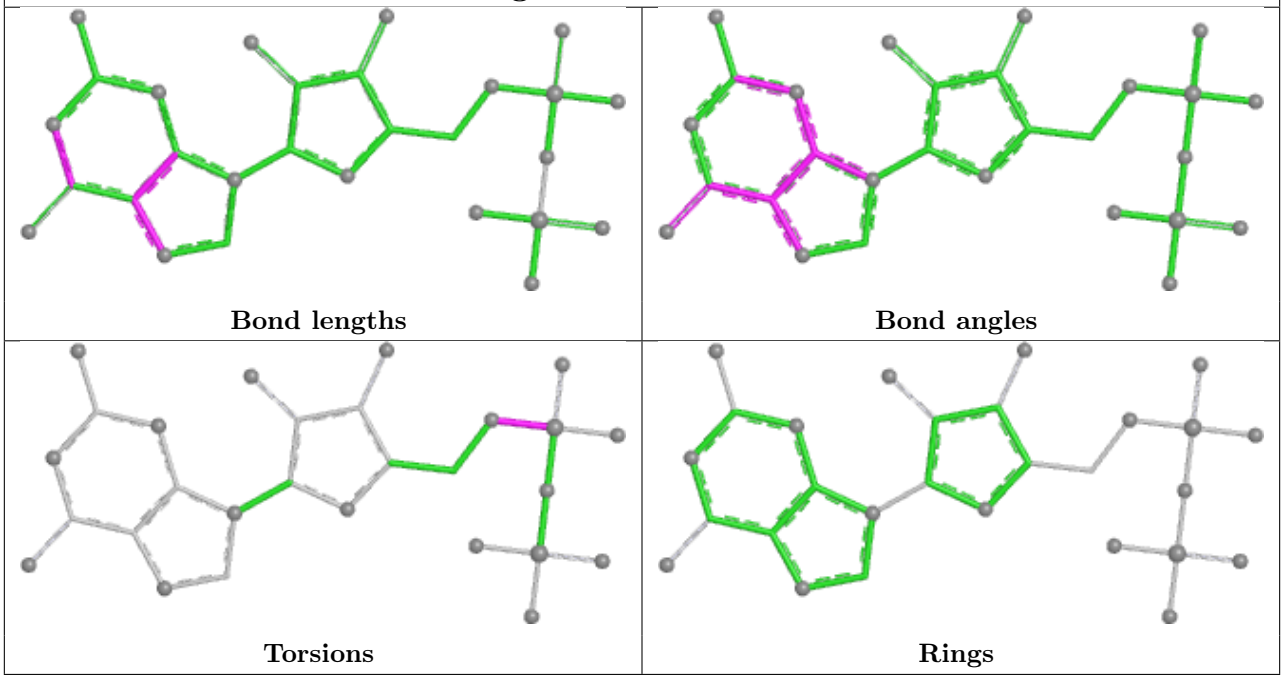


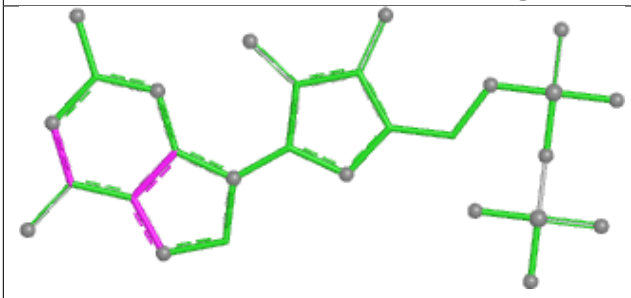
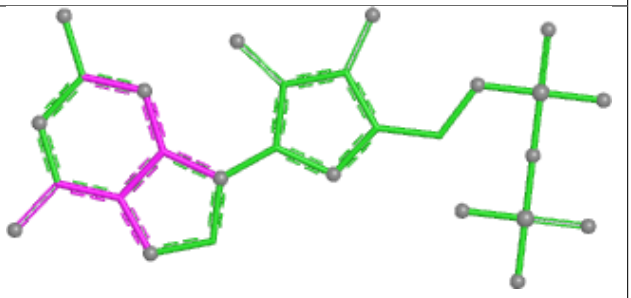
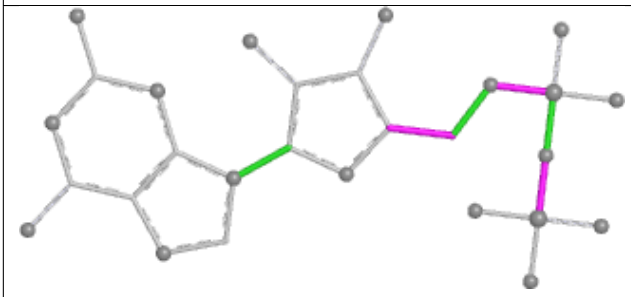
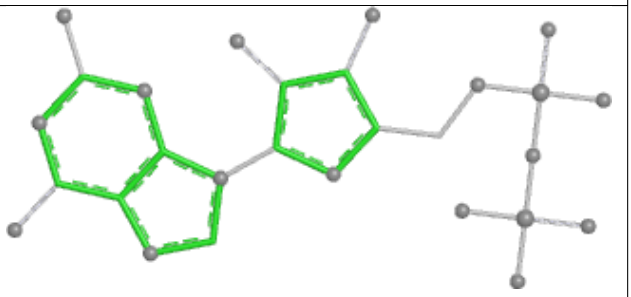
Rings

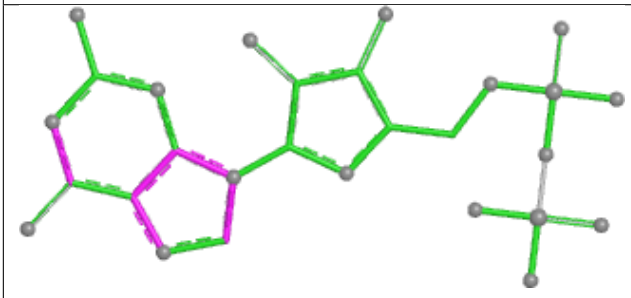
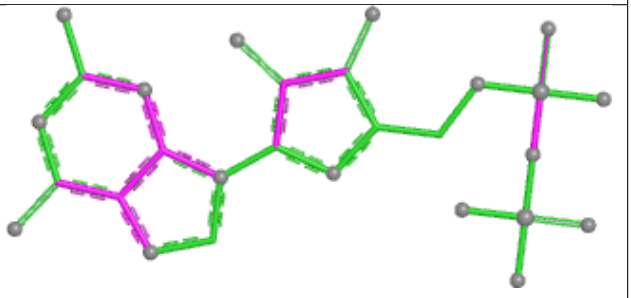
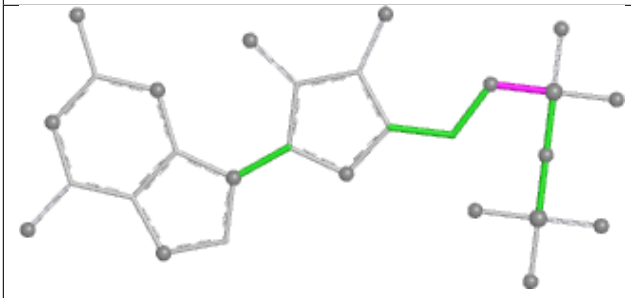
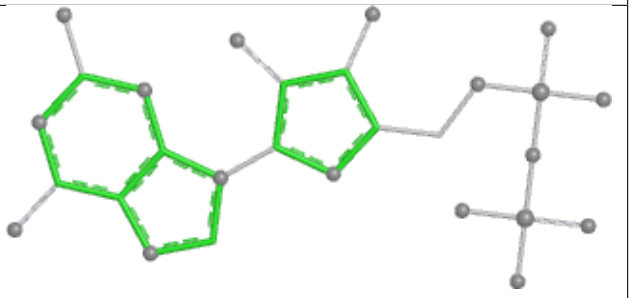
Ligand GTP FE 501



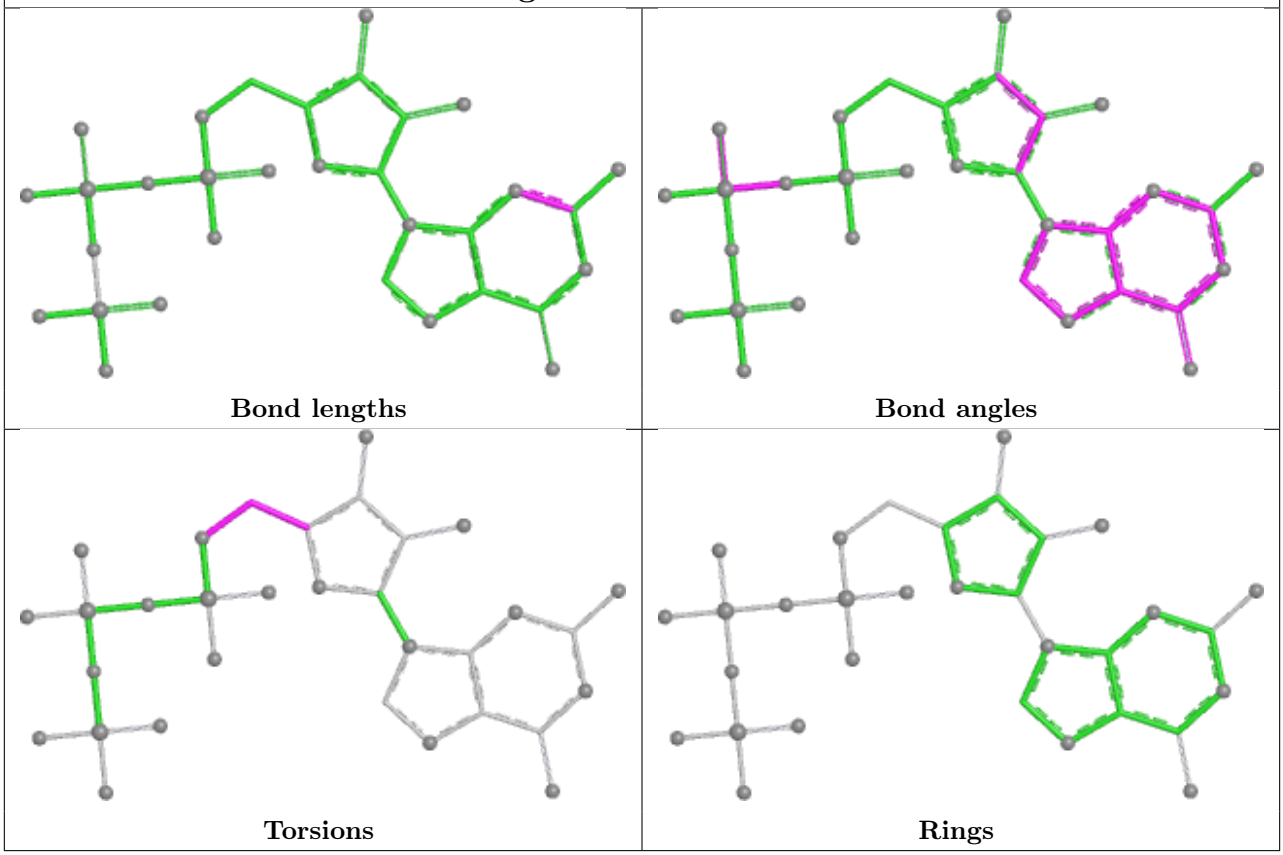
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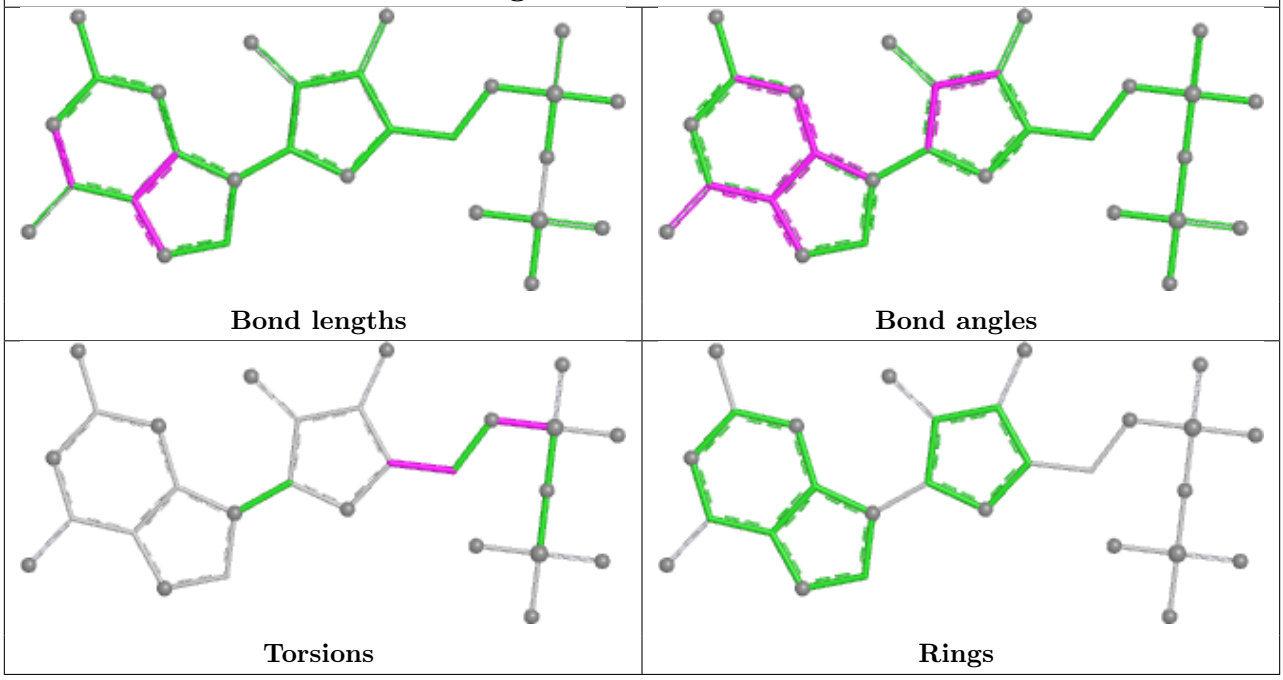
Ligand GDP JL 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP RJ 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

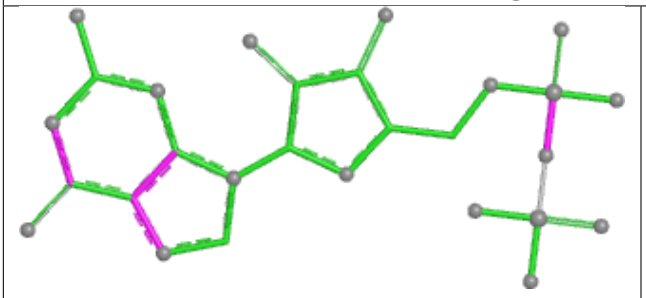
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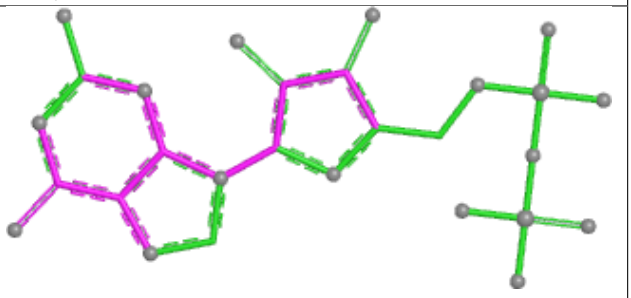
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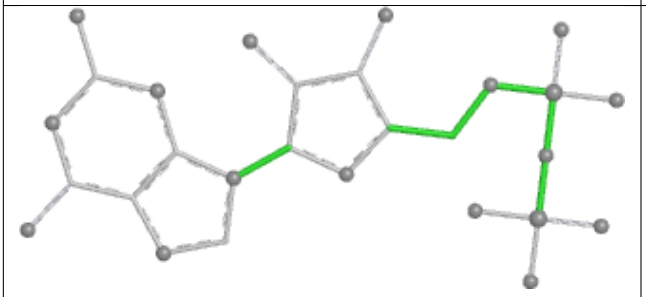
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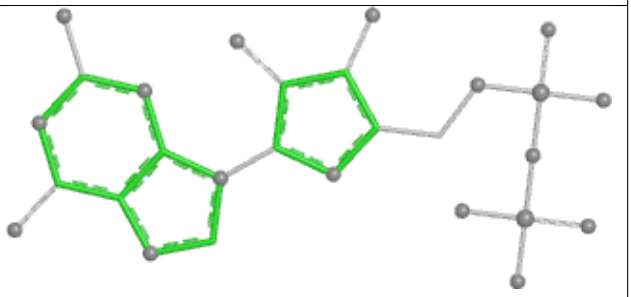
Bond lengths



Bond angles

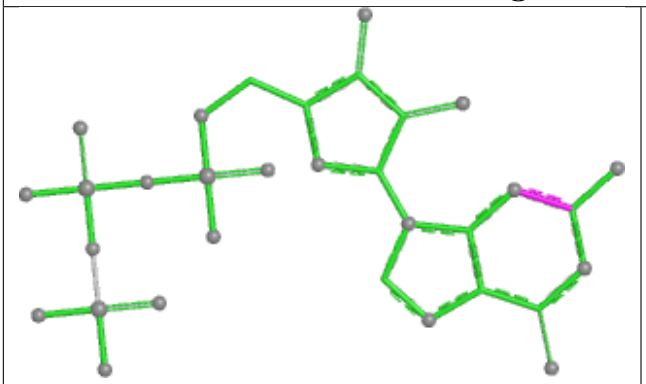


Torsions

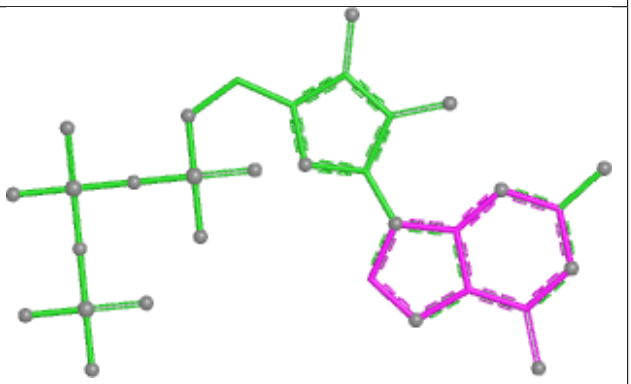


Rings

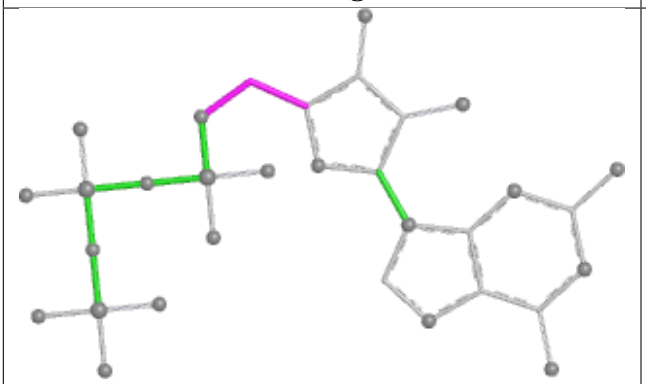
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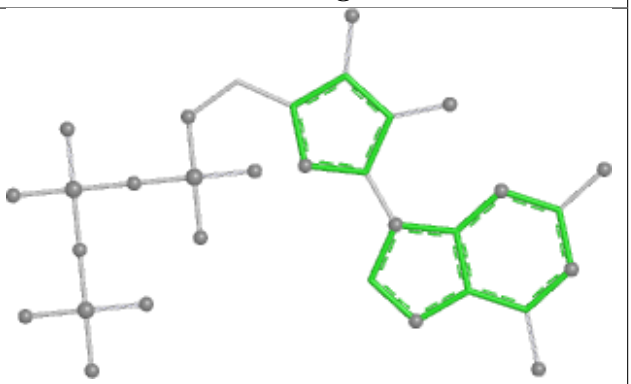
Bond lengths



Bond angles

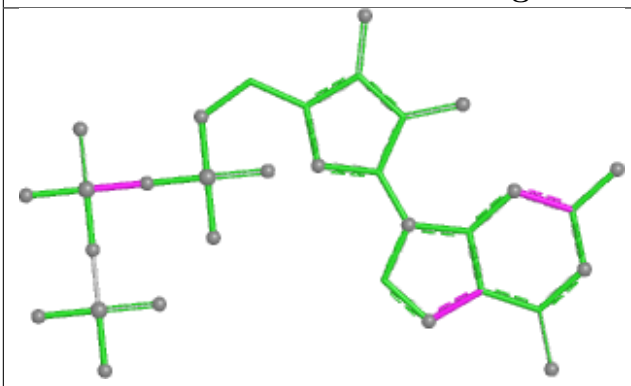


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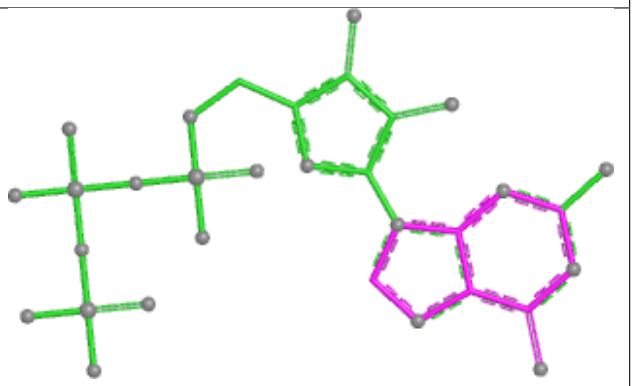


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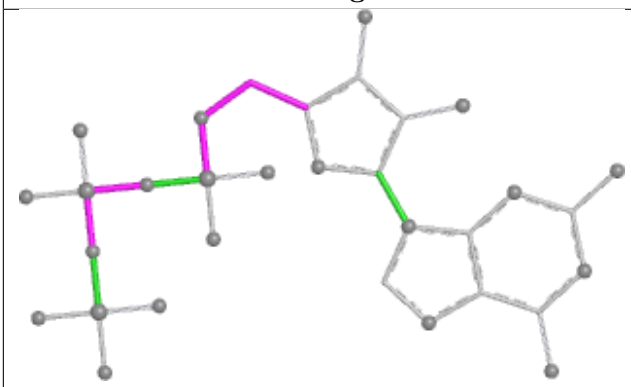
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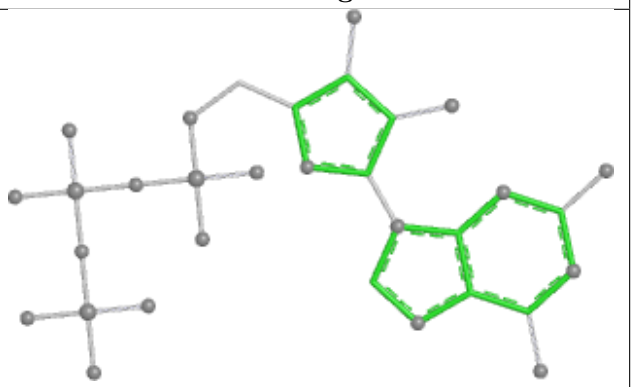
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Bond angles

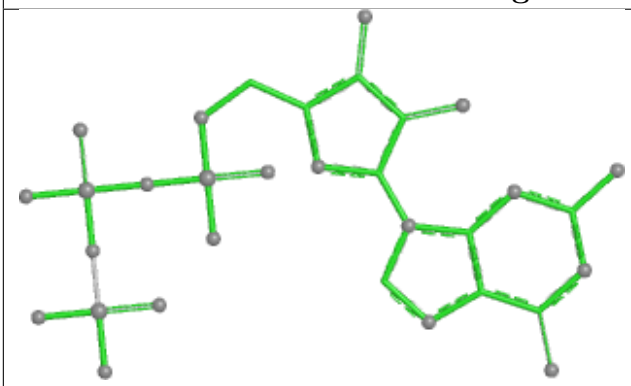


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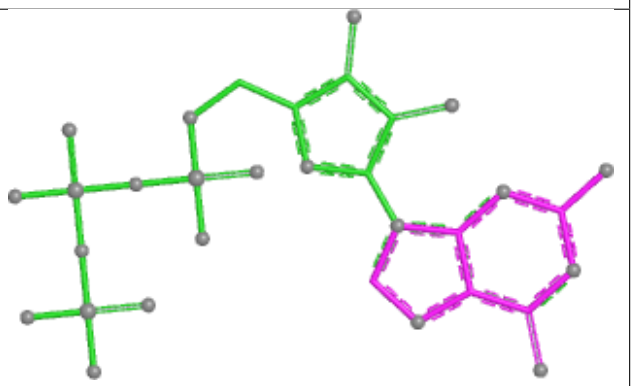


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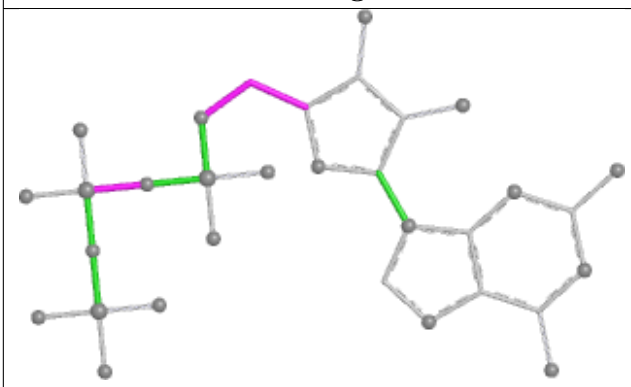
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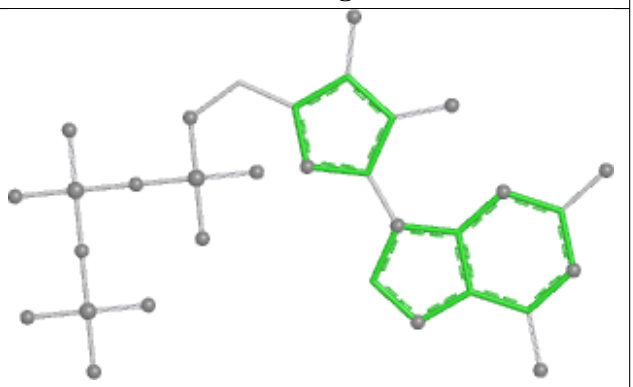
Bond lengths



Bond angles

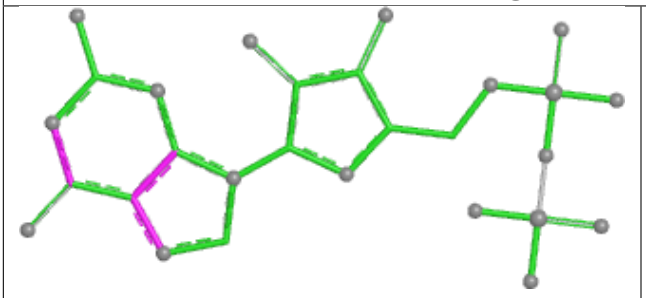


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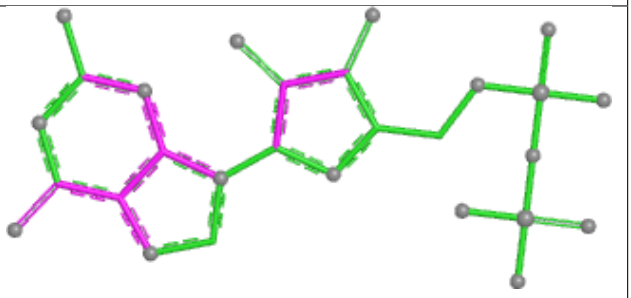


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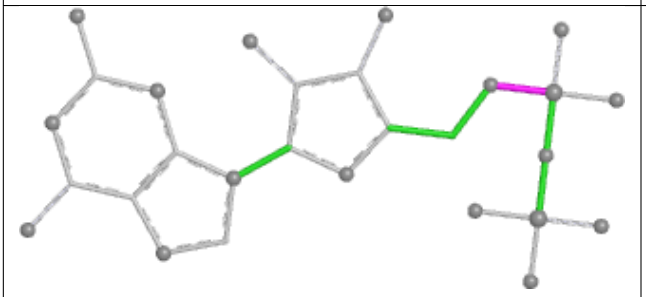
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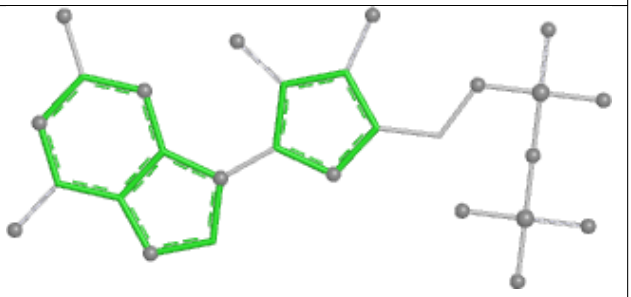
Bond lengths



Bond angles

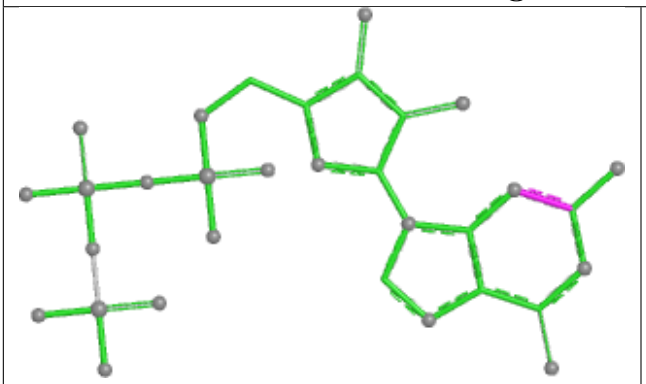


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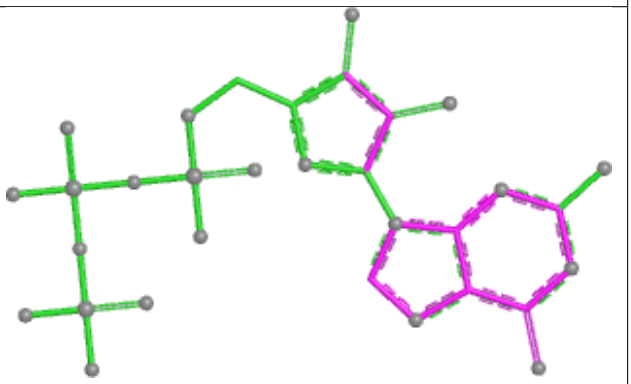


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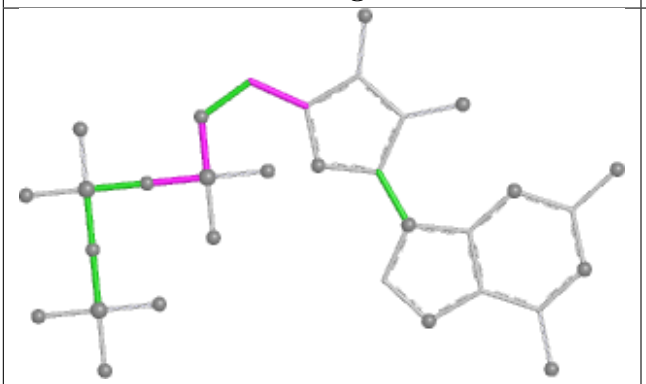
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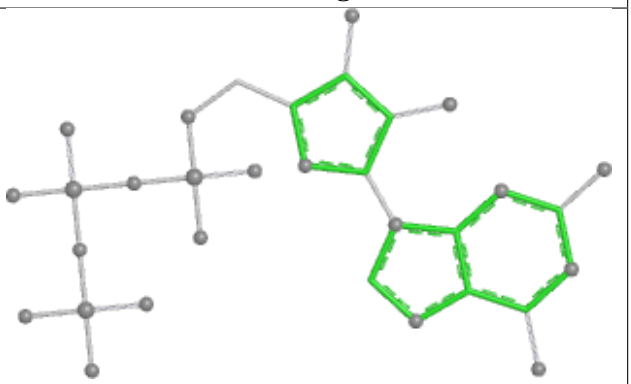
Bond lengths



Bond angles

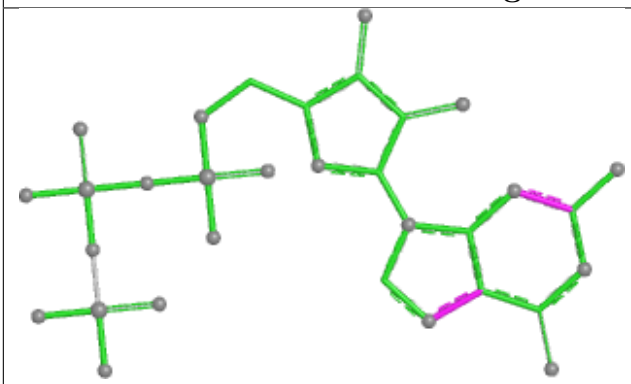


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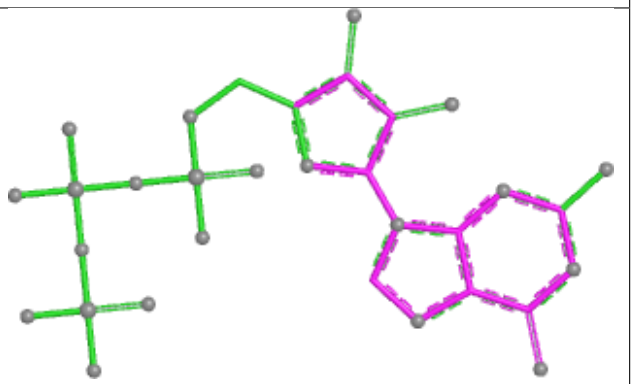


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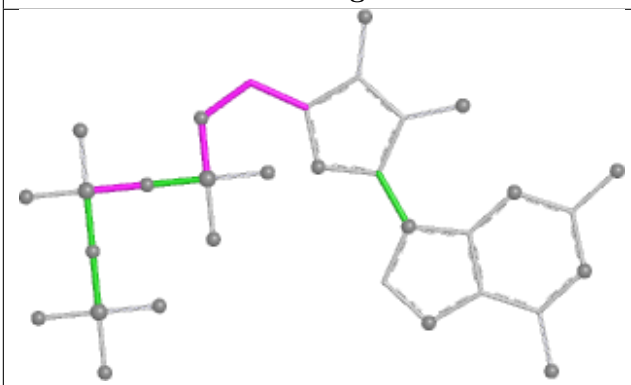
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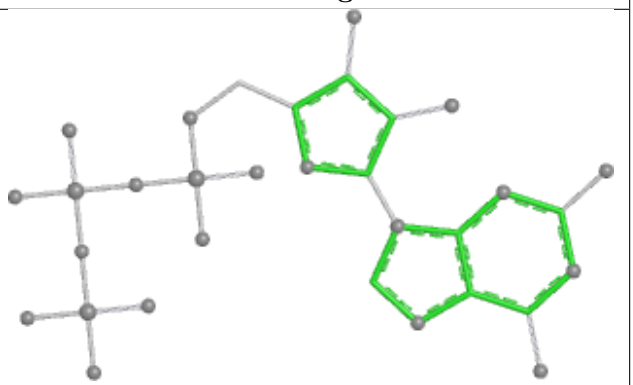
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Bond angles

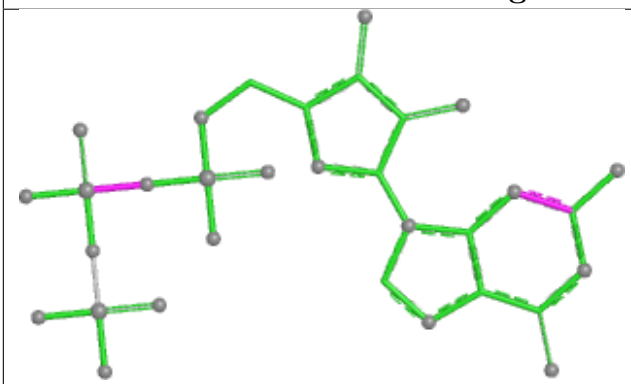


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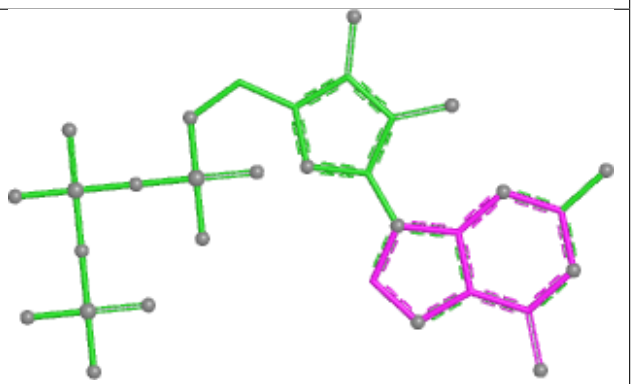


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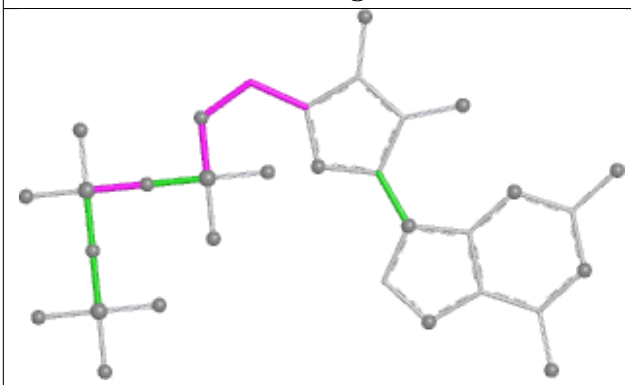
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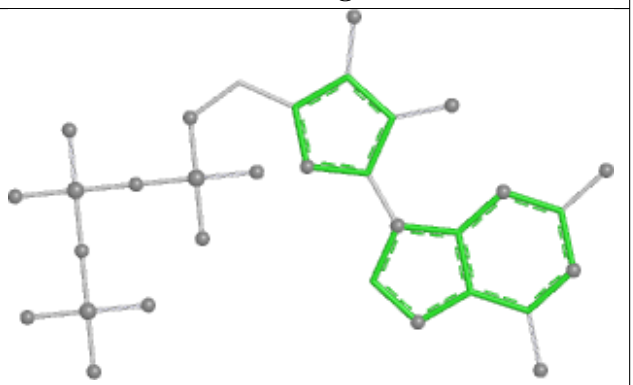
Bond lengths



Bond angles

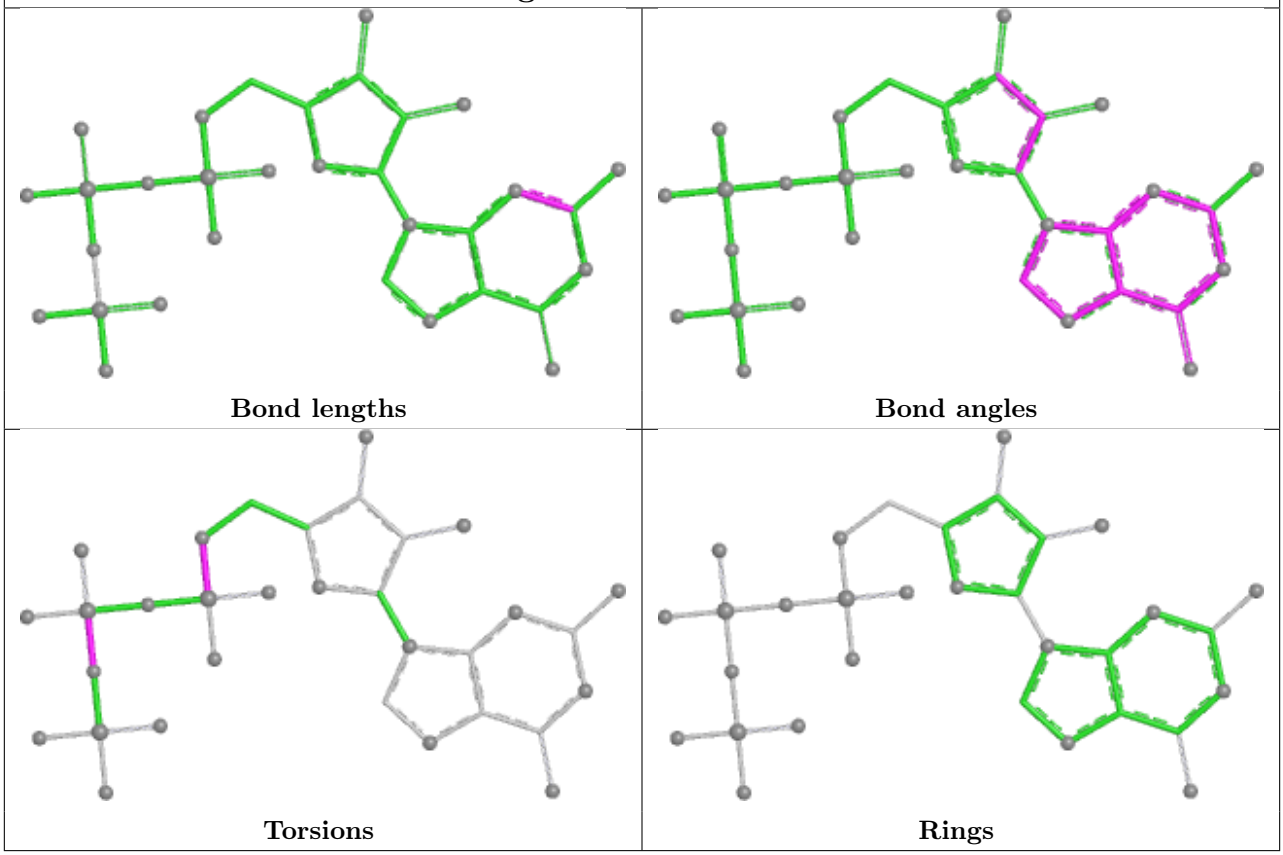


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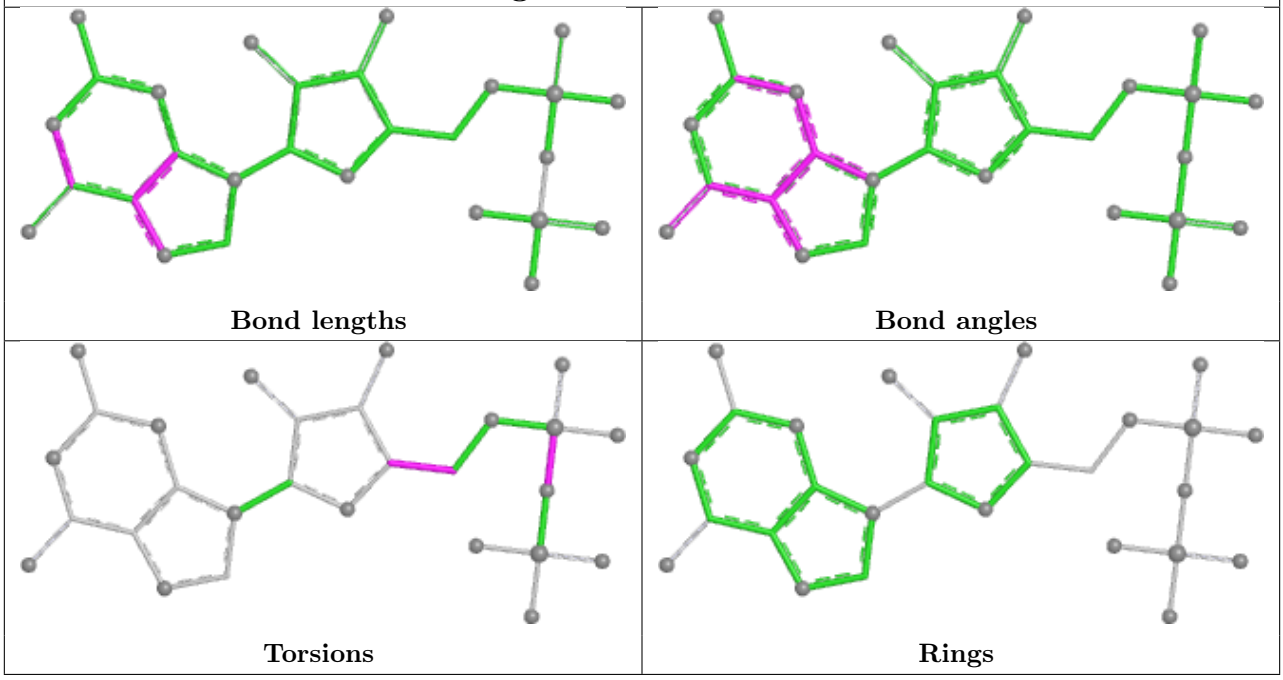


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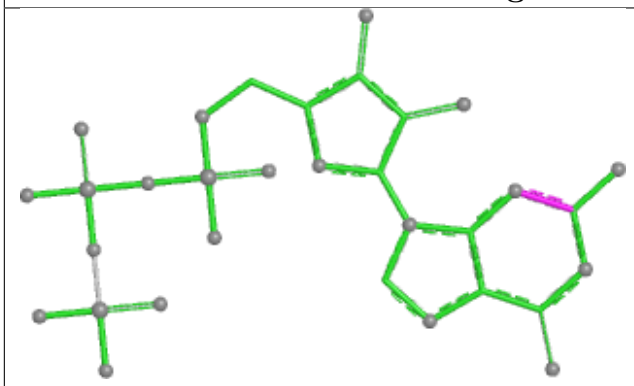
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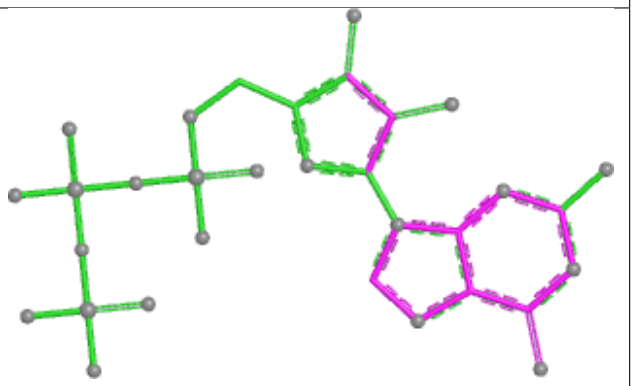
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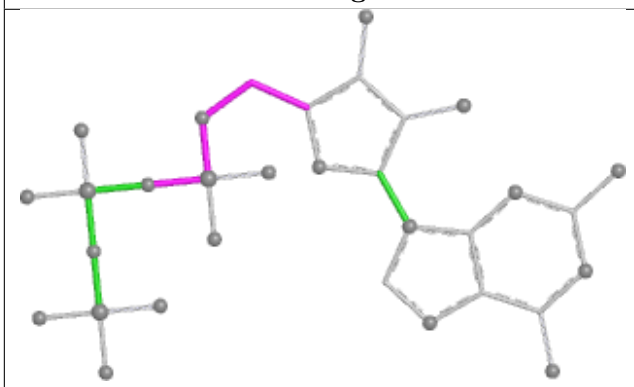
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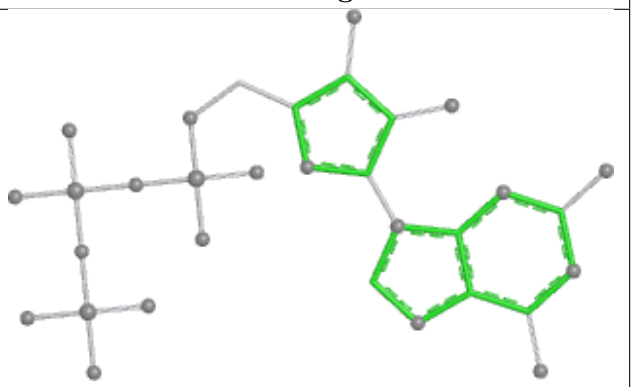
Bond lengths



Bond angles

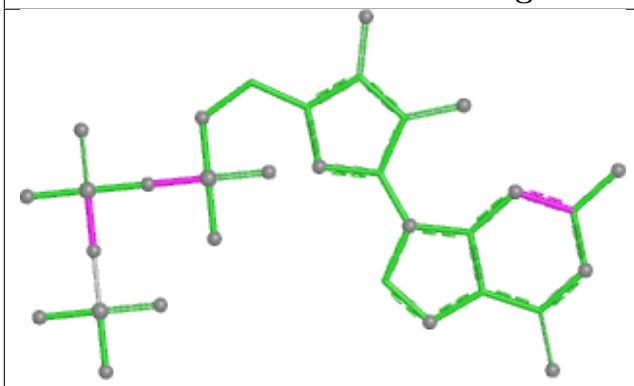


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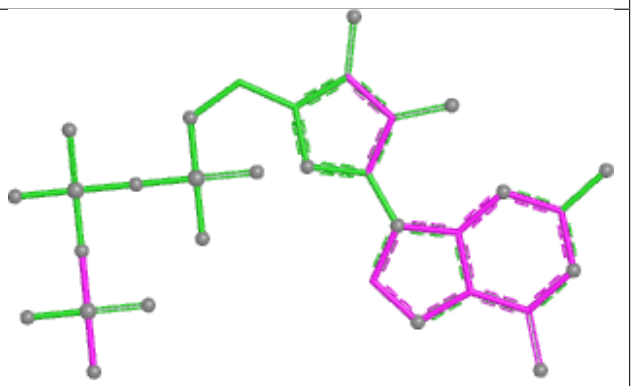


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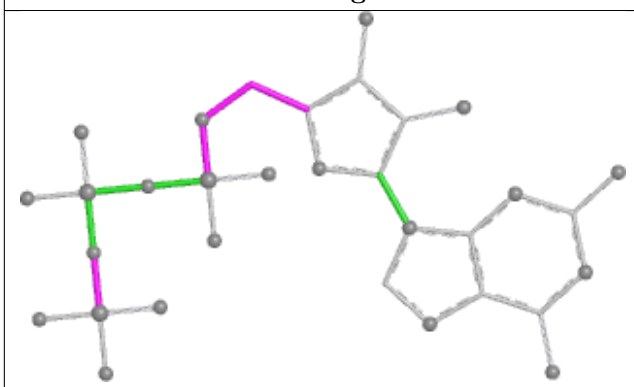
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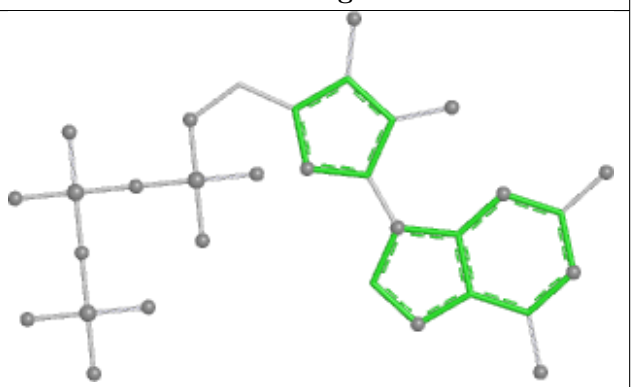
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Bond angles

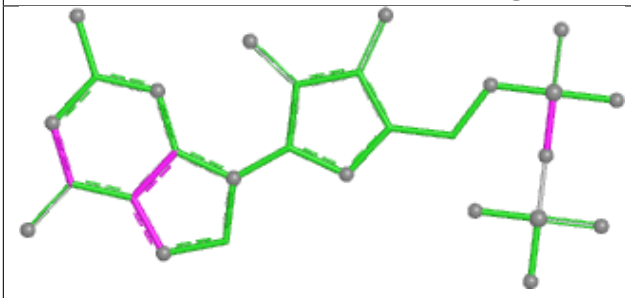


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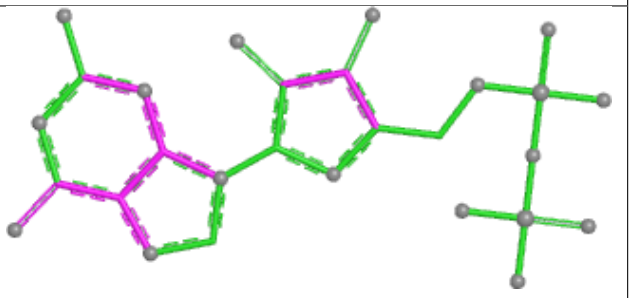


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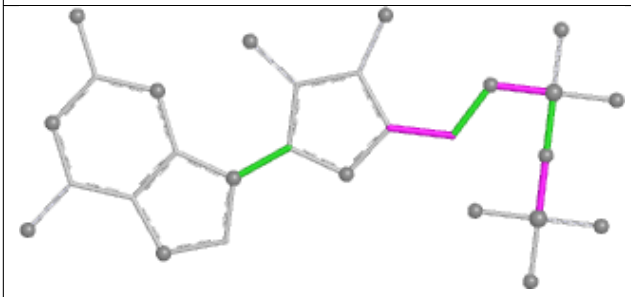
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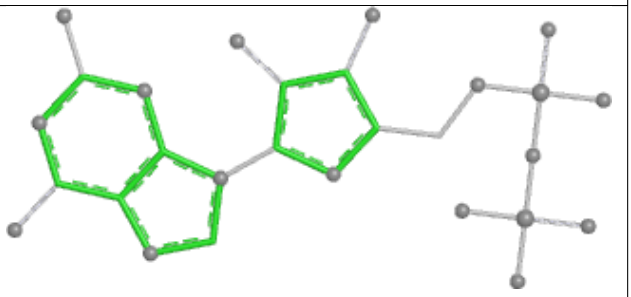
Bond lengths



Bond angles

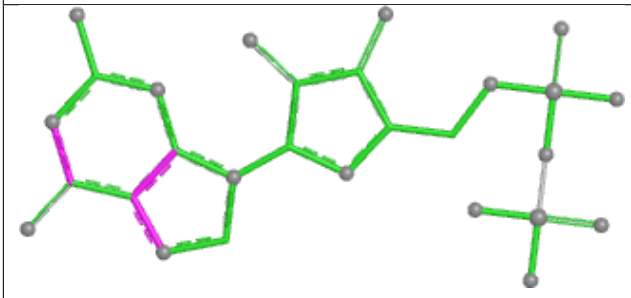


Torsions

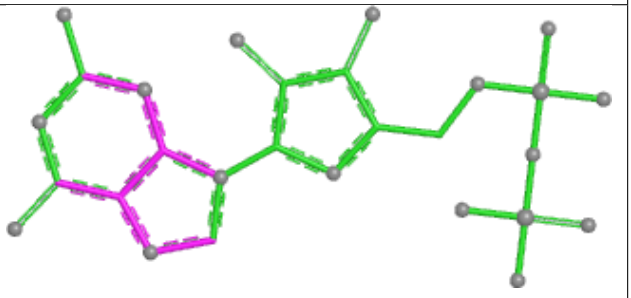


Rings

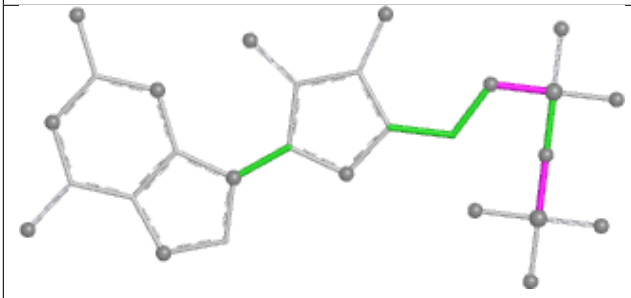
Ligand GDP FF 501



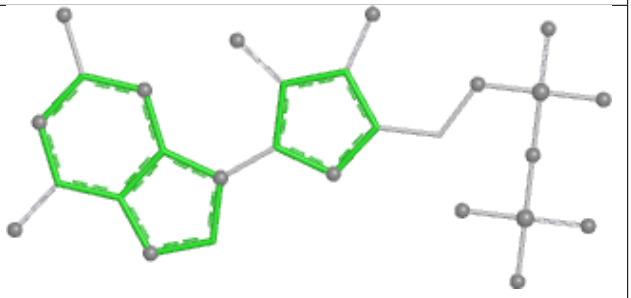
Bond lengths



Bond angles

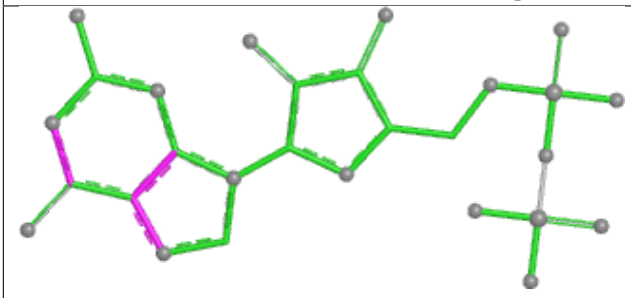


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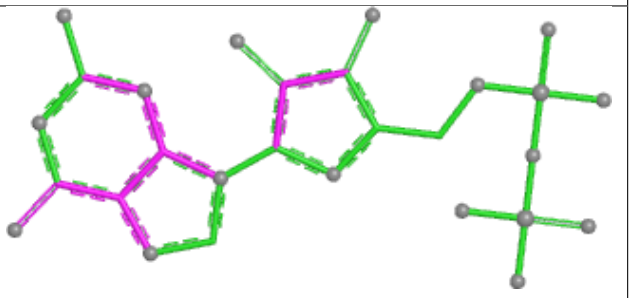


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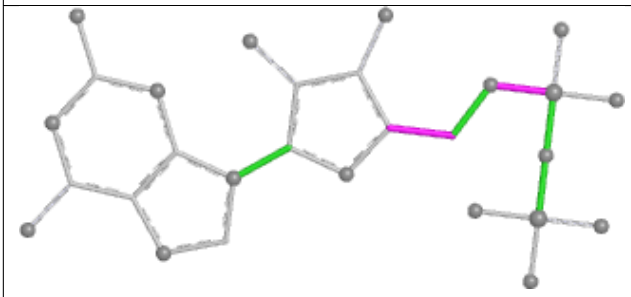
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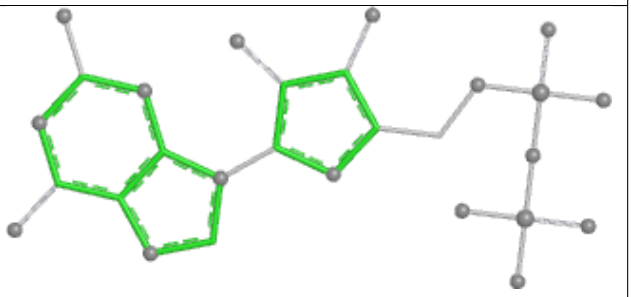
Bond lengths



Bond angles

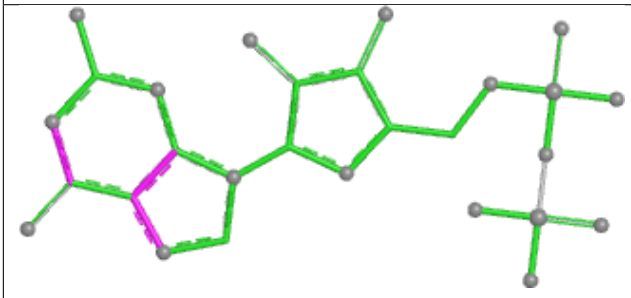


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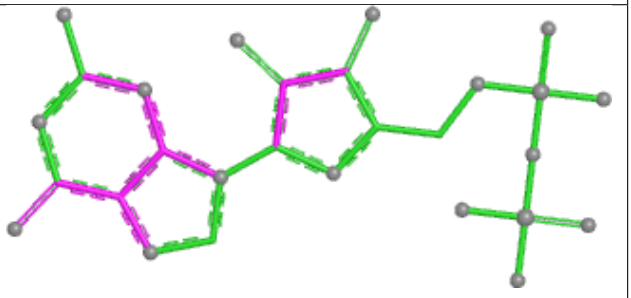


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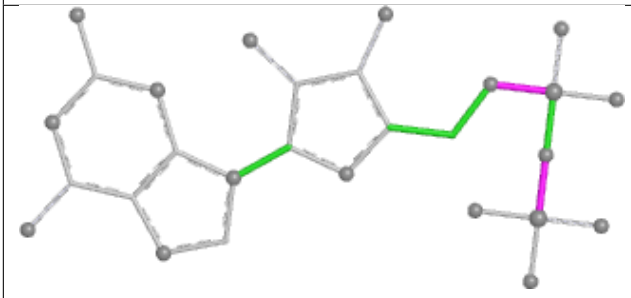
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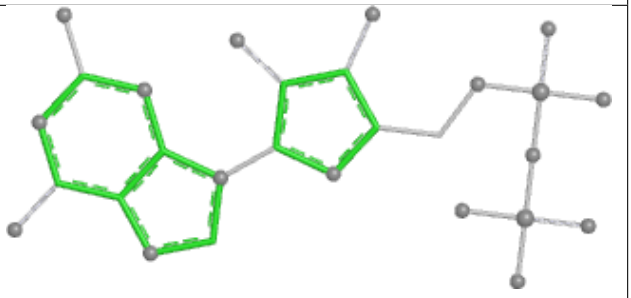
Bond lengths



Bond angles

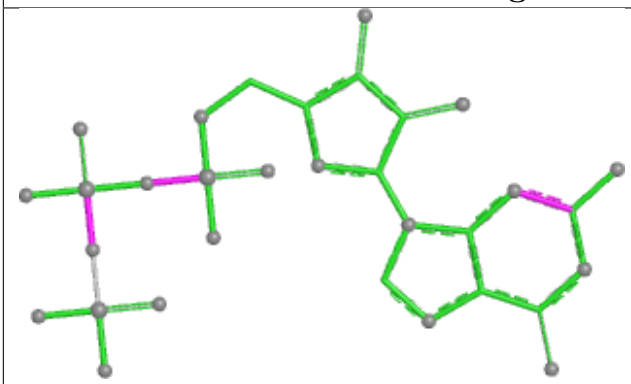


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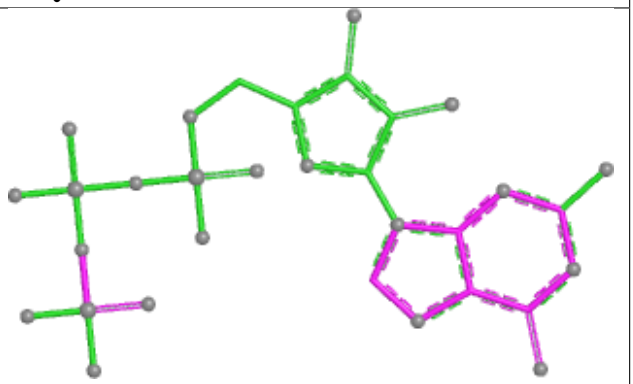


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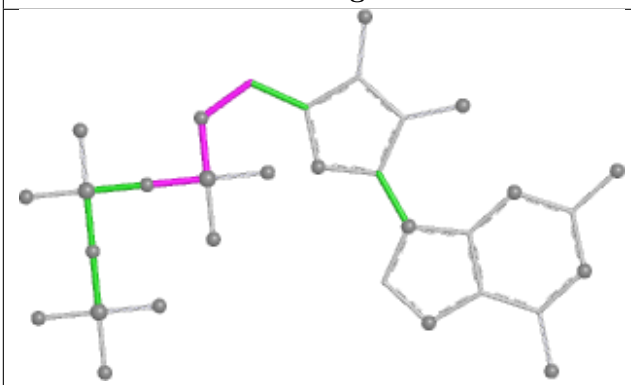
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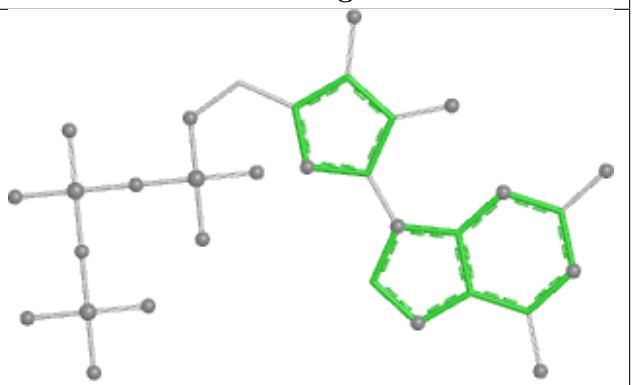
Bond lengths



Bond angles

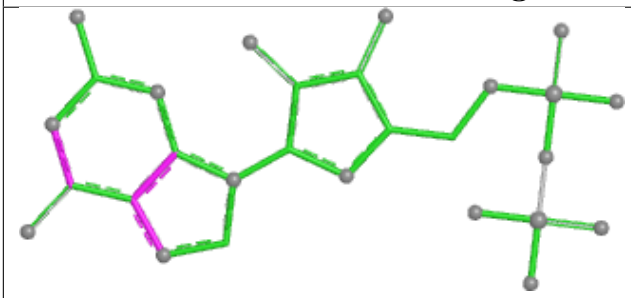


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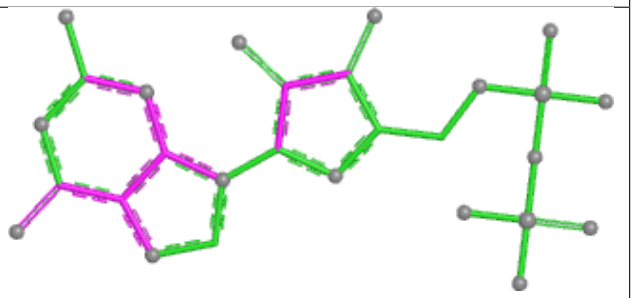


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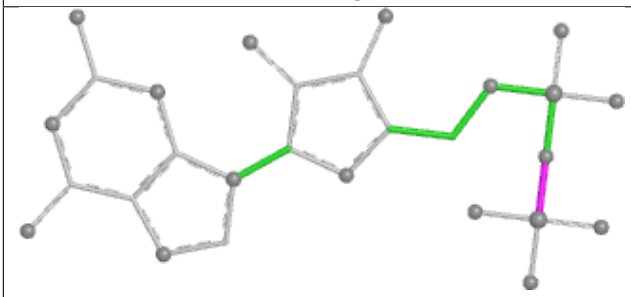
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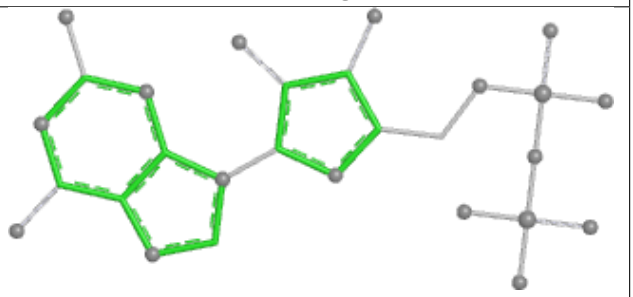
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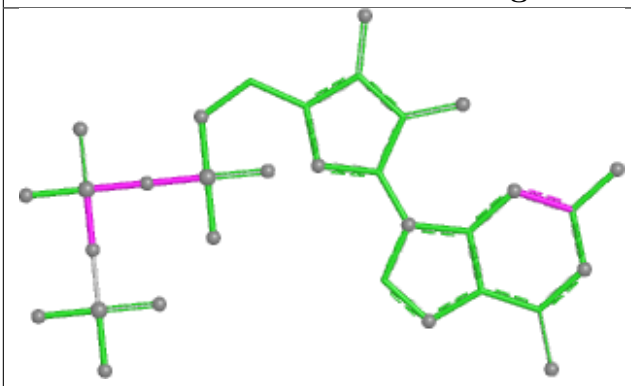


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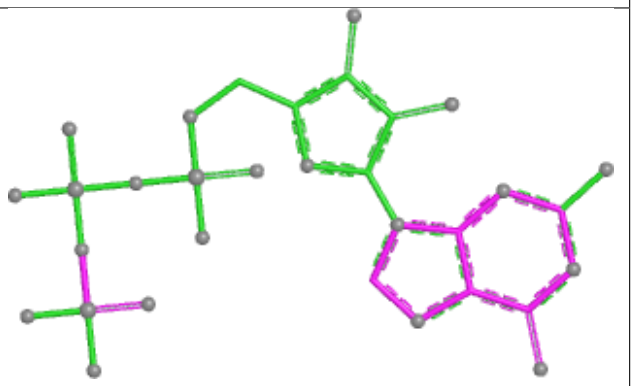


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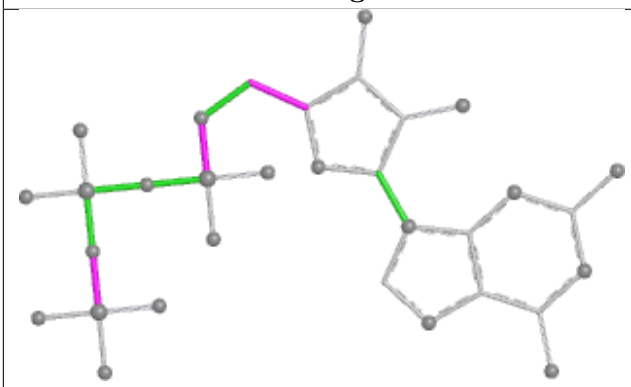
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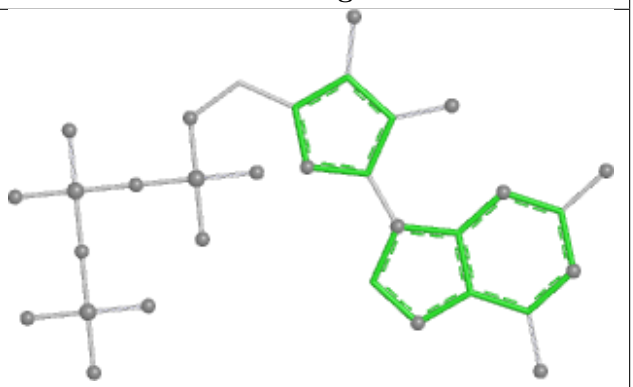
Bond lengths



Bond angles

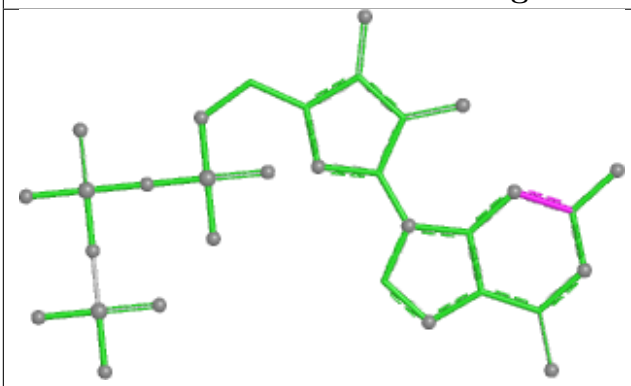


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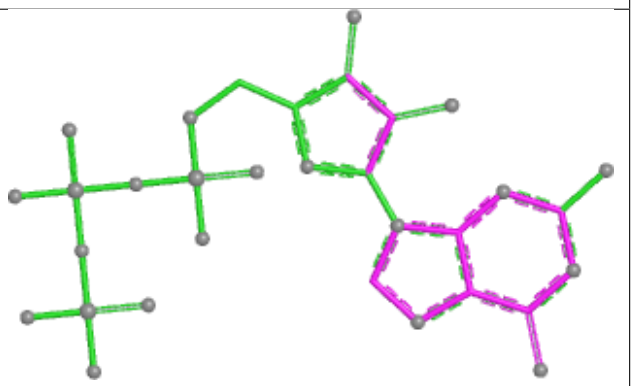


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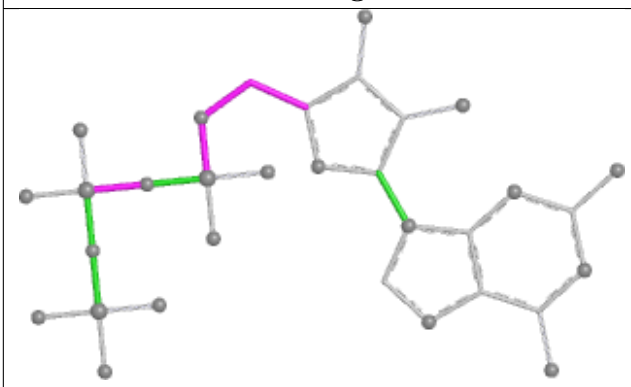
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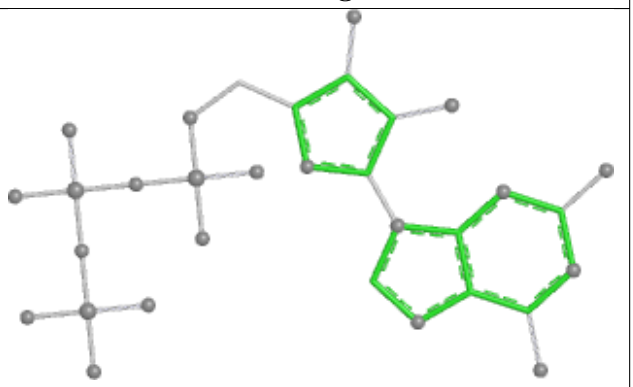
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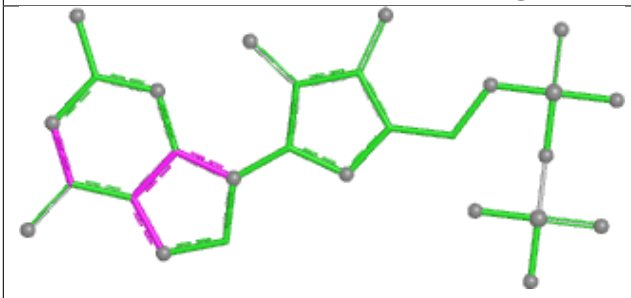


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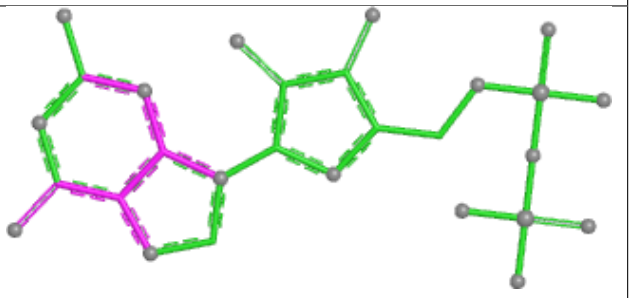


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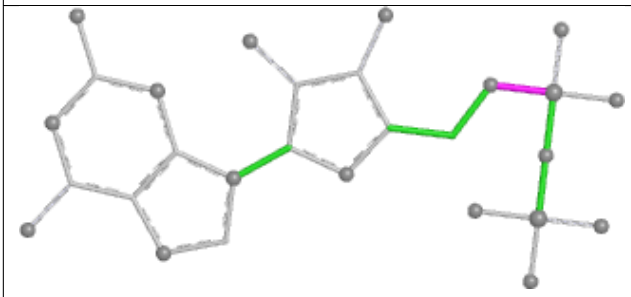
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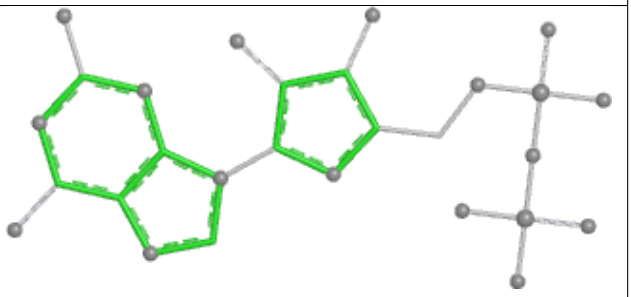
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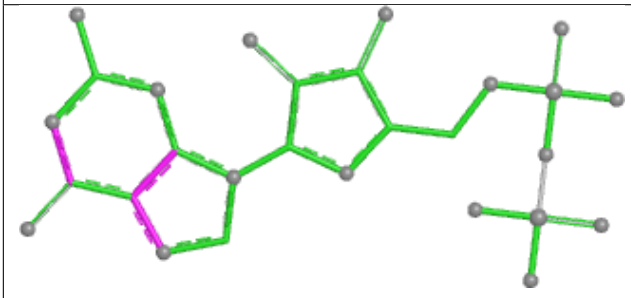


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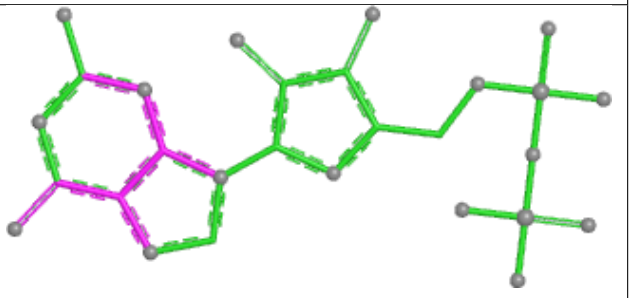


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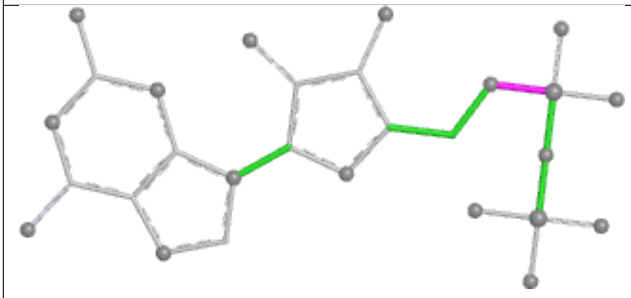
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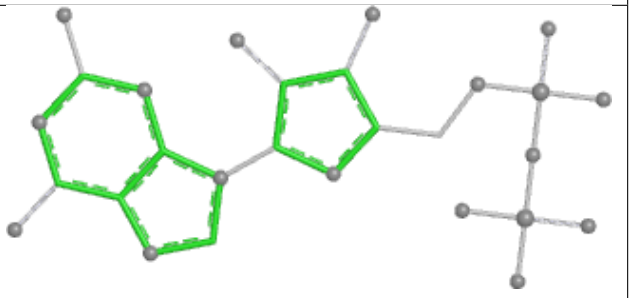
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Bond angles

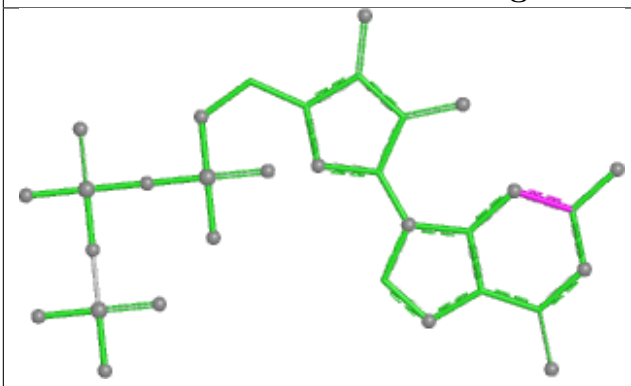


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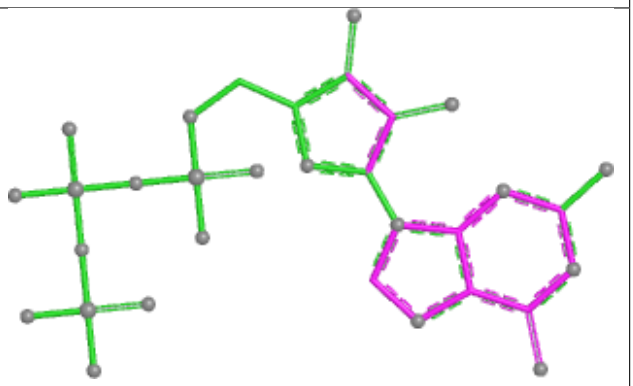


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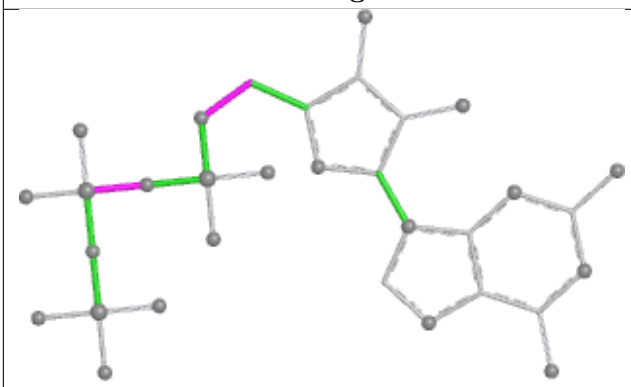
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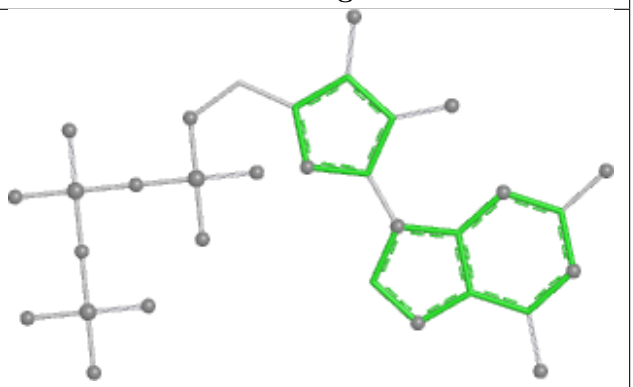
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Bond angles

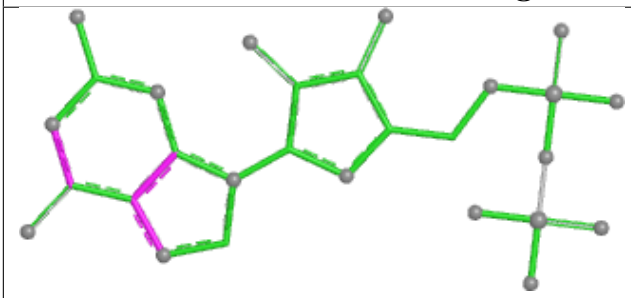


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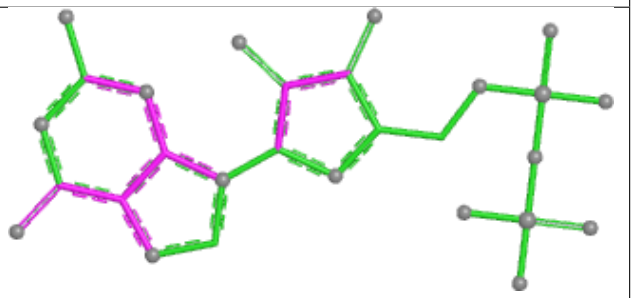


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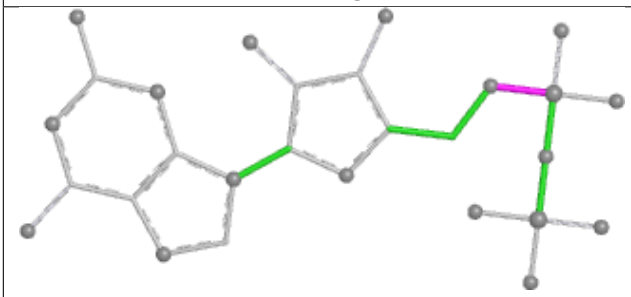
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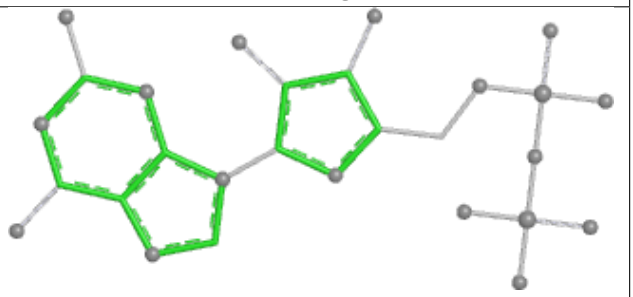
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Bond angles

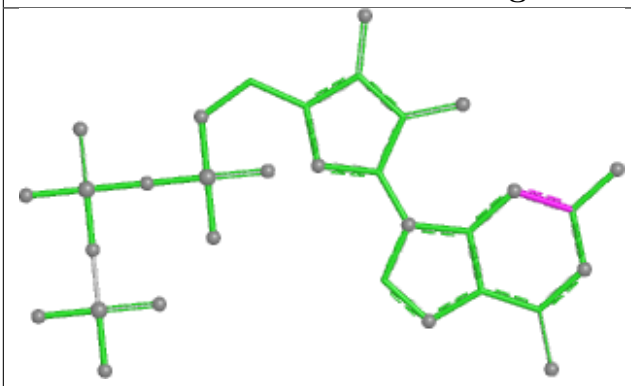


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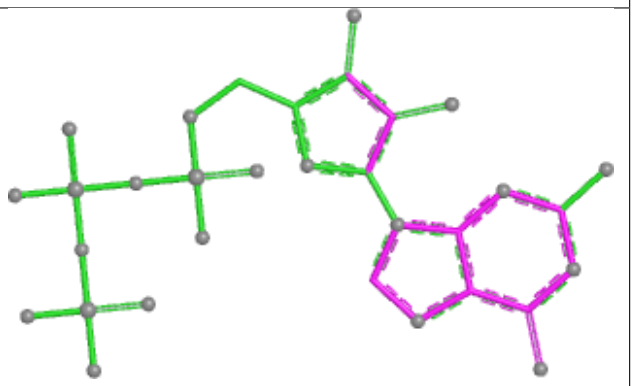


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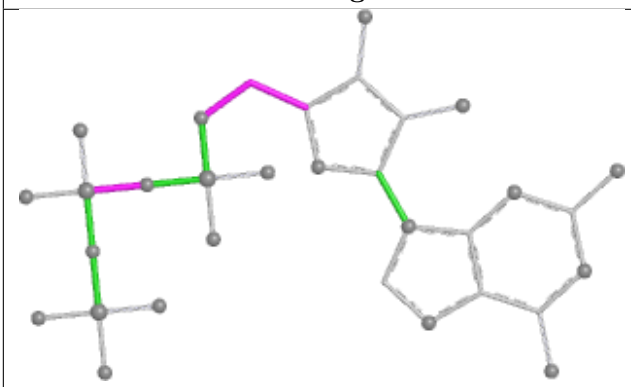
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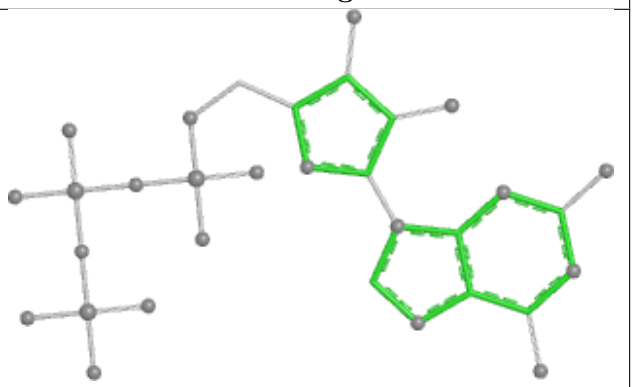
Bond lengths



Bond angles

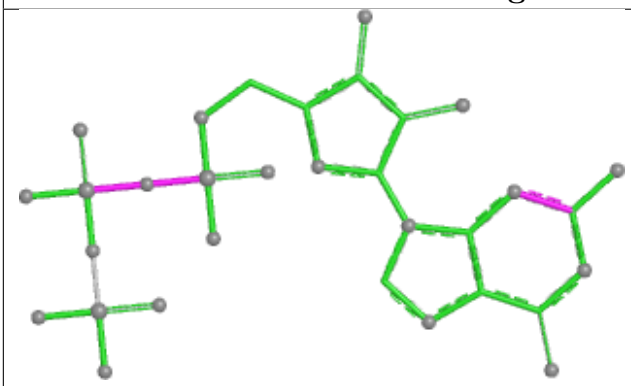


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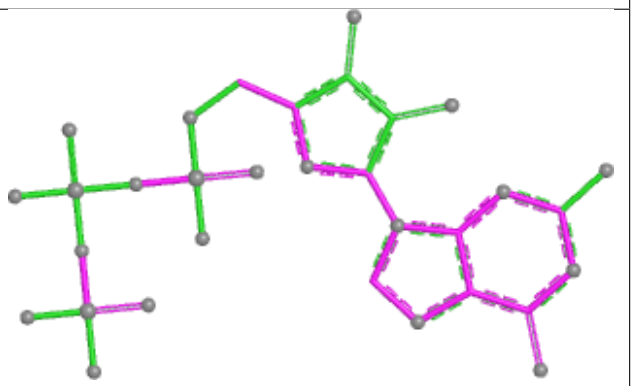


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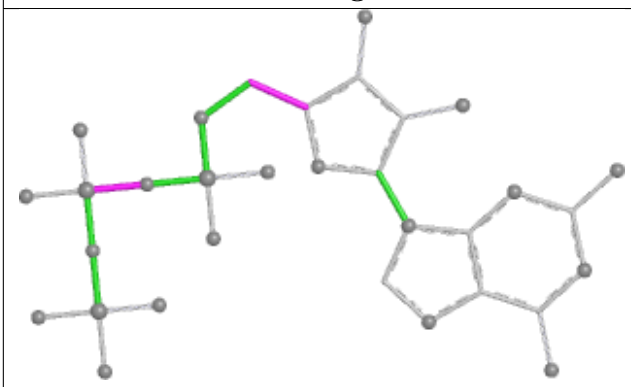
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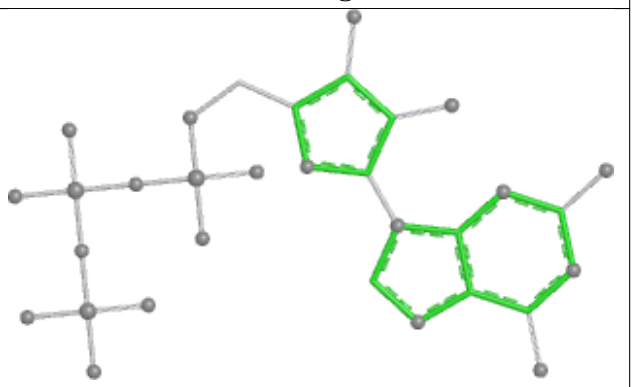
Bond lengths



Bond angles

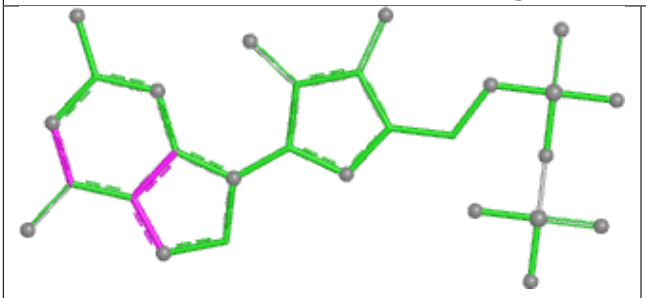


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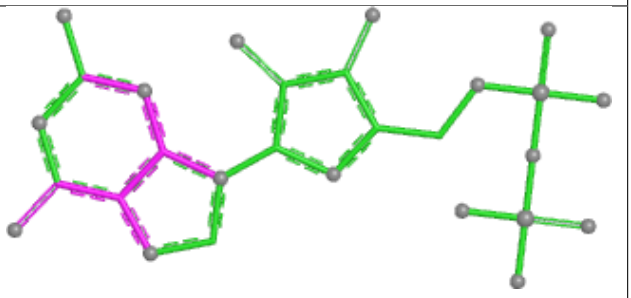


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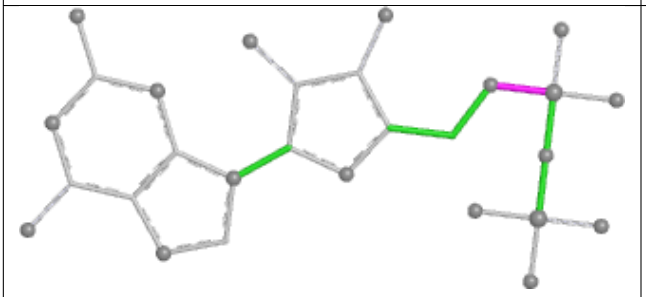
Ligand GDP AF 501



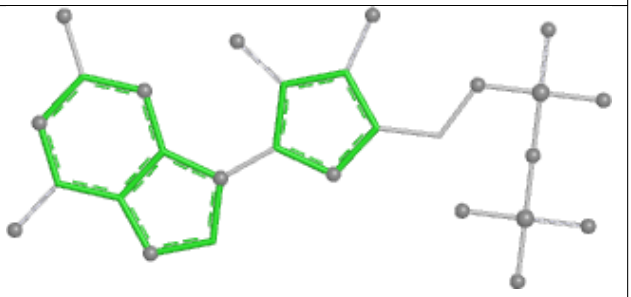
Bond lengths



Bond angles

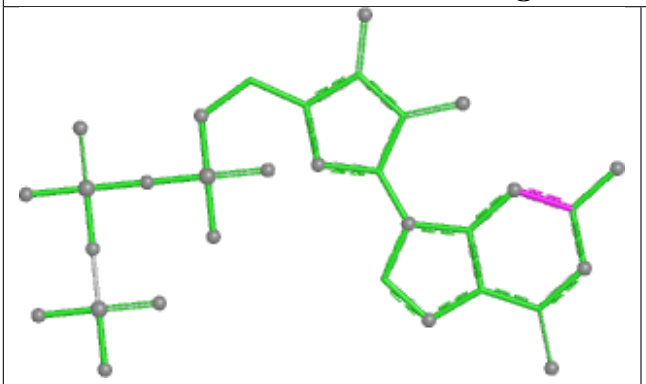


Torsions

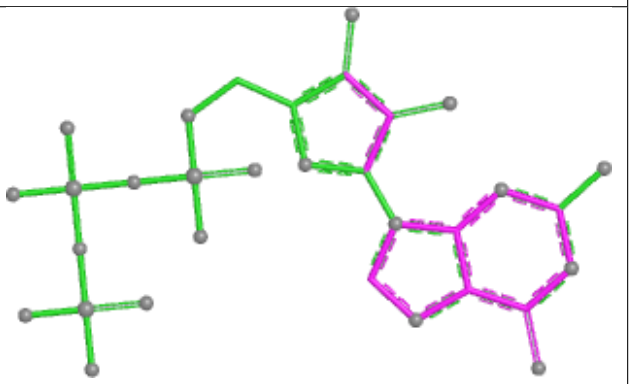


Rings

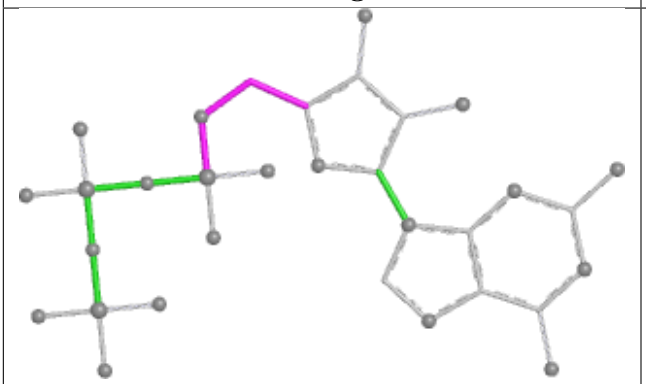
Ligand GTP HI 501



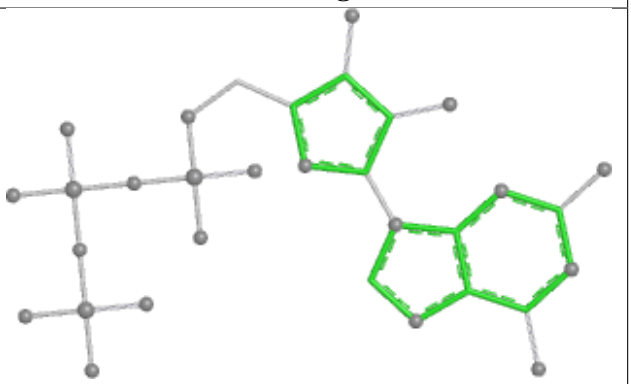
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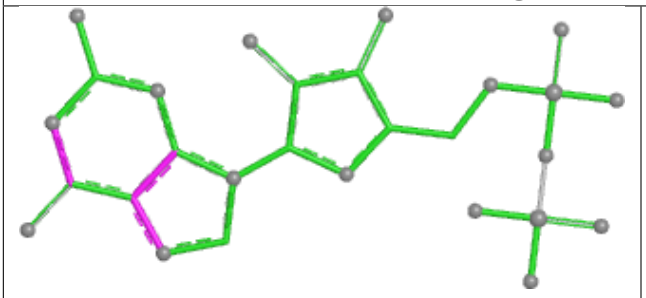


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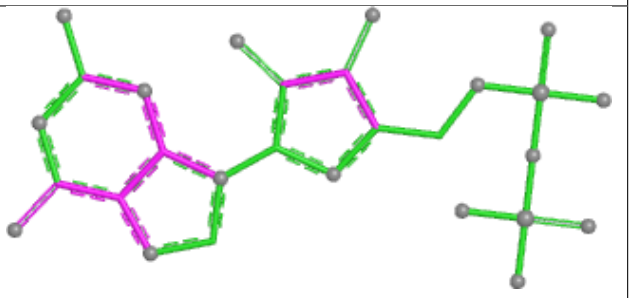


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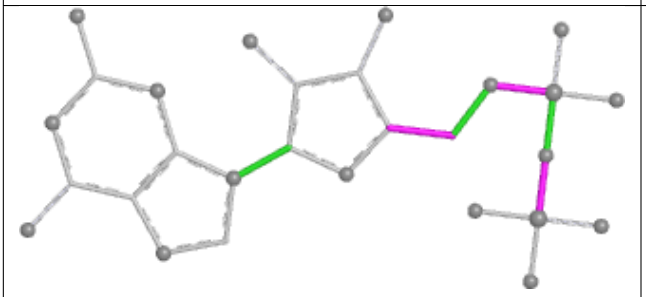
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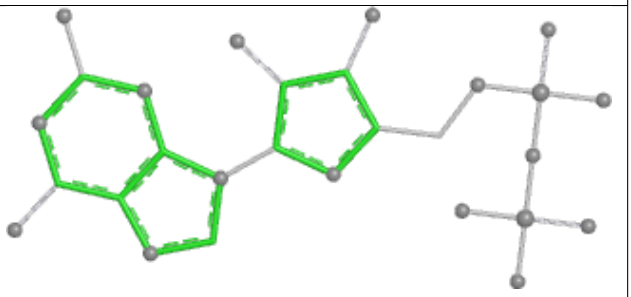
Bond lengths



Bond angles

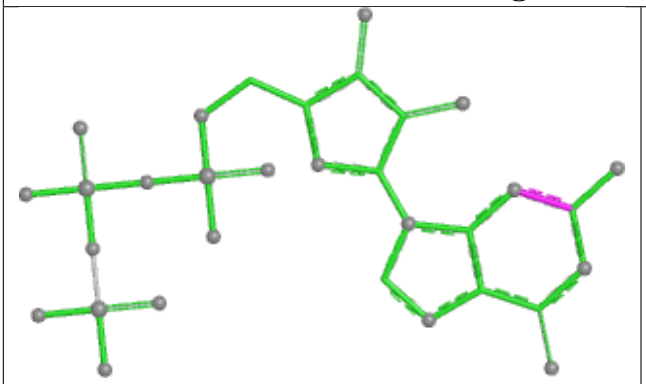


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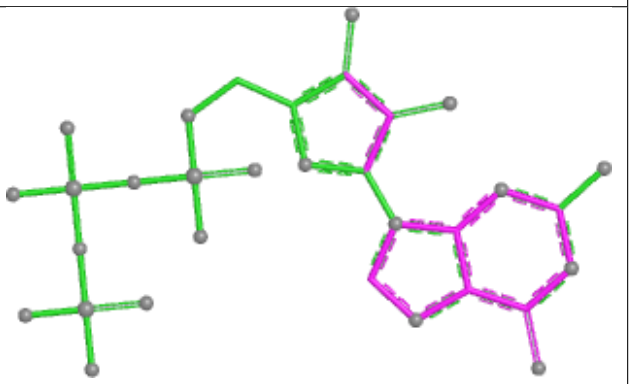


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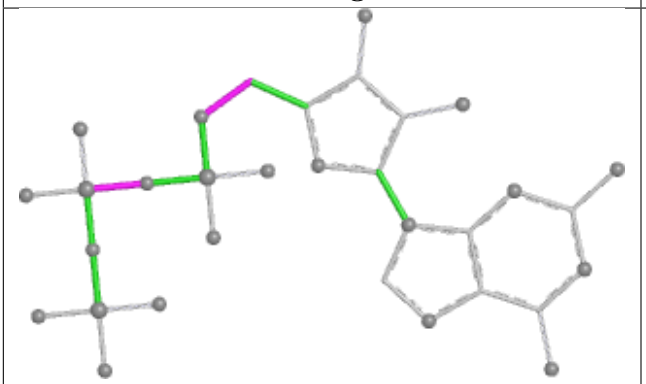
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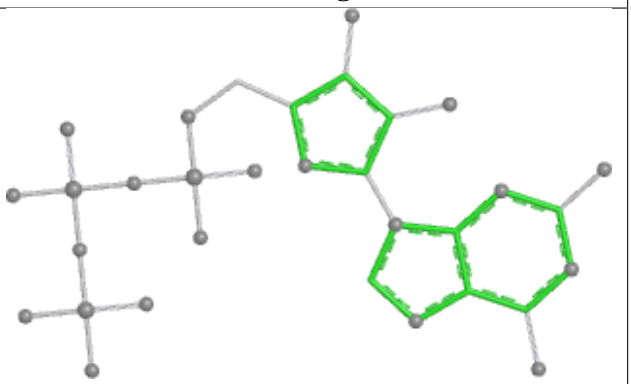
Bond lengths



Bond angles

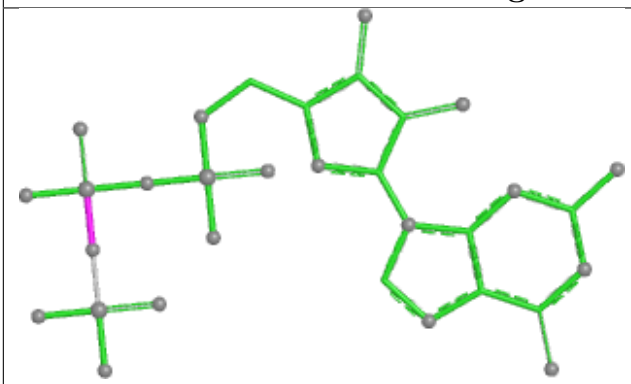


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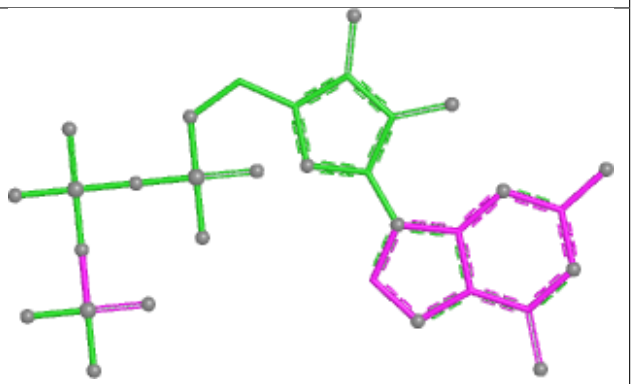


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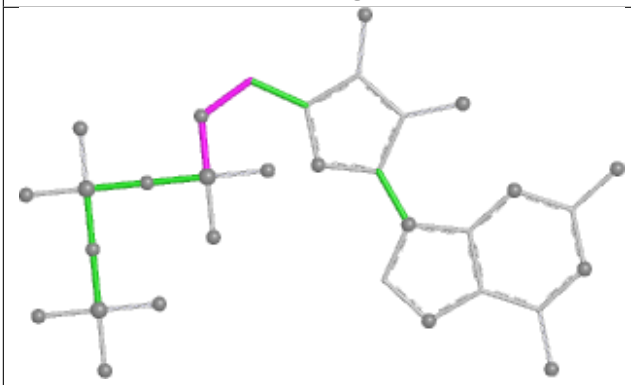
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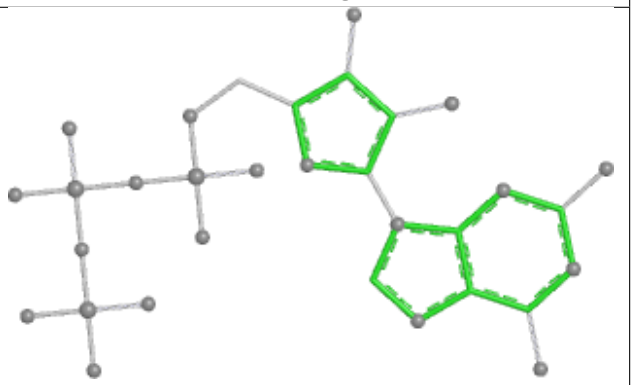
Bond lengths



Bond angles

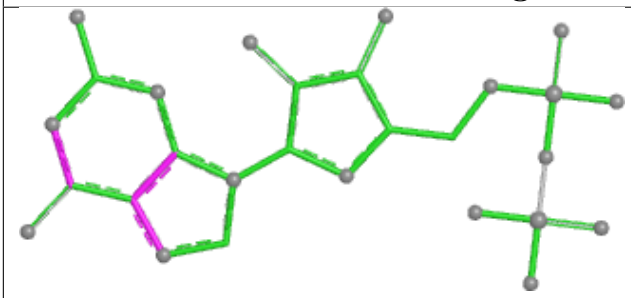


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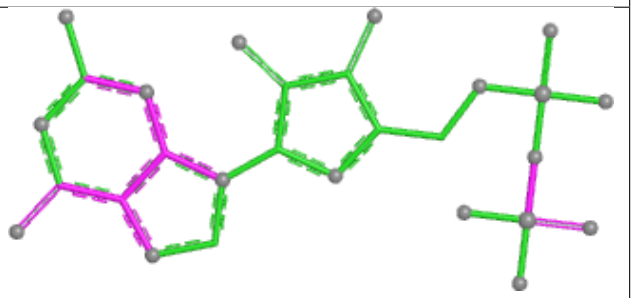


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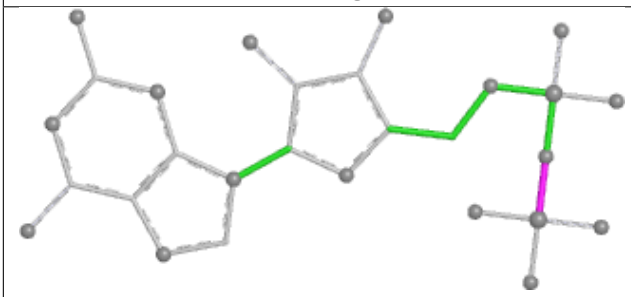
Ligand GDP VJ 501



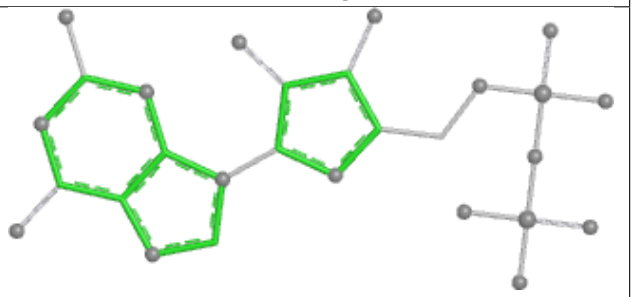
Bond lengths



Bond angles

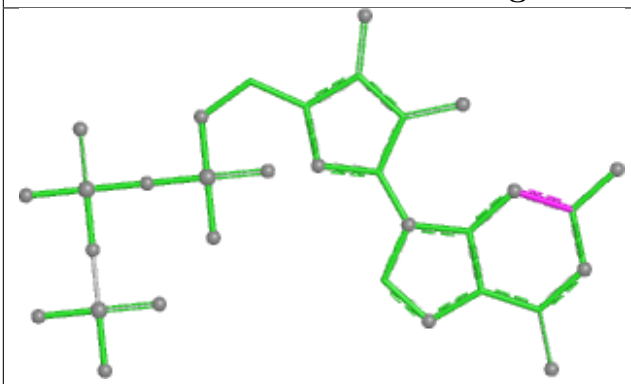


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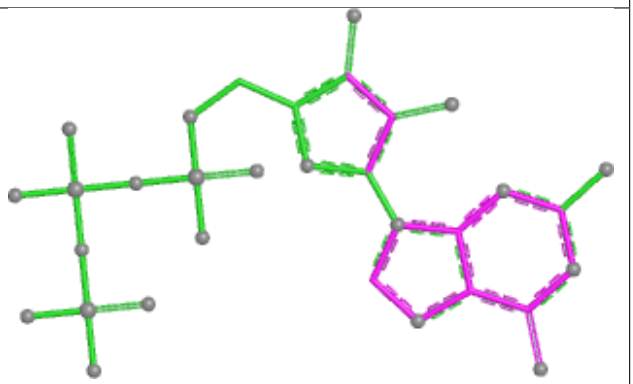


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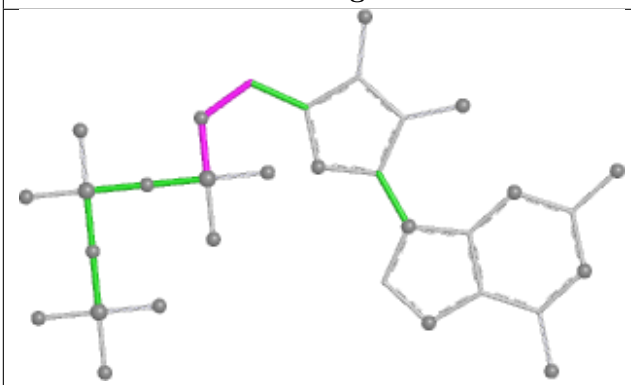
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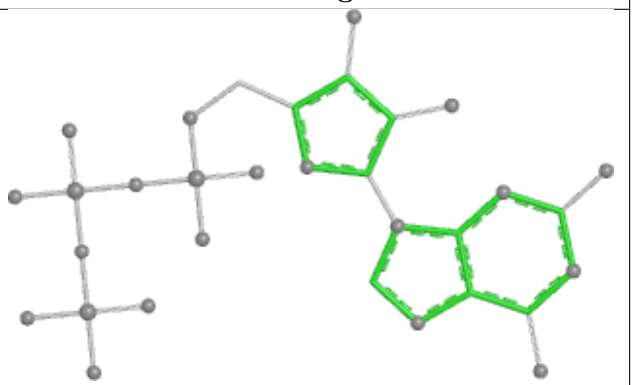
Bond lengths



Bond angles

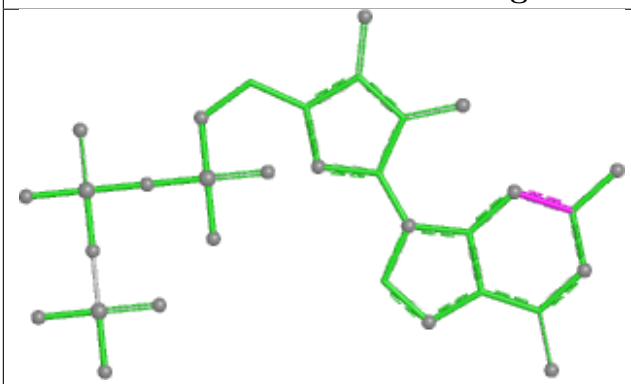


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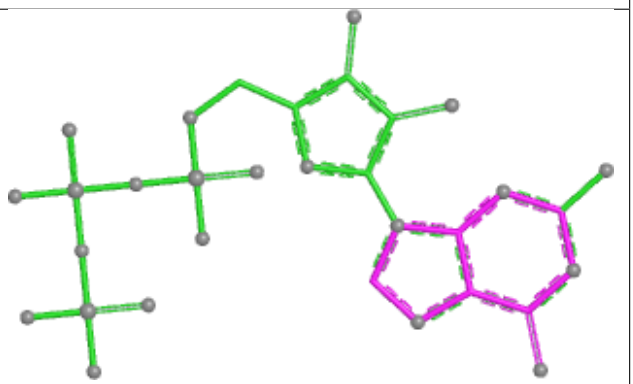


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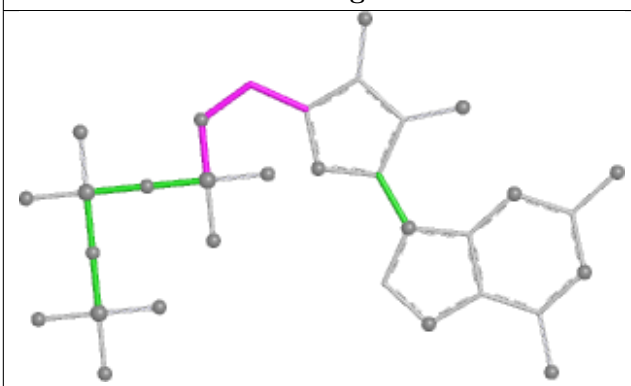
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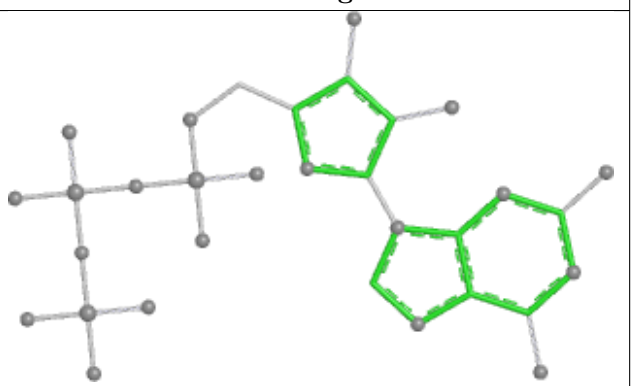
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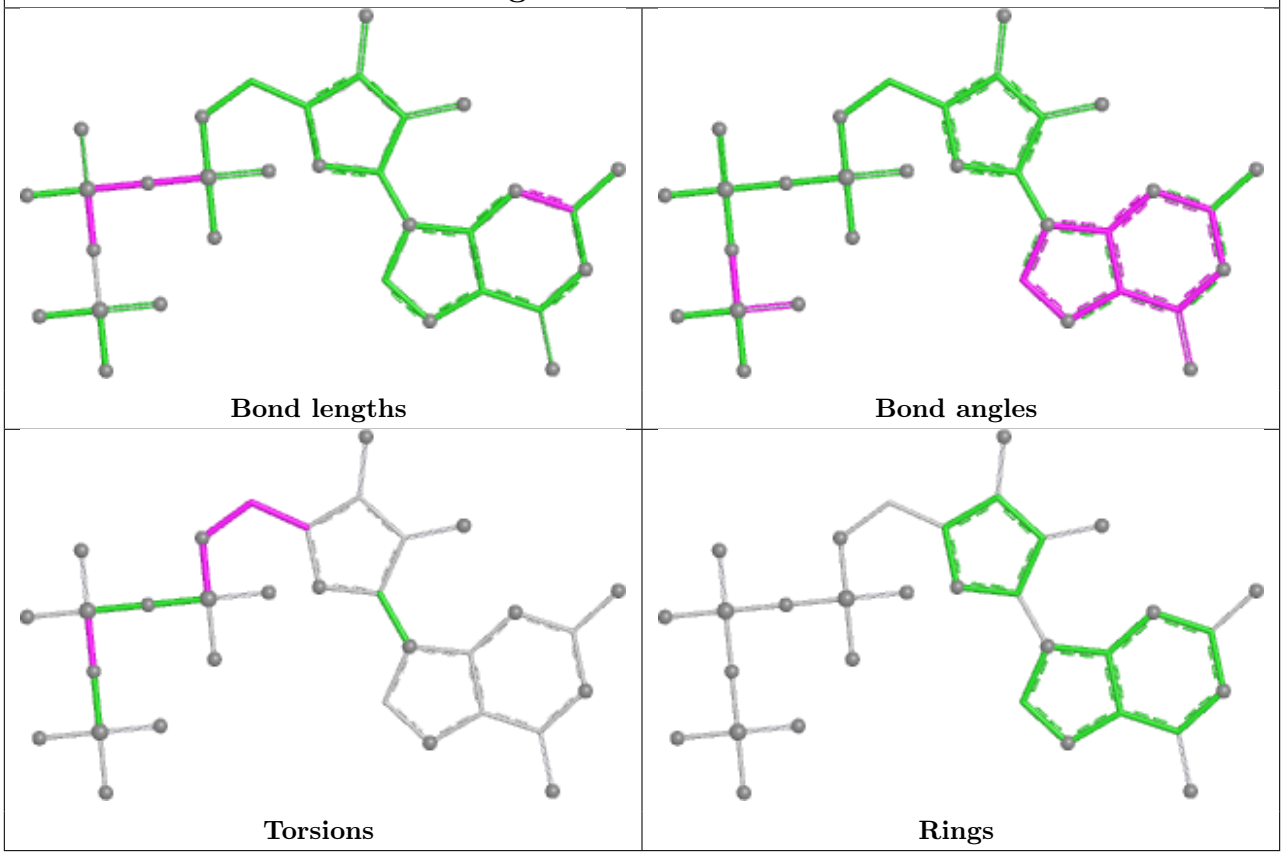


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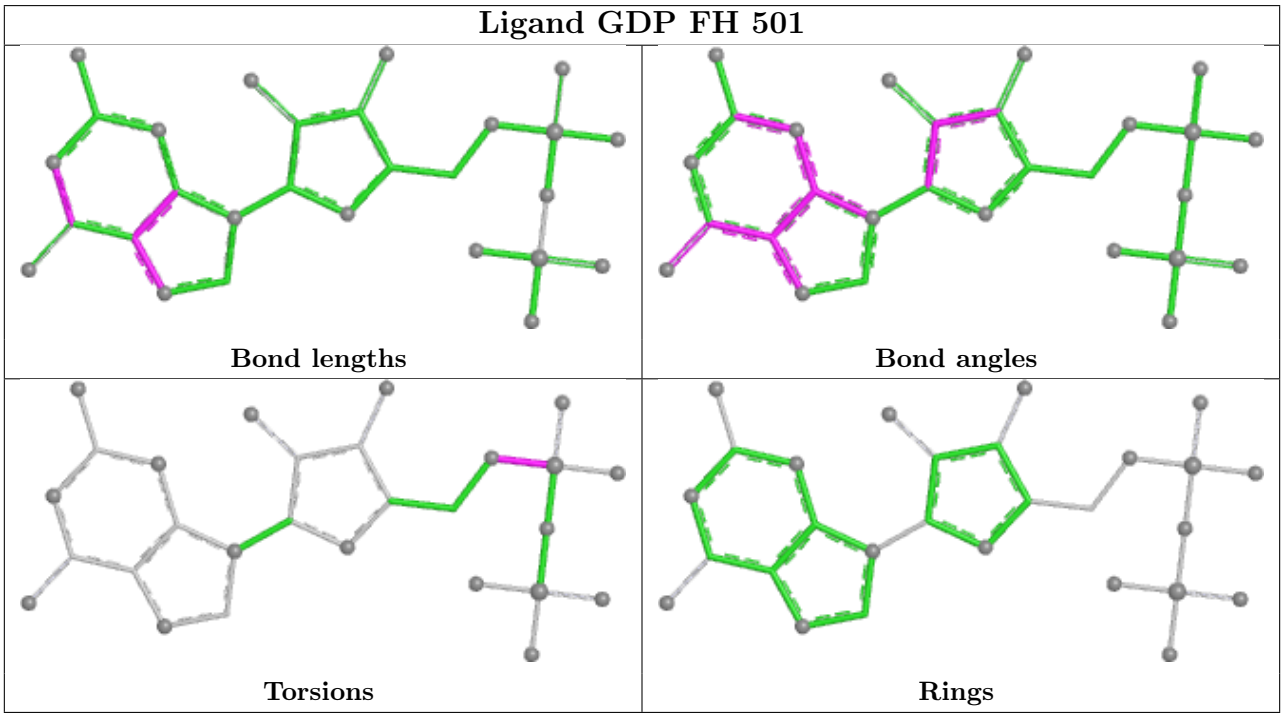


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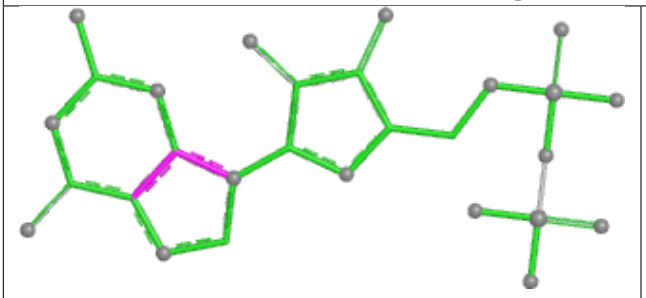
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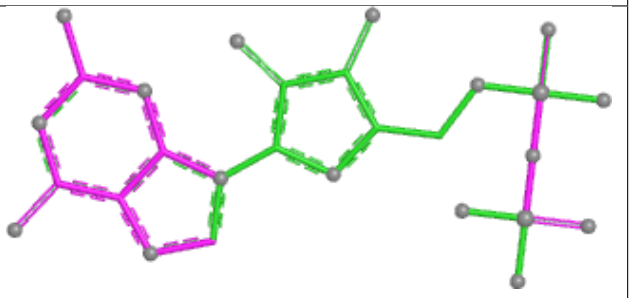
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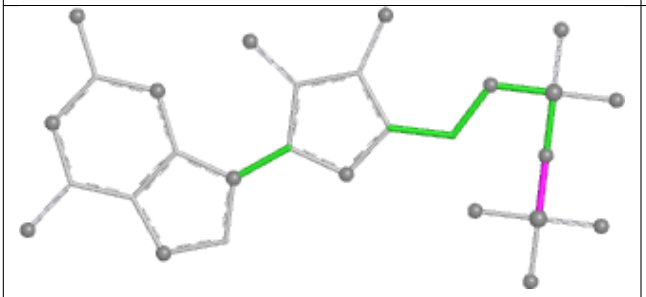
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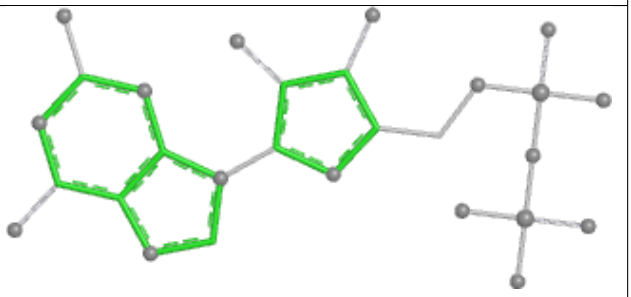
Bond lengths



Bond angles

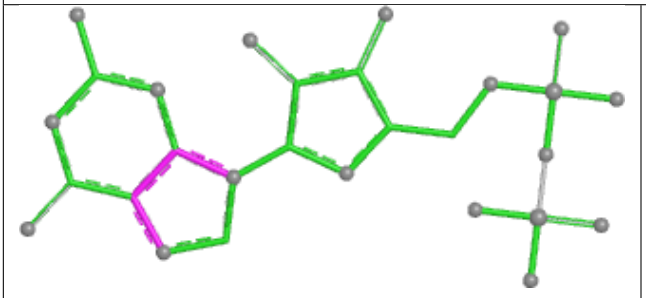


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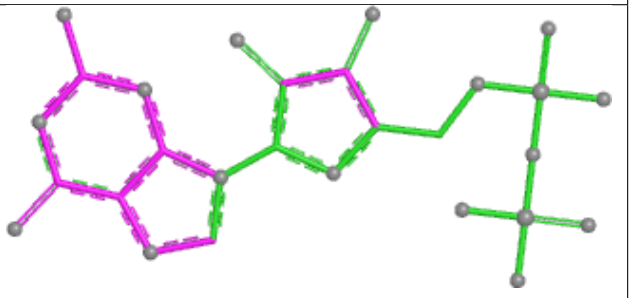


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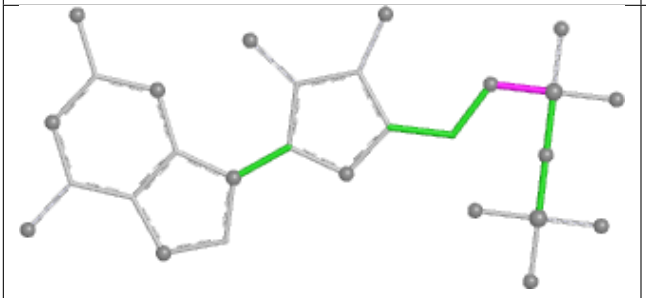
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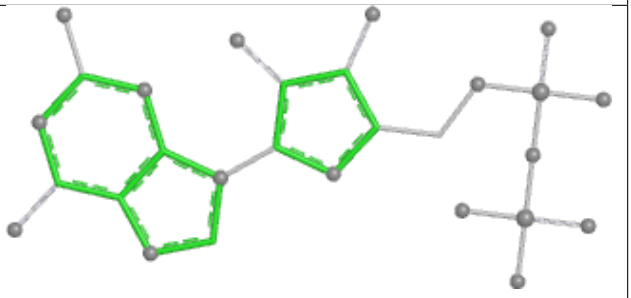
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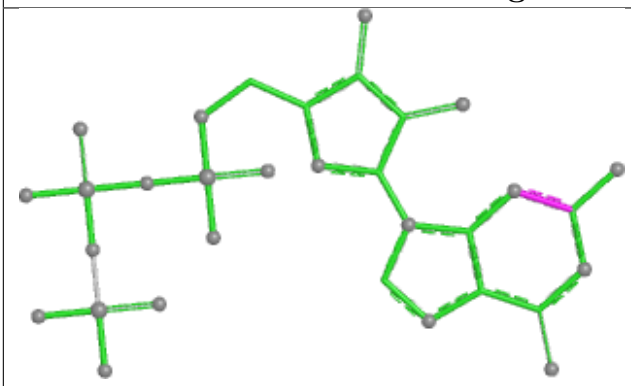


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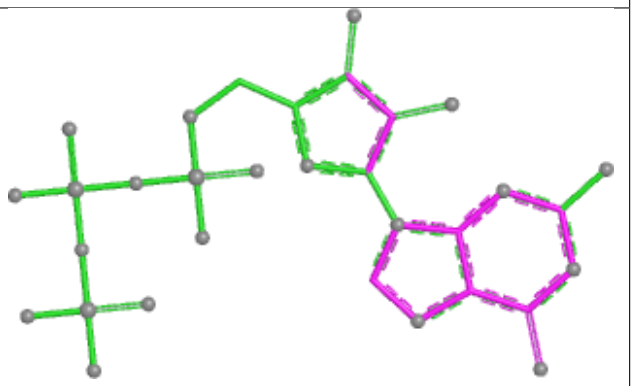


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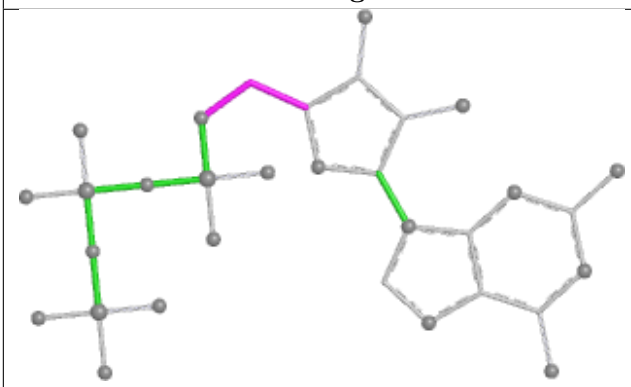
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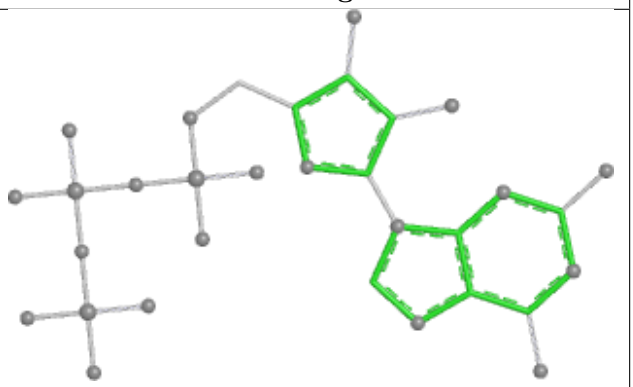
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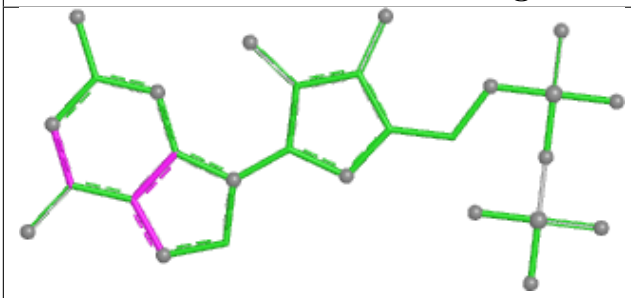


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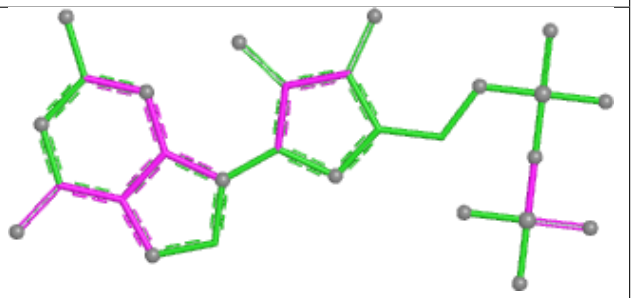


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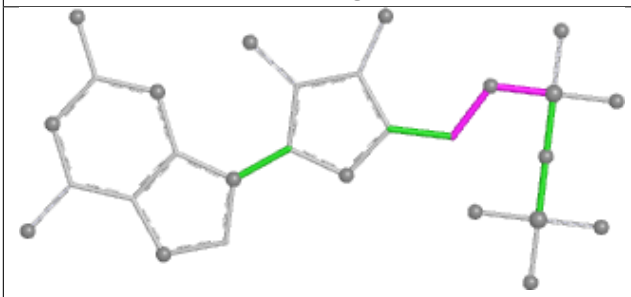
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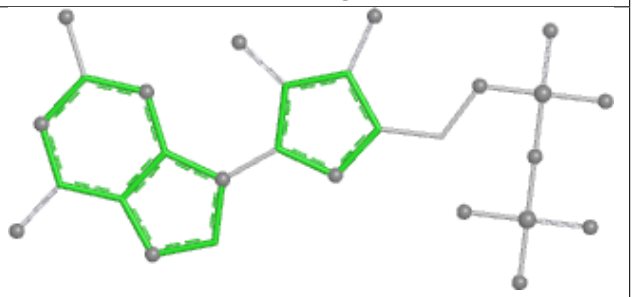
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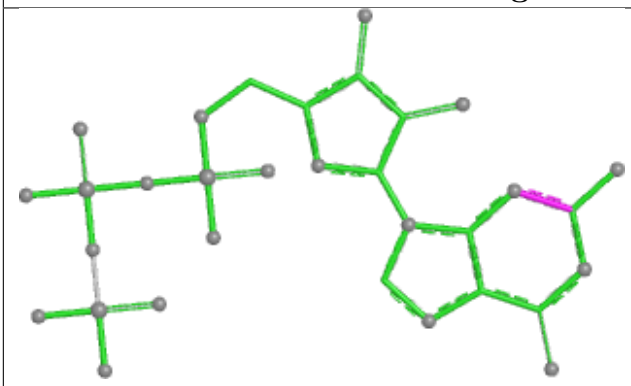


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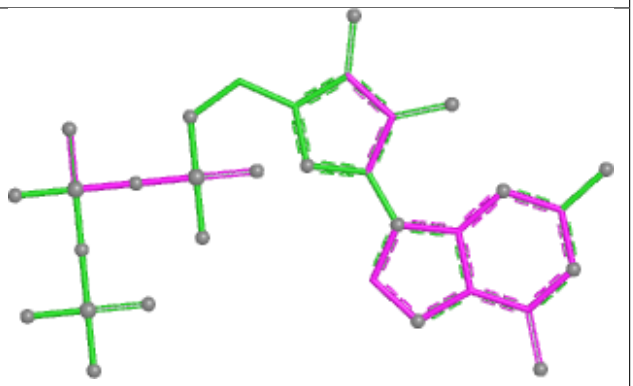


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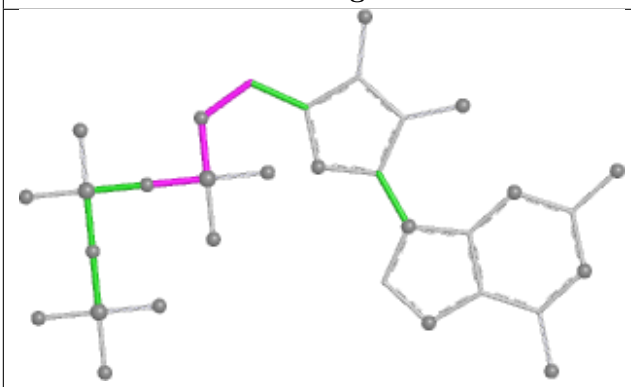
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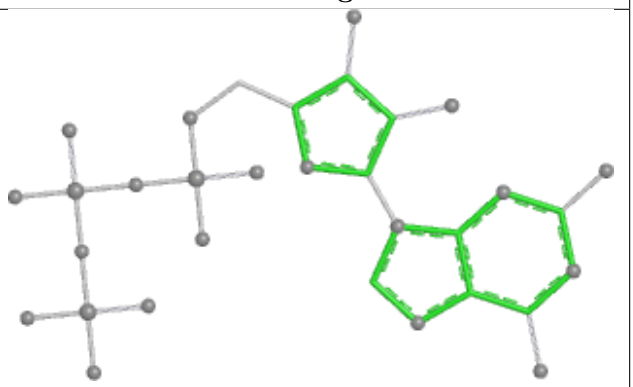
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Bond angles

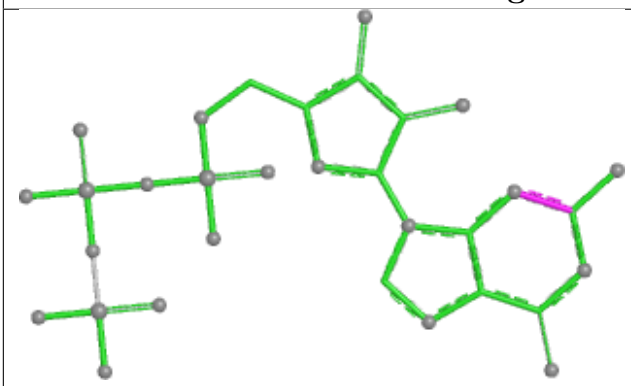


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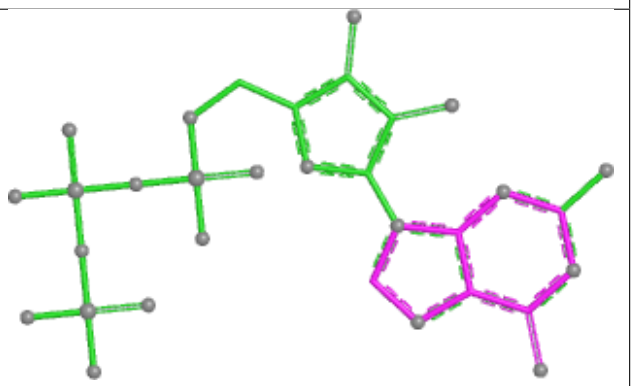


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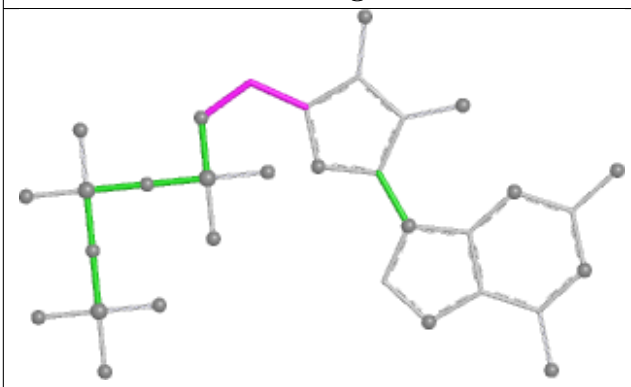
Ligand GTP UG 501



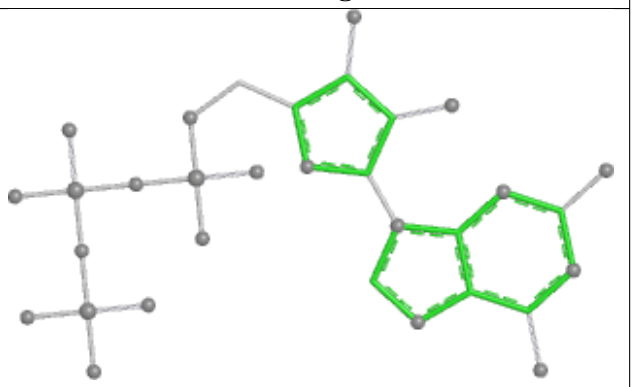
Bond lengths



Bond angles

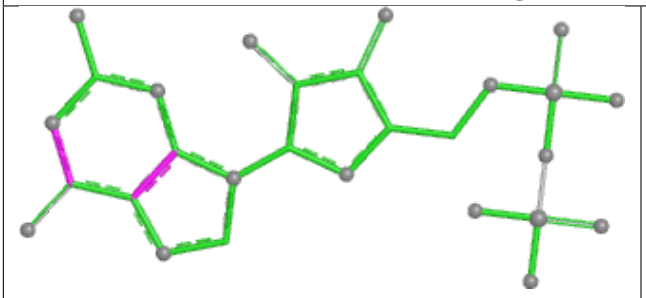


Torsions

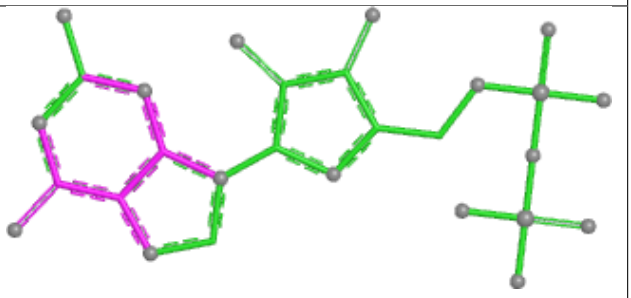


Rings

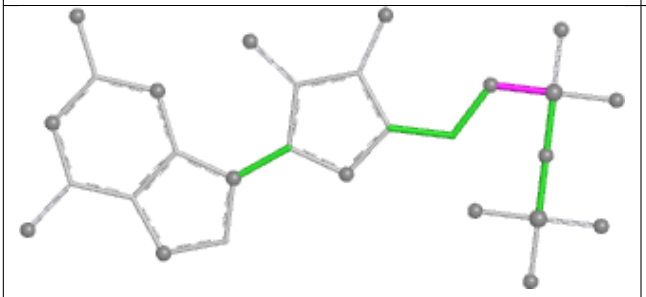
Ligand GDP NJ 501



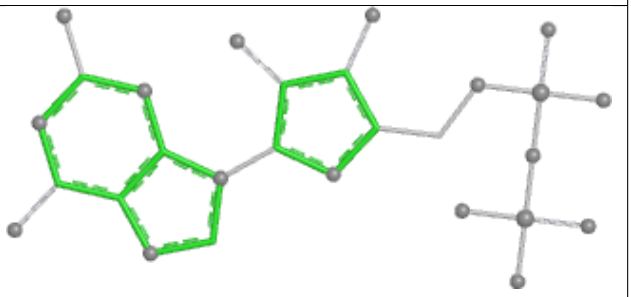
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Bond angles

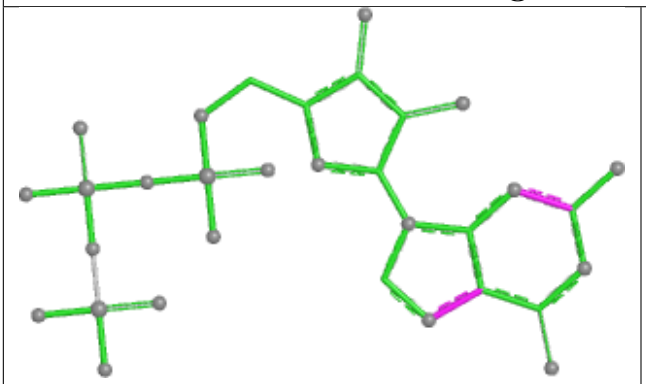


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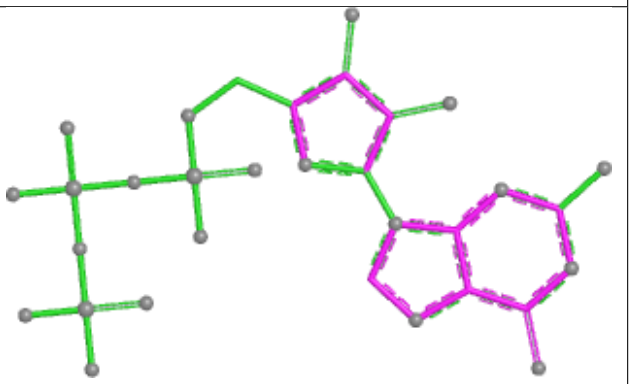


Rings

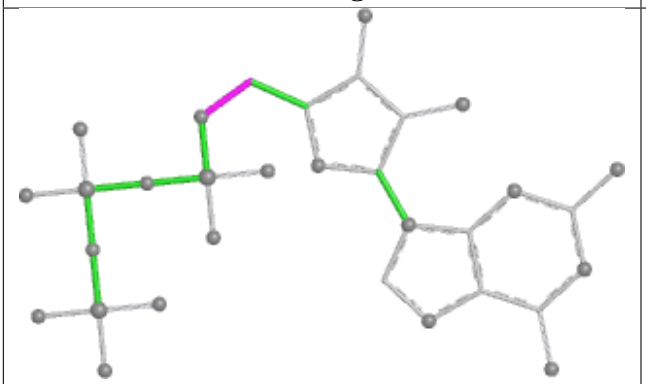
Ligand GTP DA 501



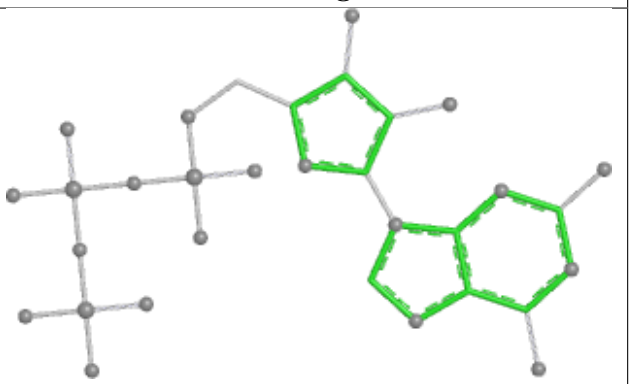
Bond lengths



Bond angles

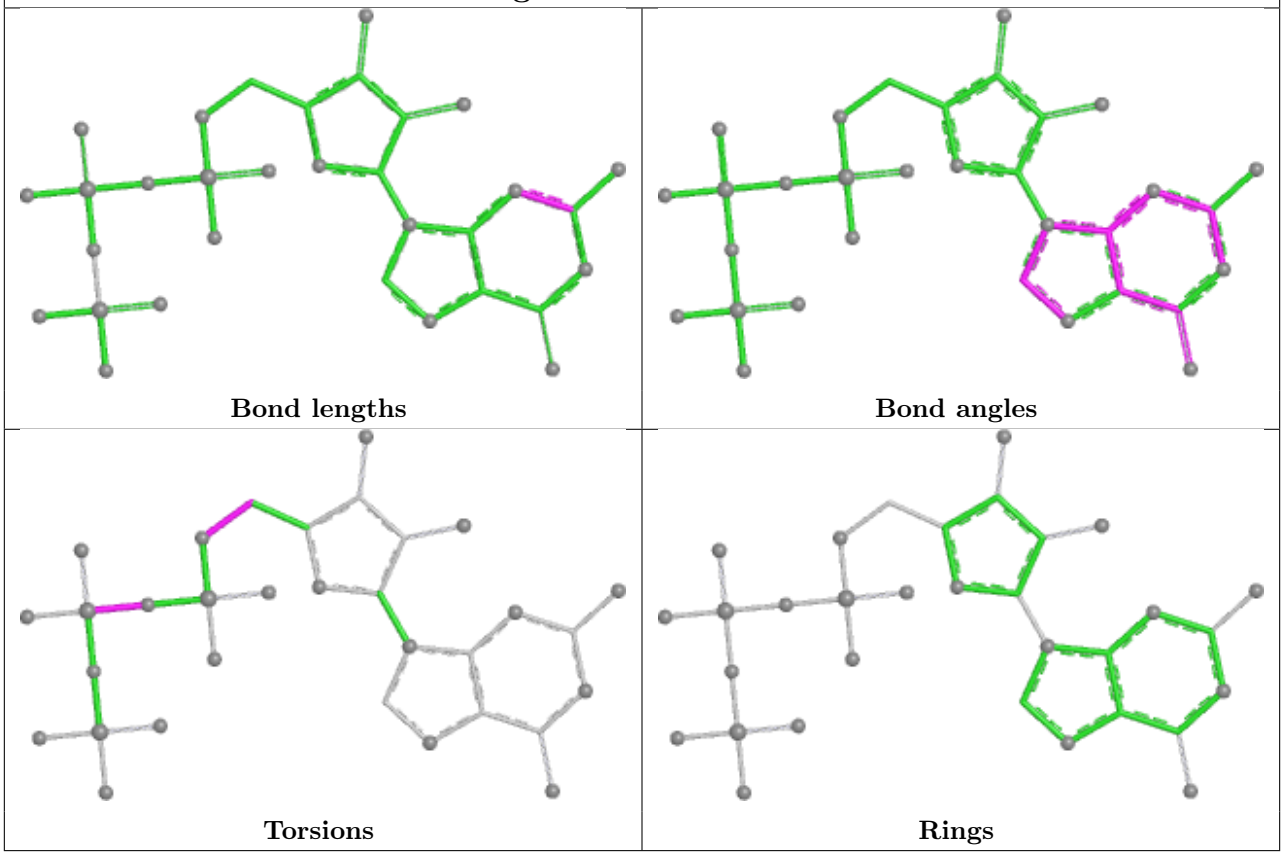


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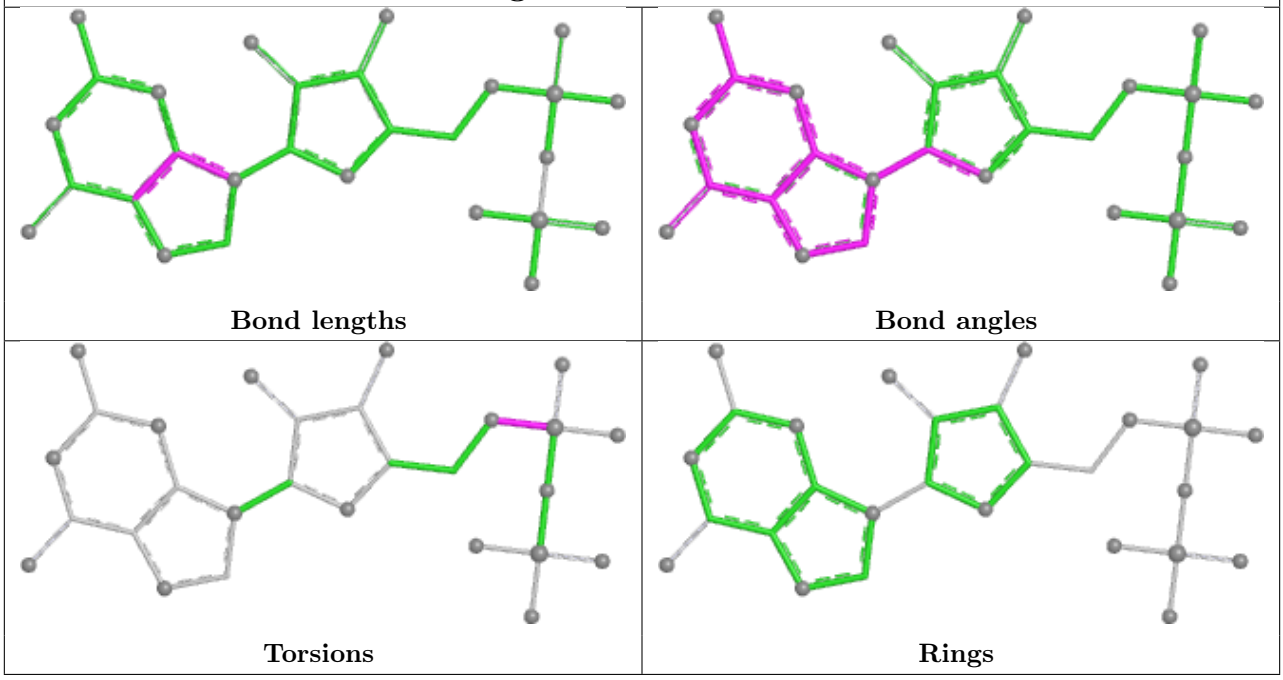


Rings

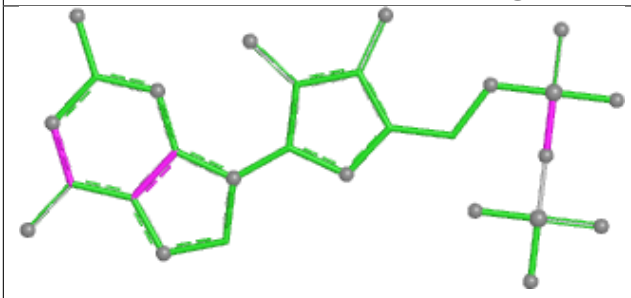
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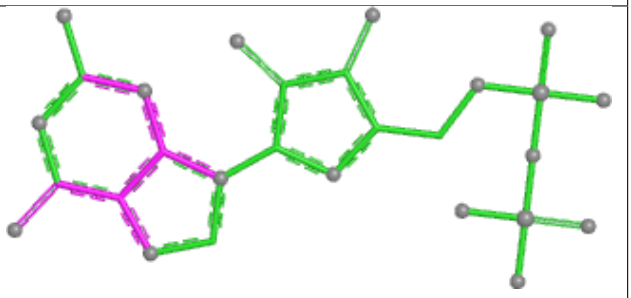
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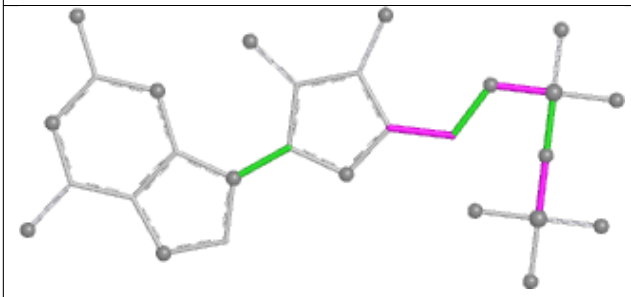
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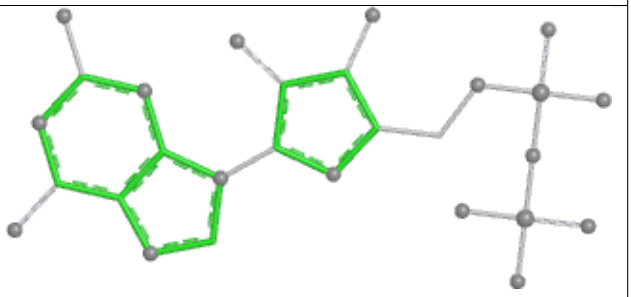
Bond lengths



Bond angles

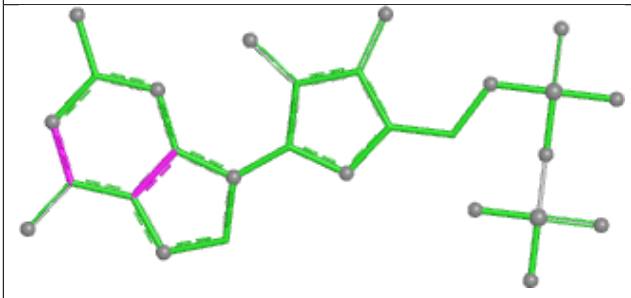


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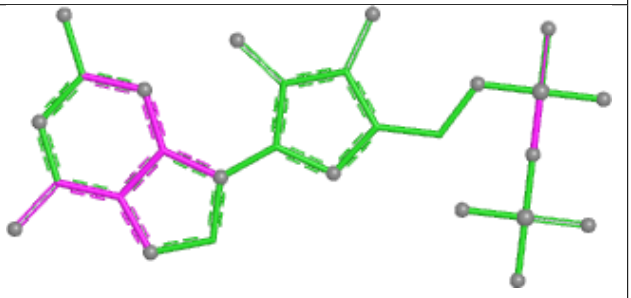


Rings

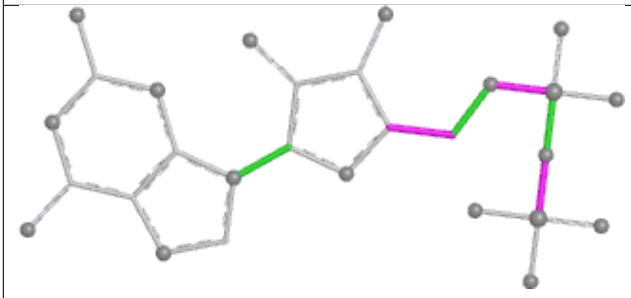
Ligand GDP MJ 501



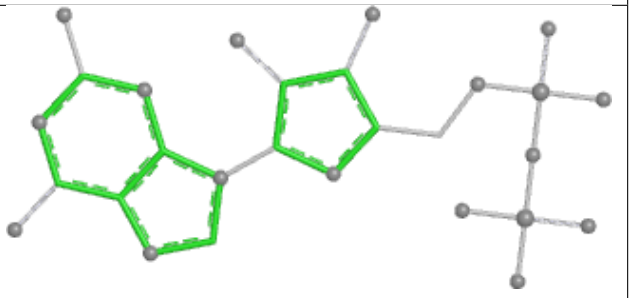
Bond lengths



Bond angles

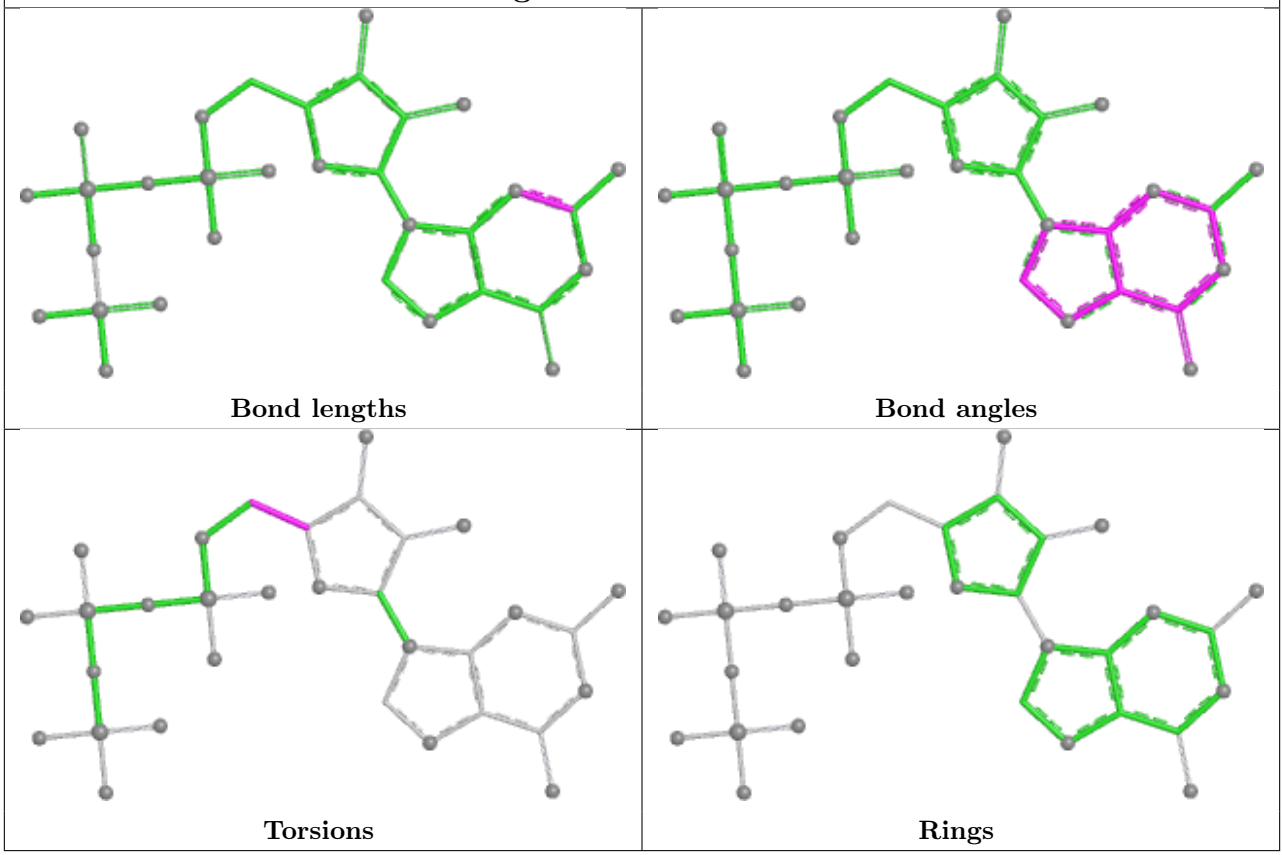


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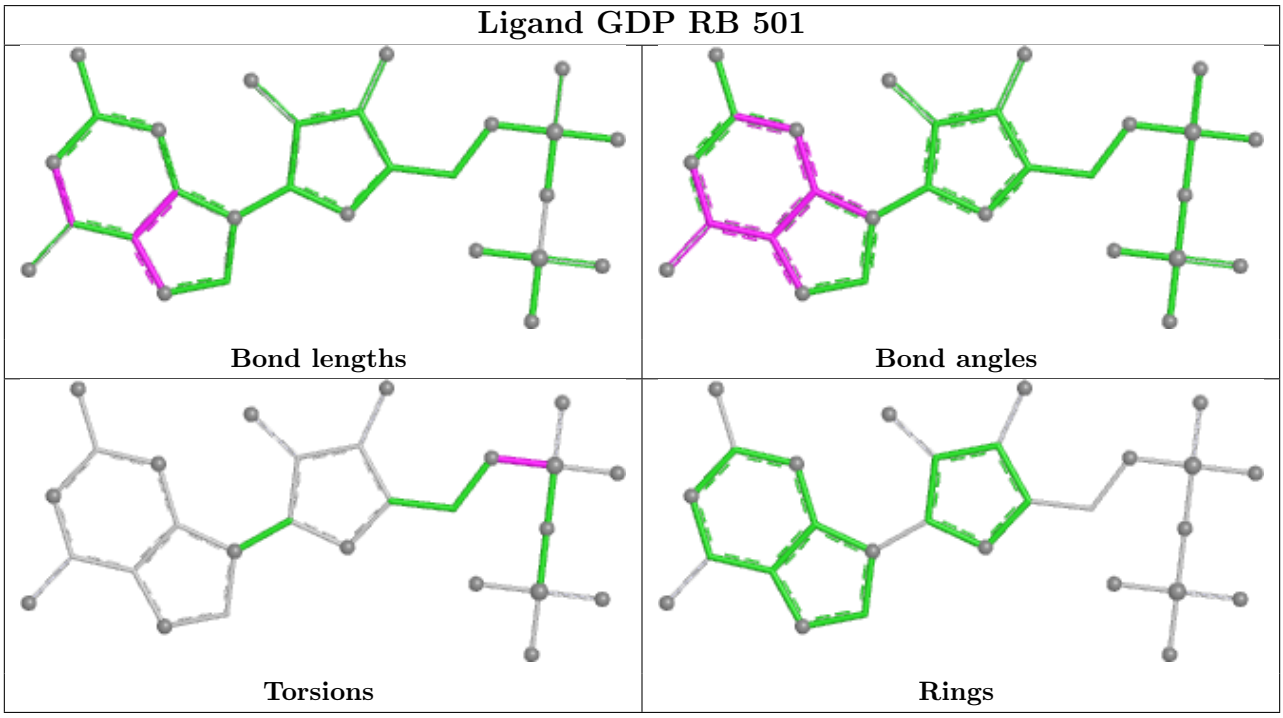


Rings

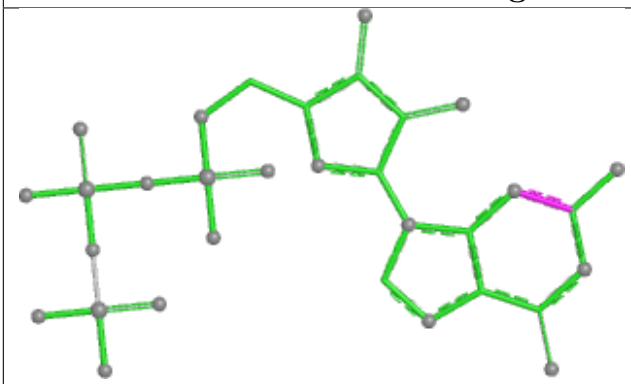
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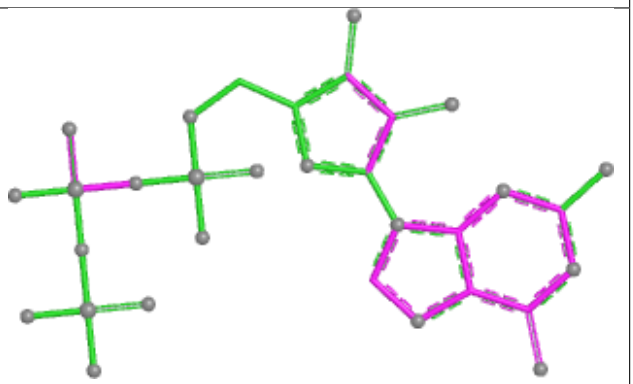
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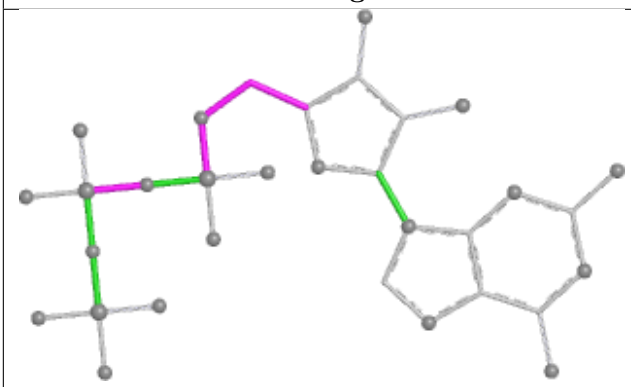
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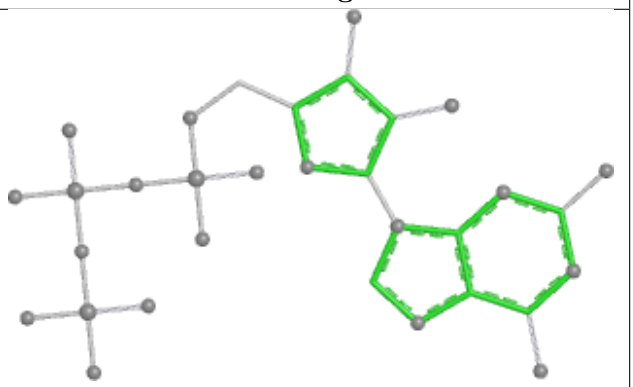
Bond lengths



Bond angles

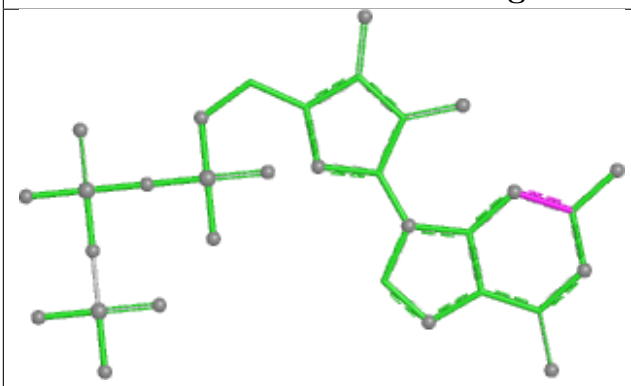


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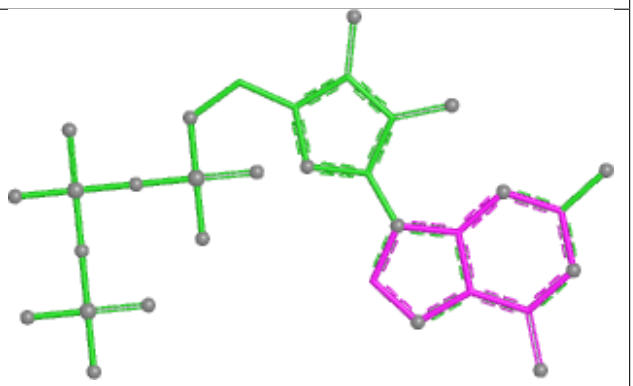


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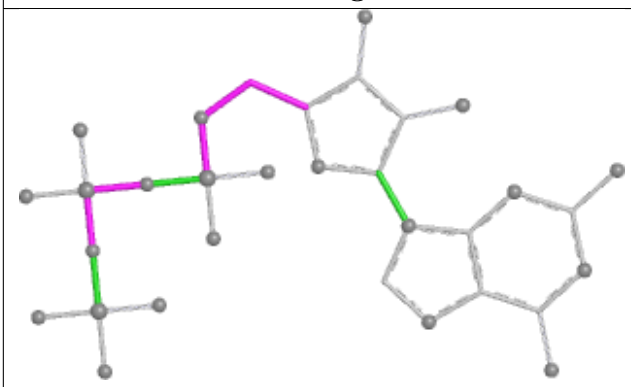
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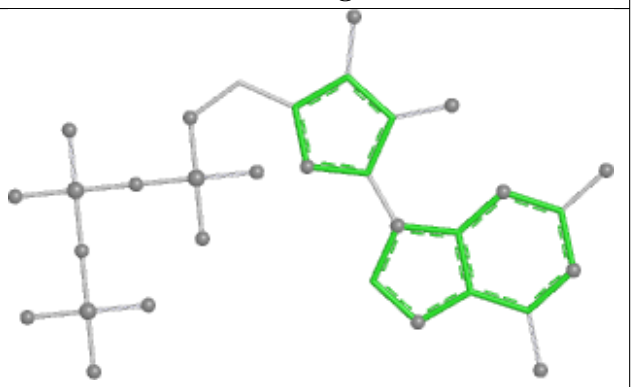
Bond lengths



Bond angles

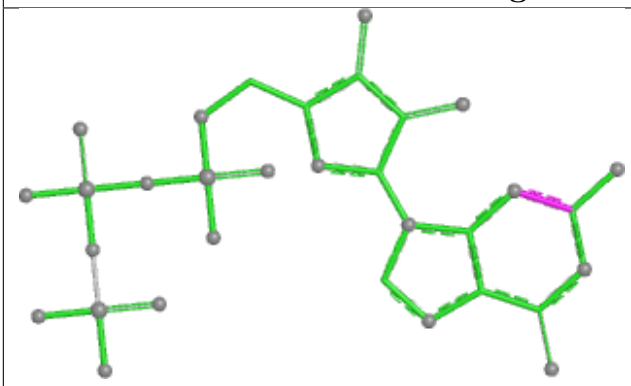


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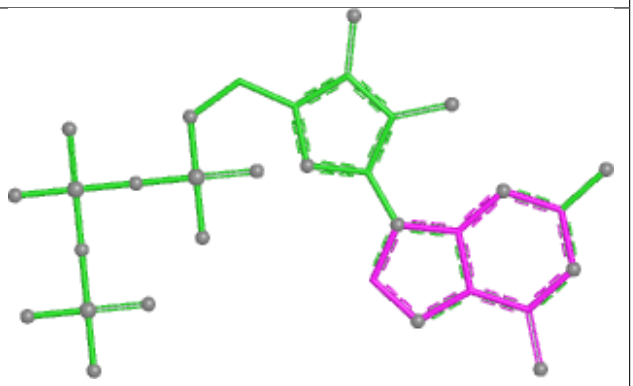


Rings

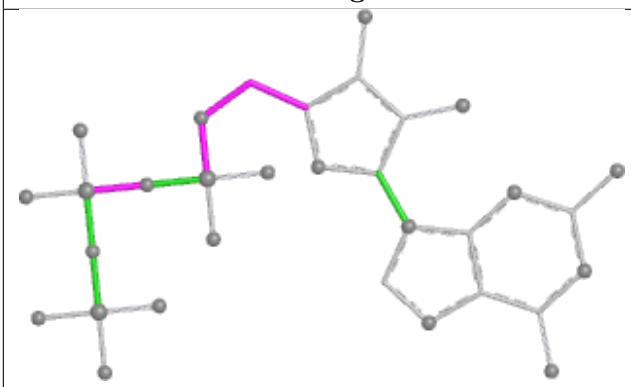
Ligand GTP OC 501



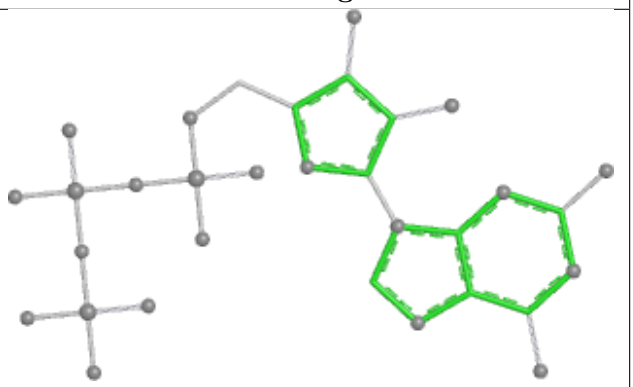
Bond lengths



Bond angles

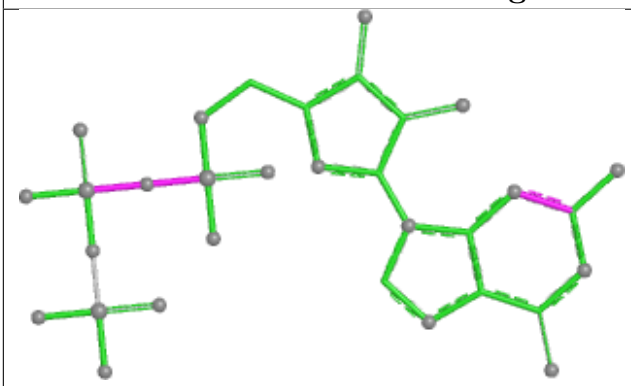


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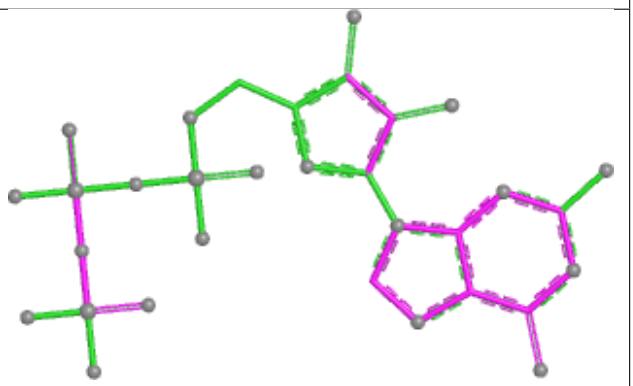


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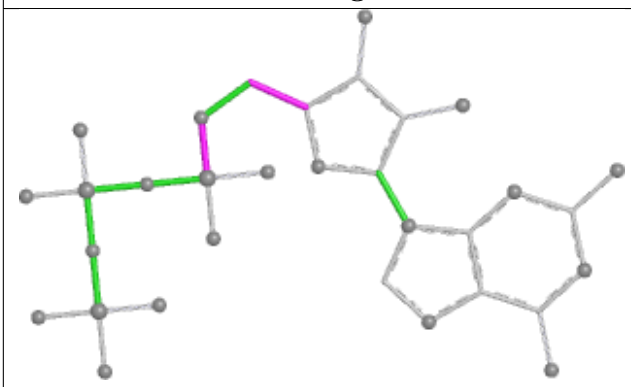
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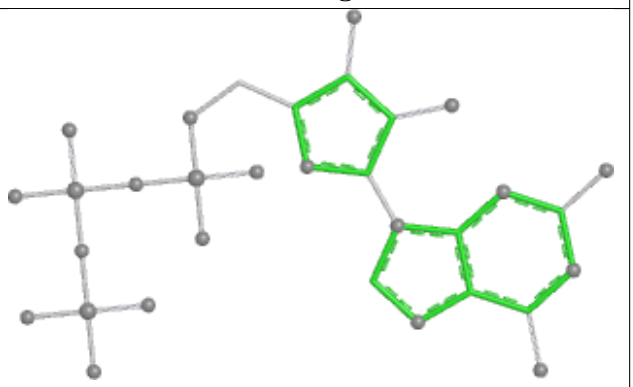
Bond lengths



Bond angles

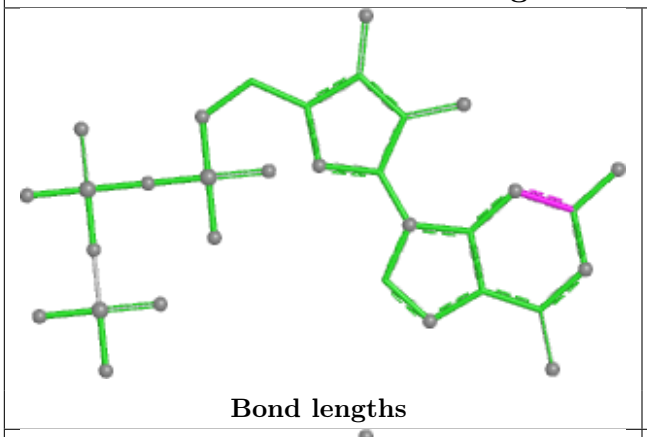


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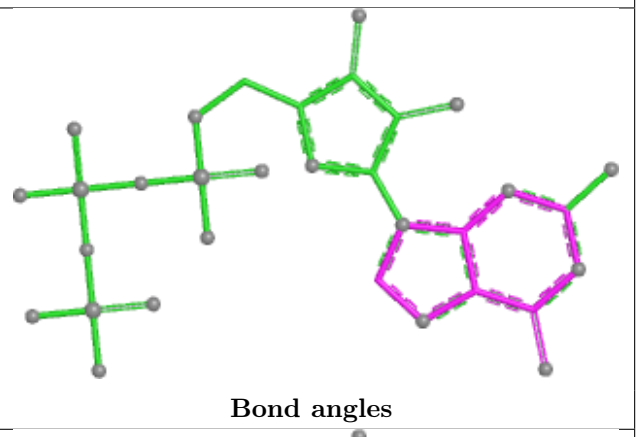


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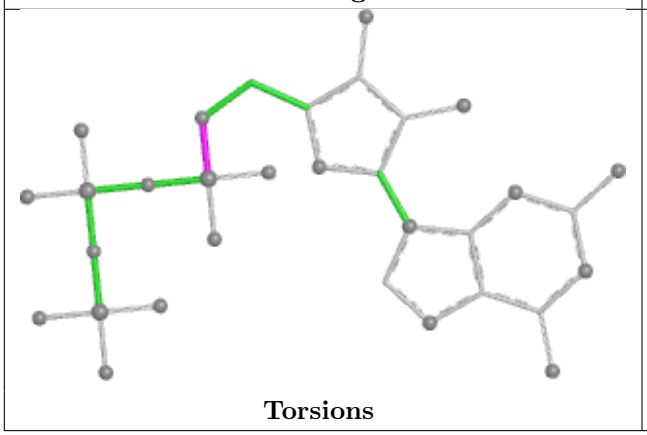
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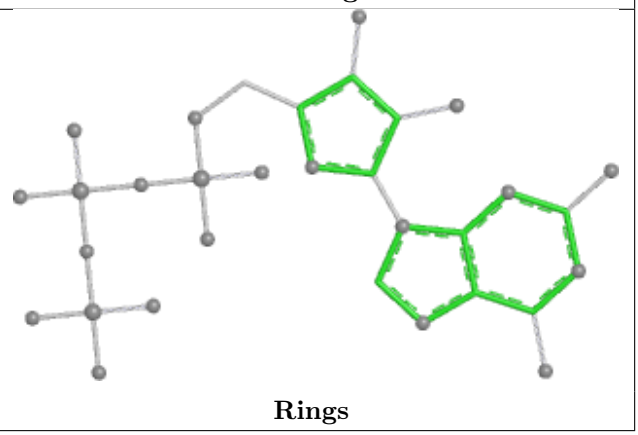
Bond lengths



Bond angles

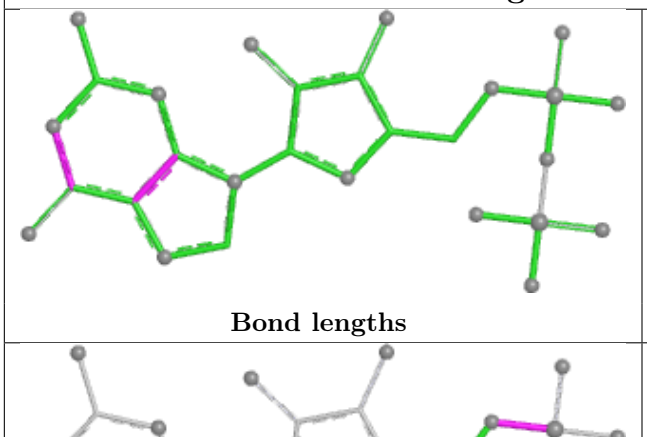


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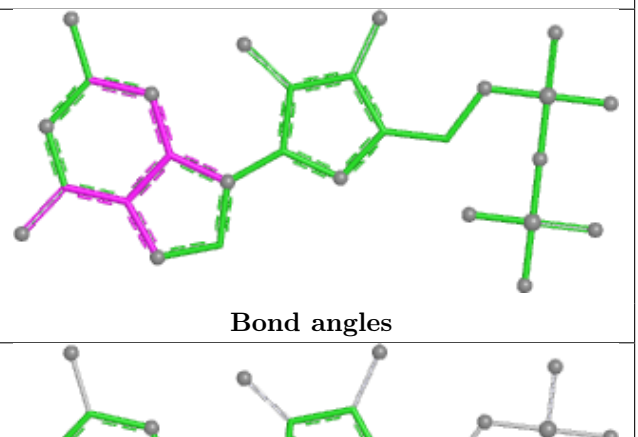


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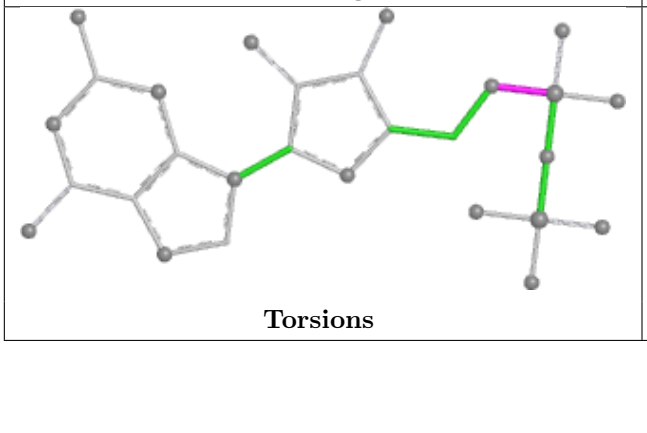
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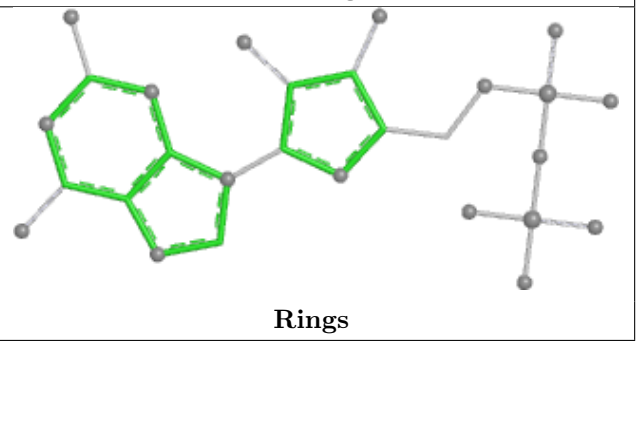
Bond lengths



Bond angles

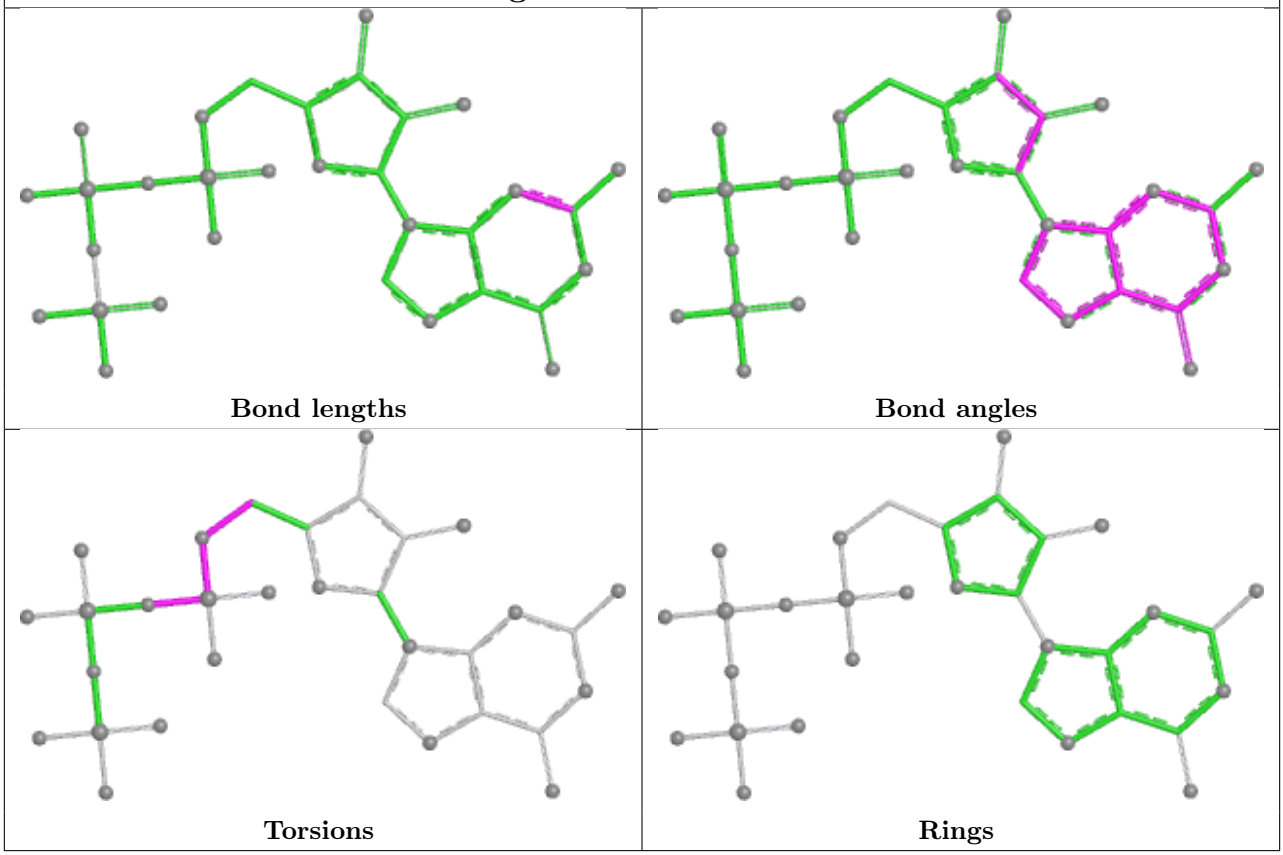


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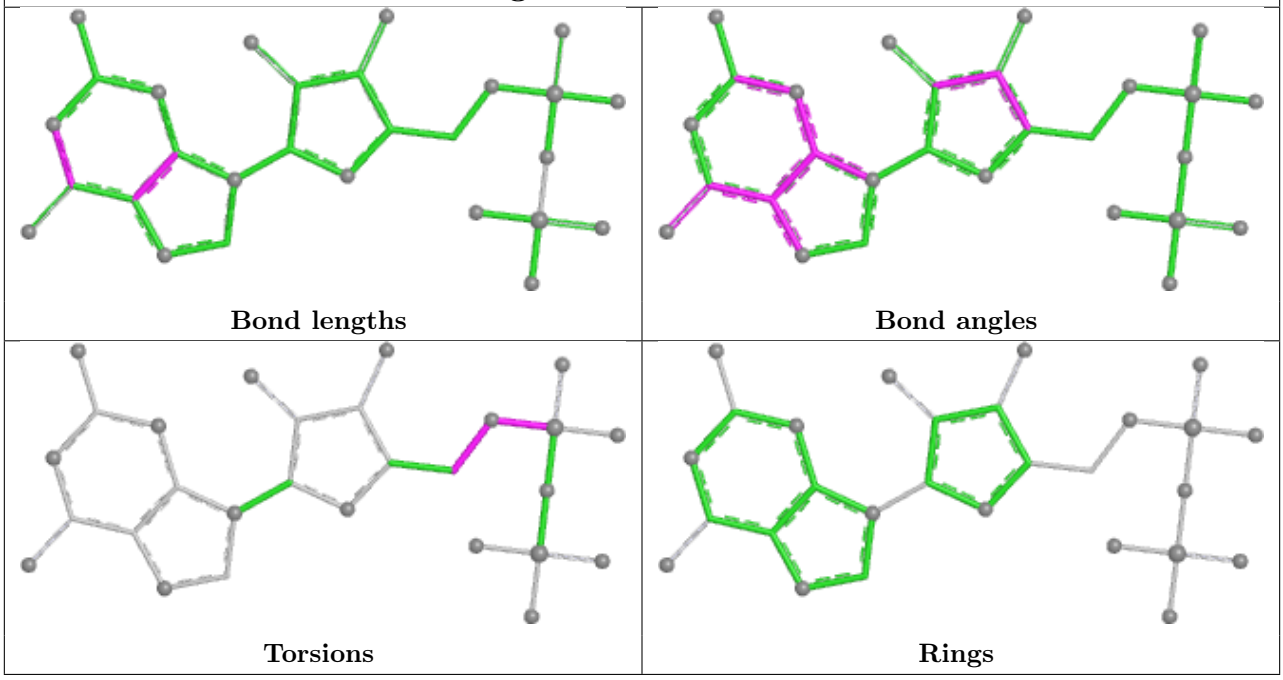


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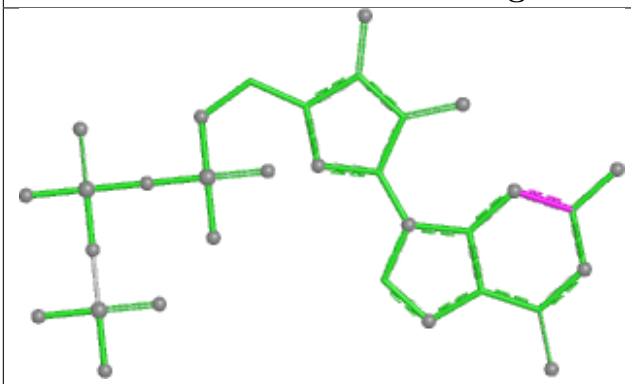
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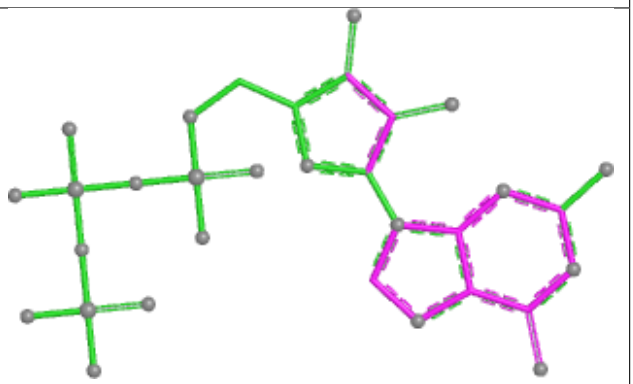
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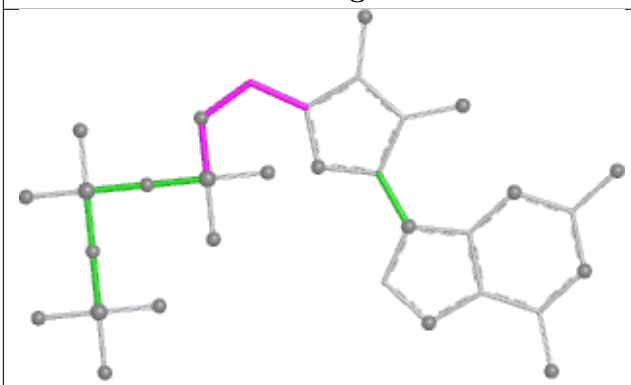
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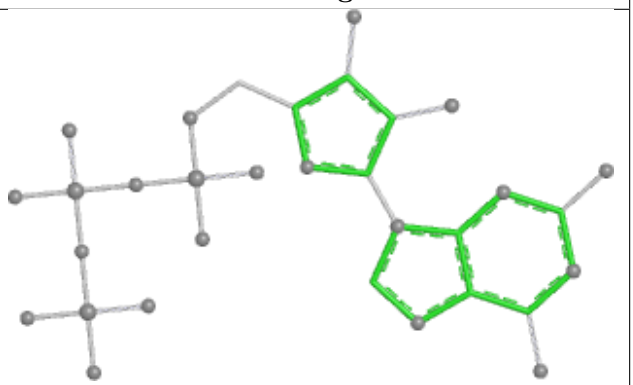
Bond lengths



Bond angles

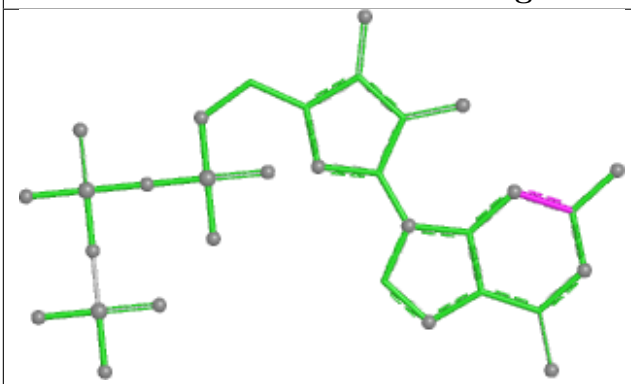


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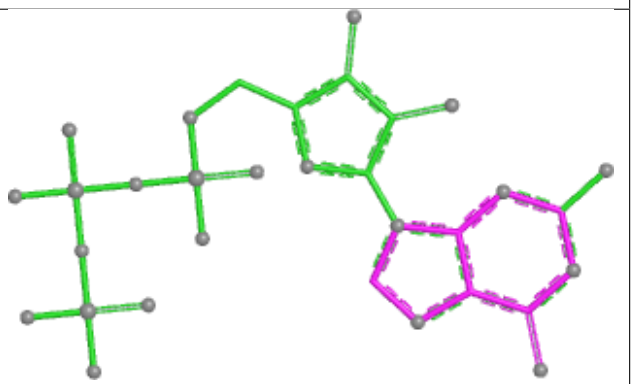


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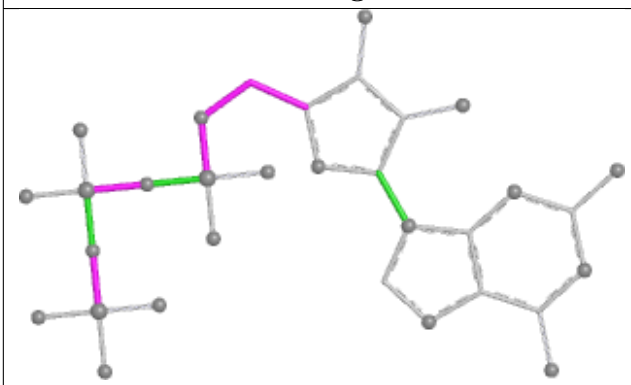
Ligand GTP KI 501



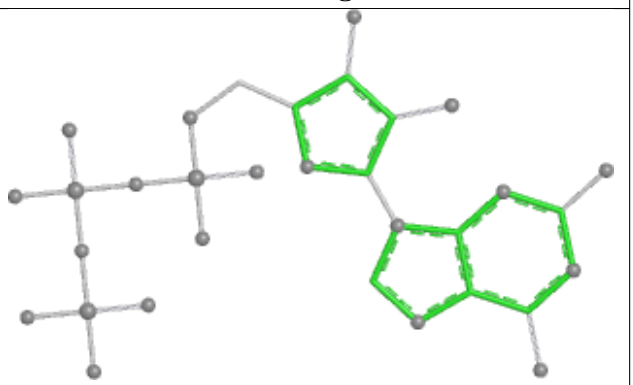
Bond lengths



Bond angles

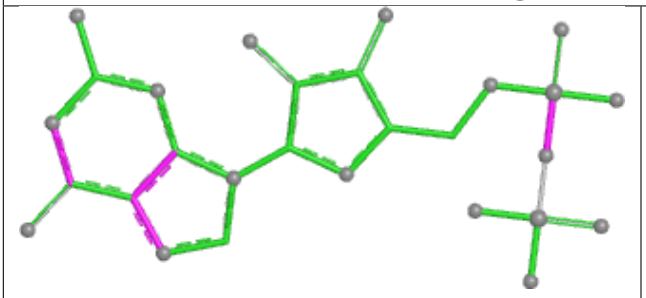


Torsions

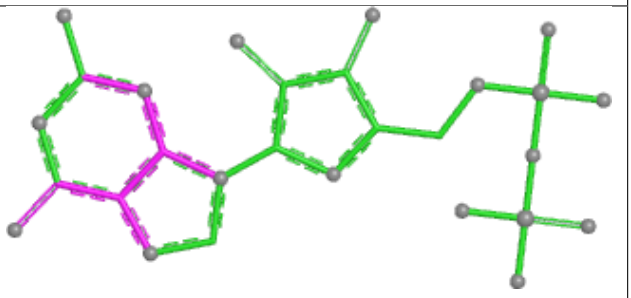


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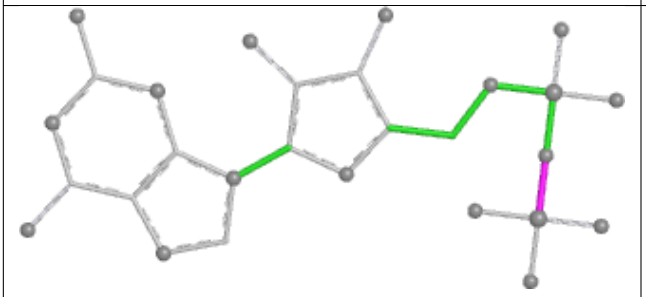
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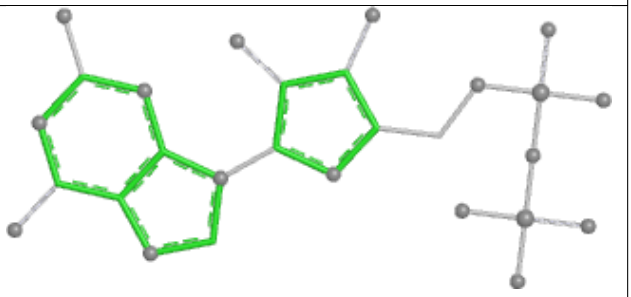
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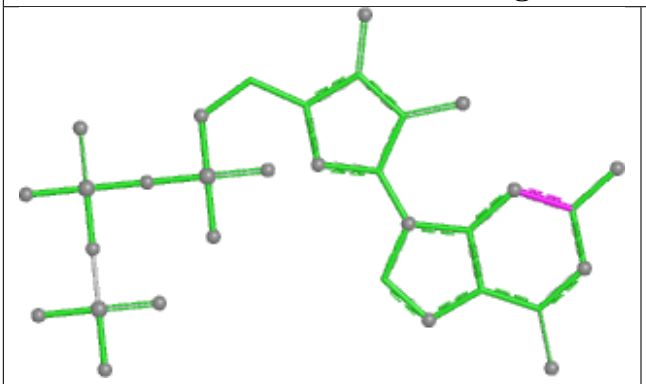


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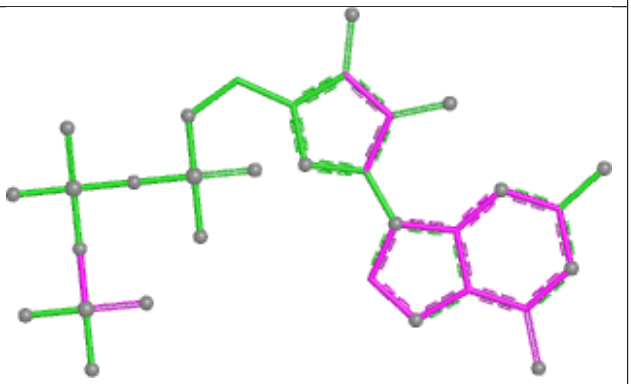


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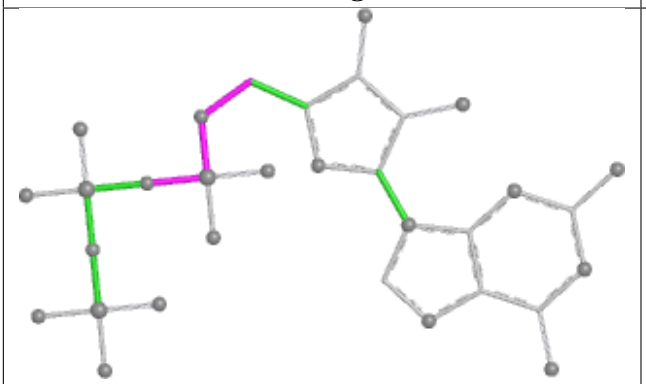
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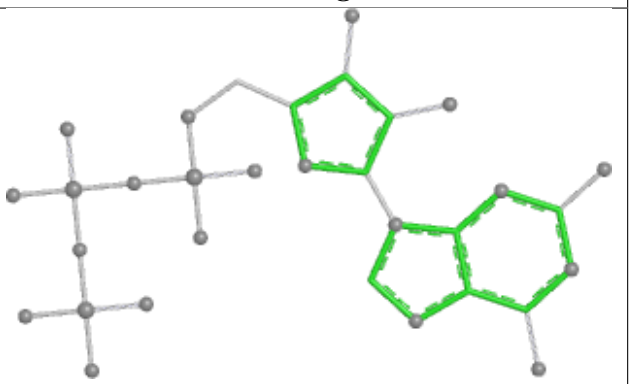
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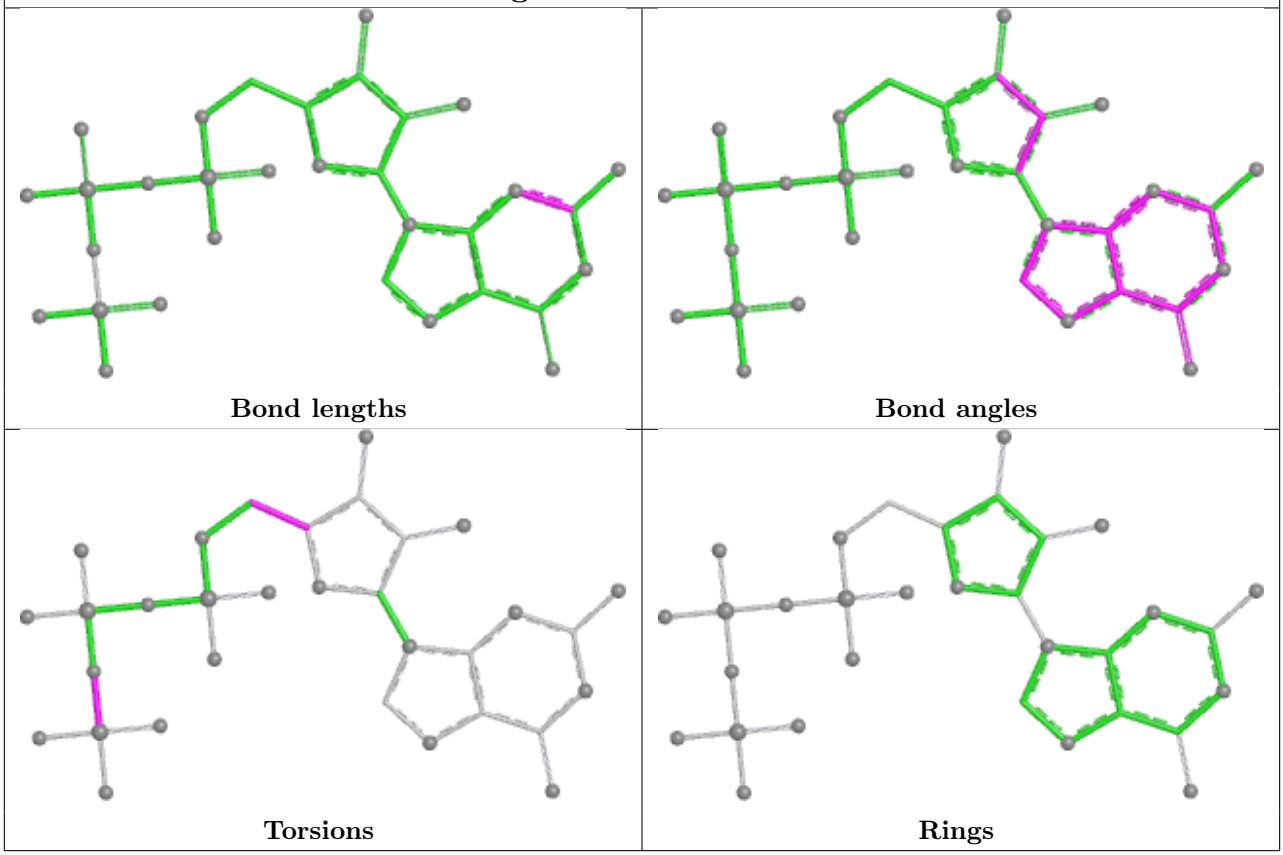


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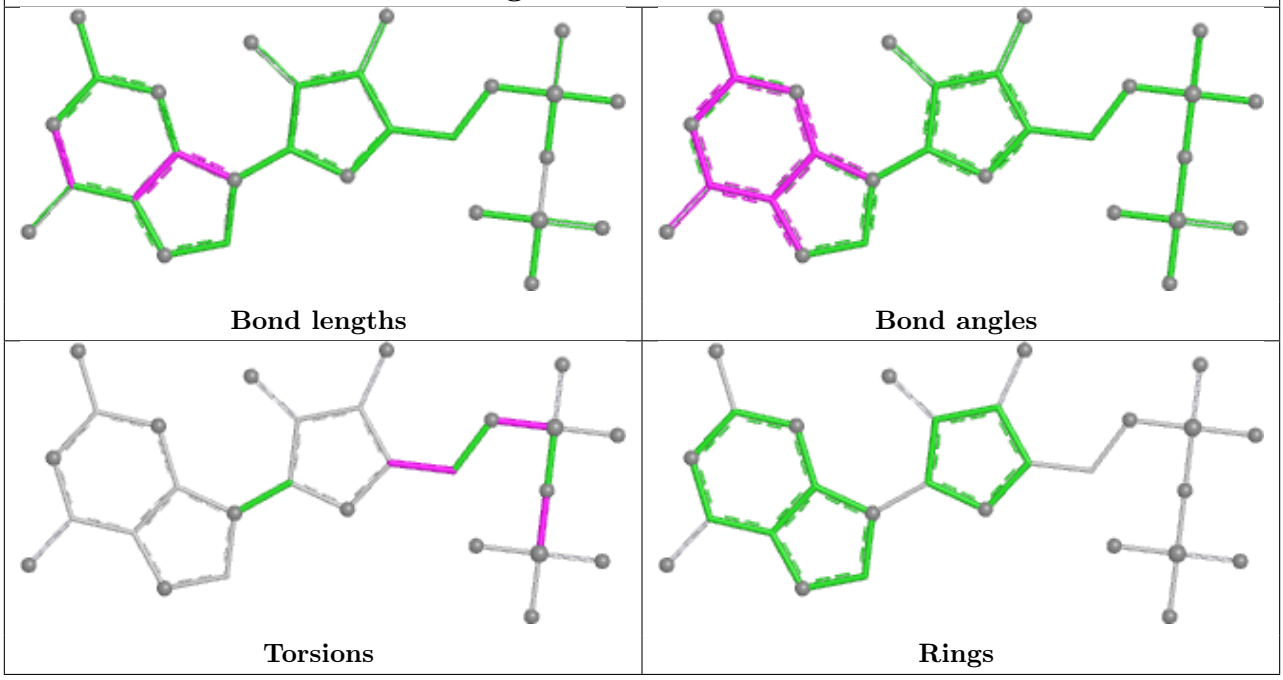


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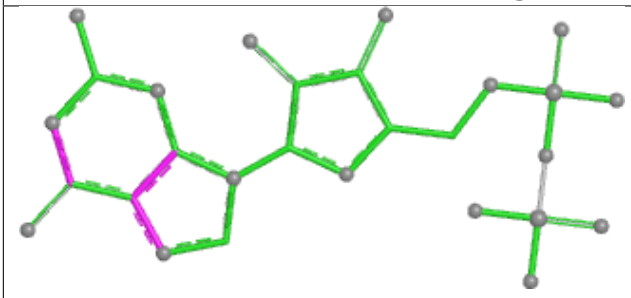
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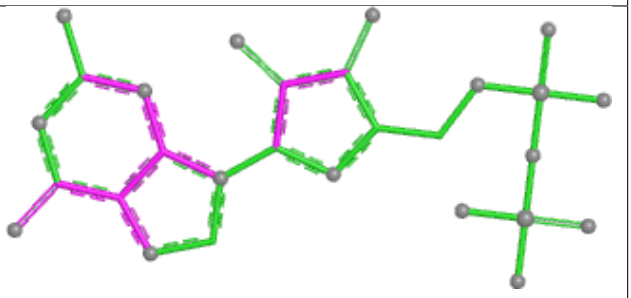
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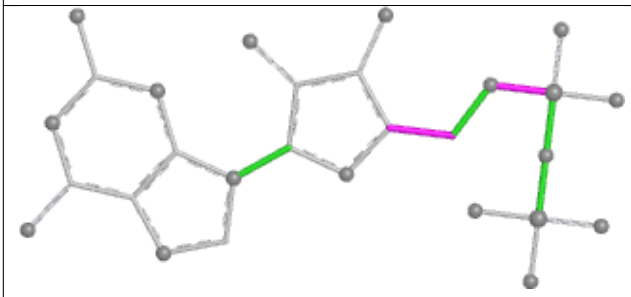
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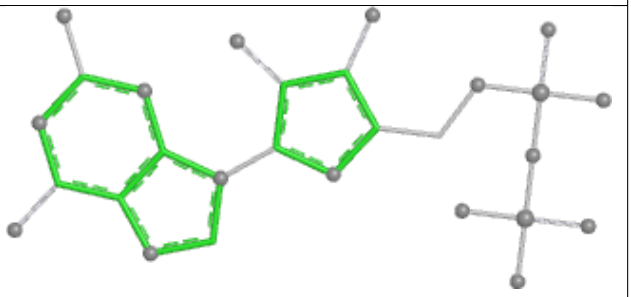
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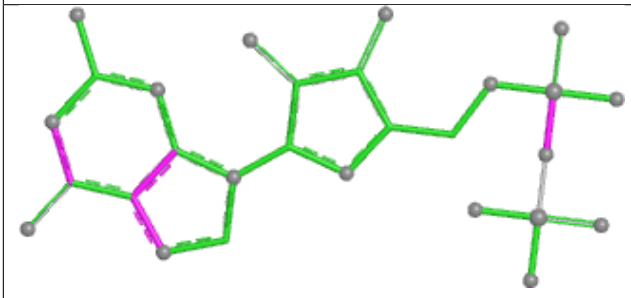


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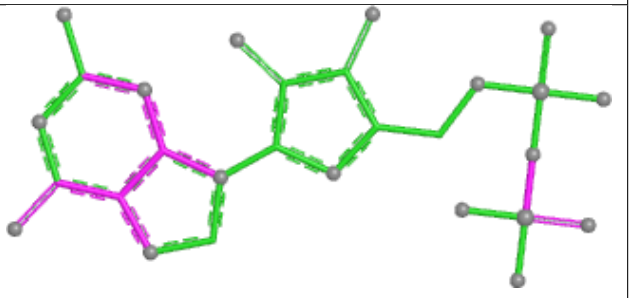


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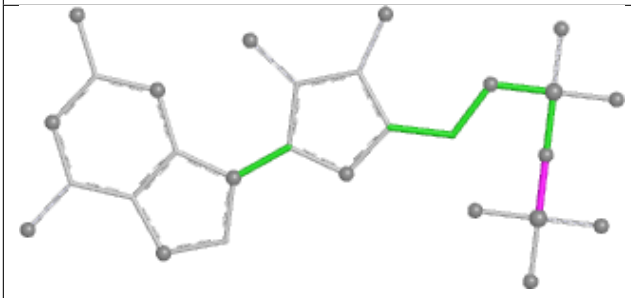
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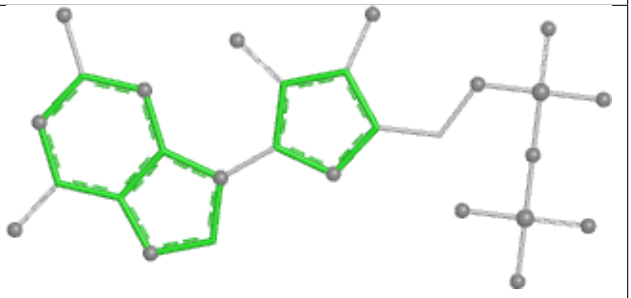
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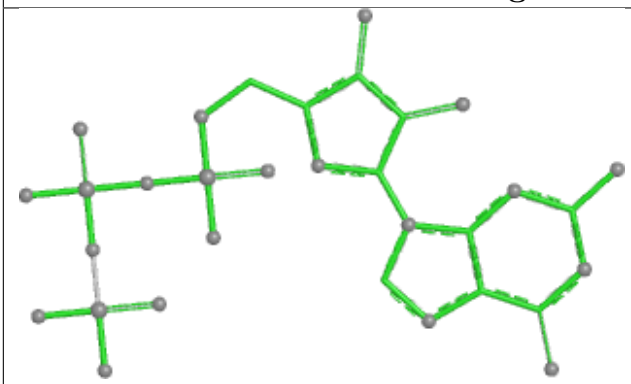


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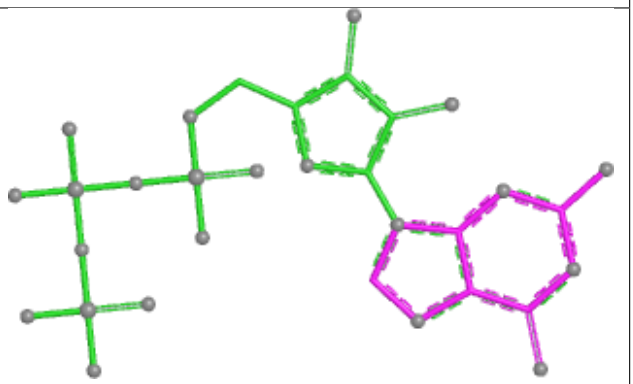


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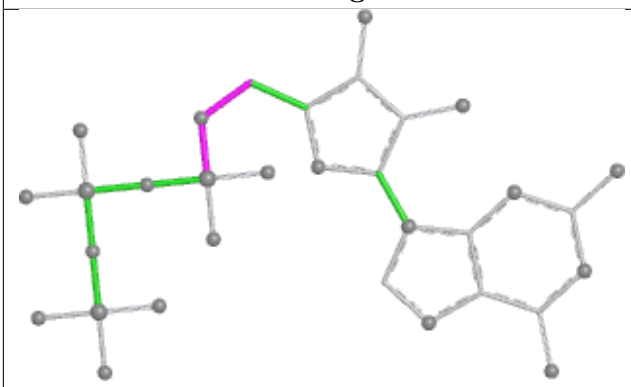
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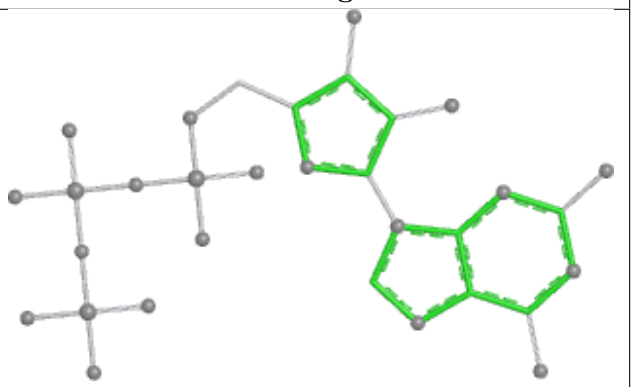
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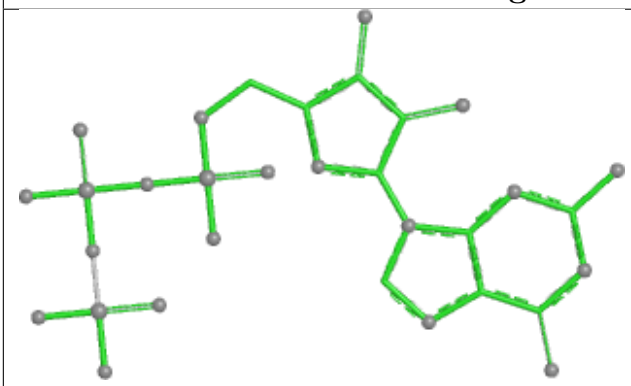


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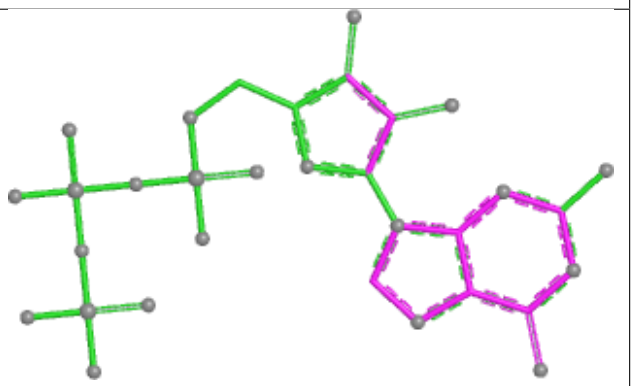


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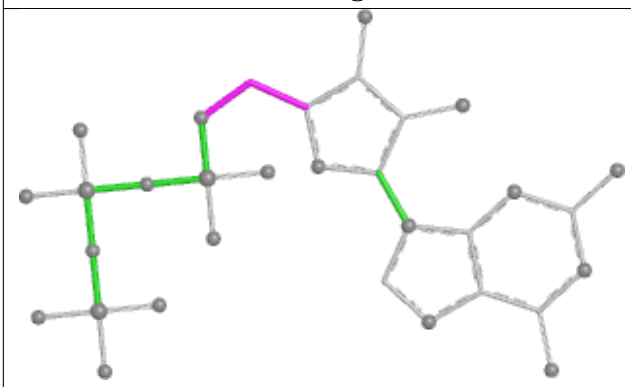
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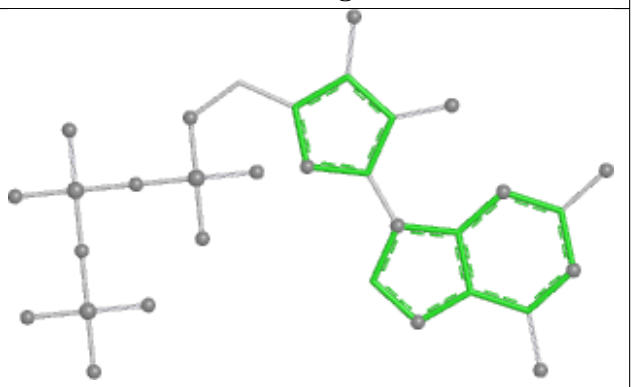
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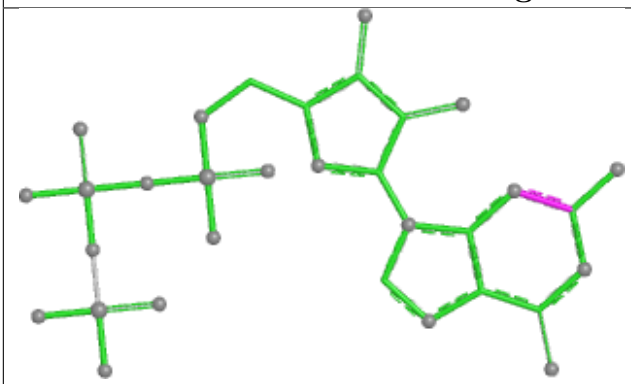


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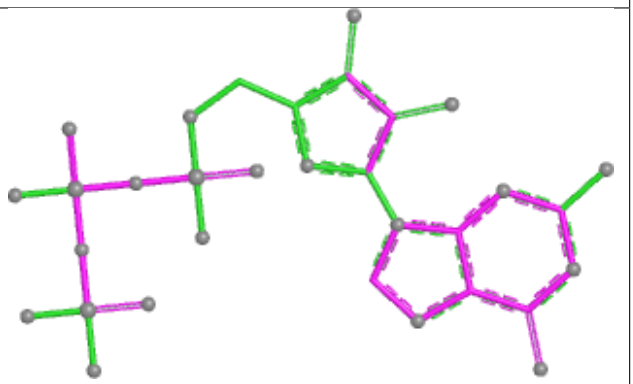


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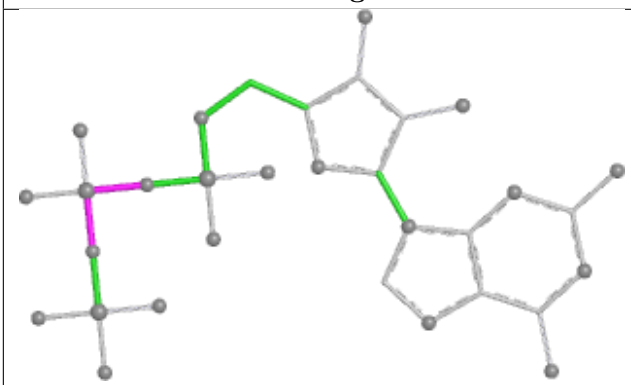
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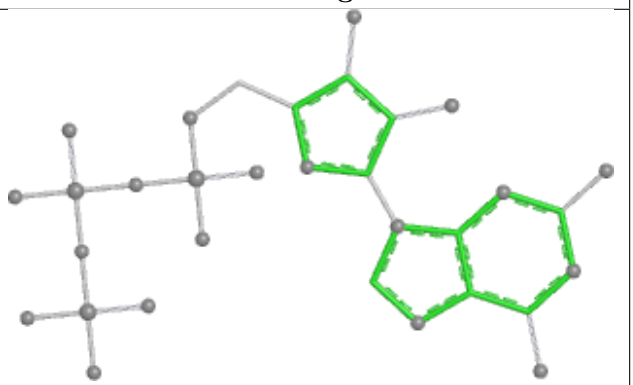
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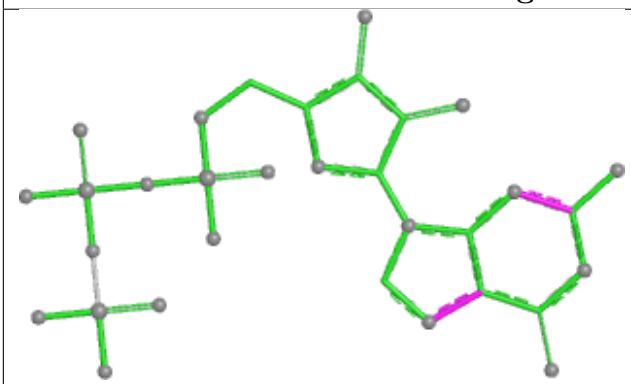


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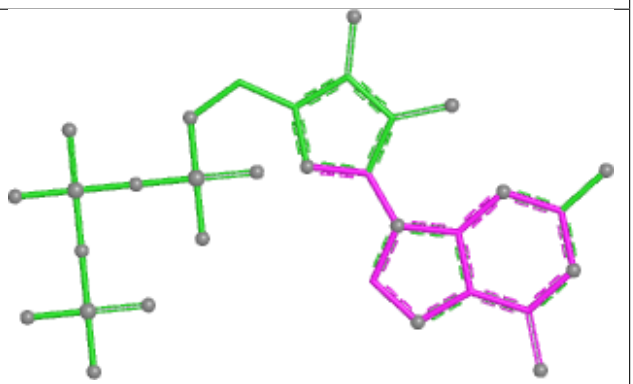


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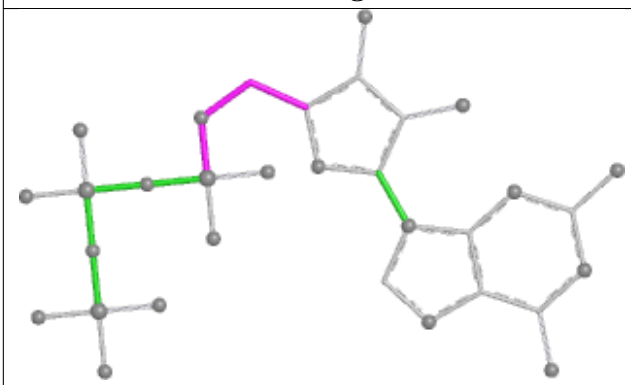
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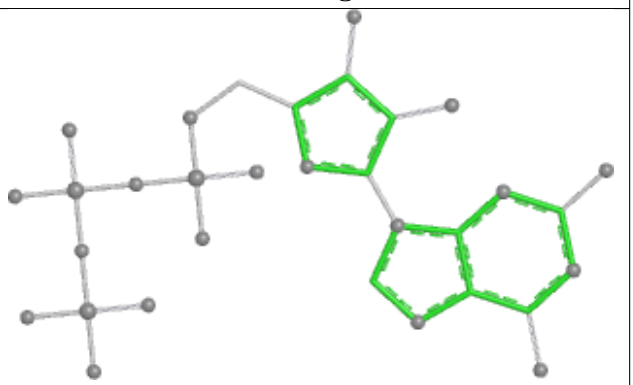
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Bond angles

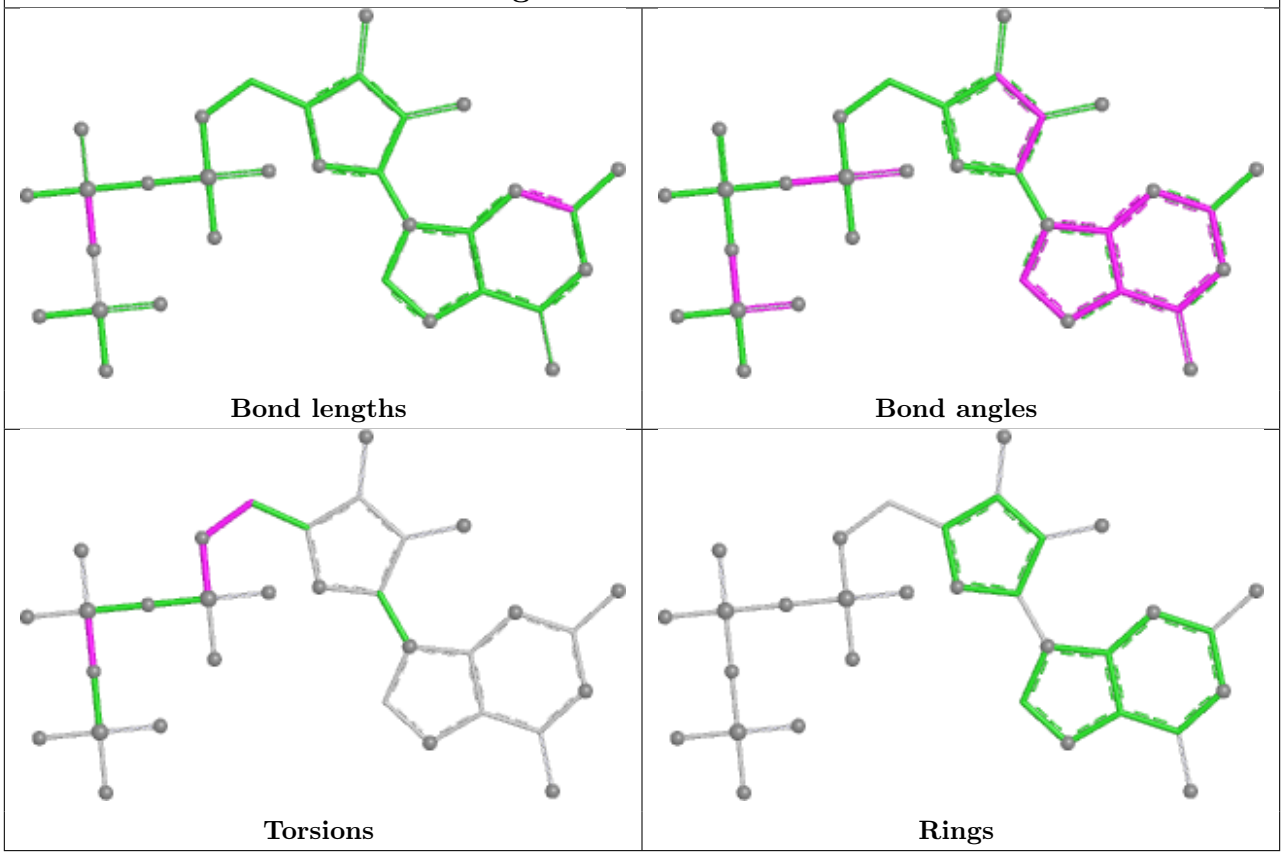


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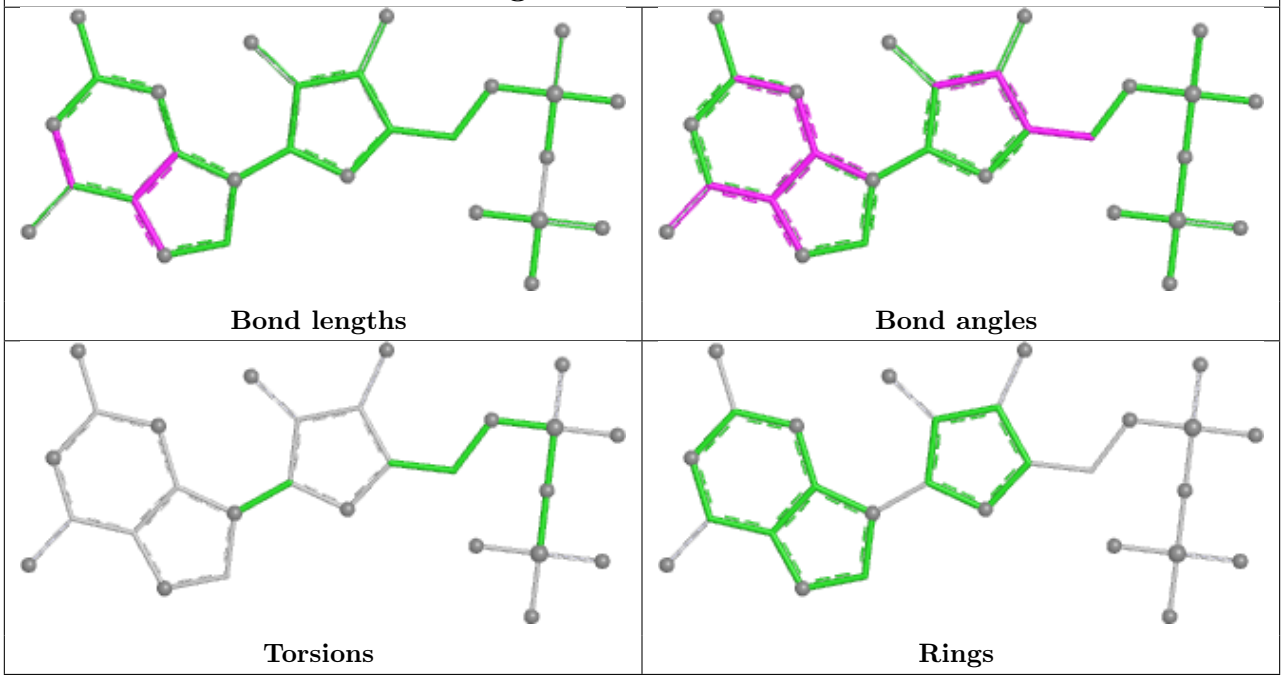


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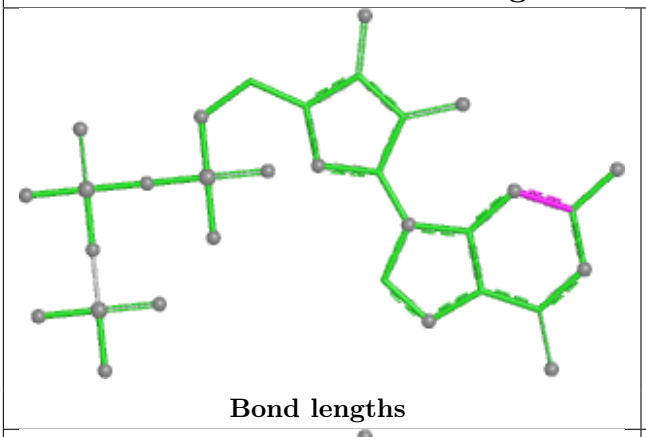
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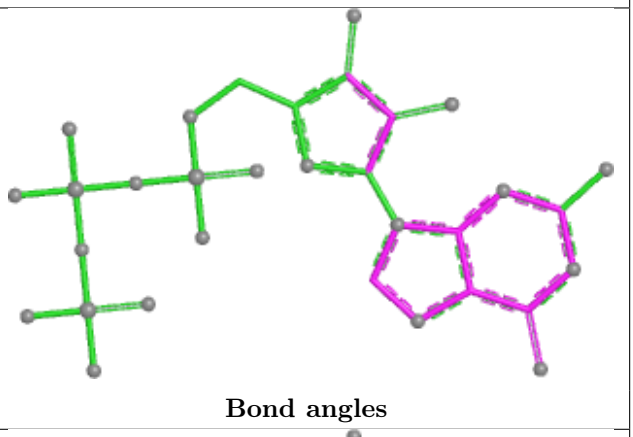
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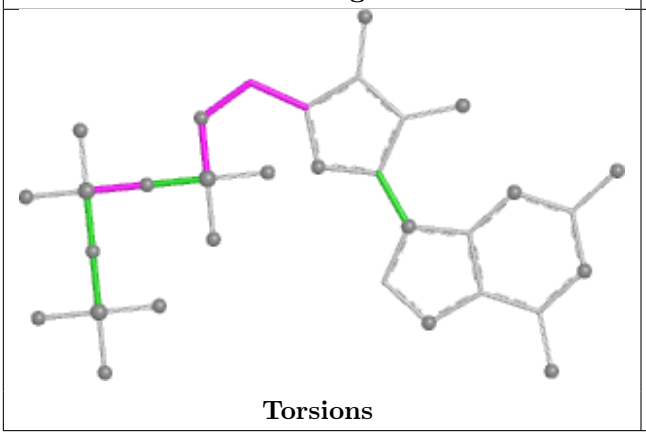
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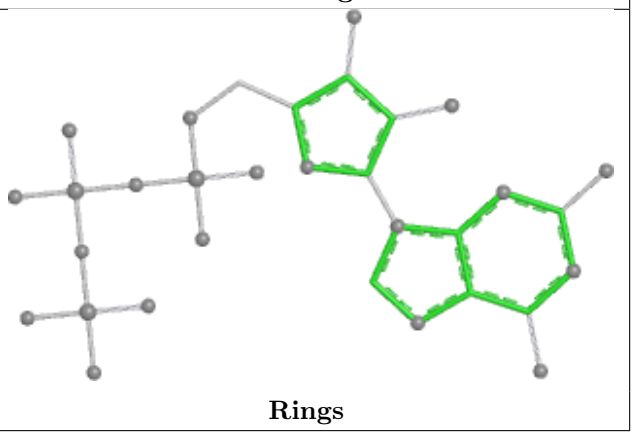
Bond lengths



Bond angles

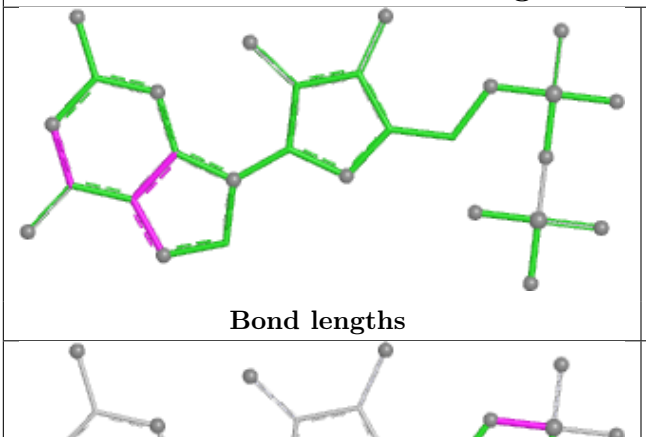


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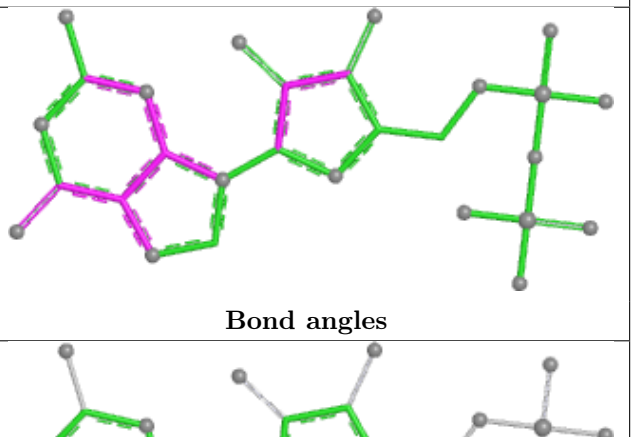


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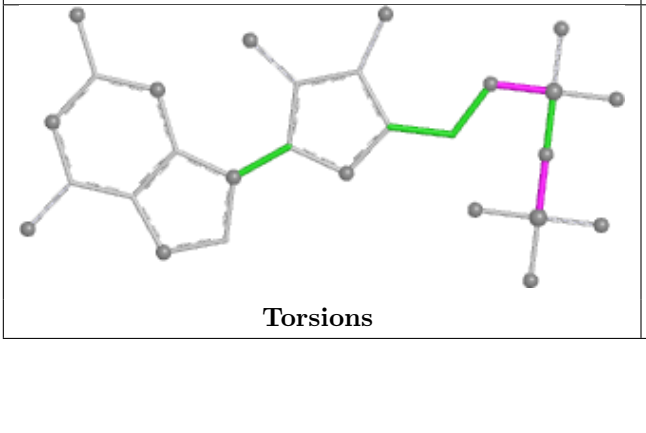
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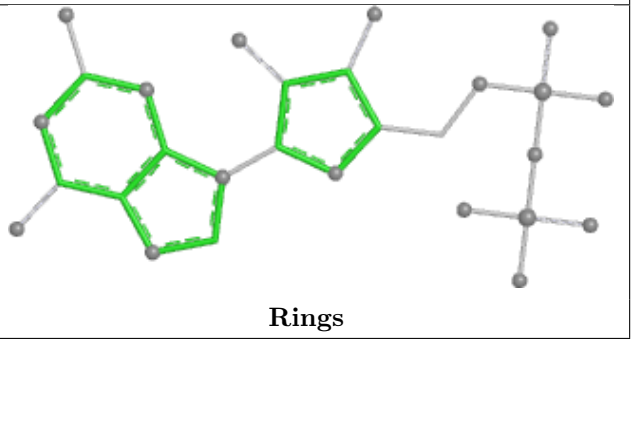
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Bond angles

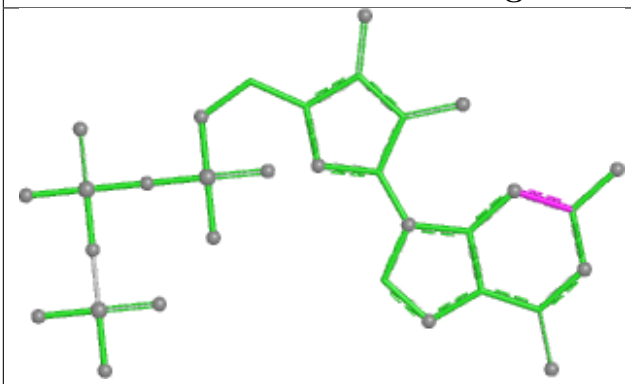


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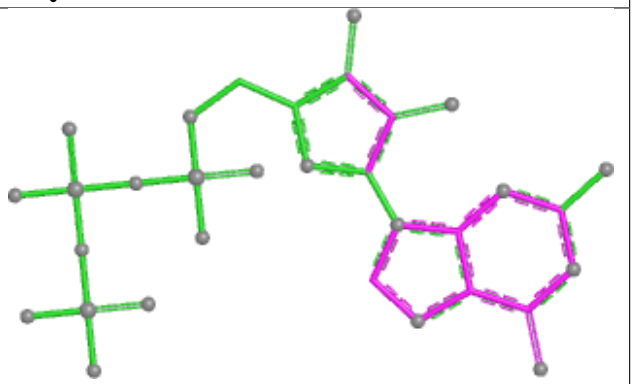


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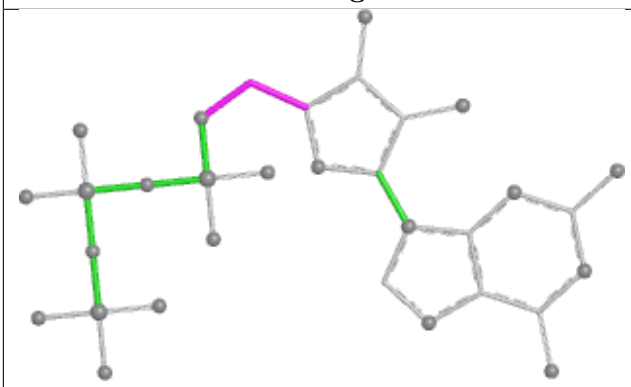
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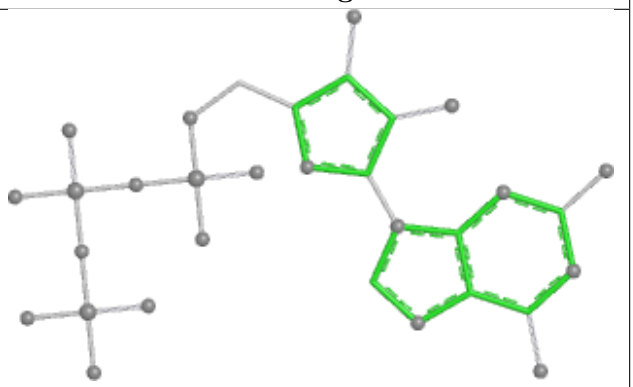
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Bond angles

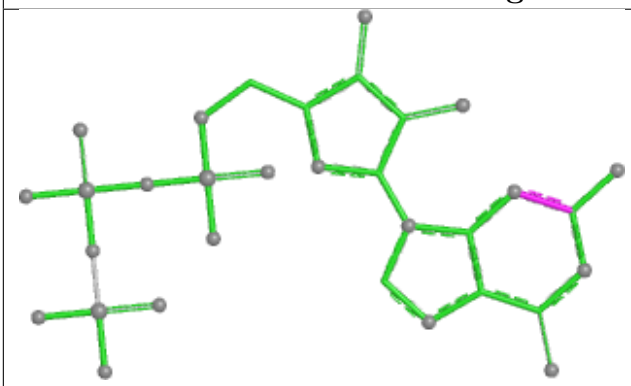


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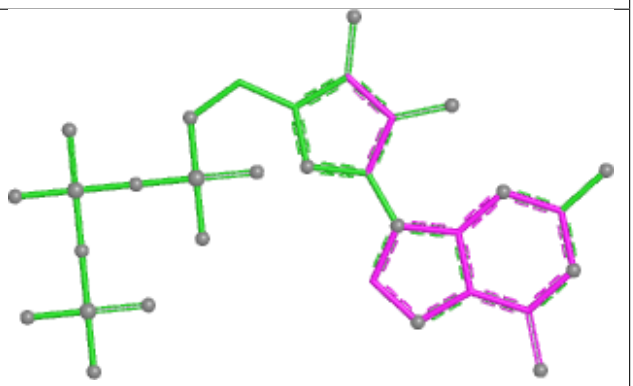


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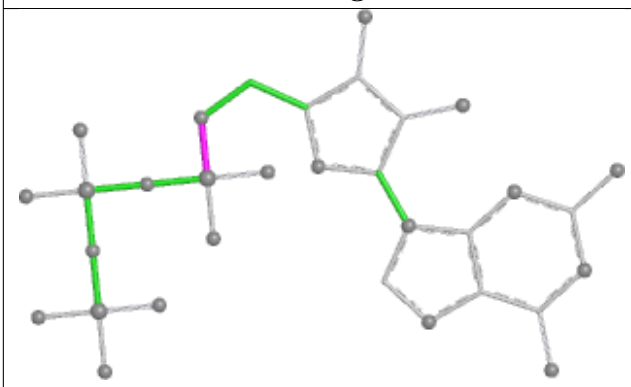
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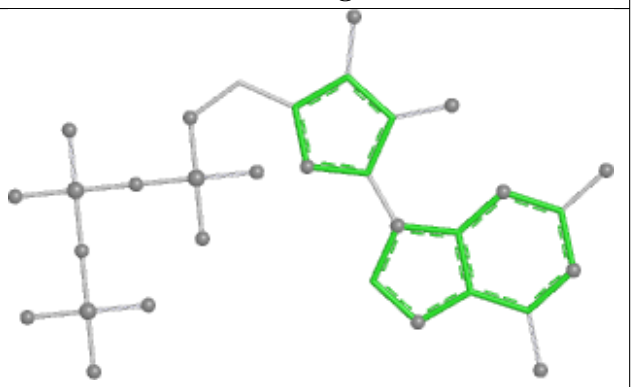
Bond lengths



Bond angles

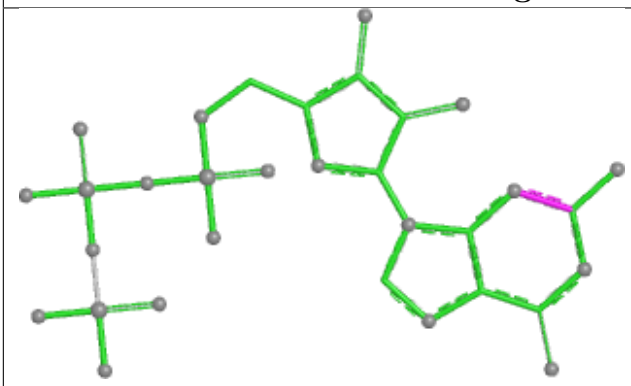


Torsions

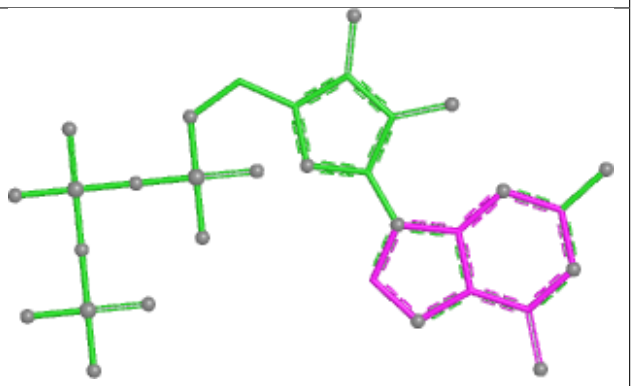


Rings

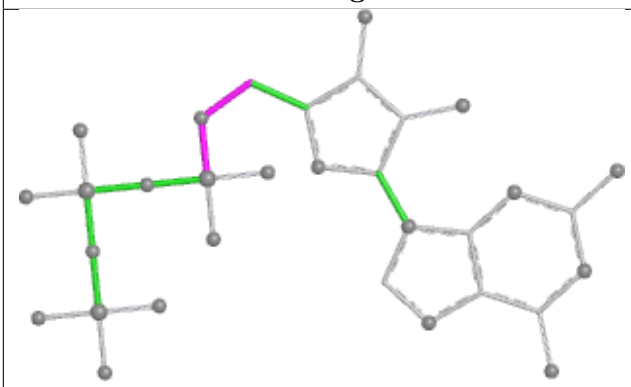
Ligand GTP SE 501



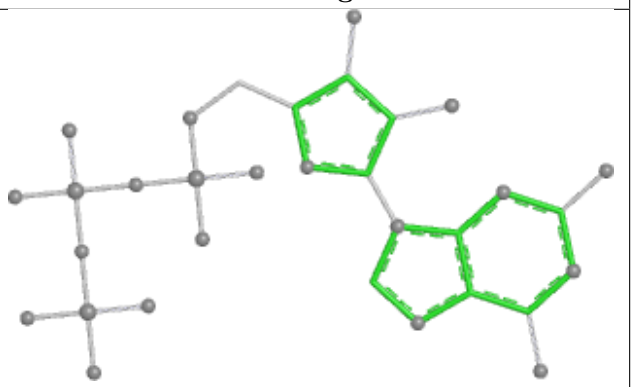
Bond lengths



Bond angles

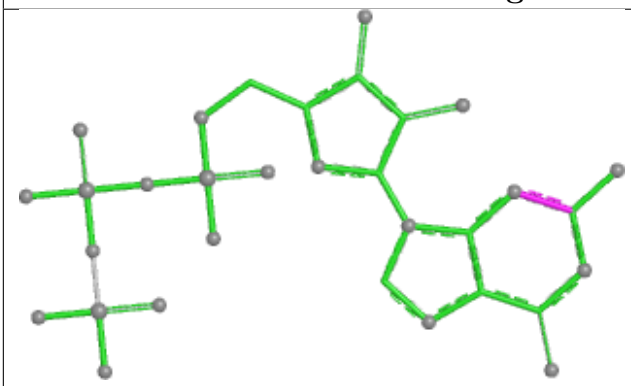


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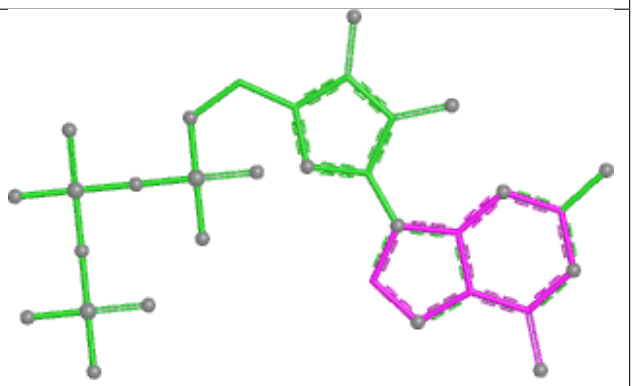


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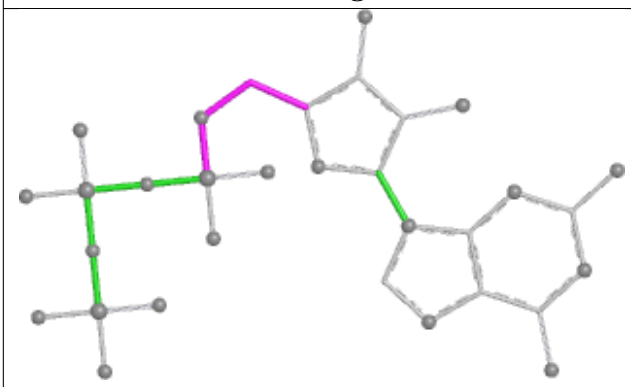
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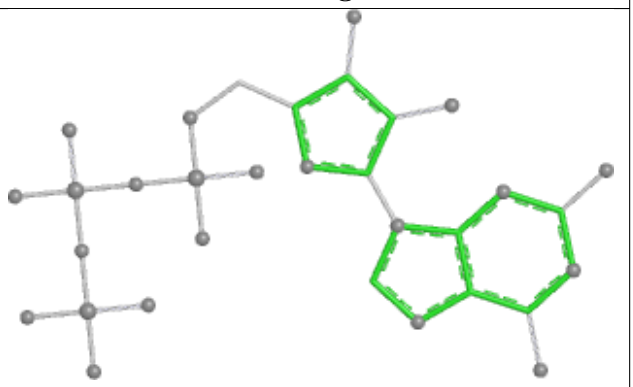
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Bond angles

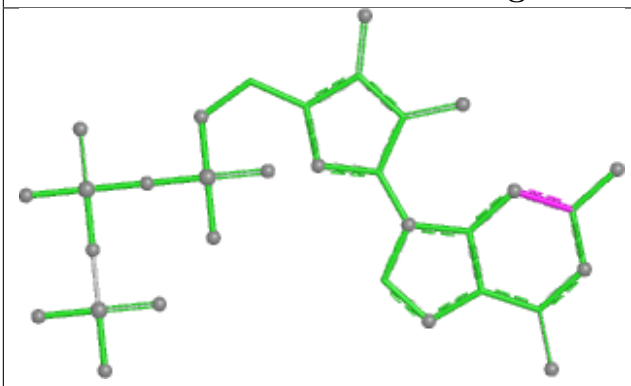


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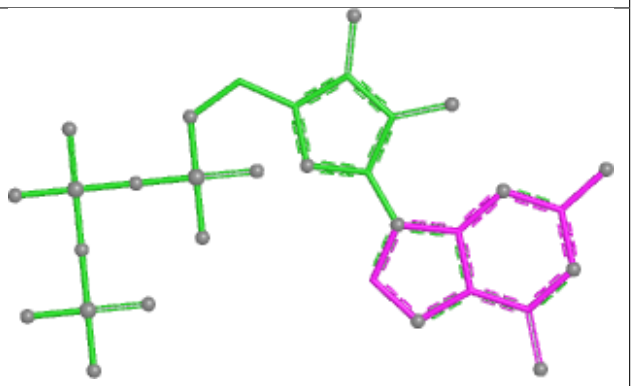


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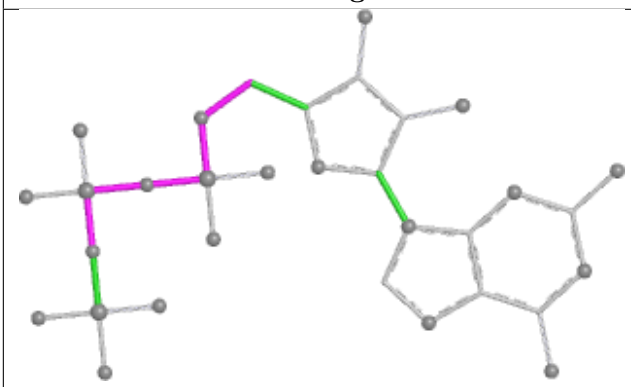
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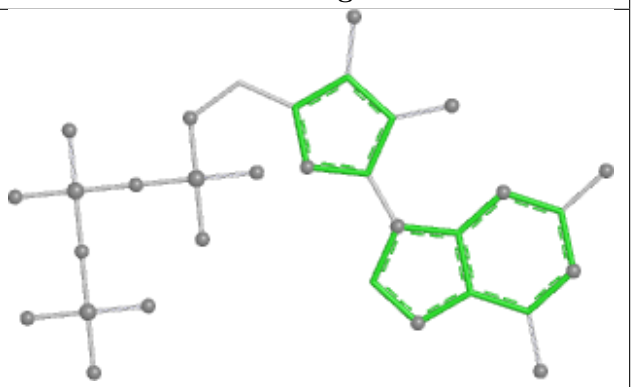
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Bond angles

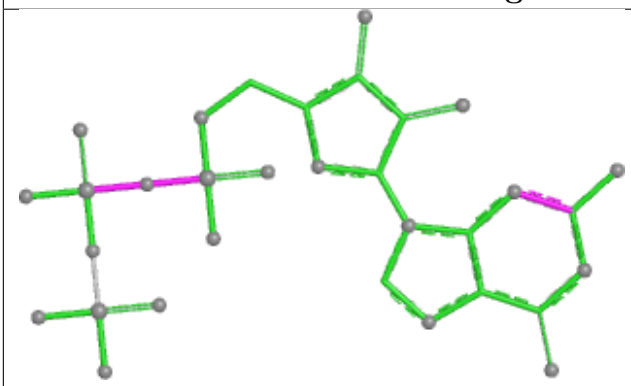


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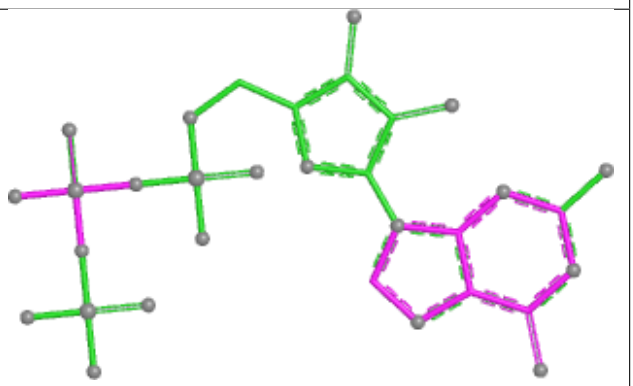


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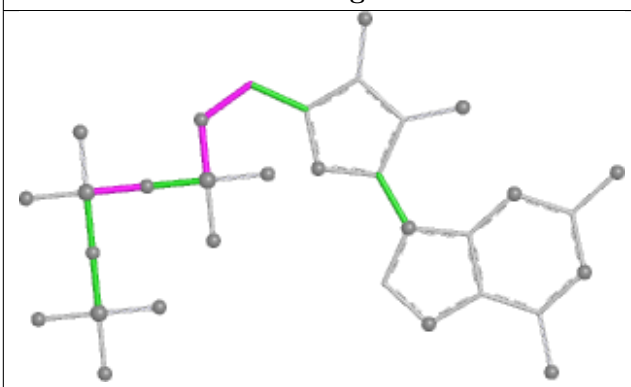
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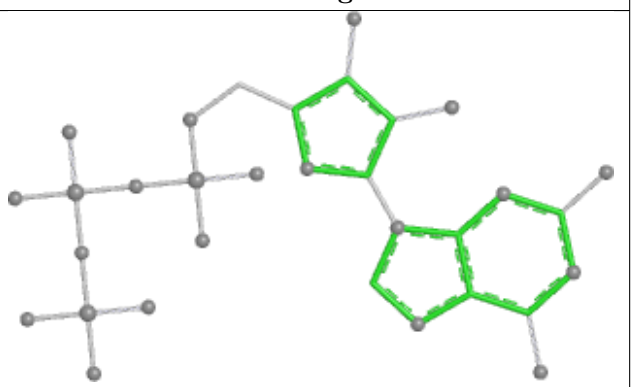
Bond lengths



Bond angles

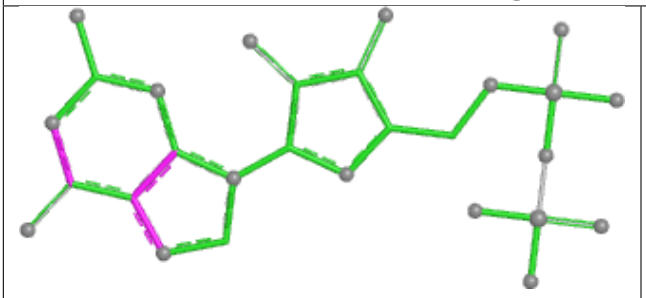


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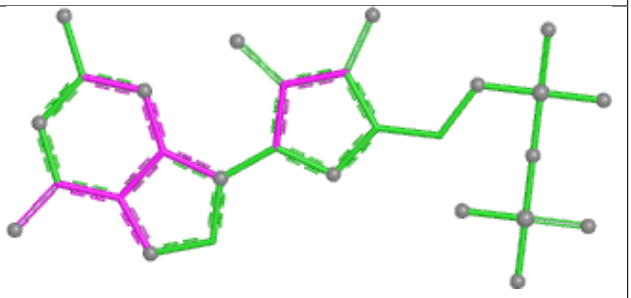


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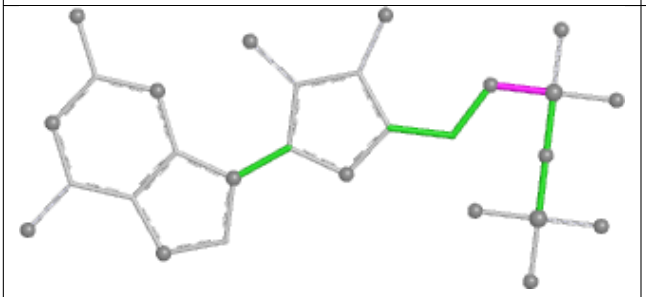
Ligand GDP AB 501



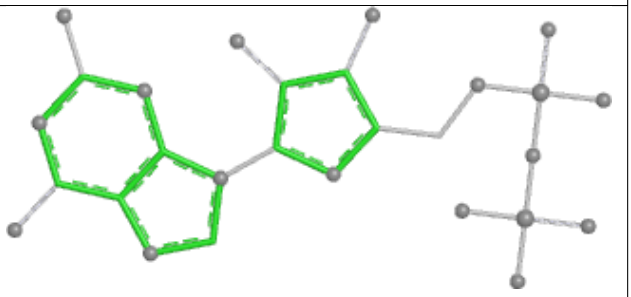
Bond lengths



Bond angles

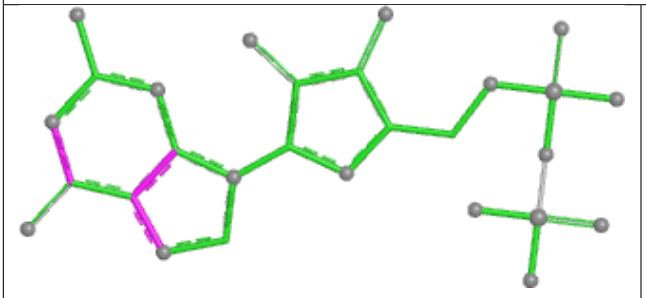


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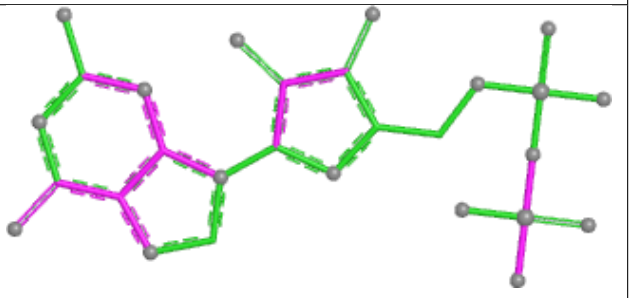


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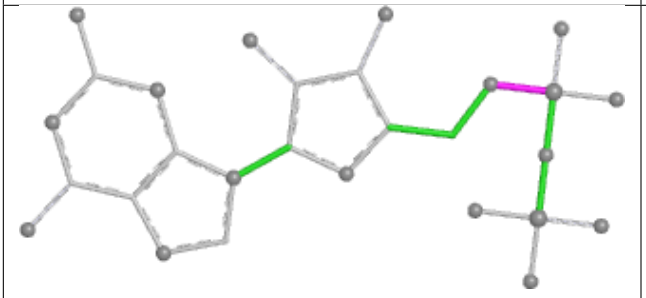
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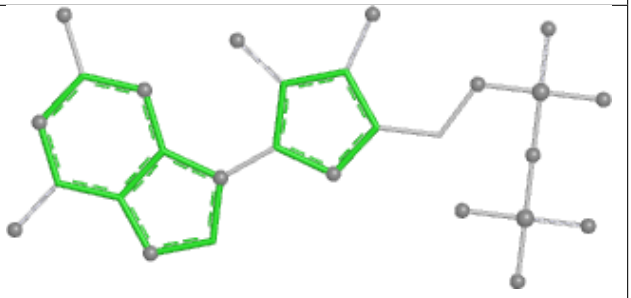
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Bond angles

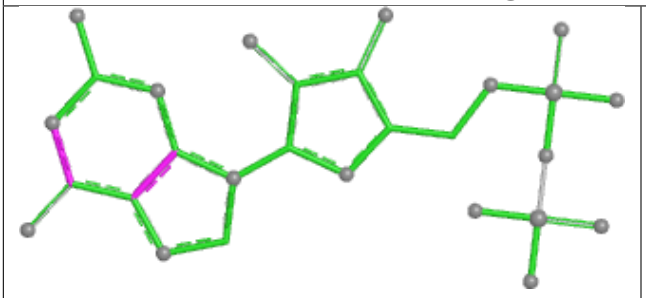


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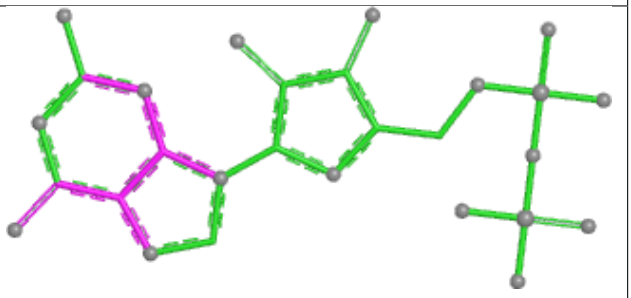


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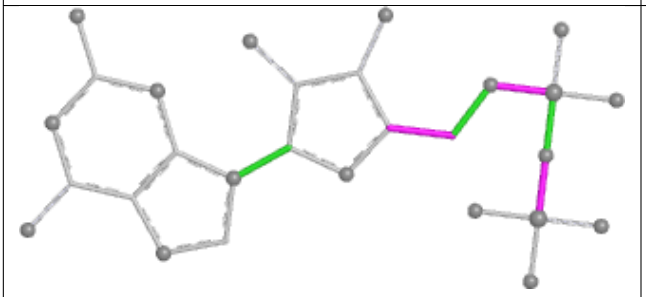
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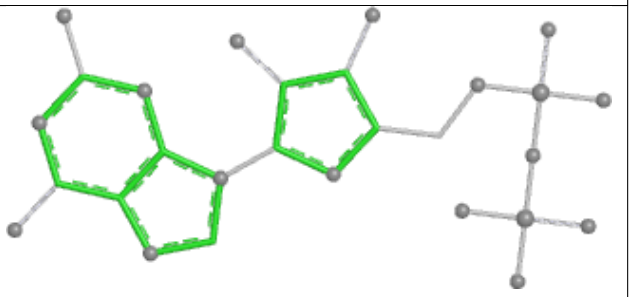
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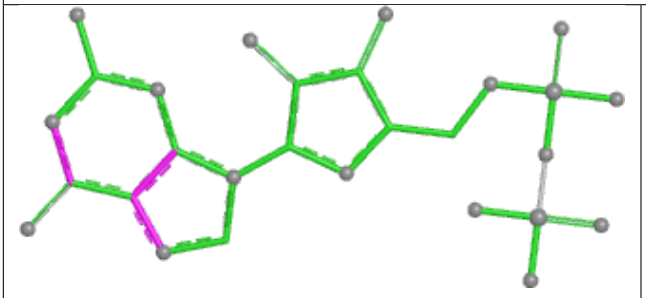


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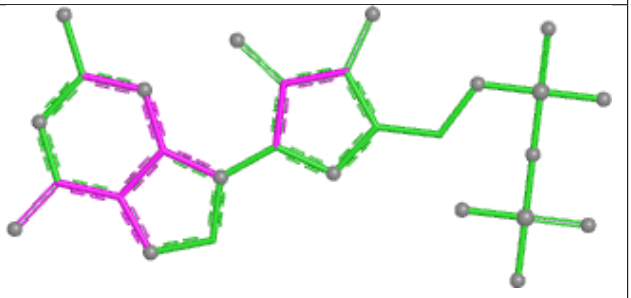


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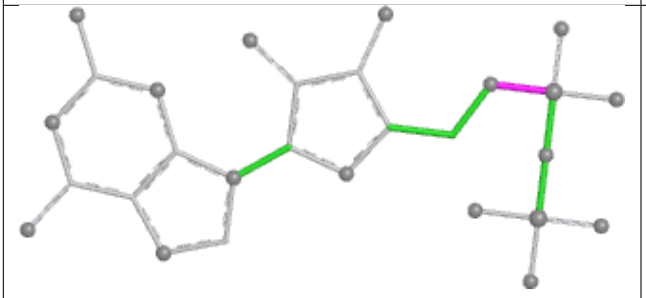
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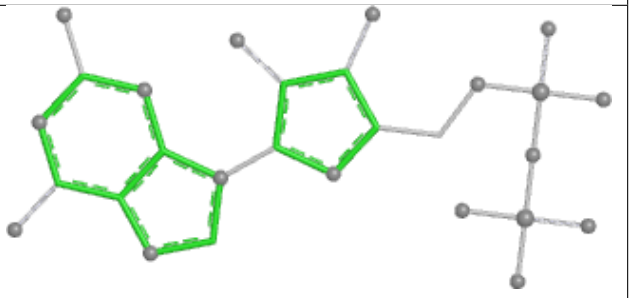
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Bond angles

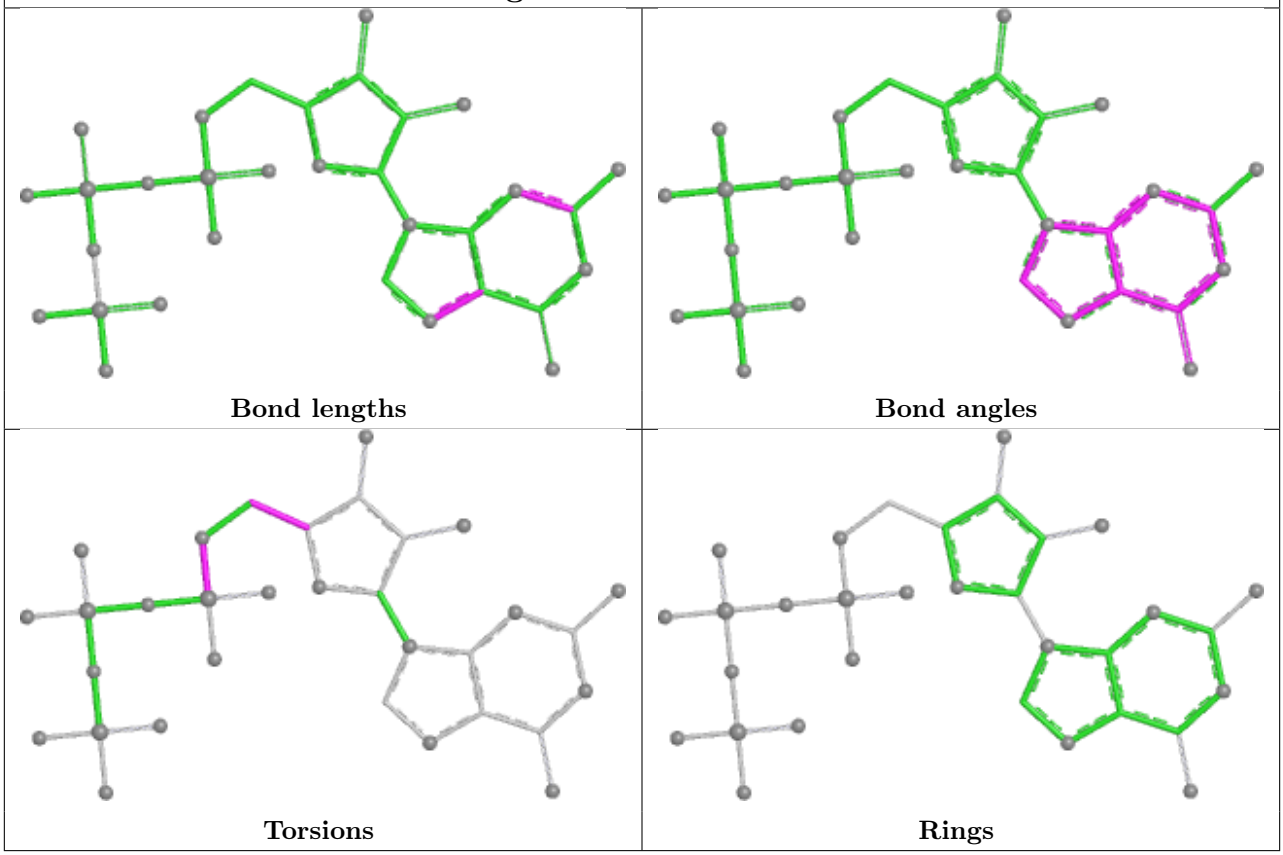


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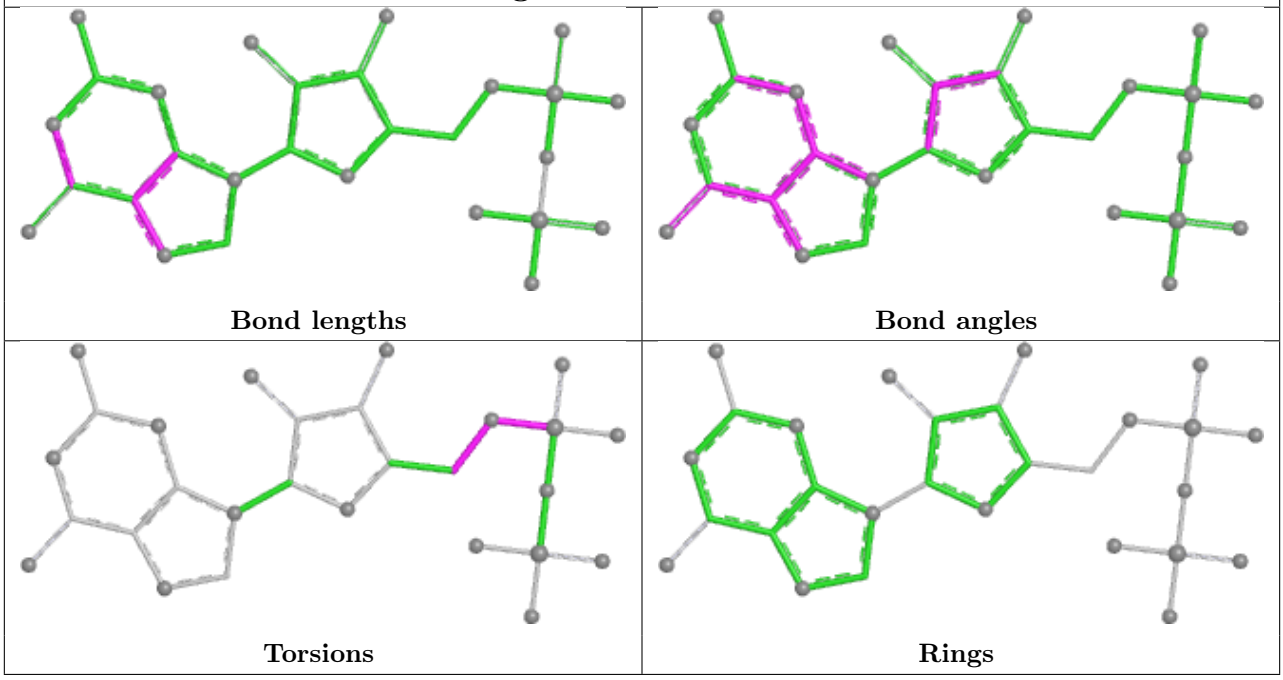


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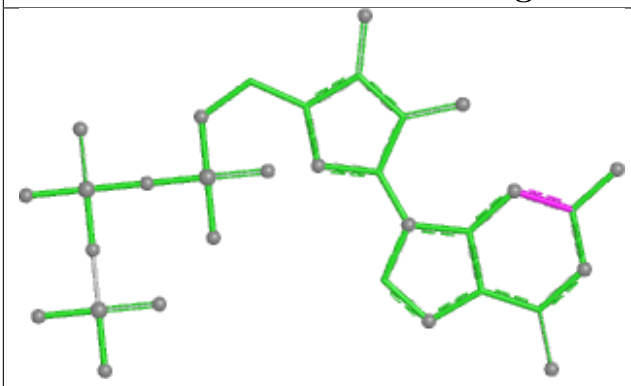
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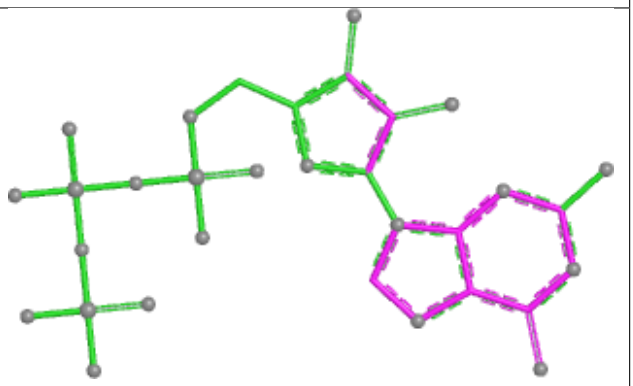
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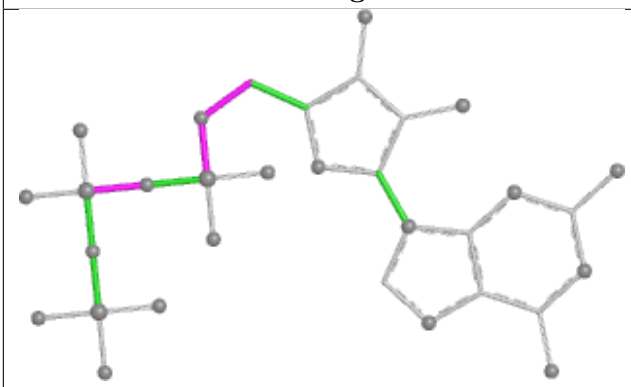
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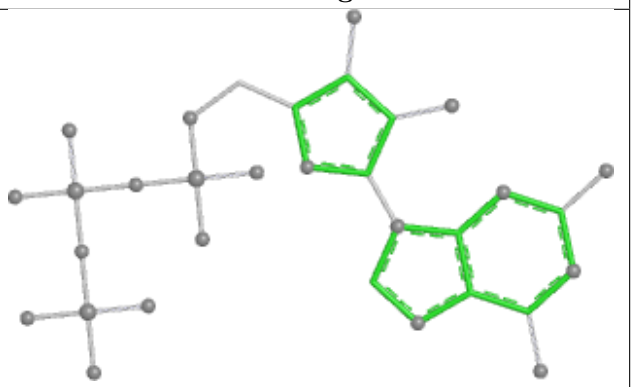
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Bond angles

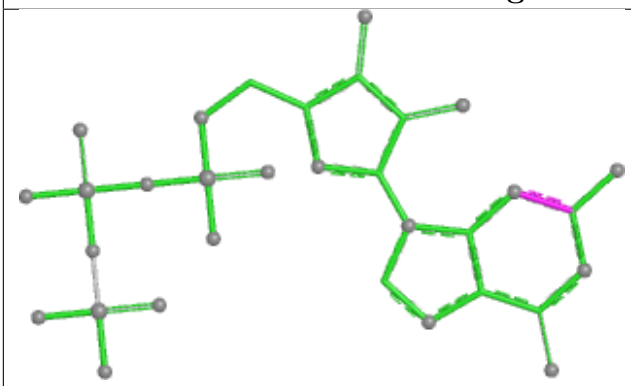


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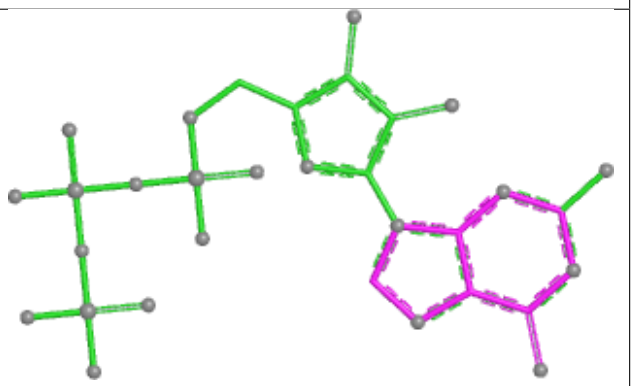


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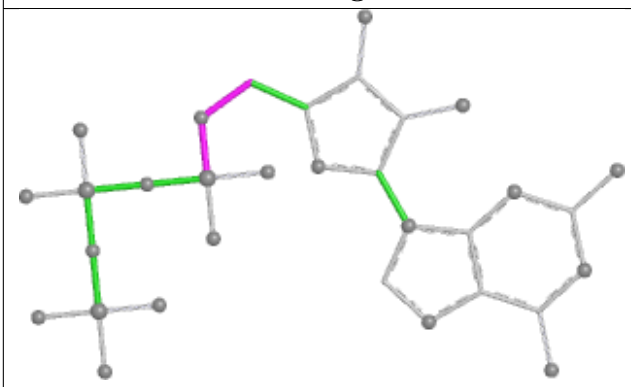
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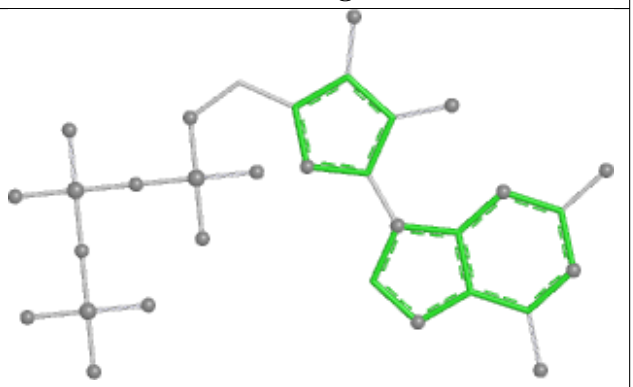
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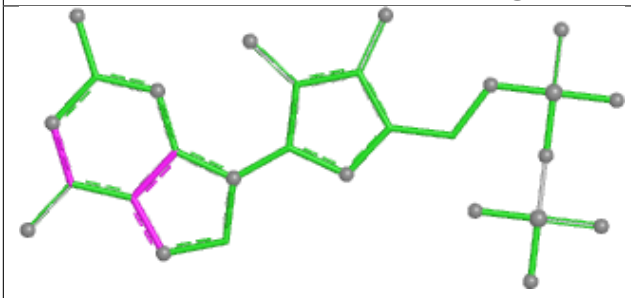


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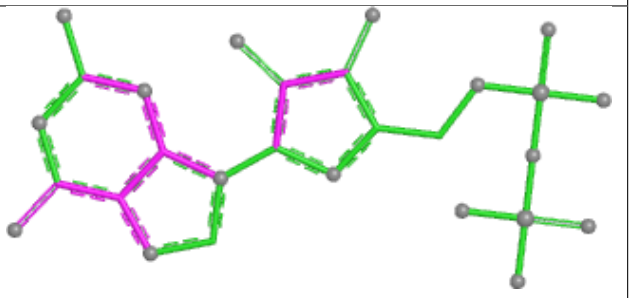


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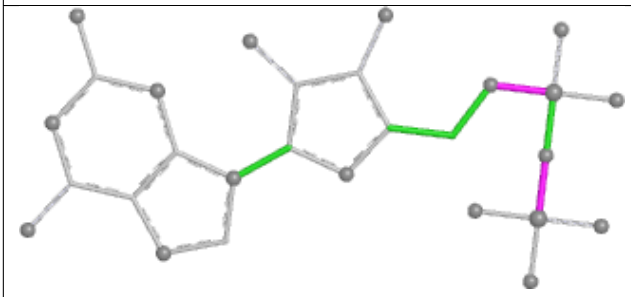
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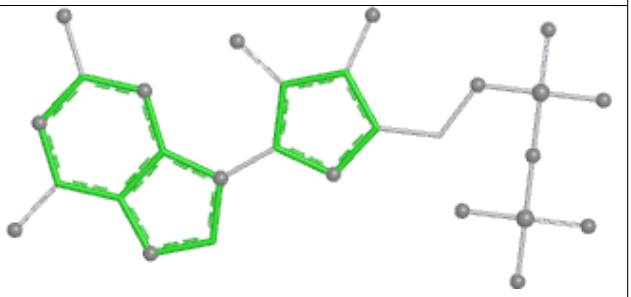
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Bond angles

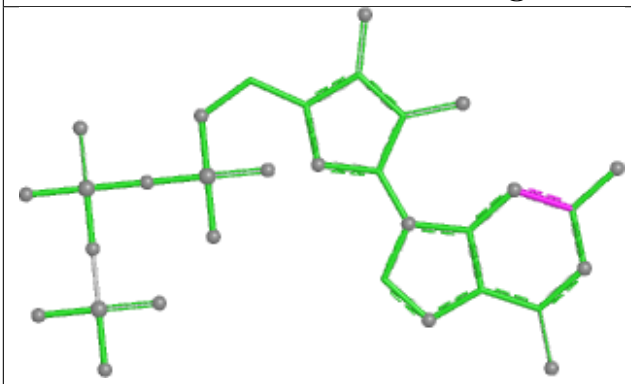


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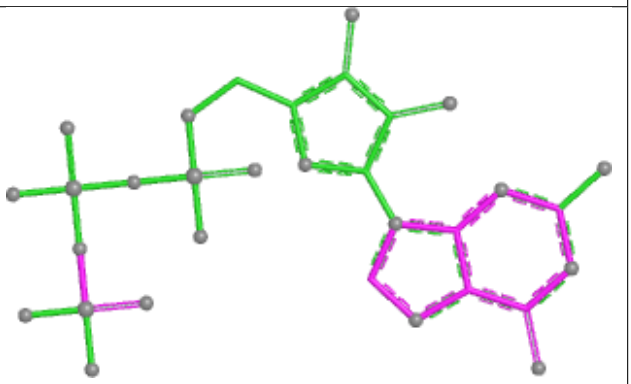


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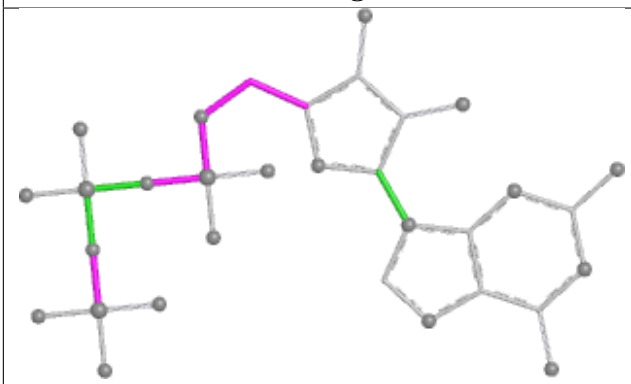
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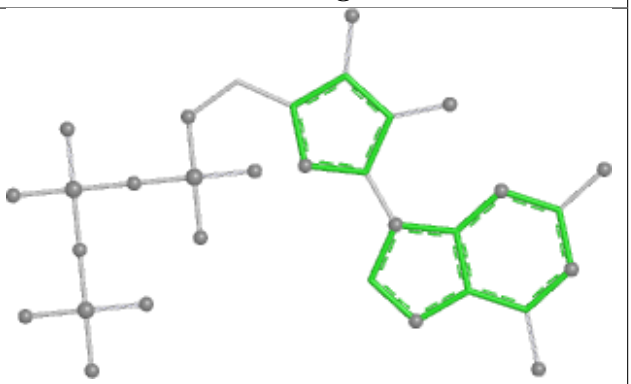
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Bond angles

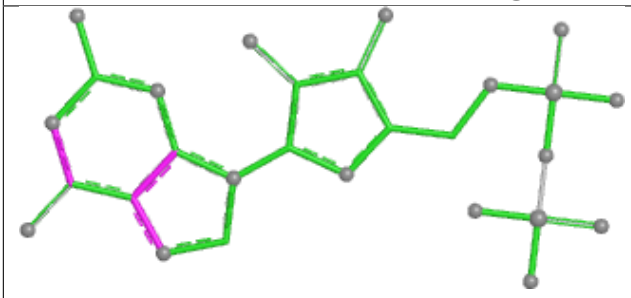


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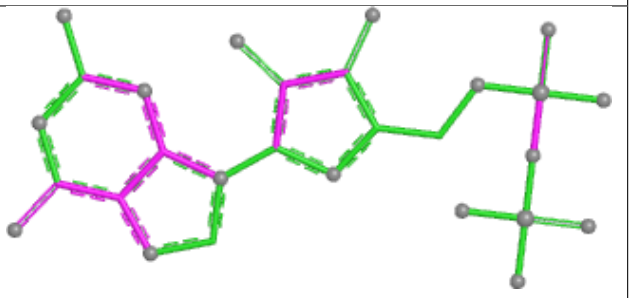


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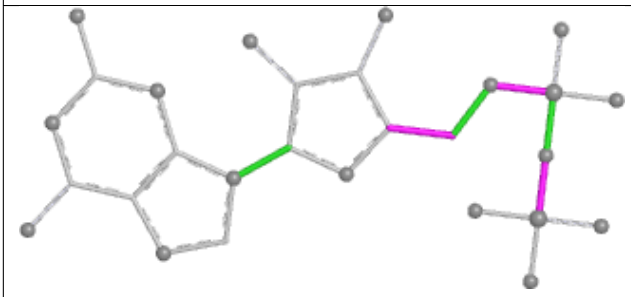
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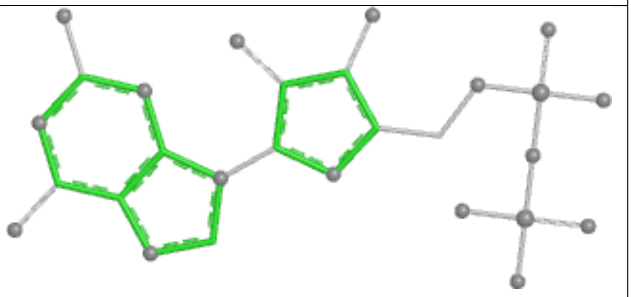
Bond lengths



Bond angles

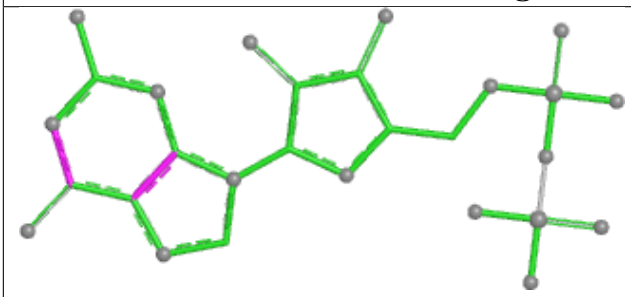


Torsions

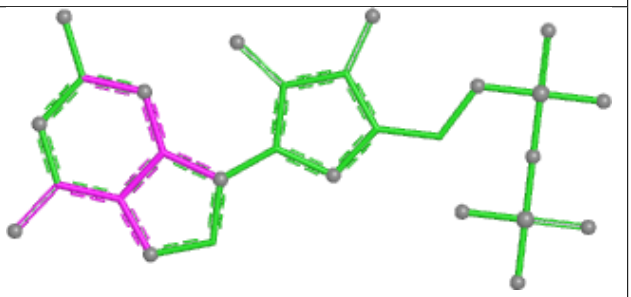


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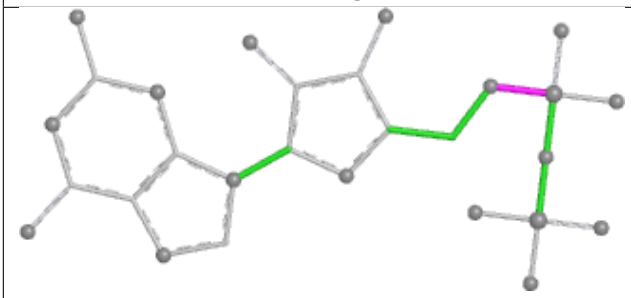
Ligand GDP ID 501



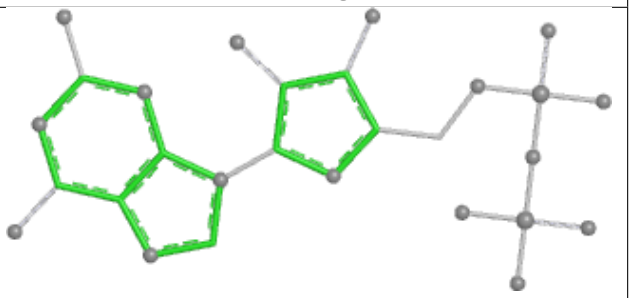
Bond lengths



Bond angles

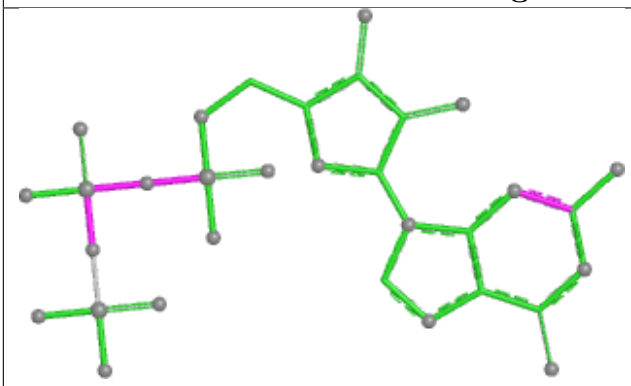


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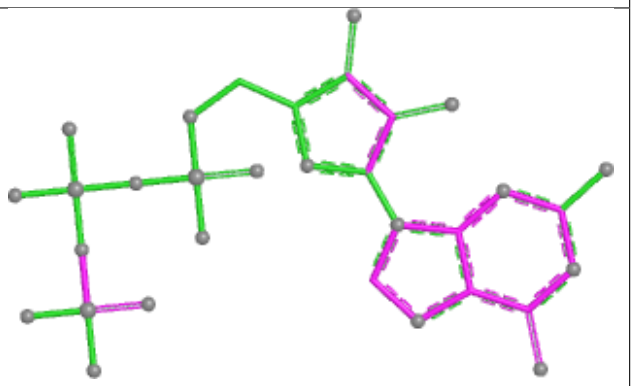


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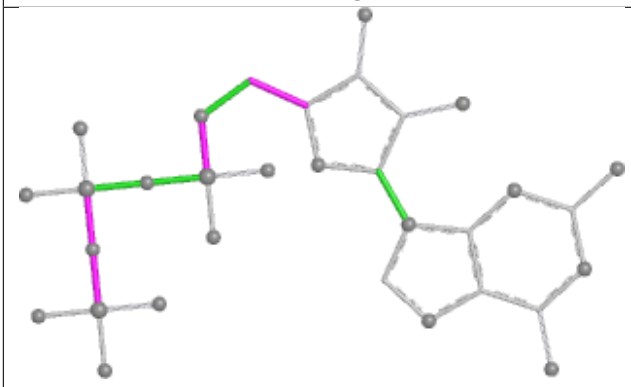
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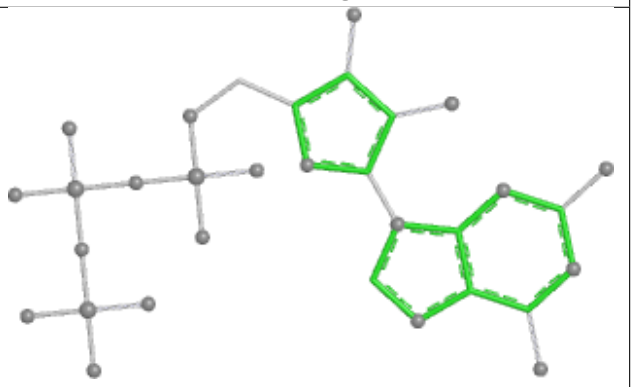
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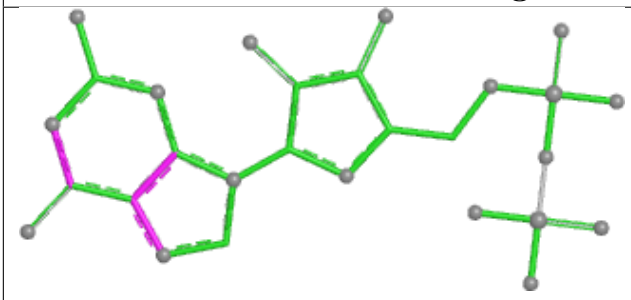


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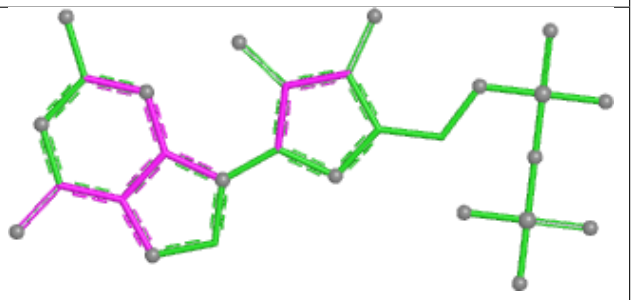


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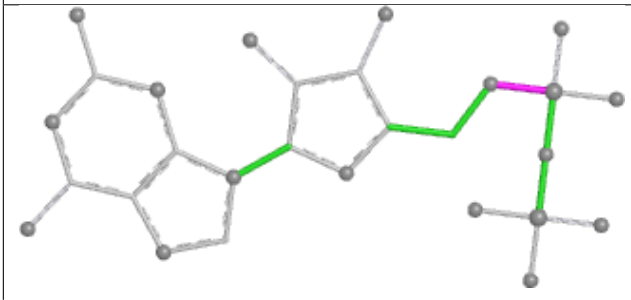
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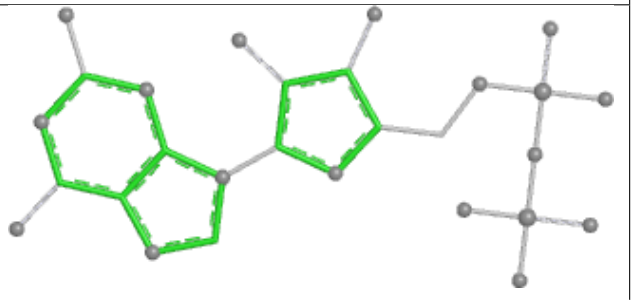
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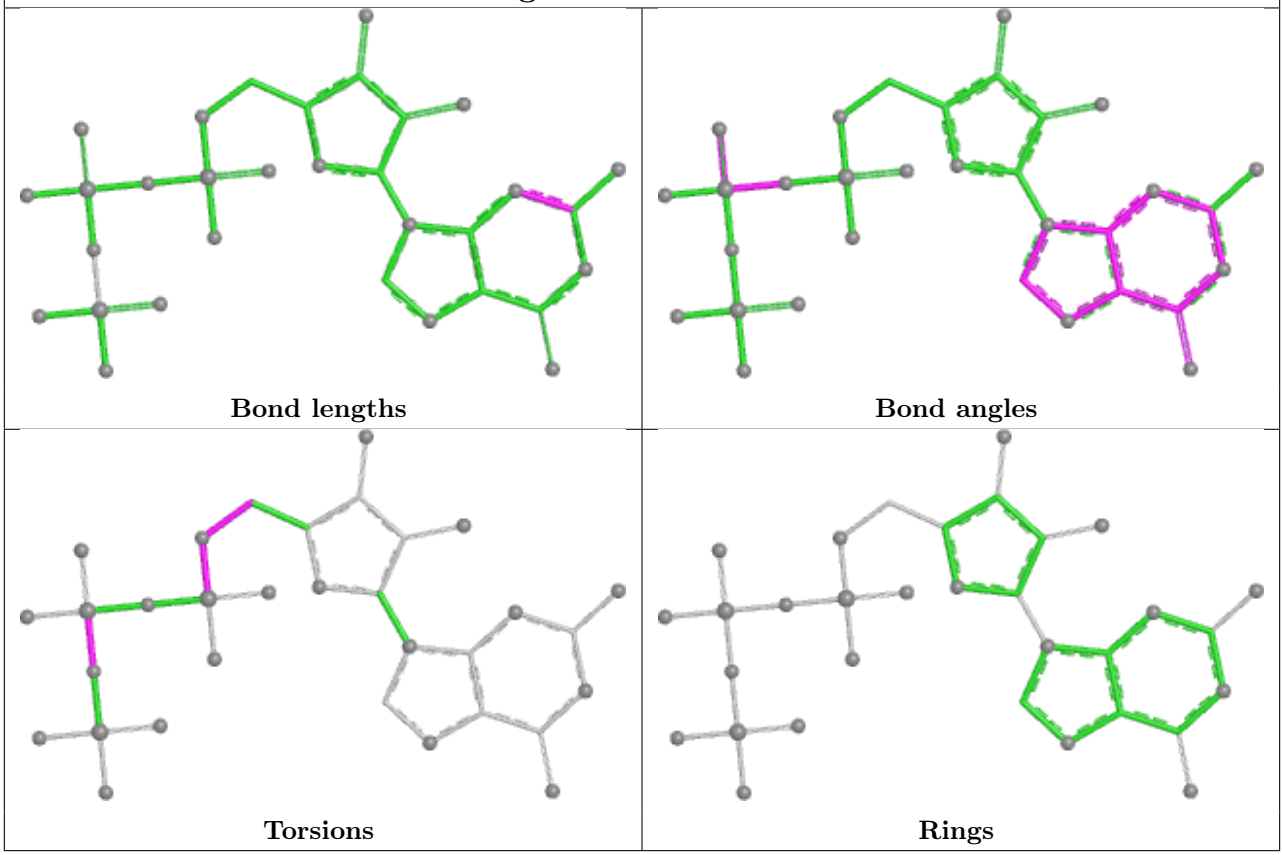


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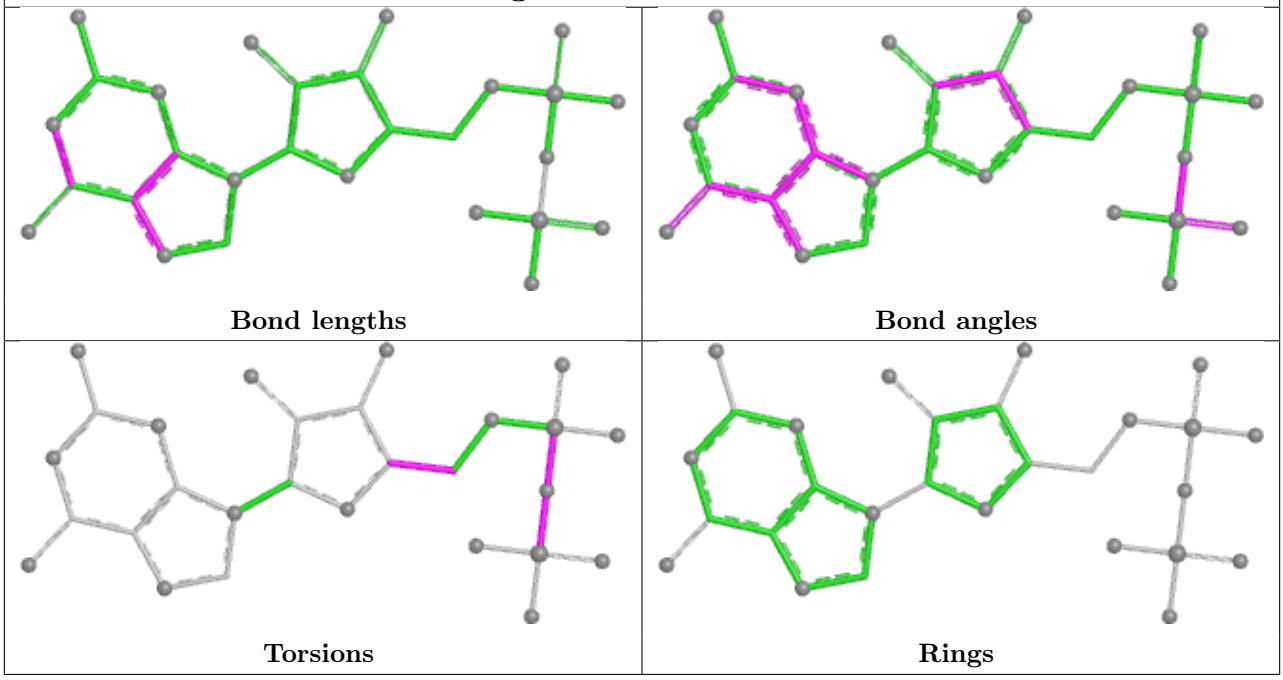


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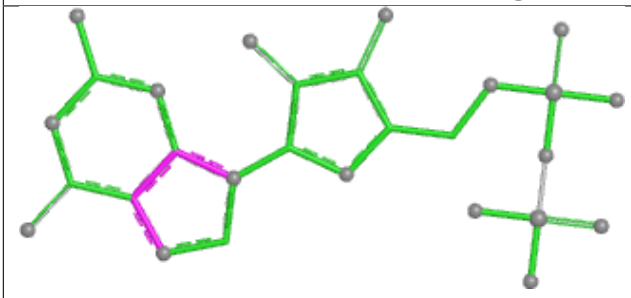
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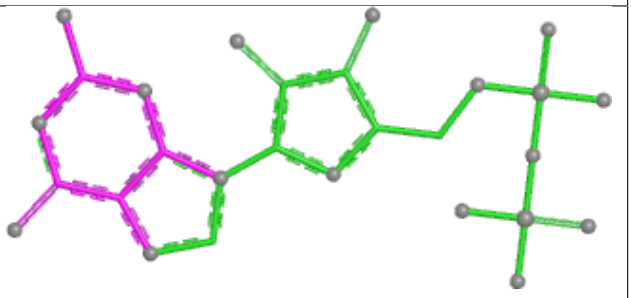
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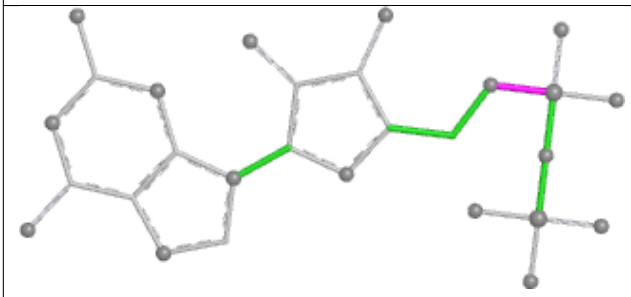
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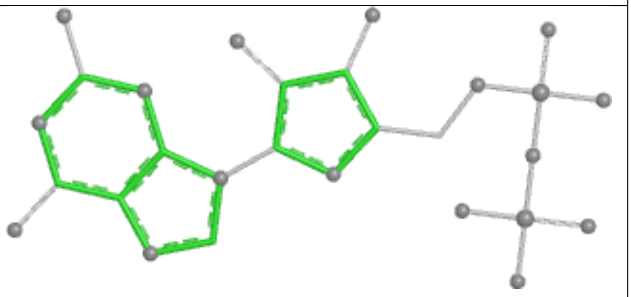
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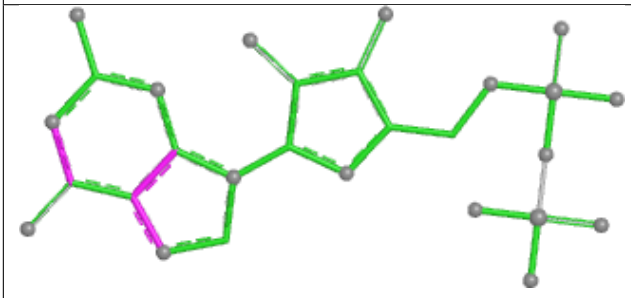


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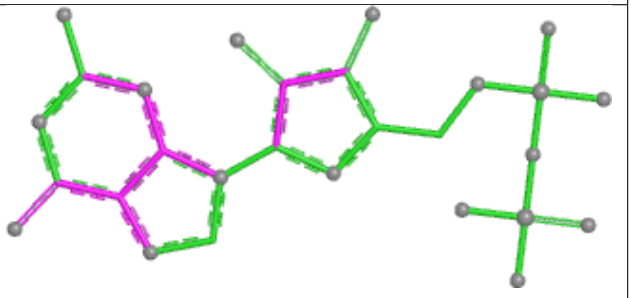


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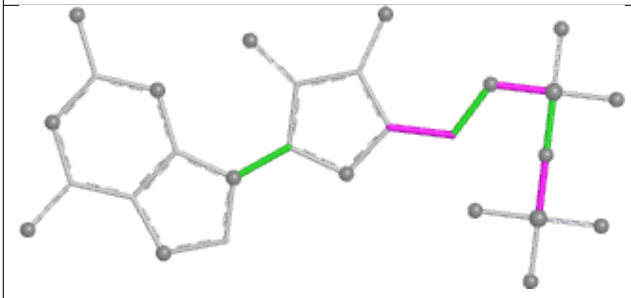
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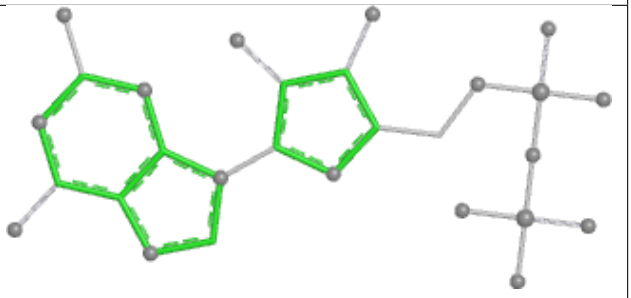
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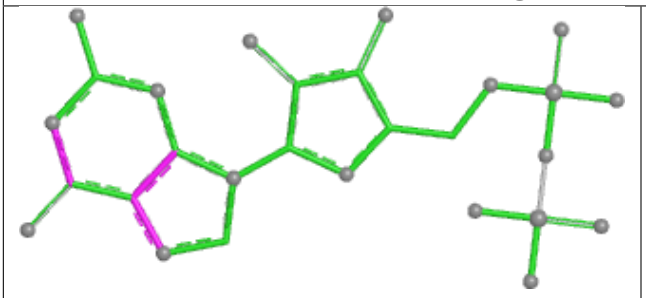


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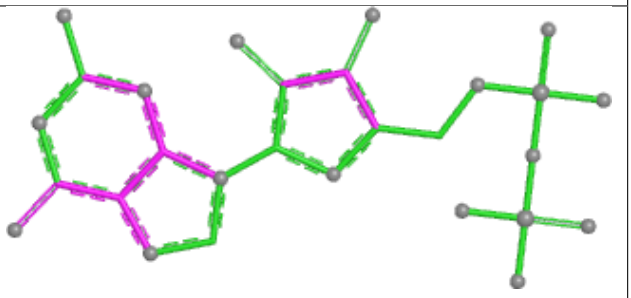


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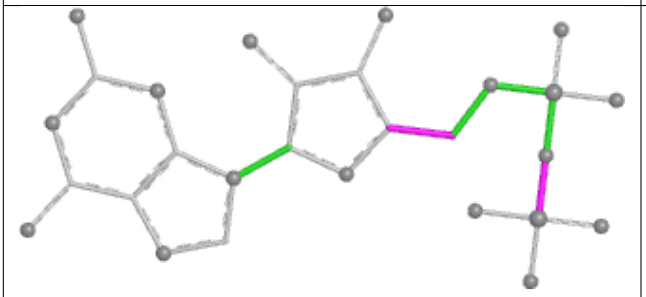
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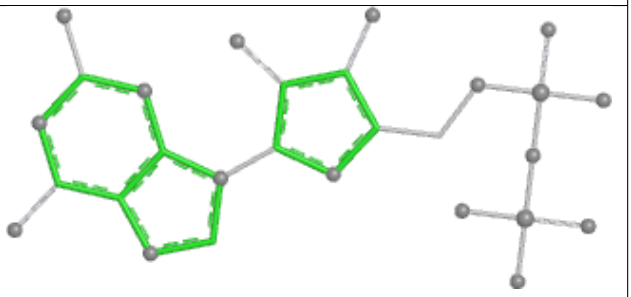
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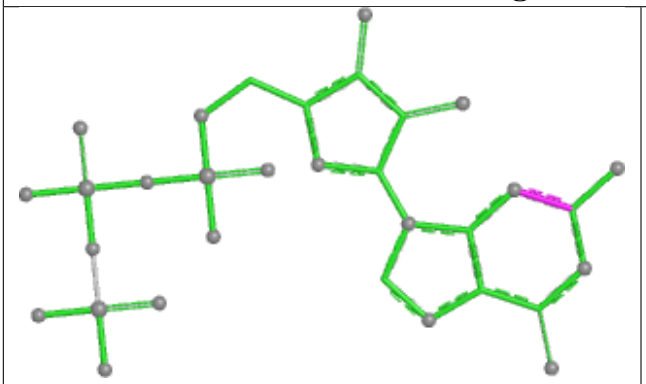


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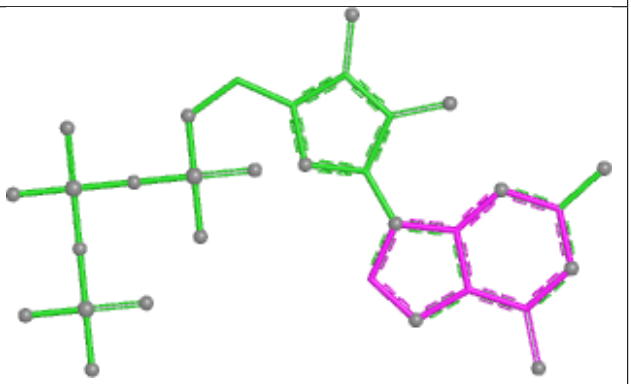


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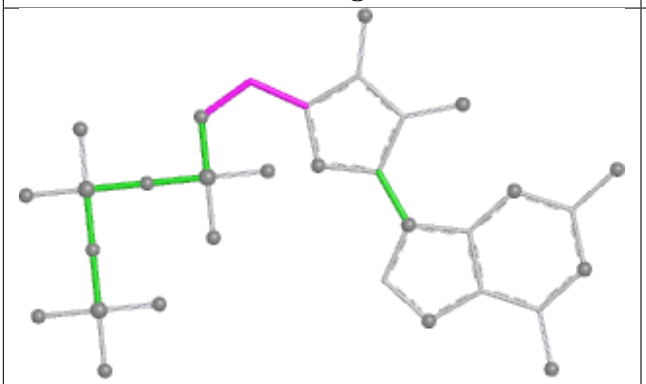
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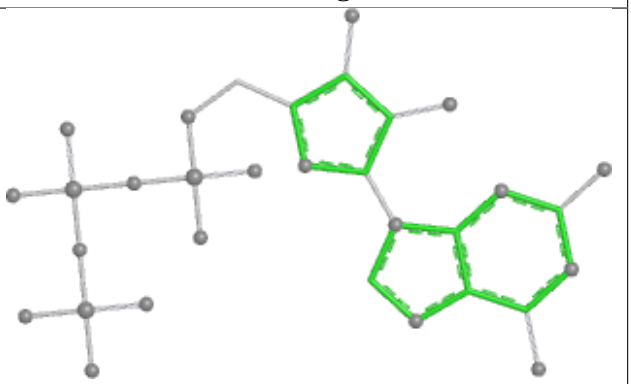
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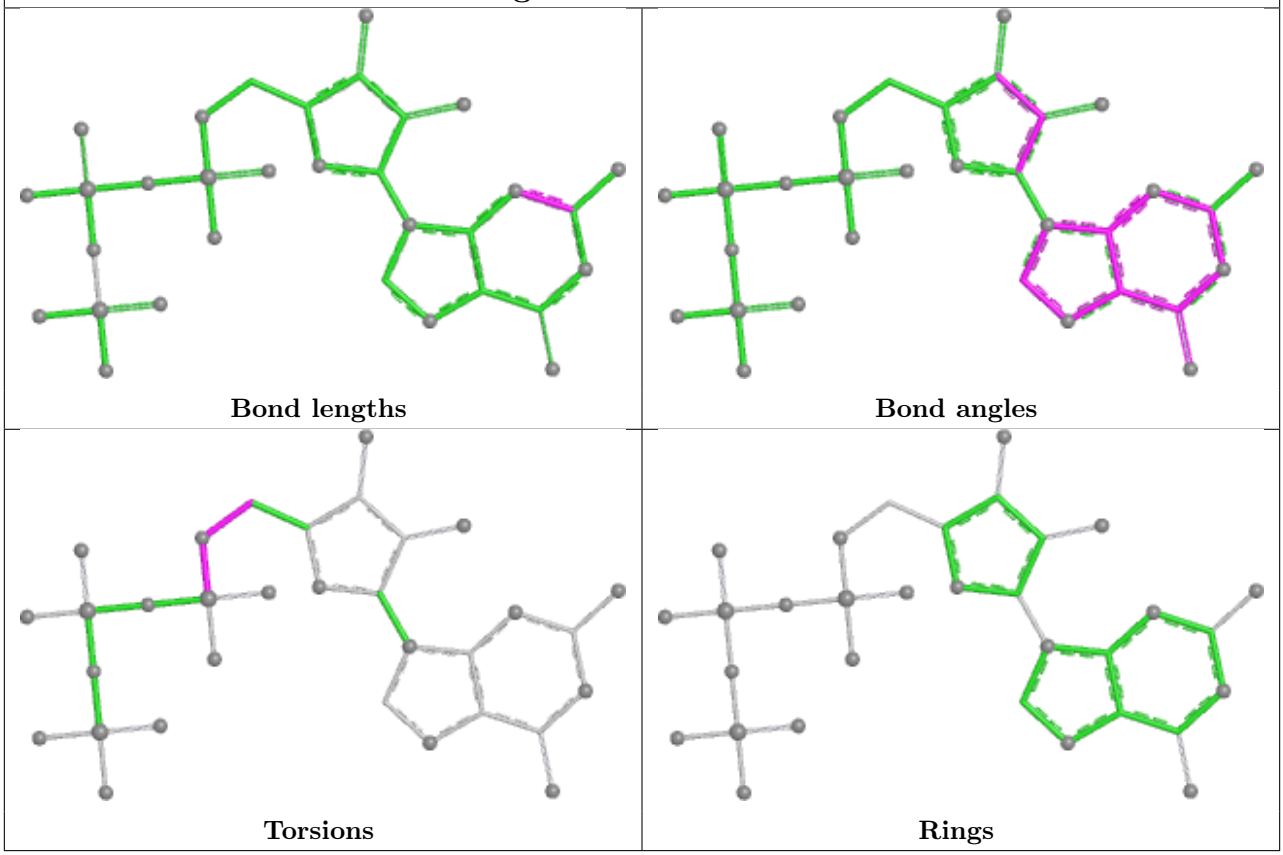


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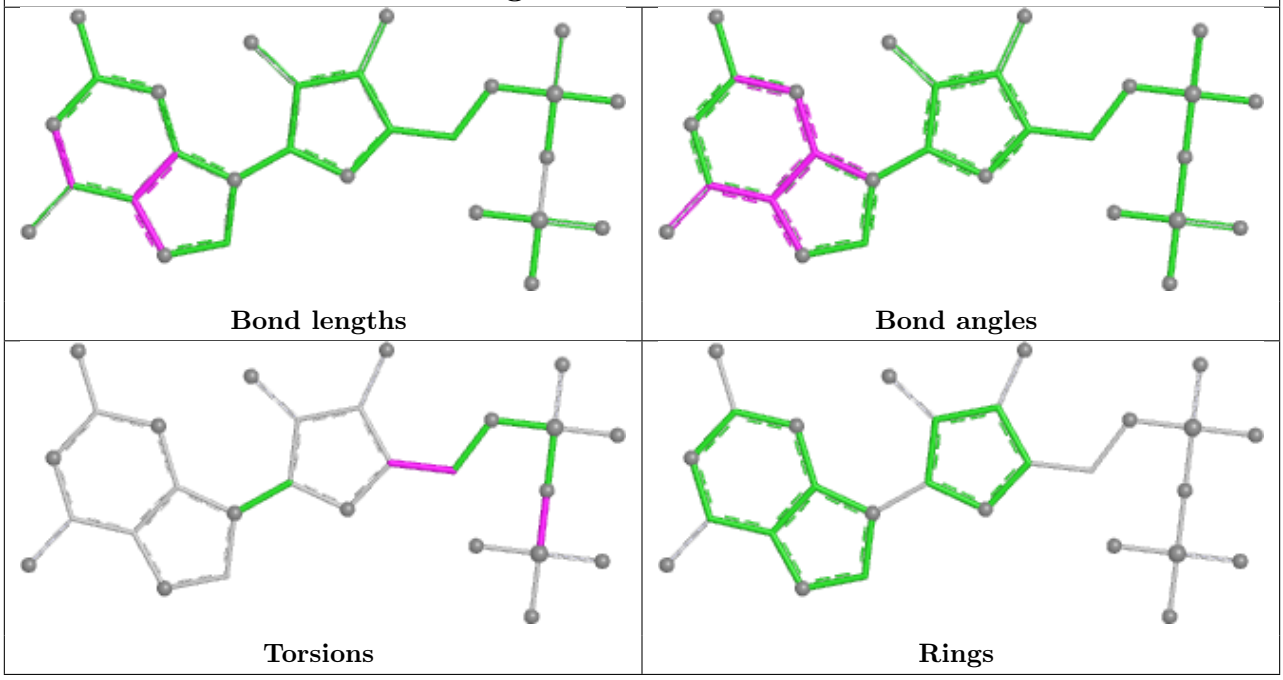


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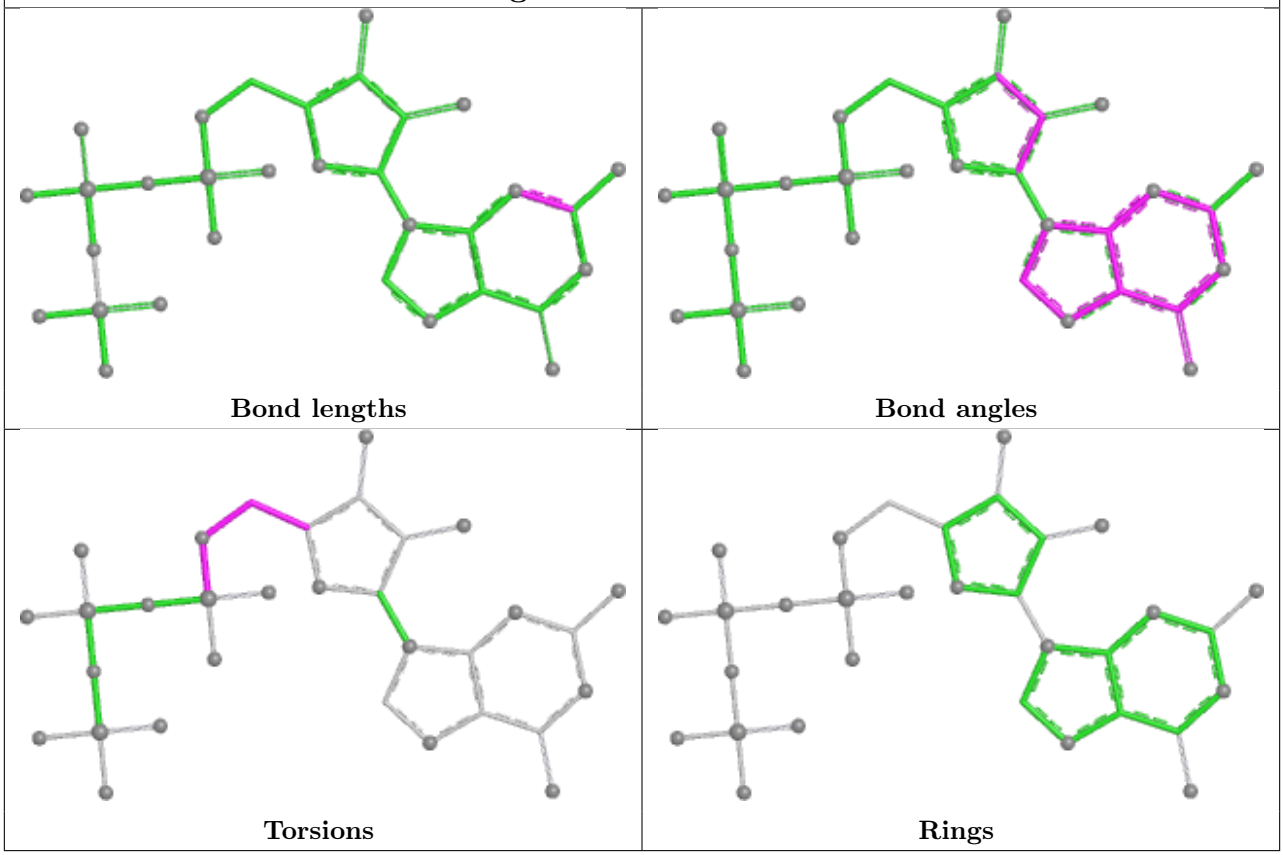
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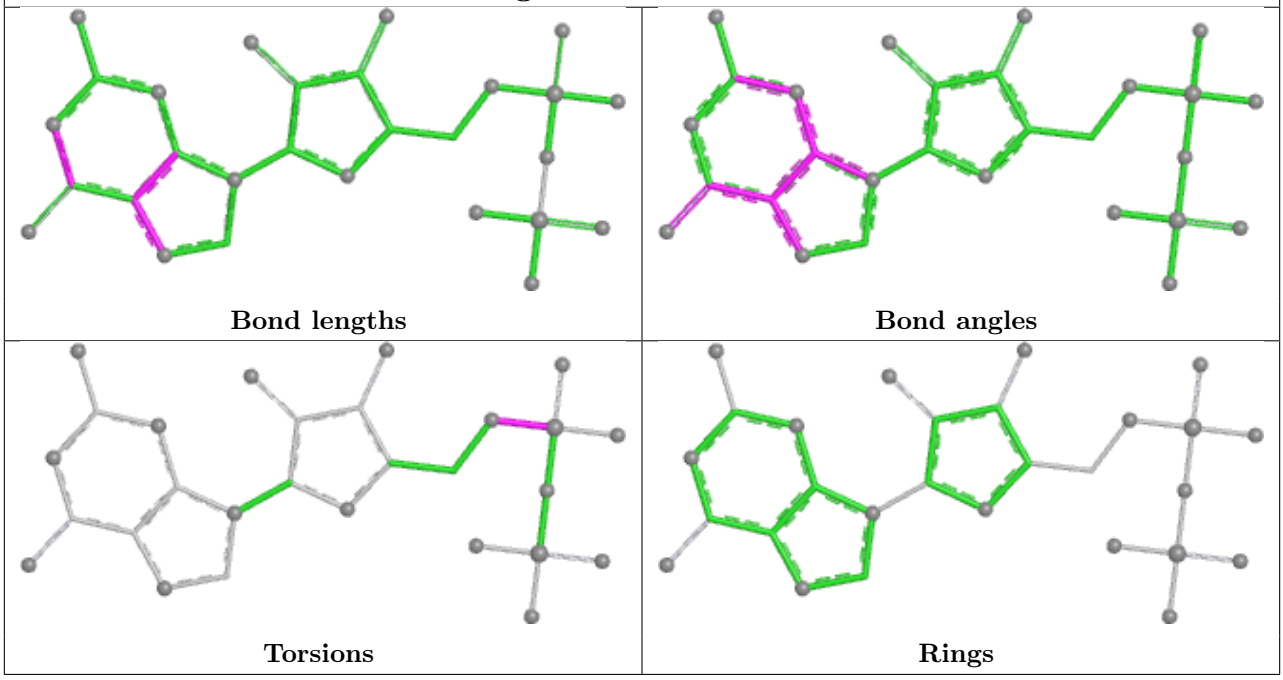
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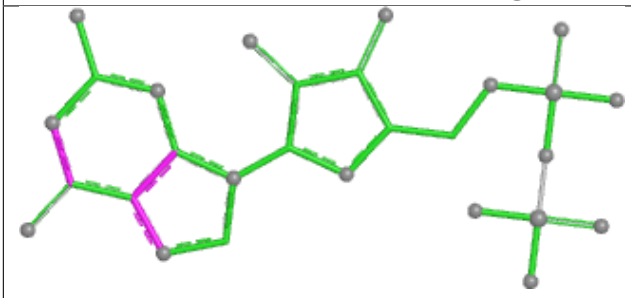
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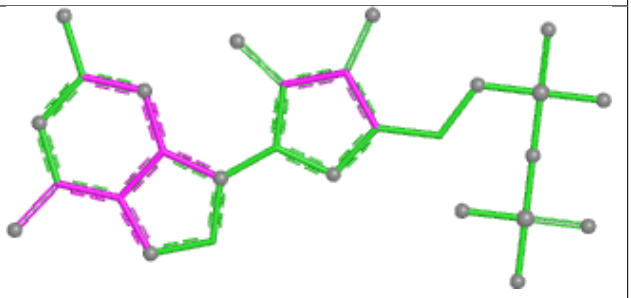
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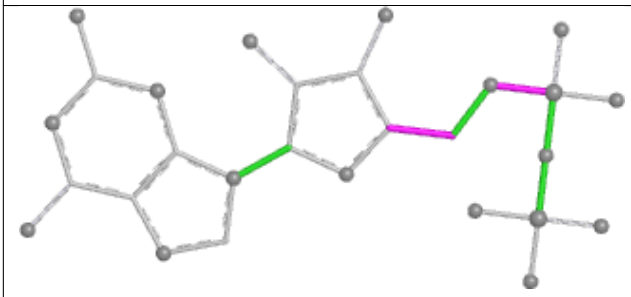
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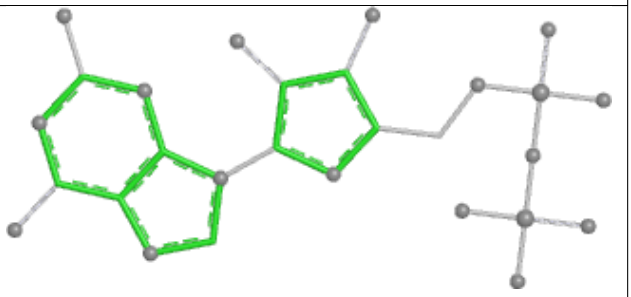
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Bond angles

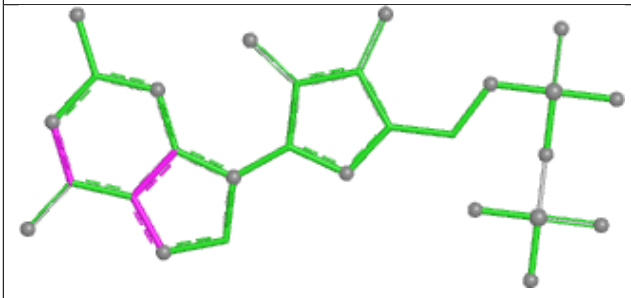


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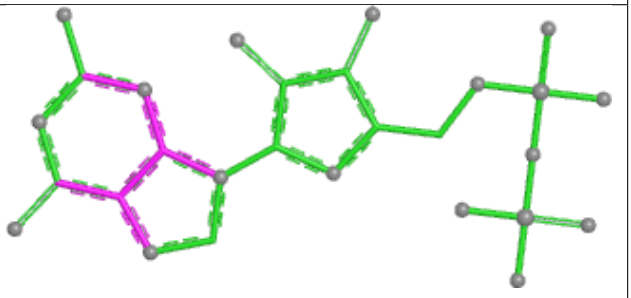


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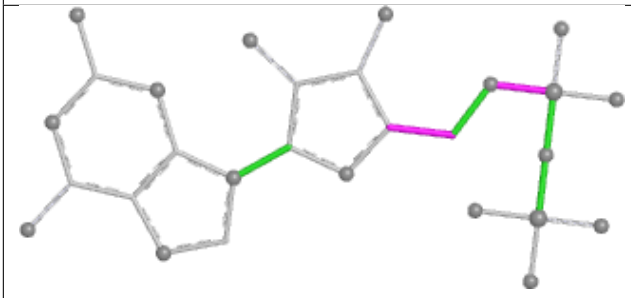
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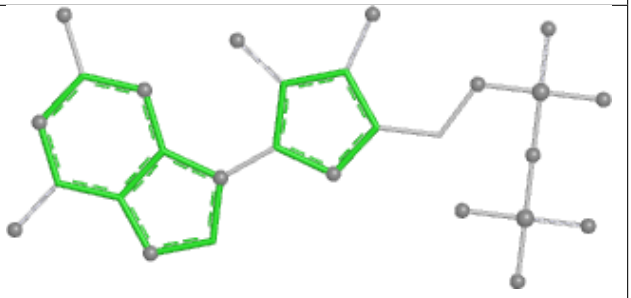
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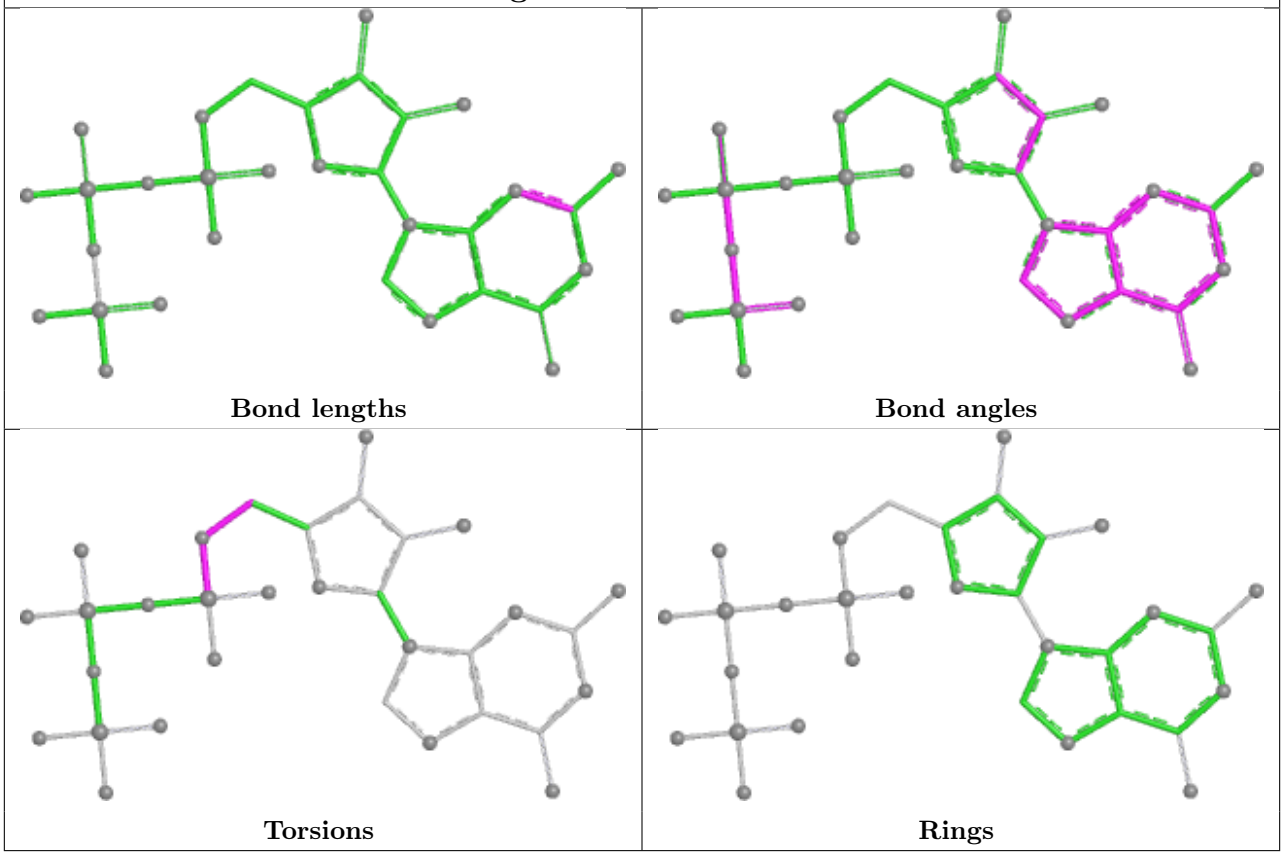


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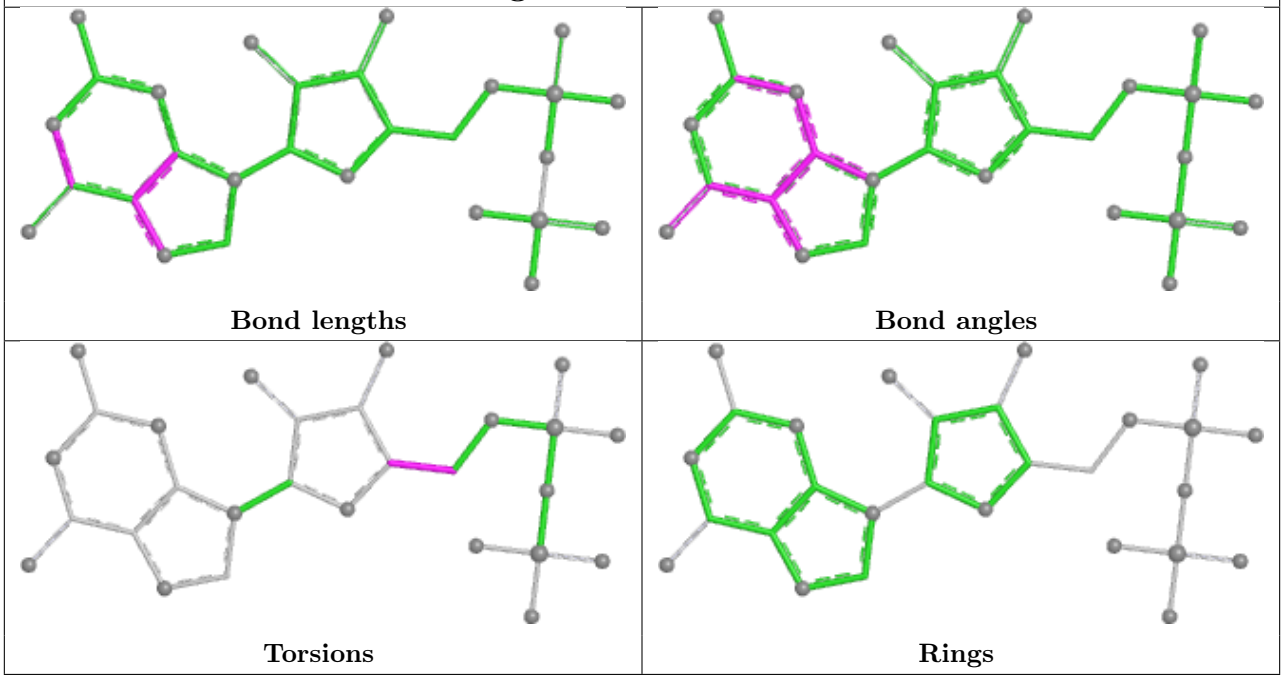


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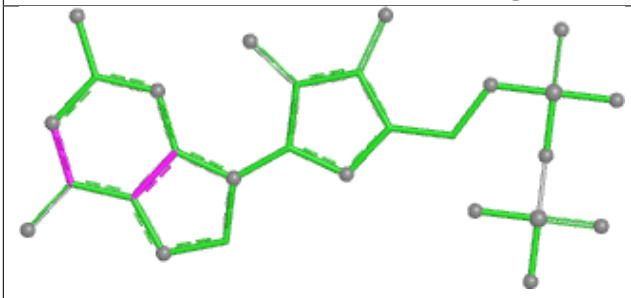
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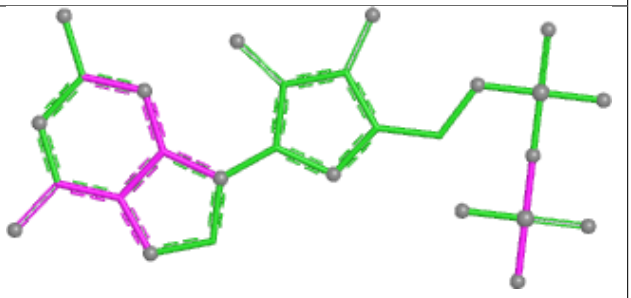
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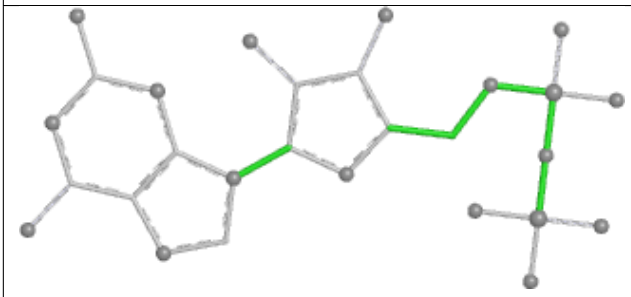
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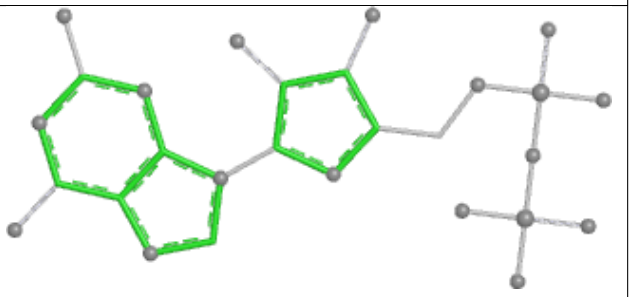
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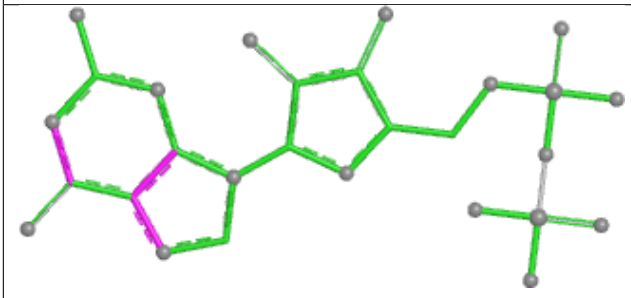


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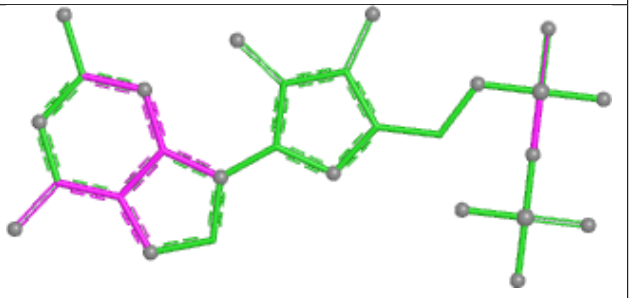


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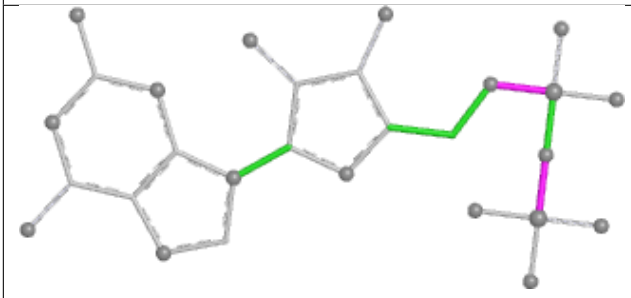
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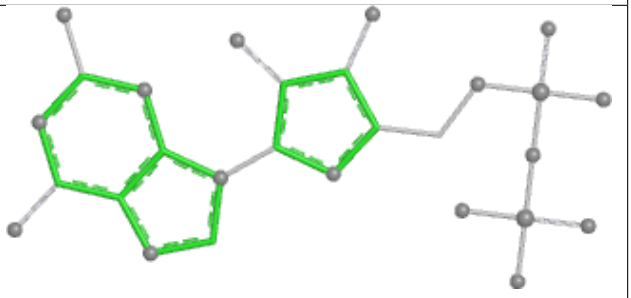
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Bond angles

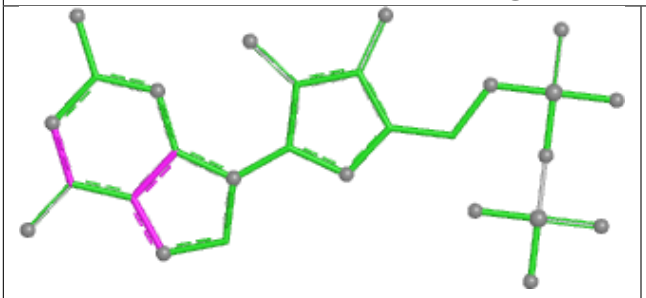


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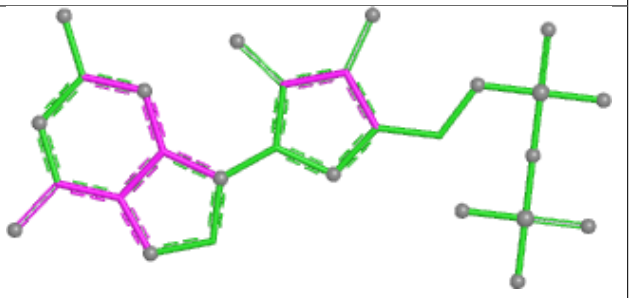


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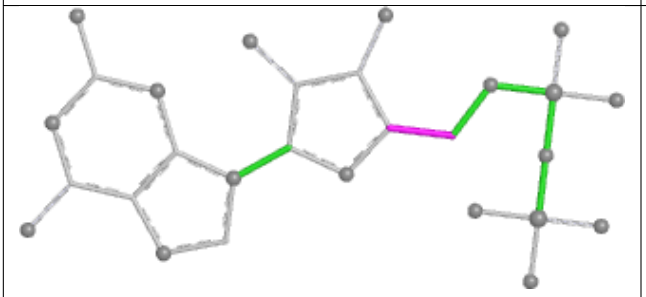
Ligand GDP WJ 501



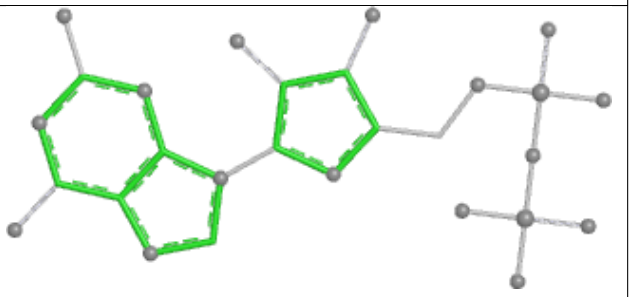
Bond lengths



Bond angles

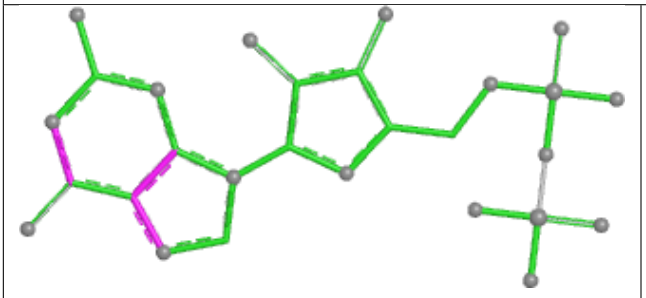


Torsions

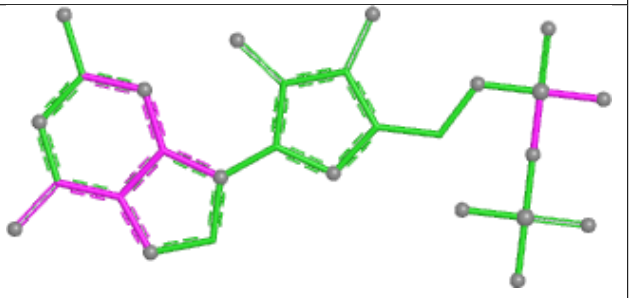


Rings

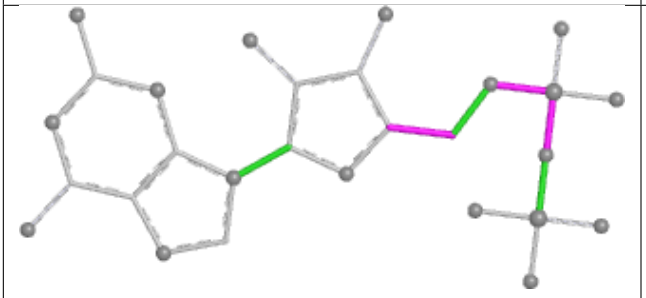
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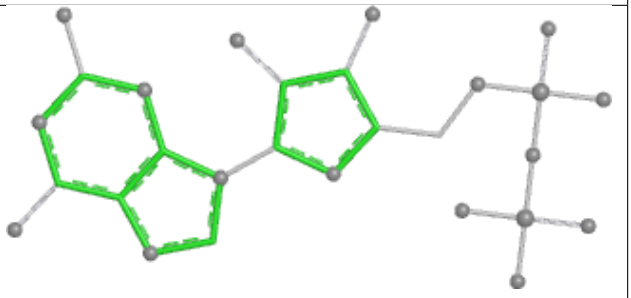
Bond lengths



Bond angles

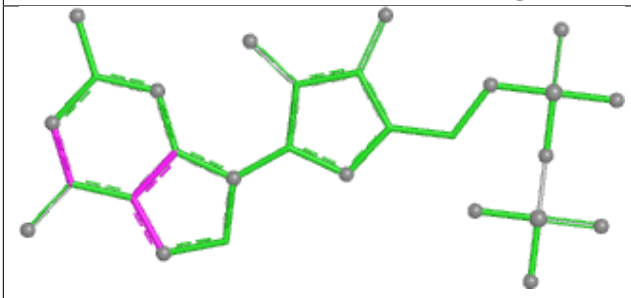


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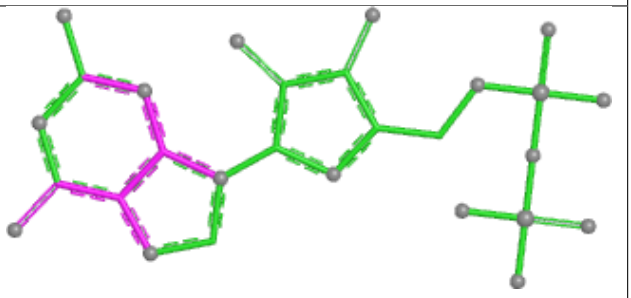


Rings

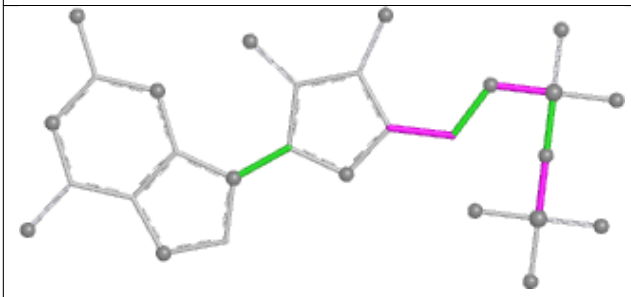
Ligand GDP JH 501



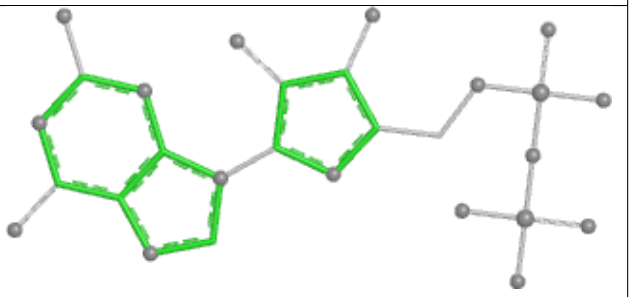
Bond lengths



Bond angles

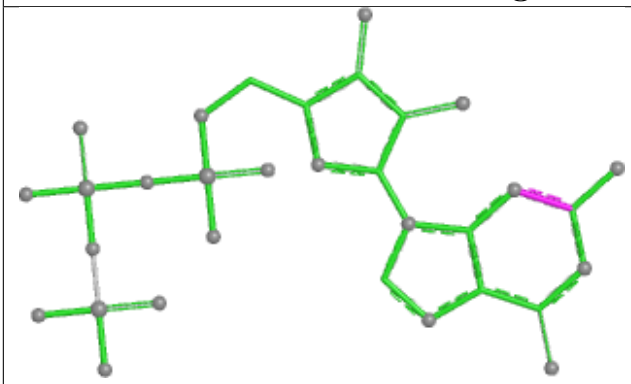


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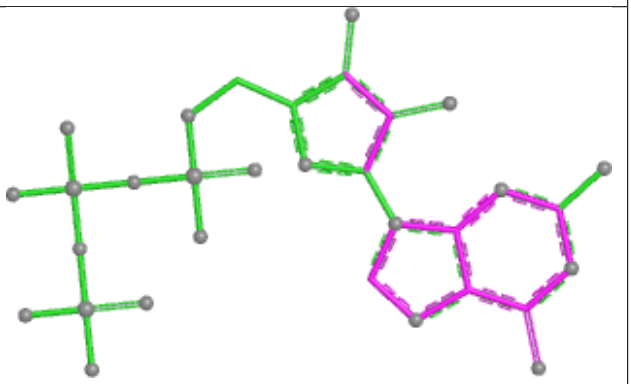


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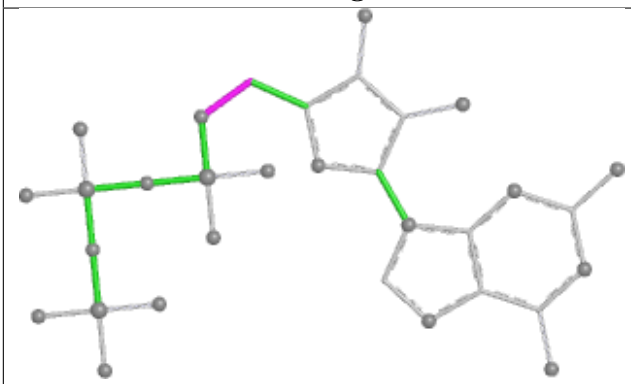
Ligand GTP CL 502



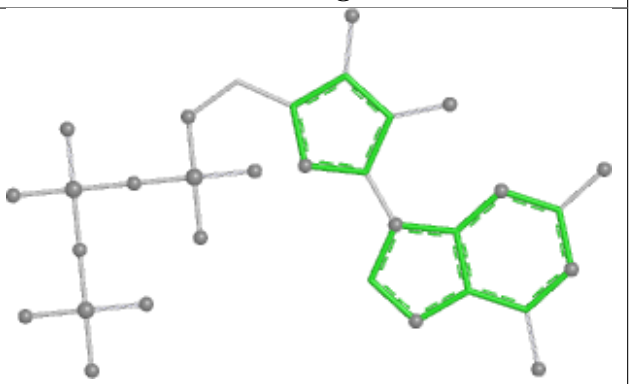
Bond lengths



Bond angles

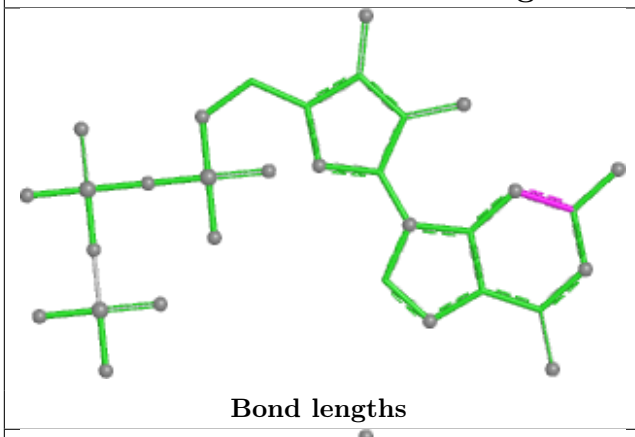


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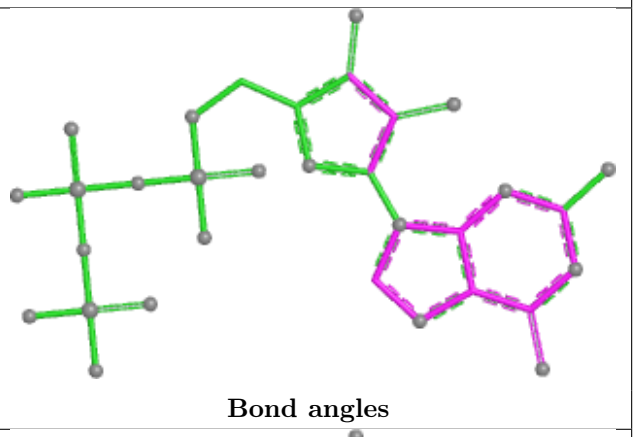


Rings

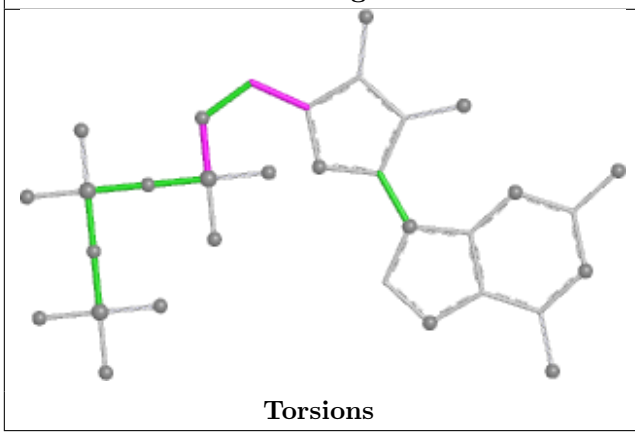
Ligand GTP IC 501



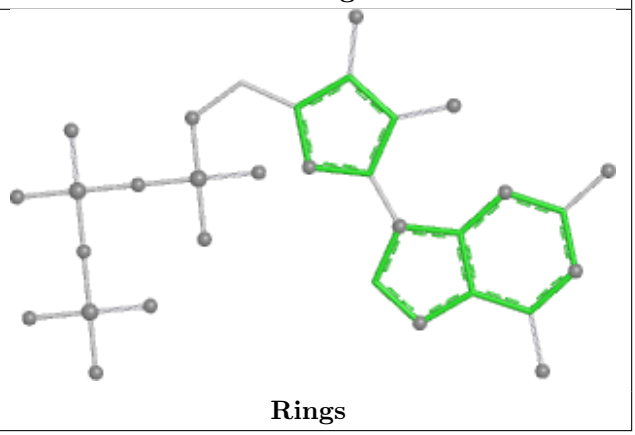
Bond lengths



Bond angles

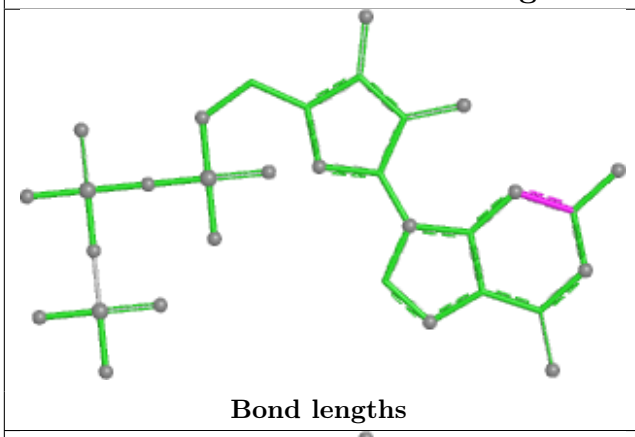


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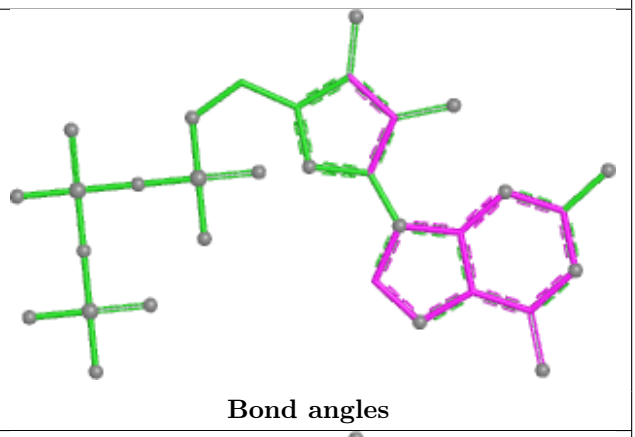


Rings

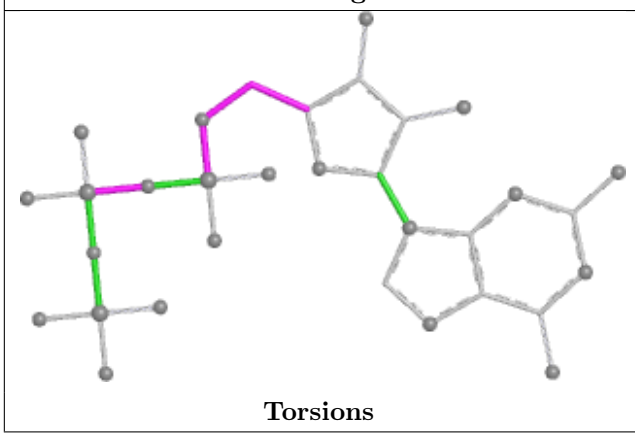
Ligand GTP LI 501



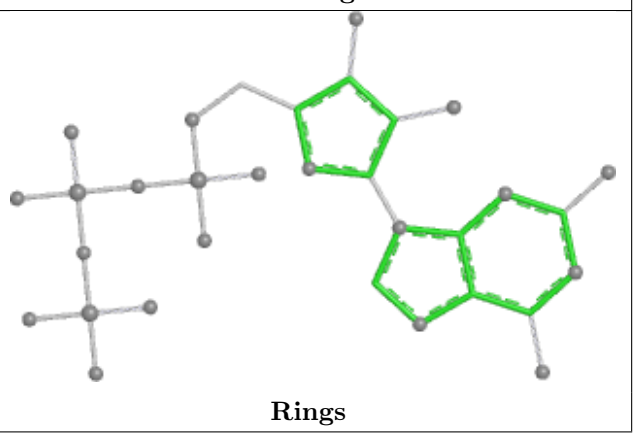
Bond lengths



Bond angles

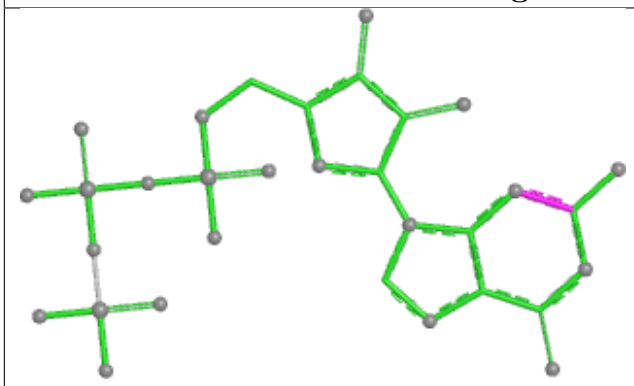


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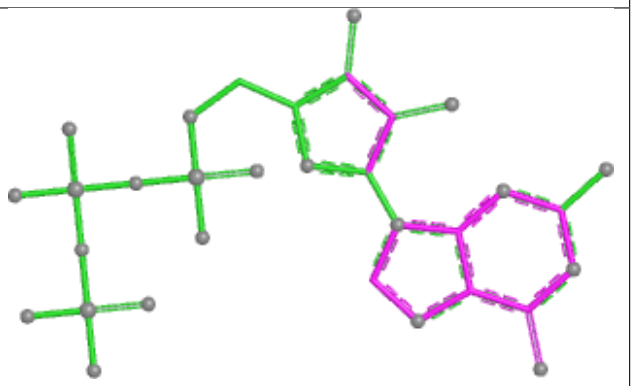


Rings

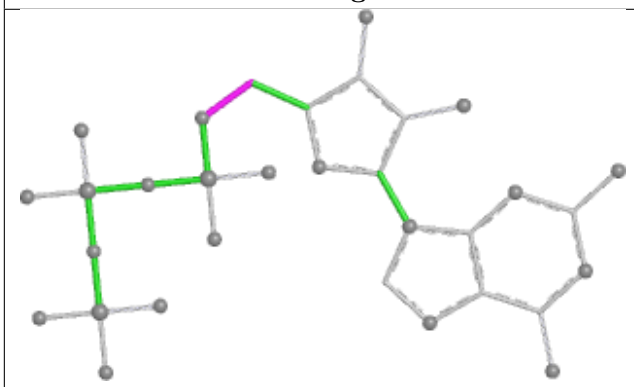
Ligand GTP DE 501



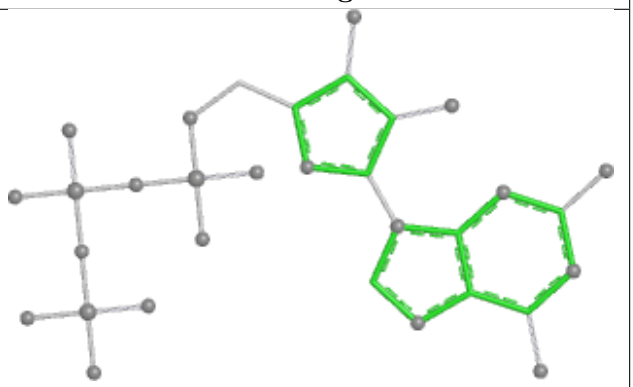
Bond lengths



Bond angles

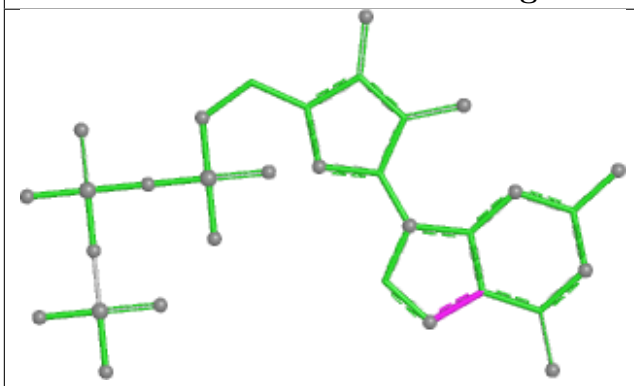


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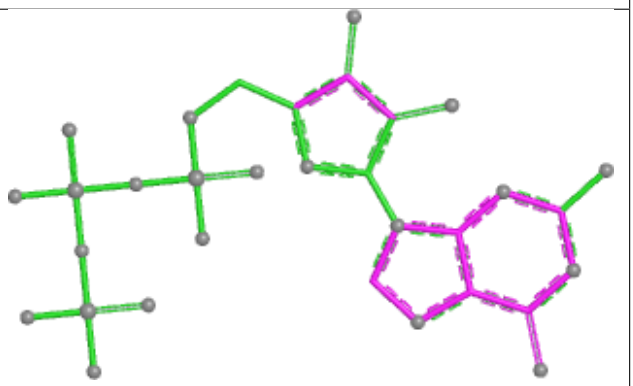


Rings

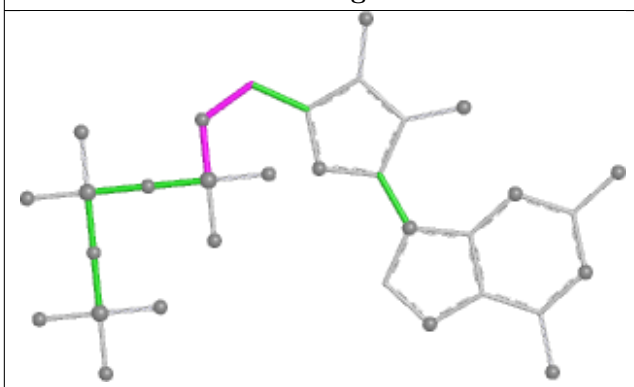
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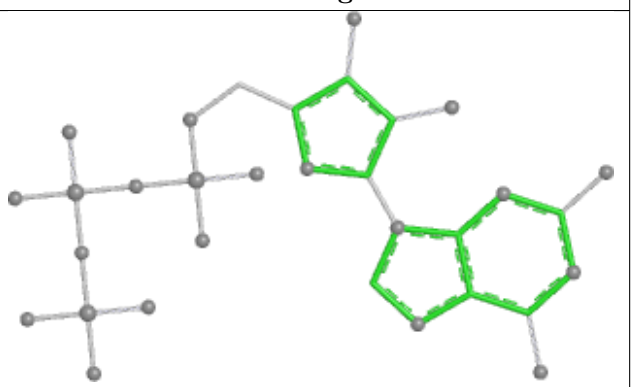
Bond lengths



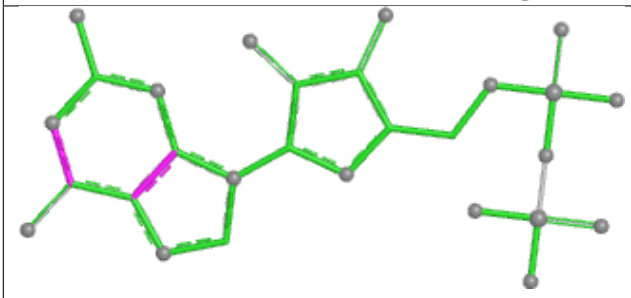
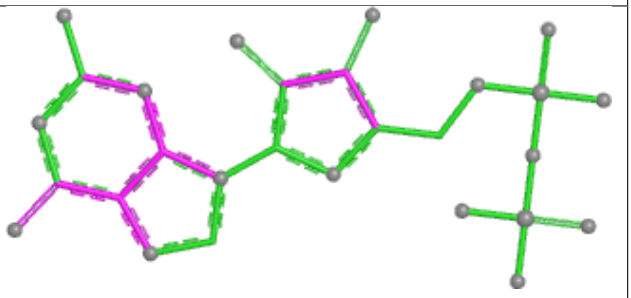
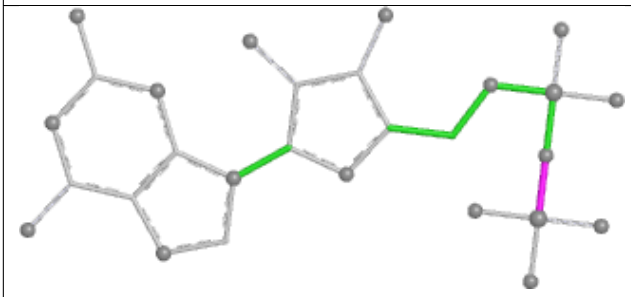
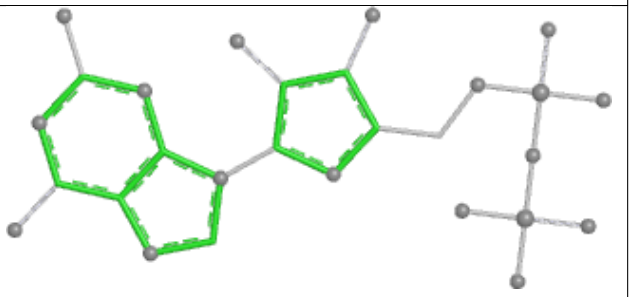
Bond angles

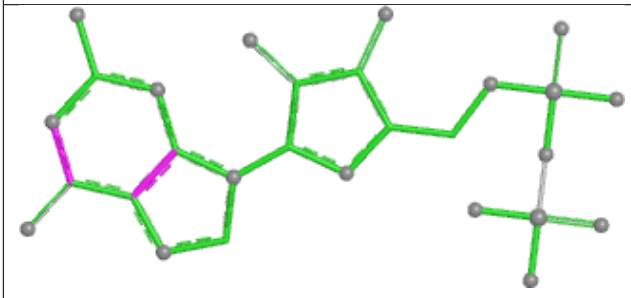
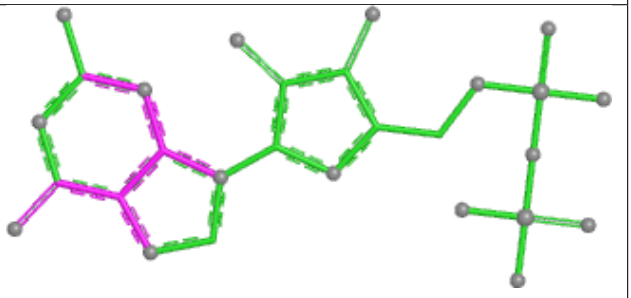
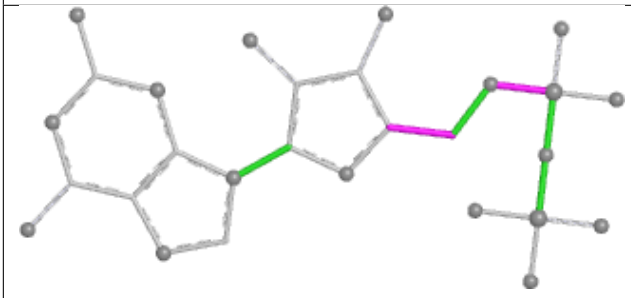
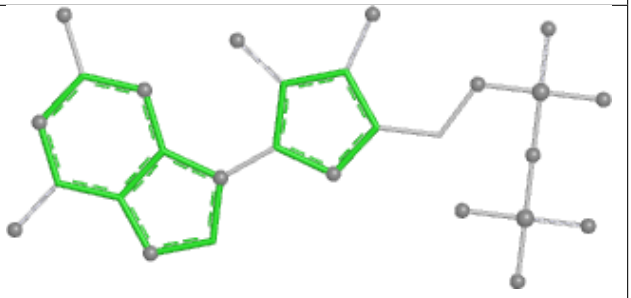


Torsions

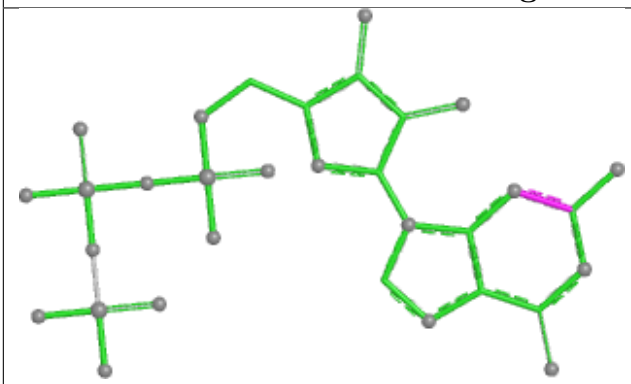


Rings

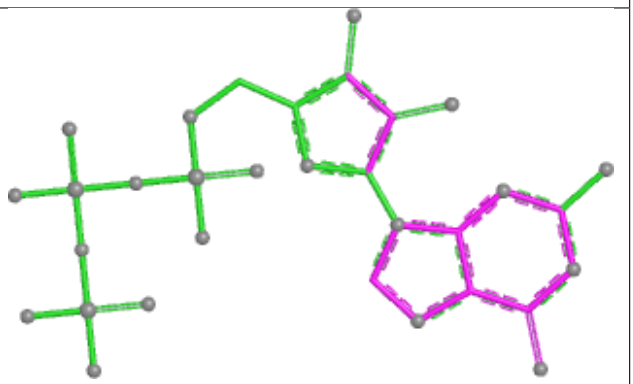
Ligand GDP IF 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP OL 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

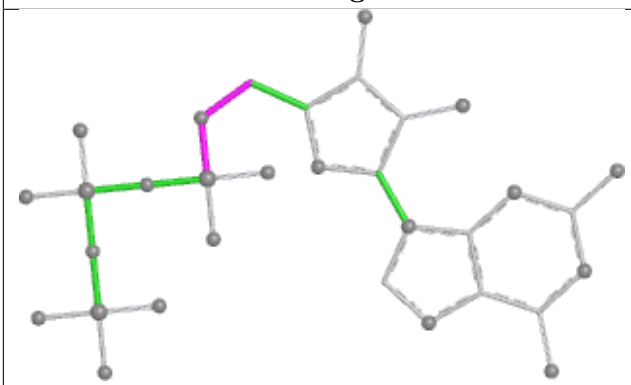
Ligand GTP JI 501



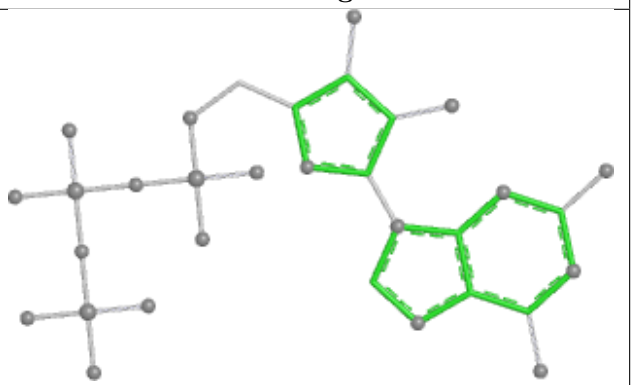
Bond lengths



Bond angles

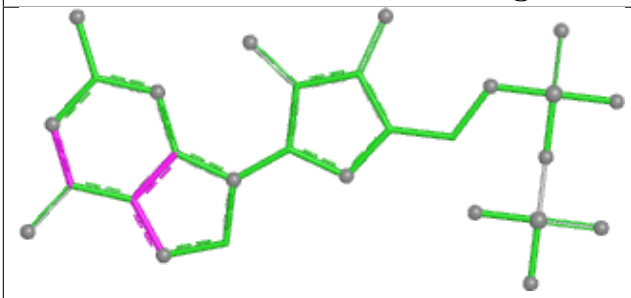


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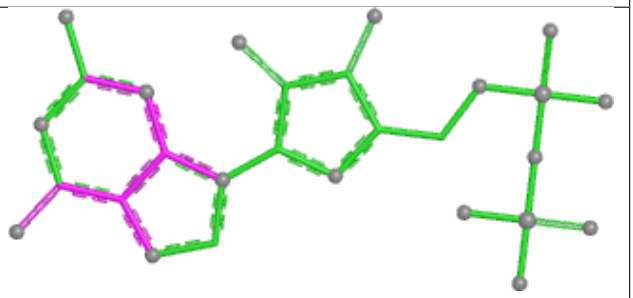


Rings

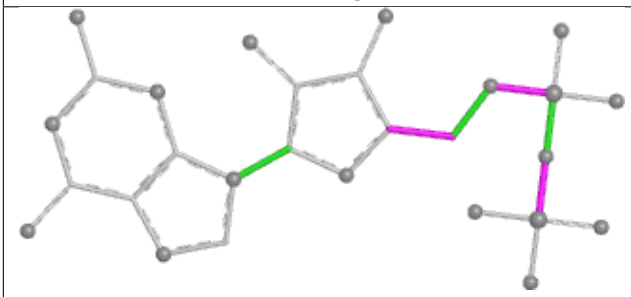
Ligand GDP JB 501



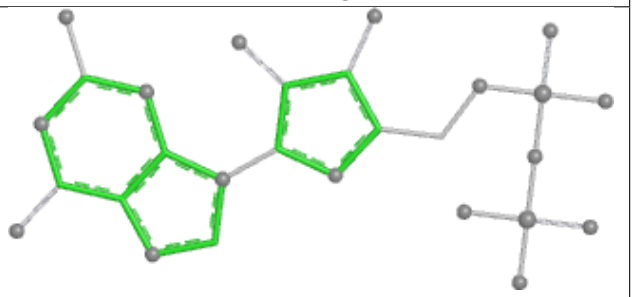
Bond lengths



Bond angles

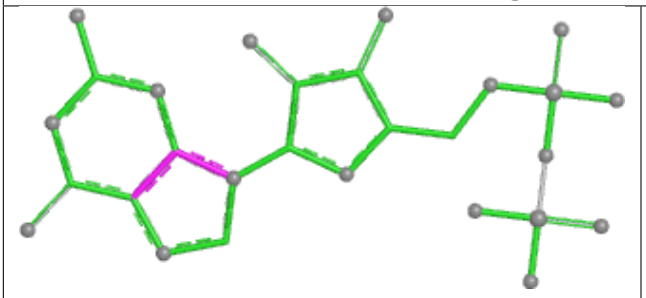


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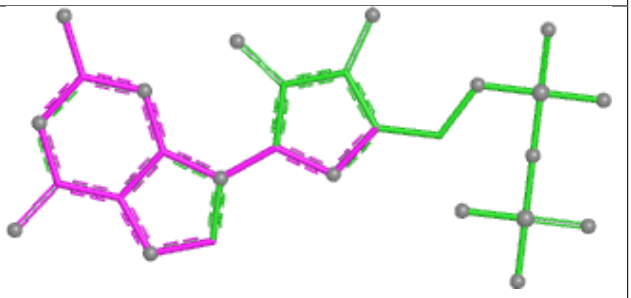


Rings

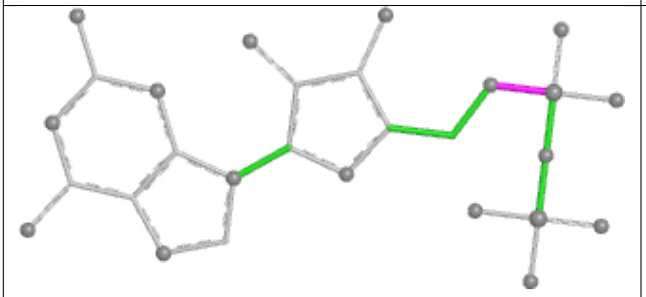
Ligand GDP NH 501



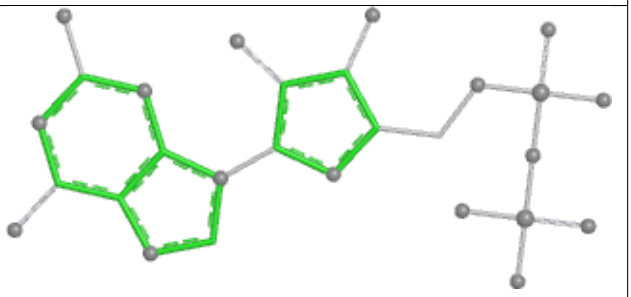
Bond lengths



Bond angles

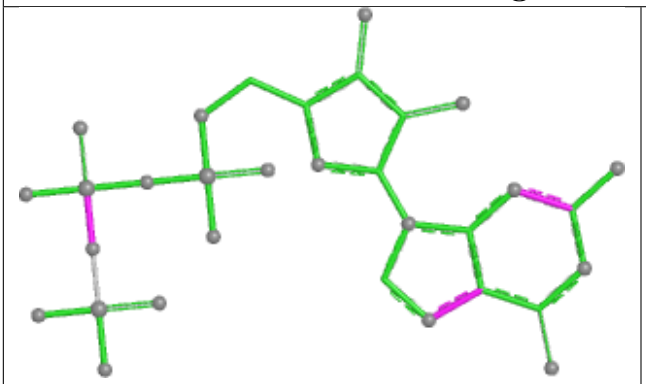


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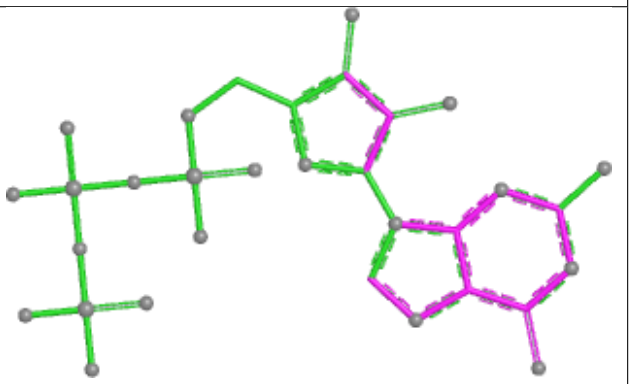


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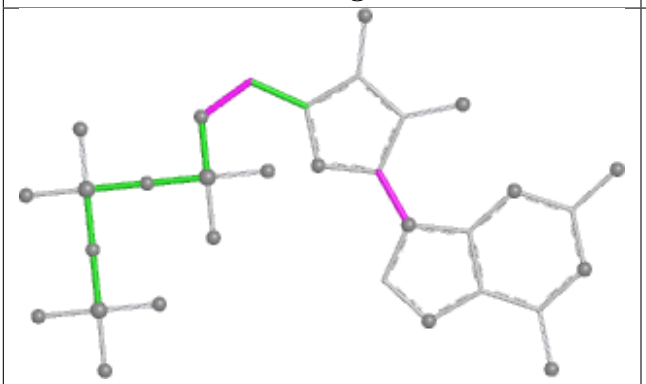
Ligand GTP FG 501



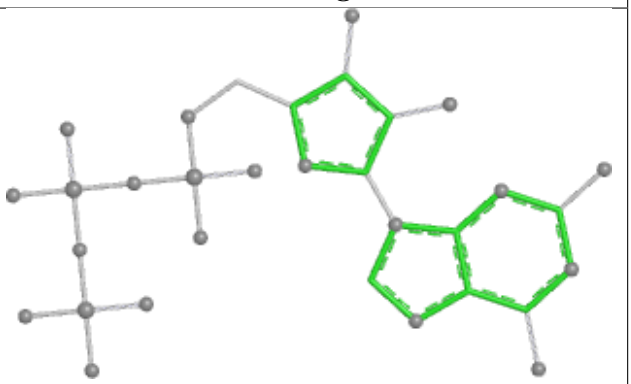
Bond lengths



Bond angles

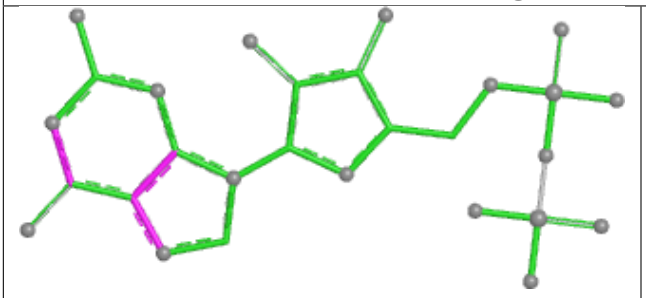


Torsions

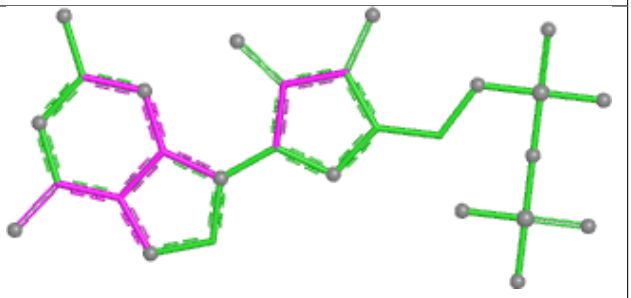


Rings

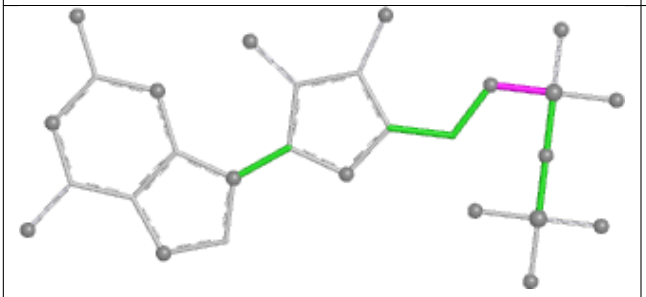
Ligand GDP NL 501



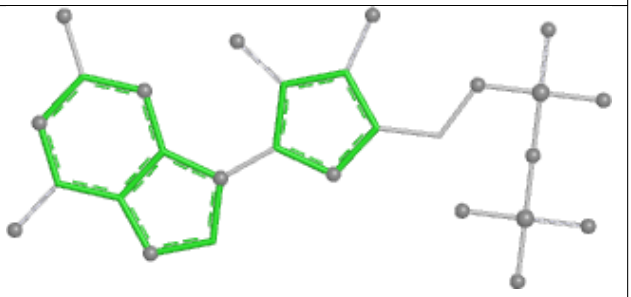
Bond lengths



Bond angles

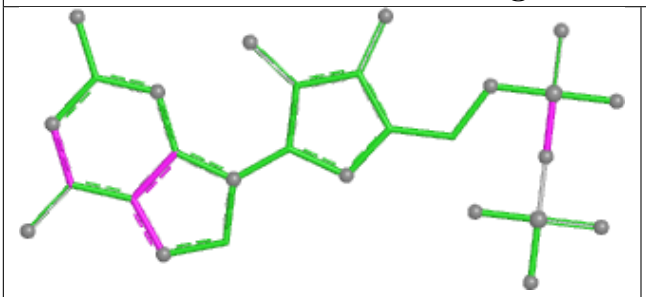


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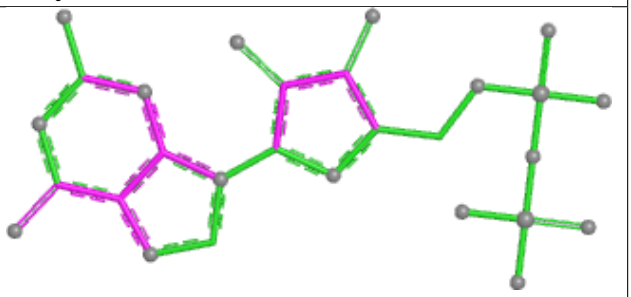


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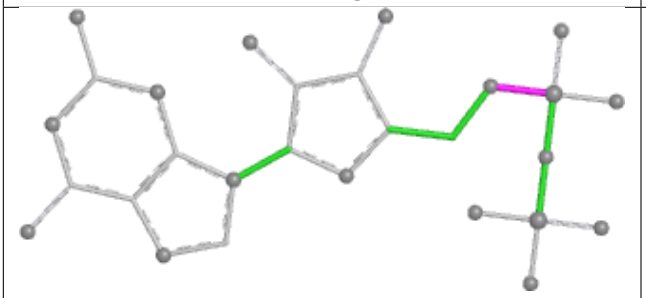
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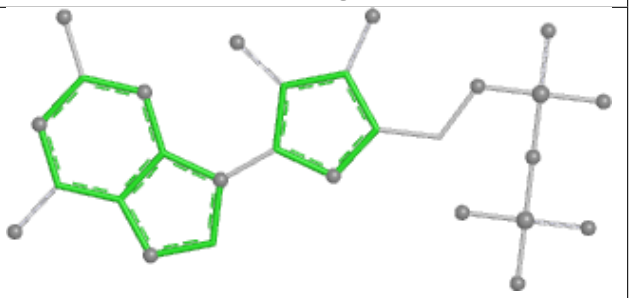
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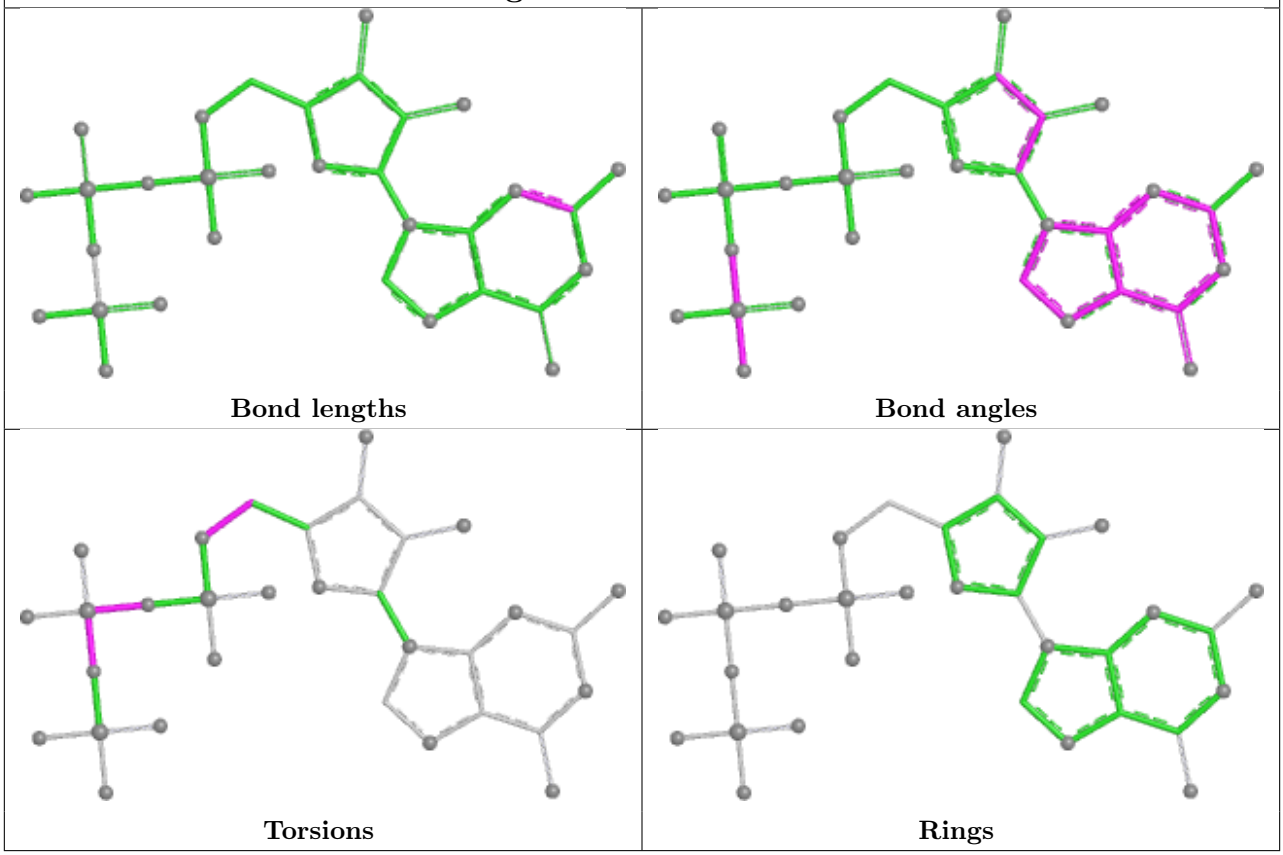


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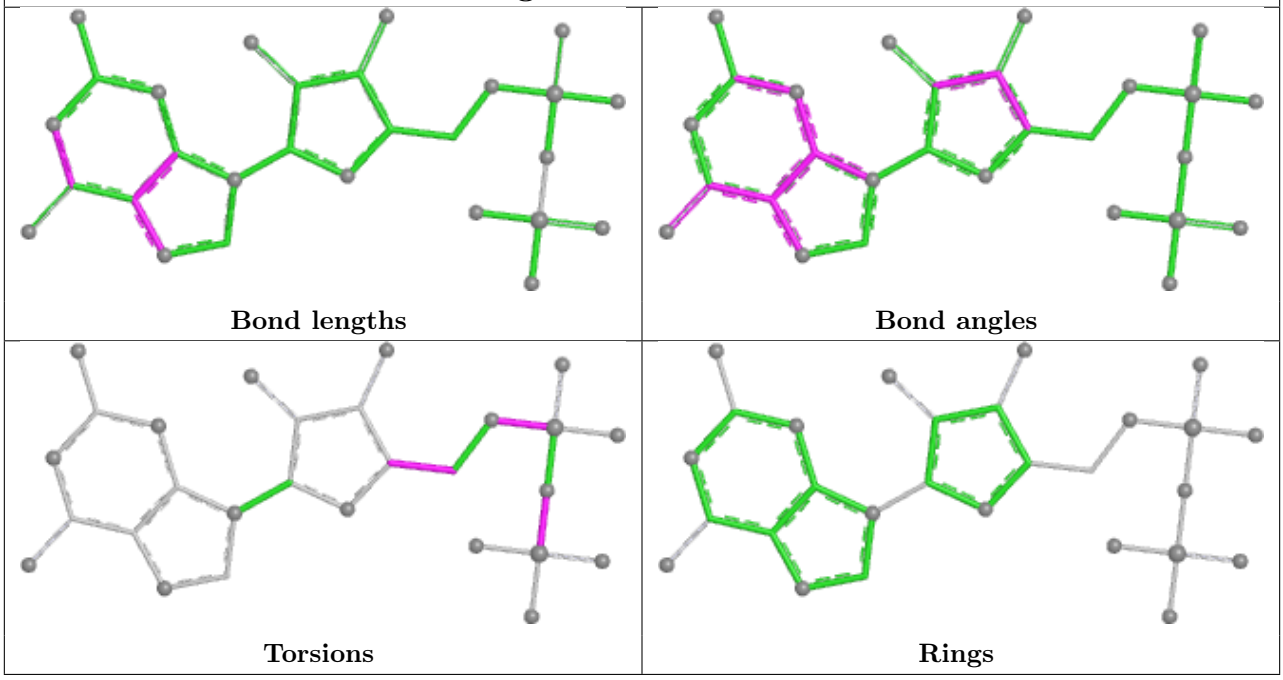


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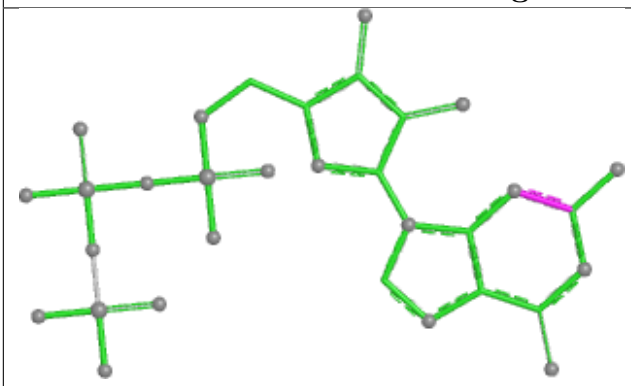
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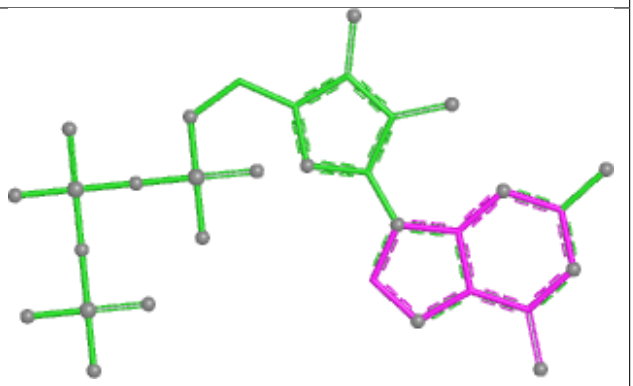
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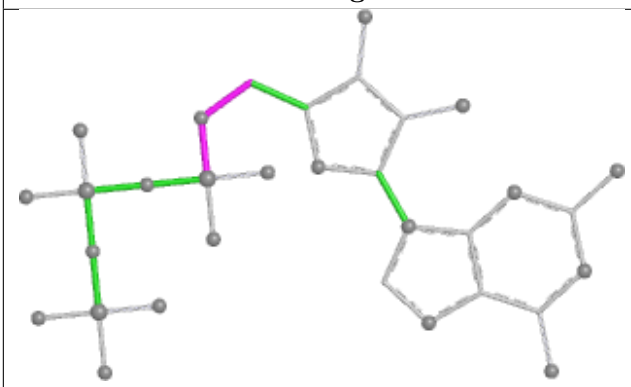
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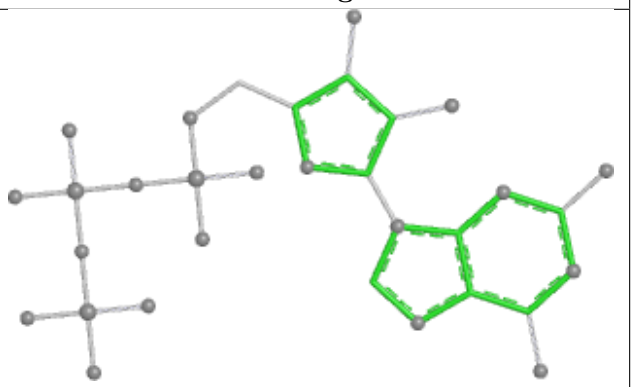
Bond lengths



Bond angles

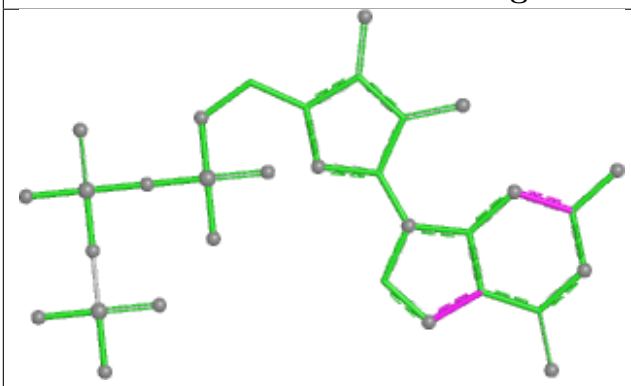


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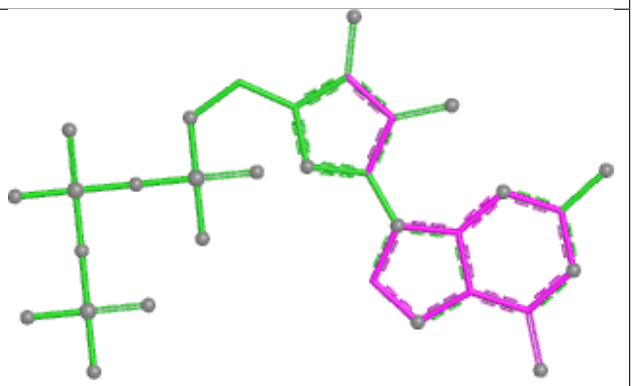


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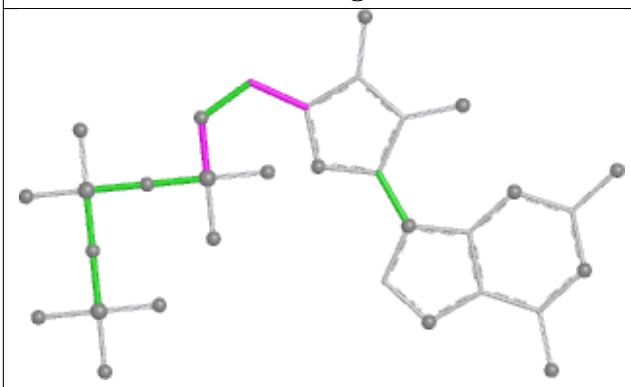
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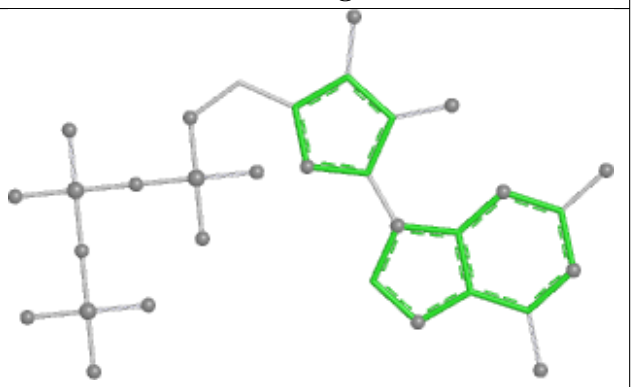
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Bond angles

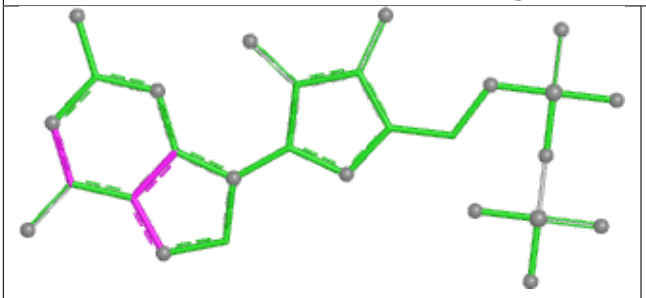


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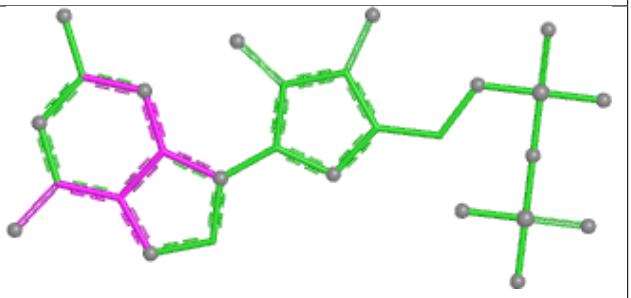


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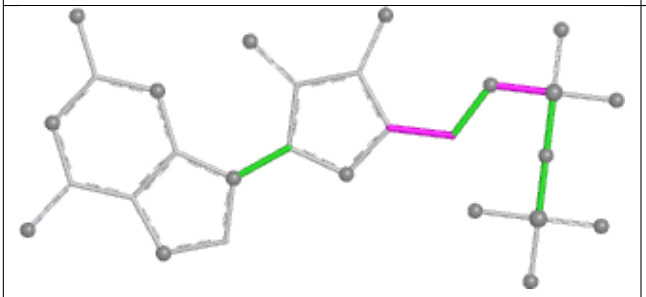
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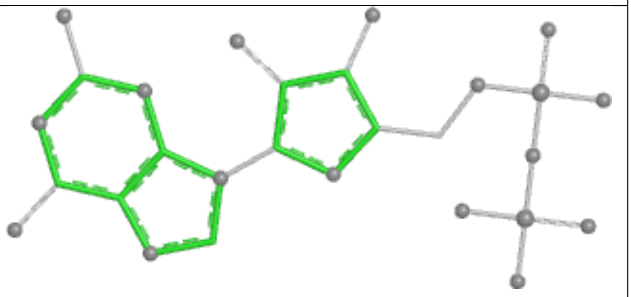
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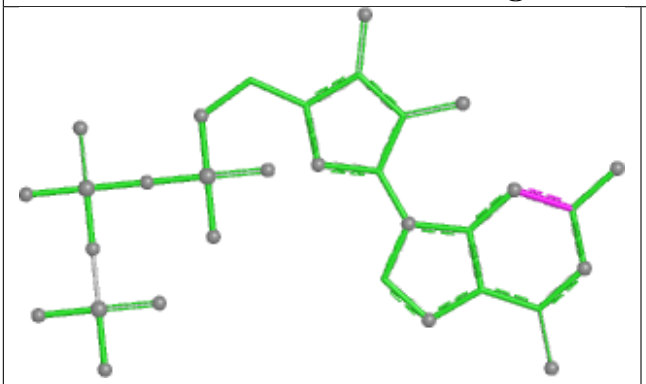


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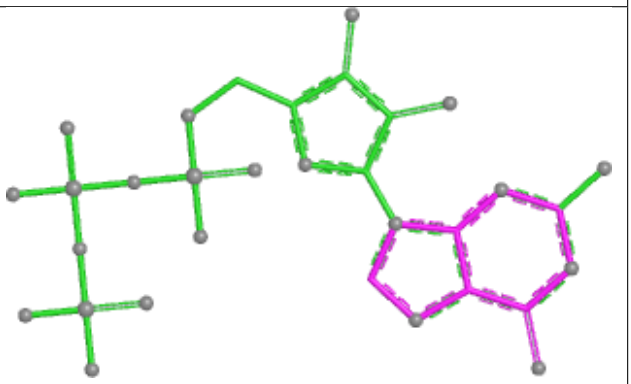


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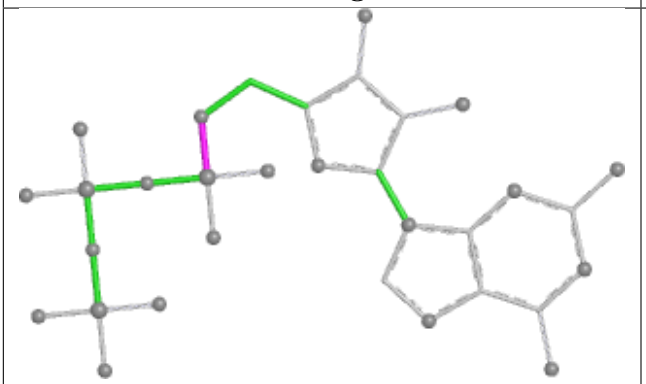
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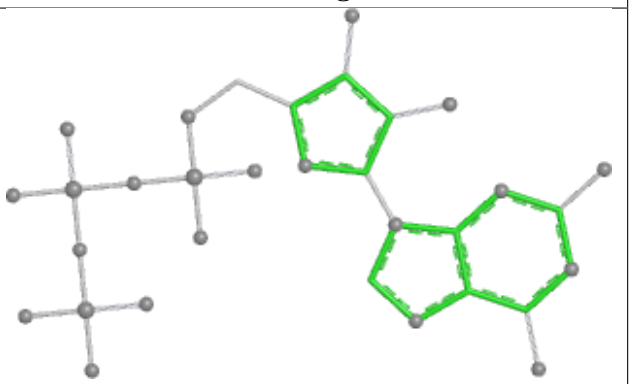
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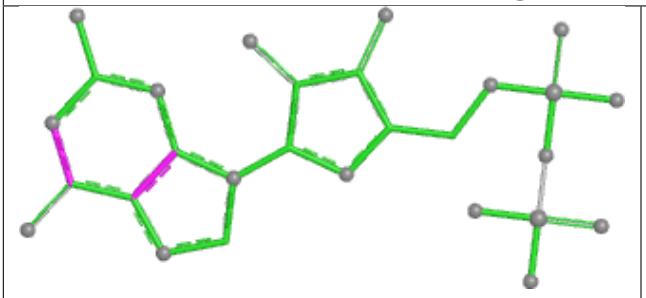


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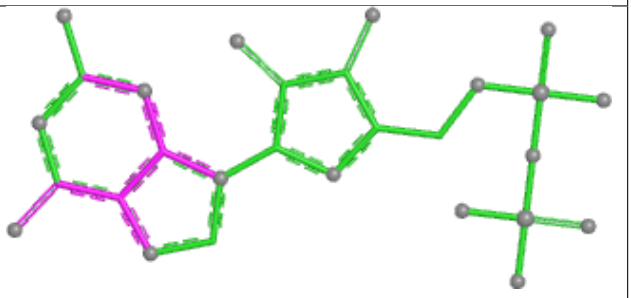


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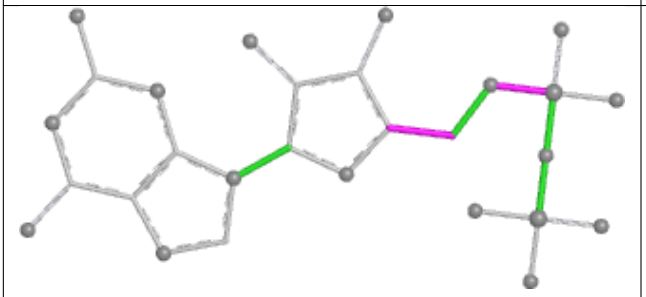
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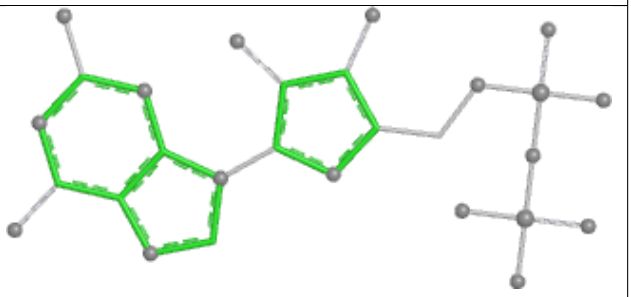
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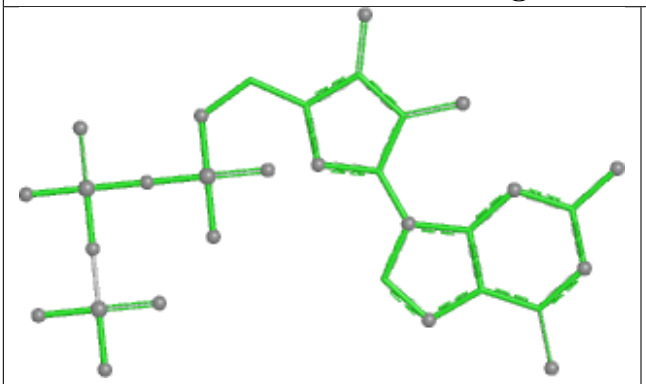


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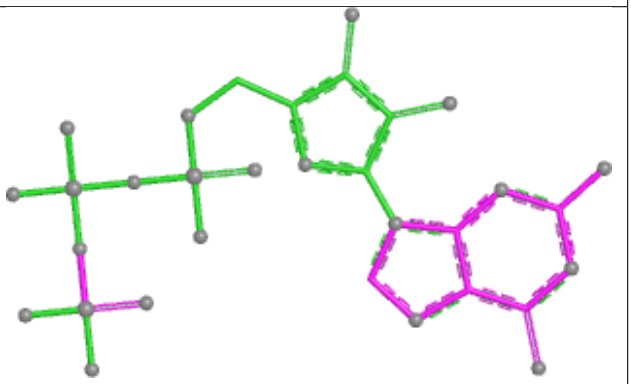


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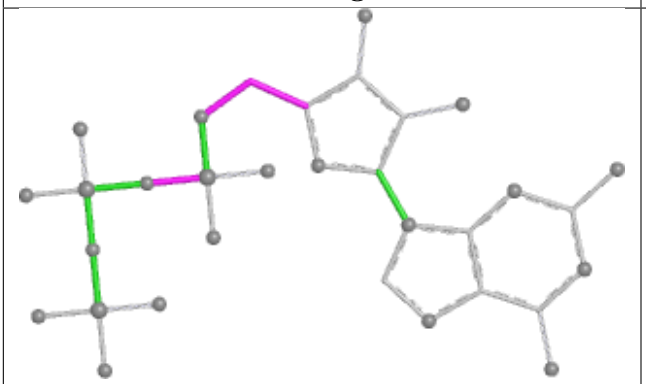
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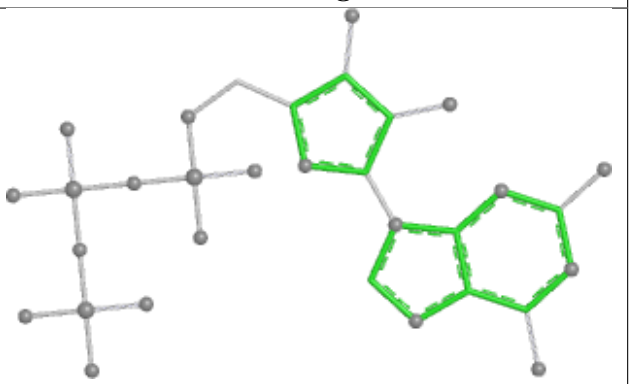
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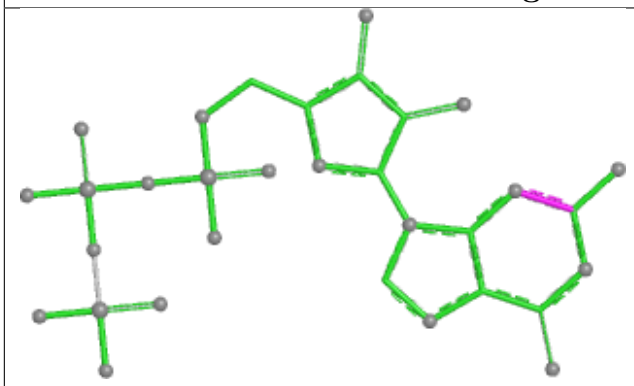


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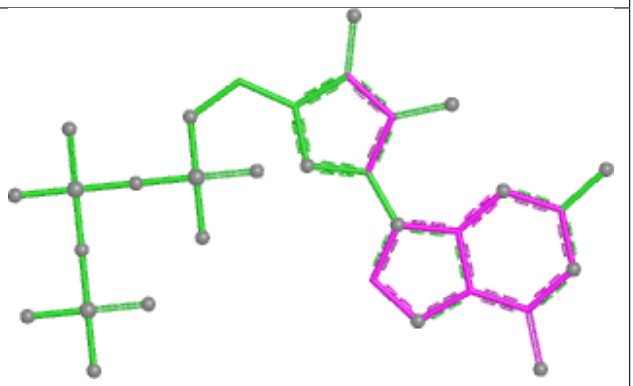


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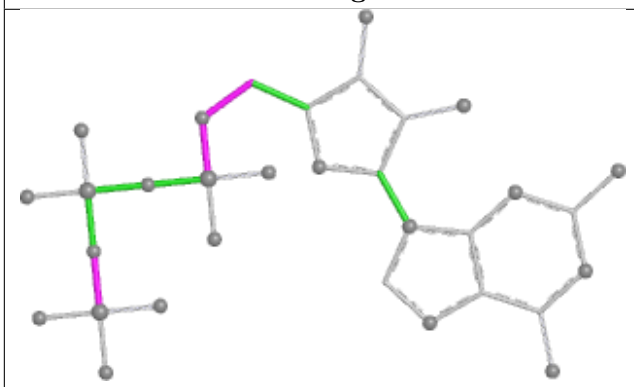
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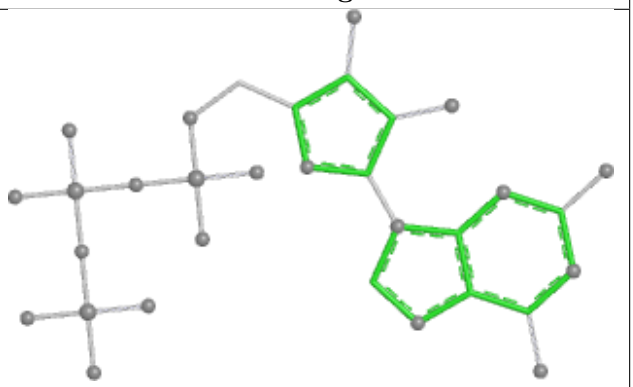
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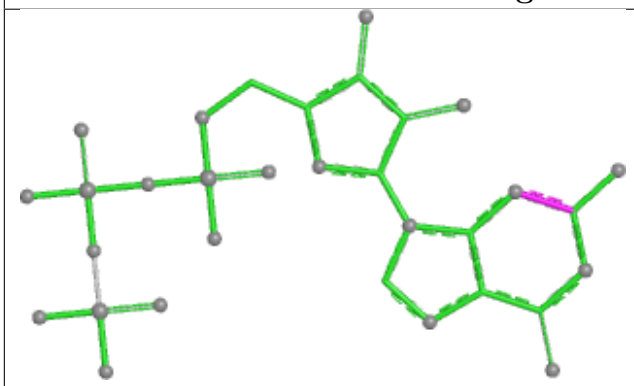


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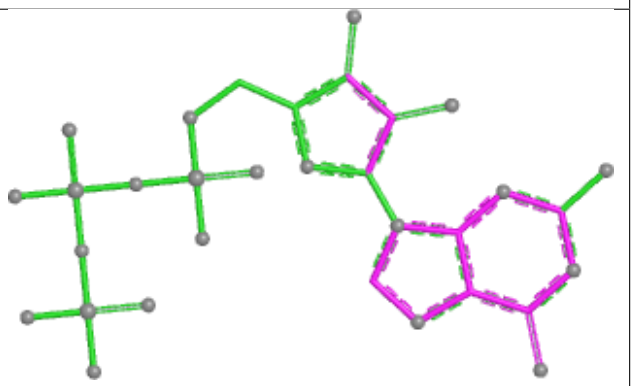


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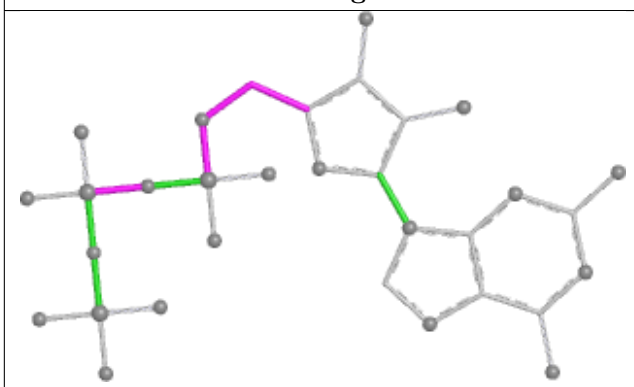
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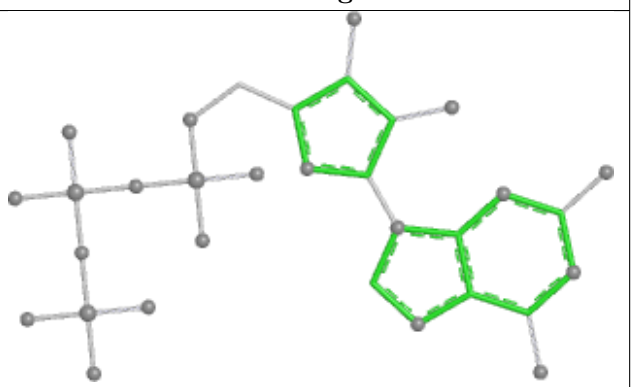
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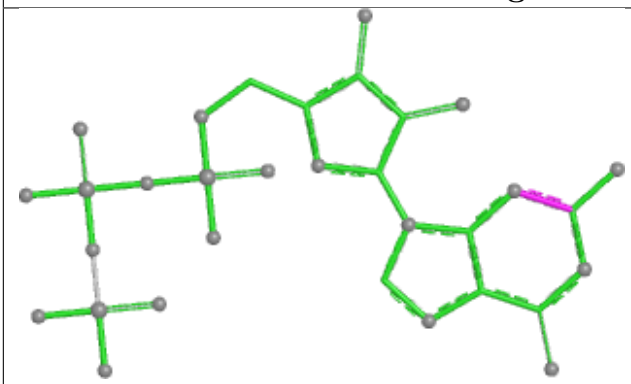


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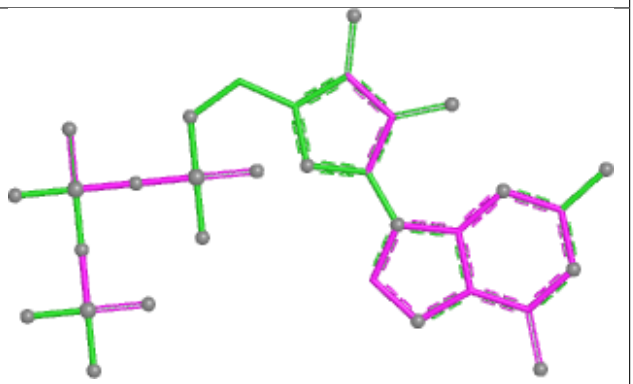


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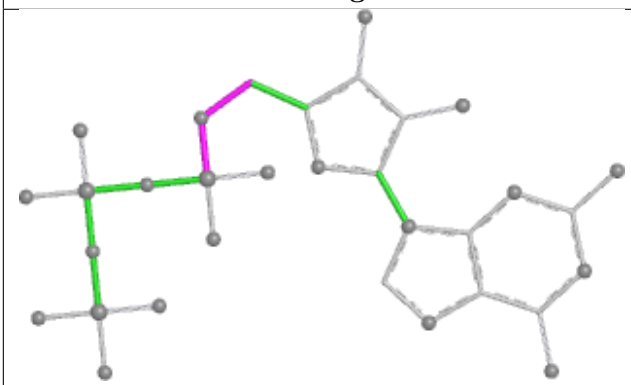
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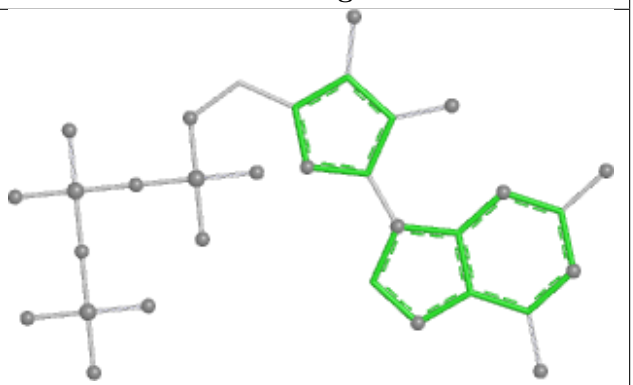
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Bond angles

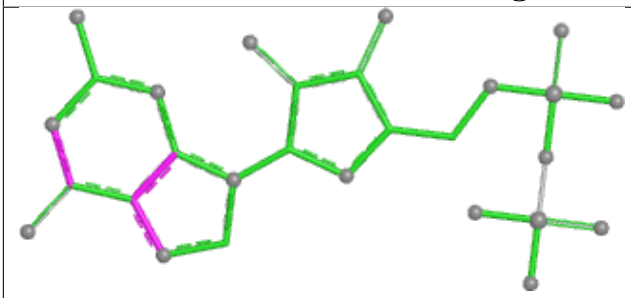


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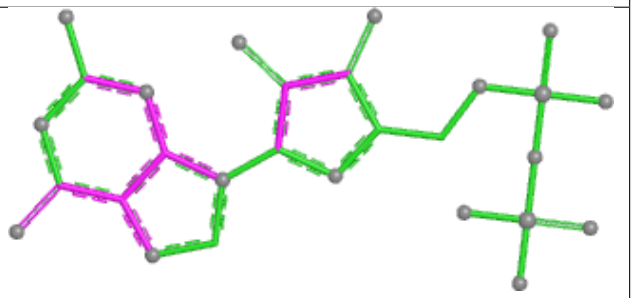


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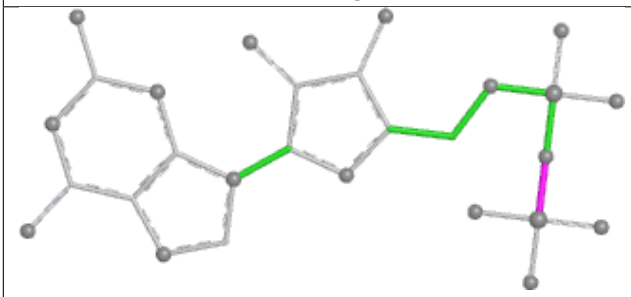
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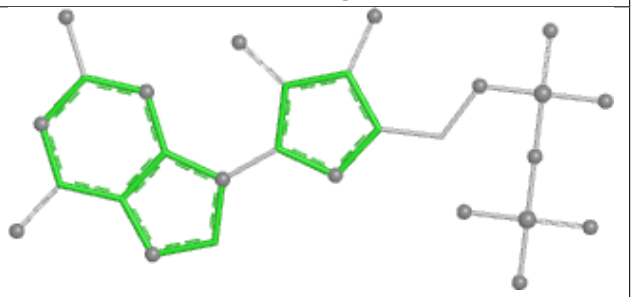
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Bond angles

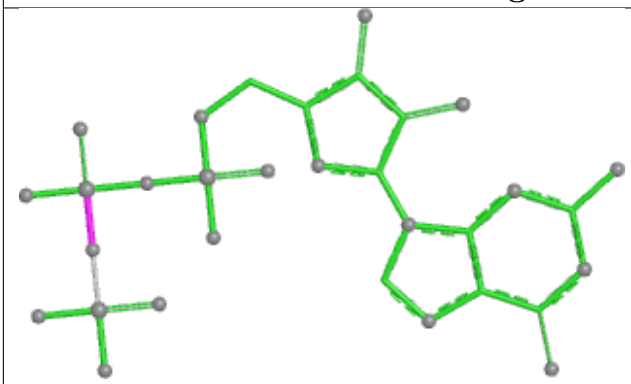


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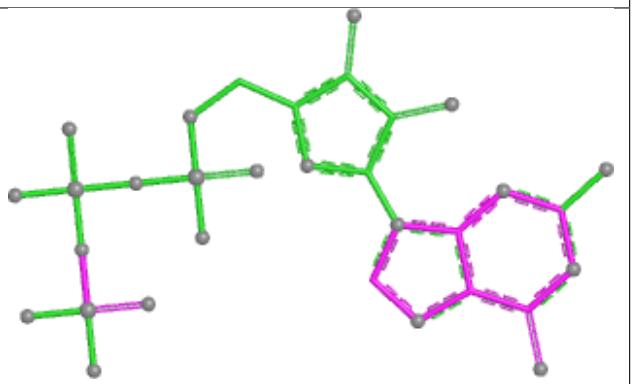


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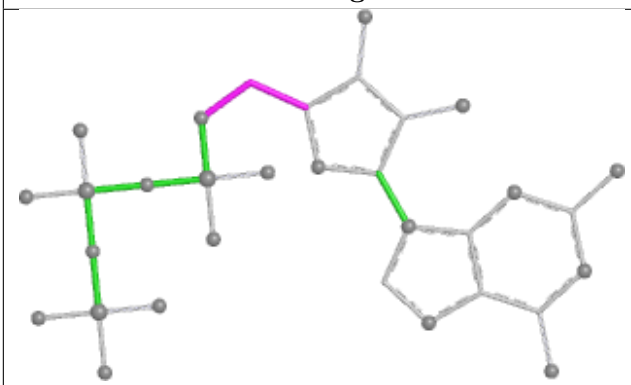
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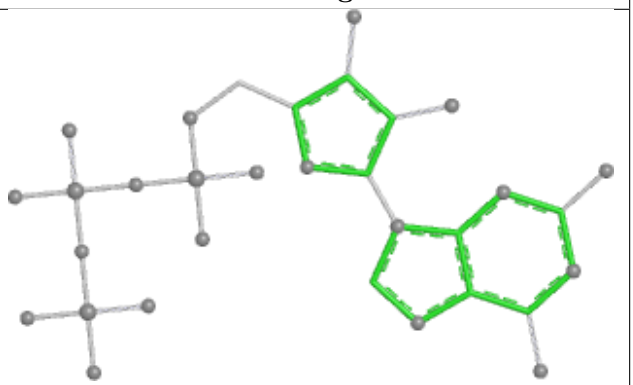
Bond lengths



Bond angles

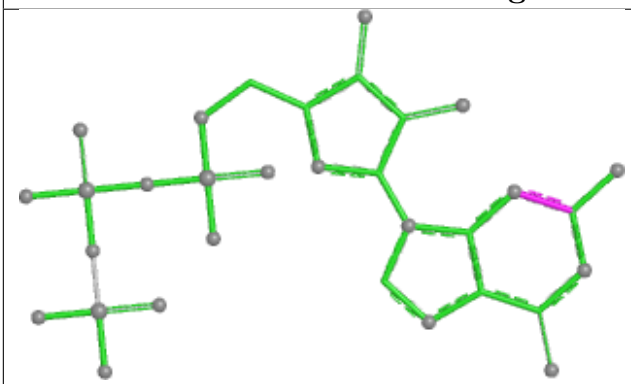


Torsions

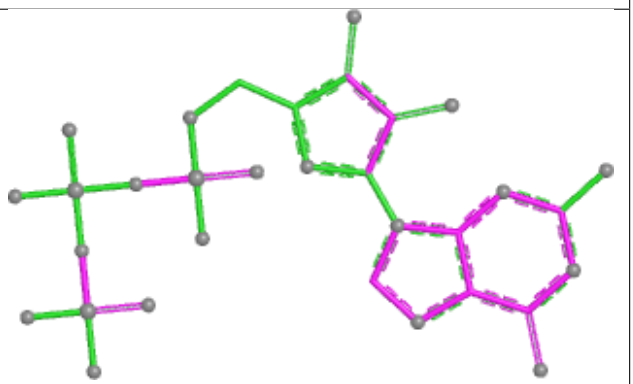


Rings

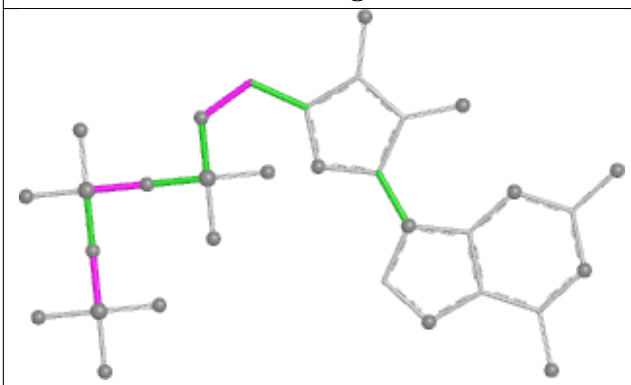
Ligand GTP OH 502



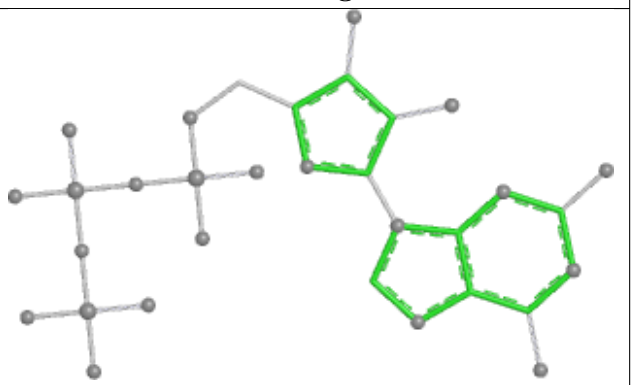
Bond lengths



Bond angles

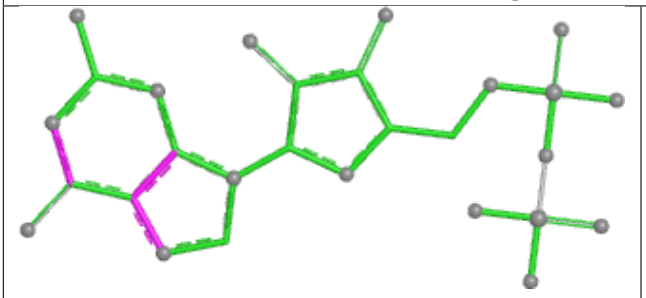


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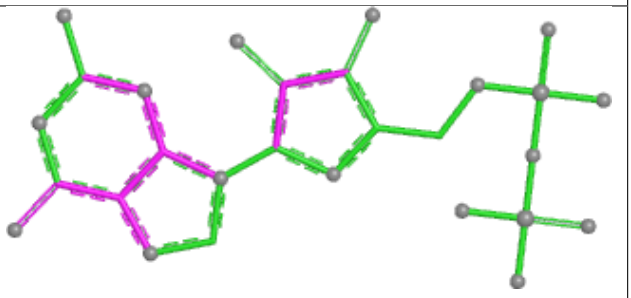


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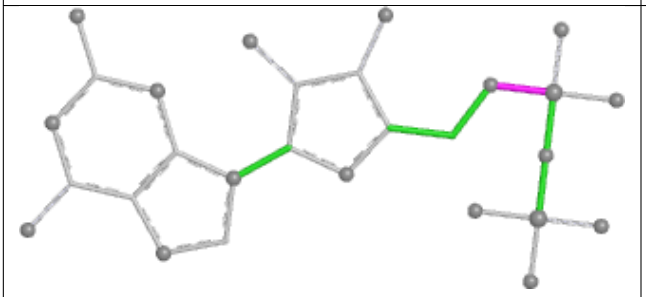
Ligand GDP AH 501



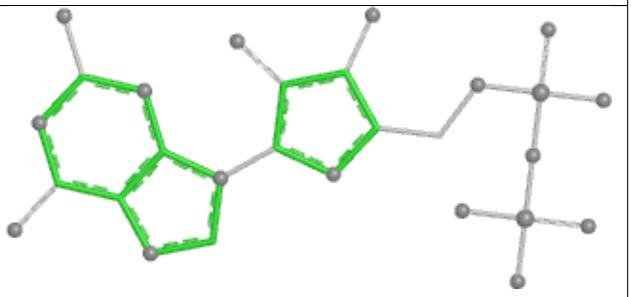
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Bond angles

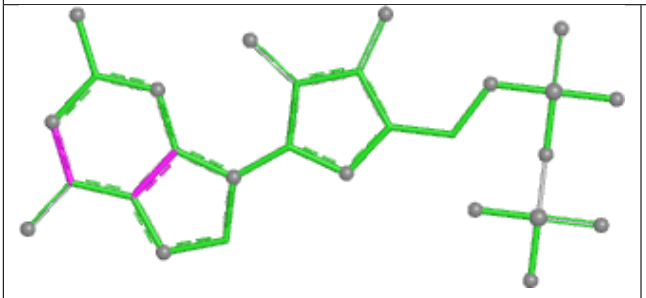


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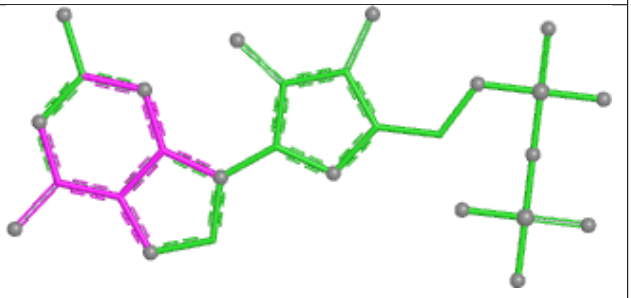


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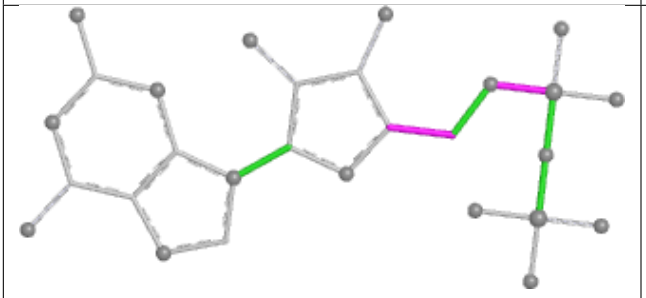
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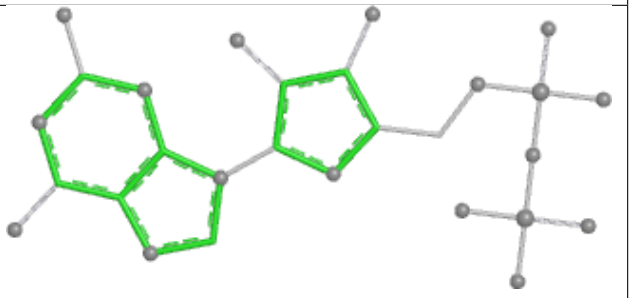
Bond lengths



Bond angles

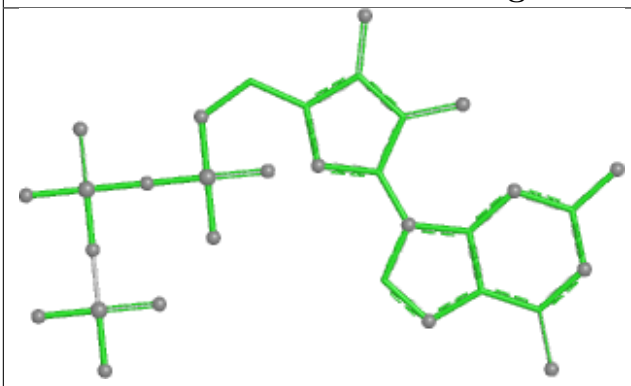


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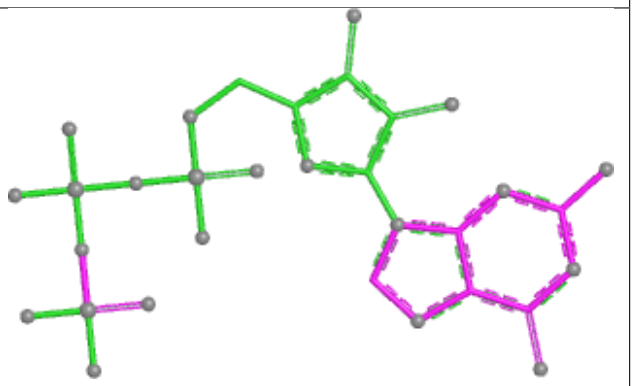


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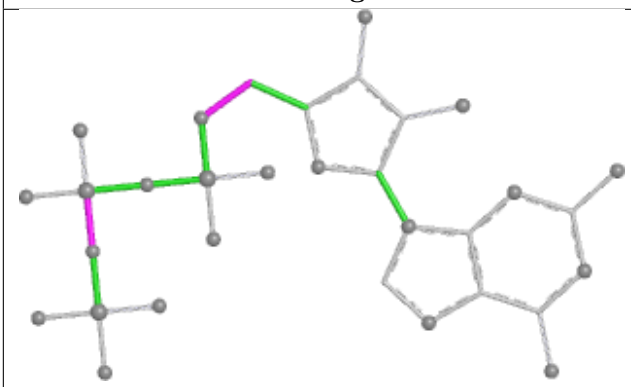
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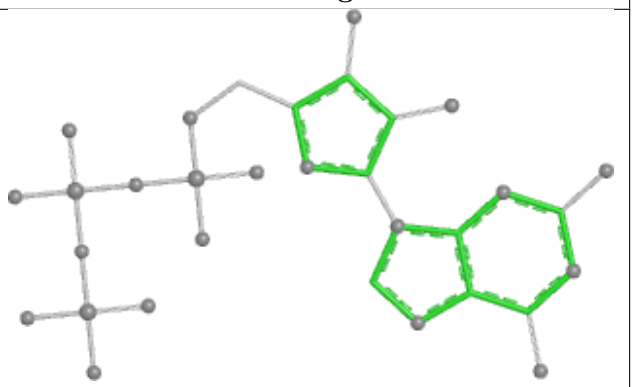
Bond lengths



Bond angles

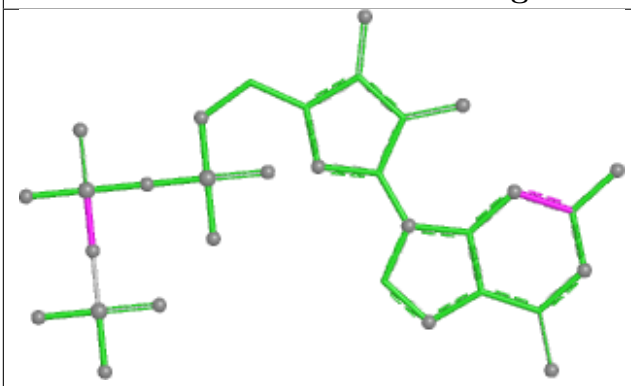


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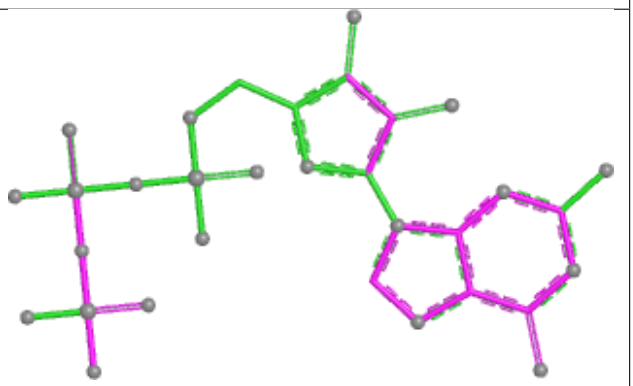


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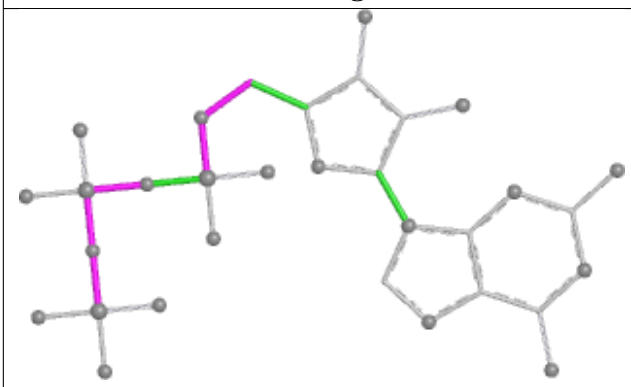
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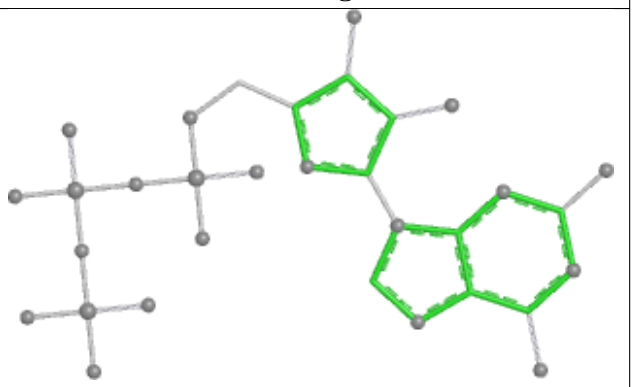
Bond lengths



Bond angles

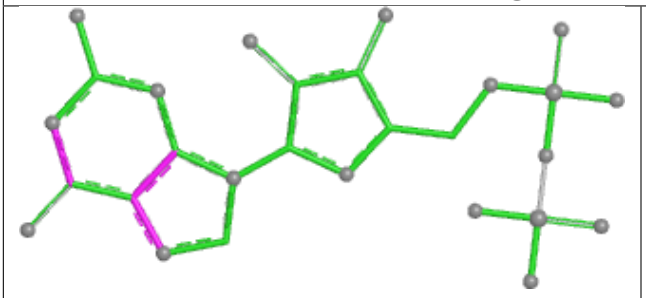


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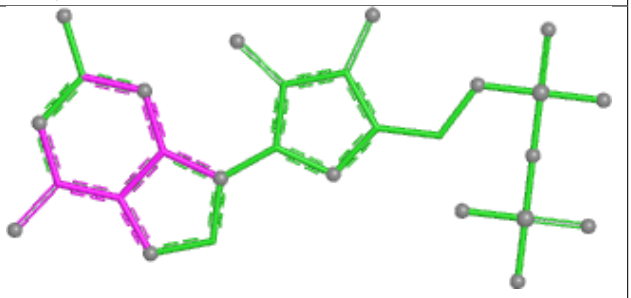


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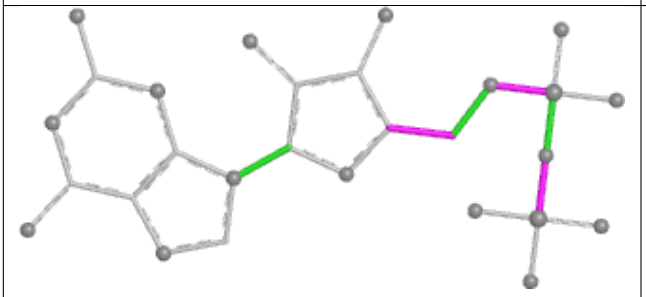
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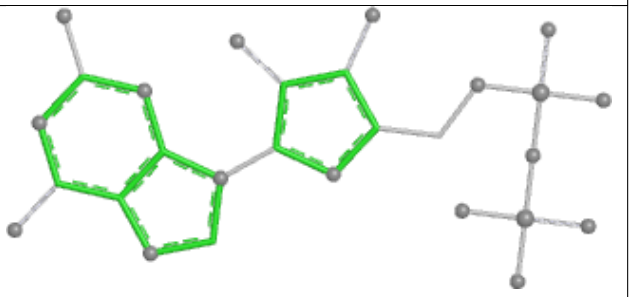
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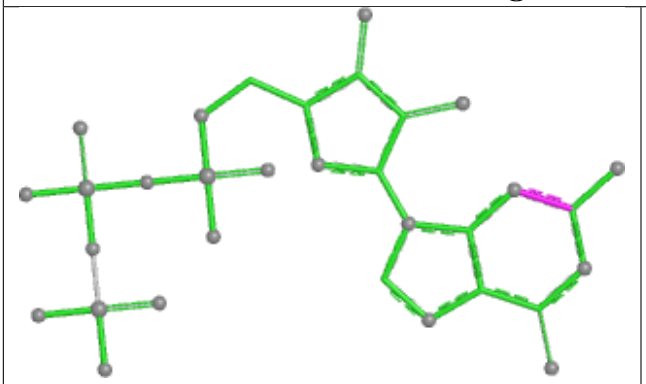


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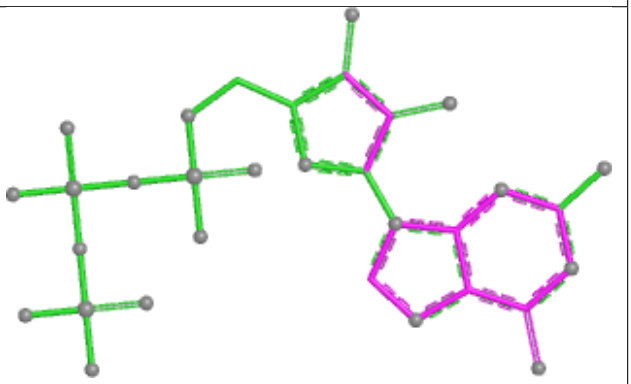


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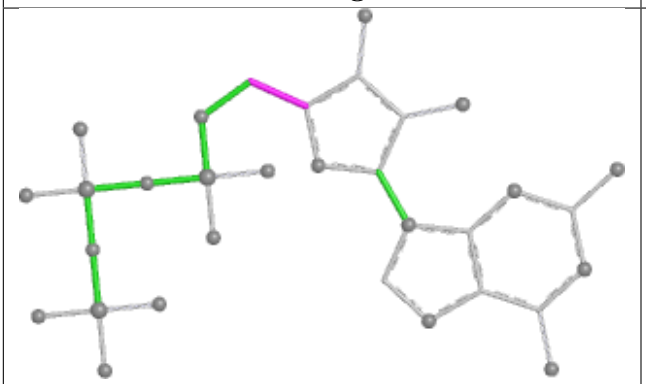
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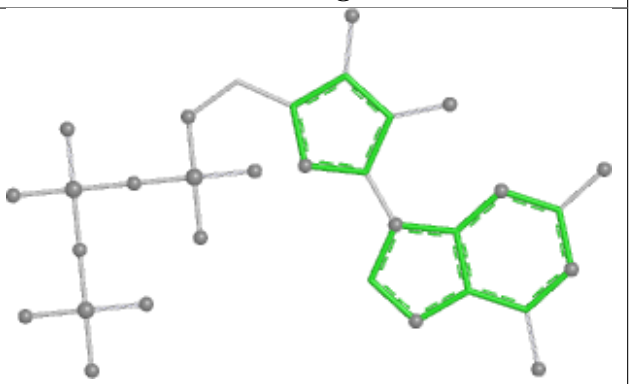
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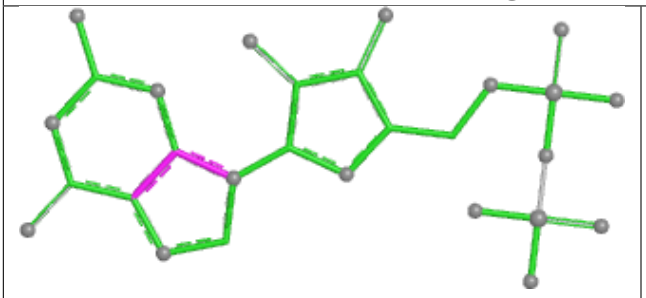


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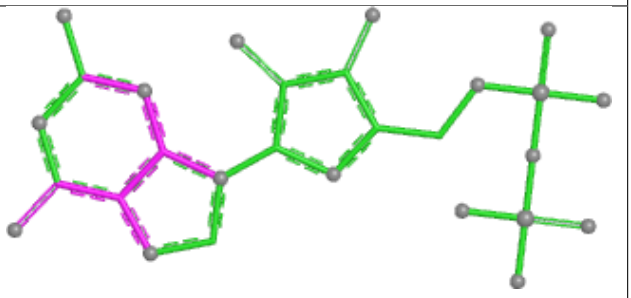


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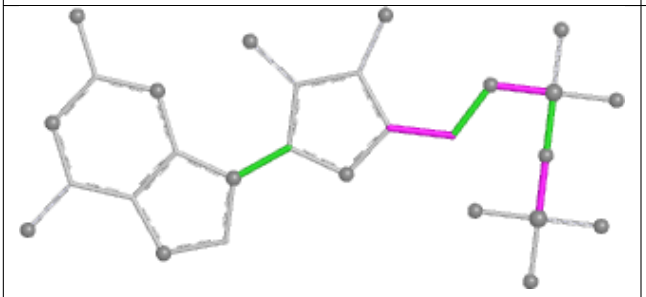
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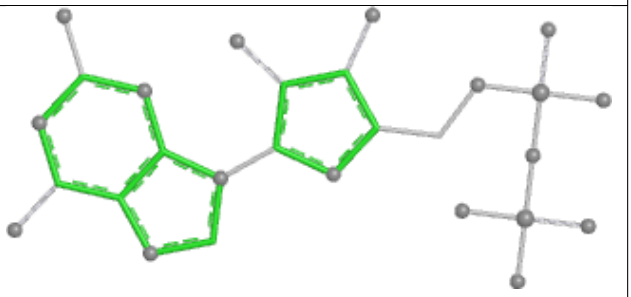
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Bond angles

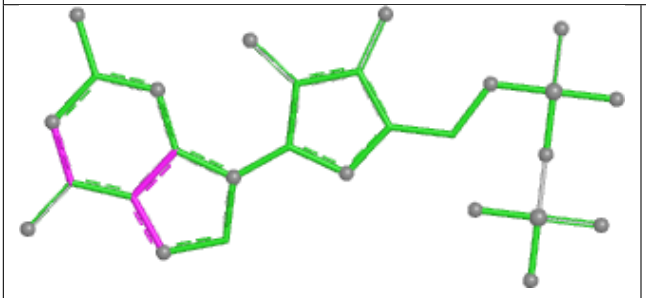


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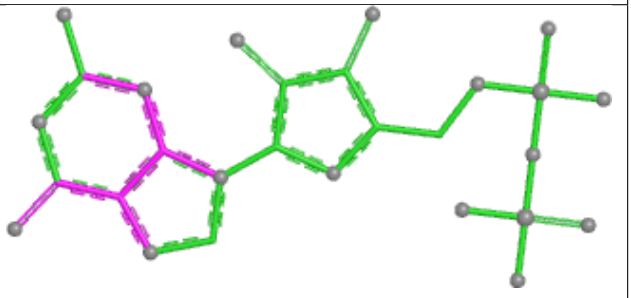


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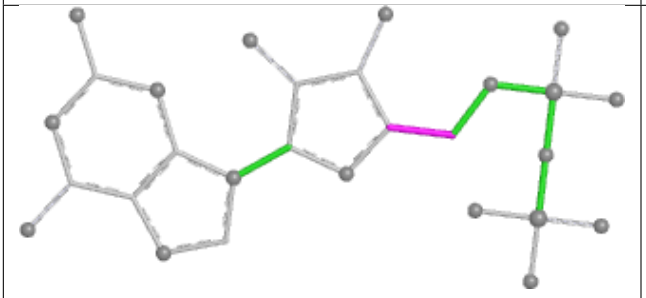
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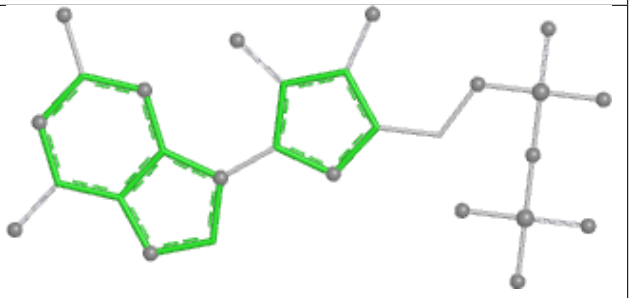
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Bond angles

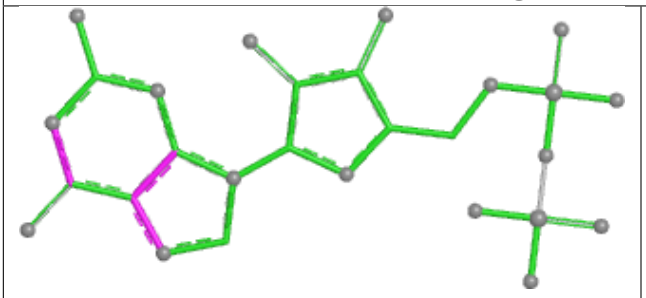


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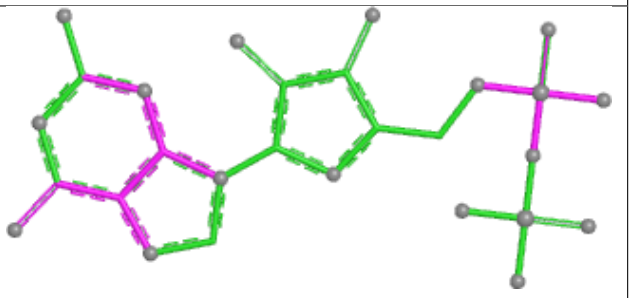


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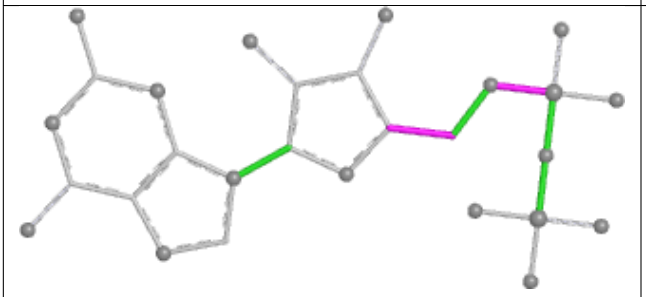
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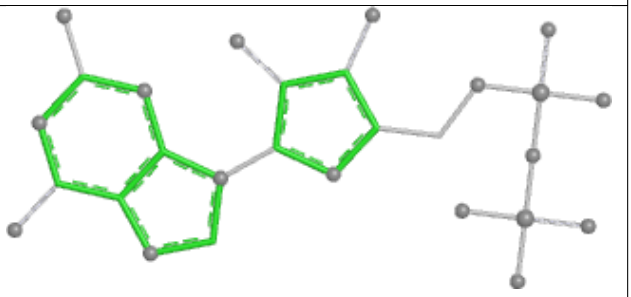
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Bond angles

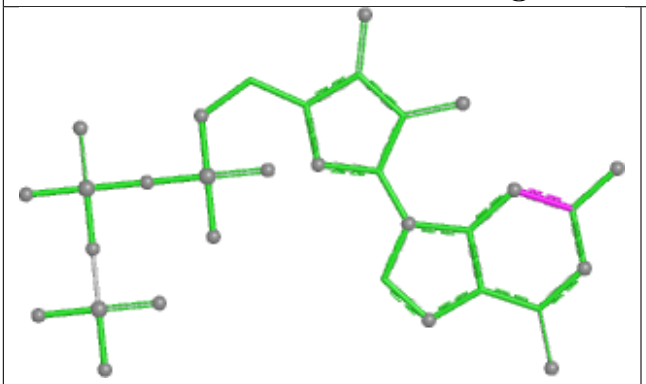


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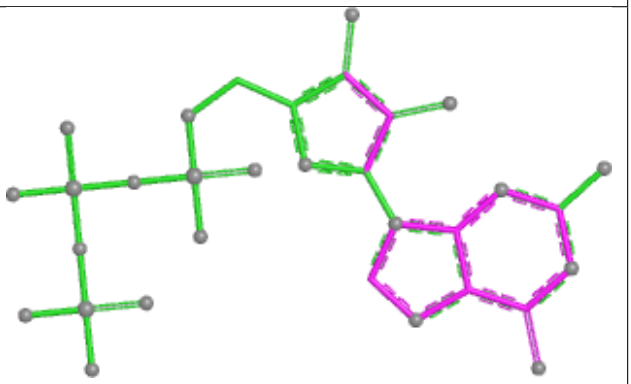


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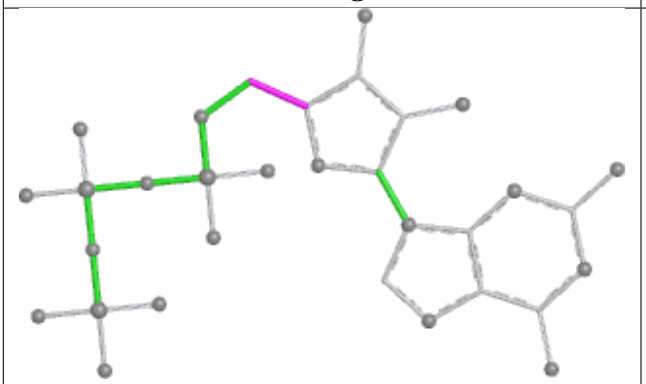
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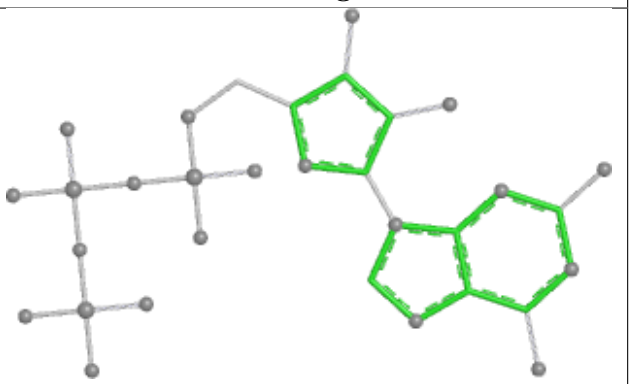
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Bond angles

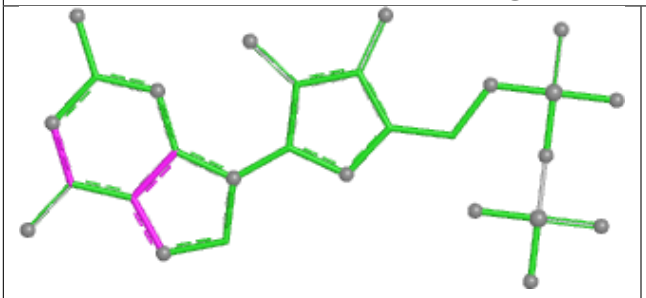


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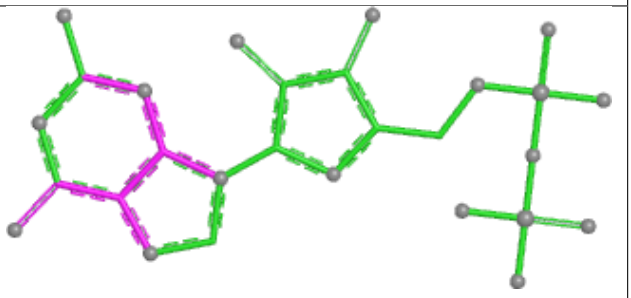


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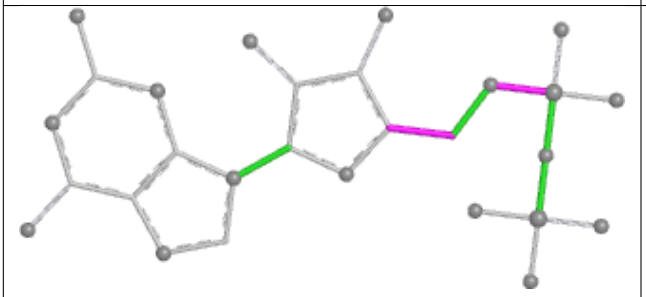
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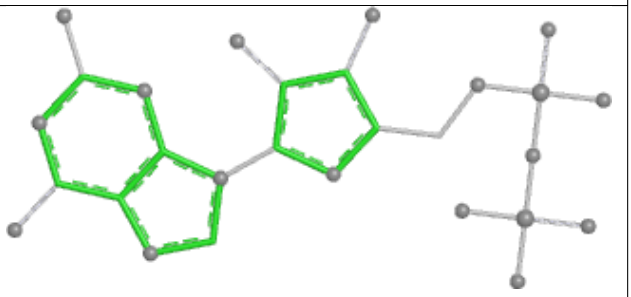
Bond lengths



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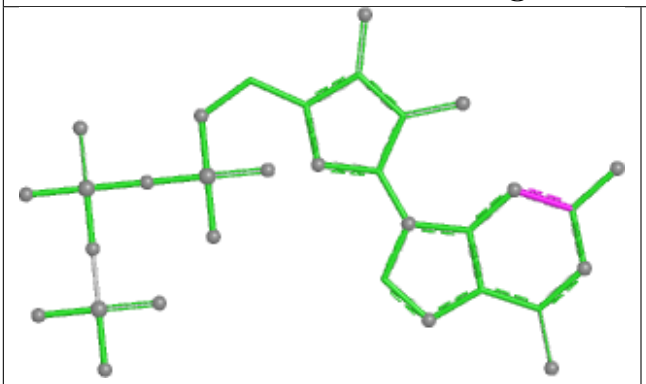


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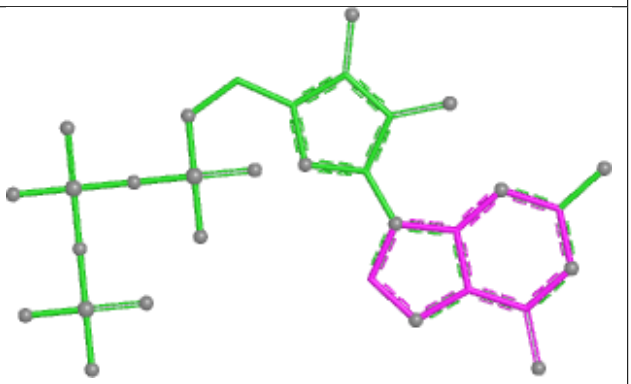


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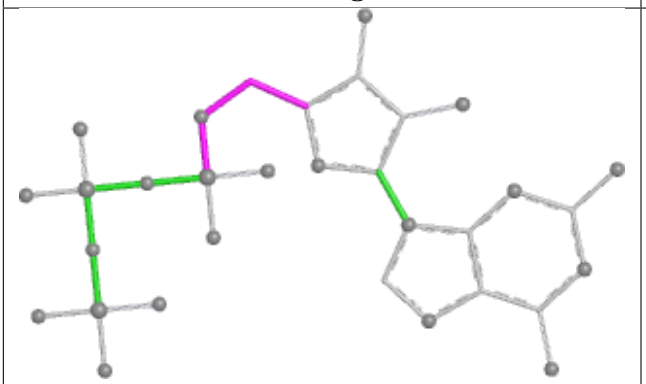
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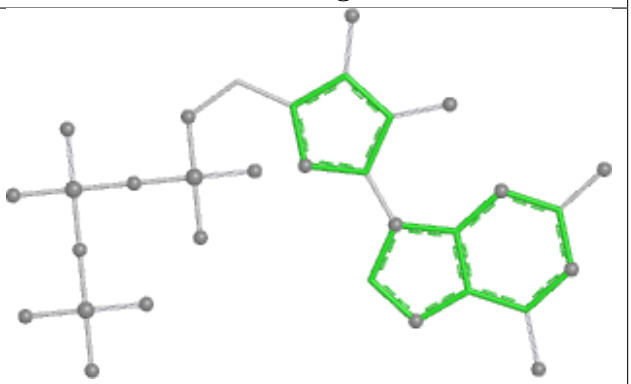
Bond lengths



Bond angles

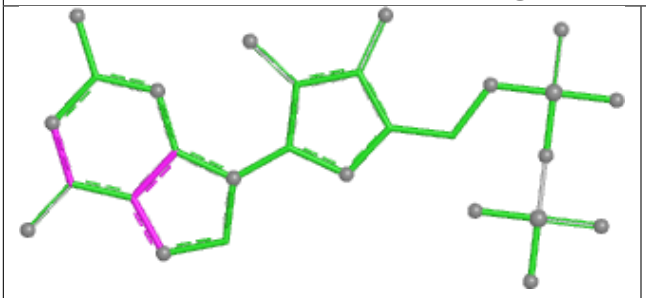


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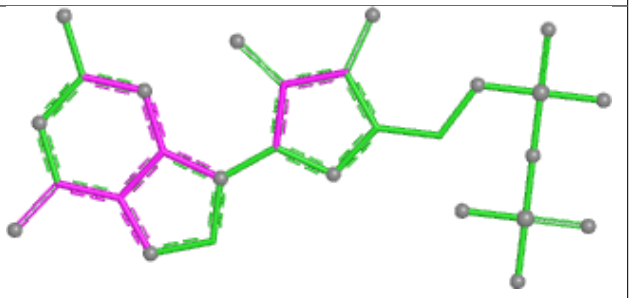


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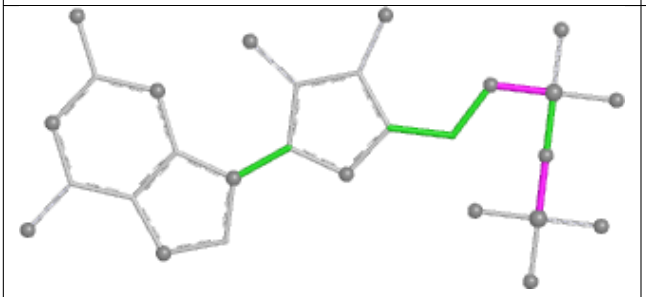
Ligand GDP EF 501



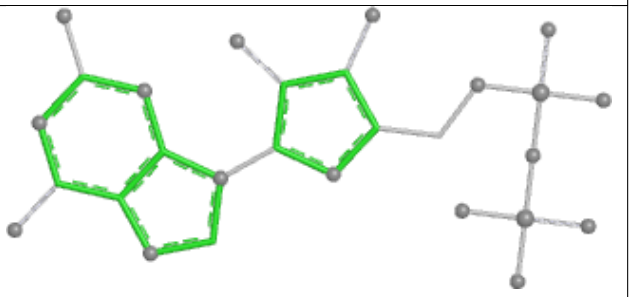
Bond lengths



Bond angles

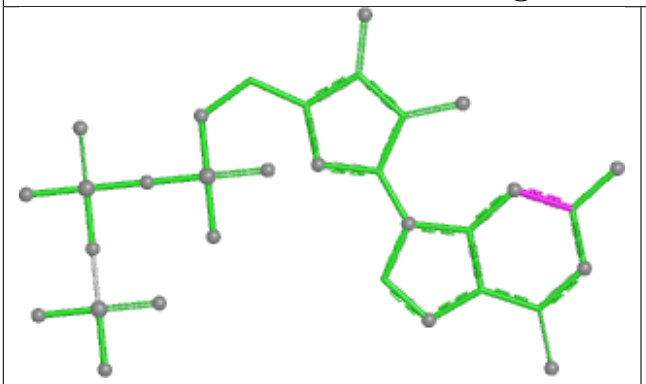


Torsions

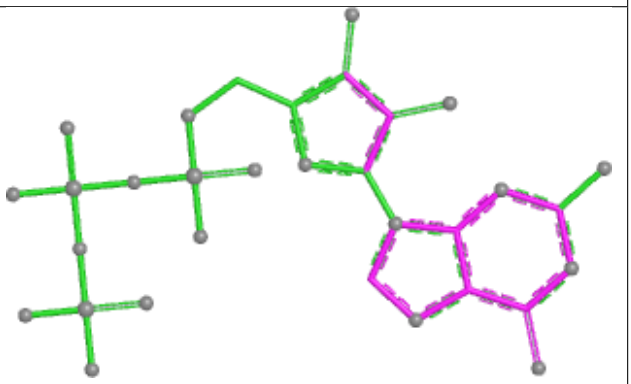


Rings

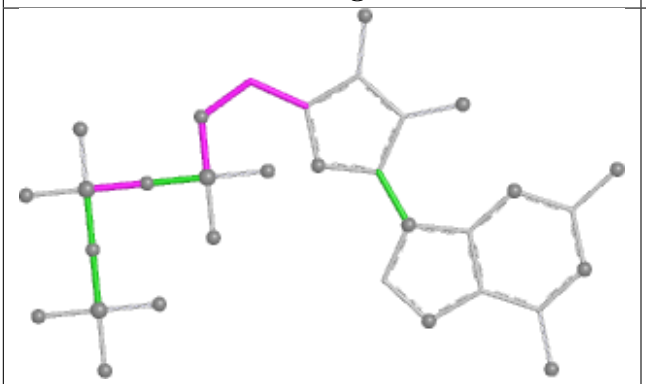
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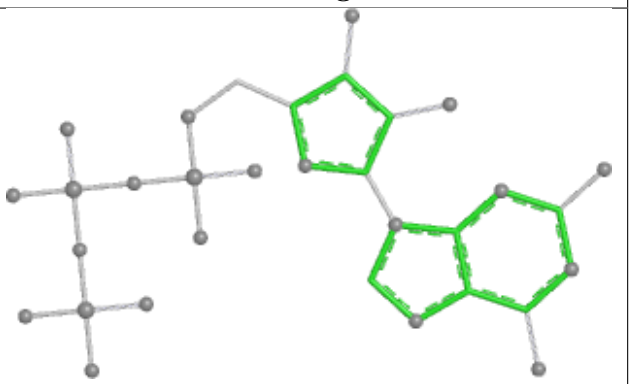
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Bond angles

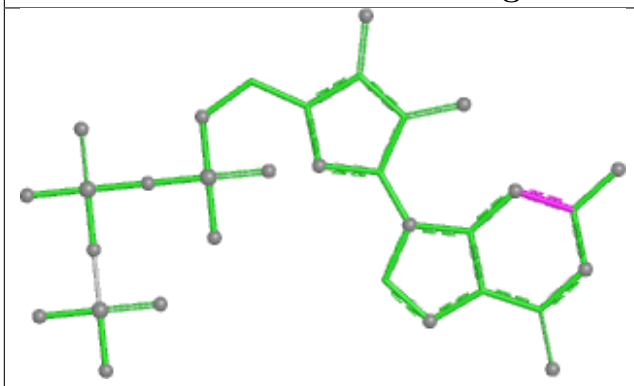


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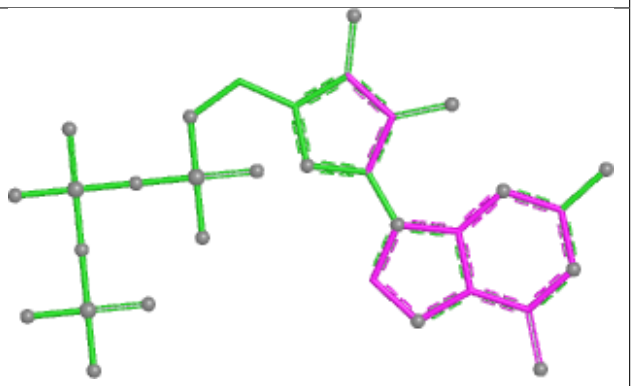


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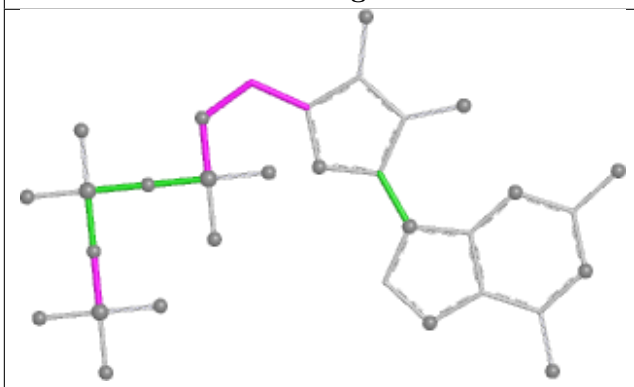
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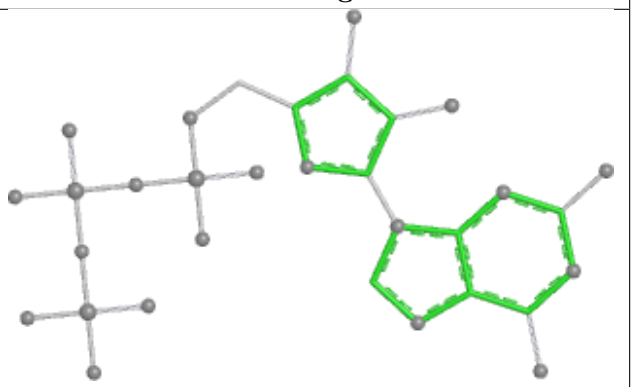
Bond lengths



Bond angles

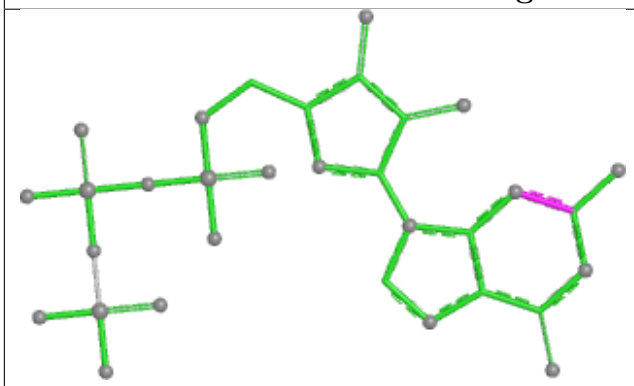


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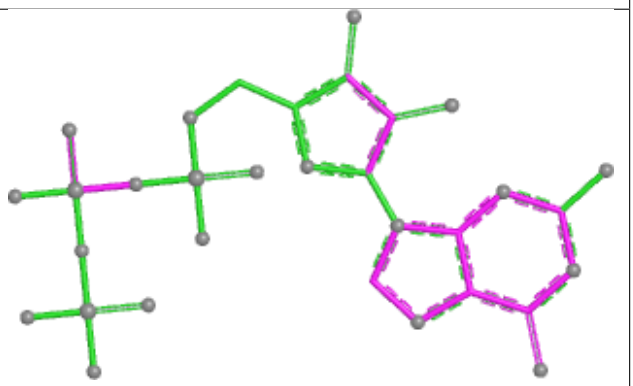


Rings

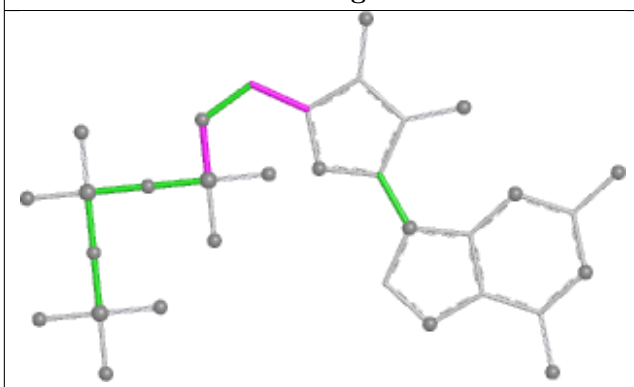
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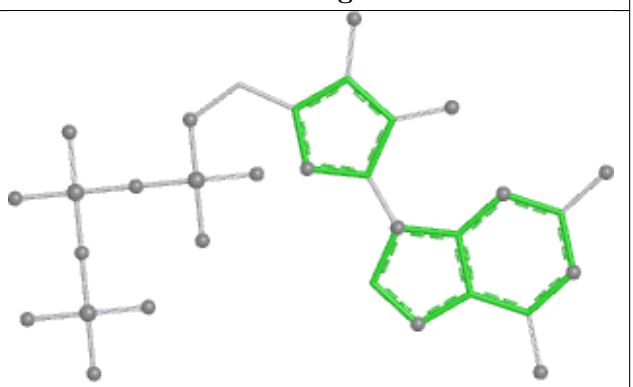
Bond lengths



Bond angles

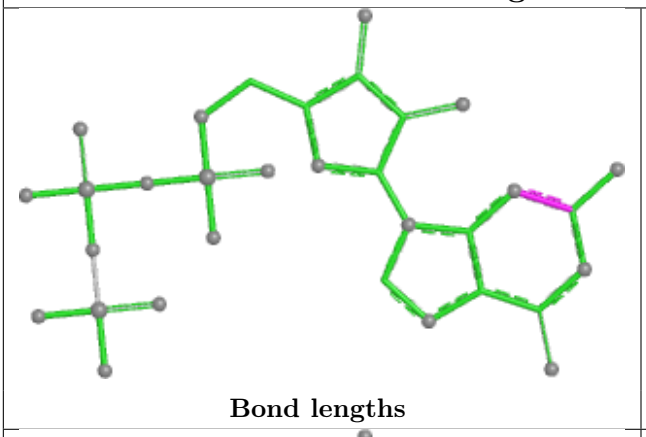


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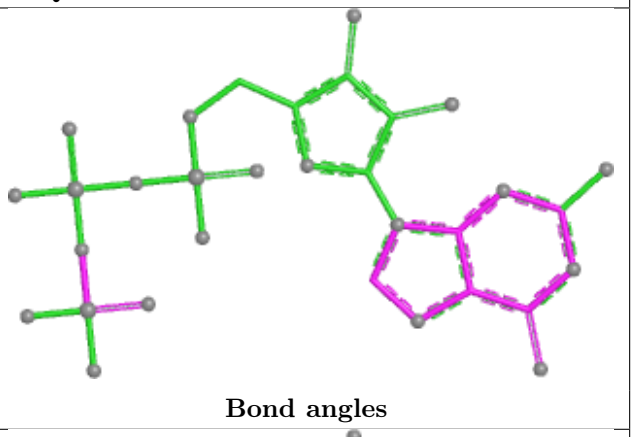


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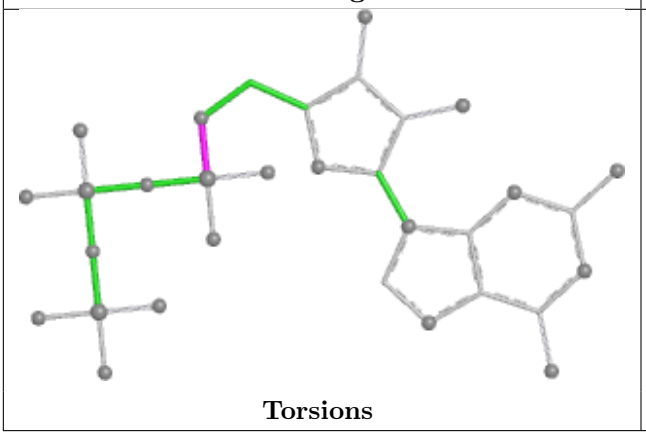
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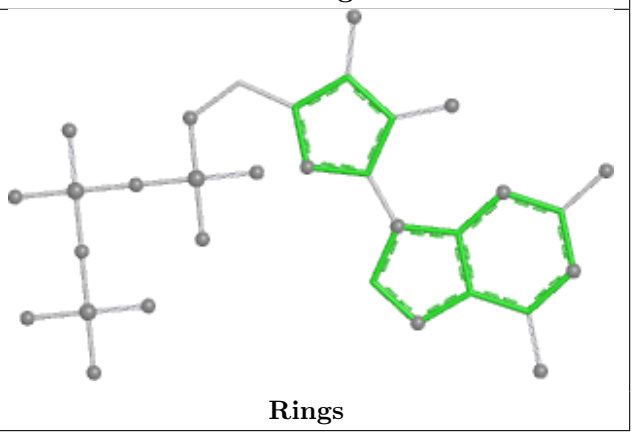
Bond lengths



Bond angles

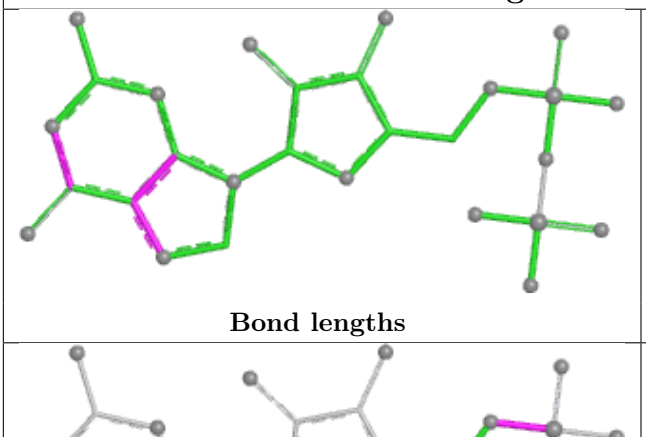


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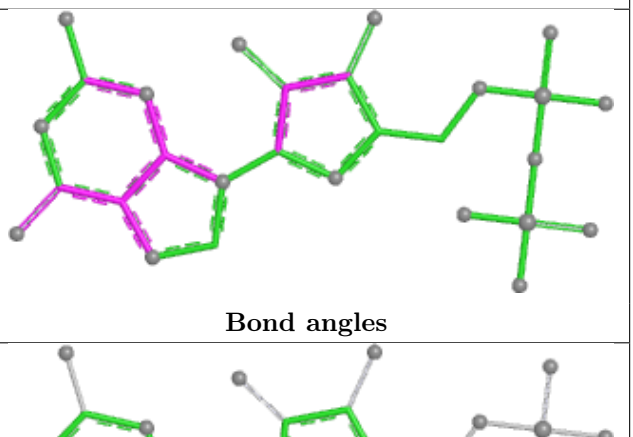


Rings

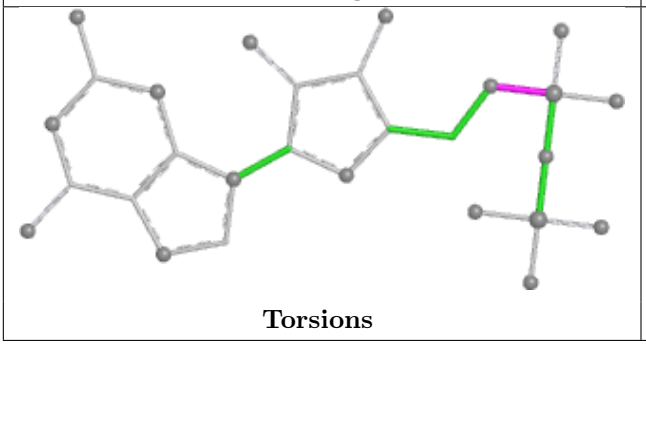
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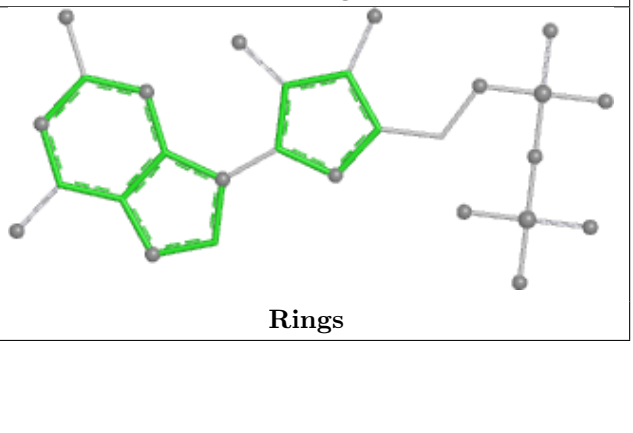
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Bond angles

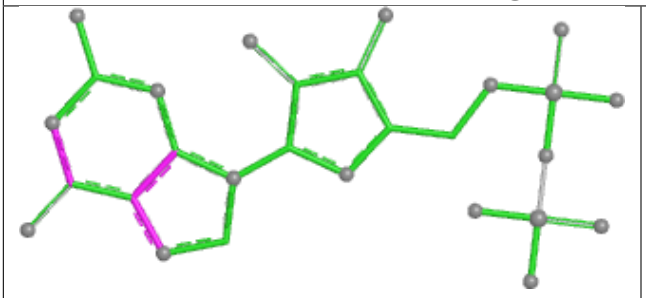


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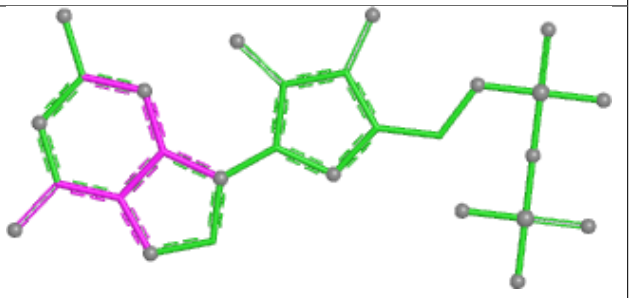


Rings

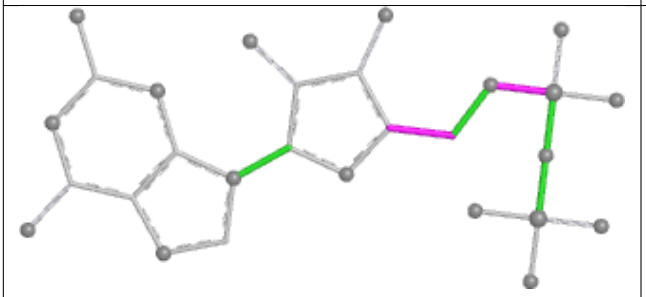
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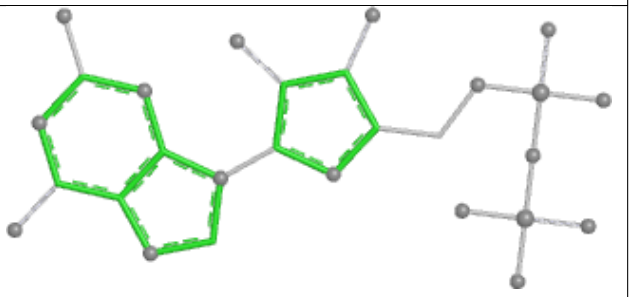
Bond lengths



Bond angles

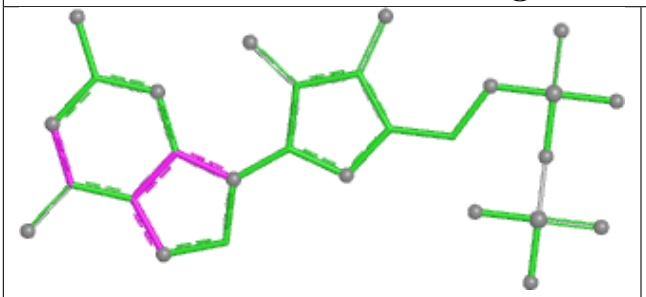


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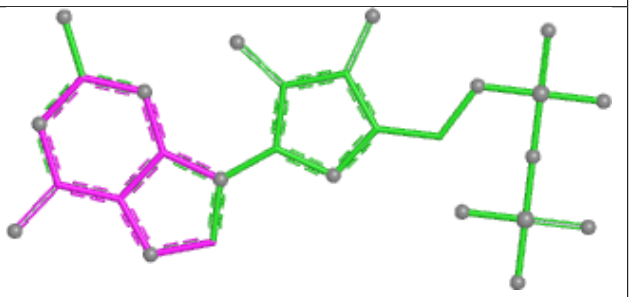


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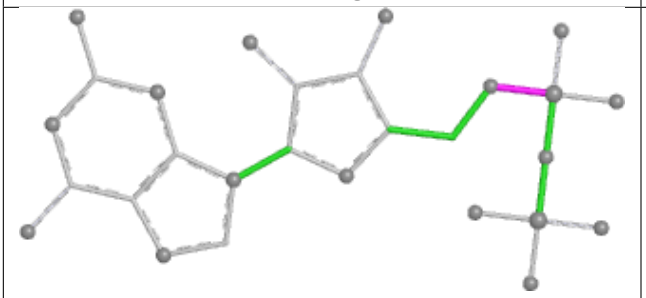
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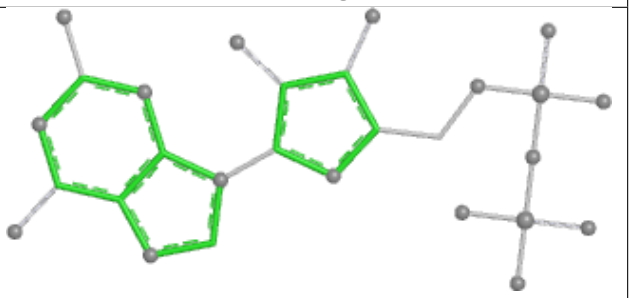
Bond lengths



Bond angles

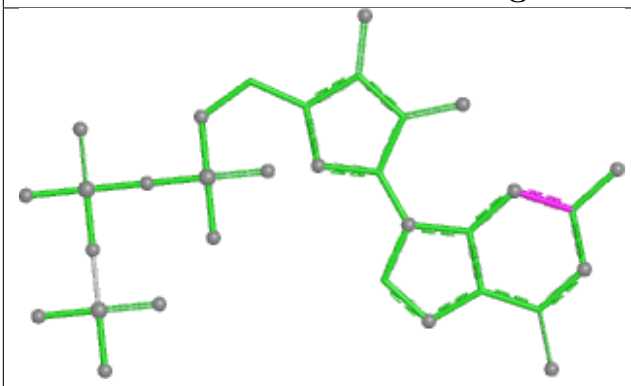


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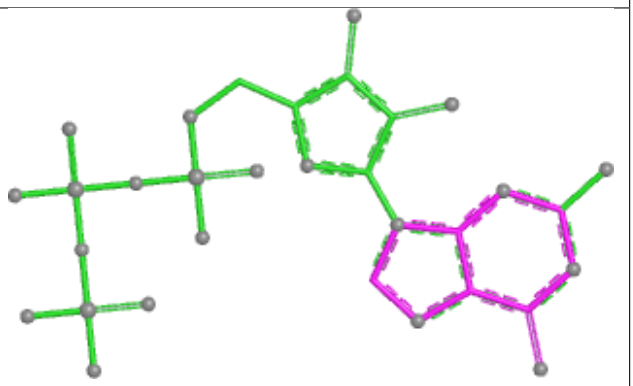


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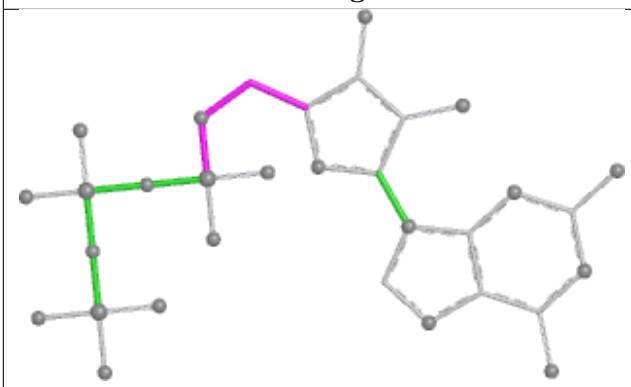
Ligand GTP JM 501



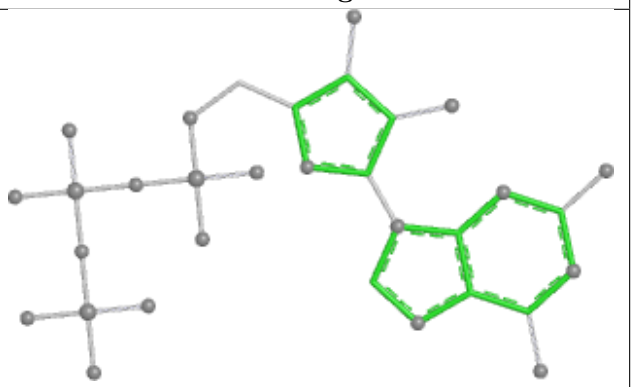
Bond lengths



Bond angles

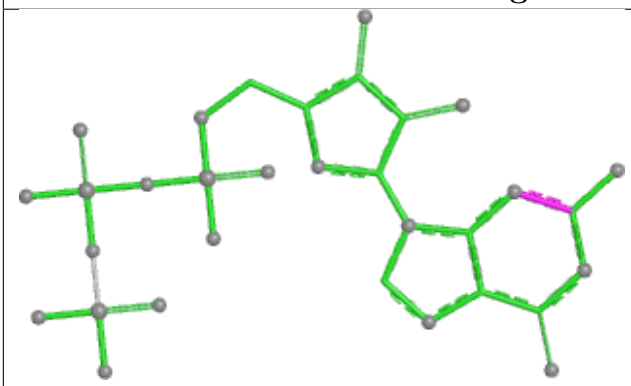


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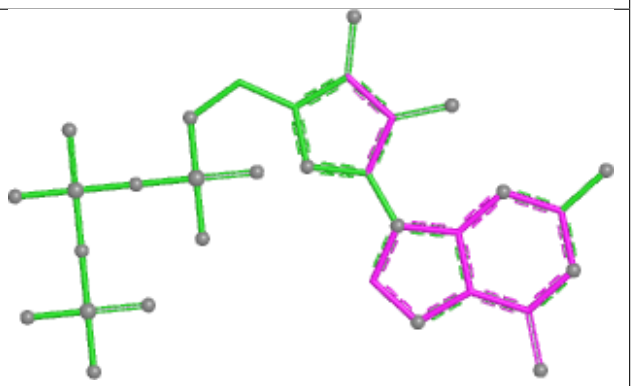


Rings

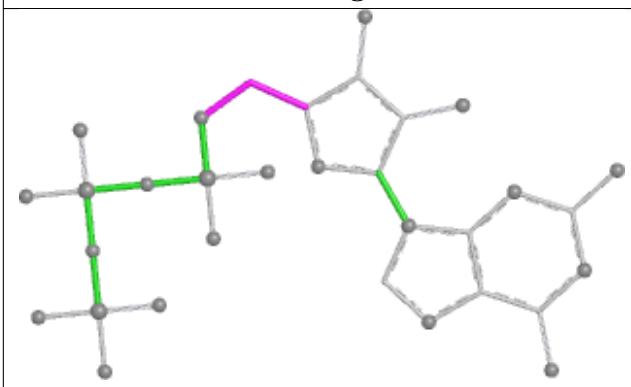
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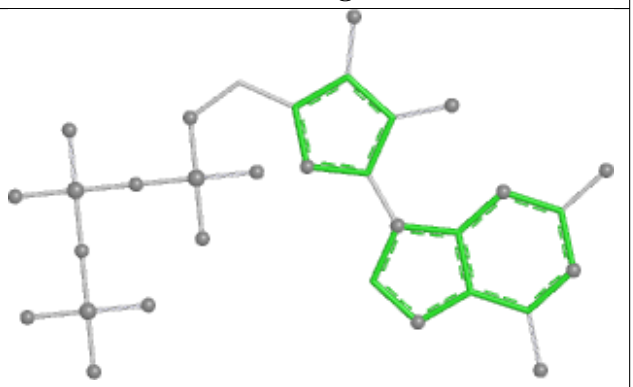
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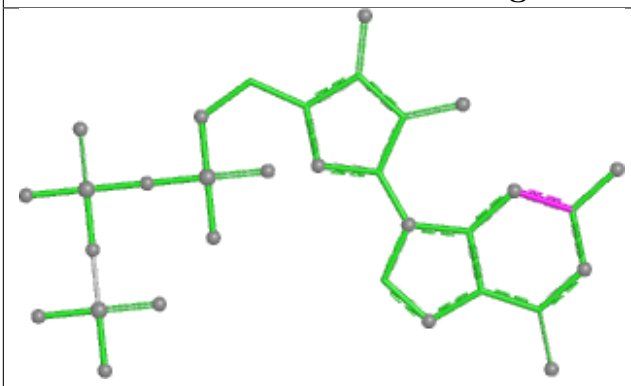


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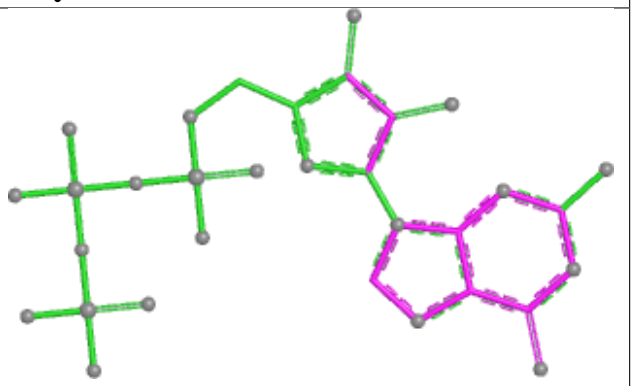


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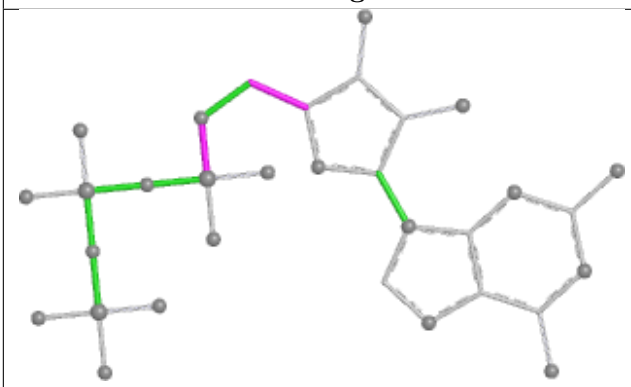
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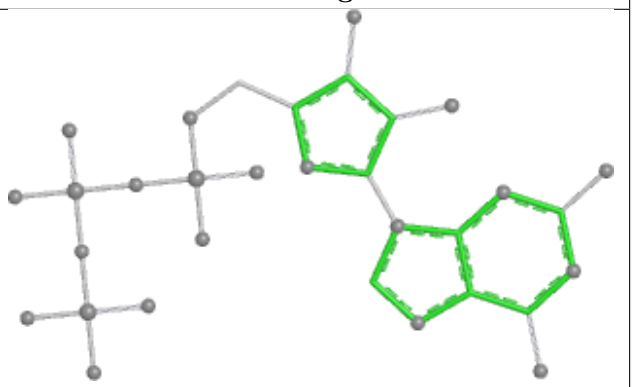
Bond lengths



Bond angles

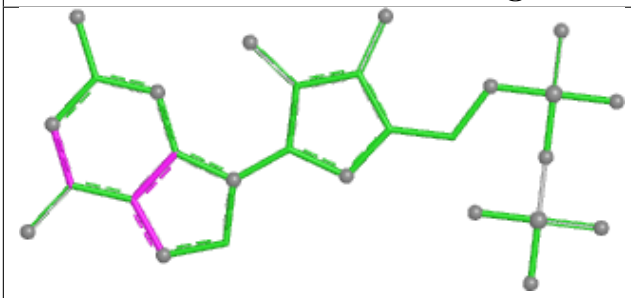


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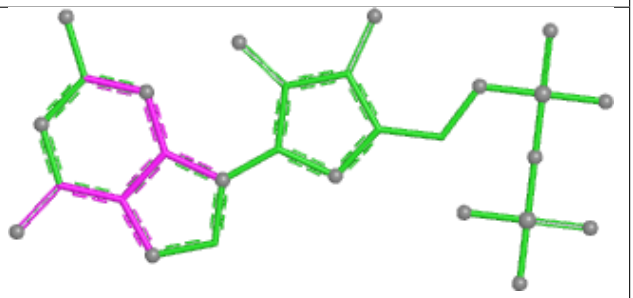


Rings

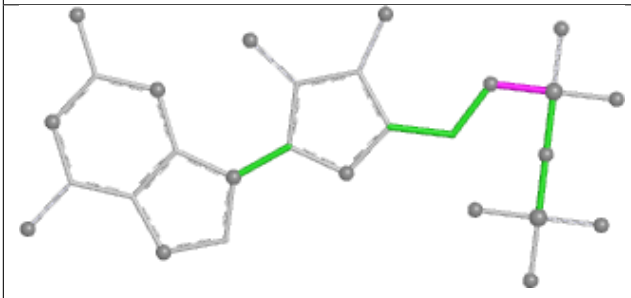
Ligand GDP KD 501



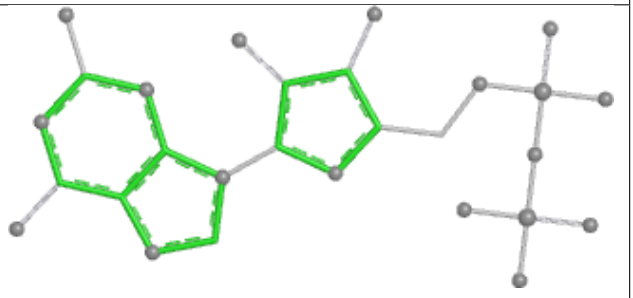
Bond lengths



Bond angles

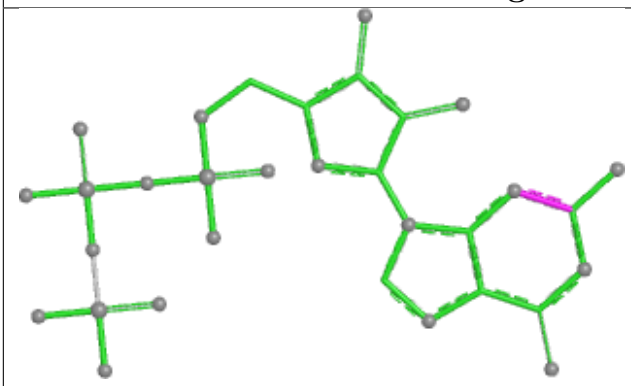


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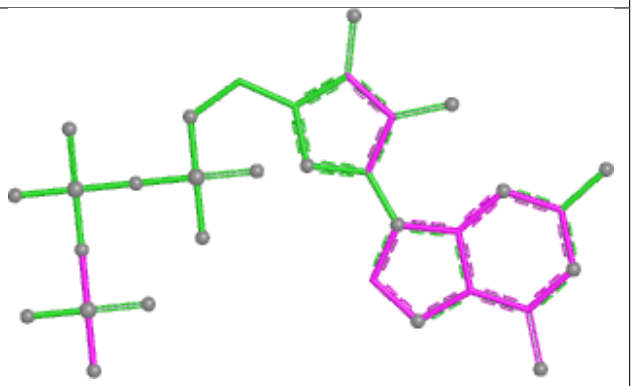


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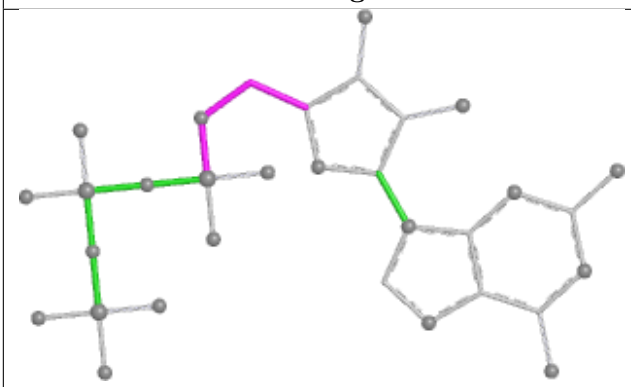
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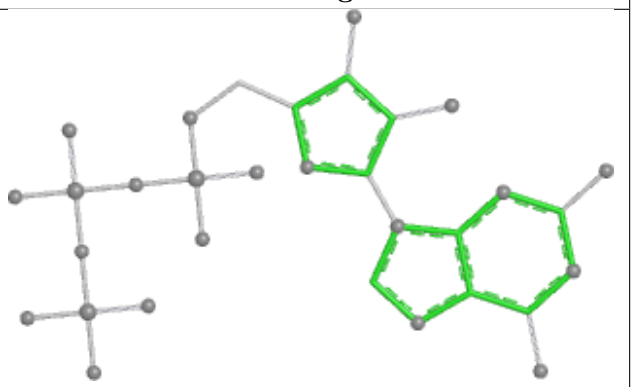
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Bond angles

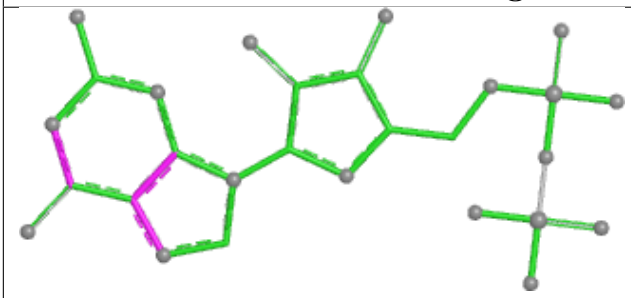


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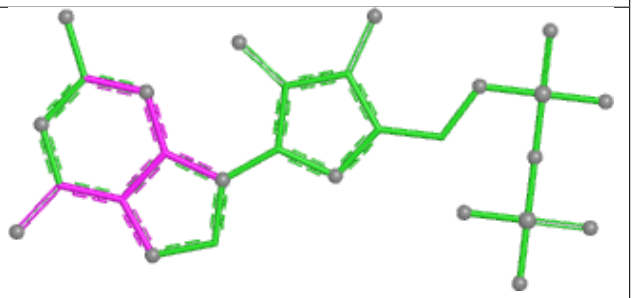


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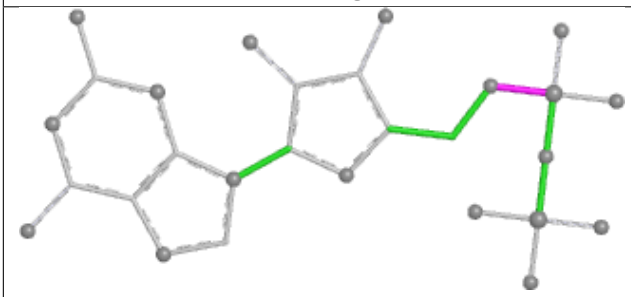
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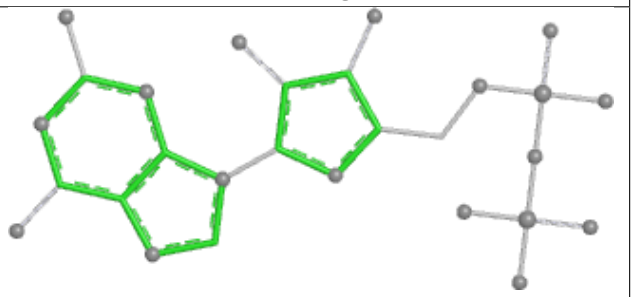
Bond lengths



Bond angles

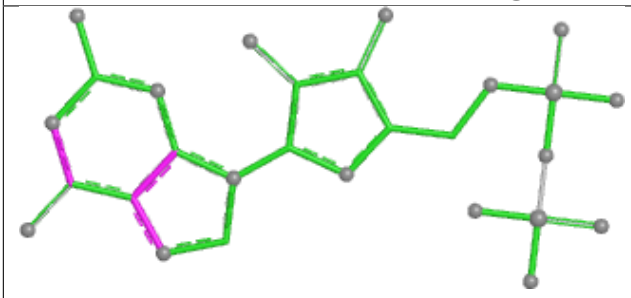


Torsions

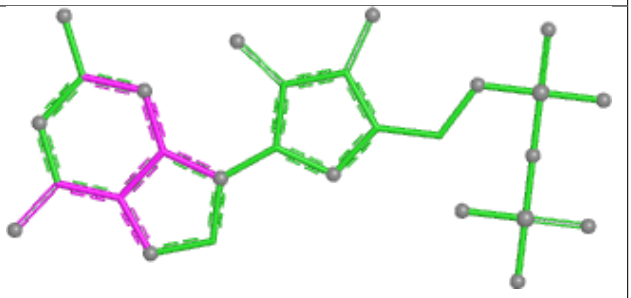


Rings

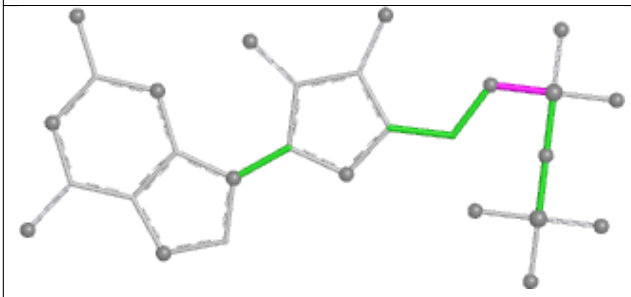
Ligand GDP HB 501



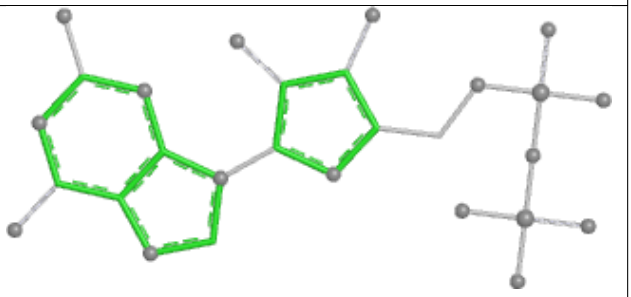
Bond lengths



Bond angles

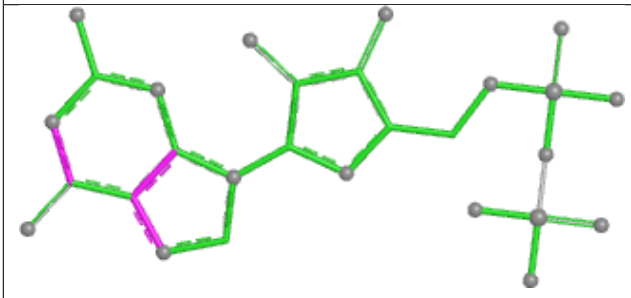


Torsions

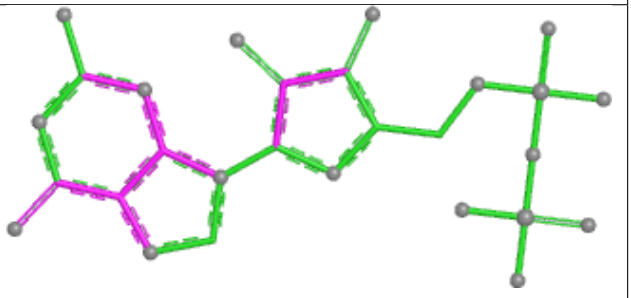


Rings

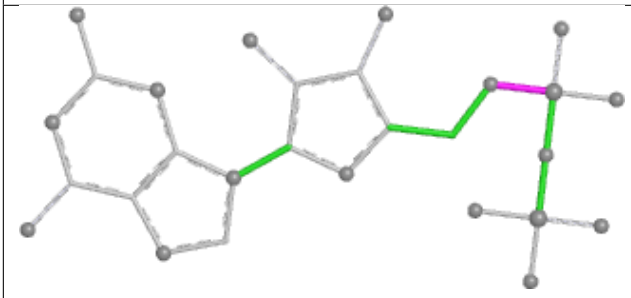
Ligand GDP AJ 501



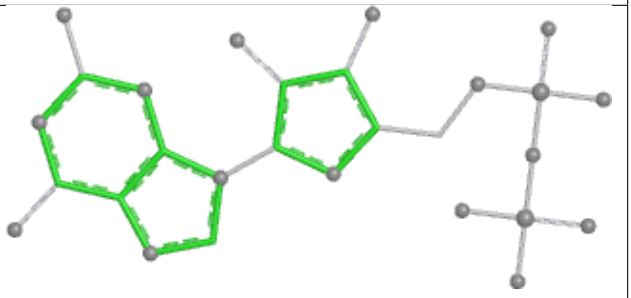
Bond lengths



Bond angles

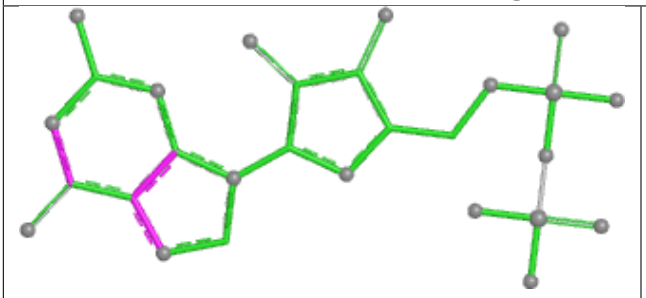


Torsions

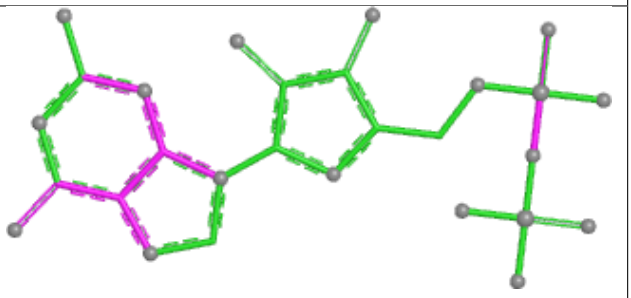


Rings

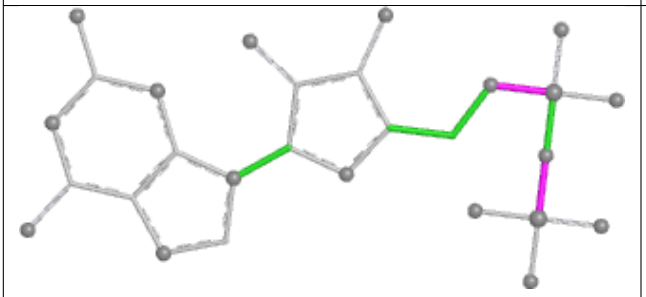
Ligand GDP PH 501



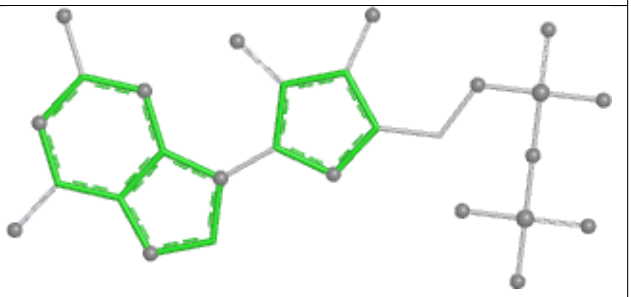
Bond lengths



Bond angles

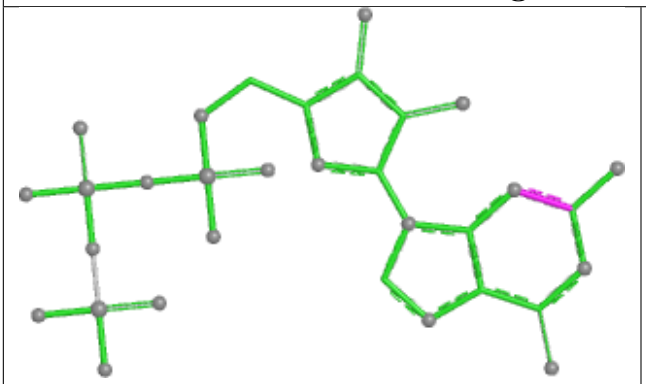


Torsions

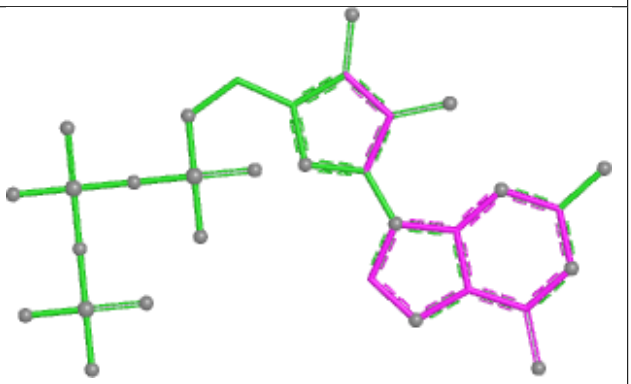


Rings

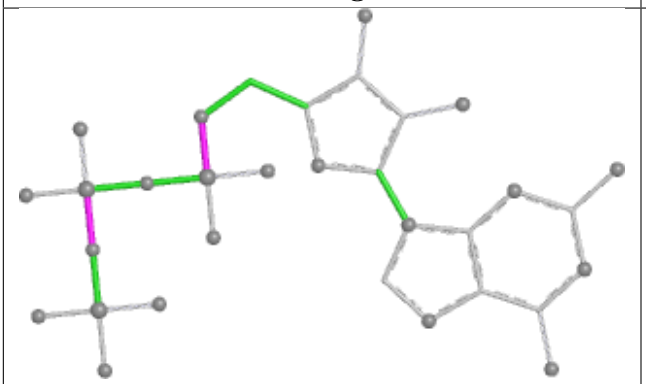
Ligand GTP VC 501



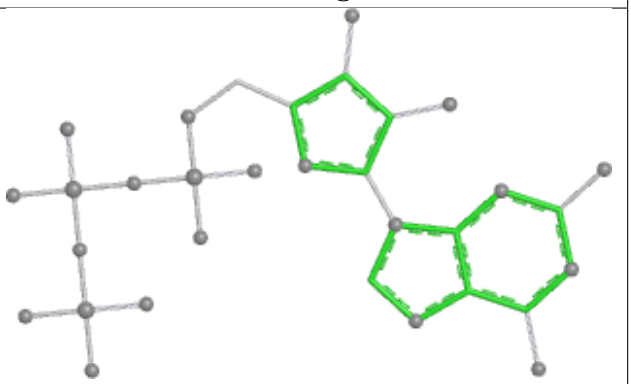
Bond lengths



Bond angles

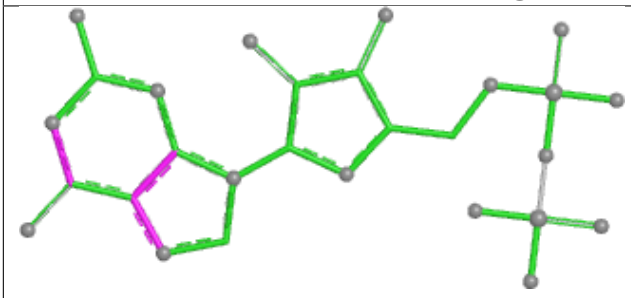


Torsions

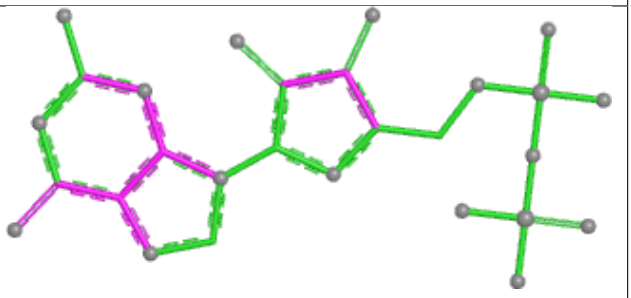


Rings

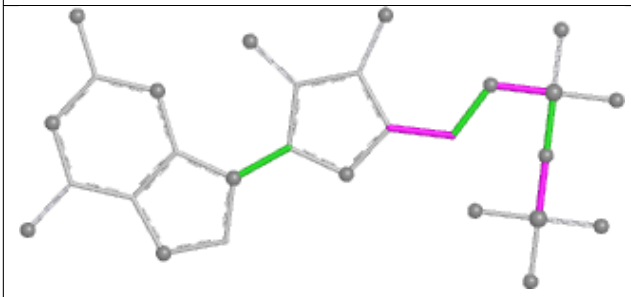
Ligand GDP BL 501



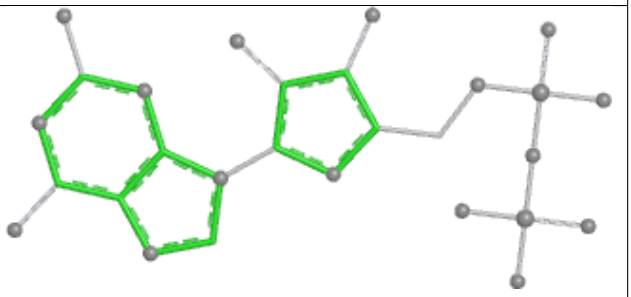
Bond lengths



Bond angles

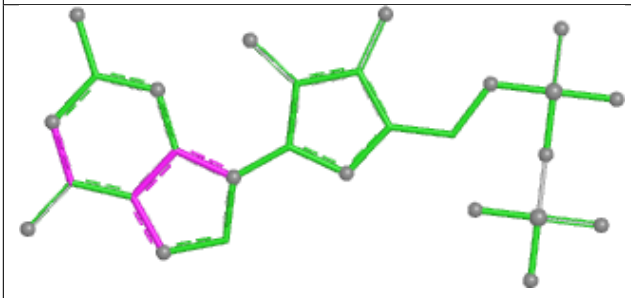


Torsions

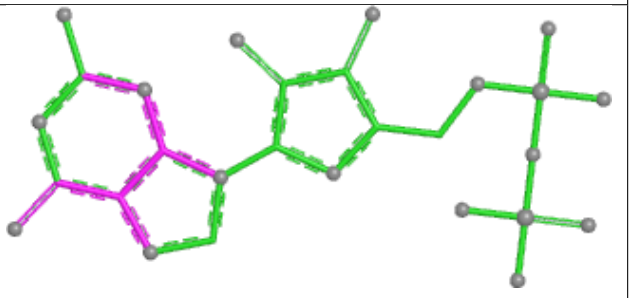


Rings

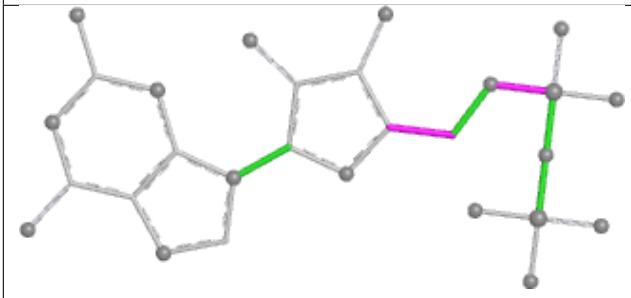
Ligand GDP MN 501



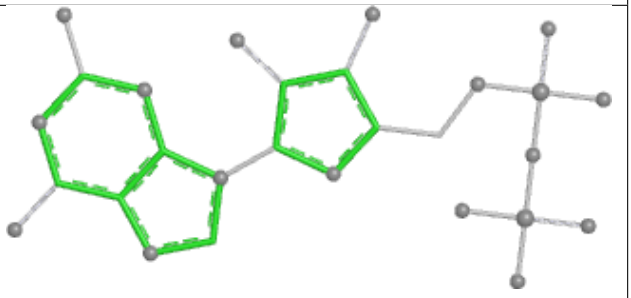
Bond lengths



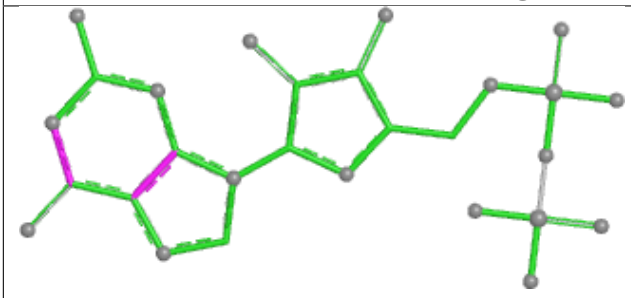
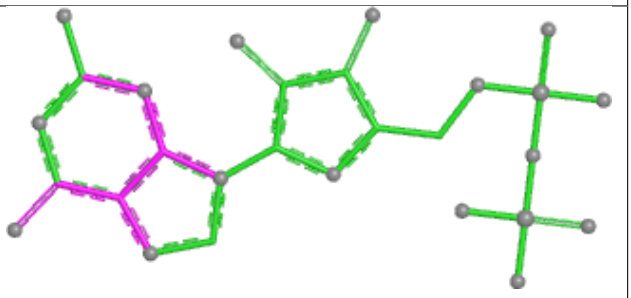
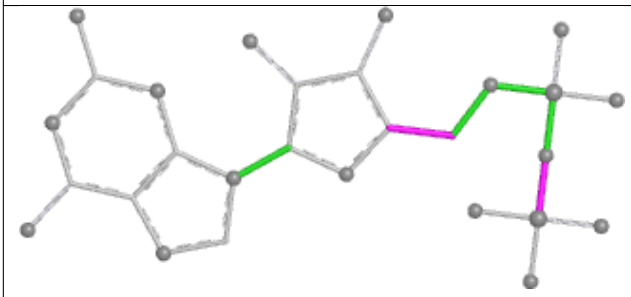
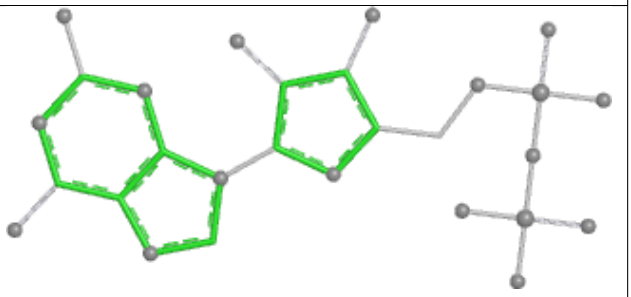
Bond angles

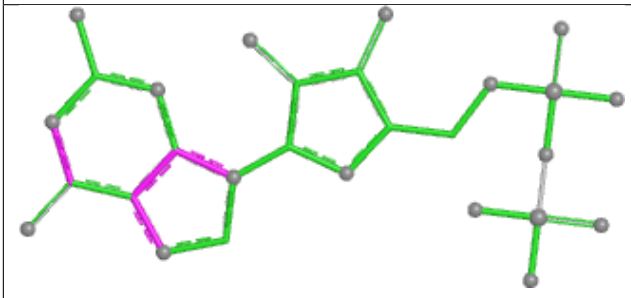
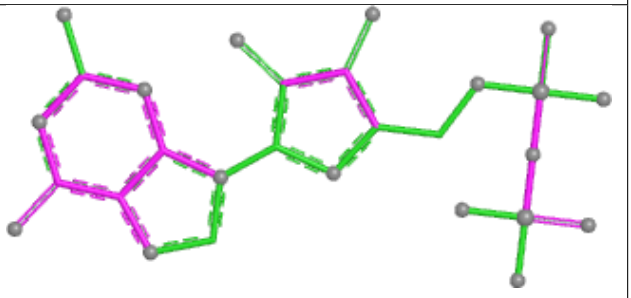
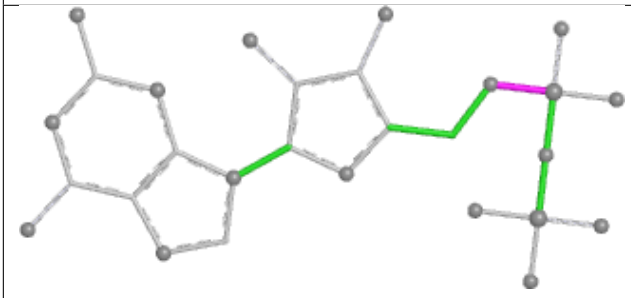
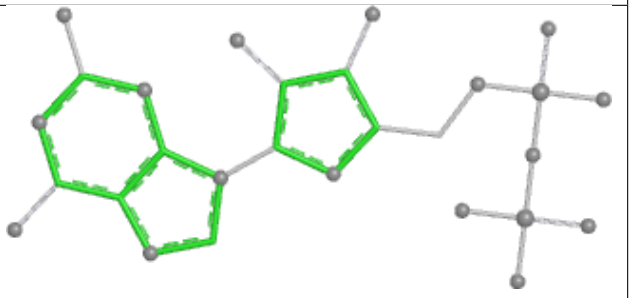


Torsions

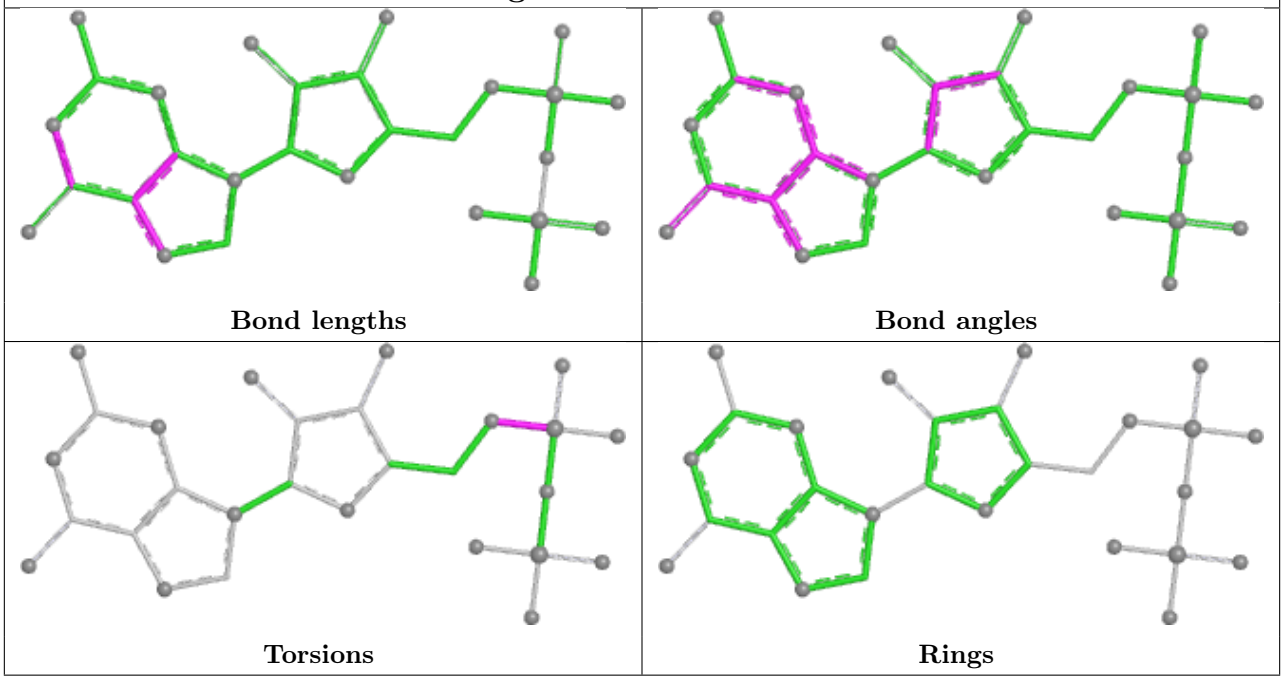


Rings

Ligand GDP JF 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP PJ 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP AD 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	Bl	6
25	Bn	6
25	Bp	6
25	Bo	6
25	Bm	6

The worst 5 of 30 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bl	83:UNK	C	103:UNK	N	55.09
1	Bl	151:UNK	C	171:UNK	N	54.90
1	Bn	151:UNK	C	171:UNK	N	54.16
1	Bp	116:UNK	C	135:UNK	N	50.17
1	Bp	218:UNK	C	236:UNK	N	49.54

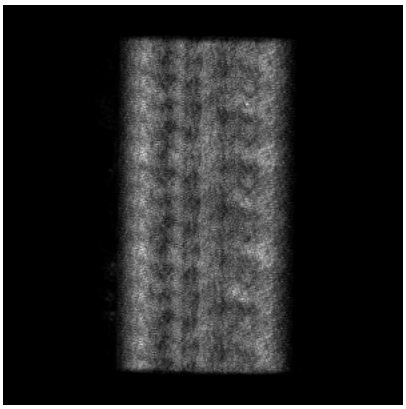
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17187. These allow visual inspection of the internal detail of the map and identification of artifacts.

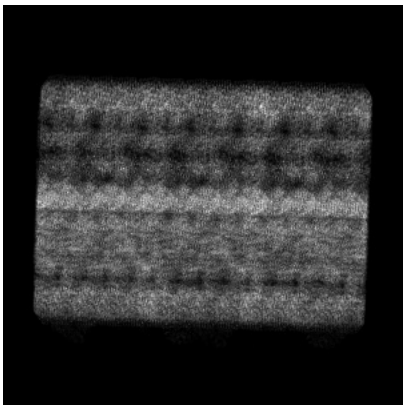
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

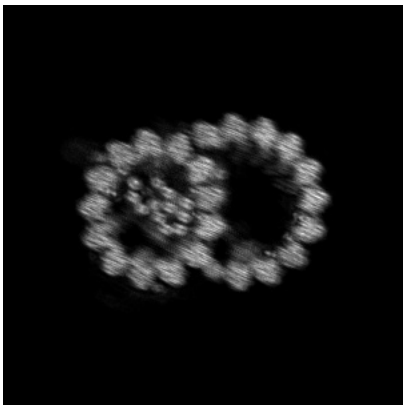
6.1.1 Primary map



X

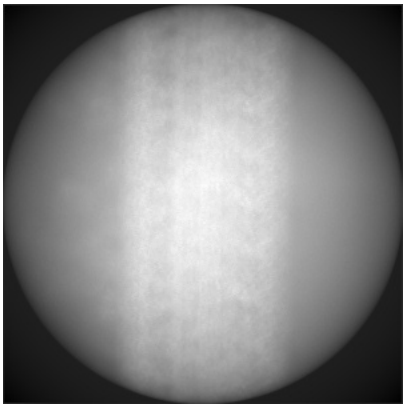


Y

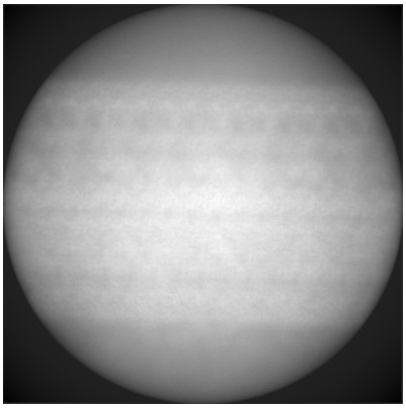


Z

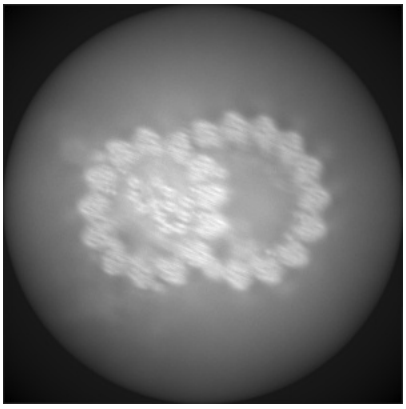
6.1.2 Raw map



X



Y

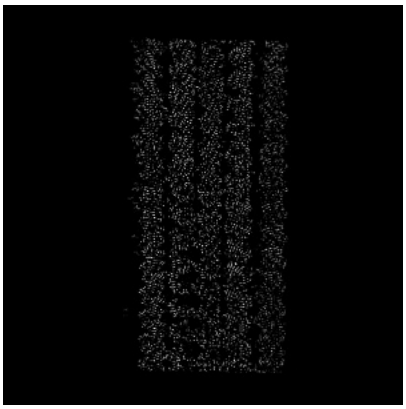


Z

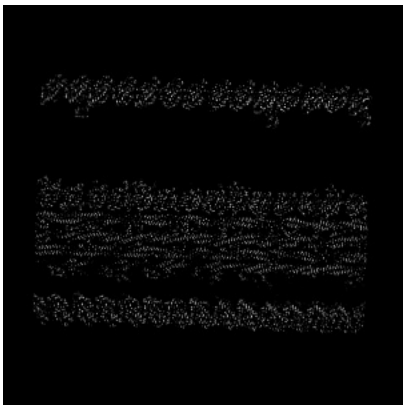
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

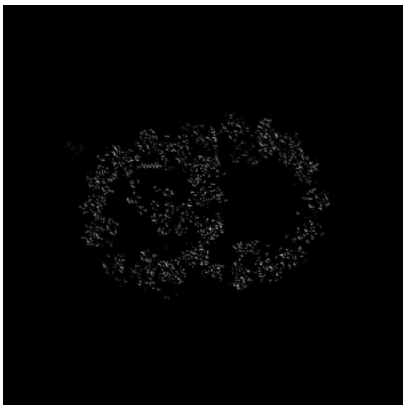
6.2.1 Primary map



X Index: 336

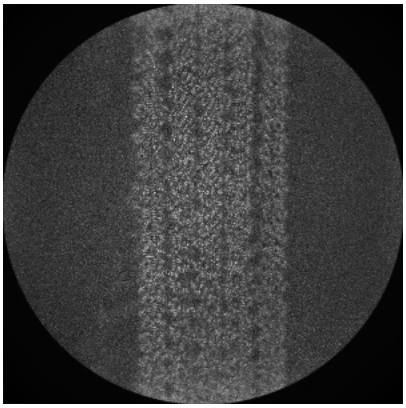


Y Index: 336

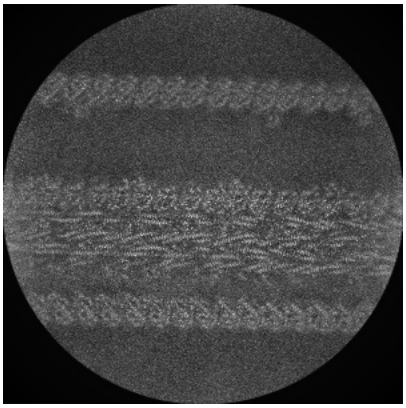


Z Index: 336

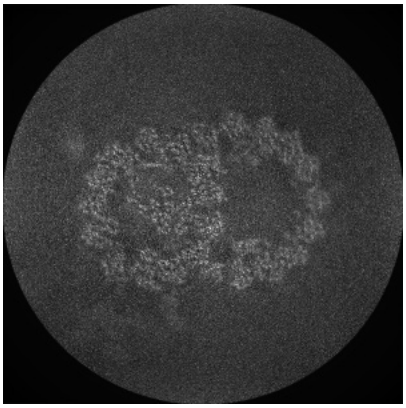
6.2.2 Raw map



X Index: 336



Y Index: 336

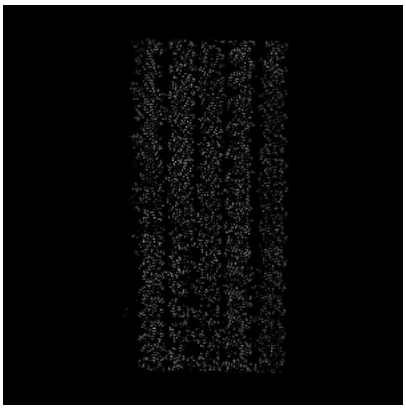


Z Index: 336

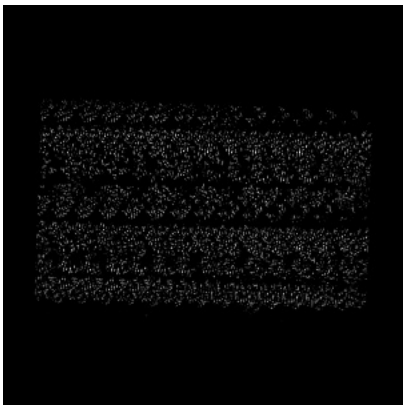
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

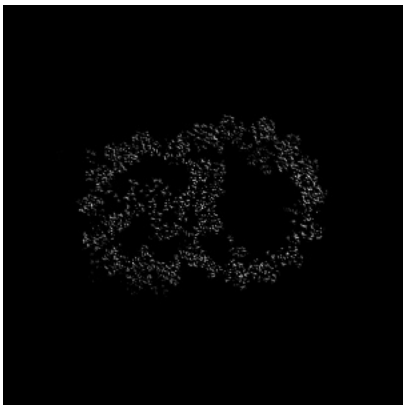
6.3.1 Primary map



X Index: 337

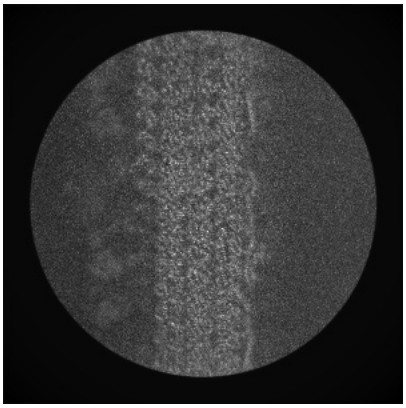


Y Index: 233

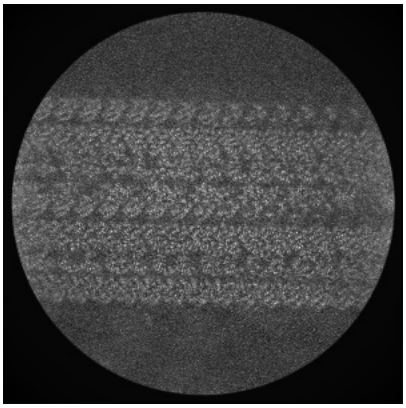


Z Index: 425

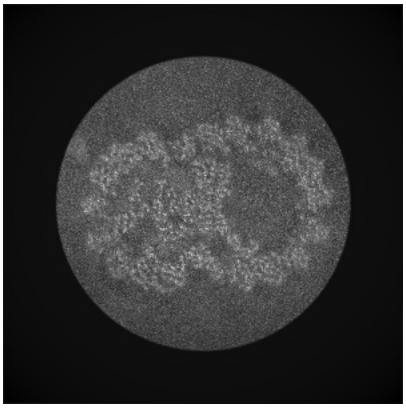
6.3.2 Raw map



X Index: 165



Y Index: 233

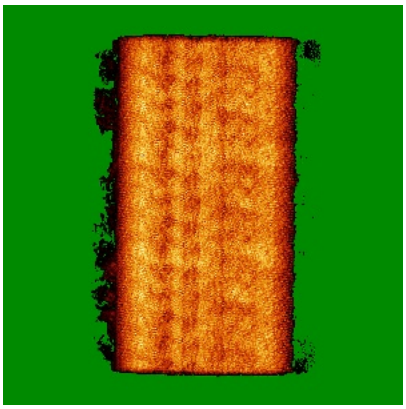


Z Index: 106

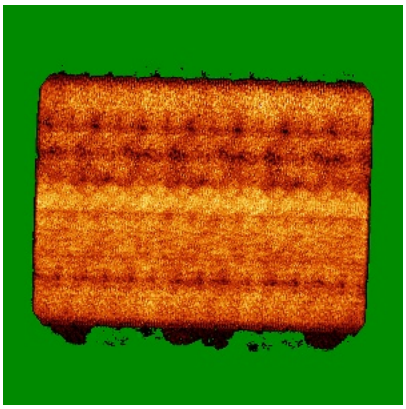
The images above show the largest variance slices of the map in three orthogonal directions.

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

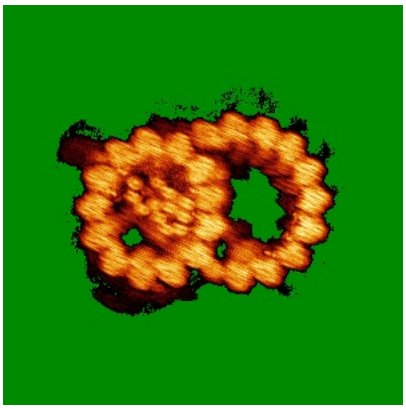
6.4.1 Primary map



X

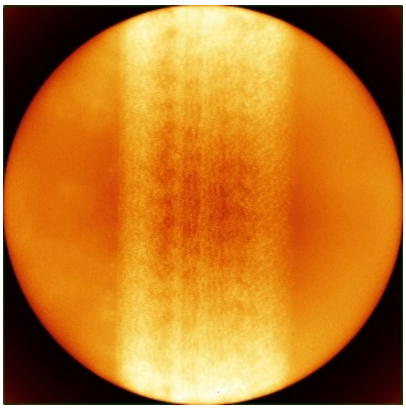


Y

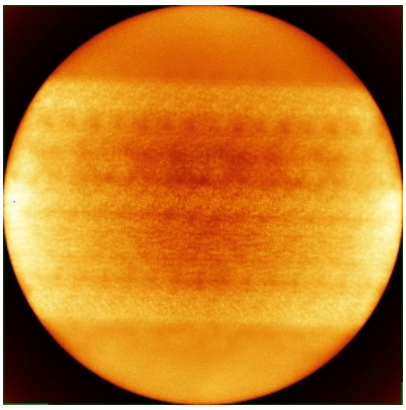


Z

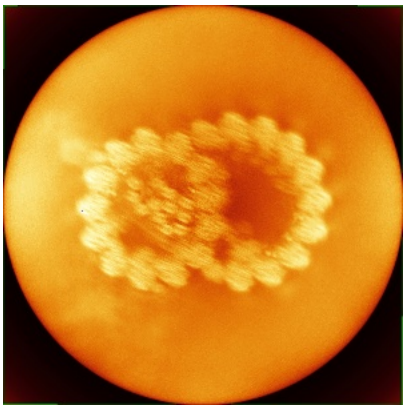
6.4.2 Raw map



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)

This section was not generated.

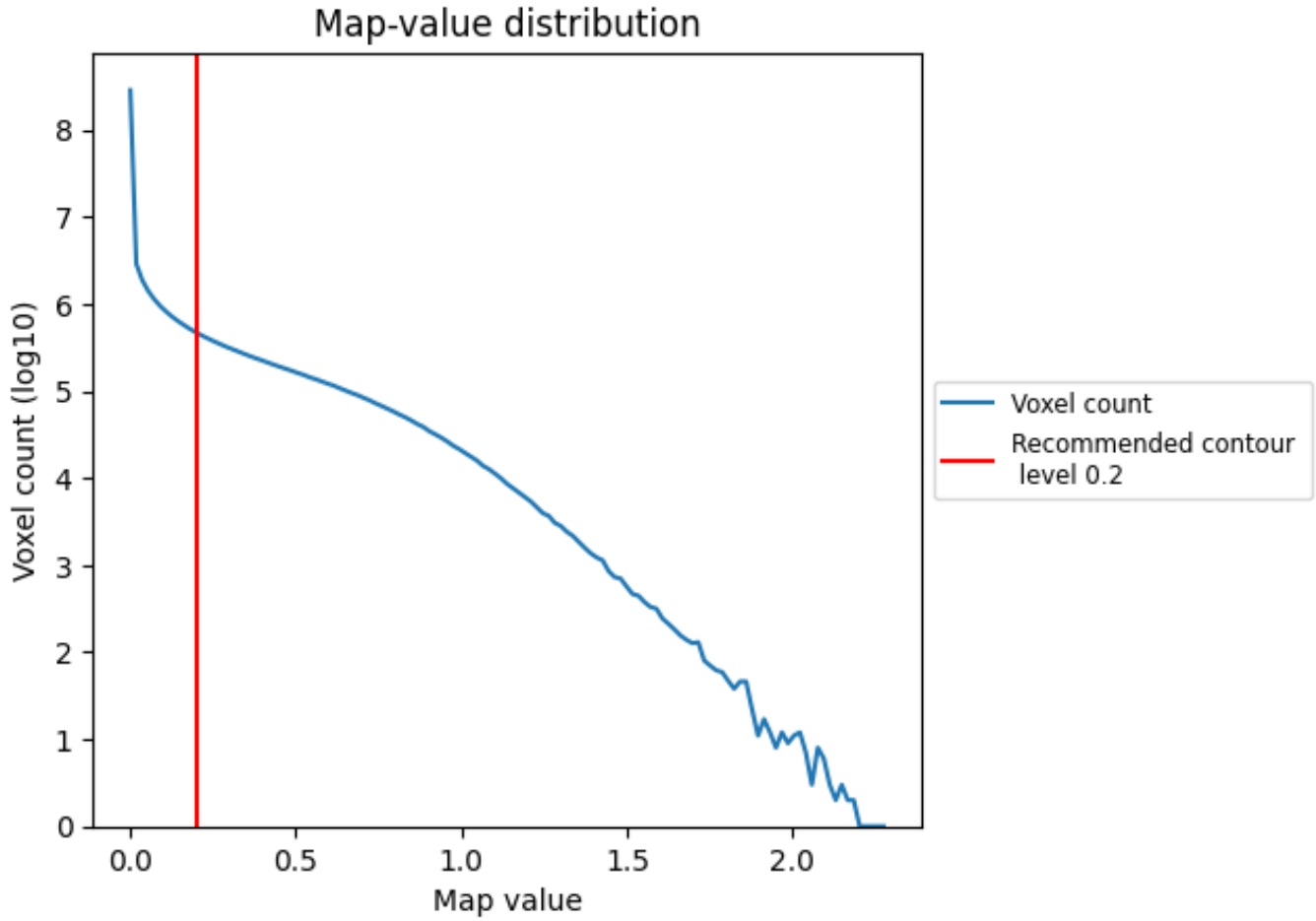
6.6 Mask visualisation (i)

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

7 Map analysis

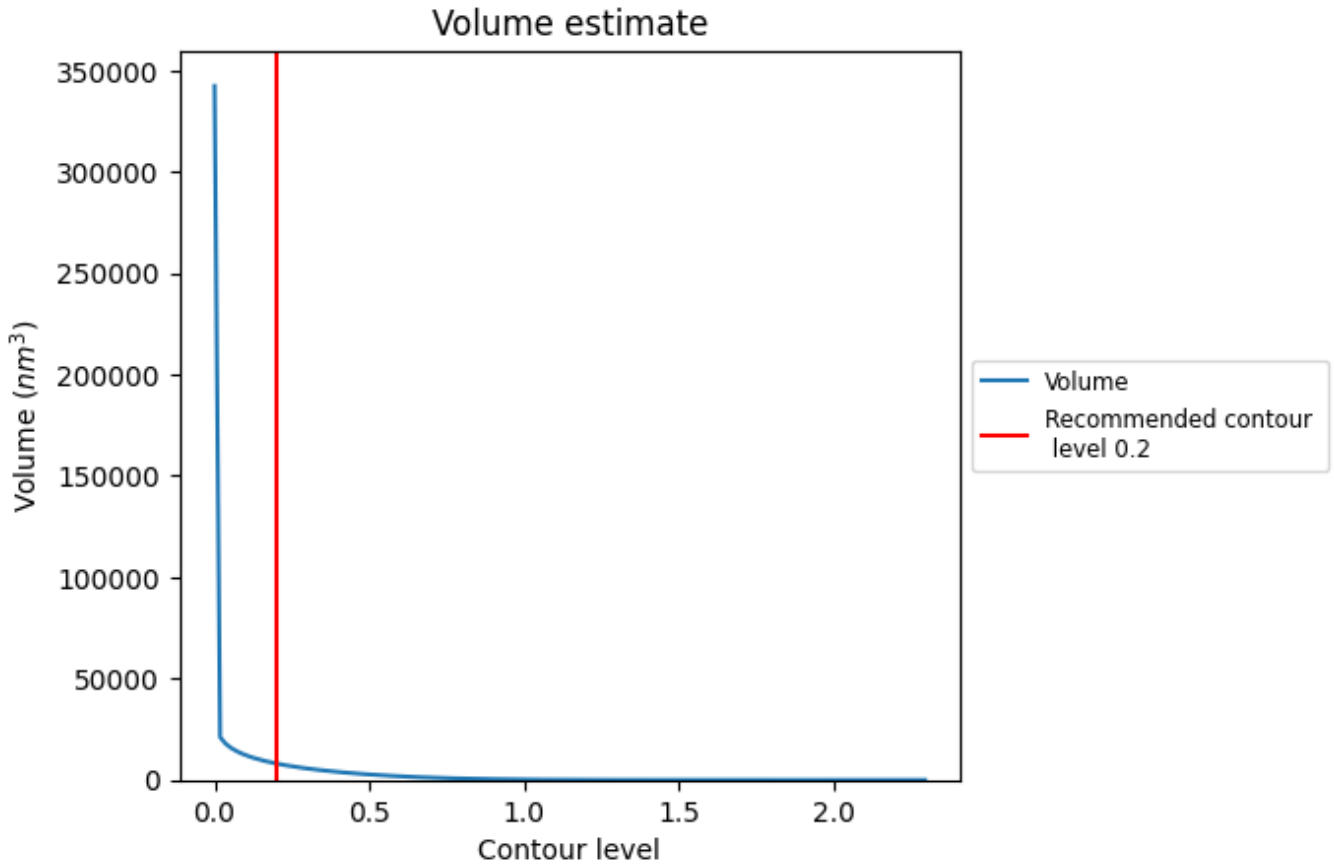
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

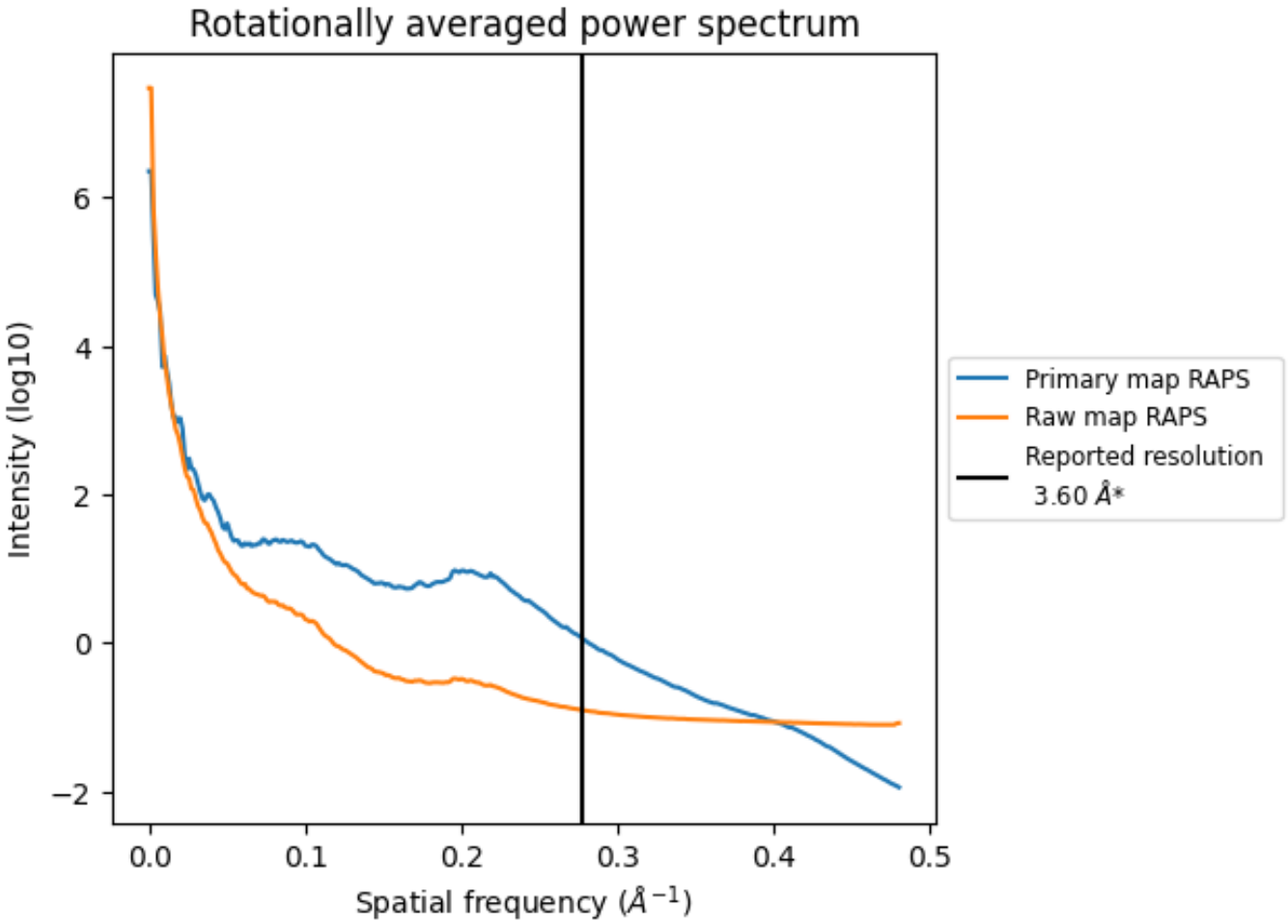
7.2 Volume estimate



The volume at the recommended contour level is 8092 nm^3; this corresponds to an approximate mass of 7310 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)

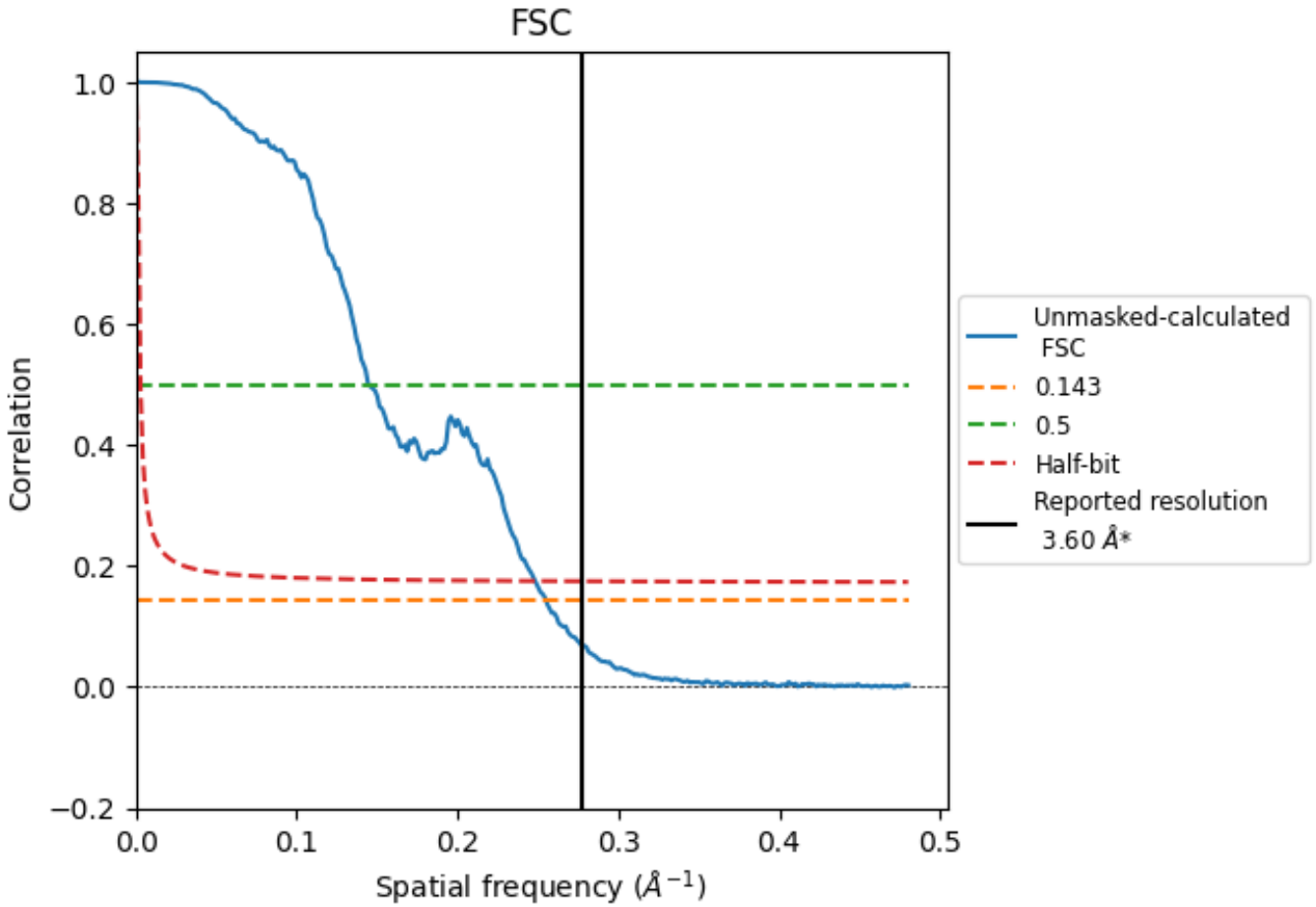


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	6.91	4.03

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

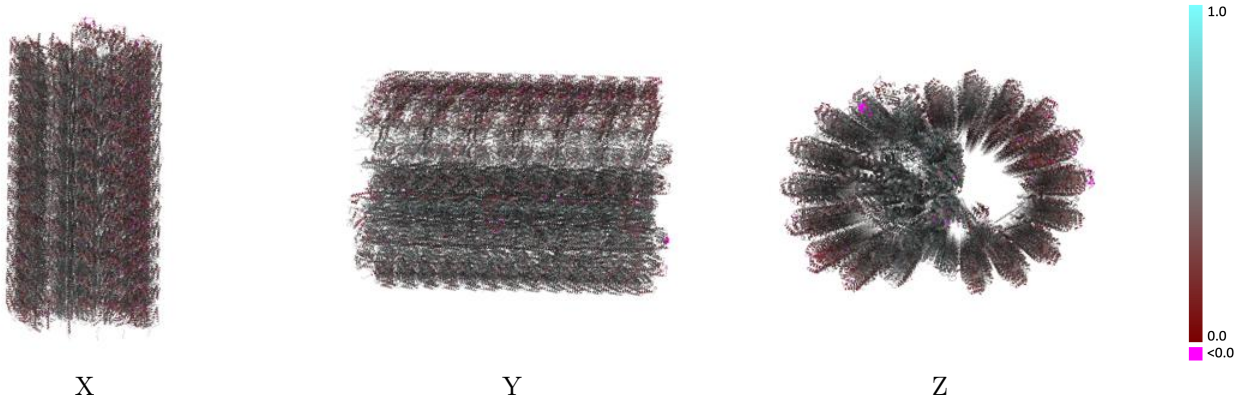
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17187 and PDB model 8OTZ. Per-residue inclusion information can be found in section 3 on page 83.

9.1 Map-model overlay

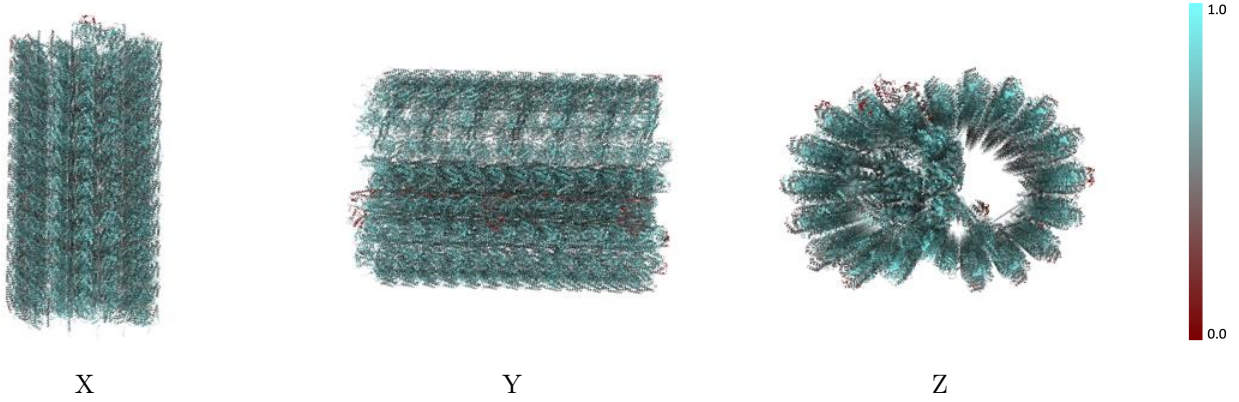
This section was not generated.

9.2 Q-score mapped to coordinate model



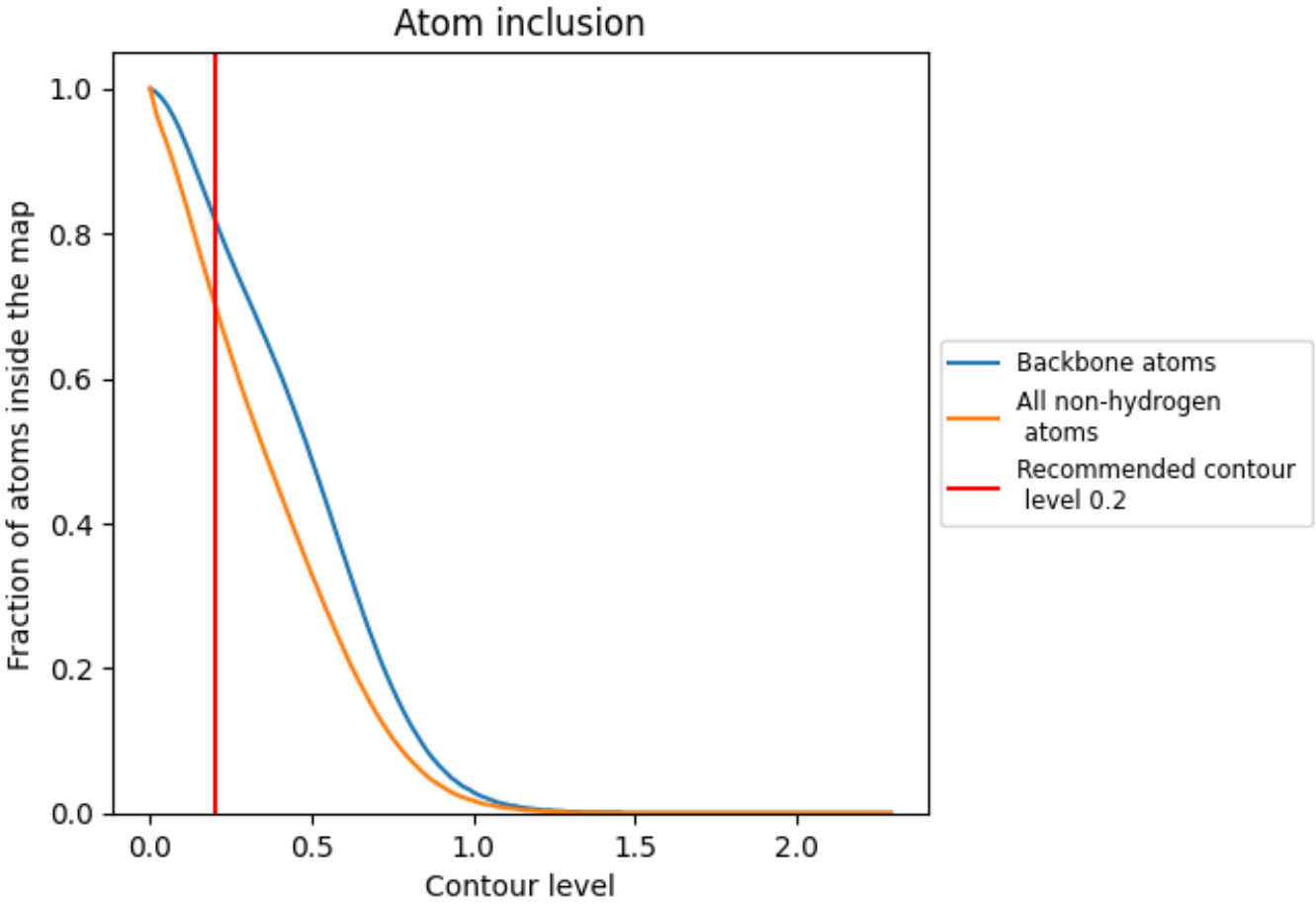
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7030	0.4380
0	0.8150	0.4950
0A	0.6410	0.3760
0C	0.5730	0.3630
0E	0.4740	0.3250
0G	0.5510	0.4050
0W	0.5900	0.4100
0Y	0.6150	0.3660
0a	0.5950	0.3580
0c	0.5520	0.3310
0e	0.6530	0.4400
0g	0.6110	0.3550
0i	0.6080	0.3360
0k	0.5270	0.2870
1	0.2550	0.2630
2	0.2450	0.2800
3	0.5620	0.3870
A	0.6710	0.4020
A0	0.6540	0.4300
A1	0.5170	0.3790
A2	0.6230	0.3500
A3	0.6280	0.3710
A4	0.6190	0.3440
A5	0.6080	0.3610
A6	0.7220	0.3920
A7	0.6710	0.3660
A8	0.6070	0.3700
A9	0.6390	0.4100
AA	0.7750	0.4890
AB	0.7690	0.4930
AC	0.7790	0.4980
AD	0.7890	0.4970
AE	0.7930	0.4970
AF	0.7730	0.4990
AG	0.7640	0.4980



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Chain	Atom inclusion	Q-score
AH	0.7610	0.5020
AI	0.8080	0.5030
AJ	0.7810	0.5000
AK	0.7690	0.4970
AL	0.7640	0.4930
AM	0.7810	0.4920
AP	0.7660	0.4970
AQ	0.7610	0.4970
AR	0.7270	0.4750
AS	0.7560	0.4930
AT	0.6560	0.3970
AU	0.6920	0.4100
AV	0.7510	0.4820
AW	0.7550	0.4740
Aa	0.7150	0.4380
Ab	0.7380	0.4540
Ac	0.7480	0.4570
Ad	0.7240	0.4370
Al	0.7860	0.4630
Am	0.8170	0.4800
An	0.8170	0.4870
Ao	0.7250	0.4740
Ap	0.7400	0.4750
Aq	0.7850	0.4930
Ar	0.7880	0.5030
At	0.5650	0.4050
Au	0.6890	0.4380
Av	0.6330	0.4220
Aw	0.6530	0.4300
Ax	0.5070	0.3810
Ay	0.6510	0.4240
Az	0.5810	0.4030
B	0.7070	0.4410
B0	0.6560	0.4170
B1	0.6420	0.4150
B2	0.7800	0.5060
B3	0.7510	0.5030
B4	0.7260	0.4750
B5	0.6420	0.4160
B6	0.6260	0.4180
B7	0.7760	0.4720
B8	0.7080	0.4620

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Chain	Atom inclusion	Q-score
B9	0.7000	0.4350
BA	0.7230	0.4400
BB	0.7460	0.4590
BC	0.7560	0.4730
BD	0.7490	0.4670
BE	0.7650	0.4640
BF	0.7400	0.4640
BG	0.7450	0.4760
BH	0.7460	0.4680
BI	0.7620	0.4660
BJ	0.7490	0.4620
BK	0.7490	0.4660
BL	0.7550	0.4710
BM	0.7470	0.4640
BN	0.6720	0.4610
BO	0.6700	0.4380
BP	0.6750	0.4680
BQ	0.6720	0.4610
BR	0.6810	0.4630
BS	0.6720	0.4430
BT	0.6820	0.4590
BU	0.6750	0.4790
BV	0.7380	0.5070
BW	0.7500	0.4890
BX	0.7060	0.4320
BY	0.7450	0.4830
BZ	0.7580	0.4740
Ba	0.7000	0.4630
Bb	0.7180	0.4560
Bc	0.7210	0.4710
Bd	0.7700	0.4870
Be	0.7600	0.4470
Bf	0.6900	0.4300
Bg	0.7580	0.4560
Bh	0.7470	0.4630
Bi	0.7350	0.4780
Bj	0.6590	0.4440
Bk	0.6440	0.4450
Bl	0.7830	0.4660
Bm	0.8160	0.4760
Bn	0.8380	0.4600
Bo	0.8620	0.4610

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Chain	Atom inclusion	Q-score
Bp	0.7890	0.5080
Bq	0.6600	0.4690
Br	0.7150	0.4320
Bs	0.7020	0.4210
Bu	0.6510	0.4760
By	0.6280	0.3840
Bz	0.6400	0.4220
C	0.7270	0.4650
C0	0.7520	0.4920
C1	0.6770	0.4640
C2	0.7370	0.5050
C3	0.7540	0.5110
C4	0.7450	0.5010
C5	0.7580	0.5110
C6	0.7880	0.4920
C7	0.7590	0.5170
C8	0.7640	0.5030
C9	0.7480	0.5010
CA	0.6110	0.3670
CB	0.6670	0.4080
CC	0.6920	0.4240
CD	0.6730	0.4140
CE	0.7130	0.4310
CF	0.7010	0.4350
CG	0.6810	0.4460
CH	0.6850	0.4370
CI	0.6950	0.4440
CJ	0.7190	0.4390
CK	0.6910	0.4420
CL	0.6900	0.4430
CM	0.6790	0.4300
CN	0.7340	0.4330
CO	0.7390	0.4620
CQ	0.6680	0.4220
CR	0.6080	0.3910
CS	0.6830	0.4380
CT	0.6620	0.3730
CU	0.6240	0.3710
CV	0.5200	0.3540
CW	0.7280	0.4900
CX	0.6590	0.3760
CY	0.5480	0.3530

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Chain	Atom inclusion	Q-score
CZ	0.6160	0.4010
Ca	0.6620	0.3760
Cb	0.6670	0.3670
Cc	0.6410	0.4060
Cd	0.6030	0.3690
Ce	0.4970	0.3790
Cf	0.5210	0.3480
Cg	0.5820	0.4000
Ch	0.6270	0.3730
Ci	0.6080	0.3610
Cj	0.5470	0.3580
Ck	0.5080	0.3110
Cl	0.6730	0.4260
Cm	0.7570	0.5100
Cn	0.7590	0.5040
Co	0.7660	0.5060
Cp	0.7590	0.4980
Cq	0.7710	0.5030
Cr	0.7660	0.5070
Cs	0.7570	0.4900
Ct	0.7680	0.5060
Cu	0.7190	0.4940
Cv	0.7270	0.5040
Cw	0.7100	0.4960
Cx	0.7240	0.4950
Cy	0.7200	0.4730
Cz	0.6210	0.4410
D	0.7330	0.4330
D0	0.7110	0.4350
D1	0.7090	0.4620
D2	0.6980	0.4680
D3	0.6940	0.4440
D4	0.6710	0.4400
D5	0.6790	0.4360
D6	0.6810	0.4310
D7	0.7110	0.4390
D8	0.6960	0.4520
D9	0.6900	0.4290
DA	0.5710	0.2960
DB	0.6320	0.3450
DC	0.6680	0.3680
DD	0.6770	0.3780

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Chain	Atom inclusion	Q-score
DE	0.6890	0.3780
DF	0.7190	0.4090
DG	0.6820	0.4180
DH	0.6870	0.4080
DI	0.6910	0.4110
DJ	0.7390	0.4150
DK	0.6770	0.3890
DL	0.6980	0.4050
DM	0.6770	0.3950
DN	0.6280	0.3350
DO	0.7950	0.5070
DP	0.6630	0.4370
DQ	0.6530	0.4430
DR	0.5250	0.3910
DS	0.5940	0.4260
DT	0.6630	0.4130
DU	0.6750	0.4400
DV	0.6400	0.4370
DW	0.6630	0.4290
DX	0.5350	0.3710
DY	0.7130	0.4600
DZ	0.7440	0.4920
Da	0.6720	0.4720
Db	0.7250	0.4430
Dc	0.7290	0.4520
Dd	0.6540	0.4140
De	0.6340	0.3830
Df	0.6430	0.4440
Dg	0.5960	0.4430
Dh	0.5990	0.4320
Di	0.6690	0.4740
Dj	0.7030	0.4870
Dk	0.6820	0.4730
Dl	0.6730	0.4670
Dm	0.7730	0.4920
Dn	0.5110	0.3670
E	0.7600	0.4570
E1	0.7560	0.4990
E2	0.7660	0.5110
E3	0.7590	0.4930
E4	0.7370	0.4850
EA	0.6900	0.4710

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Chain	Atom inclusion	Q-score
EB	0.5950	0.3500
EC	0.6500	0.3940
ED	0.6650	0.3970
EE	0.6780	0.4040
EF	0.7100	0.4260
EG	0.6860	0.4350
EH	0.6790	0.4290
EI	0.6950	0.4340
EJ	0.7300	0.4430
EK	0.6750	0.4070
EL	0.6920	0.4340
EM	0.6900	0.4280
EN	0.6350	0.3960
EO	0.6900	0.4600
EP	0.7010	0.4660
EQ	0.7040	0.4610
ER	0.7300	0.4520
ES	0.7790	0.5130
ET	0.7740	0.5090
EU	0.7650	0.5070
EV	0.7630	0.5160
EW	0.6960	0.4880
EX	0.6990	0.4910
EY	0.7040	0.4810
EZ	0.7010	0.4920
Ee	0.7840	0.5310
F	0.7710	0.4660
F2	0.7680	0.5250
F3	0.7610	0.5090
F4	0.7540	0.5140
F5	0.7570	0.5170
F6	0.7560	0.4950
FB	0.6520	0.3910
FC	0.6890	0.4260
FD	0.6890	0.4320
FE	0.7100	0.4410
FF	0.7490	0.4480
FG	0.7280	0.4580
FH	0.7270	0.4580
FI	0.7180	0.4540
FJ	0.7390	0.4470
FK	0.7190	0.4430

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Chain	Atom inclusion	Q-score
FL	0.7190	0.4560
FM	0.7360	0.4540
FN	0.6780	0.4130
G	0.6850	0.4300
GB	0.6690	0.4060
GC	0.6960	0.4240
GD	0.7100	0.4380
GE	0.7130	0.4440
GF	0.7450	0.4500
GG	0.7100	0.4470
GH	0.7200	0.4630
GI	0.7120	0.4530
GJ	0.7380	0.4620
GK	0.7330	0.4480
GL	0.7210	0.4500
GM	0.7130	0.4500
GN	0.6880	0.4210
H	0.6550	0.4060
HB	0.6190	0.3990
HC	0.6920	0.4500
HD	0.7150	0.4610
HE	0.7180	0.4660
HF	0.7170	0.4630
HG	0.7050	0.4640
HH	0.6960	0.4650
HI	0.7090	0.4700
HJ	0.7240	0.4770
HK	0.7210	0.4480
HL	0.7120	0.4690
HM	0.7170	0.4700
HN	0.6930	0.4530
HO	0.6710	0.4360
I	0.7400	0.4810
IB	0.6610	0.4120
IC	0.7430	0.4820
ID	0.7430	0.4840
IE	0.7410	0.4870
IF	0.7360	0.4740
IG	0.7460	0.4760
IH	0.7440	0.4880
II	0.7380	0.4800
IJ	0.7380	0.4920

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Chain	Atom inclusion	Q-score
IK	0.7570	0.4690
IL	0.7350	0.4700
IM	0.7330	0.4780
IN	0.7340	0.4560
IO	0.7320	0.4510
J	0.6790	0.4000
JB	0.7390	0.4870
JC	0.7390	0.4960
JD	0.7410	0.5040
JE	0.7400	0.4980
JF	0.7670	0.4970
JG	0.7470	0.5010
JH	0.7520	0.5060
JI	0.7470	0.4980
JJ	0.7740	0.5000
JK	0.7370	0.4910
JL	0.7400	0.4950
JM	0.7410	0.4890
JN	0.7390	0.4810
K	0.6970	0.4220
K1	0.7000	0.4370
KB	0.7380	0.4580
KC	0.8080	0.5150
KD	0.8100	0.5190
KE	0.7950	0.5170
KF	0.8010	0.5150
KG	0.8150	0.5240
KH	0.8090	0.5320
KI	0.8000	0.5280
KJ	0.7850	0.5180
KK	0.8290	0.5270
KL	0.7990	0.5250
KM	0.7990	0.5190
KN	0.7890	0.5100
KO	0.8160	0.5080
L	0.7310	0.4330
L1	0.6560	0.4130
L2	0.6800	0.4240
LB	0.7310	0.4900
LC	0.7550	0.5150
LD	0.7400	0.5210
LE	0.7310	0.5170

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Chain	Atom inclusion	Q-score
LF	0.7800	0.5180
LG	0.7620	0.5310
LH	0.7580	0.5380
LI	0.7430	0.5220
LJ	0.7660	0.5270
LK	0.7670	0.5210
LL	0.7590	0.5280
LM	0.7370	0.5180
LN	0.7580	0.5150
M	0.6740	0.3950
MB	0.7950	0.5000
MC	0.7930	0.5110
MD	0.7900	0.5090
ME	0.7980	0.5140
MF	0.8260	0.5170
MG	0.7990	0.5190
MH	0.7920	0.5230
MI	0.7960	0.5200
MJ	0.8110	0.5200
MK	0.7830	0.5030
ML	0.7960	0.5150
MM	0.7960	0.5160
MN	0.8070	0.5080
N	0.4530	0.3570
N0	0.6630	0.3940
NA	0.6730	0.4080
NB	0.6480	0.4190
NC	0.6490	0.4140
ND	0.7150	0.4220
NE	0.6870	0.4230
NF	0.6530	0.4110
NG	0.6570	0.4120
NH	0.6840	0.4170
NI	0.6750	0.4090
NJ	0.6530	0.4130
NK	0.6470	0.4080
NL	0.6520	0.4030
O	0.4470	0.3870
O0	0.6450	0.4100
OA	0.7000	0.4550
OB	0.6920	0.4600
OC	0.6910	0.4550

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Chain	Atom inclusion	Q-score
OD	0.7100	0.4330
OE	0.7250	0.4480
OF	0.6950	0.4380
OG	0.6810	0.4380
OH	0.6910	0.4280
OI	0.6990	0.4140
OJ	0.6820	0.4430
OK	0.7000	0.4580
OL	0.6970	0.4420
P	0.6710	0.3890
PA	0.7010	0.3900
PB	0.7180	0.4050
PC	0.6960	0.3820
PD	0.6990	0.3720
PE	0.7070	0.3570
PF	0.6820	0.3810
PG	0.6590	0.3650
PH	0.6820	0.3700
PI	0.7190	0.3620
PJ	0.7010	0.3940
PK	0.7020	0.3970
PL	0.7310	0.4170
PM	0.7020	0.3930
Q	0.7560	0.4920
QA	0.6460	0.3170
QB	0.6900	0.3510
QC	0.6470	0.3280
QD	0.6710	0.3210
QE	0.6900	0.3150
QF	0.6500	0.3220
QG	0.6520	0.3170
QH	0.6680	0.3240
QI	0.7160	0.3190
QJ	0.6810	0.3280
QK	0.6530	0.3310
QL	0.6920	0.3410
QM	0.6650	0.3270
R	0.7240	0.4820
RA	0.6370	0.3150
RB	0.6880	0.3560
RC	0.6770	0.3490
RD	0.6670	0.3390

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Chain	Atom inclusion	Q-score
RE	0.7180	0.3390
RF	0.6790	0.3590
RG	0.6390	0.3400
RH	0.6760	0.3590
RI	0.6980	0.3410
RJ	0.6920	0.3400
RK	0.6550	0.3460
RL	0.6850	0.3520
RM	0.6420	0.3410
S	0.7110	0.4720
SA	0.6160	0.3070
SB	0.6940	0.3780
SC	0.7040	0.3770
SD	0.7080	0.3810
SE	0.7540	0.3920
SF	0.7220	0.3920
SG	0.7020	0.3950
SH	0.7100	0.4030
SI	0.7180	0.3800
SJ	0.7390	0.3870
SK	0.7090	0.3980
SL	0.7200	0.3970
SM	0.7030	0.3830
T	0.7220	0.4680
TB	0.6780	0.3850
TC	0.7190	0.4110
TD	0.7120	0.4150
TE	0.7420	0.4130
TF	0.7450	0.4210
TG	0.7060	0.4330
TH	0.7230	0.4280
TI	0.7320	0.4300
TJ	0.7470	0.4070
TK	0.7080	0.4230
TL	0.7120	0.4250
TM	0.6910	0.4030
U	0.7090	0.4710
UB	0.6240	0.3750
UC	0.6590	0.4060
UD	0.6510	0.4040
UE	0.6690	0.4080
UF	0.6890	0.4070

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Chain	Atom inclusion	Q-score
UG	0.6700	0.4130
UH	0.6550	0.4120
UI	0.6520	0.4090
UJ	0.6960	0.3970
UK	0.6610	0.4140
UL	0.6440	0.4110
UM	0.6480	0.4110
UN	0.6020	0.3670
V	0.7140	0.4720
VB	0.6540	0.3950
VC	0.6740	0.4010
VD	0.6960	0.4100
VE	0.6660	0.4020
VF	0.7120	0.4040
VG	0.6670	0.3930
VH	0.6970	0.4090
VI	0.6760	0.3990
VJ	0.7090	0.4010
VK	0.6990	0.4000
VL	0.6910	0.4090
VM	0.6730	0.4010
VN	0.6520	0.3810
W	0.3360	0.2970
WB	0.6400	0.4000
WC	0.6500	0.4100
WD	0.7070	0.4430
WE	0.6740	0.4200
WF	0.7200	0.4290
WG	0.6600	0.4160
WH	0.7030	0.4330
WI	0.6880	0.4370
WJ	0.7260	0.4410
WK	0.6950	0.4300
WL	0.6930	0.4460
WM	0.6920	0.4480
WN	0.6880	0.4360
X	0.7360	0.4710
XG	0.7160	0.4580
XH	0.7320	0.4640
XI	0.7550	0.4710
XJ	0.7260	0.4690
XK	0.7470	0.4610

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Chain	Atom inclusion	Q-score
XL	0.7190	0.4620
XM	0.6850	0.4310
Y	0.7480	0.4790
YG	0.3440	0.3440
YH	0.7100	0.4580
YI	0.7030	0.4560
YJ	0.7020	0.4620
YK	0.7330	0.4530
YL	0.6830	0.4580
Z	0.2870	0.2640
a	0.5960	0.3700
b	0.5480	0.3250
c	0.5580	0.3550
d	0.5790	0.3570
e	0.7240	0.4450
f	0.7250	0.4390
g	0.7280	0.4480
h	0.7560	0.4680
i	0.7960	0.5060
j	0.7780	0.4900
k	0.6100	0.4390
ke	0.6190	0.3730
l	0.4820	0.4050
m	0.6620	0.4450
n	0.6470	0.4240
o	0.6230	0.3880
p	0.3170	0.2640
q	0.2590	0.2190
r	0.7380	0.4750
s	0.7270	0.4590
t	0.7270	0.4510
u	0.3280	0.3160
v	0.3030	0.2880
w	0.2890	0.3140
x	0.3250	0.3020
y	0.5650	0.3790
z	0.5620	0.3880